CHAPTER 8

Clustering Processes

Processes in which individuals or units form themselves into clusters have applications in a variety of fields. In Section 8.1 we shall commence investigation of these clustering processes with an example arising from the study of social behaviour. Later, in Section 8.4, we shall consider in some detail a more complex example taken from the field of polymer chemistry.

8.1 INTRODUCTION

In Section 6.2 we considered a model for social grouping behaviour based on the reversible migration processes of that chapter. A possible drawback of the model was its assumption that groups form at specific locations; this assumption might be appropriate for troops of monkeys sleeping in trees, but is less likely to apply to clusters of people at a cocktail party. An alternative model for the latter context might be as follows. Suppose there are M individuals formed into distinct groups, with m_i being the number of groups consisting of i individuals. Thus

$$\sum_{i=1}^{M} i m_i = M \tag{8.1}$$

and m_1 is the number of isolated individuals, or isolates. Suppose that a given isolate moves to join a given group of size $i (i = 1, 2, \ldots)$ at rate α and that a given individual within a group of size $i (i = 2, 3, \ldots)$ leaves that group to become an isolate at rate β. Put more precisely this is equivalent to the assumption that $\mathbf{m} = (m_1, m_2, \ldots)$ is a Markov process in which the transition rate from $(m_1, m_2, \ldots, m_i, m_{i+1}, \ldots)$ to $(m_1 - 1, m_2, \ldots, m_i - 1, m_{i+1} + 1, \ldots)$ is $\alpha m_1 m_i$ for $i \geq 2$; from $(m_1, m_2, m_3, \ldots)$ to $(m_1 - 2, m_2 + 1, m_3, \ldots)$ is $\alpha m_1 (m_1 - 1)$; from $(m_1, m_2, \ldots, m_{i-1}, m_i, \ldots)$ to $(m_1 + 1, m_2, \ldots, m_{i-1} + 1, m_i - 1, \ldots)$ is $i\beta m_i$, $i > 2$; and from $(m_1, m_2, m_3, \ldots)$ to $(m_1 + 2, m_2 - 1, m_3, \ldots)$ is $2\beta m_2$. Note that two isolates may form a group of size 2; the rate at which a group of size 2 is formed in this way while there are m_1 isolates is $\alpha m_1 (m_1 - 1)$, there being $m_1 (m_1 - 1)$ distinct ordered pairs of isolates.

The equilibrium distribution is

$$\pi(\mathbf{m}) = B \prod_{i=1}^{M} \frac{1}{m_i!} \left(\frac{\beta}{\alpha i!} \right)^{m_i} \tag{8.2}$$

for $\mathbf{m}$ satisfying restriction (8.1), where B is a normalizing constant. This can be verified by checking the detailed balance conditions, and is a special case of a more general result to be discussed in the next section. We have considered this special case separately in order to motivate the next two sections. We shall see later (Exercise 8.2.1) that from the equilibrium distribution it is possible to calculate quantities of interest such as the expected number of groups of size i or the expected proportion of individuals in groups of size i.

The process $\mathbf{m}$ has some similarities with the infinite alleles model **M** considered in the previous chapter. In each case the ith component gives the number of groups of i individuals. Like the infinite alleles model the simple clustering model described in this section can be considered as a limiting case of a reversible migration process (Exercise 8.1.1).

Exercises 8.1

1. The process described in this section is a limiting form of a reversible migration process. To see this consider a reversible migration process $(n_1, n_2, \ldots, n_J)$ with J sites and $\sum_{j=1}^{J} n_j = M$, and suppose the probability intensity an individual moves from site j to site k is $\phi(n_j)$ where $\phi(1) = \alpha$ and $\phi(n) = \beta n/J$, $n \geq 2$. Now let $\mathbf{m} = (m_1, m_2, \ldots)$ describe the system with m_i being the number of sites inhabited by i individuals. Show that as $J \to \infty$ the transition rates and the equilibrium distribution for the process $\mathbf{m}$ approach those of the model described in this section.
2. If $\mathbf{m}$ is distributed according to (8.2) with α/β an unknown parameter show that the number of groups, $\sum m_i$, is a sufficient statistic for α/β.

8.2 THE BASIC MODEL

In this section we shall discuss a fairly general clustering process. It will come as no surprise that when the process is reversible equilibrium results can be readily obtained.

Suppose there exist a countable number of possible cluster types, labelled $r = 1, 2, \ldots$. Two clusters may join together to form a single cluster or a cluster may break up into two clusters. Let m_r be the number of r-clusters, i.e. clusters of type r, and let $\mathbf{m} = (m_1, m_2, \ldots)$. Define the operators R_u^{rs} and R_{rs}^u by

$$R_u^{rs}\mathbf{m} = (m_1, m_2, \ldots, m_r - 1, \ldots, m_s - 1, \ldots, m_u + 1, \ldots)$$

and

$$R_{rs}^u\mathbf{m} = (m_1, m_2, \ldots, m_r + 1, \ldots, m_s + 1, \ldots, m_u - 1, \ldots)$$

so that they correspond respectively to the union of an r-cluster and an s-cluster to form a u-cluster and the break up of a u-cluster into an r-cluster

and an s-cluster. Similarly define

$$R_u^{rr}\mathbf{m} = (m_1, m_2, \ldots, m_r - 2, \ldots, m_u + 1, \ldots)$$

and

$$R_{rr}^{u}\mathbf{m} = (m_1, m_2, \ldots, m_r + 2, \ldots, m_u - 1, \ldots)$$

We shall suppose that the process $\mathbf{m}$ is Markov with transition rates

$$\begin{aligned} q(\mathbf{m}, R_u^{rs}\mathbf{m}) &= \lambda_{rsu} m_r m_s \qquad r \neq s \\ q(\mathbf{m}, R_u^{rr}\mathbf{m}) &= \lambda_{rru} m_r (m_r - 1) \\ q(\mathbf{m}, R_{rs}^{u}\mathbf{m}) &= \mu_{rsu} m_u \end{aligned} \tag{8.3}$$

where $\lambda_{rsu} = \lambda_{sru}$ and $\mu_{rsu} = \mu_{sru}$. The parameter μ_{rsu} can be regarded as the probability intensity a given u-cluster breaks up into an r-cluster and an s-cluster; similarly, λ_{rsu} for $r \leq s$ can be regarded as the probability intensity a given r-cluster attaches itself to a given s-cluster to form a u-cluster. Let $\mathcal{S}$ be the state space of the process $\mathbf{m}$. For the moment we shall assume $\mathcal{S}$ is finite and irreducible. In this case call $\mathbf{m}$ a closed clustering process.

Theorem 8.1. *If there exist positive numbers $c_1, c_2, \ldots$ satisfying*

$$c_r c_s \lambda_{rsu} = c_u \mu_{rsu} \tag{8.4}$$

then in equilibrium the closed clustering process $\mathbf{m}$ is reversible with equilibrium distribution

$$\pi(\mathbf{m}) = B \prod_r \frac{c_r^{m_r}}{m_r!} \tag{8.5}$$

where B is a normalizing constant.

Proof. The detailed balance conditions

$$\pi(\mathbf{m}) q(\mathbf{m}, R_u^{rs}\mathbf{m}) = \pi(R_u^{rs}\mathbf{m}) q(R_u^{rs}\mathbf{m}, \mathbf{m}) \tag{8.6}$$

are readily verified; the theorem follows from these.

