## 5.2 Continuum limit

5.2.1 Drift and diffusion

Let us now consider evolving probabilities for a generic situation where the states are ordered along a line, such as in the previous examples with population size $n = 0, 1, 2 \cdots, N$. The general form of the Master equation is

$$\frac{dp_n}{dt} = + \sum_{m \neq n} R_{nm} p_m - \sum_{m \neq n} R_{mn} p_n \,. \tag{5.2.1}$$

In many relevant circumstances the number of states is large, and the probability varies smoothly from one value of n to the next. In such cases it is reasonable to replace the discrete index n with a continuous variable x, the probabilities $p_n(t)$ with a probability density $p(x, t)$, and the rates R_{mn} with a rate function $R(x', x)$. The rate function R depends on two variables x and x', denoting respectively the start and end positions for a transition along the line. We have the option of redefining the two arguments of this function, and it is useful to reparameterize it as $\tilde{R}(x' - x, x) \equiv R(x', x)$ indicating the rate at which, starting from the position x, a transition is made to a position $\Delta x = x' - x$ away. As in the case of mutations, there is usually a preference for changes that are *local*, i.e. with rates that decay rapidly when the separation $x' - x$ becomes large.
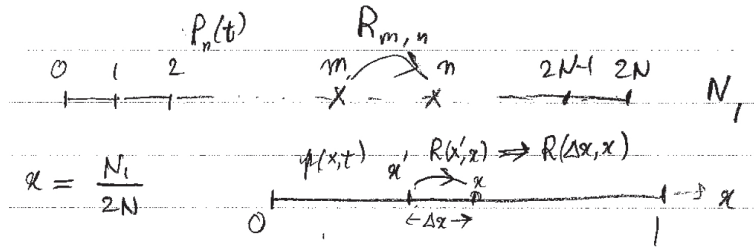
These transformations and relabelings,

$$n \to x, \ p_n(t) \to p(x, t), \ R_{mn} \to \tilde{R}(x' - x, x) \,, \tag{5.2.2}$$

enable us to transform Eq. (5.2.1) to the continuous integral equation

$$\frac{\partial}{\partial t} p(x, t) = + \int^* dx' \tilde{R}(x - x', x') p(x', t) - \int^* dx' \tilde{R}(x' - x, x) p(x, t) \,. \tag{5.2.3}$$

Some care is necessary in replacing the sums with integrals, as the summations in Eq. (5.2.1) exclude the term with $m = n$. To treat this restriction in the continuum limit, we focus on an interval y around any point x, and consider the change in probability due to incoming flux from $x - y$ and the outgoing flux to $x + y$, thus arriving at[3]

$$\frac{\partial}{\partial t} p(x, t) = \int dy \left[\tilde{R}(y, x - y) p(x - y) - \tilde{R}(y, x) p(x) \right] \,. \tag{5.2.4}$$

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[3] In Eq. (5.2.3) this amounts to change of variable from x' to $(x - y)$ in the first integral, and to $(x + y)$ in the second.

Note that the contribution for $y = 0$ is now clearly zero. The flux difference for small y is now estimated by a Taylor expansion of the first term in the square bracket, *but only with respect to the location of the incoming flux*, treating the argument pertaining to the separation of the two points as fixed, i.e.

$$\tilde{R}(y, x-y)p(x-y) = \tilde{R}(y, x)p(x) - y\frac{\partial}{\partial x}\left(\tilde{R}(y, x)p(x)\right) + \frac{y^2}{2}\frac{\partial^2}{\partial x^2}\left(\tilde{R}(y, x)p(x)\right) + \cdots . \quad (5.2.5)$$

While formally correct, the above expansion is useful only in cases where typical values of y are small (i.e. when only almost *local* transitions occur). Keeping terms up to the second order, Eq. (5.2.4) can be rewritten as

$$\frac{\partial}{\partial t}p(x, t) = -\int dy\, y\frac{\partial}{\partial x}(\tilde{R}(y, x)p(x)) + \frac{1}{2}\int dy\, y^2\frac{\partial^2}{\partial x^2}(\tilde{R}(y, x)p(x)). \quad (5.2.6)$$

