Modelling population processes with random initial conditions

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ABSTRACT

Population dynamics are almost inevitably associated with two predominant sources of variation: the first, *demographic variability*, a consequence of chance in progenitive and deleterious events; the second, *initial state uncertainty*, a consequence of partial observability and reporting delays and errors. Here we outline a general method for incorporating random initial conditions in population models where a deterministic model is sufficient to describe the dynamics of the population. Additionally, we show that for a large class of stochastic models the overall variation is the sum of variation due to random initial conditions and variation due to random dynamics, and thus we are able to quantify the variation not accounted for when random dynamics are ignored. Our results are illustrated with reference to both simulated and real data.

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1. Introduction

Often the initial state of population processes is not known with certainty. This can happen because of delays and inaccuracies in reporting, partial observability, and difficulties in assessing the actual population size. The initial state is often assumed to be known, or approximated and then treated as known, in which case mathematical models can give only partial information about dynamics and do not describe the full range of behaviour that may be exhibited. This may lead to inaccurate predictions and result in the implementation of non-optimal control actions.

Kegan and West [25] addressed this issue, in the context of the SI (*susceptible-infectious*) epidemic model, by investigating the effect of random initial conditions on the state of the deterministic SI model. Using the Beta distribution to model the initial proportion of infectives, they obtained explicit information about the distribution of the proportion of susceptibles at any time during the epidemic, as well as the distribution of the time until a given proportion of the population remains susceptible. We explain how their approach can be extended to allow initial state uncertainty to be incorporated in general population processes where a deterministic model is sufficient to describe the dynamics of the population, thus allowing one to model variability in dynamics, at any point in time, due solely to uncertainty in the initial state. For one-dimensional processes, such as those used for modelling sexually transmitted infections [2] and hospital-acquired infections [36], and a range of single-species population models, we demonstrate how this can be effected without the need to exhibit the trajectories explicitly. We illustrate our results with reference to several population models.

We also consider a wide class of stochastic models, called *density-dependent processes*, for which there are natural deterministic analogues, and summarise results that quantify variation not accounted for when demographic variability is ignored. Many models appearing in the ecology and epidemiology literature belong to this class. Our purpose here is simply to delineate and quantify variation due to initial state uncertainty and variation due to random dynamics, rather than to study the approximations in detail. The ability to delineate variability in this way has been shown to be of great importance in understanding both population and disease dynamics [13,17,20,32]. We illustrate these results for several population models, including a detailed study of simulated data from a model for disease spread in metapopulations, and real data on the prevalence of HIV antibodies in homosexual men [3,25].

2. Initial state uncertainty in deterministic models

We outline how to account for initial state uncertainty in a general population modelling context. Let n_t be the state of our process at time t, and assume that n_t lies in some subset S of $\mathbb{Z}^D$ (the D-dimensional integer lattice). This would typically be a vector of numbers of individuals of various types (D in total). Suppose also that there is a parameter N, which would usually be related to the size of the system (for example N might be a population ceiling), such that $x_t = n_t/N$ can be interpreted as a vector of population *densities*, and that we have identified an appropriate deterministic model for x_t.

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We will suppose that $x_t = x_t(x_0)$ satisfies the ordinary differential equation

$$x'_s = F(x_s) \quad (x_s \in E, 0 \leqslant s \leqslant t), \tag{1}$$

where the function $F : E \to \mathbb{R}^D$ is specified and E is an appropriate subset of $\mathbb{R}^D$ (D-dimensional Euclidean space). For example, if the state x_t were a vector of proportions, such as the proportions of individuals of various types, then it would be natural to take $E = [0, 1]^D$.

We will exploit the standard change of variable technique to assess the effect of assuming that the initial state is random. Let $X = (X_1, \ldots, X_D)$ be a D-dimensional random vector whose probability density function (pdf) f_X is specified, and let $g : \mathbb{R}^D \to \mathbb{R}^D$ be an injective (one-to-one) map with continuous first partial derivatives. Denote by $\partial g(x)$ the Jacobian matrix $(\partial g_i(x)/\partial x_j)$. Then, the pdf of $Y = (Y_1, \ldots, Y_D)$, where $Y = g(X)$, is given by $f_Y(y) = |J(y)|f_X(g^{-1}(y))$, $y \in \mathbb{R}^D$, where $J(y)$ is the Jacobian of $g^{-1}(y)$ (the determinant of $\partial g^{-1}(y)$) and $|J(y)|$ is its absolute value (see for example [21, Section 4.7]). If the map is not injective, then it is usually possible to partition the domain into regions over which the map *is* injective.

Now think of the initial state as being a random variable X_0 with a specified pdf f_0. In determining the action of the map $g_t(x_0) = x_t(x_0)$ (for simplicity, assumed to be injective) on f_0, we obtain a pdf f_t that summarises the effect of random initial conditions in our population: for any $t > 0$,

$$f_t(y) = |J_t(y)|f_0(g_t^{-1}(y)) \quad (y \in \mathscr{R}_t), \tag{2}$$

where $J_t(y)$ is the Jacobian of $g_t^{-1}(y)$ and $\mathscr{R}_t = g_t(E)$ is the image of E under g_t. We emphasise that f_t is the pdf of the state of our process at time t, assuming deterministic dynamics with an initial pdf f_0.