Often the clusters are made up of basic units which cannot be created or destroyed. In this case if $k(r)$ is the number of units in an r-cluster then $c_r \theta^{k(r)}$, $r = 1, 2, \ldots$, will also satisfy equation (8.4). The distribution (8.5) is, however, unaltered—a factor θ^M is incorporated into the constant B, where M is the total number of units in the system. In the example described in the last section $k(r) = r$ and so the number of units, or individuals, in a cluster defines it completely. This will often be the case but a process for which it is not true will be discussed in Section 8.4. The normalizing constant B is, as in closed queueing systems, straightforward but tedious to calculate (Exercise

8.2.1). As might be expected we can avoid difficulties with B by making the system open. One way to do this is as follows. Define the operators

$$R_1^{+}\mathbf{m} = (m_1 + 1, m_2, m_3, \ldots)$$
$$R_1^{-}\mathbf{m} = (m_1 - 1, m_2, m_3, \ldots)$$

and suppose that one-clusters may enter or leave the system with corresponding transition rates

$$\begin{aligned} q(\mathbf{m}, R_1^{+}\mathbf{m}) &= \nu \\ q(\mathbf{m}, R_1^{-}\mathbf{m}) &= \mu m_1 \end{aligned} \tag{8.7}$$

Assume that every state $(m_1, m_2, \ldots)$ with $\sum m_r$ finite can be reached from every other such state.

Theorem 8.2. *If there exist positive numbers $c_1, c_2, \ldots$ satisfying*

$$\begin{aligned} \nu &= c_1 \mu \\ \lambda_{rsu} c_r c_s &= c_u \mu_{rsu} \end{aligned} \tag{8.8}$$

and

$$\sum_{r=1}^{\infty} c_r < \infty \tag{8.9}$$

then the open clustering process $\mathbf{m}$ *with transition rates* (8.3) *and* (8.7) *has equilibrium distribution*

$$\pi(\mathbf{m}) = \prod_{r=1}^{\infty} e^{-c_r} \frac{c_r^{m_r}}{m_r!} \tag{8.10}$$

In equilibrium $\mathbf{m}$ *is reversible and $m_1, m_2, \ldots$ are independent random variables; m_r has a Poisson distribution with mean c_r.*

Proof. For the open process there is in addition to conditions (8.6) the extra detailed balance condition

$$\pi(\mathbf{m})\nu = \pi(R_1^{-}\mathbf{m})\mu(m_1 + 1)$$

and it is readily checked that the form (8.10) satisfies all of these equations. The additional assumption (8.9) is necessary to ensure that the form (8.10) assigns probability one to the countable set $\mathcal{S}$ consisting of states $\mathbf{m}$ with $\sum m_r$ finite.

It is often not apparent from the transition rates (8.3) whether equations (8.4) have a non-zero solution; the following lemma, a partial converse to Theorem 8.1, can sometimes be used to establish this.

Lemma 8.3. *Let* $\mathbf{m}$ *be a closed clustering process with transition rates* (8.3), *and suppose the parameters* μ_{rsu} *permit a sequence of dissociations by which an r-cluster can break up into one-clusters. If* $\mathbf{m}$ *is reversible then there exists a solution to equations* (8.4) *with the property that* $c_r > 0$ *if in equilibrium there is a positive probability that an r-cluster is present.*

Proof. Let $\mathbf{m}^1$ be a state in which $m_r > 0$, and let $\mathbf{m}^1, \mathbf{m}^2, \ldots, \mathbf{m}^{k(r)}$ be a sequence of states produced by the dissociation of an r-cluster into one-clusters. Thus $\mathbf{m}^{k(r)}$ is the state obtained from $\mathbf{m}^1$ by removing an r-cluster and replacing it with $k(r)$ one-clusters. The condition on the parameters μ_{rsu} ensures that there exists such a sequence with $q(\mathbf{m}^i, \mathbf{m}^{i+1}) > 0$ for $i = 1, 2, \ldots, k(r)-1$. Define

$$c_r = \frac{m_r m_1!}{(m_1 + k(r))!} \prod_{i=1}^{k(r)-1} \frac{q(\mathbf{m}^{i+1}, \mathbf{m}^i)}{q(\mathbf{m}^i, \mathbf{m}^{i+1})}$$

Observe that the first factor has been chosen so that terms involving $m_1, m_2, \ldots$ cancel, leaving c_r as the product of ratios λ_{rsu}/μ_{rsu}. Further, since $\mathbf{m}$ is reversible Kolmogorov's criteria establishes that c_r does not depend on the sequence of states $\mathbf{m}^1, \mathbf{m}^2, \ldots, \mathbf{m}^{k(r)}$ used to define it. Note that c_r will be positive unless the numerator is zero, in which case an r-cluster could not exist in equilibrium. It now remains to check that c_r, $r = 1, 2, \ldots$, satisfy equations (8.4). This can be most readily verified by defining c_u using the sequence $\mathbf{m}^1, \mathbf{m}^2, \ldots$ in which after the u-cluster has separated into an r-cluster and an s-cluster the r-cluster completely breaks up into one-clusters before the s-cluster begins to dissociate.

Exercises 8.2

1. Consider a closed clustering process in which the total number of units present in the system is fixed at M, with r units present in each r-cluster. Let B_M be the normalizing constant appearing in expression (8.5). Thus

$$B_M^{-1} = \sum_{\mathbf{m}} \prod_r \frac{c_r^{m_r}}{m_r!}$$

where the summation runs over all $\mathbf{m}$ satisfying $\sum r m_r = M$. Show that the expected number of clusters of size r is $c_r B_M / B_{M-r}$ and that the probability a randomly chosen unit lies in a cluster of size r is $r c_r B_M / M B_{M-r}$. Deduce the recursive formula for $B_1, B_2, \ldots,$

$$M B_M^{-1} = \sum_{r=1}^{M} r c_r B_{M-r}^{-1} \tag{8.11}$$

where $B_0 = 1$.

2. For the process considered in the previous exercise show that B_M^{-1} is the

coefficient of θ^M in the power series expansion of

$$G(\theta) = e^{F(\theta)} = \exp\left(\sum_r c_r \theta^r\right)$$

Deduce the recursion (8.11) from the identity

$$\theta G'(\theta) = G(\theta) \sum_r r c_r \theta^r$$

3. There are many ways a closed clustering process can be amended to produce an open clustering process. For example, suppose that r-clusters may enter or leave the system at rates

$$\begin{aligned} q(\mathbf{m}, R_r\mathbf{m}) &= \nu_r \\ q(\mathbf{m}, R_r'\mathbf{m}) &= \mu_r m_r \end{aligned} \tag{8.12}$$

Show that if

$$\nu_r = c_r \mu_r$$

and

$$c_r c_s \lambda_{rsu} = c_u \mu_{rsu}$$

then the system with transition rates (8.3) and (8.12) is reversible with equilibrium distribution (8.10), provided condition (8.9) holds and any state with $\sum m_r$ finite can be reached from any other such state.

