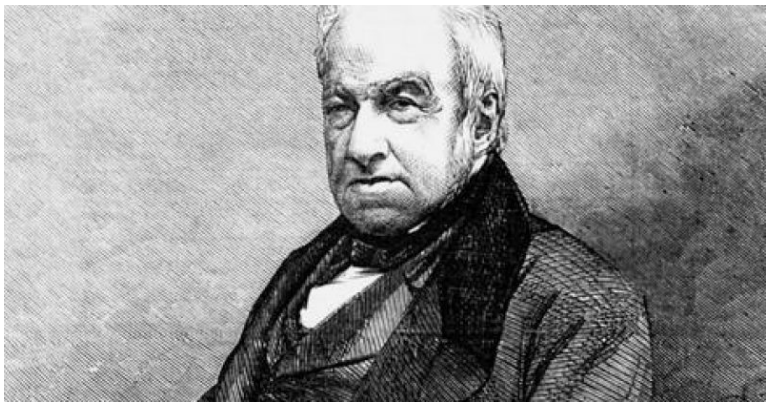
Lecture 1 – Stochastic processes

February 7, 2020

Outline

1. Brownian motion: from Einstein to Langevin.
2. Introduction to the theory of stochastic processes.
3. Markov chains.
4. How to deal with fluctuations: the urn model.
5. Theory predictions vs. numerical simulations.

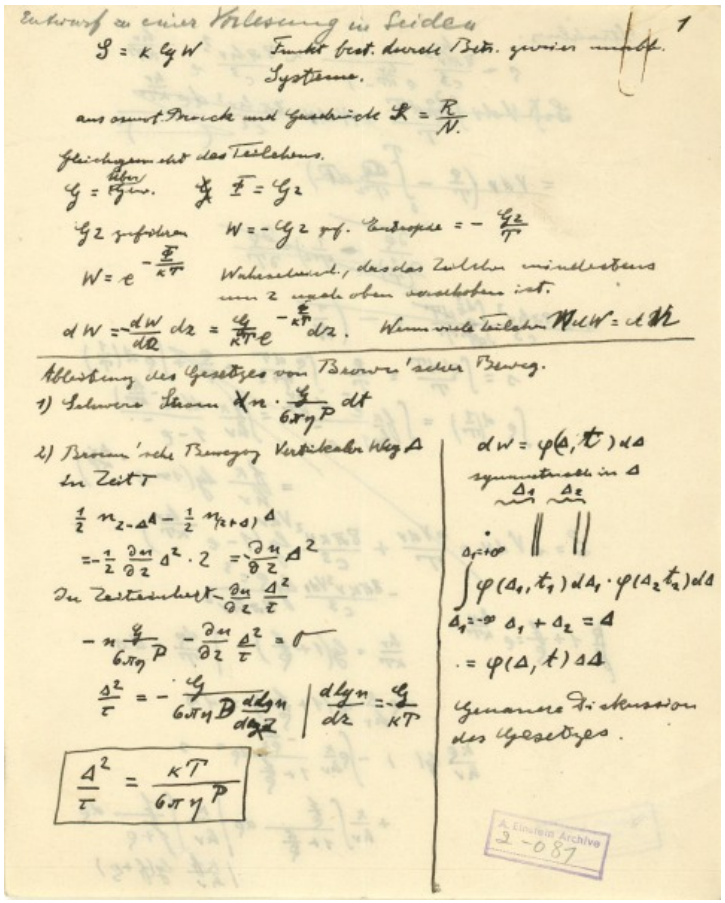
Brownian motion



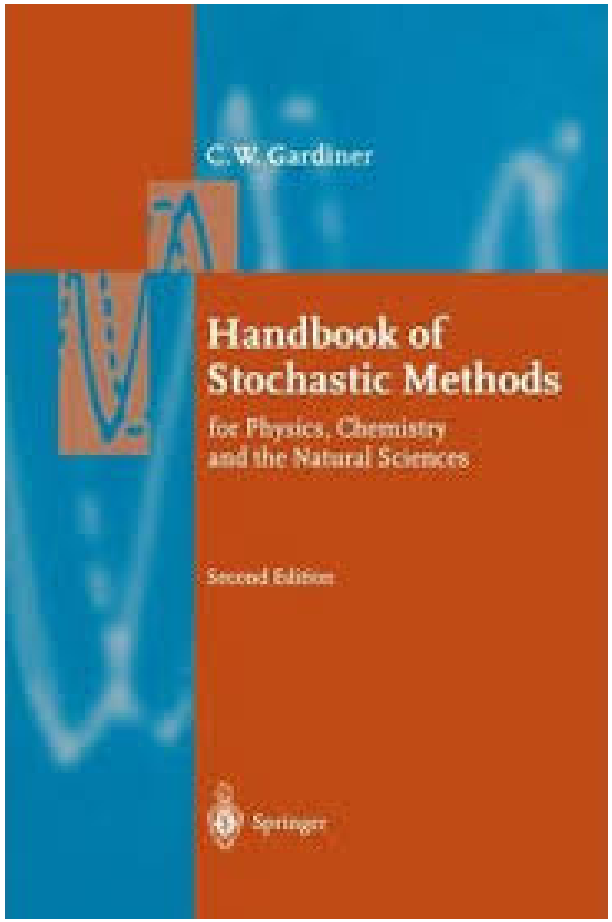
Small pollen grains in water move continuously and randomly. Why?

Water molecules hit pollen grains

Einstein explanation (1905): the birth of stochastic modeling of natural phenomena.



1. The motion is caused by the impact on the pollen grain of incessantly moving molecules of liquid.
2. The motion of these molecules is so complicated that the effects produced can be solely accessed probabilistically.
3. Assume exceedingly frequent statistically independent impacts


C. W. Gardiner
Handbook of
Stochastic Methods
for Physics, Chemistry
and the Natural Sciences
Second Edition
Springer

An extended excerpt of Einstein's paper (Gardiner's translation).

"It must clearly be assumed that each individual particle executes a motion which is independent of the motion of all other particles; it will also be considered that the movements of one and the same particle in the different time intervals are independent processes, as long as these time intervals are not chosen too small."

