S5B.2. Linear Birth-Death Processes

Setting

$$b_n = \beta n \text{and} \qquad d_n = \gamma n$$

turns the master equation (5.100) into

$$\frac{\partial P(n, t)}{\partial t} = \beta (n-1) P(n-1, t) + \gamma (n+1) P(n+1, t) - (\beta n + \gamma n) P(n, t) \qquad (5.104)$$

which describes a linear process since the coefficients of P are all linear in n.

Note that since the bacteria number $n \geq 0$, the flow of P must never enter the region $n < 0$. We can prove that (5.104) satisfies this requirement. To begin,

$$\frac{\partial P(0, t)}{\partial t} = -\beta \; P(-1, t) + \gamma \; P(1, t)$$

$$\frac{\partial P(-1, t)}{\partial t} = -2 \beta P(-2, t) + (\beta + \gamma) P(-1, t)$$

$$\vdots$$

$$\frac{\partial P(-n, t)}{\partial t} = -\beta (n+1) P(-(n+1), t) - \gamma (n-1) P(-(n-1), t) + (\beta n + \gamma n) P(-n, t)$$

Thus, $\dfrac{\partial P(n, t)}{\partial t}$ for $n < 0$ depend only on $P(m, t)$ with $m < 0$. If we start with

$$P(m, t) = 0 \qquad \forall \; m < 0 \qquad \text{(a)}$$

then

$$\frac{\partial P(m, t)}{\partial t} = 0 \qquad \forall \; m < 0$$

and (a) holds forever. In which case, we need only concern with

$$\frac{\partial P(0, t)}{\partial t} = \gamma \; P(1, t)$$

$$\frac{\partial P(1, t)}{\partial t} = 2 \gamma \; P(2, t) - (\beta + \gamma) P(1, t)$$

$$\vdots$$

Since the probability current never flows into the $n < 0$ region, (5.104) is said to have a natural boundary at $n = 0$.

Linear master equations for discrete stochastic variables are often easily solved by means of a generating function defined as

$$F(z, t) \equiv \sum_{n=-\infty}^{\infty} z^n P(n, t) \qquad (5.105)$$

$$= \sum_{n=0}^{\infty} z^n P(n, t)$$

The inclusion of $n < 0$ terms in the sum does not contribute to its value because of (a). However, it frees us from the necessity to adjust the lower bound of n in subsequent calculations [see, e.g., derivation of (5.108)].

$F(z, t)$ is called a generating function since it generates various moments of $n(t)$ by differentiation at the limit $z \to 1$. For example,

$$\begin{aligned}\lim_{z\to 1}\frac{\partial F(z,t)}{\partial z} &= \lim_{z\to 1}\sum_{n=-\infty}^{\infty} n\, z^{n-1}\, P(n,t)\\ &= \sum_{n=-\infty}^{\infty} n\, P(n,t)\\ &= \langle n(t)\rangle \end{aligned} \tag{5.106}$$

$$\begin{aligned}\lim_{z\to 1}\frac{\partial^2 F(z,t)}{\partial z^2} &= \lim_{z\to 1}\sum_{n=-\infty}^{\infty} n(n-1)\, z^{n-2}\, P(n,t)\\ &= \sum_{n=0}^{\infty} n^2\, P(n,t) - \sum_{n=0}^{\infty} n\; P(n,t)\\ &= \langle n^2(t)\rangle - \langle n(t)\rangle \end{aligned} \tag{5.107}$$

$\sum_{n=-\infty}^{\infty} z^n \times (5.104)$ will give us a differential equation for $F(z,t)$. Using

$$\begin{aligned}\sum_{n=-\infty}^{\infty} z^n\,(n-1)\,P(n-1,t) &= z^2\,\frac{\partial}{\partial z}\sum_{n=-\infty}^{\infty} z^{n-1}\,P(n-1,t)\\ &= z^2\,\frac{\partial}{\partial z}\sum_{n=-\infty}^{\infty} z^{n}\,P(n,t)\\ &= z^2\,\frac{\partial F(z,t)}{\partial z}\end{aligned}$$