4. Suppose that an r-cluster contains $k(r)$ units. Show that if c_r, $r = 1, 2, \ldots$, is a solution to equations (8.4) then $c_r \theta^{k(r)}$, $r = 1, 2, \ldots$, is a solution to equations (8.8) where $\theta^{k(1)} = \nu/\mu c_1$.
5. Even when clusters are made up of units the condition imposed on the dissociation rates in Lemma 8.3 may not be satisfied. For example if an r-cluster contains r units and if $\lambda_{rsu} = \mu_{rsu}$, $\lambda_{112} = \lambda_{224} = \lambda_{246} = \lambda_{336} = 1$ with all other $\lambda_{rsu} = 0$ then a three-cluster can only be formed by the breakup of a six-cluster. In fact the condition imposed in Lemma 8.3 is unnecessary. Show that if a process $\mathbf{m}$ with transition rates (8.3) is reversible then there exists a non-zero solution $c_1, c_2, \ldots$ to equations (8.4).
6. Suppose that the function $F(\theta)$ defined in Exercise 8.2.2 has radius of convergence θ_0. Deduce that $G(\theta)$ has the same radius of convergence, and that if B_M/B_{M-1} tends to a limit as $M \to \infty$ the limiting value is θ_0. Consider now the effect of letting $M \to \infty$ on the equilibrium distribution of the clustering process. Deduce from Exercise 8.2.1 that if B_M/B_{M-1} converges then the expected number of r-clusters tends to $c_r \theta_0^r$.
7. Generalize the results contained in Exercises 8.2.1, 8.2.2, and 8.2.6 to allow an r-cluster to contain $k(r)$ units.

8.3 EXAMPLES

In general the rates λ_{rsu} and μ_{rsu} will not allow a solution to equations (8.4): in this section we shall give some examples where they do. In most of these examples the number of units in a cluster will define it completely, with $k(r) = r$. Initially we shall consider clustering processes in which only a single unit can join on to or break off from a cluster, and we shall write λ_r and μ_r for $\lambda_{1,r,r+1}$ and $\mu_{1,r-1,r}$ respectively. For such processes equations (8.4) always have a solution: it can be built up from the recursion

$$c_r\mu_r = c_{r-1}c_1\lambda_{r-1} \tag{8.13}$$

with c_1 chosen arbitrarily. The solution to equations (8.8) is given by the same recursion, with c_1 set equal to ν/μ.

Example 1. The simplest case occurs when

$$\lambda_r = \alpha \qquad \mu_r = \beta$$

so that size does not affect the propensity of clusters to associate or dissociate. From the recursion (8.13) we find that a solution to equations (8.4) is

$$c_r = \frac{\beta}{\alpha}$$

Thus for a closed clustering process in which the total number of units is fixed at M the equilibrium distribution is

$$\pi(\mathbf{m}) = B_M\left(\frac{\beta}{\alpha}\right)^{\Sigma_r m_r} \prod_r \frac{1}{m_r!} \tag{8.14}$$

where B_M can be calculated from the recursion (8.11). Observe that if β is much smaller than α then we can expect $\sum m_r$ to be small and hence we can expect the M units to be concentrated in a few large clusters. Suppose now the process is made open using transition rates (8.7). The solution to equations (8.8) is $c_r = (\beta/\alpha)\theta^r$ where

$$\theta = \frac{\alpha\nu}{\beta\mu}$$

(Exercise 8.2.4). Define formally the function

$$F(\theta) = \sum_{r=1}^{\infty} c_r$$

so that for this example

$$F(\theta) = \sum_{r=1}^{\infty} \frac{\beta}{\alpha}\theta^r$$

To satisfy (8.9) we require $F(\theta)<\infty$ and thus $\theta<1$. Provided $\theta<1$,

$$F(\theta)=\frac{\beta}{\alpha}\frac{\theta}{1-\theta}$$

is the expected number of clusters. As θ approaches unity the expected number of clusters approaches infinity.

Example 2. The case

$$\lambda_r=\alpha \qquad \mu_r=\beta r$$

was considered in Section 8.1; the closed process has equilibrium distribution (8.2). Figure 8.1 plots the expected number of units in clusters of size r against r, for certain values of the parameters. The open process has

$$c_r=\frac{\beta}{\alpha}\frac{\theta^r}{r!}$$

and thus

$$F(\theta)=\frac{\beta}{\alpha}(e^{\theta}-1)$$

The radius of convergence of the function $F(\theta)$ is infinite: no matter how large θ becomes the open process has an equilibrium distribution.

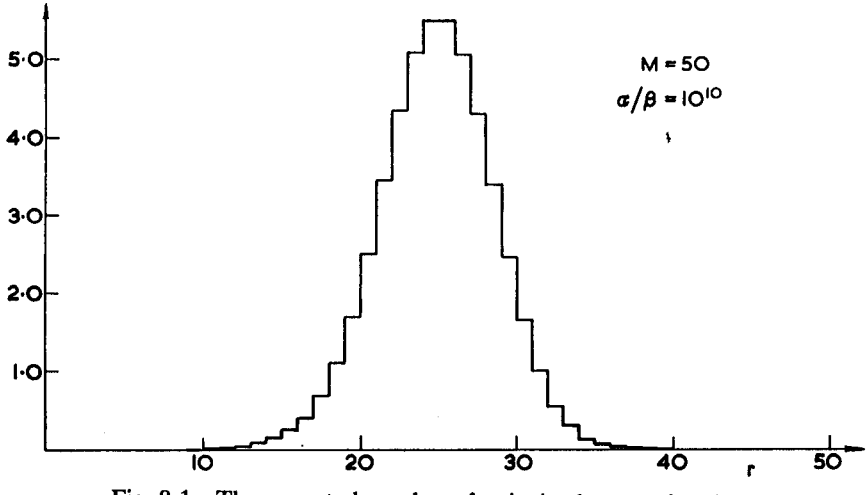

Fig. 8.1 The expected number of units in clusters of various sizes

Example 3. Consider the case

$$\lambda_r=\alpha r \qquad \mu_r=\beta$$

The association rate αr will arise if a given isolate is attracted to each individual of a group at a constant rate α. The closed process has $c_r = (\beta/\alpha)(r-1)!$. The open process does not have an equilibrium distribution for any positive value of θ since $\theta^r(r-1)!$ diverges as r tends to infinity.

Example 4. If

$$\lambda_r = \alpha r \qquad \mu_r = \beta r$$

then the closed process has $c_r = \beta/\alpha r$. For this case the normalizing constant can be written in a closed form and the equilibrium distribution is

$$\pi(\mathbf{m}) = \binom{(\beta/\alpha)+M-1}{M}^{-1} \prod_r \frac{1}{m_r!}\left(\frac{\beta}{\alpha r}\right)^{m_r} \tag{8.15}$$

the same as for the infinite alleles model of Chapter 7. For the open process

$$c_r = \frac{\beta\theta^r}{\alpha r}$$

and so

$$F(\theta) = -\frac{\beta}{\alpha}\log(1-\theta)$$

provided $\theta < 1$.