"We introduce a time interval τ into consideration, which is very small compared to the observable time intervals, but nevertheless so large that in two successive time intervals τ, the motion executed by the particle can be thought of as events which are independent of each other. "

Now let there be a total of n particles suspended in a liquid. In a time interval τ, the x-coordinate of the individual particle will increase of an amount Δ, where for each particle Δ has a different (positive or negative) value. There will be a certain frequency law for Δ; the number dn of the particles which experience a shift which is between Δ and $\Delta + d\Delta$ will be expressible by an equation of the form:

$$dn = n\phi(\Delta)d\Delta$$

where:

1. $\int_{-\infty}^{\infty} \phi(\Delta)d\Delta = 1$
2. ϕ is different from zero only for very small values of Δ.
3. ϕ is symmetric: $\phi(\Delta) = \phi(-\Delta)$.

Let $\nu = f(x,t)$ be the number of particles per unit volume. We compute the distribution of particles at the time $t+\tau$ from the distribution at time t. From the definition of the function $\phi(\Delta)$ it is easy to find the number of particles which at time $t+\tau$ are found between two planes perpendicular to the x-axis and passing through points x and $x+dx$. One obtains:

$$f(x,t+\tau)dx = dx\int_{-\infty}^{\infty} f(x+\Delta,t)\phi(\Delta)d\Delta \tag{1}$$

But since τ is small, $f(x,t+\tau) \simeq f(x,\tau) + \tau\frac{\partial f}{\partial t}$. Furthermore:

$$f(x+\Delta,t) \simeq f(x,t) + \Delta\frac{\partial f(x,t)}{\partial x} + \frac{\Delta^2}{2}\frac{\partial^2 f(x,t)}{\partial^2 x}$$

We can use this series under the integral, because only small values of Δ contribute to this equation. We obtain:

$$f + \frac{\partial f}{\partial t}\tau = f\int_{-\infty}^{\infty}\phi(\Delta)d\Delta + \frac{\partial f}{\partial x}\int_{-\infty}^{\infty}\Delta\phi(\Delta)d\Delta + \frac{\partial^2 f}{\partial^2 x}\int_{-\infty}^{\infty}\frac{\Delta^2}{2}\phi(\Delta)d\Delta$$

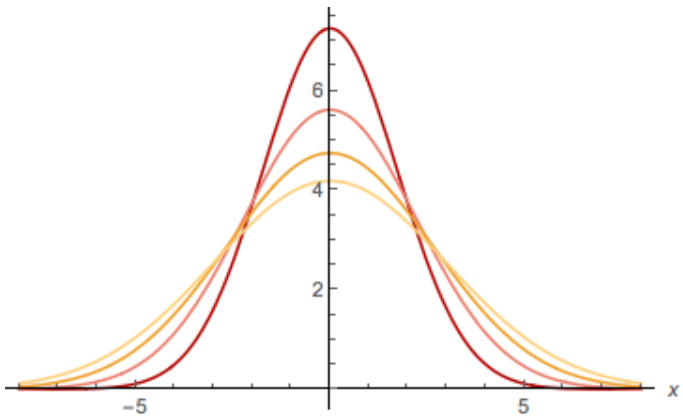
Because $\phi(\Delta) = \phi(-\Delta)$, then $\int_{-\infty}^{\infty} \Delta\phi(\Delta) = 0$. Recalling that $\int_{-\infty}^{\infty} \phi(\Delta)d\Delta = 1$ and setting:

$$\frac{1}{\tau}\int_{-\infty}^{\infty} \frac{\Delta^2}{2}\phi(\Delta)d\Delta \equiv D$$

yields:

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

$$f(x,t) = \frac{n}{\sqrt{4\pi D}}\frac{-x^2/4Dt}{\sqrt{t}}$$



A lot of smart ideas

1. The Chapman-Kolmogorov equation occurs as Einstein's equation (1). It states that the probability of the particle being at position x at time $t + \tau$ is given by the sum of the probability of all possible "jumps" Δ from position $x + \Delta$, multiplied by the probability of being at $x + \Delta$ at time t. Independence of the jumps on the previous history of the particles (Markov hypothesis).

2. The Fokker-Planck equation. The diffusion equation is a very special case of the so called Fokker-Planck equation which is encountered in a large class of interesting stochastic processes with continuous sample path.

3. The Kramers-Moyal and analogous expansion are similar to that used by Einstein to go from the Chapman-Kolmogorov equation to the diffusion equation.

Langevin: looking at individual trajectories.

From statistical mechanics, the mean kinetic energy of the Brownian particles is $\langle \frac{1}{2} m v^2 \rangle = \frac{1}{2} \kappa_B T$ where T is the absolute temperature and κ_B the Boltzmann 's constant. The forces acting on the particle should be:

1. A viscous drag: this is $-6\pi\eta a dx/dt$, η being the viscosity and a the diameter of the particles, assumed spherical.
2. A fluctuating force X which represents the impacts of the molecules of the liquid on the Brownian particle. It should be positive and negative with equal probability.

Hence:

$$m\frac{d^2x}{dt^2} = -6\pi\eta a\frac{dx}{dt} + X$$

After multiplying by x, the above equation can be cast in the form:

$$\frac{m}{2}\frac{d^2}{dt^2}\left(x^2\right) - mv^2 = -3\pi\eta a\frac{d\left(x^2\right)}{dt} + Xx$$

and averaging over a large set of particles yields an equation for $\langle x^2 \rangle$:

$$\frac{m}{2}\frac{d^2\langle x^2\rangle}{dt^2} + 3\pi\eta a\frac{d\langle x^2\rangle}{dt} = \kappa_B T$$

where $\langle Xx \rangle = 0$ because "of the irregularity of quantity X" (Langevin). One then finds:

$$\frac{d\langle x^2\rangle}{dt} = \kappa_B T/(3\pi\eta a) + C\exp\left(-6\pi\eta a t/m\right)$$

Langevin estimated that the time constant of the exponential is of the order 10^{-8} s. Thus one can neglect the exponential term to get:

$$\langle x^2\rangle - \langle x^2\rangle_0 = \left[\kappa_B T/\left(3\pi\eta a\right)\right] t$$

$$D = \kappa_B T/\left(6\pi\eta a\right)$$

1. The Einstein approach returns an equation for the evolution of the probability density function ($f \rightarrow P$) of seeing the Brownian particle in position x at time t.
2. The Langevin approach returns a stochastic differential equation for accessing the trajectory of individual Brownian particles.
3. Averaging over independent trajectories returns the probability density function P.
4. Determination of Avogadro constant by Perrin (atomic hypothesis): $N_A = R/\kappa_B$.

