

Counting the Heads: Population Kinetics and Chemical Reactions

7.1 Simple population kinetics with birth and death

Let us consider a single population, with a constant per capita birth rate u and death rate v . Therefore, the conventional differential equations for the population size at time t is

$$\frac{1}{x(t)} \left(\frac{dx(t)}{dt} \right) = b - d. \quad (7.1)$$

In the classic population biology, this equation is true simply because the *definition* of *per capita* birth and death rates!

But we now know that this equation can not be really true! The population size does not grow by a continuous value, it has to be by integers; and furthermore, the per capita birth and death rates are only “average” concepts. There are a great deal of randomness in the birth and death processes.

So, instead of using real valued $x(t)$ as the population size at time t , we shall now study the *probability of the population having n individuals at time t : $p_n(t)$* . Then this $p_n(t)$ satisfies the following equation:

$$\frac{dp_n(t)}{dt} = (n-1)bp_{n-1}(t) - (b+d)np_n(t) + (n+1)dp_{n+1}(t). \quad (7.2)$$

The assumption here is that all the individuals in the population, though are different, they are statistically identical, and independent in their giving birth and going death; and the birth and death events for a person has an exponential distributed time.

One can draw a number line ...

The Eq. 7.2 looks complicated; but we can have the following two important results. First,

$$\begin{aligned} \frac{d}{dt} \sum_{n=0}^{\infty} p_n(t) &= \sum_{n=1}^{\infty} \left[(n-1)bp_{n-1}(t) - (b+d)np_n(t) + (n+1)dp_{n+1}(t) \right] \\ &= 0. \end{aligned} \quad (7.3)$$

This is of course expected: The total probability should always be 1 and this does not change with time.

More interestingly,

$$\begin{aligned}
 \frac{d}{dt}\langle n \rangle(t) &= \frac{d}{dt} \sum_{n=0}^{\infty} n p_n(t) \\
 &= \sum_{n=0}^{\infty} n \left[(n-1)b_1 p_{n-1}(t) - (b_1 + d_1)n p_n(t) + (n+1)d_{n+1} p_{n+1}(t) \right] \\
 &= \sum_{n=1}^{\infty} (n-1)b p_{n-1}(t) - \sum_{n=0}^{\infty} (n+1)d p_{n+1}(t) \\
 &= b \sum_{k=0}^{\infty} k p_k(t) - d \sum_{k=0}^{\infty} k p_k(t) = (b-d)\langle n \rangle(t) \tag{7.4}
 \end{aligned}$$

If one identifies the $\langle n \rangle(t)$ as the $x(t)$ in Eq. 7.2), then we have just *proved* the earlier equation; together with a better understanding the meaning of “per capita birth rate” and “per capita birth rate” in a probabilistic sense. There is even an real practical value: One can measure the b and d from data collected from individuals.

7.1.1 Stationary distribution of dynamics of a single species

The general dynamics for the probability distribution of single specie system is

$$\frac{d}{dt} p_n(t) = u_{n-1} p_{n-1} - (u_n + w_n) p_n + w_{n+1} p_{n+1}, \tag{7.5}$$

in which $n = 0, 1, 2, \dots$. u_n and w_n are the birth rate and death rate of the population when there are n individuals. u_n and w_n are not per capita rates; if all the individuals are independent and identically distributed, then $u_n = n u_1$ and $w_n = n w_1$. This recovers the Eq. 7.2. If all $u_n = \lambda$ and all $w_n = 0$, this becomes the Poisson process.

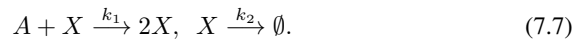
Just as we always look for the fixed points of a system of ODEs, we again are interested in the *stationary solution* to the differential equation in (7.5). Note there are infinitely many equations here; the solution is

$$\begin{aligned}
 \frac{p_n^s}{p_0^s} &= \frac{p_n^s}{p_{n-1}^s} \times \frac{p_{n-1}^s}{p_{n-2}^s} \times \dots \times \frac{p_1^s}{p_0^s} \\
 &= \frac{u_{n-1}}{w_n} \times \frac{u_{n-2}}{w_{n-1}} \times \dots \times \frac{u_0}{w_1} \\
 &= \prod_{m=1}^n \left(\frac{u_{m-1}}{w_m} \right). \tag{7.6}
 \end{aligned}$$

What is the shape of the distribution p_n^s as a function of n ? Does it have peaks and troughs? And where are they?

7.2 Chemical reactions and law of mass action

The form of population kinetics can be applied not just to biological organisms and ecology; it is equally valued to the molecules in a test tube and inside a cell - e.g., chemistry and biochemistry. In this case, birth is called “autocatalytic synthesis” and death is called “degradation”:



We now introduce the *Law of Mass Action* for rapidly stirred chemical reaction:

The instantaneous rate of a chemical reaction is proportional to the product of the masses of the reacting substances, with each mass raised to a power equal to the coefficient that occurs in the chemical equation. The proportional constant is called a rate constant.

Applying this principle to the reactions in (7.7), we have the concentration of the X at time t , $x(t)$, satisfies

$$\frac{dx(t)}{dt} = J_1(t) - J_2(t), \quad J_1 = k_1 a x, \quad J_2 = k_2 x. \quad (7.8)$$

k_1 and k_2 , are the rate constants for the two reactions. We used a for the concentration of A . The first reaction in (7.7) is called a second-order reaction, and the second reaction is called a first-order reaction. Therefore,

$$\frac{dx(t)}{dt} = k_1 a x - k_2 x = (k_1 a - k_2) x. \quad (7.9)$$

To arrive at Eq. 7.9, we have used the three equations in (7.8): The first equation is absolutely true, since it is just a matter of counting head; or *mass conservation*; or the definition of what instantaneous rate is. The second and third equations are based on the law of mass action. This part can always be improved when dealing with a real system. The situation is completely parallel to the idea of Newton’s law $m(d^2x/dt^2) = F(x)$ and the need for a realistic “force field” $F(x)$, as in molecular dynamics (MD).