Example 5. Let

$$\lambda_r = \alpha r \qquad \mu_r = \beta(r+1)$$

The dissociation rate in this and the next example are a little artificial; the purpose of the examples is to introduce a phenomenon which will arise naturally in Section 8.4. For the open process

$$c_r = \frac{2\beta\theta^r}{\alpha r(r+1)}$$

and so an equilibrium distribution exists provided $\theta \leq 1$. As θ approaches unity the expected number of clusters does *not* diverge; in fact the expected number of clusters approaches $F(1) = 2\beta/\alpha$ (Exercise 8.3.1). However, the expected number of units in the system is $\sum rc_r$, and thus as θ approaches unity the expected number of units *does* diverge. When $\theta = 1$ an equilibrium distribution exists, and it has the property that the mean cluster size is infinite (Exercise 8.3.1).

Example 6. Let

$$\lambda_r = \alpha r \qquad \mu_r = \beta(r+2)$$

For the open process

$$c_r = \frac{6\beta\theta^r}{\alpha r(r+1)(r+2)}$$

and so an equilibrium distribution exists provided $\theta \leq 1$. When $\theta = 1$ the expected number of clusters, $\sum c_r$, and the expected number of units, $\sum rc_r$, are both finite. However, $\sum r^2 c_r$ is infinite, a fact which can be interpreted in various ways (Exercise 8.3.2). It shows that the size of a randomly chosen cluster has infinite variance. Suppose there exists a link between two units if they are in the same cluster; thus an r-cluster contains $\frac{1}{2}r(r-1)$ links. When $\theta = 1$ the expected number of links is infinite.

The next examples allow clusters of any size to associate. Write λ_{rs} and μ_{rs} for $\lambda_{r,s,r+s}$, and $\mu_{r,s,r+s}$ respectively. If equations (8.4) have a solution then it can be built up from the recursion

$$c_r \mu_{1,r-1} = c_{r-1} c_1 \lambda_{1,r-1}$$

with c_1 chosen arbitrarily provided $\lambda_{1r} > 0$ for $r \geq 1$. The solution to equations (8.8) is given by the same recursion with c_1 set equal to ν/μ.

Example 7. The obvious generalization of Example 1 is given by the choice of parameters

$$\lambda_{rs} = \alpha \qquad \mu_{rs} = \beta$$

Once again a solution to equations (8.4) is $c_r = \beta/\alpha$, and the equilibrium distribution for the closed system is given by expression (8.14). The open system also has the same equilibrium distribution as for Example 1.

Example 8. One possible generalization of Example 2 which allows a solution to equations (8.4) is obtained by letting

$$\lambda_{rs} = \alpha \qquad \mu_{rs} = \beta\binom{r+s}{r}$$

This dissociation rate arises if the rate at which an $(r+s)$-cluster breaks up to leave a given r units in one cluster and the other s units in another cluster is β, since with the units identified in this way there are $\binom{r+s}{r}$ distinct ways in which an $(r+s)$-cluster can break up to form an r-cluster and an s-cluster. The closed and open equilibrium distributions are the same as for Example 2.

Following the definition of the transition rates (8.3) the parameter λ_{rsu}, $r \leq s$, was interpreted as the probability intensity a given r-cluster attaches itself to a given s-cluster. This interpretation occasionally requires a minor modification when $r = s$. For $r \leq s$ the number of distinct ordered pairs of

clusters in which the first cluster is an r-cluster and the second cluster is an s-cluster is $n_r n_s$ (for $r<s$) or $n_r(n_r-1)$ (for $r=s$). However, the number of distinct *unordered* pairs is $n_r n_s$ (for $r<s$) or $\frac{1}{2}n_r(n_r-1)$ (for $r=s$). In the model considered in Section 8.1 (and again as Example 2) it was reasonable to count ordered pairs of clusters with $r \leq s$, and it was therefore reasonable to set $\lambda_{112}=\alpha$. When it is more suitable to count unordered pairs a factor of $\frac{1}{2}$ must be incorporated in the definition of λ_{rru}. To illustrate this consider the following example.

Example 9. Suppose that an r-cluster represents a molecule made up of a string of r atoms arranged along a line with a bond between adjacent atoms. Imagine that the molecules are milling around in a confined space. Molecules combine when they come into close proximity and a molecule breaks into two when a bond breaks. Ignoring spatial considerations it may be reasonable to assume that any given unordered pair of molecules comes into close proximity at rate α and hence to set

$$\lambda_{rs}=\begin{cases}\alpha & r\neq s\\ \frac{1}{2}\alpha & r=s\end{cases}$$

If we suppose that each bond breaks at rate $\frac{1}{2}\beta$ then

$$\mu_{rs}=\begin{cases}\beta & r\neq s\\ \frac{1}{2}\beta & r=s\end{cases}$$

since if $r\neq s$ there are two bonds in an $(r+s)$-cluster whose severance would produce an r-cluster and an s-cluster. The solution to equations (8.4) is $c_r=\beta/\alpha$, and the equilibrium distribution in the open and closed cases are as for Examples 7 and 1.

Occasionally clusters may be constructed from more than one type of basic unit. As an example consider the following elaboration of Example 9.

Example 10. Suppose there are two types of atom, A-atoms and B-atoms. Molecules consist of a chain of atoms with a bond between adjacent atoms. A-atoms can be bonded to up to two other atoms, but B-atoms can only occur at the ends of a chain. Call a chain consisting of just r A-atoms an $r0$-cluster, r A-atoms and one B-atom an $r1$-cluster, and r A-atoms and two B-atoms an $r2$-cluster. Suppose the probability intensity a given (unordered) pair of clusters combine is α if neither of them contain any B-atoms, $\frac{1}{2}\alpha$ if between them they contain one B-atom, and $\frac{1}{4}\alpha$ if they both contain one B-atom. Suppose the rate at which a given bond breaks is $\frac{1}{2}\beta_0$ if it links two A-atoms, $\frac{1}{2}\beta_1$ if it links an A-atom and a B-atom, and $\frac{1}{2}\beta_2$ if it links two B-atoms. It is readily checked that the resulting association and dissociation

rates allow the solution

$$c_{r0}=\frac{\beta_0}{\alpha} \qquad c_{r1}=\frac{\beta_0}{\alpha} \qquad c_{r2}=\frac{\beta_0}{4\alpha} \qquad r\geq 1$$

$$c_{01}=\frac{\beta_1}{\alpha} \qquad c_{02}=\frac{\beta_1^2}{4\alpha\beta_2}$$

to equations (8.4).

Exercises 8.3

1. Check that for Example 5,

$$F(\theta)=\frac{2\beta}{\alpha}\left[1+\frac{1-\theta}{\theta}\log(1-\theta)\right]$$

and that $F(1)=2\beta/\alpha$. Show that conditional on the event $\sum m_r=N$ the expected size of a randomly chosen cluster is $\theta F'(\theta)/F(\theta)$, for all $N\geq 1$. Show that when $\theta=1$ the expected size of a cluster chosen at random is infinite. (If $\sum m_r=0$ regard the size of the chosen cluster as zero.)

2. Check that for Example 6,

$$F(\theta)=\frac{3\beta}{2\alpha\theta^2}[3\theta^2-2\theta-2(1-\theta)^2\log(1-\theta)]$$

and that the radius of convergence of $F(\theta)$ is unity. When $\theta=1$ show that the expected number of clusters is $3\beta/2\alpha$, and that, conditional on $\sum m_r>0$, the expected size of a randomly chosen cluster is 2. Show that the expected number of links is $\frac{1}{2}\theta^2F''(\theta)$, and observe that this diverges as $\theta\to 1$. Check that when $\theta=1$ the size of a randomly chosen cluster has infinite variance.

