

Master Equation and Population Dynamics

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1 Introduction

The aim of this text is to present an introduction to a way by which we can derive a theory of population dynamics from "first principles". The focus will be more on arguments and less on mathematical details, although the main equations are laid out and explained. The kind of theoretical construction we will follow is akin to statistical mechanics, where we define collections of elements subject to local behavior laws and that, as a collective, give rise to global patterns observed in the larger scale of populations. Thus, "first principles" is referring to the fact that we understand population dynamics as an emergent behavior with underlying mechanisms happening at the scale of individuals, and instead of describing population behavior as perceived (i.e. phenomenologically), the goal is to describe population behavior as the mechanistic principles dynamically governing it. In this way, population dynamics is to individuals' interactions as thermodynamics is to energetic interacting molecules.

Central to this discussion is the concept of a model. What does it mean to build a mathematical model of a system? In the most general sense, a "model" of a system A is another system that is intended to behave as A behaves. If one can control a model of A , then the observation of the model is an indirect observation of A itself, and knowledge given by the model potentially translate into knowledge about A . Of course, models can't and shouldn't try to be exact

representations of systems. In creating models, the aim is to craft a clever perspective of a system and then model by this perspective. What constitutes a clever perspective is an important question, and mathematics has a lot to say about this. It should strike a balance between simplicity (i.e. control, analytical power) and accuracy (i.e. being right, able to represent something in the system). Interestingly, accuracy of a model is not mainly about realism, it's about mechanisms. To "behave the same" in the context of modeling is not to emulate the perception of a system or "fit" the system; it is to "live by the same rules". In that way, a model aims to produce data by the same generating process that the system itself produces data. We can only harness such kind of power while using incomplete models of nature if we are able to define a quantitative understanding. A good model can capture dominant behaviors while leaving out "details". Think of the ideal gas. No real gas is composed of non-interacting point-particles, as the model assumes, so it lacks realism. However, it captures dominant behaviors and is extremely insightful. When the model breaks in a given context, it is because that context asks for more mechanisms, more precision, and the model leads the way to the correction; as an anchor from which we can depart. Thus, the general aim of models is to lay out mechanisms that capture dominant patterns or first-order behaviors as emergent phenomena arising from those mechanisms. The mechanisms are then considered to be explanations for the behavior of the modeled system or data.

2 Motivation

We then begin with a familiar model of population dynamics, the logistic growth. Suppose a population of size $x(t)$ at a given instant t that has a growth rate r

and a carrying capacity K . Then

$$\frac{dx}{dt} = rx \left(1 - \frac{x}{K}\right). \quad (1)$$

First of all, why do we always represent behavior as differential equations instead of directly writing $x(t) = f(t)$? Because behavior laws represent mechanisms of how objects change, and what/where objects are in fact is a consequence of how they change (like how, in physics, forces are about $\frac{d^2x}{dt^2}$ and not about x). The logistic equation above is a statement on the behavior of a population that evolves (i.e. progresses) in time according to the law $rx(1 - \frac{x}{K})$. As we discussed, a model should ultimately aim to uncover mechanisms, and population mechanisms lie at the level of individuals. Then, what does this law say about individuals? It can be that individuals are simply reproducing at a rate r , but can it be that individuals reproduce at a rate $1000r$ and die at a rate $999r$? The carrying capacity is the maximum size of the population before the saturation of growth, but what does K mean at the individual level? This is the kind of question to which we'll provide an answer, and it begins with master equations for stochastic processes.

3 Master equation

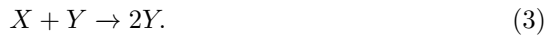
To build individual interactions, let's imagine and define the system as the following situation: populations are each comprised of a set of individuals that will share the same ways of interaction (the same behavior), then all individuals of all populations are put inside a place of size Ω (this parameter is the relevant size or generalized volume, and it can be for example an area or the spatial volume). Each individual will go about its own trajectory and, at first, we assume to know nothing about where individuals are. Therefore, we imagine

them being placed inside the system with uniform probability distribution at every time instant. We then assume a constant passage of time (i.e. time is represented by real numbers). We can picture this situation as a field filled with individuals, and we don't have a clue about where they are in the field. At first, they never interact with each other and they never change their state, thus nothing happens. By introducing interactions, we allow the system to change state. We track the state of the system by following the total amount of individuals in each population. If the system contains N different populations, then $\mathbf{n} = (n_1, n_2, \dots, n_N)$ is the state variable containing the set of all population sizes. Each n_i counts the number of individuals of the i -th population.

