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# 19

# Pair Approximations for Different Spatial Geometries

Minus van Baalen

## 19.1 Introduction

The standard assumption underlying the formulation of models for population dynamics (such as the logistic growth equation, the Lotka–Volterra predator–prey model, and the Kermack and McKendrick epidemiological equations, to name a few) is that populations spread homogeneously through space and that individuals mix rapidly. It is not a new insight that spatial structure is often an essential component of the ecological (and evolutionary) dynamics of populations, and there have been many approaches to understanding the various consequences of spatial structure. In this chapter I address one of the more recently developed techniques for modeling spatial population dynamics.

The oldest approach is to assume that populations are subdivided into different discrete subpopulations that are linked through migration (the "metapopulation" approach). This may be a reasonable assumption for certain systems (groups of parasites living in different hosts, for example), but space often has a more a continuous aspect. For example, a forest may be highly structured without having clear boundaries between subpopulations. Such situations are often modeled using a diffusion formalism, but this approach has its shortcomings as well. In particular, when one considers spatial spread of a population (or gene), individuality (discreteness) and its associated stochasticity may be important (Durrett and Levin 1994b). In a diffusion model, the rate of population growth is determined by the spread of "nano-individuals" at the wave front, whereas in reality it is often determined by the more erratic process of dispersal and subsequent successful settlement of individuals. Not only might this give quantitatively wrong estimates [e.g., the conditions under which an epidemic can arise; see Chapter 6 and Jeltsch *et al.* (1997)], it can also yield qualitatively wrong predictions (the term “atto-foxes” has been used to describe some spurious results from diffusion-based population models; see Mollison 1991).

By their very nature, diffusion models do not incorporate individuality. There exists, however, a suite of powerful mathematical techniques to deal with models that are based on stochastic, discrete events (Durrett and Levin 1994b). In some variants, individuals are represented as points and inhabit a continuous spatial domain (see Chapters 20 and 21; Pacala and Tilman 1994; Dieckmann *et al.* 1997); in others, individuals inhabit a discretized spatial domain, that is, a lattice of sites. This chapter focuses on the latter of these.

Even if localized, discrete and stochastic events make it difficult to study the exact dynamics of a system. However, the rates of change of certain average quantities (macroscopic spatial statistics) can be predicted with some accuracy. The fundamental approach is to derive the expected rate of change of an average quantity $f$ (such as the proportion or number of sites in a particular state) by averaging all possible events over the entire lattice; that is,

$$\frac{dE(f)}{dt} = E\left(\frac{df}{dt}\right) = \sum_{\text{All sites } x} \; \sum_{\text{All events } e_x} r(e_x)(f_{e_x} - f) \ , \tag{19.1}$$

where $r(e_x)$ gives the probability per unit time that an event $e$ occurs at location $x$ changing the average from $f$ to $f_{e_x}$. The main technical problem that we need to address in this chapter originates with the fact that rates $r(e_x)$ usually depend on the full spatial configuration.

When $f$ stands for a quantity such as the proportion of sites occupied by a given species, classical (nonspatial) models can be obtained. However, $f$ can just as easily stand for a configuration statistic involving more than one site. In that case, Equation (19.1) describes the dynamics of this configuration statistic and allows us, in principle, to work out how spatial structure changes over time. The simplest spatial “configuration” to which to apply this technique is pairs of nearest neighbors. In other words, instead of having as average quantity the proportion of sites in a given state (which yields the “density” of that state), the formalism is applied to the states of pairs of neighboring sites. The density concept is thus extended to pairs of nearest neighbors (or pairs for short).

The main advantage of knowing pair densities is that they provide information about the spatial distribution of states on the lattice. I will explain how they do so in some detail in this chapter. Pair-dynamics models originated in theoretical physics and were introduced into theoretical biology by Matsuda *et al.* (1992) to analyze spatial dynamics of predator–prey systems. They subsequently have been applied to host–parasite systems (Satō *et al.* 1994; Keeling 1995), models for plant competition (Harada and Iwasa 1994), and the evolution of altruism (Matsuda *et al.* 1992; Harada *et al.* 1995; Nakamaru *et al.* 1997; van Baalen and Rand 1998).

A minor note for the connoisseur of spatial models may be appropriate here. In the simplest pair-dynamics models, events change the state of only a single site at a time. For some applications this may be sufficient, but in many ecologically interesting systems, events change two sites at a time. Maybe the most important example of such a two-site event is movement of an individual from one site to another: an occupied site is vacated as another becomes occupied. In addition, other types of events cause simultaneous changes in a pair of neighboring sites. For example, in a predator–prey model, a predation event is modeled as one in which a "prey"–"hungry predator" pair becomes a "satiated predator"–"empty site" pair (de Roos *et al.* 1991). Models that allow simultaneous changes in neighboring sites are called "artificial ecologies" by Rand *et al.* (1995). To account for processes such as movement of individuals, in this chapter I use this formalism to allow events that change *pairs* of neighboring sites, instead of just single sites. Because movement is allowed, the method can be used to describe "viscous" populations, a term introduced by Hamilton (1964) to characterize populations that do not exhibit panmixis, but do not have a sharply subdivided spatial structure either.

A major incentive for developing pair-dynamics models has been the limited usefulness of probabilistic cellular automata, an increasingly popular way of studying spatial dynamics. It is relatively straightforward to model a spatial ecological system by setting up a lattice of sites and defining a set of rules that change the state of sites depending on their state and that of their environment. The advantage of this approach is that spatial phenomena are explicitly included. A disadvantage, however, is that simulating these models is rather time consuming. More seriously, the results are sometimes difficult to interpret and are not easily generalized. One is effectively limited to observing what happens in the simulation. Often, for example, it is difficult to explain *why* some species persist in spatial simulations and others do not. Pair-dynamics models provide analytical insight into this question. Used this way, pair-dynamics models are tools for capturing the essence of more-detailed, explicitly spatial models.

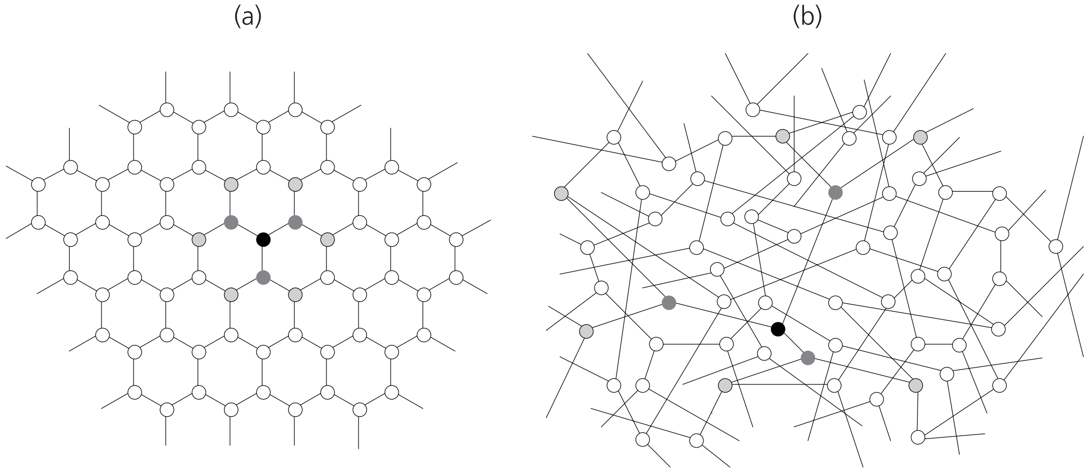


**Figure 19.1** Examples of (a) a regular two-dimensional lattice and (b) a random network, both with a neighborhood size of three. In both graphs, a focal site (black) and its neighbors up to two links away (dark and light gray) are indicated.

Pair-dynamics models sometimes cannot account for all features of the full spatial dynamics, particularly when the dynamics give rise to large-scale spatial structures (these cannot be accurately described on the basis of nearest-neighbor correlations alone). Nonetheless, the analytical insight pair-dynamics models provide is valuable. In this chapter I demonstrate that, even if pair-dynamics models do not describe the exact dynamics of a full system, they can provide good approximations for invasion and equilibrium conditions. Moreover, pair-dynamics models provide analytical insight into the relationship between lattice structure and population dynamics.

Computer simulations are usually defined on square grids where every site is connected to either four or eight neighbors. This is of practical convenience, as such lattices can easily be implemented in a program and displayed on a screen. However, it should be realized that such square lattices are quite special; even with a fixed number of connections per site, sites can be arranged in many ways. For example, with four connections per site, the sites can be laid out geometrically in a flat lattice (the usual case), but also in a lattice (based on tetrahedrons) that fills three-dimensional space, and of course in many other, less regular lattices.

That the structure of a lattice has consequences for population dynamics becomes apparent once one realizes that growing clusters of individuals have different overall shapes on different lattices: expanding foci are roughly circular on two-dimensional lattices such as the lattice depicted in Figure 19.1a, roughly spherical on three-dimensional lattices; and more tree-like in random lattices (Figure 19.1b). Obviously, for a model of plant population dynamics the choice of a two-dimensional lattice can be justified. However, a case can be made for more random lattices to describe other systems, such as parasites that transmit themselves across the social network of their host. Such a network does not necessarily correspond to the host individuals' spatial arrangement and may resemble a random network such as shown in Figure 19.1b (see also Watts and Strogatz 1998).

