5 Stochastic dynamics (Murray, Ch. 11)

So far we have considered simplified mathematical models for growth and interaction of populations, as well as chemical reactions. These have been deterministic models: the populations|concentrations are uniquely determined by the initial conditions. But in reality population sizes and chemical concentrations do not follow deterministic laws. More realistic stochastic models take into account of stochastic fluctuations of the population size and chemical concentrations.

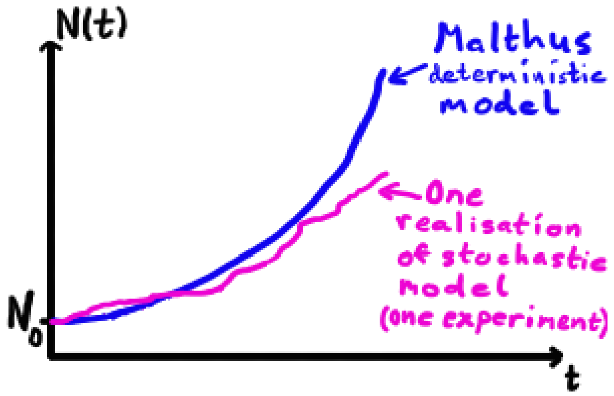
5.1 Deterministic versus stochastic growth models (Okubo, Chapter 1.3)

As an illustrative example, consider Malthus' growth model due to births only (per capita birth rate r, no deaths nor migration)

$$\dot{N} = rN \qquad \Rightarrow \qquad N(t) = N_0 e^{rt} \,.$$

If r is constant, then $N(t)$ is uniquely determined by the initial size N_0.

Now consider an experiment (numerical or real-world) where the population increases due to births. Let $r \cdot \delta t$ denote the probability that in a small time interval, δt, one individual gives birth to another individual (r is an average per capita birth rate). In this formulation the size evolution $N(t)$ varies from experiment to experiment, even though r and N_0 are kept fixed:



Let $Q_N(t)$ be the probability to have N individuals at discrete time steps $t \in n\delta t$ with integer n. The following stochastic model determines how this probability changes with time:

$$Q_N(t) = Q_N(t - \delta t) + r\delta t(N-1)Q_{N-1}(t - \delta t) - r\delta t N Q_N(t - \delta t)\,.$$

The second term on the right-hand side is the gain in probability from the previous time step due to births causing transitions $N - 1 \to N$. The third term is the loss in probability due to births, $N \to N + 1$.

Move the term $Q_N(t - \delta t)$ to the left-hand side, divide by δt and take limit $\delta t \to 0$ to form a differential equation (Master equation)

$$\frac{\mathrm{d}Q_N}{\mathrm{d}t} = r(N-1)Q_{N-1}(t) - rNQ_N(t) \tag{1}$$

with initial condition $Q_N(0) = \delta_{N,N_0}$.

As seen in the figure above, a realisation of the stochastic model in general differ from the deterministic model. To obtain the average result of the stochastic model, multiply Eq. (1) with N and sum over N

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\sum_{N=0}^{\infty} NQ_N &= r\sum_{N=0}^{\infty} N(N-1)Q_{N-1}(t) - r\sum_{N=0}^{\infty} N^2 Q_N(t)\\
&\quad\text{[Change of variable } N = N' + 1 \text{ in the first sum]}\\
&= r\sum_{N'=-1}^{\infty}(N'+1)N'Q_{N'}(t) - r\sum_{N=0}^{\infty} N^2 Q_N(t)\\
&\quad\text{[First term is zero in first sum. Relabel } N' \to N\text{]}\\
&= r\sum_{N=0}^{\infty} NQ_N(t)\,.
\end{aligned}$$

Using that the expectation value of the population size N at time t is

$$\langle N(t)\rangle = \sum_{N=0}^{\infty} NQ_N(t)$$

we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle N(t)\rangle = r\langle N(t)\rangle\,.$$