$$\begin{aligned}\sum_{n=-\infty}^{\infty} z^n\,(n+1)\,P(n+1,t) &= \frac{\partial}{\partial z}\sum_{n=-\infty}^{\infty} z^{n+1}\,P(n+1,t)\\ &= \frac{\partial}{\partial z}\sum_{n=-\infty}^{\infty} z^{n}\,P(n,t)\\ &= \frac{\partial F(z,t)}{\partial z}\end{aligned}$$

$$\sum_{n=-\infty}^{\infty} n\,z^n\,P(n,t) = z\,\frac{\partial}{\partial z}\sum_{n=-\infty}^{\infty} z^{n}\,P(n,t) \;= z\,\frac{\partial F(z,t)}{\partial z}$$

(5.104) becomes

$$\begin{aligned}\frac{\partial F}{\partial t} &= \beta\, z^2\,\frac{\partial F}{\partial z} + \gamma\,\frac{\partial F}{\partial z} - (\beta+\gamma)\, z\,\frac{\partial F}{\partial z}\\ &= (z-1)\,(\beta\, z - \gamma)\,\frac{\partial F}{\partial z}\end{aligned} \tag{5.108}$$

which can be solved by the method of characteristics [see §(Method of Characteristics)].

Setting

$$g(z) = -(z-1)\,(\beta\, z - \gamma) \qquad\qquad h(z) = 0$$

we have [see §Code]

$$\int\frac{d\,z}{g(z)} = -\int\frac{d\,z}{(z-1)\,(\beta\, z-\gamma)} \;= -\frac{1}{\beta-\gamma}\ln\frac{z-1}{\beta\, z-\gamma} \;= \ln\left(\frac{z-1}{\beta\, z-\gamma}\right)^{-\frac{1}{\beta-\gamma}}$$

$$\exp\left(\int\frac{d\,z}{g(z)} - t\right) = \left(\frac{z-1}{\beta\, z-\gamma}\right)^{-\frac{1}{\beta-\gamma}} e^{-t} \;= \left(\frac{z-1}{\beta\, z-\gamma}\, e^{(\beta-\gamma)\,t}\right)^{-\frac{1}{\beta-\gamma}}$$

(4) of §(Method of Characteristics) becomes

$$F(z,\ t) = F\left(\frac{z-1}{\beta z - \gamma} e^{(\beta-\gamma)t} \right) \tag{5.109}$$

The exact form of $F(z,\ t)$ can be determined by initial conditions.

Consider the case where we start with m bacteria at $t = 0$. Then

$$P(n,\ 0) = \delta_{n\,m} \qquad \to \qquad F(z,\ 0) = z^m \qquad \text{[(5.105) used.]}$$

Combing with (5.109) gives

$$F(z,\ 0) = F\left(\frac{z-1}{\beta z - \gamma} \right) = z^m \tag{5.110}$$

The functional form of F is obtained by setting

$$u = \frac{z-1}{\beta z - \gamma} \qquad \to \qquad z = \frac{\gamma u - 1}{\beta u - 1}$$

so that (5.10) becomes

$$F(z,\ 0) = F(u) = z^m = \left(\frac{\gamma u - 1}{\beta u - 1} \right)^m \tag{5.111}$$

(5.109) then gives

$$\begin{aligned} F(z,\ t) &= F\left(u\, e^{(\beta-\gamma)t} \right) \\ &= \left(\frac{\gamma \frac{z-1}{\beta z-\gamma} e^{(\beta-\gamma)t} - 1}{\beta \frac{z-1}{\beta z-\gamma} e^{(\beta-\gamma)t} - 1} \right)^m \qquad \text{[(5.111) used.]} \\ &= \left(\frac{\gamma (z-1) e^{(\beta-\gamma)t} - \beta z + \gamma}{\beta (z-1) e^{(\beta-\gamma)t} - \beta z + \gamma} \right)^m \end{aligned} \tag{5.112}$$

By (5.105), $P(n,\ t)$ is just the coefficient of z^n in a Taylor expansion of $F(z,\ t)$, i.e.,

$$P(n,\ t) = \frac{1}{n!} \left. \frac{\partial^n F}{\partial z^n} \right|_{z=0}$$

On the other hand, (5.106) gives the 1st moment as [see §Code]

$$\langle n(t) \rangle = \left. \frac{\partial F}{\partial z} \right|_{z=1} = m\, e^{(\beta-\gamma)t} \tag{5.113}$$

The population thus grows exponentially if $\beta > \gamma$ or dies out if $\beta < \gamma$.