3. The phenomenon observed in Examples 5 and 6 can also arise in quite simple queueing systems. Consider a queue at which arrivals occur at rate $\nu(n+1)/(n+2)$ and customers depart at rate $(n+1)/n$, where n is the number in the queue. Show that an equilibrium distribution exists when $\nu=1$ but the mean number in the queue is infinite.

4. Observe that the equilibrium distribution for Example 8 is unaltered if λ_{rr} is set to $\frac{1}{2}\alpha$ and μ_{rr} to $\frac{1}{2}\beta\binom{2r}{r}$. Show that the resulting dissociation rates arise if u-clusters receive shocks at rate $2^{u-1}\beta$ and if after a cluster has received a shock each of its units assigns itself independently and at random to one of two new clusters. Show that if shocks are received by a u-cluster at rate $f(u)$ then equations (8.4) have a solution only when $f(u)$ takes the form $2^{u-1}\beta$.

8.4 POLYMERIZATION PROCESSES

In this section we shall consider a model of the way in which organic molecules form themselves into polymers. We shall assume that a cluster is constructed from single units linked together by bonds in such a way that the graph formed by regarding units as vertices and bonds as edges is a tree. A cluster breaks up into two clusters by the severance of a single bond, and two clusters join together to form one cluster by the establishment of a single additional bond between two units, one from each cluster. Two clusters are to be regarded as of the same type if the graphs associated with them are isomorphic. Thus when we refer to an r-cluster r identifies the graph associated with the cluster.

Typical clusters are illustrated in Fig. 8.2. There are two simplifications implicit in this model of polymer chains which are worth noting. First, the assumption that clusters correspond to trees rules out cycles, which can of course occur in organic molecules. Second, the assumption that the tree associated with a cluster defines it completely ignores the fact that the angles between bonds are sometimes important.

Suppose that any existing bond breaks at rate κ. This implies that the parameter μ_{rsu} is equal to κ times the number of bonds in a u-cluster whose severance would result in an r-cluster and an s-cluster. The association rate is more difficult to define and arises in the following way. Each unit has f sites (or functionalities, to use the polymer science term) at which a bond can be based. A bond appears at unit rate between any two given vacant sites provided they are on units in different clusters. With this in mind set λ_{rsu} (or $2\lambda_{rru}$ in the case $r=s$) equal to

$$\sum_{x,y} h_x h_y$$

where x and y mark units in an r-cluster and an s-cluster respectively, and the summation runs over all units x and y such that the introduction of a bond between x and y would cause the r-cluster and the s-cluster to form a u-cluster. Let

$$h_x = f - j$$

where j is the number of other units to which x is bonded in the r-cluster and f is a fixed positive integer. Note that the case $f=2$ corresponds to Example 9 of the previous section, with $\alpha = \frac{1}{4}$ and $\beta = 2\kappa$.

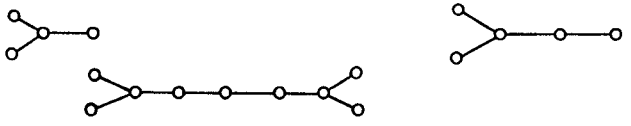

Fig. 8.2 Typical clusters when $f=3$

For given r, s, and u the parameters λ_{rsu} and μ_{rsu} can be explicitly calculated. For example if $f=3$ and r, s, and u are as in Fig. 8.2, then $\lambda_{rsu}=12$ and $\mu_{rsu}=2\kappa$. The precise form of the parameters λ_{rsu} and μ_{rsu} for general r, s, and u involve rather complicated combinational coefficients depending on the shape of r-, s-, and u-clusters. Our first objective will be to show that these parameters allow a non-zero solution to equations (8.4); we shall achieve this by an appeal to Lemma 8.3, after we have shown that the process $\mathbf{m}=(m_1, m_2, \ldots)$, where m_r is the number of r-clusters, is reversible.

Suppose there are in total M units and that these units are distinguishable. Suppose further that each of the f sites on each unit is distinguishable. Redefine the possible cluster types so that the type of a cluster gives not only the graph associated with the cluster but also which unit is at each vertex of the graph, and which sites are used on units for each bond. Use r', s', and u' and primes generally when dealing with clusters described at this level of detail; note that there can exist at most one r'-cluster. Usually it will not be possible for a u'-cluster to be formed from an r'-cluster and an s'-cluster since even if the graphs are compatible the particular units and sites used may not be. In this case $\lambda'_{r's'u'}$ and $\mu'_{r's'u'}$ are both zero. If a u'-cluster can be formed from an r'-cluster and an s'-cluster there will be just one way of doing it; in this case $\lambda'_{r's'u'}=1$ and $\mu'_{r's'u'}=\kappa$. There are no combinatorial coefficients involved in the definition of $\lambda'_{r's'u'}$ and $\mu'_{r's'u'}$, and it is clear that a solution to the equations

$$c'_{r'}c'_{s'}\lambda'_{r's'u'}=c'_{u'}\mu'_{r's'u'}$$

is given by

$$c'_{r'}=\kappa$$

Hence by Theorem 8.1 the process $\mathbf{m}'=(m'_1, m'_2, \ldots)$, where $m'_{r'}$ is the number (zero or one) of r'-clusters, is reversible.

Now $\mathbf{m}$ is a function of $\mathbf{m}'$; m_r is obtained by summing $m'_{r'}$ over all r' whose graph is compatible with r. Hence $\mathbf{m}$ is reversible (Exercise 1.2.9). Further, $\mathbf{m}$ is a Markov process with transition rates of the form (8.3) where λ_{rsu} and μ_{rsu} have been defined earlier. Thus Lemma 8.3 shows that the rates λ_{rsu} and μ_{rsu} allow a non-zero solution $c_1, c_2, \ldots$ to the equations

$$c_r c_s \lambda_{rsu}=c_u \mu_{rsu} \tag{8.16}$$

and we have achieved our first objective.

We shall not obtain a solution $c_1, c_2, \ldots$ to equations (8.16); the expression for c_r would be complicated, involving the combinatorial coefficients appearing through λ_{rsu} and μ_{rsu}. Instead we shall determine $c^*_{r^*}$ where

$$c^*_{r^*}=\sum_{r:k(r)=r^*} c_r$$

We shall see that the mere fact that equations (8.16) have a solution allows us to deduce a recursion for $c_{r^*}^*$ and that from this we can calculate quantities such as the expected number of clusters containing r^* units.