The average of the stochastic variable $N(t)$ follows the deterministic growth law (true for linear systems, but may fail for non-linear ones). As a result $\langle N(t)\rangle = N_0 e^{rt}$. A similar calculation gives the standard deviation:

$$\mathrm{std}(N(t)) \equiv \sqrt{\langle N(t)^2\rangle - \langle N(t)\rangle^2} = \sqrt{N_0} e^{rt}\sqrt{1-e^{-rt}}\,.$$

For large t the relative standard deviation becomes

$$\frac{\mathrm{std}(N(t))}{\langle N(t)\rangle} \sim N_0^{-1/2}\,.$$

Thus, a larger initial population gives better agreement between the deterministic law and one realization of the stochastic process. This latter result holds quite generally (also for non-linear systems). However, there are also critical differences between the models. If deaths were included in the models such that

$$r = \text{'rate of births'} - \text{'rate of deaths'} > 0$$

the population increases monotonously in the deterministic model. In a stochastic model with births and deaths there is always a finite (but in general small) probability that the population becomes extinct. Later in the course we will consider stochastic effects of finite population sizes in the context of disease spreading.

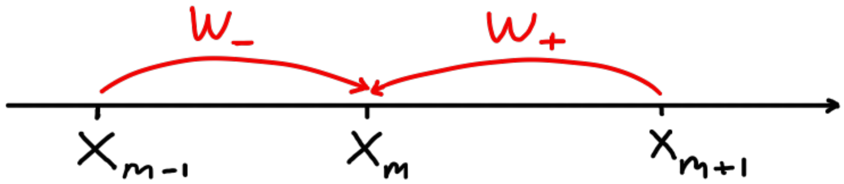
5.2 One-dimensional diffusion (M 11.1)

In the example above, a stochastic model was introduced to model temporal fluctuations in births. If the population size is large enough, this is not a problem and we can treat the growth deterministically.

Another stochastic aspect of the evolution of a population is spatial spread. As a simplest example the individuals of a population move randomly and independent of each other, a random walk.

5.2.1 One-dimensional random walk

Consider an individual, or a particle in general, moving at discrete coordinates $x_m \equiv m\delta x$ along the x-axis:



Assume that at each time step δt the particle makes a jump to a neighbouring discrete coordinate. Let w_- be the probability that the jump is $+\delta x$, i.e. w_- is the transition probability to move from $x_{m-1} \to x_m$. Analogously, w_+ is the transition probability from $x_{m+1} \to x_m$. The assumption that the particle jumps either $-\delta x$ or $+\delta x$ each time step gives $w_+ + w_- = 1$.

This process gives the possible particle positions $-n\delta x, \ldots, n\delta x$ at time $n\delta t$. However, one should expect the probability to be higher close to $x = 0$. To find the time evolution of the spatial probability distribution, let $Q(x,t)$ be the probability to find the particle at discrete position $x \in m\delta x$ at discrete time steps $t \in n\delta t$ (m and n integers), given it was at $x = 0$ at $t = 0$. For the random walk we have:

$$Q(x,t) = w_- Q(x-\delta x, t-\delta t) + w_+ Q(x+\delta x, t-\delta t)\,. \tag{2}$$

We want to find an equation for Q in the continuous limit $\delta t \to 0$ and $\delta x \to 0$. Series expand the Q:s on the r.h.s. in Eq. (2)

$$Q(x\pm\delta x, t-\delta t) = Q \pm \delta x\frac{\partial Q}{\partial x} - \delta t\frac{\partial Q}{\partial t} + \frac{\delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} \mp \delta x\delta t\frac{\partial^2 Q}{\partial x\partial t} + \frac{\delta t^2}{2}\frac{\partial^2 Q}{\partial t^2} + \ldots$$

where $Q \equiv Q(x,t)$. Insert this expansion into Eq. (2), using $w_+ = 1 - w_-$ and define $\epsilon \equiv w_- - w_+$:

$$\begin{aligned}
Q &= Q - \epsilon\delta x\frac{\partial Q}{\partial x} - \delta t\frac{\partial Q}{\partial t} + \frac{\delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} + \epsilon\delta x\delta t\frac{\partial^2 Q}{\partial x\partial t} + \frac{\delta t^2}{2}\frac{\partial^2 Q}{\partial t^2} + \ldots\\
\Rightarrow \frac{\partial Q}{\partial t} &= -\frac{\epsilon\delta x}{\delta t}\frac{\partial Q}{\partial x} + \frac{\delta x^2}{2\delta t}\frac{\partial^2 Q}{\partial x^2} + \epsilon\delta x\frac{\partial^2 Q}{\partial x\partial t} + \frac{\delta t}{2}\frac{\partial^2 Q}{\partial t^2} + \ldots
\end{aligned}$$

Take δt, δx and ϵ to zero such that

$$\frac{\delta x^2}{2\delta t} \to D \tag{3}$$
$$\frac{\delta x \epsilon}{\delta t} \to v\,, \tag{4}$$

where $D > 0$ and v are constants. This gives the continuous probability $Q(x,t)$ to find a particle at (continuous) position x and time t

$$\frac{\partial Q}{\partial t} = \underbrace{-v\frac{\partial Q}{\partial x}}_{\text{Advection (Drift)}} + \underbrace{D\frac{\partial^2 Q}{\partial x^2}}_{\text{Diffusion}} . \tag{5}$$

This is an example of an advection-diffusion equation. Eq. (5) is also satisfied for concentrations $n(x,t) = Q(x,t)N/V$ (here N is the total number of entities enclosed in a volume V).

5.2.2 Probability moments

To investigate Eq. (5), consider the moments

$$m_p(t) \equiv \langle x^p \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, x^p Q(x,t)\,.$$

$Q(x,t)$ is a probability distribution $\Rightarrow m_0(t) = 1$ at all times.
Assume that particle is initially localized at $x = 0$:

$$Q(x, t=0) = \delta(x)$$
$$\Rightarrow\ m_p(0) = \begin{cases} 0 & \text{if } p > 0 \\ 1 & \text{if } p = 0 \text{ (normalisation)} \end{cases}$$

Multiply Eq. (5) by x^p and integrate over x

$$\underbrace{\int_{-\infty}^{\infty} \mathrm{d}x\, x^p \frac{\partial Q}{\partial t}}_{\frac{\partial m_p}{\partial t}} = -v\int_{-\infty}^{\infty} \mathrm{d}x\, x^p \frac{\partial Q}{\partial x} + D\int_{-\infty}^{\infty} \mathrm{d}x\, x^p \frac{\partial^2 Q}{\partial x^2} = [\text{P.I.}]$$

$$= \underbrace{\left[-vx^pQ + x^p\frac{\partial Q}{\partial x}\right]_{-\infty}^{\infty}}_{0} + pv\underbrace{\int_{-\infty}^{\infty} \mathrm{d}x\, x^{p-1}Q}_{m_{p-1}} - pD\int_{-\infty}^{\infty} \mathrm{d}x\, x^{p-1}\frac{\partial Q}{\partial x}$$

$$= pvm_{p-1} - pD\underbrace{\left[x^{p-1}Q\right]_{-\infty}^{\infty}}_{0} + p(p-1)D\underbrace{\int_{-\infty}^{\infty} \mathrm{d}x\, x^{p-2}Q}_{m_{p-2}}$$

$$\Rightarrow \partial_t m_p = pvm_{p-1} + p(p-1)Dm_{p-2}$$

Case $p = 0$: $\partial_t m_0 = 0 \Rightarrow m_0 = 1$ (normalisation)

Case $p = 1$: $\partial_t m_1 = 1 \cdot v \cdot 1 + 0 \Rightarrow m_1 = vt$

(average position moves with const. velocity v)