Stochastic processes

Suppose that a system has properties which can be described in terms of a single stochastic variable Y, for example, the number of molecules in a given volume of air, the number of people in a queue,..

Then we introduce the following quantities:

$$p(y,t) \equiv \quad \text{(the probability density that the stochastic variable } Y \text{ has value } y \text{ at time } t\text{)}$$

The expectation value of Y at time t is

$$\langle Y(t) \rangle = \int_{\text{all } y} dy\, y\, p(y,t)$$

Similarly

$$\langle Y^n(t) \rangle = \int_{\text{all } y} dy\, y^n\, p(y,t)\,, \qquad \langle f(Y(t)) \rangle = \int_{\text{all } y} dy\, f(y)\, p(y,t)\,,$$

$p(y_2, t_2; y_1, t_1) \equiv$ (the joint probability density that the stochastic variable Y has value y_1 at time t_1 and y_2 at time t_2)

So, for example, the expectation value of $Y(t_2)Y(t_1)$ is

$$\langle Y(t_2)Y(t_1)\rangle = \int dy_2\, dy_1\, y_2 y_1\, p(y_2, t_2; y_1, t_1)$$

If the value of Y at time t_2 is completely independent of the value of Y at time t_1, then

$$p(y_2, t_2; y_1, t_1) = p(y_2, t_2)p(y_1, t_1)\,,$$

and we find that

$$\langle Y(t_2)Y(t_1)\rangle = \int dy_2\, y_2\, p(y_2,t_2) \int dy_1\, y_1\, p(y_1,t_1) = \langle Y(t_2)\rangle\langle Y(t_1)\rangle$$

$$\Rightarrow \quad \langle Y(t_2)Y(t_1)\rangle - \langle Y(t_2)\rangle\langle Y(t_1)\rangle$$

is a measure of the *correlation* between Y at time t_2 and time t_1

$p(y_n, t_n; \ldots; y_2, t_2; y_1, t_1) \equiv$ (the joint probability density that the stochastic variable Y has value y_1 at time t_1, y_2 at time $t_2, \ldots, y_n$ at time t_n)

Marginal and conditional probabilities may be defined as follows:

$$\int dy_n \dots dy_{m+1}\, p(y_n, t_n; \dots; y_2, t_2; y_1, t_1)$$
$$= p(y_m, t_m; \dots; y_2, t_2; y_1, t_1) \quad [\text{marginal pdf }]$$

$$p(y_n, t_n; \dots; y_{m+1}, t_{m+1} | y_m, t_m; \dots; y_1, t_1)$$
$$= \frac{p(y_n, t_n; \dots; y_1, t_1)}{p(y_m, t_m; \dots; y_1, t_1)} \quad [\text{conditional pdf }]$$

Define two special types of stochastic process.

- A process is called stationary when all the probability densities depend on the time differences alone:

$$\begin{aligned} & p(y_n, t_n + \tau; \ldots; y_2, t_2 + \tau; y_1, t_1 + \tau) \\ & = p(y_n, t_n; \ldots; y_2, t_2; y_1, t_1) \quad \text{for all } n \text{ and } \tau \end{aligned}$$

So, for example, taking $\tau = -t_1$, then

$$p(y_1, t_1 - t_1) = p(y_1, t_1) \quad \Rightarrow \quad p(y_1, t_1) = p(y_1, 0) \equiv p(y_1)$$

is time-independent

Similarly by taking different values for τ,

$$p(y_2, t_2; y_1, t_1) = p(y_2, t_2 - t_1; y_1, 0) = p(y_2, 0; y_1, t_1 - t_2)\,,$$

and so depends only on the time difference

But

$$\langle Y(t_2)Y(t_1)\rangle = \int dy_2\, dy_1\, y_2 y_1\, p(y_2, t_2; y_1, t_1)$$

is symmetric under $t_1 \leftrightarrow t_2$ and so $\langle Y(t_2)Y(t_1)\rangle$ depends only on $|t_2 - t_1|$ when the process is stationary

- A process is called Gaussian if all the cumulants beyond the second vanish

$\Rightarrow$ A Gaussian process is fully specified by $\langle\langle Y(t_2)Y(t_1)\rangle\rangle$ and $\langle Y(t_1)\rangle$, or equivalently by $\langle Y(t_2)Y(t_1)\rangle$ and $\langle Y(t_1)\rangle$

Markov processes

A process is Markov if $p(y_{k+1}, t_{k+1}|y_k, t_k; \ldots; y_1, t_1)$ depends on the *state* $Y(t_k) = y_k$, but not on $Y(t_{k-1}) = y_{k-1}, \ldots, Y(t_1) = y_1$

i.e., $p(y_{k+1}, t_{k+1}|y_k, t_k; \ldots; y_1, t_1) = p(y_{k+1}, t_{k+1}|y_k, t_k) \, \forall k$

So the conditional pdfs are affected only by the state of the system at a given time, and not by the state of the system at times prior to this.

$$
\begin{aligned}
\text{(a)} \qquad & p(y_n, t_n; \ldots; y_1, t_1) \\
& = p(y_n, t_n|y_{n-1}, t_{n-1}; \ldots; y_1, t_1) p(y_{n-1}, t_{n-1}; \ldots; y_1, t_1) \\
= \quad & p(y_n, t_n|y_{n-1}, t_{n-1}) p(y_{n-1}, t_{n-1}|y_{n-2}, t_{n-2}; \ldots; y_1, t_1) \\
& \times p(y_{n-2}, t_{n-2}; \ldots; y_1, t_1) \\
& = \ldots = \prod_{i=1}^{n-1} p(y_{i+1}, t_{i+1}|y_i, t_i) p(y_1, t_1)
\end{aligned}
$$