A u-cluster contains $k(u)$ units and hence has $k(u)-1$ bonds. The rate at which a u-cluster breaks up is thus

$$\sum_{r,s} \mu_{rsu} = \kappa(k(u)-1) \tag{8.17}$$

where the summation runs over all unordered pairs (r, s). An r-cluster contains $k(r)$ units, has $k(r)-1$ bonds, and hence has $(f-2)k(r)+2$ vacant sites. The rate at which a given r-cluster and a given s-cluster associate is thus

$$\sum_u \lambda_{rsu} = [(f-2)k(r)+2][(f-2)k(s)+2] \qquad r \neq s$$

or

$$2\sum_u \lambda_{rru} = [(f-2)k(r)+2]^2 \qquad r = s \tag{8.18}$$

From equation (8.16)

$$c_r\theta^{k(r)} c_s\theta^{k(s)}\lambda_{rsu} = c_u\theta^{k(u)}\mu_{rsu}$$

Summing this over u and unordered pairs (r, s) and substituting from equations (8.17) and (8.18) gives

$$\frac{1}{2}\sum_r\sum_s c_r\theta^{k(r)}[(f-2)k(r)+2]c_s\theta^{k(s)}[(f-2)k(s)+2]$$

$$= \kappa\sum_u c_u\theta^{k(u)}(k(u)-1) \tag{8.19}$$

Notice that the double summation over r and s and the introduction of the factor $\frac{1}{2}$ in equation (8.19) deal adequately with both of the forms appearing in equation (8.18). In terms of the quantities $c_{r^*}^*$ equation (8.19) becomes

$$\frac{1}{2}\sum_{r^*}\sum_{s^*} c_{r^*}^*\theta^{r^*}[(f-2)r^*+2]c_{s^*}^*\theta^{s^*}[(f-2)s^*+2] = \kappa\sum_{u^*} c_{u^*}^*\theta^{u^*}(u^*-1)$$

Equating coefficients of θ^{u^*} produces the recursion

$$\kappa c_{u^*}^*(u^*-1) = \frac{1}{2}\sum_{r^*=1}^{u^*-1} c_{r^*}^*[(f-2)r^*+2]c_{u^*-r^*}^*[(f-2)(u^*-r^*)+2] \tag{8.20}$$

from which $c_{r^*}^*$, $r^* = 1, 2, \ldots$, can be built up. Setting $c_1^* = \kappa$ the recursion can be shown to produce

$$c_{r^*}^* = \kappa\frac{f^{r^*}[(f-1)r^*]!}{r^*![(f-2)r^*+2]!} \tag{8.21}$$

What is the statistical interpretation of $c^*_{r^*}$? Well we know that $\mathbf{m}$ has the equilibrium distribution $\pi(\mathbf{m})$ given by expression (8.5). Let $\mathbf{m}^* = (m^*_1, m^*_2, \ldots)$ where

$$m^*_{r^*} = \sum_{r:k(r)=r^*} m_r$$

the number of clusters of size r^*. The description r^* of a cluster tells us how many units are in the cluster, but no more. If $f > 2$ the process $\mathbf{m}^*$ is not Markov; the number of units in a cluster does not give enough information about the various ways the cluster can associate or dissociate. Nevertheless, the equilibrium distribution for $\mathbf{m}^*$ can be calculated from $\pi(\mathbf{m})$ (Exercise 8.4.1) and is given by

$$\pi^*(\mathbf{m}^*) = B \prod_{r^*} \frac{c^{*m^*_{r^*}}_{r^*}}{m^*_{r^*}!} \tag{8.22}$$

for $\mathbf{m}^*$ such that $\sum_i i m^*_i = M$. This expression gives the distribution of clusters of various sizes, but does not give more detailed information about the shapes of clusters of a given size. The expected number of clusters of size r^* and the expected number of units in clusters of size r^* can be calculated using Exercise 8.2.1 (see Fig. 8.3).

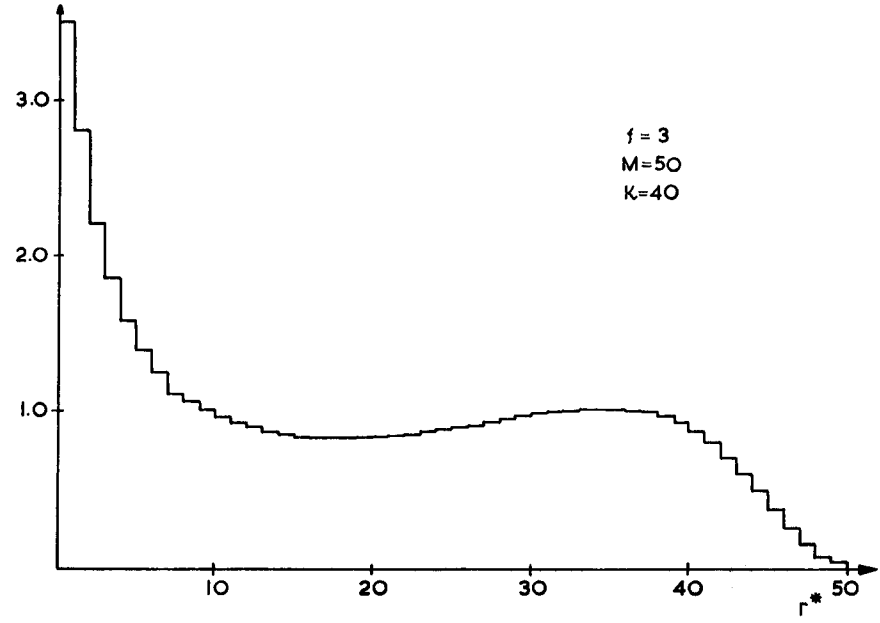

Fig. 8.3 The expected number of units in clusters of various sizes

An important physical phenomenon exhibited by polymers is gelation: when the density is increased above a critical value an observable change takes place in the physical properties of the system. We shall now discuss an elaboration of the above polymerization process which casts some light on this phenomenon. Suppose that a large volume of space consists of J unit sized boxes, and let $\mathbf{m}$ describe the clusters present in a typical box. Suppose that the clusters present in a box associate and dissociate in accordance with rates (8.3) and that in addition each cluster moves from its present box to an adjacent box at rate γ. Suppose, further, that one of the boxes is open to the outside environment with one-clusters emigrating from it and immigrating to it at rates (8.7). The detailed balance conditions allow it to be readily checked that in equilibrium the contents of the J boxes are independent and for each box

$$\pi(\mathbf{m}) = \prod_r e^{-c_r} \frac{c_r^{m_r}}{m_r!}$$

provided conditions (8.8) and (8.9) are satisfied. Thus $m_1, m_2, \ldots$ are independent random variables and m_r has a Poisson distribution with mean c_r. In the polymerization context we can deduce that the number of clusters of size r^* in a typical box has a Poisson distribution with mean

$$c_{r^*}^* = \kappa \frac{(f\theta)^{r^*}[(f-1)r^*]!}{r^*![(f-2)r^*+2]!}$$

where $\theta = \nu/\mu\kappa$, provided $F(\theta) = \sum c_{r^*}^* < \infty$. The radius of convergence of $F(\theta)$ is

$$\theta_0 = \frac{(f-2)^{f-2}}{f(f-1)^{f-1}} \tag{8.23}$$

for $f > 2$ (Exercise 8.4.2). The number of units is independent from box to box with expectation $\sum i c_i^*$. Define the density ρ to be the total number of units divided by the total volume J. For finite J the density is a random variable but from now on we shall consider the limiting case of J infinitely large when the density becomes a constant, $\rho = \sum i c_i^*$. As θ increases towards θ_0 the density increases monotonically to the limiting value

$$\rho_0 = \frac{\kappa(f-1)}{f^2(f-2)}$$

and the sum $\sum i^2 c_i^*$ increases monotonically to infinity (Exercise 8.4.6). Consider now how the equilibrium distribution alters as the density is varied. As the density ρ approaches ρ_0 the parameter θ approaches θ_0 and so the expression $\sum i^2 c_i^*$ approaches infinity. The divergence of $\sum i^2 c_i^*$ corresponds to the physical phenomenon of gelation, whereby as the density passes through a critical value the system moves from the sol to the gel state.