The aim of this chapter is twofold. First, I outline how to derive and use pair-dynamics equations, that is, differential equations that describe the rate of change of the density of pairs of neighbors (instead of only the densities of singlets, as is usually done). I then indicate how pair dynamics depend on the geometric structure of the lattice.

Working out the derivation in some detail is useful because it makes explicit the types of assumptions that must be made to "close" the set of equations. This term refers to the fact that the differential equations depend on quantities outside their scope (the densities of "triplets" and more complicated configurations). "Closure" means adopting an assumption that allows the differential equations to be completely expressed in terms of the quantities whose dynamics are described by the differential equations (in our case, pair densities). This is an important step, because pair dynamics turn out to depend on the densities of triplets and even larger configurations. The standard approach is to approximate triplets using pairs. However, as I show, knowledge of the geometrical structure of the lattice can be used to provide better estimates. A limitation of the approach adopted here is that it applies only to lattices with a fixed number of neighbors. Morris (1997) and Rand (1999) provide discussions of possible approaches for lattices that have variable numbers of connections per site.

Because the first part of this chapter is quite technical, it is accompanied by a parallel series of boxes in which a pair-dynamics model is derived and analyzed for a simple example. The example is the spatial equivalent of the well-known logistic growth model, where in addition to the birth and death of individuals, movement is also included. I compare the pair-dynamics model with explicit simulations and outline how invasion conditions can be derived. (Such invasion conditions give valuable insight into the conditions for persistence of a given population, because persistence requires that a population must bounce back when it is brought to low densities.) In this analysis, particular attention again is paid to how the spatial dynamics depend on the geometrical structure of the lattice.

## 19.2 The Dynamics of Pair Events

The set of sites that belong to the lattice (which is assumed to be finite but large) is denoted by $S$. Every site is assumed to have $n$ neighbors. Let $L \subset S \times S$ represent the set of connections (or *pairs* of sites) on the lattice. That is, two sites $x$ and $y$ form a pair if $xy \in L$.

Every site $x \in S$ is in a state $\sigma_x$, where $\Omega$ is the set of all possible states. The state of the entire lattice is denoted by $\sigma$; the state of a pair $xy$ is denoted by $\sigma_x \sigma_y$.

In an artificial ecology, the state of the lattice $\sigma$ changes over time because events change the state of sites or pairs of sites. Here, all events are defined in terms of pairs:

$$\sigma_x \sigma_y \to \sigma'_x \sigma'_y \ , \tag{19.2}$$

where the state of the lattice changes from $\sigma_x$ to $\sigma'_x$ at site $x$ and from $\sigma_y$ to $\sigma'_y$ at site $y$ simultaneously. (Notice that this formalism also includes all "single-site" events. Single-site events can be analyzed separately, but for the moment we consider a single-site event a special pair event.)

Any event $\sigma_x \sigma_y \to \sigma'_x \sigma'_y$ has an associated rate (probability per unit time)

$$r_\sigma(\sigma_x \sigma_y \to \sigma'_x \sigma'_y) \ . \tag{19.3}$$

Usually, it is assumed that all interactions are local: therefore, rates affecting a pair $xy$ depend only on the state of the pair's immediate environment $E_{xy}$:

$$r_\sigma(\sigma_x \sigma_y \to \sigma'_x \sigma'_y) = r(\sigma_x \sigma_y \to \sigma'_x \sigma'_y | \sigma_{E_{xy}}) \ , \tag{19.4}$$

where $E_{xy}$ is a list of all pairs in the local environment of the pair at $xy$ (see Figure 19.2).

A specific example of a simple artificial ecology is given in Box 19.1.

### Pair densities

The initial state of the lattice, $\sigma(0)$, together with the event rates specify a stochastic dynamical system: the state of the lattice follows a stochastic trajectory $\sigma(t)$. However, if the lattice is large enough, some quantities (such as the average number of pairs in a particular state) change almost deterministically. Here, I explain how differential equations can be found that (approximately) describe the expected dynamics of these quantities.

One can derive the expected rate of change in $p_a$, the probability that a given site is in state $a$. This is basically the classical "density" concept, and indeed the differential equations that result are of the type commonly used in population biology. The disadvantage is that all information with

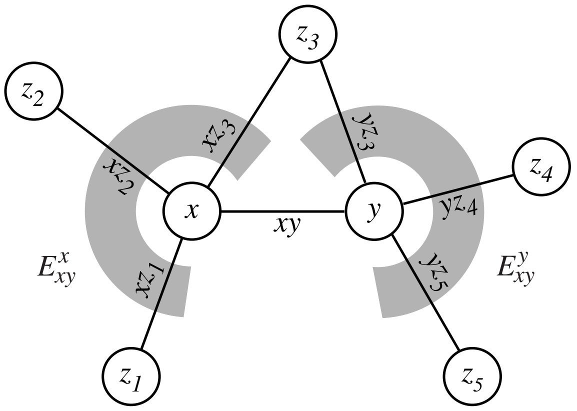


**Figure 19.2** An example of a pair at $xy$ and its "left" ($xz_i \in E^x_{xy}$) and "right" ($yz_i \in E^y_{xy}$) environments. The combination of the two specifies the entire environment $E_{xy}$ of the pair.

regard to spatial structure is lost: one is forced to assume that populations are "well mixed."

Some spatial information is retained if the states of *pairs* of nearest neighbors are traced instead of the states of single sites. One can work out the expected rate of change in the "pair densities" $p_{ij}$, where $p_{ij}$ gives the probability of finding a given pair in state $ij$. Knowing the pair densities permits computation of the conditional probabilities

$$q_{j|i} = p_{ij}/p_i \ . \tag{19.5}$$

These conditional probabilities give the density of $j$ sites as "experienced" by sites in state $i$: effectively, $q_{j|i}$ is the *local* density of $j$ in the environment of $i$ [Matsuda *et al.* (1992), use the term "environs densities" for these quantities].

## Pair dynamics of simple birth–death–movement process

Consider a particular pair combination $ab$. Obviously, its density $p_{ab}$ will change when pair events directly create or destroy both partners of $ab$ pairs. In other words, $p_{ab}$ increases with all $ij \rightarrow ab$ events (see Figure 19.3a) and $p_{ab}$ decreases with all $ab \rightarrow kl$ events. In addition, the density of $ab$ pairs will be affected by events that occur in $ab$'s neighborhood; for example, $ab$ pairs will be created if $ij \rightarrow bl$ events occur next to an $ai$ pair (such an event indirectly changes the $ai$ into an $ab$ pair; see Figure 19.3b). Throughout this chapter, I use the symbols $a$ and $b$ to refer to the pair combination of states whose dynamics are in focus. The indices $i$, $j$, $k$, and $l$ are used to sum over other states.

The contribution of direct events to the rate of change of $p_{ab}$ is straightforward. For example, the creation of $ab$ pairs from $ij$ pairs occurs at rate $p_{ij}\bar{r}_\sigma(ij \rightarrow ab)$, which is just the density of $ij$ pairs multiplied by the

**Box 19.1** A simple example of a birth–death–movement process

The simple artificial ecology analyzed in this chapter is defined on a lattice where every site is connected to $n$ other sites. The sites may be either empty (o) or occupied by a single individual (×), so $\Omega = \{\mathrm{o}, \times\}$. The spatial dynamics are determined by birth, death, and movement.

"Birth events" that change o× and ×o pairs into ×× pairs occur with rate (i.e., probability per unit time)

$$r(\times\mathrm{o} \to \times\times) = r(\mathrm{o}\times \to \times\times) = \phi b \ .$$

The factor $\phi = 1/n$ has been introduced for convenience: it allows $b$ to be interpreted as a *per capita* rate instead of a *per neighbor-pair* rate. Note that "mirror image" events (like the two above) always have the same rates.

"Death events" change × sites into o sites, or in terms of pairs, $\times j$ pairs into $\mathrm{o}j$ pairs (where $j \in \Omega$). They occur with rate

$$r(\times j \to \mathrm{o}j) = r(j\times \to j\mathrm{o}) = \phi d \ .$$

"Movement events" swap × and o sites in ×o and o× pairs (the individual moves to the empty neighbor site). They occur with rate

$$r(\times\mathrm{o} \to \mathrm{o}\times) = r(\mathrm{o}\times \to \times\mathrm{o}) = \phi m \ .$$

Notice that in this model the rates do not depend on the environment of the pairs. Such a dependency would arise if, for example, an individual's rate of reproduction were dependent on how many occupied neighbors it has. In that case, $b$ would not be constant but would be given by a function $b(n_{\times\times})$, where $n_{\times\times}$ is the number of × neighbors of the × in the ×o pair. Such environment-dependent rates result, for example, from altruistic behavior, where altruistic individuals help their neighbors at their own cost (Matsuda *et al.* 1992; van Baalen and Rand 1998). Intra- and interspecific competition also lead to environment-dependent rates.

average event rate. We must sum over all possible source pairs $ij$ to compute the total rate of direct $ab$ creation. [Calculating average rates such as $\bar{r}_\sigma(ij \to ab)$ is discussed below.]