Case $p = 2$: $\partial_t m_2 = 2 \cdot v \cdot (vt) + 2 \cdot 1 \cdot D \cdot 1 \Rightarrow m_2 = v^2t^2 + 2Dt$

The mean square displacement (when $x_0 = 0$) becomes

$$\mathrm{var}(x) = \langle (x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = m_2 - m_1^2 = 2Dt\,. \qquad (6)$$

Eq. (6) is the characteristic law of diffusion, the mean square displacement grows linearly in time. The constant D is the diffusion coefficient. Note that Eq. (6) is a macroscopic equation (valid at macroscopic length and time scales), while Eq. (3) is a microscopic law.

5.2.3 Diffusion equation

For the special case $v = 0$ in Eq. (5) we get the diffusion equation:

$$\frac{\partial Q}{\partial t} = D\frac{\partial^2 Q}{\partial x^2}\,. \qquad (7)$$

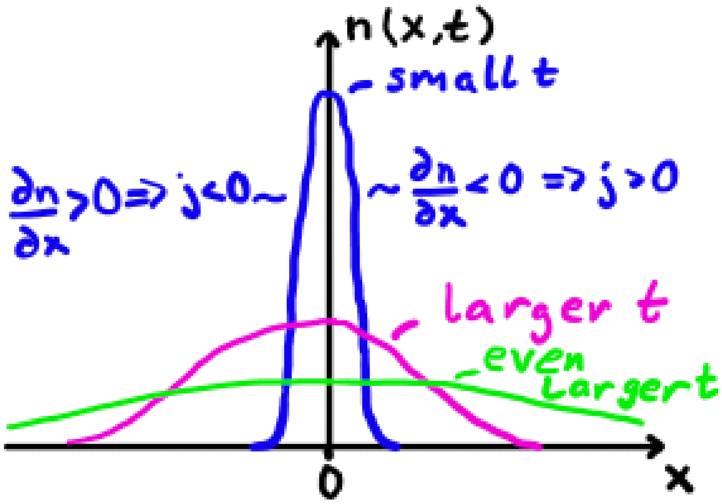
When $v = 0$, there is no net drift, $\langle x\rangle = 0$, but the mean square displacement increases with time: $\langle x^2\rangle = 2Dt$ (diffusion).

5.3 Macroscopic view of diffusion

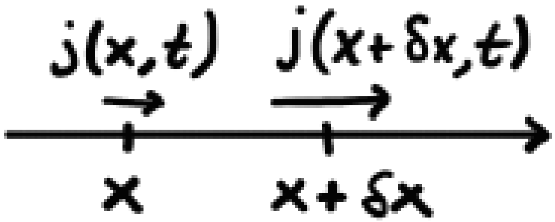
The diffusion equation in the previous section was derived from a microscopic viewpoint, where the detailed motion of individual particles (the random walk) led to an equation for the macroscopic probability distribution Q. It is also possible to derive the diffusion equation starting from a macroscopic viewpoint. According to Fick's law matter is transported from high concentrations to low concentrations:

$$j(x,t) = -D\frac{\partial n}{\partial x}\,.$$

Here n is particle concentration, $n(x,t) = Q(x,t)N/V$ and the matter flux $j(x,t)$ denotes the transport of matter in the x-direction per 'unit area' and unit time. The effect of Fick's law is to spread out sharp concentration gradients:



The change of concentration in a small interval δx



is

$$\frac{\partial}{\partial t}\int_x^{x+\delta x} \mathrm{d}x' n(x',t) = j(x,t) - j(x+\delta x,t)\,.$$

Divide by δx and let $\delta x \to 0$ to get

$$\frac{\partial n}{\partial t} = -\frac{\partial j}{\partial x} = D\frac{\partial^2 n}{\partial x^2}\,.$$

i.e. same as the diffusion equation Eq. (7).