The phenomenon can only occur where $f>2$; when $f=2$ the expressions $\sum ic_i^*$ and $\sum i^2c_i^*$ both increase to infinity as θ approaches θ_0.

Exercises 8.4

1. By summing $\pi(\mathbf{m})$, given by expression (8.5), over all states $\mathbf{m}$ consistent with the reduced description $\mathbf{m}^*$ obtain the distribution (8.22).
2. Use Stirling's formula

$$n!\sim\sqrt{2\pi}n^{n+1/2}e^{-n}$$

(where $\sim$ indicates that the ratio of the two sides tends to unity as $n\to\infty$) to show that the radius of convergence of $F(\theta)=\sum c_r^*$ is given by expression (8.23) for $f>2$. Show that when $\theta=\theta_0$,

$$c_i^*\sim\frac{\kappa(f-1)^{1/2}}{\sqrt{2\pi}(f-2)^{5/2}}\frac{1}{i^{5/2}}$$

3. Show that in the limit of large J the cluster a randomly chosen unit belongs to has mean size $\sum i^2c_i^*/\sum ic_i^*$. It is possible to relate this quantity to the physically observable characteristic, viscosity. The model then predicts that as the density approaches ρ_0 the viscosity becomes infinite.
4. Show that in the limit of large J the probability a randomly chosen site is occupied is

$$\frac{2}{f}\left(1-\frac{F(\theta)}{\theta F'(\theta)}\right)$$

5. To obtain $F(\theta)$ and its derivatives in a closed form it is helpful to change variable from θ to α, where α is the smallest positive root of the equation

$$f\theta=\alpha(1-\alpha)^{f-2}$$

Using this transformation to define α as a function of θ show that

$$\rho=\theta F'(\theta)=\frac{\kappa\alpha}{(1-\alpha)^2f^2}$$

Deduce that

$$F(\theta)=\frac{\kappa\alpha(2-\alpha f)}{2(1-\alpha)^2f}$$

6. Show that the probability a randomly chosen site is occupied, calculated in Exercise 8.4.4, is in fact equal to the variable α of Exercise 8.4.5. Show that as θ approaches θ_0 the probability α approaches $(f-1)^{-1}$. Deduce that as θ increases towards θ_0 the sum $\sum ic_i^*$ increases monotonically to the limiting value ρ_0 and the sum $\sum i^2c_i^*$ increases monotonically to infinity.

7. An alternative approach to the modelling of polymerization yields some results more readily. Suppose that a large vessel contains $2M$ units each with f sites for bonds. From the $2Mf$ sites available select at random $2Mf\alpha$ sites and form these randomly into $Mf\alpha$ pairs of sites. Now introduce a bond between the two sites in each pair. Observe that a proportion α of the sites will be occupied. Suppose now that M is arbitrarily large. Check that the probability a given unit is bonded to itself is zero and that the f sites on a given unit are independently occupied, each with probability α. Check further that the probability r units are linked together by r or more bonds, given they are linked by $r-1$ bonds, is zero. Now choose a unit at random and call the units to which it is directly linked its descendants. Observe that the number of descendants of the initial unit is binomial with parameters f and α, and that each descendant has a further set of descendants, whose number is binomial with parameters $f-1$ and α. Deduce that the expected number of units in the cluster of a randomly chosen unit is

$$\frac{1+\alpha}{1-(f-1)\alpha}$$

Observe that as α increases to $(f-1)^{-1}$ this diverges.

The above model is consistent with that developed in the preceding section. Note that its starting point is α, the proportion of occupied sites, while α is a derived quantity for the model of the preceding section.

8. Suppose that a closed vessel is divided up into J compartments, that in each compartment the clusters present associate and dissociate with rates

$$\begin{aligned} q(\mathbf{m}, R_u^{rs}\mathbf{m}) &= J\lambda_{rsu}m_r m_s \qquad r \neq s \\ &= J\lambda_{rru}m_r(m_r-1) \\ &= \mu_{rsu}m_u \end{aligned}$$

and that each cluster moves from its present box to an adjacent box at rate $\gamma(J)$. Let $\mathbf{m}^+ = (m_1^+, m_2^+, \ldots)$, where m_r^+ is the total number of r-clusters in the vessel. Note that $\mathbf{m}^+$ is not a Markov process. Show that if $c_1, c_2, \ldots$ are positive numbers satisfying equations (8.4) then $\mathbf{m}^+$ has equilibrium distribution given by expression (8.5). Observe that for large J we obtain a model in which clusters perform random walks, possibly merging when they collide.

9. We have used the equilibrium distribution for an open clustering process to investigate the behaviour of a polymerization process as the density approaches the critical value. The open equilibrium distribution is not available when the density exceeds the critical value, but we can use the closed equilibrium distribution. Consider the equilibrium distribution when M units are confined within a fixed finite volume. Exercise 8.2.6

suggests that as $M \to \infty$ the expected number of clusters of size r^* tends to the value $c_{r^*}^*$ obtained with $\theta = \theta_0$. In the limit $(m_1^*, m_2^*, \ldots, m_i^*)$ are independent Poisson random variables for all finite i. Physically this can be interpreted in the following way. As more units are added to the system they increase the gel component but leave unaffected the sol component, which does not depend on density provided this exceeds the critical value. Above the critical point the predictions obtained from the clustering process model and the branching process model of Exercise 8.4.7 differ. When $\alpha > (f-1)^{-1}$ the branching process model relates the expected number of r-clusters to the probability that a unit finds itself in a cluster of size r conditional on the cluster it belongs to being finite, and thus predicts that the sol component depends on α even when this exceeds the critical value. Above the critical density both models are suspect, since the assumption that clusters must correspond to trees becomes untenable.

8.5 GENERALIZATIONS

In this section we shall briefly indicate the results that can be obtained for processes with more general transition rates than those allowed in Section 8.2.

Define the operator $R_v^u\mathbf{m}$ to correspond to the transformation of a cluster of type u into a cluster of type v, so that

$$R_v^u\mathbf{m} = (m_1, m_2, \ldots, m_u - 1, \ldots, m_v + 1, \ldots)$$

Occasionally it may be useful to allow clusters to spontaneously transmute from one form to another. Suppose

$$q(\mathbf{m}, R_v^u\mathbf{m}) = \gamma_{uv} m_u \tag{8.24}$$

It is clear that with an equilibrium distribution of the form (8.5) the detailed balance conditions are satisfied provided $c_1, c_2, \ldots$ satisfy

$$c_u \gamma_{uv} = c_v \gamma_{vu} \tag{8.25}$$

in addition to equations (8.4). To illustrate this consider the following elaboration of Example 7 from Section 8.3, in which $\lambda_{rs} = \alpha$, $\mu_{rs} = \beta$. Suppose that $\gamma_{r,r+1} = \gamma r$ and $\gamma_{r,r-1} = \delta(r-1)$, with $\gamma < \delta$. The first of these rates arises naturally if we suppose that a unit gives birth at rate γ. The second rate is a little contrived, since the obvious choice would be δr. An advantage of $\delta(r-1)$ is that it prevents one-clusters from disappearing, and so allows a non-trivial equilibrium distribution in the absence of immigration. The solution to equations (8.4) and (8.25) is

$$c_r = \frac{\beta}{\alpha}\left(\frac{\gamma}{\delta}\right)^r$$

Any state $\mathbf{m}$ with $\sum m_j < \infty$ is accessible from any other such state; hence in equilibrium $m_1, m_2, \ldots$ are independent, and m_r has a Poisson distribution with mean c_r.