(b)
$$
\begin{aligned}
& p(y_{k+\ell}, t_{k+\ell}; \ldots; y_{k+1}, t_{k+1} | y_k, t_k; \ldots; y_1, t_1) \\
&= \frac{\prod_{i=1}^{k+\ell-1} p(y_{i+1}, t_{i+1} | y_i, t_i) p(y_1, t_1)}{\prod_{i=1}^{k-1} p(y_{i+1}, t_{i+1} | y_i, t_i) p(y_1, t_1)} \\
&= \prod_{i=k}^{k+\ell-1} p(y_{i+1}, t_{i+1} | y_i, t_i)
\end{aligned}
$$

(a) tells us that for Markov processes all joint pdfs can be written down in terms of the functions $p(y', t' | y, t)$ and $p(y, t)$ and (b) tells us that for Markov processes all conditional pdfs can be written down in terms of $p(y', t' | y, t)$

Using (a) and (b) we can show that the hierarchy of pdfs related through the definition of marginal and conditional pdfs collapse down to just two relations between the functions $p(y', t' | y, t)$ and $p(y, t)$

These are:

$$(i) \qquad p(y_2, t_2) = \int dy_1 \, p(y_2, t_2 | y_1, t_1) p(y_1, t_1)$$

$$\begin{aligned} \underline{\textit{Proof}} \quad p(y_2, t_2) &= \int dy_1 \, p(y_2, t_2; y_1, t_1) \\ &= \int dy_1 \, p(y_2, t_2 | y_1, t_1) p(y_1, t_1) \end{aligned}$$

In fact we have not used the Markov assumption to derive the, rather obvious, result above

$$(ii) \qquad p(y_3, t_3 | y_1, t_1) = \int dy_2 \, p(y_3, t_3 | y_2, t_2) p(y_2, t_2 | y_1, t_1)$$

$$\begin{aligned} \underline{\textit{Proof}} \qquad & p(y_3, t_3; y_2, t_2; y_1, t_1) \\ & = p(y_3, t_3 | y_2, t_2) p(y_2, t_2 | y_1, t_1) p(y_1, t_1) \end{aligned}$$

Integrating over y_2 leads to

$$p(y_3, t_3; y_1, t_1) = \left\{ \int dy_2 \, p(y_3, t_3|y_2, t_2) p(y_2, t_2|y_1, t_1) \right\} p(y_1, t_1)$$

But $p(y_3, t_3; y_1, t_1) = p(y_3, t_3|y_1, t_1) p(y_1, t_1)$ and the result is proved

The result (ii) is called the *Chapman-Kolmogorov (CK) equation*. It is the starting point for the study of Markov processes

For a Markov process the functions $p(y', t'|y, t)$ and $p(y, t)$ are not arbitrary; they must satisfy conditions (i) and (ii)

Conversely, any two non-negative functions $p(y', t'|y, t)$ and $p(y, t)$ that obey (i) and (ii) uniquely define a Markov process

The CK equation tells us that we can break up the probability of transition from state y_1 at time t_1 to state y_3 at time t_3 into a process involving two successive steps which are statistically independent; the probability of the transition from y_2 to y_3 is not affected by the fact that it was preceded by a transition from y_1 to y_2

Markov chains

In this case the stochastic variables are discrete and will be labelled by an integer n

Then the two equations (i) and (ii) governing Markov processes take the form

$$p(n_2, t_2) = \sum_{n_1} p(n_2, t_2|n_1, t_1)p(n_1, t_1)$$

$$p(n_3, t_3|n_1, t_1) = \sum_{n_2} p(n_3, t_3|n_2, t_2)p(n_2, t_2|n_1, t_1) \quad t_1 < t_2 < t_3$$

In addition, we take time to be discrete, so that t also takes on integer values $t = 0, 1, \ldots$

If time is discrete, the Chapman-Kolmogorov (CK) equation tells us that the conditional probability at any time, $p(n, t'|m, t) \equiv p(n, t + \ell|m, t)$ $(\ell = 2, 3, \ldots)$, can be found if the function $p(n, t + 1|m, t)$ is known for all t

This follows because

$$p(n,t+2|m,t) = \sum_{n'} p(n,t+2|n',t+1)p(n',t+1|m,t)\,,$$
$$p(n,t+3|m,t) = \sum_{n'} p(n,t+3|n',t+1)p(n',t+1|m,t)\,, \quad \text{etc}$$

This fundamental conditional pdf can be thought of as a matrix:

$$Q_{nm}(t) \equiv p(n,t+1|m,t)$$

Such pdfs are called *transition probabilities* since they give the probability of the system making a transition from state m to state n

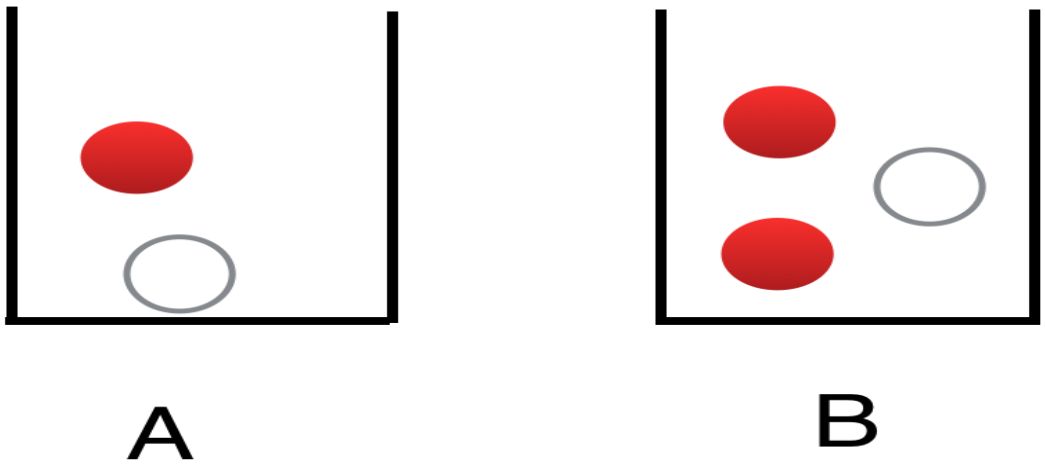
If we also write $p(n,t)$ as $P_n(t)$, then the first equation for Markov processes can be written as