The contribution of indirect events is a bit more complicated. First, the contribution of, say, $ij \to bl$ events depends on how many $j$ neighbors an $ai$ pair has on average. This average is given by $(n-1)q_{j|ia}$: the $i$ in an $ai$ pair has $n-1$ neighbors, and the likelihood of finding any one of them in state $j$ is given by the conditional probability $q_{j|ia}$. Note that this conditional probability depends on *triplet* densities: $q_{j|ia} = p_{aij}/p_{ia}$. Thus the set of differential equations for pairs depends on quantities outside its scope. (I return to this problem in Section 19.4.) The average rate of neighborhood events is given by $\bar{r}_\sigma(ij \to bl|aij)$; note that this is not the

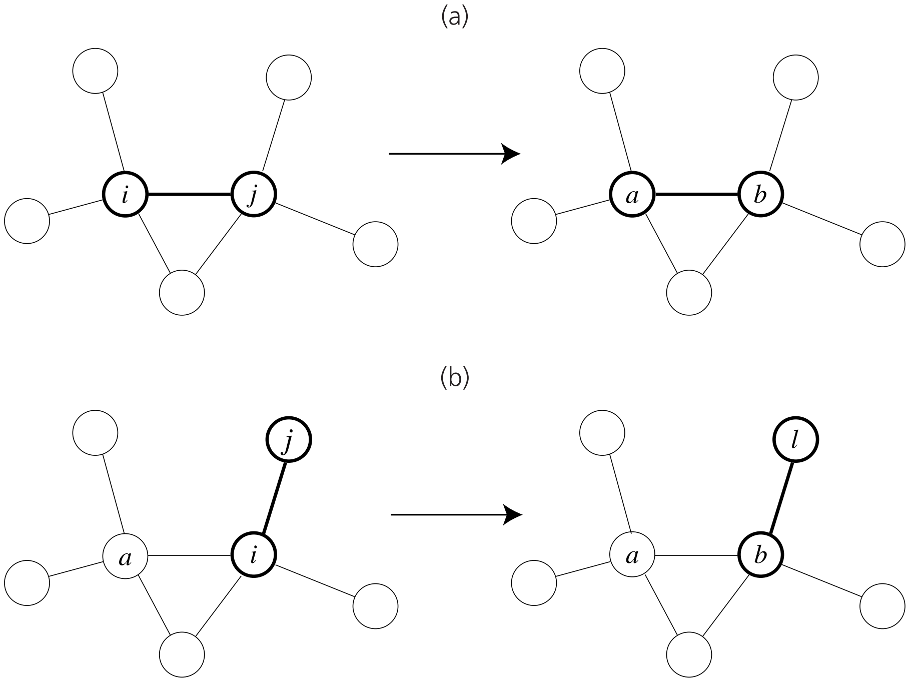


**Figure 19.3** The bookkeeping of pairs can depend both directly and indirectly on pair events. For example, (a) $ab$ pairs are created directly from $ij \to ab$ events, whereas (b) they are created indirectly when an $ij \to bl$ event changes the $i$ of an $ai$ pair into a $b$.

average rate of these events over the entire lattice, but the average rate of these events in $ij$ pairs in the neighborhood of $ai$ pairs. If the event rates are constant, conditional and unconditional averages are the same; if they are dependent on the environment, these averages are different.

Putting together all direct and indirect events that create as well as destroy $ab$ pairs yields the following "master equation":

$$\begin{aligned}\frac{dp_{ab}}{dt} = &- p_{ab}\sum_{kl}\Big[\bar{r}_\sigma(ab \to kl)+\sum_i (n-1)q_{i|ab}\bar{r}_\sigma(ia \to kl|iab)\\ &\qquad + \sum_j (n-1)q_{j|ba}\bar{r}_\sigma(bj \to kl|abj)\Big]\\ &+ \sum_{ij}\Big[p_{ij}\bar{r}_\sigma(ij \to ab)+p_{jb}\sum_k (n-1)q_{i|jb}\bar{r}_\sigma(ij \to ka|ijb)\\ &\qquad + p_{ai}\sum_l (n-1)q_{j|ia}\bar{r}_\sigma(ij \to bl|aij)\Big]\,.\end{aligned} \tag{19.6}$$

Note that this equation itself does not contain any specific references to the actual locations of $ab$ pairs on this lattice (there is no summation over all pairs $xy$ in the lattice). In other words, Equation (19.6) does not explicitly depend on space. It depends, however, on average event rates, and these

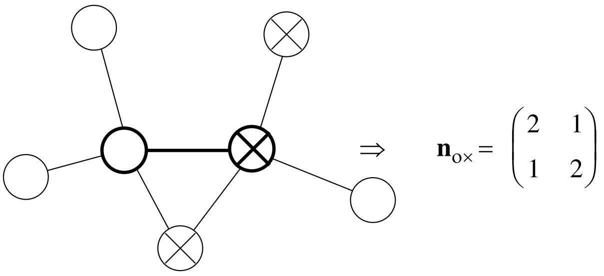


**Figure 19.4** Example of how to characterize the state $n_{\text{o}\times}$ of the local environment of a pair in state o×.

average rates depend on the state of the lattice. For this reason I have given the average rates a subscript $\sigma$.

A specific example of how to apply Equation (19.6) to the simple birth–death–movement process introduced in Box 19.1 is given in Box 19.2.

## 19.3 Average Event Rates

In the simplest models, pair event rates are constants. Often, however, such rates depend on the local environment of a pair. For example, if $a$ is an altruistic individual and $b$ is an empty site, the probability of an $ab \to aa$ (birth) event may depend on the number of other $a$s in $a$'s neighborhood. The mean rate of $ab \to aa$ events therefore depends on the mean number of $a$s next to $ab$ pairs. Of course, more complicated schemes are possible, such as in hypercycle dynamics where $a$ helps the reproduction of $b$, $b$ helps the reproduction of $c$, and so on, until eventually there is a type that helps $a$ (Boerlijst *et al.* 1993; see also Chapters 9 and 10). The approach I present here allows all such schemes; it even allows for nonlinear effects (when the effect of two $i$s is not equal to twice the effect of a single $i$).

Consider a pair event $ab \to kl$. When the event rate depends on the environment of the pair (say it increases with every neighbor in state $i$ in $a$'s neighborhood), the rates must be averaged over all possible configurations (i.e., over all configurations with zero $i$s, with one $i$, with two $i$s, etc.).

To be as general as possible, I represent the entire neighborhood of a given pair $ab$ at $xy$ using two vectors,

$$n^a_{ab} = \begin{pmatrix} \vdots \\ n_{ia} \\ \vdots \end{pmatrix} \qquad \text{and} \qquad n^b_{ab} = \begin{pmatrix} \vdots \\ n_{jb} \\ \vdots \end{pmatrix} , \tag{19.7}$$

with $i, j \in \Omega$. The vector $n^a_{ab}$ simply counts the different types of neighbors around $a$ in the $ab$ pair, while $n^b_{ab}$ does the same around $b$. These two vectors together give a two-column matrix,

$$n_{ab} = \begin{pmatrix} n_{ab}^{a} & n_{ab}^{b} \end{pmatrix} \; , \tag{19.8}$$

which therefore fully characterizes the state of the environment $n_{ab}$ of the $ab$ pair (see Figure 19.4). While the environment $E_{xy}$ itself simply specifies the geometrical *connections* around two sites $x$ and $y$, the neighborhood $n_{ab}$ specifies the *state* of this environment around a pair of sites in states $a$ and $b$. The assumption that all interactions occur only among neighbors and are not dependent on the actual configuration (i.e., whether a neighbor is located to the north or to the south, or to any other direction, is irrelevant) implies that this configuration completely determines the rate of events $ab \to kl$.

In principle, we could calculate the average event rate $\bar{r}_\sigma(ij \to kl)$ by averaging over the environments of all $ij$ pairs on the lattice. An equivalent and conceptually advantageous alternative, however, is to work out the frequency distribution of all possible neighborhoods $n_{ij}$ on the lattice. If the proportion of a given neighborhood $n_{ij}$ (relative to all possible configurations) is denoted by $F_\sigma(n_{ij})$, the average rate is given by

$$\bar{r}_\sigma(ij \to kl) = \sum_{n_{ij}} F_\sigma(n_{ij})\, r(ij \to kl|n_{ij}) \; . \tag{19.9}$$

The only component on the right-hand side that still depends on the state of the lattice is $F_\sigma(n_{ij})$. This quantity can be interpreted as a (local) density, this time not of a simple pair but of a larger spatial configuration. Thus, the pair equations may depend not only on the densities of triplets (which are needed to calculate local densities $q_{i|jk}$), but also on the densities of more complicated local configurations.