The integrals over y can be taken inside the derivatives with respect to x,

$$\frac{\partial}{\partial t}p(x, t) = -\frac{\partial}{\partial x}\left[p(x)\left(\int dy\, y\tilde{R}(y, x)\right)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[p(x)\left(\int dy\, y^2\tilde{R}(y, x)\right)\right], \quad (5.2.7)$$

after which we obtain

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x}\left[v(x)\, p(x, t)\right] + \frac{\partial^2}{\partial x^2}\left[D(x)p(x, t)\right]. \quad (5.2.8)$$

We have introduced

$$v(x) \equiv \int dy\, y\tilde{R}(y, x) = \frac{\langle\Delta(x)\rangle}{\Delta t}, \quad (5.2.9)$$

and

$$D(x) \equiv \frac{1}{2}\int dy\, y^2\tilde{R}(y, x) = \frac{1}{2}\frac{\langle\Delta(x)^2\rangle}{\Delta t}. \quad (5.2.10)$$

Equation (5.2.8) is a prototypical description of *drift* and *diffusion* which appears in many contexts. The *drift* term $v(x)$ expresses the rate (velocity) with which transitions change (on average) the position from x. Given the probabilistic nature of the process, there are variations in the rate of change of position captured by the position dependent *diffusion* coefficient $D(x)$.[4] The drift–diffusion equation is known as the *forward Kolmogorov* equation in the context of populations. As a description of random walks it appeared earlier in physics literature as the *Fokker–Planck* equation.

5.2.2 Steady states

While it is usually hard to solve a general drift–diffusion equation as a function of time, it is relatively easy to find the steady state solution to which it settles after a long time. Let us denote the steady-state probability distribution by $p^*(x)$, which by definition must satisfy

$$\frac{\partial p^*(x)}{\partial t} = 0. \quad (5.2.11)$$

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[4]The diffusion coefficient is usually associated with the *variance*, $\langle\Delta(x)^2\rangle_c \equiv \langle\Delta(x)^2\rangle - \langle\Delta(x)\rangle^2$. However, in the limit of $\Delta t \to 0$, the squared mean is of second order in Δt, and can be ignored.

Therefore, setting the right-hand side of Eq. (5.2.8) to zero, we get

$$-\frac{\partial}{\partial x}\left[v(x)p^*(x)\right] + \frac{\partial^2}{\partial x^2}\left[D(x)p^*(x)\right] = 0. \tag{5.2.12}$$

The most general solution admits steady states in which there is an overall current and the integral over x of the last equation leads to a constant flow in probability. It is not clear how such a circumstance may arise in the context of population genetics, and we shall therefore focus on circumstances where there is no probability current, such that

$$-v(x)p^*(x) + \frac{\partial}{\partial x}(D(x)p^*(x)) = 0. \tag{5.2.13}$$

We can easily rearrange this equation to

$$\frac{1}{D(x)p^*}\frac{\partial}{\partial x}(D(x)p^*(x)) = \frac{\partial}{\partial x}\ln\left(D(x)p^*(x)\right) = \frac{v(x)}{D(x)}. \tag{5.2.14}$$

This equation can be integrated to

$$\ln D(x)p^*(x) = \int^x dx' \frac{v(x')}{D(x')} + \text{constant}, \tag{5.2.15}$$

such that

$$p^*(x) \propto \frac{1}{D(x)}\exp\left[\int^x \frac{v(x')}{D(x')}\right], \tag{5.2.16}$$

with the proportionality constant set by boundary conditions.

5.2.3   Evolving composition of a population of fixed size

Let us examine the case of the dynamics of a fixed population of N individuals which can come in two variants (alleles) A_1 and A_2. At a particular time, there can be n individuals of type 1, and $(N-n)$ individuals of type 2. For $N \gg 1$, it is convenient to introduce the composition $x = n/N$, which in the continuum limit x is limited to the interval $[0,1]$. We shall consider the following two processes contributing to the change of population over time:

Mutations:

In an infinitesimal time interval, the number n increases or decreases by 1, at rates given in Eq. (5.1.15) as $R_{n,n+1} = \mu_2(n+1)$ and $R_{n,n-1} = \mu_1(N-n+1)$. This leads to

$$v_{\text{mutation}}(x) = \frac{\langle\Delta n\rangle}{N} = \frac{R_{n+1,n}(+1) + R_{n-1,n}(-1)}{N} = \frac{1}{N}\left[\mu_1(N-n) - \mu_2 n\right] = \mu_1(1-x) - \mu_2 x, \tag{5.2.17}$$

while

$$D_{\text{mutation}}(x) = \frac{\langle\Delta n^2\rangle}{2N^2} = \frac{R_{n+1,n} + R_{n-1,n}}{2N^2} = \frac{1}{2N^2}\left[\mu_1(N-n) + \mu_2 n\right] = \frac{\mu_1(1-x) + \mu_2 x}{2N}. \tag{5.2.18}$$

Binary competition

Let us consider another form of population change, in which one individual is randomly chosen to die, and another chosen to reproduce (thus keeping the population fixed).[5] If the two individuals are from the same group there will be no change in composition, which if one individual in taken from group 1 and the other from group 2, the number n will change by ± 1. The probability for latter is proportional to $n(N - n)$, accounting to the number of possible choices of individuals from the two groups. In principle, and the corresponding changes can be assigned rates

$$R_{n,n+1} = \alpha n(N - n), \quad \text{and} \quad R_{n,n-1} = \alpha' n(N - n). \tag{5.2.19}$$

In principle, the two rates α and α' can be different, providing a competitive edge that will allow one group to expand at the expense of the other. However, here we shall consider the symmetric case with $\alpha = \alpha'$ which leads to

$$v_{\text{competition}}(x) = \frac{\langle \Delta n \rangle}{N} = \alpha \frac{n(N - n)(+1) + n(N - n)(-1)}{N} = 0, \tag{5.2.20}$$

and

$$D_{\text{competition}}(x) = \frac{\langle \Delta n^2 \rangle}{2N^2} = \alpha \frac{n(N - n) + n(N - n)}{2N^2} = \alpha x(1 - x). \tag{5.2.21}$$

Adding both contributions results in

$$v(x) = \mu_1(1 - x) - \mu_2 x, \tag{5.2.22}$$

dominated by mutation, and

$$D(x) = \alpha x(1 - x) + \frac{\mu_1(1 - x) + \mu_2 x}{2N} \approx \alpha x(1 - x). \tag{5.2.23}$$

The last approximation of ignoring the contribution from mutations to diffusion is justified as long N is large, while mutation and competition rates are comparable. It enables a closed form solution to the steady state, as

$$
\begin{aligned}
\log D(x)p^*(x) &= \int^x dx' \frac{v(x')}{D(x')} \\
&= \frac{1}{\alpha} \int^x dx' \left[\frac{\mu_1}{x'} - \frac{\mu_2}{1 - x'} \right] \\
&= \frac{1}{\alpha} \left[\mu_1 \ln x + \mu_2 \ln(1 - x) \right] + \text{constant},
\end{aligned}
$$

resulting in

$$p^*(x) \propto \frac{1}{x(1 - x)} \times x^{\mu_1/\alpha} \times (1 - x)^{\mu_2/\alpha}. \tag{5.2.24}$$

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[5]In population dynamics, this is known as a *Moran process*.

Setting for convenience $\mu_1 = \mu_2 = \mu$, the steady-state solution in Eq. (5.2.24) simplifies to

$$p^*(x) \propto [x(1-x)]^{\mu/\alpha-1} . \tag{5.2.25}$$

The shape of the solution is determined by the ration μ/α. If $\mu > \alpha$, then the distribution has a peak at $x = 1/2$ and diminishes to the sides, while for $\mu < \alpha$, $p^*(x)$ has peaks at either extreme. This can be understood by considering the limit of no mutations ($\mu = 0$): I this case fluctuations due to diffusion may randomly bring the population to a uniform state with $n = 0$ or $n = N$. In the absence of mutation, there can then be no further change to the population. These two limiting states then act as sinks of probability and in the final state the discrete probabilities will be zero, expect for p_0^* and p_N^*. The absence of a proper continuum limit is then signaled by a $p^*(x)$ in Eq. (5.2.24) that can not be normalized to unity.