$$P_n(t+1) = \sum_m Q_{nm}(t)P_m(t)$$

Urn model: balls of various colours in a pot

Suppose two pots, A and B, each contain 3 red balls and 2 white balls between them so that A always has 2 balls and B always has 3 balls.
Note: this is Exercise 5.1. of Reichl

What are the states of the system?



What are the transition probabilities?

To find these have to define the rules that govern the model.

Dynamical rule: at each time step pick a ball out of pot A at random and one out of pot B at random, and interchange them

- Start from state 1. It can only go to state 2.

$$\Rightarrow \quad Q_{11} = 0\,, \;\; Q_{21} = 1\,, \;\; Q_{31} = 0$$

- Start from state 2.

$$\begin{aligned}
&\text{To go to } n = 1 \quad : \quad \text{probability} \;\; = \frac{1}{2} \times \frac{1}{3} = \frac{1}{6} \\
&\text{To go to } n = 3 \quad : \quad \text{probability} \;\; = \frac{1}{2} \times \frac{2}{3} = \frac{1}{3} \\
&\text{To go to } n = 2 \quad : \quad \text{probability} \;\; = 1 - \frac{1}{6} - \frac{1}{3} = \frac{1}{2} \\
&n = 2 \text{ directly} \quad : \quad \text{probability} \;\; = \frac{1}{2} \times \frac{1}{3} + \frac{1}{2} \times \frac{2}{3} = \frac{1}{2}
\end{aligned}$$

$$\Rightarrow \quad Q_{12} = \frac{1}{6}\,, \;\; Q_{22} = \frac{1}{2}\,, \;\; Q_{32} = \frac{1}{3}$$

- Start from state 3.

$$\begin{aligned}
\text{To go to } n=1 \quad &: \quad \text{probability} \quad = 0 \\
\text{To go to } n=2 \quad &: \quad \text{probability} \quad = 1 \times \frac{2}{3} = \frac{2}{3} \\
\text{To go to } n=3 \quad &: \quad \text{probability} \quad = 1 \times \frac{1}{3} = \frac{1}{3}
\end{aligned}$$

$$\Rightarrow \quad Q_{13} = 0\,, \; Q_{23} = \frac{2}{3}\,, \; Q_{33} = \frac{1}{3}$$

So the transition probability matrix is:

$$Q = \begin{pmatrix} 0 & \frac{1}{6} & 0 \\ 1 & \frac{1}{2} & \frac{2}{3} \\ 0 & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

Notice that each of the columns add up to 1. Matrices which have this property and in addition have entries which are all non-negative, are called stochastic matrices.

So suppose we are given $P(0)$ — say that the system starts in state 2 at $t = 0$. This means that

$$P(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Then

$$P(1) = QP(0)\,;\ P(2) = QP(1) = Q^2P(0)\,;\ldots;\ P(3) = Q^3P(0)\ \ldots$$

Continuing in this way we arrive at the general result

$$P(t) = Q^tP(0)$$

We will discuss later how to study this for general t, but for the moment let's just look at what happens after one and two time steps in this example

Since

$$Q^2 = \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{9} \\ \frac{1}{2} & \frac{23}{36} & \frac{20}{36} \\ \frac{1}{3} & \frac{10}{36} & \frac{1}{3} \end{pmatrix},$$

we find that if we start in state 2, then after one step

$$P(1) = \begin{pmatrix} 0 & \frac{1}{6} & 0 \\ 1 & \frac{1}{2} & \frac{2}{3} \\ 0 & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{6} \\ \frac{1}{2} \\ \frac{1}{3} \end{pmatrix}$$

and after two steps

$$P(2) = \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{9} \\ \frac{1}{2} & \frac{23}{36} & \frac{20}{36} \\ \frac{1}{3} & \frac{10}{36} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{12} \\ \frac{23}{36} \\ \frac{10}{36} \end{pmatrix}$$

So, for example, the probability of being in state 2 having started in state 2 two time steps earlier, is 23/36

General solution of a Markov chain

Let us return to the general equation for Markov chains, when the transition probability is time-independent:

$$P(t) = Q^t P(0)$$

How do we solve it for general t?

Answer: We need to find the eigenvalues and eigenvectors of the matrix Q.

We first need to have an aside on the eigenvalues and eigenvectors of a (typically non-symmetric) matrix.

Let us look at the specific example:

$$M = \begin{pmatrix} -1 & 2 \\ -3 & 4 \end{pmatrix},$$

which clearly is not a stochastic matrix (its columns don't sum to unity, and it has negative entries).

So, we compute its eigenvalues in the usual way; subtract λ from the diagonals, and set the determinant to zero;

$$\begin{vmatrix} -1-\lambda & 2 \\ -3 & 4-\lambda \end{vmatrix} = 0 \quad \Rightarrow \quad \lambda^2 - 3\lambda + 2 = 0.$$

Thus, the characteristic equation (the one on the right, above) has solutions

$$\lambda^{(1)} = 1, \quad \lambda^{(2)} = 2.$$

We find what we will now call the *right eigenvectors* the way we "normally" find eigenvectors. That is, by solving

$$\begin{pmatrix} -1 & 2 \\ -3 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$$

for each of the cases $\lambda = 1, \lambda = 2$ separately

We shall denote the right eigenvector as $\psi^{(i)}$, corresponding to eigenvalue $\lambda^{(i)}$.