Many chemical reactions are actually reversible:



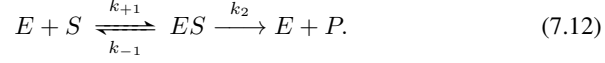
If we denote the instantaneous rate of the forward and backward reactions at time t as $J_+(t)$ and $J_-(t)$, then

$$-\frac{dc_A(t)}{dt} = -\frac{dc_B(t)}{dt} = \frac{dc_C(t)}{dt} = \frac{dc_D(t)}{dt} = J_+(t) - J_-(t), \quad (7.11)$$

and Law of Mass Action states that $J_+(t) = k_{+1}c_Ac_B$ and $J_-(t) = k_{-1}c_Cc_D$.

7.3 Enzyme kinetics: Deterministic and stochastic models

Michaelis-Menten kinetics for an enzymatic reaction is



Using x , y and z for the concentrations of the biochemical species S , ES and P , we have

$$\frac{dx(t)}{dt} = -k_{+1}(e_0 - y)x + k_{-1}y, \quad (7.13a)$$

$$\frac{dy(t)}{dt} = k_{+1}(e_0 - y)x - (k_{-1} + k_2)y, \quad (7.13b)$$

$$\frac{dz(t)}{dt} = k_2y. \quad (7.13c)$$

The initial condition is $x(0) = x_0$, $y(0) = 0$ and $z(0) = 0$. The first two equations can be solved independent of the z , afterward $z(t)$ can be computed

$$z(t) = z(0) + k_2 \int_0^t y(s) ds.$$

If one makes an assumption that the concentration of total enzyme E , e_0 , is much smaller than the concentration of the substrate $x_0 \gg e_0$, then the concentration of ES goes to steady rapidly. This implies

$$k_{+1}(e_0 - y)x - (k_{-1} + k_2)y = 0$$

from which we can solve

$$y = \frac{k_{+1}e_0x}{k_{-1} + k_2 + k_{+1}x}.$$

Substituting this into Eq. 7.13a, we have

$$\frac{dx(t)}{dt} = \frac{k_2k_{+1}e_0x}{k_{-1} + k_2 + k_{+1}x} = \frac{v_{max}[S]}{K_M + [S]}, \quad (7.14)$$

in which $[S] = x$ is the concentration of the substrate, $v_{max} = k_2e_0$ is called the maximal velocity, and $K_M = \frac{k_{-1} + k_2}{k_{+1}}$ is called Michaelis constant. Eq. 7.14 is called Michaelis-Menten equation.

7.3.1 Stochastic model for a single enzyme

If there is only a single enzyme, then a complete enzyme cycle is from the left of (7.12) to the right of the (7.12). The mean value of this random time T is

$$\langle T \rangle = \frac{1}{k_{+1}[S]} + \frac{1}{k_{-1} + k_2} + \frac{0 \times k_2}{k_{-1} + k_2} + \frac{\langle T \rangle \times k_{-1}}{k_{-1} + k_2}. \quad (7.15)$$

Solving $\langle T \rangle$ we obtain

$$\langle T \rangle = \frac{k_{-1} + k_2}{k_2} \left(\frac{1}{k_{+1}[S]} + \frac{1}{k_{-1} + k_2} \right) = \frac{k_{-1} + k_2}{k_2 k_{+1}[S]} + \frac{1}{k_2}. \quad (7.16)$$

Comparing this with Eq. 7.14 we see that the velocity is the e_0 multiple of the reciprocal of the mean time, as expected.

7.4 Nonlinear kinetics: Bistability and bifurcation

Let us again consider the population kinetics of a single species: In addition to logistic growth, let us consider also the presence of a predator to which the species under consideration is not the necessary source of food. In other words, the predator can live perfect normal no matter what is the ecological situation of the species. Therefore we have

$$\frac{dN}{dt} = rN \left(1 - \frac{N}{K} \right) - p(N), \quad (7.17)$$

Note we have assumed that the population of the predator is not changing with time; it is a constant. Otherwise, there would be one more equation describing the dynamics of the predator population.

The function $p(N)$ is called predation function. What should it look like? Certainly, when $N = 0$, $p(N)$ has to be zero. Furthermore, with increasing N , the $p(N)$ increases. But for $N \rightarrow \infty$, the $p(N)$ approaches to a constant value. Therefore, here are two reasonable predation functions:

$$p_1(N) = \frac{CN}{D + N}, \quad p_2(N) = \frac{BN^2}{A^2 + N^2}. \quad (7.18)$$

The $p_2(N)$ represents the situation in which when N is sufficiently small, the predator can not find them.

Let us consider the problem with $p_2(N)$. In this case, we expect that the population can stable at a rather low, stable level, almost as the predation is non-existent; or it the population survives at a rather high level, that the loss from predation is balanced by the growth. This is indeed the case, as shown by the figure:

[On the white board]

7.4.1 Bifurcation diagram

We now introduce two very important types of nonlinear phenomena: *transcritical* and *blue-sky* (also called saddle-node) bifurcations.

$$\frac{dx}{dt} = f(x; r) = x(r - x); \quad (7.19)$$