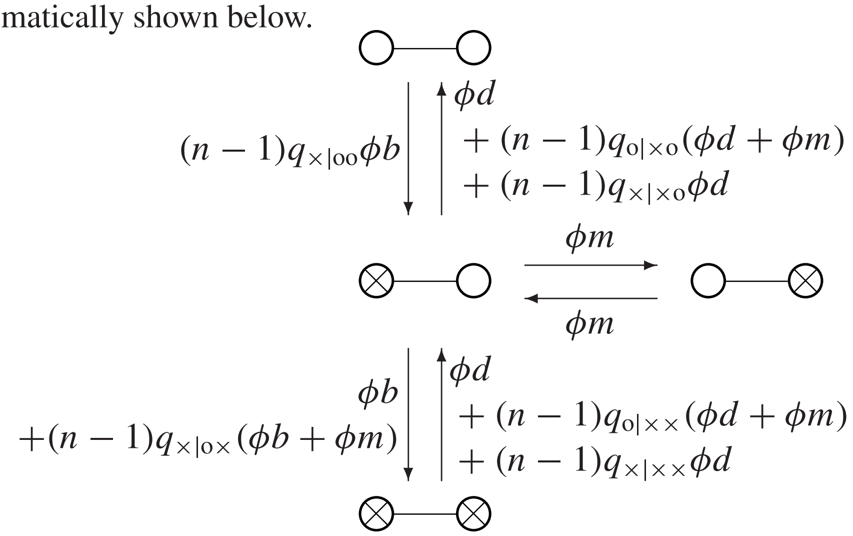
Conditional average rates are calculated in a similar fashion. The complicating factor here is that they depend on one of the pair's neighbors (they are the mean rate over triplets, not pairs). Writing down the expression is straightforward:

$$\bar{r}_\sigma(bj \to kl|abj) = \sum_{n_{abj}} F_\sigma(n_{abj})\, r(bj \to kl|n_{abj}) \; , \tag{19.10}$$

where $F_\sigma(n_{abj})$ is the frequency distribution of the neighborhoods $n_{abj}$ of $abj$ triplets ($n_{abj}$ are three-column matrices that count the number of neighbors of $a$, $b$, and $j$ similar to the way $n_{ab}$ describes the neighborhood of an $ab$ pair). Note that in the case of environment-independent pair event rates, calculating the densities of the larger local configurations is not necessary.

**Box 19.2** Pair dynamics of the simple birth–death–movement process

In the artificial ecology defined in Box 19.1, there are four different pair combinations: o o, $\times$o, o$\times$, and $\times\times$. As an example of the dynamics of their densities, the differential equation for $dp_{\times\mathrm{o}}/dt$ is worked out in detail. Setting up the bookkeeping, using all direct and indirect (neighbor) pair events that affect the density of $\times$o pairs, yields the transitions schematically shown below.



Contributions of direct and indirect events affecting the density of $\times$o pairs. To calculate net transition rates, the rates indicated in the diagram have to be multiplied by the density of the source pairs.

Summing all terms in this figure and simplifying the ensuing expression using $q_{\mathrm{o}|ij} + q_{\times|ij} = 1$, $(n-1)\phi = (n-1)/n = 1-\phi$, and $p_{\mathrm{o}\times} = p_{\times\mathrm{o}}$ yields

$$\begin{aligned}\frac{dp_{\times\mathrm{o}}}{dt} = &- p_{\times\mathrm{o}}\left[\phi b + d + (1-\phi)q_{\mathrm{o}|\times\mathrm{o}}m + (1-\phi)q_{\times|\mathrm{o}\times}(b+m)\right]\\ &+ p_{\mathrm{oo}}\,(1-\phi)q_{\times|\mathrm{oo}}(b+m)\\ &+ p_{\times\times}\left[d + (1-\phi)q_{\mathrm{o}|\times\times}m\right].\end{aligned}$$

The first term, incorporating all events that destroy $\times$o pairs, has four components. The first component represents the $\times$ individual giving birth into the o site, the second represents the death of the $\times$ individual, the third represents the departure of the $\times$ individual through movement (note that this depends on the proportion of empty sites surrounding it), and the fourth represents the arrival of another $\times$ individual at the empty site (which may happen if a neighboring $\times$ individual reproduces or moves).

Similar considerations for $dp_{\mathrm{oo}}/dt$ and $dp_{\times\times}/dt$ yield the other two differential equations that describe the pair dynamics of this system:

$$\begin{aligned}\frac{dp_{\mathrm{oo}}}{dt} = &- p_{\mathrm{oo}}\,2(1-\phi)q_{\times|\mathrm{oo}}(b+m)\\ &+ p_{\times\mathrm{o}}\,2\left[d + (1-\phi)q_{\mathrm{o}|\times\mathrm{o}}m\right],\end{aligned}$$

*continued*

**Box 19.2** *continued*

$$\begin{aligned}\frac{dp_{\times\times}}{dt} &= + p_{\times \mathrm{o}}\, 2\big[\phi b + (1-\phi) q_{\times|\mathrm{o}\times}(b+m)\big] \\ &\quad - p_{\times\times}\, 2\big[d + (1-\phi) q_{\mathrm{o}|\times\times} m\big]\ .\end{aligned}$$

The factor 2 arises in these expressions because oo and ×× are symmetric, so that all events can happen "on both sides."

Thus we have obtained a set of three differential equations that describe the pair dynamics of the artificial ecology defined in Box 19.1. Note that because the sum of the $p_{ij}$ equals 1, one of the differential equations is actually redundant: we could do away with, for example, the differential equation for $p_{\mathrm{oo}}$ and substitute $p_{\mathrm{oo}} = 1 - 2p_{\times\mathrm{o}} - p_{\times\times}$ in the remaining two equations for $p_{\times\mathrm{o}}$ and $p_{\times\times}$.

Because we must analyze the dynamics without keeping track of the entire lattice, the densities of triplets (and in the case of density-dependent rates, the densities of the larger local configurations) have to be estimated from the distribution of pairs. This estimation "closes" the system of differential equations because they are now entirely defined in terms of pairs. How to close the system is dealt with in Section 19.4.

Here we summarize our understanding developed so far: given

- a lattice $L$,
- a set of states $\Omega$, and
- a list of possible events $ij \rightarrow kl$ and their rates $r(ij \rightarrow kl|n_{ij})$,

differential equations can be constructed for the expected rates of change in the frequency $p_{ab}$ of all pair combinations $ab$, as a function of all

- pair frequencies $p_{ab}$,
- conditional probabilities $q_{i|ab}$, and
- frequencies $F_\sigma(n_{ab})$ and $F_\sigma(n_{iab})$ of configurations surrounding pairs and triplets, respectively.

Of these, only the pair frequencies are known, because the differential equations keep track of the numbers of pair combinations. The conditional probabilities $q_{k|ij}$ and the frequencies of larger configurations either have to be calculated from the explicit state of the lattice (which would require explicit simulations) or have to be worked out by other means.

In principle, differential equations can be derived for the dynamics of triplets (and of more complex configurations) analogously to the derivation of the differential equations for pairs. However, there are various reasons for not pursuing this avenue. First, the bookkeeping is much more complicated, as all transitions from one configuration to another must be incorporated. Second, the dynamics of configurations will depend on “configurations of configurations,” which means that the problem has only been carried to the next level. We therefore estimate the frequencies of more complex configurations from the simpler ones (pairs); this is the essence of a solution to what is often called the “moment-closure” problem.

## 19.4 Pair Approximations for Special Geometries

The pair equations that we have derived so far are exact (on infinitely large lattices); no simplifying assumptions have been made. The problem is that they depend on the density of configurations that are outside their scope. To avoid a cascade of dependency on ever more complex configurations, the system of differential equations has to be “closed.” That is, if the aim is to describe the dynamics of pairs, everything has to be expressed in terms of configurations no more complex than pairs. This implies that the frequencies of all configurations larger than pairs have to be approximated.

Consider the conditional probability $q_{i|ab}$. This gives the probability that a site next to the $a$ of an $ab$ pair is in state $i$. The most straightforward approximation for the conditional probability $q_{i|ab}$ is based on the simple heuristics that the more distant site of the pair (in this case $b$) might not influence the probability of finding an $i$ next to the $a$; that is,

$$q_{i|ab} \approx q_{i|a} \tag{19.11}$$

(Matsuda *et al.* 1992; see also Chapters 13 and 18). The error this assumption introduces may be considerable. For example, if $b$ is rare globally, $q_{b|a}$ is likely to be small for $a \neq b$. However, if $b$ is clustered on the lattice, $q_{b|ab}$ may be much larger, because the $ab$ pair is likely to be picked from within such a cluster and then more $b$s are likely to be nearby.

Any approximation introduces errors and information is inevitably lost. In this section I discuss how knowledge of the geometrical structure of the lattice can be used to derive improved “closure” assumptions (i.e., expressions for $q_{i|ab}$ in terms of pair densities). The basic method is outlined first for “random” lattices – lattices in which every site is connected to $n$ other sites, but with no overall spatial structure, such as depicted in Figure 19.1b. I then discuss how to correct for lattices that are more regular and that do have an overall spatial structure – such as the flat lattice in Figure 19.1a.

## Random lattices

On a random lattice like that depicted in Figure 19.1b, sites are randomly connected to $n$ other sites. Consequently, if the number of sites is large, the probability that the members of a pair have neighbors in common is negligible. Thus, for the probability that a given triplet is in state $iab$ one can write

$$p_{iab} = p_i p_a p_b C_{ia} C_{ab} T_{iab} \ , \tag{19.12}$$

where $p_i$ denotes the probability of finding a site in state $i$,

$$p_i = \sum_j p_{ij} \ , \tag{19.13}$$

$C_{ij}$ denotes the *pair correlation* between $i$ and $j$ sites,

$$C_{ij} = \frac{p_{ij}}{p_i p_j} \ , \tag{19.14}$$

and $T_{ijk}$ denotes the *triple correlation* of $ijk$ chains, which is basically the error in the estimate based only on pairs. Notice that there is no correlation factor $C_{ib}$; the only way $b$ can "influence" the probability distribution of $a$'s other neighbors is through the triple correlation.