We find that

$$\lambda^{(1)} = 1 \quad \Rightarrow \quad \psi^{(1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

and

$$\lambda^{(2)} = 2 \quad \Rightarrow \quad \psi^{(2)} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}.$$

Now, to find the left eigenvectors $\chi^{(i)}$, which correspond to eigenvector $\lambda^{(i)}$, we solve

$$(x \quad y) \begin{pmatrix} -1 & 2 \\ -3 & 4 \end{pmatrix} = \lambda^{(i)} (x \quad y),$$

for each $\lambda^{(i)}$. So, for $\lambda^{(1)} = 1$, we see that

$$-x - 3y = x \quad \Rightarrow \quad \text{left eigenvector is} \quad (3 \quad -2),$$

and that for $\lambda^{(2)} = 2$, we see that

$$x = -y \quad \Rightarrow \quad \text{left eigenvector is} \quad (1 \quad -1).$$

Note that these eigenvectors are rows, rather than columns. We therefore denote them as $(\chi^{(i)})^T$. That is,

$$(\chi^{(1)})^T = (3 \quad -2) \quad \Leftrightarrow \quad \chi^{(1)} = \begin{pmatrix} 3 \\ -2 \end{pmatrix}$$

$$(\chi^{(2)})^T = (1 \quad -1) \quad \Leftrightarrow \quad \chi^{(2)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Now, by way of convenient notation, we denote right eigenvectors as kets $|\psi^{(i)}\rangle$, and left eigenvectors as bras $\langle\chi^{(i)}|$. Thus, notice the orthogonality of the two sets of eigenvectors:

$$\langle\chi^{(1)}|\psi^{(2)}\rangle = 6 - 6 = 0, \quad \langle\chi^{(2)}|\psi^{(1)}\rangle = 1 - 1 = 0.$$

They can also be normalised:

$$\langle\chi^{(1)}|\psi^{(1)}\rangle = 3 - 2 = 1,$$

so this set is already normalised, and

$$\langle\chi^{(2)}|\psi^{(2)}\rangle = 2 - 3 = -1,$$

so we simply multiply $\chi^{(2)}$ by -1.

Summary

$$\psi^{(1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad , \quad \psi^{(2)} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

$$\chi^{(1)} = \begin{pmatrix} 3 \\ -2 \end{pmatrix} \quad , \quad \chi^{(2)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$(\chi^{(1)})^T = (3 \quad -2) \quad , \quad (\chi^{(2)})^T = (-1 \quad 1)$$

Warning: M is not a stochastic matrix, so do not read anything into the nature of the eigenvalues or eigenvectors. In particular, the fact that one of the eigenvalues happens to be 1 and one of the eigenvectors $(1 \quad 1)^T$ will not be true for another choice of matrix.

With this, let us return to the study of Markov chains, and stochastic matrices (whose entries are all non-negative and where the entries in any one column add up to unity). We saw this latter property in the urn model example, but this is obviously true in general, since "something must happen".

Mathematically, this idea that some event must happen can be formulated by using the definition of Q. We see that it corresponds to

$$\sum_n Q_{nm} = \sum_n P(n, t+1|m, t) = 1,$$

so that the probability that the state transitions from state m at time t, to all other states n at time $t+1$, is unity.

Properties of stochastic matrices

- If Q_1 and Q_2 are stochastic matrices, so is $Q_1 Q_2$.
- If Q is a stochastic matrix, then so is any power of that matrix, Q^t.
- In our brief example, we saw that an eigenvalue $\lambda = 1$ appeared. This is a general property of stochastic matrices. All stochastic matrices have one eigenvalue which is unity. Corresponding to that eigenvalue, the left eigenvector is "unit". That is,

$$\lambda^{(1)} = 1, \quad (\chi^{(1)})^T = (1 \quad 1 \quad \dots \quad 1).$$

This follows just by writing the condition $\sum_n Q_{nm} = 1$ as

$$\sum_n \chi_n^{(1)} Q_{nm} = 1.\chi_m^{(1)},$$

where $\chi_n^{(1)} = 1$ for all n. Note that our example during the brief aside, was not a stochastic matrix, and therefore this left eigenvector did not appear.

- Suppose that Q is time-independent. Then at large times $P(t)$ may approach a time-independent value called P^{st} — the *stationary state*. In that case $P(t+1)$ and $P(t)$ both equal P^{st}, so that

  $$P(t+1) = QP(t),$$

  becomes

  $$P^{st} = QP^{st},$$

  which is merely an eigenvalue equation, corresponding to eigenvalue 1. That is,

  $$QP^{st} = 1.P^{st}.$$

  so that P_n^{st} is a right-eigenvector of Q with eigenvalue 1

Note that

$$(1 \quad 1 \quad \dots \quad 1) \begin{pmatrix} P_1^{st} \\ P_2^{st} \\ \vdots \end{pmatrix} = \sum_n P_n^{st} = 1,$$

so that the correct normalisation of P^{st} implies that $(\chi^{(1)})^T \psi^{(1)} = 1$ and visa-versa.

- All eigenvalues of a stochastic matrix have modulus ≤ 1,

$$|\lambda^{(i)}| \leq 1, \quad \forall i.$$

(see Reichl p236 for a proof).

Finally, if the matrix is symmetric, $Q^T = Q$, then the left- and right-eigenvectors are the same.

Example 3 red balls and 2 white balls in urns A and B (continued)

Let us compute the right & left eigenvectors for our previous transition matrix for the urn model:

$$Q = \begin{pmatrix} 0 & 1/6 & 0 \\ 1 & 1/2 & 2/3 \\ 0 & 1/3 & 1/3 \end{pmatrix}.$$

We compute eigenvalues via

$$\begin{vmatrix} -\lambda & 1/6 & 0 \\ 1 & 1/2-\lambda & 2/3 \\ 0 & 1/3 & 1/3-\lambda \end{vmatrix} = 0,$$

which results in the characteristic equation

$$\lambda^3 - \tfrac{5}{6}\lambda^2 - \tfrac{2}{9}\lambda + \tfrac{1}{18} = 0.$$

To solve this cubic, we first note that we know that one factor is $\lambda = 1$ (it being a stochastic matrix implies that there is one unit eigenvalue). Thus, we factorise, correctly choosing the λ^3 and λ^0 coefficients:

$$(\lambda - 1)(\lambda^2 + a\lambda - \tfrac{1}{18}) = 0.$$

If we expand this out, and compare the powers of λ^2 with the original characteristic equation, we find that $a = \frac{1}{6}$.