The variance is [see §Code],

$$\begin{aligned} \left\langle n^2(t) \right\rangle - \langle n(t) \rangle^2 &= \left[\frac{\partial^2 F}{\partial z^2} + \frac{\partial F}{\partial z} - \left(\frac{\partial F}{\partial z} \right)^2 \right]_{z=1} \\ &= \frac{m (\beta + \gamma)\ e^{t(\beta-\gamma)} \left(-1 + e^{t(\beta-\gamma)}\right)}{\beta - \gamma} \end{aligned} \tag{5.114}$$

Code

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A = ∫ 1/((z - 1) (β z - γ)) ⅆ z
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$$\frac{\text{Log}[-1+z]-\text{Log}[z\,\beta-\gamma]}{\beta-\gamma}$$

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Solve[u == (z - 1)/(β z - γ), z]
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$$\left\{\left\{z\to\frac{-1+u\,\gamma}{-1+u\,\beta}\right\}\right\}$$

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F[z_, t_] := ((γ (z - 1) ⅇ^((β-γ) t) - β z + γ)/(β (z - 1) ⅇ^((β-γ) t) - β z + γ))^m
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$$F[z\_, t\_] := \left(\frac{\gamma\,(z-1)\,e^{(\beta-\gamma)\,t}-\beta\,z+\gamma}{\beta\,(z-1)\,e^{(\beta-\gamma)\,t}-\beta\,z+\gamma}\right)^{m}$$

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∂_z F[z, t] /. z → 1 // Simplify
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$$e^{t\,(\beta-\gamma)}\,m$$

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(∂_{z,z} F[z, t] + ∂_z F[z, t] - (∂_z F[z, t])^2) /. z → 1 // Simplify
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$$\frac{e^{t\,(\beta-\gamma)}\left(-1+e^{t\,(\beta-\gamma)}\right)m\,(\beta+\gamma)}{\beta-\gamma}$$

Method of Characteristics

Consider the 1st order linear differential equation for $F(z,\,t)$,

$$\frac{\partial F}{\partial t}+g(z)\,\frac{\partial F}{\partial z}+h(z)\,F=0 \tag{1}$$

Let

$$F(z,\,t)=\exp\left(-\int d\,z\,\frac{h(z)}{g(z)}\right)\Phi(z,\,t) \tag{2}$$

$$\rightarrow\qquad \frac{\partial F}{\partial t}=\exp\left(-\int d\,z\,\frac{h(z)}{g(z)}\right)\frac{\partial\Phi}{\partial t}$$

$$\frac{\partial F}{\partial z}=\exp\left(-\int d\,z\,\frac{h(z)}{g(z)}\right)\left(-\frac{h(z)}{g(z)}\Phi+\frac{\partial\Phi}{\partial z}\right)$$

(1) thus becomes

$$\frac{\partial\Phi}{\partial t}+g(z)\,\frac{\partial\Phi}{\partial z}=0 \tag{3}$$

The characteristics of (3) are curves in the t-z plane along which $\Phi=\text{const}$, i.e., they are the contour lines of Φ. Therefore, they satisfy

$$d\,\Phi=\frac{\partial\Phi}{\partial t}d\,t+\frac{\partial\Phi}{\partial z}d\,z=0$$

Comparing with (3), we have

$$d\,t - \frac{d\,z}{g(z)} = 0$$

$$\rightarrow \qquad t - \int \frac{d\,z}{g(z)} = C \qquad\qquad C = \text{const} \qquad\qquad \text{(a)}$$

Consider now any function

$$f = f(\xi) \text{ where } \qquad \xi = t - \int \frac{d\,z}{g(z)}$$

$$\rightarrow \qquad \frac{\partial f}{\partial t} = \frac{\partial \xi}{\partial t}\frac{d\,f}{d\,\xi} = \frac{d\,f}{d\,\xi}$$

$$\frac{\partial f}{\partial z} = \frac{\partial \xi}{\partial z}\frac{d\,f}{d\,\xi} = -\frac{1}{g(z)}\frac{d\,f}{d\,\xi}$$

$$\therefore \qquad \frac{\partial f}{\partial t} + g(z)\frac{\partial f}{\partial z} = 0$$

i.e., $f(\xi)$ is a solution to (3).