The values of triple correlations $T_{iab}$ are determined by the full spatial dynamics of the system under consideration. Unless they are estimated from full stochastic simulations, however, their values are unknown. Therefore, to arrive at a closed set of differential expressions for pairs, assumptions have to be made with respect to the triple correlations. The simplest approach is to assume that they are constant. That is, we substitute an estimate $\tau_{ijk}$ for every triple correlation $T_{ijk}$. In fact, the standard pair approximation follows from the assumption that all $T_{iab} = 1$. One then obtains

$$q_{i|ab} = \frac{p_{iab}}{p_{ab}} = \frac{p_i p_a p_b C_{ia} C_{ab}}{p_a p_b C_{ab}} = p_i C_{ia} = q_{i|a} \ . \tag{19.15}$$

Thus for chain-like triplets the simplest estimate for $q_{i|ab}$ is indeed simply $q_{i|a}$; the fact that the $a$ has a $b$ neighbor becomes irrelevant.

Some authors (Harada *et al.* 1995; Keeling 1995) have analyzed improved pair approximations that are based on the assumption that these triple correlations have values not equal to 1, particularly for $bab$-type triplets (see Chapter 18). The reason for doing so is best understood by considering a biological example. Let $b$ stand for a site that is occupied by a member of a rare population and let $a$ stand for an empty site. What is the likelihood that in an *ab* pair the *a* becomes occupied and becomes a *b*? There are two ways for this to happen: the *b* in the pair reproduces or another *b* neighboring *a* reproduces. The probability of the latter happening is proportional to $q_{b|ab}$. However, under the classical pair approximation, this would be approximated by $q_{b|a}$, which is very small when *b* is rare. Analysis of simulations have shown that if *b* is rare and tends to form clusters, *within* such clusters $q_{b|a}$ is not small at all. By setting $\tau_{bab}$ to a value larger than 1, we assume that, if an *a* has one *b* neighbor, it is likely to have more. In other words, increasing the triple correlations increases the degree of crowding on the lattice, which may have various consequences.

It should be noted that the estimates $\tau_{iab}$ for the triple correlations are not independent, as they have to satisfy the consistency condition

$$\sum_i q_{i|ab} = \sum_i q_{i|a}\tau_{iab} = 1 \ . \tag{19.16}$$

If all $\tau_{iab}$ are equal to 1, this condition is satisfied. But if a value not equal to 1 is chosen for one $\tau_{iab}$, the others have to be corrected such that Equation (19.16) holds for all $q_{i|a}$.

## Triangular lattices

Most cellular automata assume square lattices, but the way to improve on the classical pair approximation is most easily understood by first considering a triangular lattice – that is, a lattice in which every site has six neighbors arranged in a hexagon.

On such a lattice, a triplet can be in one of two different configurations, "chain-like" (or *open*) or "triangular" (or *closed*). In fact, there is a 2/5 chance that a randomly picked triplet is in a closed configuration and a 3/5 chance that it is open (see Figure 19.5). We can take this information into account when calculating conditional probabilities.

For open triplets, denoted by $\angle iab$, we can still write

$$p_{\angle iab} = p_i p_a p_j C_{ia} C_{ab} T_{\angle iab} \ , \tag{19.17}$$

but for closed triplets we must take into account an extra correlation factor $C_{bi}$:

$$p_{\triangle iab} = p_i p_a p_j C_{ia} C_{ab} C_{bi} T_{\triangle iab} \ . \tag{19.18}$$

Then, if $\theta$ denotes the probability of finding the triplet in closed form ($\theta = 2/5$), one obtains

$$q_{i|ab} = q_{i|a}\left((1-\theta)T_{\angle iab} + \theta C_{ib} T_{\triangle iab}\right) \ . \tag{19.19}$$

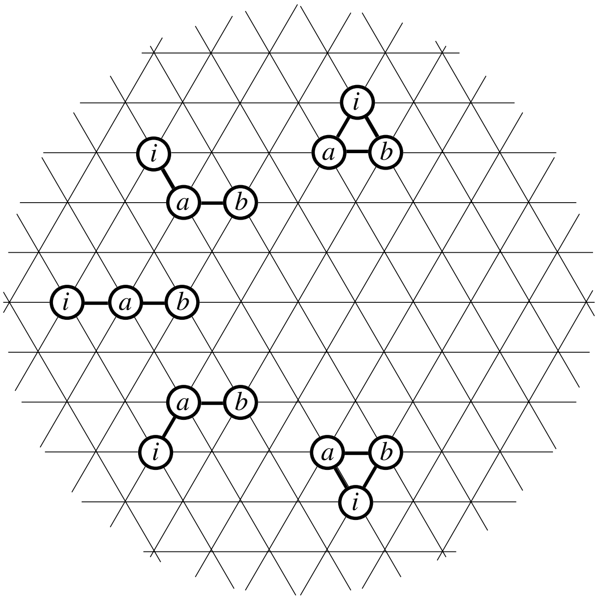


**Figure 19.5** The five different configurations for an $iab$ triplet on a triangular lattice.

On a triangular lattice there are *two* kinds of triple correlation, $T_{\angle iab}$ for open triangles and $T_{\triangle iab}$ for closed triangles. There is no *a priori* reason these should be the same. Let $\tau_{\angle iab}$ and $\tau_{\triangle iab}$ be our estimates for the triple correlations $T_{\angle iab}$ and $T_{\triangle iab}$. The consistency condition then becomes

$$\sum_i q_{i|ab} = \sum_i q_{i|a} \big((1-\theta)\tau_{\angle iab} + \theta C_{ib}\tau_{\triangle iab}\big) = 1 \ . \tag{19.20}$$

With $\tau_{\angle iab} = \tau_{\triangle iab} = 1$, this holds (for all $q_{i|a}$ and $\theta > 0$) *only* if all $C_{ib} = 1$, in which case the pairs are entirely uncorrelated. Therefore, we cannot simply set $\tau_{\angle iab} = \tau_{\triangle iab} = 1$. The simplest assumption that satisfies condition (19.20) is that all $\tau_{\angle iab} = 1$ and all $\tau_{\triangle iab} = 1/C_{ib}$. Note, however, that this implies that we have "uncorrected" the correlation for closed triplets (because we divide by the correlation among the far ends of the triplet). In fact, we have recovered the classical pair approximation, because now the proportion of triangles $\theta$ disappears from our estimate.

To arrive at more sophisticated approximations, one must take into account a number of facts. The first is that open triple correlations should be symmetric (i.e., $\tau_{\angle iab} = \tau_{\angle bai}$); the second is that all closed triple correlations should also be rotationally symmetric (i.e., $\tau_{\triangle iab} = \tau_{\triangle abi} = \tau_{\triangle bia} = \tau_{\triangle bai} = \tau_{\triangle aib} = \tau_{\triangle iba}$). Thus our estimates for $\tau_{\triangle iab}$ have to satisfy the set of Equations (19.20) under these symmetry conditions: the same triple correlation estimate $\tau_{\triangle iab}$ may occur in up to three different equations (i.e., in those for $\sum_i q_{i|ab}$, $\sum_a q_{a|bi}$, and $\sum_b q_{b|ai}$). It is always possible to find solutions, that is, approximations for the $\tau$s. Actually, there are many more triple correlation estimates to be solved for than there are equations: if $N$ is the number of states in $\Omega$, the number of equations to be satisfied is of order $N^2$ while the number of triple correlations is of order $N^3$. (Incidentally, this also shows that many more differential equations would be needed to track triplets in addition to pairs).

I have found no simple expressions for $\tau_{\triangle iab}$ on the basis of the scheme $\tau_{\angle iab} = 1$. The simplest consistent approximation that I have found is based on the assumption that closed and open triple correlations are equal (i.e., $\tau_{\triangle iab} = \tau_{\angle iab} = \tau_{iab}$). The resulting set of equations

$$\sum_i q_{i|a}\big((1-\theta)+\theta C_{ib}\big)\tau_{iab} = 1 \tag{19.21}$$

is satisfied by

$$\tau_{iab} = \begin{cases} 1 & \text{if } i \neq b \\ \frac{1}{q_{b|a}}\big[1 - \sum_{i \neq b} q_{i|a}\big((1-\theta)+\theta C_{ib}\big)\big] & \text{if } i = b \end{cases}, \tag{19.22}$$

which leads to the simple estimate

$$q_{i|ab} \approx \begin{cases} q_{i|a}\big((1-\theta)+\theta C_{ib}\big) & \text{if } i \neq b \\ 1 - \sum_{j \neq b} q_{j|ab} & \text{if } i = b \end{cases}. \tag{19.23}$$

In a later section, this approximation is compared with explicit simulations of the artificial ecology described in Box 19.1. Keeling *et al.* (1997a) and Rand (1999) also provide examples of pair-dynamics models that are based on this approach. (Notice, however, that these authors did not apply the correction terms $\tau_{iab}$ to their estimates, which may have caused a small error in their results.)

## Square lattices

Configurations other than triangles can be taken into account in a similar manner. Take, for example, an $iab$ triplet on a square lattice ($n = 4$). There is no *direct* connection between the $b$ and the $i$, but there is an indirect one through an intermediate site. In other words, the $iab$ triplet may form part of an $iabj$ square quadruplet. Given the square configuration, the probability of finding it in state $iabj$ is

$$p_{\square iabj} = p_i p_a p_b p_j \, C_{ia} C_{ab} C_{bj} C_{ij} \, T_{\square iabj} \ . \tag{19.24}$$

One can arrive at an estimate for $q_{i|ab}$ in a fashion similar to that for triangular lattices. Averaging over all $j$ configurations and using the fact that on a square lattice 1/3 of the triplets are straight and 2/3 form part of a square, one arrives at the estimate

$$q_{i|ab} \approx q_{i|a}\left(\tfrac{1}{3}\tau_{\angle iab} + \tfrac{2}{3}\sum_j q_{j|b}C_{ij}\tau_{\square iabj}\right) , \tag{19.25}$$

where the estimates $\tau_{\angle iab}$ and $\tau_{\square iabj}$ again have to be chosen such that the conditional probabilities sum to 1.