Therefore,

$$(\lambda - 1)(\lambda^2 + \tfrac{1}{6}\lambda - \tfrac{1}{18}) = 0,$$

which further factorises to

$$(\lambda - 1)(\lambda + \tfrac{1}{3})(\lambda - \tfrac{1}{6}) = 0.$$

So the three eigenvalues are

$$\lambda^{(1)} = 1, \quad \lambda^{(2)} = -\tfrac{1}{3}, \quad \lambda^{(3)} = \tfrac{1}{6}.$$

Now, corresponding to $\lambda^{(1)} = 1$, we know that the left eigenvector is just

$$(\chi^{(1)})^T = (1 \quad 1 \quad 1), \quad \lambda^{(1)} = 1.$$

So, to find the corresponding right eigenvector, $\psi^{(1)}$, we solve in the usual way:

$$\begin{pmatrix} 0 & 1/6 & 0 \\ 1 & 1/2 & 2/3 \\ 0 & 1/3 & 1/3 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 1. \begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

to give

$$\psi^{(1)} = \begin{pmatrix} 1 \\ 6 \\ 3 \end{pmatrix}.$$

This is the stationary state; but, to correctly normalise it so that $\langle \chi^{(1)} | \psi^{(1)} \rangle = 1$, we note that

$$(1 \quad 1 \quad 1) \begin{pmatrix} 1 \\ 6 \\ 3 \end{pmatrix} = 10; \quad \psi^{(1)} = P^{st} = \begin{pmatrix} 1/10 \\ 3/5 \\ 3/10 \end{pmatrix}.$$

And thus, we have found the stationary state. The other eigenvectors are fairly easily found to be

$$\lambda^{(2)} = -\tfrac{1}{3} \quad \Rightarrow \quad \psi^{(2)} = \begin{pmatrix} 1/6 \\ -1/3 \\ 1/6 \end{pmatrix}, \quad \chi^{(2)} = \begin{pmatrix} 3 \\ -1 \\ 1 \end{pmatrix}$$

and

$$\lambda^{(3)} = \tfrac{1}{6} \quad \Rightarrow \quad \psi^{(3)} = \begin{pmatrix} -4/15 \\ -4/15 \\ 8/15 \end{pmatrix}, \quad \chi^{(3)} = \begin{pmatrix} -3/2 \\ -1/4 \\ 1 \end{pmatrix}.$$

Remember that we get the $\chi^{(i)}$ in the form of a row vector, $(\chi^{(i)})^T$. To continue, we make the identification

$$\psi^{(i)} \longmapsto |\psi^{(i)}\rangle, \quad (\chi^{(i)})^T \longmapsto \langle\chi^{(i)}|,$$

and so, using this notation, we see orthonormality:

$$\langle\chi^{(1)}|\psi^{(3)}\rangle = 0.$$

Also note, as $\psi^{(2),(3)}$ are orthogonal to $\chi^{(1)}$, their entries must sum to zero (which they do).

General theory of eigenvectors of Q

We now prove various relations, in a very similar fashion to quantum mechanics. This theory does not rely on the matrix being stochastic; it is true for any matrix.

So suppose Q is a (time-independent) $M \times M$ matrix. It will have M eigenvalues in general. If Q is symmetric the eigenvalues will be real, otherwise they may be complex

Corresponding to the ith eigenvalue $\lambda^{(i)}$, there will be a right-eigenvector (or eigenstate) $|\psi^{(i)}\rangle$ and a left-eigenvector (or eigenstate) $\langle\chi^{(i)}|$ such that

$$Q|\psi^{(i)}\rangle = \lambda^{(i)}|\psi^{(i)}\rangle \quad \text{and} \quad \langle\chi^{(i)}|Q = \lambda^{(i)}\langle\chi^{(i)}|$$

Orthogonality

Forming the product of the above eigenvalue equations, with a bra-state on the first, and a ket-state on the second, we have that

$$\langle\chi^{(j)}|Q|\psi^{(i)}\rangle = \lambda^{(i)}\langle\chi^{(j)}|\psi^{(i)}\rangle, \quad \langle\chi^{(i)}|Q|\psi^{(j)}\rangle = \lambda^{(i)}\langle\chi^{(i)}|\psi^{(j)}\rangle.$$

Interchanging indices in the second expression gives

$$\langle \chi^{(j)} | Q | \psi^{(i)} \rangle = \lambda^{(j)} \langle \chi^{(j)} | \psi^{(i)} \rangle.$$

Subtracting the two expressions now gives

$$0 = (\lambda^{(i)} - \lambda^{(j)}) \langle \chi^{(j)} | \psi^{(i)} \rangle.$$

So, if $\lambda^{(i)} \neq \lambda^{(j)}$, then this simply reads

$$\langle \chi^{(j)} | \psi^{(i)} \rangle = 0, \quad \lambda^{(i)} \neq \lambda^{(j)}.$$

If we have chosen to normalise the eigenvectors, then

$$\langle \chi^{(j)} | \psi^{(i)} \rangle = \delta_{ij}, \tag{2}$$

which is the statement of orthonormality: right and left eigenvectors corresponding to different eigenvalues are orthonormal to each other.