Since our trajectory satisfies (1) with F specified, we can often take this a step further. In the one-dimensional case ($D = 1$) we can exhibit f_t explicitly. Let $L(u)$ be the primitive $L(u) = \int^u dw/F(w)$. Suppose L is injective, so that L^{-1} is well defined (it is sufficient that F be everywhere positive or everywhere negative). Then, the solution to (1) can be written $x_t(x_0) = L^{-1}(t + L(x_0))$. The Jacobian can also be evaluated. Since $g_t(x) = y$ if and only if $L(y) - t = L(x)$, we get $g_t^{-1}(y) = L^{-1}(L(y) - t)(= g_{-t}(y))$, and so

$$J_t(y) = \frac{d}{dy}L^{-1}(L(y) - t) = (L^{-1})'(L(y) - t)L'(y) = \frac{L'(y)}{L'(L^{-1}(L(y) - t))}$$
$$= \frac{F(L^{-1}(L(y) - t))}{F(y)},$$

where here we have used the inverse function theorem, $(L^{-1})'(y) = 1/(L'(L^{-1}(y)))$, together with $L' = 1/F$. Therefore, from (2),

$$f_t(y) = \left| \frac{F(L^{-1}(L(y) - t))}{F(y)} \right| f_0(L^{-1}(L(y) - t)). \tag{3}$$

We will illustrate these results in Section 5.

The corresponding expected value m_t and covariance matrix V_t of the state of the process at time t can be evaluated either directly from (2) or from (3), or via the trajectory $x_t(x_0)$:

$$m_t = \mathbb{E}x_t(X_0) = \int_E x_t(u)f_0(u)\,du \tag{4}$$

and, taking $x_t(u)$ and m_t to be row vectors,

$$V_t = \mathrm{Cov}(x_t(X_0)) = \int_E x_t(u)^\top x_t(u)f_0(u)\,du - m_t^\top m_t, \tag{5}$$

where $^\top$ denotes transpose.

One might expect that in most instances f_t would be a poor model for the state of the population at time t, because randomness in the dynamics of the process (*demographic variability*) is not taken into account. The effect of ignoring random dynamics

would be particularly pronounced when t becomes large, for it quickly becomes the *only* source of variation. Suppose that the trajectory $x_t(x_0)$ approaches an equilibrium point x_{eq} of (1) (that is, $F(x_{eq}) = 0$ and x_{eq} is stable). Then, it is clear from (4) and (5) that, under mild conditions (for example, $x_t(u)$ monotonic in t, $\mathbb{E}x_t(X_0) < \infty$ or E finite), $m_t \to x_{eq}$ and $V_t \to 0$ as $t \to \infty$ (that is, the randomness induced by the initial distribution disappears). Thus, it would be useful to quantify demographic variation and to be able to delineate this and initial state uncertainty. This will be achieved for a wide class of stochastic population models, termed *density dependent*, using properties of conditional expectation coupled with the idea of a diffusion approximation, whereby the process is approximated by a simpler one (a Gaussian diffusion) whose properties can be exhibited explicitly in terms of the parameters of the original model.

3. Density-dependent population models

Our population process $(n_t, t \geqslant 0)$ is now assumed to be a continuous-time Markov chain with state space $S \subseteq \mathbb{Z}^D$. We let $q(m, n)$ denote the rate at which the process moves from state m to state n for $n \neq m$ and set $q(m, m) = -q(m)$, where $q(m) = \sum_{n \neq m} q(m, n)$ ($< \infty$) is the total rate at which the process leaves state m.

We will suppose that population process is *density dependent* in the sense of Kurtz [26]: there is a parameter N with the property

$$q(n, n + l) = Nf\left(\frac{n}{N}, l\right) \quad (n, n + l \in S), \tag{6}$$

for suitable functions $f(x, l)$, $x \in E$, where E is a subset of $\mathbb{R}^D$. As before, N will usually be related to the size of the system and n/N will usually be interpreted as a population density (or vector of population densities). Condition (6) stipulates that n_t changes at a rate that depends on n_t only *through* (the density) $X_t = n_t/N$, a property shared by a wide variety of models that arise in areas as diverse as ecology [39,41,42,44], epidemiology [6,12,24,47], parasitology [37], chemical kinetics [4,28,34,40], telecommunications [38,45] and random graphs [14,51]. Notice that the density *process* $(X_t, t \geqslant 0)$, being itself a Markov chain, takes values in the set E no matter what the value of N.

Before proceeding, we note that there is a larger class of models termed *asymptotically density dependent* [37], where more general dependence on N is permitted, but which disappears in the limit as N gets large. All of the results presented below carry over without change.

Now, a formal argument based on the forward equations (the master equation) for state probabilities shows that $(d/dt)\mathbb{E}X_t = \mathbb{E}F(X_t)$, where

$$F(x) = \sum_{l \neq 0} lf(x, l) \quad (x \in E), \tag{7}$$

suggesting that (6) entails a law of motion of the kind (1) for the mean path $m_t = \mathbb{E}X_t$. However, it is not generally true that $m'_t = F(m_t)$. For example, the SI model has $F(x) = -\beta x(1 - x)$, $x \in E$, where β is the transmission rate (see Section 5), and therefore $m'_t = F(m_t) + \beta\mathrm{Var}(X_t)$. This was observed by Isham [23] and exploited in West and Thompson's study [50], where they argued that the variance is small when the initial number of susceptibles is large. In fact this is true in great generality, being a consequence of the basic limit theorems of Kurtz [26,27], which we will now describe. These results allow us to identify the most appropriate approximating deterministic model and to quantify variation not accounted for when random dynamics are ignored. As N will vary, we need to make the dependence on N explicit in our notation; we write $X_t^{(N)} = n_t/N$.

Suppose that F, given by (7), is Lipschitz on E, that is, for some positive constant K_E, $|F(x) - F(y)| < K_E|x - y|$, $x, y \in E$ (true for