(2) thus becomes

$$F(z,\,t) = \exp\left(-\int d\,z\,\frac{h(z)}{g(z)}\right)\Phi\left(t - \int \frac{d\,z}{g(z)}\right)$$

Since Φ is any function, we can also write

$$F(z,\,t) = \exp\left(-\int d\,z\,\frac{h(z)}{g(z)}\right)\Phi\left[\exp\left(\int \frac{d\,z}{g(z)} - t\right)\right] \qquad (4)$$

which ensures Φ behaves nicely as $t \to \infty$.

Chemical Reaction

Consider the reaction

$$A + X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A + Y$$

where k_1 (k_2) is the probability per unit time that a reaction takes place if an X (Y) molecule collides with an A molecule.

In the forward reaction, an X molecule collides with an A molecule and turns into an Y molecule, while the A molecule merely scatters off. The changes in the numbers of molecules are therefore

$$\Delta\,n_A = 0 \qquad \Delta\,n_X = -1 \qquad \Delta\,n_Y = +1 \qquad \text{for forward reaction}$$

In the backward reaction, the roles of X and Y are reversed so that

$$\Delta\,n_A = 0 \qquad \Delta\,n_X = +1 \qquad \Delta\,n_Y = -1 \qquad \text{for backward reaction}$$

Since for all reactions,

$$\Delta\,n_X + \Delta\,n_Y = 0 \rightarrow \qquad n_X + n_Y = N = \text{const}$$

there is only 1 independent stochastic variable, which we choose to be n_X.

As all reactions involve only $\Delta\,n_X = \pm 1$, the reaction is a birth-death process.

Let $P(n,\,t)$ be the probability at time t that $n_X = n$, and hence $n_Y = N - n$.

Consider first reactions that have $n_X = n$ as the final state.

The relevant forward reactions satisfy

$$n_A\, A + (n+1)\, X + (N-n-1)\, Y \underset{k_1}{\longrightarrow} n_A\, A + n\, X + (N-n)\, Y$$

The corresponding transition rate w_1 is proportional to the number of collisions between A & X molecules, and hence to the initial value of the product $n_A\, n_X$. Therefore,

$$w_1 = n_A\, k_1 (n+1)$$

Similarly, the relevant backward reactions satisfy

$$n_A\, A + (n-1)\, X + (N-n+1)\, Y \underset{k_2}{\longrightarrow} n_A\, A + n\, X + (N-n)\, Y$$

with transition rate

$$w_2 = n_A\, k_2\, (N-n+1)$$

Next, for reactions that have $n_X = n$ as the initial state, the forward reactions satisfy

$$n_A\, A + n\, X + (N-n)\, Y \underset{k_1}{\longrightarrow} n_A\, A + (n-1)\, X + (N-n+1)\, Y$$

with transition rate

$$w_1{}' = n_A\, k_1\, n$$

while the backward reactions satisfy

$$n_A\, A + n\, X + (N-n)\, Y \underset{k_2}{\longrightarrow} n_A\, A + (n+1)\, X + (N-n-1)\, Y$$

with transition rate

$$w_2{}' = n_A\, k_2\, (N-n)$$

The master equation is therefore

$$\begin{aligned} \frac{\partial P(n,t)}{\partial t} &= P(n+1,t)\, w_1 + P(n-1,t)\, w_2 - P(n,t)\,(w_1{}' + w_2{}') \\ &= P(n+1,t)\, n_A\, k_1 (n+1) + P(n-1,t)\, n_A\, k_2\, (N-n+1) \\ &\qquad - P(n,t)\, n_A \left(k_1\, n + k_2 (N-n)\right) \end{aligned} \tag{5.115}$$