Another extension which springs naturally to mind in view of the migration processes considered in Chapter 2 is the substitution of $\phi_r(m_r)$ for m_r in the transition rates. Consider then the rates

$$\begin{aligned} q(\mathbf{m}, R_u^{rs}\mathbf{m}) &= \lambda_{rsu}\phi_r(m_r)\phi_s(m_s) \qquad r \neq s \\ q(\mathbf{m}, R_u^{rr}\mathbf{m}) &= \lambda_{rru}\phi_r(m_r)\phi_r(m_r - 1) \\ q(\mathbf{m}, R_{rs}^{u}\mathbf{m}) &= \mu_{rsu}\phi_u(m_u) \\ q(\mathbf{m}, R_v^{u}\mathbf{m}) &= \gamma_{uv}\phi_u(m_u) \end{aligned} \tag{8.26}$$

and the possible equilibrium distribution

$$\pi(\mathbf{m}) = B\prod_r \frac{c_r^{m_r}}{\prod_{l=1}^{m_r}\phi_r(l)} \tag{8.27}$$

where it is assumed that B can be chosen to make the distribution sum to unity. It is readily checked that if $c_1, c_2, \ldots$ are a non-zero solution of equations (8.4) and (8.25) then $\pi(\mathbf{m})$ satisfies the detailed balance conditions. Indeed $\pi(\mathbf{m})$ will be the equilibrium distribution under even weaker conditions. If $c_1, c_2, \ldots$ are a non-zero solution of

$$\begin{aligned} c_r c_s \sum_u \lambda_{rsu} &= \sum_u c_u \mu_{rsu} \\ \sum_{r,s} c_r c_s \lambda_{rsu} + \sum_v c_v \gamma_{vu} &= c_u\left(\sum_{r,s}\mu_{rsu} + \sum_v \gamma_{uv}\right) \end{aligned} \tag{8.28}$$

then $\pi(\mathbf{m})$ satisfies the equilibrium equations, even though in this case the process may not be reversible (Exercise 8.5.2).

To illustrate these results consider the following simple example. Suppose that a one-cluster and a two-cluster are single units of different types, and a three-cluster contains one unit of each type. Write λ and μ for λ_{123} and μ_{123} respectively. Then equations (8.4) have the solution $c_1 = c_2 = 1$, $c_3 = \lambda/\mu$, and so the equilibrium distribution is of the form (8.27) whatever the form of the functions ϕ_r, $r = 1, 2, 3$. A special case is

$$\begin{aligned} &\phi_1(n) = \phi_3(n) = n \\ &\phi_2(0) = 0 \\ &\phi_2(n) = 1 \qquad n > 0 \end{aligned} \tag{8.29}$$

This might correspond to a reversible chemical reaction in which the rate of association between molecules of types 1 and 2 is independent of the

number of molecules of type 2, provided the number is positive. Alternatively, the model might be appropriate for a social occasion, with three-clusters regarded as dancing couples and the functions ϕ_1 and ϕ_2 reflecting cultural conventions.

In the above example a cluster containing two units survives for an exponentially distributed period before breaking up. Suppose now that such a cluster passes through two stages: call it a three-cluster during the first stage and a four-cluster during the second stage. Consider then a process in which $\lambda_{123} = \lambda$, $\gamma_{34} = 2\mu$, $\mu_{124} = 2\mu$. Equations (8.28) have the solution $c_1 = c_2 = 1$, $c_3 = c_4 = \lambda/2\mu$, and so the equilibrium distribution again takes the form (8.27). If $\phi_3(n) = \phi_4(n) = n$ then it is readily shown that in equilibrium $(n_1, n_2, n_3 + n_4)$ has the same distribution as had (n_1, n_2, n_3) in the previous process. Indeed the only difference between the two processes is that now the overall lifetime of a cluster containing two units is not exponentially distributed. The method of stages can be used, as in Chapter 3, to obtain results when the overall lifetime of a cluster containing two units is arbitrarily distributed (Exercise 8.5.4).

Exercises 8.5

1. Extend Example 4 of Section 8.3 to allow clusters of any size to associate; show that if $\lambda_{rs} = \alpha rs$ and $\mu_{rs} = \beta(r+s)$ then expression (8.15) remains the equilibrium distribution of the closed process. Suppose now that individuals give birth at rate λ and die at rate μ, so that $\gamma_{r,r+1} = \lambda r$, $\gamma_{r,r-1} = \mu r$, and single individuals immigrate at rate ν. Show that in equilibrium $m_1, m_2, \ldots$ are independent Poisson random variables provided $\alpha\nu = \beta\lambda$.
2. Check that expression (8.27) satisfies the equilibrium equations provided $c_1, c_2, \ldots$ satisfy equations (8.28). Observe that a form of partial balance obtains.
3. Show that if $\lambda_{124} = \mu_{234} = \lambda_{235} = \mu_{125} = 1$ with all other λ_{rsu} and μ_{rsu} zero, then equations (8.28) have a solution. Observe that association with a two-cluster transforms a one-cluster into a three-cluster, and vice versa. Show that the process is dynamically reversible.
4. Consider a clustering process with transition rates (8.26) for which equations (8.28) are satisfied and for which the equilibrium distribution has the form (8.27). Suppose that r'-clusters cannot associate with other clusters, that is $\lambda_{r'su} = 0$ for all s, u, and that $\phi_{r'}(m) = m$. Thus r'-clusters survive for an exponentially distributed period with mean μ^{-1}, say. Show that the equilibrium distribution $\pi(\mathbf{m})$ will remain the same if the period for which r'-clusters survive has a distribution with mean μ^{-1} which can be expressed as a mixture of gamma distributions.
5. Check that the final example of this section which used the functions (8.29) is equivalent to the finite population telephone exchange model of

Exercise 1.3.5. Observe that allowing three-clusters to survive for an arbitrarily distributed period is equivalent to allowing arbitrarily distributed call lengths, an extension discussed in Section 4.4.

6. In Chapter 6 we considered migration processes in which the rate of migration into colony j was affected by the number of individuals already there, through a function ψ_j. Extend the transition rates (8.26) in an analogous manner and find the equilibrium distribution when equations (8.4) and (8.25) are satisfied.
7. Produce a clustering process analogous to the basic model of Section 8.2, but in which three or more clusters can associate to form, or can result from the dissociation of, a single cluster. Produce the equations analogous to equations (8.4). Develop a finite population telephone exchange model similar to that mentioned in Exercise 8.5.5 but where the subscribers call each other, so that when a call is successfully connected two subscribers and one line become engaged. Show that the form of the equilibrium distribution is unaltered.
8. Consider the garage described in Section 4.6. Suppose the garage and an infinite-server queue form a closed network of queues; interpret the time a car spends in the infinite-server queue as the time between repairs. Describe the resulting system as a clustering process, allowing possible clusters to be a car, a mechanic, or a car plus a mechanic.