Completeness

Since $\{|\psi^{(i)}\rangle\}$ are a complete set of states, we can expand any probability vector in terms of them:

$$|P\rangle = \sum_{i=1}^{M} \alpha_i |\psi^{(i)}\rangle.$$

So, forming the product of this with a bra-state gives

$$\langle\chi^{(j)}|P\rangle = \sum_{i=1}^{M} \alpha_i \langle\chi^{(j)}|\psi^{(i)}\rangle,$$

which, by our orthonormality statement, is simply

$$\langle\chi^{(j)}|P\rangle = \sum_{i=1}^{M} \alpha_i \langle\chi^{(j)}|\psi^{(i)}\rangle = \sum_{i=1}^{M} \alpha_i \delta_{ij} = \alpha_j.$$

This identifies the α_i:

$$\alpha_i = \langle\chi^{(i)}|P\rangle.$$

Then, using this in our original expansion,

$$|P\rangle = \sum_{i=1}^{M} |\psi^{(i)}\rangle \alpha_i = \left\{ \sum_{i=1}^{M} |\psi^{i}\rangle\langle\chi^{(i)}| \right\} |P\rangle.$$

But this is true for any $|P\rangle$, so that

$$\sum_{i=1}^{M} |\psi^{(i)}\rangle\langle\chi^{(i)}| = I, \tag{3}$$

where I is the $M \times M$ identity matrix.

We note the following important relation which follows by multiplying (3) by Q:

$$\begin{aligned} Q &= \sum_{i=1}^{M} Q|\psi^{(i)}\rangle\langle\chi^{(i)}| \\ &= \sum_{i=1}^{M} \lambda^{(i)}|\psi^{(i)}\rangle\langle\chi^{(i)}| \end{aligned}$$

How does all this help us to solve $P(t) = Q^t P(0)$?

Well, if Q has eigenvalues $\lambda^{(i)}$ and eigenvectors $\langle\chi^{(i)}|$ and $|\psi^{(i)}\rangle$, then Q^t has eigenvalues $(\lambda^{(i)})^t$ and also has eigenvectors $\langle\chi^{(i)}|$ and $|\psi^{(i)}\rangle$

This is easy to prove by induction: assume Q^N has eigenvalues $(\lambda^{(i)})^N$ and eigenvectors $\langle\chi^{(i)}|$ and $|\psi^{(i)}\rangle$. Then $Q^{N+1}|\psi^{(i)}\rangle = Q.Q^N|\psi^{(i)}\rangle$ which equals $Q(\lambda^{(i)})^N|\psi^{(i)}\rangle = (\lambda^{(i)})^{N+1}|\psi^{(i)}\rangle$. So if it is true for N, it is true for $N+1$. Since it is true for $N=1$, it is true for all N. A similar proof holds for the left eigenvector.

Now just as we obtained an important relation above by multiplying (3) by Q, we can obtain a generalisation by multiplying (3) by Q^t:

$$\begin{aligned} Q^t &= \sum_{i=1}^{M} Q^t|\psi^{(i)}\rangle\langle\chi^{(i)}| \\ &= \sum_{i=1}^{M} (\lambda^{(i)})^t|\psi^{(i)}\rangle\langle\chi^{(i)}| \end{aligned} \tag{4}$$

Equation (4) is a key result, because it shows that if we can find the eigenvalues and eigenvectors of Q, we can calculate Q^t.

Notice that this implies that

$$P(t) = Q^t P(0) = \sum_{i=1}^{M} (\lambda^{(i)})^t |\psi^{(i)}\rangle\langle\chi^{(i)}|P(0)\rangle.$$

All the quantities on the right-hand side can be found from a knowledge of Q.

Example The urn model, Exercise 5.1 from Reichl, continued.

Let us return to the urn models matrix & eigenvectors, to compute an arbitrary power of the matrix.
For $\lambda^{(1)} = 1$, we see that

$$|\psi^{(1)}\rangle\langle\chi^{(1)}| = \begin{pmatrix} 1/10 \\ 3/5 \\ 3/10 \end{pmatrix} (1 \quad 1 \quad 1) = \begin{pmatrix} 1/10 & 1/10 & 1/10 \\ 3/5 & 3/5 & 3/5 \\ 3/10 & 3/10 & 3/10 \end{pmatrix} \equiv Q_1.$$

For $\lambda^{(2)} = -1/3$, we see that

$$|\psi^{(2)}\rangle\langle\chi^{(2)}| = \begin{pmatrix} 1/6 \\ -1/3 \\ 1/6 \end{pmatrix} (3 \quad -1 \quad 1) = \begin{pmatrix} 1/2 & -1/6 & 1/6 \\ -1 & 1/3 & -1/3 \\ 1/2 & -1/6 & 1/6 \end{pmatrix} \equiv Q_2.$$

And finally, for $\lambda^{(3)} = 1/6$, we see that

$$|\psi^{(3)}\rangle\langle\chi^{(3)}| = \begin{pmatrix} 2/5 & 1/15 & -4/15 \\ 2/5 & 1/15 & -4/15 \\ -4/5 & -2/15 & 8/15 \end{pmatrix} \equiv Q_3.$$

So, an arbitrary power of Q may be found from

$$Q^t = Q_1 + (-\tfrac{1}{3})^t Q_2 + (\tfrac{1}{6})^t Q_3.$$

Thus, we have a way of computing

$$P(t) = Q^t P(0).$$

Now, we can notice a few things from this. First, note that the smallest eigenvalue will have little effect on the late-time behaviour of the system. That is, for high t, the last term will be negligible. The next largest eigenvalue gives the dominant large t behaviour. Second, notice that if any of the eigenvalues had been > 1, then the system would have diverged. Finally, the very-large t behaviour is completely determined by Q_1.

If the initial state of the system is, for instance, $P(0)^T = (1\ 0\ 0)$, then multiplying the above expression for Q^t into this gives

$$P(t) = \begin{pmatrix} 1/10 \\ 3/5 \\ 3/10 \end{pmatrix} + \left(-\frac{1}{3}\right)^t \begin{pmatrix} 1/2 \\ -1 \\ 1/2 \end{pmatrix} + \left(\frac{1}{6}\right)^t \begin{pmatrix} 2/5 \\ 2/5 \\ -4/5 \end{pmatrix}$$

From this we can calculate, for example, the mean

$$\langle n(t) \rangle = \sum_{n=1}^{3} nP(n,t) = P(1,t) + 2P(2,t) + 3P(3,t) = \frac{11}{5} - \frac{6}{5}\left(\frac{1}{6}\right)^t$$