In this formulation, the $b$ from the example above can be thought of as modifying the probability distribution of the intermediate site, which in turn modifies the probability distribution of $a$'s other neighbor. This way, the influence of $b$ "percolates" through the intermediate site and so modifies $q_{i|a}$.

However, the influence of $b$ may percolate through many more routes. This suggests that we need not confine ourselves to triangles or squares. Actually, every closed chain that goes through $iab$ will contribute to the conditional probability $q_{i|ab}$. It should therefore be possible to find increasingly sophisticated estimates for $q_{i|ab}$ by including closed loops (and other closed structures) of greater length while still using only pairs as building blocks.

Notice, however, that this approach still assumes that higher-order correlations ($T_{\square ijkl}$ etc.) are all either fixed or expressed in terms of pair frequencies. There is no *a priori* reason these correlations should not have dynamics of their own, and it may well be that for an adequate description of configurations, higher-order correlations *must* be included. Then either specific assumptions can be made as to the size of some of these correlations, or the analysis should be extended to include the dynamics of more complex configurations. As an example of the first approach, one can set $T_{\angle ijk}$ to a value not equal to 1, and work out the consequences. This is basically the underlying strategy of the improved pair approximations (see Chapter 18; Satō *et al.* 1994; Harada *et al.* 1995; Keeling 1995). If this scheme does not work, the higher-order correlations have to be derived from the dynamics of the system. Thus differential equations for configurations more complex than pairs have to be derived and analyzed; not surprisingly, this is a difficult undertaking (see Morris 1997 for an example).

## Toward higher-order approximations

At this point we have expressed the conditional probabilities $q_{i|ab}$ in terms of pair densities. If the model that is studied has constant pair event rates, the differential equations are now fully closed. However, if event rates are density dependent, another approximation step is necessary.

As we have seen, with density-dependent event rates, the differential equation for $ab$ depends on averages over neighborhoods surrounding the $ab$ pairs ($n_{ab}$ and $n_{iab}$). In a spatially explicit simulation, these frequency distributions [$F_\sigma(n_{ab})$ and $F_\sigma(n_{iab})$] can be measured. Because we want to avoid simulations of the full lattice and develop a model purely in terms of pairs, we have to approximate these frequency distributions in terms of pairs. Thus, to calculate the average event rates, estimates for the likelihood of larger configurations [i.e., $\Pr(n_{ab})$ for $F_\sigma(n_{ab})$ and $\Pr(n_{abj})$ for $F_\sigma(n_{iab})$] must be formulated.

The average rate $\bar{r}_\sigma(ab \to kl)$ depends on the frequency distribution of the configurations $\Pr(n_{ab})$. This can be approximated in much the same way we approximate triplet frequencies, using pair correlations as building blocks. The main difficulty is that many more correlations have to be taken into account.

As a start, consider a random lattice, so that members of a pair are unlikely to have common neighbors. The assumption then is that the neighbors of $a$ and $b$ are independently distributed; that is,

$$\Pr(n_{ab}) = \Pr(n^a_{ab})\Pr(n^b_{ab}) \ . \tag{19.26}$$

Recall that a neighborhood $n_{ab}$ consists of two vectors giving the number of $ia$ and $bj$ pairs. Having no neighbors in common means that the pairs in the left and right environments do not share sites and can be treated independently. A simple assumption then is that probabilities follow a multinomial distribution

$$\Pr(n^a_{ab}) = (n-1)! \prod_i \frac{(q_{i|a})^{n_{ia}}}{n_{ia}!} \ , \tag{19.27}$$

where $\sum_{ia} n_{ia} = n - 1$ (there are $n - 1$ neighbors to be distributed, because one of the neighbors, namely, the other member of the pair, is already given). If $a$ and $b$ share neighbors, or if there are chains of connections between the neighbors of each, this method introduces an error, because $a$'s neighbors and $b$'s neighbors can no longer be considered independent.

For example, if a pair forms part of only one triangle, both sites have $n - 2$ "independent" neighbors and one shared neighbor. The probability distribution of the independent neighbors can still be represented by a multinomial, except that the $n_{ia}$ (or $n_{bj}$) should sum to $n - 2$. If it is assumed that open triplets are uncorrelated, the probability distribution of the shared neighbor can be estimated by

$$\Pr(\text{common neighbor of type } i|ab) = q_{i|a} C_{ib} \tau_{\triangle iab} \ , \tag{19.28}$$

as we have seen in the section on estimating the frequencies of closed triplets. Although it would involve some cumbersome combinatorics, in principle both probability distributions can be calculated to find the probability distribution of the entire configuration around the pair.

However, all these calculations become simpler if it is assumed that event rates are linear functions of their environment, that is, if the effect of one neighbor is independent of that of the other neighbors. In this case, the rate averaged over the configurations equals the rate for the mean configuration. That is,

$$\begin{aligned}\bar{r}_\sigma(ab \to kl) &= \sum_{n_{ab}} F_\sigma(n_{ab})\, r(ab \to kl|n_{ab}) \\ &= r(ab \to kl, \overline{n_{ab}})\ ,\end{aligned} \tag{19.29}$$

where

$$\overline{n_{ab}} = \sum_{n_{ab}} F_\sigma(n_{ab}) n_{ab}\ . \tag{19.30}$$

I do not attempt to further discuss the complexities that arise in trying to incorporate density-dependent event rates in pair-dynamics models. In particular, overlap among the neighbors of a pair introduces all sorts of extra correlations to be taken into account. Most likely, the only feasible approach is to assume multinomial distributions [Equation (19.27)] and accept the fact that some error will remain if the system under study is defined on a regular lattice.

## 19.5 Pair Approximations versus Explicit Simulations

We have seen in the previous section that it is possible to improve on classical pair approximation by introducing new correlations to incorporate knowledge of the geometrical structure of the lattice. The resulting expressions are cumbersome, however, and substituting them into the differential equations leads to complicated sets of expressions that are still rather difficult to analyze.

More important, at this stage it is not known to what extent these refinements actually improve the accuracy of the differential equations for pairs. When is classical pair approximation sufficient? When do we need to incorporate extra correlations? Is it really worth the trouble? In other words, some estimate of the errors associated with the various approximations is needed. Error analysis can be used to assess the accuracy of the approximation (Morris 1997), but as this approach is worthy of a chapter in itself, in this section the accuracy of pair-dynamics models is assessed merely by comparing their results with explicit spatial simulations.

**Box 19.3** Singlet dynamics and the mean-field equation

To calculate local densities $q_{j|i}$, the singlet densities should be known. These can be derived from the differential equations for the dynamics of pairs. Because it is assumed that all sites have the same number of neighbors, we have $p_i = \sum_j p_{ij}$ (which is a standard relationship from probability theory). Thus, from the pair equations derived in Box 19.2, we can derive the equation for $dp_\times/dt$ by summing $dp_{\times \mathrm{o}}/dt$ and $dp_{\times\times}/dt$. This yields

$$\frac{dp_\times}{dt} = (bq_{\mathrm{o}|\times} - d)p_\times \ . \tag{a}$$

Ignoring spatial structure implies assuming $q_{\mathrm{o}|\times} = p_\mathrm{o} = 1 - p_\times$, which then leads to

$$\frac{dp_\times}{dt} = \big(b(1 - p_\times) - d\big)p_\times \ . \tag{b}$$

This is the well-known model for logistic population growth. It can be verified that this model results from the spatially explicit one under mean-field conditions, that is, if the population is well connected ($n$ is large) and/or well mixed (the rate of movement $m$ is very large). If $b > d$, a small population will grow logistically toward a carrying capacity $\bar{p}_\times = 1 - d/b$.

(A note of caution: if the number of neighbors is *not* constant across the lattice, $p_\times = p_{\times \mathrm{o}} + p_{\times\times}$ does not hold, and the differential equation for singlets has to be derived separately.)

Consider the system introduced in Boxes 19.1 to 19.3. This system models a population of individuals inhabiting a lattice (so the sites may be either empty or occupied, $\Omega = \{\mathrm{o}, \times\}$). The events that change the distribution are birth, death, and movement (see Box 19.1). Notice that the rates are constant (i.e., they do not depend on the environment of a pair), so that we do not have to average over configurations. The resulting pair-dynamics equations are given in Box 19.2.

Stochastic, event-based simulations of the artificial ecology have been run for two types of lattices, a random lattice (2500 sites with six neighbors per site) and a triangular lattice (also 2500 sites with six neighbors per cell and with periodic boundary conditions), starting with a low number of randomly distributed individuals [expected initial density $p_\times(0) = 0.001$]. The parameters chosen for the simulations are as follows: per capita birth rate $b = 2$; per capita mortality rate $d = 1$; and per capita movement rate $m = 1$. These runs can be compared with results obtained by numerical integration of the pair-approximation model.

Figure 19.6 shows a run for the random lattice case and the corresponding pair-approximation model (classical pair approximation

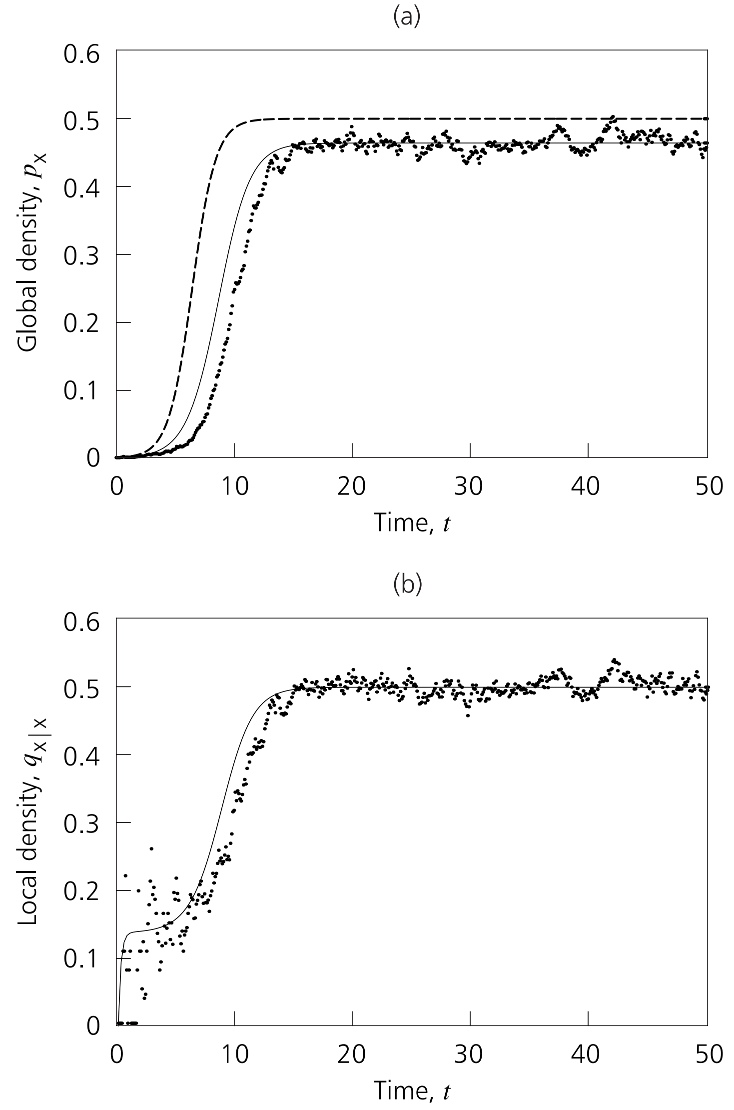


**Figure 19.6** Logistic growth on a random lattice. (a) Global density $p_\times$ of the simulation (dots), the trajectory predicted by the pair approximation (continuous line), and the trajectory predicted by the equivalent mean-field model (nonspatial logistic growth; dashed line). (b) Local densities $q_{\times|\times}$ in the simulation (dots) and as predicted by the pair-approximation model (continuous line). Notice that the local density $q_{\times|\times}$ equilibrates much faster than the global density $p_\times$; this fact is very useful for deriving invasion conditions.

with $\theta = 0$). Because in the simulation the lattice is finite, the population density fluctuates at first due to demographic stochasticity. Such demographic stochasticity is inevitable. However large the lattice, if the initial population consists of only a few individuals, it will be a matter of chance whether they reproduce before they die. There is always a probability that the population goes extinct even if its expected rate of growth is positive. Also note that the simulation lags a bit behind the prediction made by the pair-dynamics model. This lag is a direct consequence of demographic stochasticity, since at low overall densities random events can have a considerable effect, either accelerating or decelerating population growth.

In the trajectory that follows the initial fluctuations, the fit is striking. What can be seen is that during the initial phase of exponential growth, the local density $q_{\times|\times}$ converges to a constant value (much larger than the global density $p_\times$ at this initial stage; the significance of this effect is discussed by Matsuda *et al.* 1992). Only when the lattice fills up and different clusters start to mingle does the local density rise again. Both the exponential phase and the end phase, where the population has settled at its carrying capacity, are well predicted by the pair-approximation model. Notice that this carrying capacity is somewhat lower than that of the nonspatial model; this is caused by the nonhomogeneous distribution of the population, which causes individuals to "experience" a higher density of conspecifics than exists globally.

For the regular, triangular lattice, the situation is a bit different. As can be seen by comparing Figure 19.6 and Figure 19.7, population growth is much slower on the regular lattice. This is no surprise because on a two-dimensional lattice, growth of a focus of individuals is confined to its boundary (consequently, the area covered by a cluster increases roughly in proportion to $t^2$). What can also be seen is that the pair approximation does not perform as well. The classical pair approximation (with $\theta = 0$) is widely off the mark. The pair approximation that was derived earlier (with $\theta = 2/5 = 0.4$) predicts local densities $q_{i|\times}$ fairly well, but its global density $p_\times$ increases much faster than in the simulation. It may come as a surprise that increasing $\theta$ even further (to 0.6) produces an approximation that is reasonably accurate. There is no *a priori* reason to assume a high value of $\theta$, but doing so apparently captures the consequences of clustering quite well, particularly in the early phase of cluster formation (where $q_{\times|\times}$ equilibrates while $p_\times$ increases) and for the final equilibrium. Only during the intermediate phase where the lattice fills up does the approximation fail to perform as well.

## 19.6 Invasion Dynamics

Studies based on a probabilistic cellular automaton framework have shown that results of classical game theory (which is based on random encounters between individuals) can be significantly affected by spatial structure (see Chapter 8; Axelrod 1984; Nowak and May 1992; Boerlijst *et al.* 1993). Pair approximation provides a tool for understanding these effects.

One of the basic concepts in biological game theory (as in any branch of evolutionary theory) is that of fitness. Fitness should be defined as the invasion capacity of a rare mutant (Metz *et al.* 1992; Rand *et al.* 1994). In a well-mixed, nonspatial system this poses no theoretical problems, but

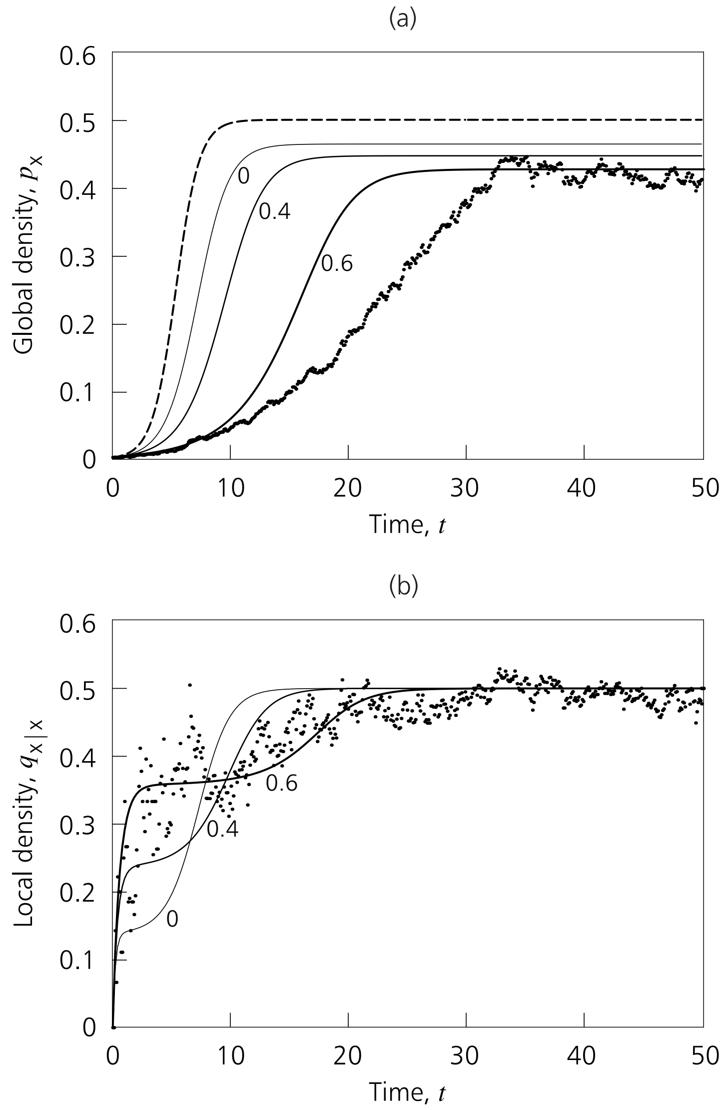


**Figure 19.7** Logistic growth on a triangular lattice. (a) Global density $p_\times$ of the simulation (dots); trajectories (continuous lines) as predicted by the pair approximation based on different values of $\theta$ (indicated in the graph), the proportion of triplets that are in closed form; and trajectory (dashed line) predicted by the equivalent mean-field model (nonspatial logistic population growth). (b) Local densities $q_{\times|\times}$ in the simulation (dots) and as predicted by the pair-approximation models (continuous lines).

deriving the "invasion exponent" of a rare mutant in an explicitly spatial system is no trivial matter. This problem has been investigated in more detail by van Baalen and Rand (1998); here, the basic approach is illustrated using the simpler problem of a population's invasion of an "empty" world. Apart from evolutionary considerations, this gives insight into the factors that determine a population's persistence (since extinction is basically the reverse of invasion).

Using $q_{\times|\mathrm{oo}}p_{\mathrm{oo}} = p_{\times\mathrm{oo}} = q_{\mathrm{o}|\mathrm{o}\times}p_{\mathrm{o}\times}$, the dynamics of an invading population can be written in matrix form:

$$\frac{dP_\times}{dt} = M(Q_\times)P_\times \ , \tag{19.31}$$

where

$$P_\times = \begin{pmatrix} p_{\mathrm{o}\times} \\ p_{\times\times} \end{pmatrix} \quad \text{and} \quad Q_\times = \begin{pmatrix} q_{\mathrm{o}|\times} \\ q_{\times|\times} \end{pmatrix} \ . \tag{19.32}$$

Because the "invasion matrix" $M(Q_\times)$ depends only on local densities that equilibrate relatively quickly (Matsuda *et al.* 1992), the invasion dynamics are given by

$$\frac{dP_\times}{dt} = c\tilde{Q}_\times e^{\lambda t} \ , \tag{19.33}$$

where $\lambda$ is the dominant eigenvalue of $M$ and $\tilde{Q}_\times$ is its normalized eigenvector (which is a vector of local densities $q_{i|\times}$). In this case, the invasion condition becomes obvious: $\lambda$ should be positive. Van Baalen and Rand (1998) argue that by extending this approach to the dynamics of a rare mutant in a lattice dominated by a resident population, $\lambda$ can be interpreted as a fitness measure, while $\tilde{Q}_\times$ gives information about the associated "unit of selection" (i.e., the entity whose fitness is maximized).

For the specific model considered above, the invasion matrix is

$$M(Q_x) = \begin{pmatrix} \begin{matrix} (b+m)(1-\phi)q_{\mathrm{o}|\mathrm{o}\times} - b\phi \\ -(b+m)(1-\phi)q_{\times|\mathrm{o}\times} \\ -d-(1-\phi)q_{\mathrm{o}|\times\mathrm{o}} \end{matrix} & 2b\phi + 2(b+m)(1-\phi)q_{\times|\mathrm{o}\times} \\ \\ d+(1-\phi)mq_{\mathrm{o}|\times\times} & -2d+2(1-\phi)mq_{\mathrm{o}|\times\times} \end{pmatrix} \tag{19.34}$$

From this, the condition for invasion [$M(Q_\times)$ has a positive dominant eigenvalue] can be calculated:

$$b(1-\phi)\tilde{q}_{\mathrm{o}|\mathrm{o}\times} - d + m(1-\phi)(\tilde{q}_{\mathrm{o}|\mathrm{o}\times} - \tilde{q}_{\mathrm{o}|\times\mathrm{o}}) > 0 \ . \tag{19.35}$$

Using improved pair approximation, Equation (19.23), this yields

$$\begin{aligned} & b(1-\phi) - d - m(1-\phi)\tilde{q}_{\times|\times} \\ & \qquad > \theta\tilde{q}_{\times|\times}\big[(b+m)(1-\phi) + m(1-\phi)\tilde{q}_{\times|\times}\big] \ , \end{aligned} \tag{19.36}$$

where $\tilde{q}_{\times|\times} = 1 - \tilde{q}_{\text{o}|\times} = 1 - d/b$. That $\tilde{q}_{\text{o}|\times}$ equals $d/b$ follows readily from the singlet equation (a) in Box 19.3.

On a random lattice, $\theta$ equals zero, in which case the right-hand side of inequality (19.35) vanishes. Thus, a non-moving population can invade a random lattice if $b(1 - \phi) > d$. Invasion is thus more difficult the lower the number of connections per site (because this reduces the factor $1 - \phi = 1 - 1/n$). This result is in accordance with the conclusion of Matsuda *et al.* (1992) that, for a focus to grow on a lattice, the birth rate must exceed the death rate by a certain amount. It can also be concluded that movement facilitates invasion: if $m$ becomes very large, the invasion condition will become $b > d$, which is the invasion condition for the nonspatial model.

Triangular lattices are even more difficult to invade, because the right-hand side of the invasion condition will be positive, so that higher values of $b$ or $m$ are necessary. The ecological reason for this is that competition for space is more intense on regular lattices than on random lattices. Even if a lattice is totally empty, members of the invading population will crowd together, effectively competing for space with each other (which is indicated by $q_{\times|\text{o}\times} > 0$). On a random lattice this effect is almost absent because there an expanding focus of individuals has many more sites to grow into.

## 19.7 Concluding Comments

Simulations of probabilistic cellular automata are excellent for developing intuition regarding spatial processes (see, for example, Chapters 6 to 9; Crawley and May 1987; Boerlijst *et al.* 1993; Claessen and de Roos 1995). The drawback, however, is that they take much computer time to simulate (transient behavior persists) and they are difficult to analyze and compare with classical models for population dynamics (de Roos *et al.* 1991; Claessen and de Roos 1995). Pair-dynamics models fill the gap between unwieldy spatially explicit models and nonspatial models that are easy to analyze but fail to capture the spatial effects.

Even though a fairly simple pair-dynamics model may still involve a substantial number of differential equations, there are far fewer than in an equivalent cellular automaton model (whose dynamical dimension equals the number of sites on the lattice). The first advantage of pair-dynamics models is therefore purely practical: even if the model turns out to be too complex to obtain analytical results, within the same amount of computer time a much greater region of parameter space can be explored with a pair-dynamics model than with a probabilistic cellular automaton. In addition, pair-dynamics models do not "suffer" from demographic stochasticity, but whether this is actually an advantage will depend on the system under consideration – demographic stochasticity may be the dominant process on smaller lattices. A third, more important advantage is that pair-dynamics models allow direct insight into the effect of space, because classical population-dynamical models result in the limiting case of high movement rates. Finally, analytical insight often *is* possible. For example, in this chapter, explicit persistence conditions are derived that indicate how persistence of an artificial ecology depends on individual-based properties. Related to the persistence problem is the problem of fitness in "viscous populations": both require an understanding of invasion conditions (van Baalen and Rand 1998).

Although pair-dynamics models incorporate an essential aspect of spatial structure, they ignore other aspects: in particular, the standard "closure assumption" of pair approximation underestimates the consequences of spatial clustering. The assumption that triple correlations are simply absent (i.e., that the probability of encountering a particular triplet configuration is fully given by pair densities) fails to incorporate certain aspects of population clustering. For example, the simulations presented in this chapter show that local competition for space reduces the rate of population growth on a two-dimensional lattice. A number of improved approximations have been published (see Chapter 18; Satō *et al.* 1994; Harada *et al.* 1995; Keeling 1995) that incorporate this effect. They presuppose that certain kinds of triplets (in particular $bab$-type triplets) are more common than expected on the basis of pairs. This increase in triple correlations implies that if $a$ has one rare neighbor $b$, it is likely to have more (which would not be the prediction of classical pair approximation). For example, if $b$ stands for an infected host and $a$ for a susceptible host, this would lead to increased clustering and hence increased competition for hosts among the infecting parasites.

Here, an improved approximation is proposed that is not based on such *a priori* assumptions of triple correlations of *certain* types of triplets, but rather on an evaluation of how triple correlations may arise as a consequence of the lattice structure itself. In contrast to random lattices, on regular lattices (for example, the triangular lattice considered in this chapter) the members of a pair often have common neighbors. This introduces extra correlations, and when these are taken into account one can *predict* that, for example, $bab$-type triple correlations may be larger than 1.

An important limitation of the analysis presented here is that the number of neighbors per site should be constant. If this assumption is relaxed, and there are good reasons for wanting to do so – for example, to model a network of social relations in which some individuals have more contacts than others – the analysis becomes more complex (Morris 1997; Keeling *et al.* 1997a; Rand 1999). Not only does one have to introduce additional equations for the dynamics of single sites (which can no longer be derived from the pairs), one may also have to make assumptions about many more higher-order correlations.

The extent to which pair-dynamics models are satisfactory depends on the goal of the modeler. As we have seen, these models do not capture all of the phenomena that can be observed in simulations of fully spatial probabilistic cellular automata. Basically, the approximation fails whenever spatial structures arise that are difficult to "describe" using pairs alone. More technically, the method fails whenever significant higher-order correlations arise – that is, whenever the frequency of particular triplets (or triangles, squares, or all sorts of star-like configurations) starts to diverge from what one would expect on the basis of pair densities. Thus, pair-dynamics models satisfactorily describe probabilistic cellular automata in which only "small-scale" patterns arise. Larger, "meso-scale" patterns such as spirals are difficult to capture using this method.

However, probabilistic cellular automata occupy only one end of the spectrum; models for classical nonspatial population dynamics are at the other end, and it is there, in particular, that pair-dynamics models can be valuable tools. In the first place, pair-dynamics models can be used to test the assumptions underlying mean-field models. If a pair-dynamics model does not behave significantly differently from the equivalent mean-field model, it is probably not worth bothering about space. Second, and more important, because they are more open to mathematical analysis, pair-dynamics models may give real insight into *why* spatial models behave differently from nonspatial mean-field models. This way, pair-dynamics models can be used "to add space" to a well-understood but nonspatial model without having to resort to analyzing explicitly spatial models.

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*References in the book in which this chapter is published are integrated in a single list, which appears on pp. 517–552. For the purpose of this reprint, references cited in the chapter have been assembled below.*

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