Suppose, for example, that individuals from a population X are now able to replicate themselves. This is an event, and we classify it as an interaction; it is able to change the state of the system. If the replication means that an individual can become two at some point, we can represent this interaction as



We can ask ourselves: by which detailed mechanism this replication can occur? And the full answer to this question is outside the scope of dynamics, so we consider the word 'mechanism' in dynamical modeling as the type of individual event giving rise to populational observations. What we should do here is provide a clear connection to detailed scope-specific mechanisms in the form of interpretable free parameters (more on this later). If now there is a population Y , we can add an interaction where an individual from Y consumes an individual from X and, by doing this, reproduces itself in the same manner. This would be represented as



This means that, whenever an individual from X encounters one from Y , there is a chance by which the interaction occurs, resulting in two Y individuals. Note that, defined in this way as a single interaction, this assumes the reproduction to occur jointly with the consumption event. Whether this is a valid approximation or not is a pertinent question and can be further evaluated depending on the context. The general form of an interaction r can be represented as

$$\sum_{i=1}^N s_{ir} X_i \rightarrow \sum_{i=1}^N s'_{ir} X_i, \quad (4)$$

where s_{ir} is the number of individuals from X_i necessary for the interaction r and s'_{ir} is the number of individuals from X_i that result from the interaction. The number $S_{ir} = s'_{ir} - s_{ir}$ is defined as the jump of population X_i associated with interaction r , i.e. the increase or decrease of individuals updated to n_i . In the predation interaction above, population X loses an individual, so the jump is -1 , whereas population Y gains an individual, so the jump is $+1$.

We then say that each interaction r can occur periodically at a given rate W_r that is a function of the present state: $W_r = W_r(\mathbf{n})$. This means that, during a tiny interval of time dt , we should expect the interaction to occur with probability $W_r(\mathbf{n})dt + \mathcal{O}(dt^2)$. If an interaction changes the state of the system from \mathbf{n} to \mathbf{n}' , we can write $W_r(\mathbf{n}) = W_{\mathbf{n} \rightarrow \mathbf{n}'}^r$. The whole situation we just described is called, in stochastic calculus, a Markov jump process (MJP). It turns out that we are able to derive an equation that is the time-evolution law of the probability distribution associated with the system state. It describes how the probability of being in state \mathbf{n} , $P_{\mathbf{n}}(t)$, changes in time as a function of the transition rates. This equation is called the master equation of MJPs:

$$\frac{dP_{\mathbf{n}}(t)}{dt} = \sum_r (W_{\mathbf{n}' \rightarrow \mathbf{n}}^r P_{\mathbf{n}'}(t) - W_{\mathbf{n} \rightarrow \mathbf{n}'}^r P_{\mathbf{n}}(t)). \quad (5)$$

The sum over r runs over all possible interactions included in the system. For each interaction, we have two terms. The first, $W_{\mathbf{n}' \rightarrow \mathbf{n}}^r P_{\mathbf{n}'}(t)$, measures the increase in probability from jumps that lead to state \mathbf{n} , coming from another state \mathbf{n}' . The second, $W_{\mathbf{n}, \mathbf{n}''}^r P_{\mathbf{n}}(t)$, measures the decrease in probability from jumps that move away from state \mathbf{n} , into another state \mathbf{n}'' . The jumps $\mathbf{n}' \rightarrow \mathbf{n}$ and $\mathbf{n} \rightarrow \mathbf{n}''$ are determined by the jump sizes S_{ir} defined above.

The master equation (ME) can be solved, given an initial state $P_{\mathbf{n}}(0)$. Analytical solutions exist for very few simple systems, but they can be approximated or indirectly analyzed. Importantly, they can be exactly simulated using a stochastic simulation algorithm, such as the standard Gillespie algorithm.

As stated above, the ME doesn't require individuals to be modeled by a uniform probability distribution as we assumed. But this assumption allows us to derive a fairly simple equation for the transition rates $W_{\mathbf{n}}^r$ in terms of the system state. We define that an interaction can occur in two steps: 1) individuals gather in an encounter event where they are within an interaction range, and 2) given the encounter happening during the interval dt , individuals will in fact engage in the interaction with a probability $k_r^0 dt$. The parameter k_r^0 is the domain-specific rate of interactions, and it can be calculated as the expected fraction of encounters of the relevant type to result in the interaction or by evaluation of individual attributes and behaviors. Of course, it can also be state-dependent, $k_r^0(\mathbf{n})$, and reflect dynamical aspects happening locally in a different time-scale (as e.g. in quasi-steady state approximations and type II or type III functional responses). If we define ω_r as a mean interaction volume where individuals can be considered as encountering each other, i.e. an effective range of interactions, then the probability of an individual being inside a particular encounter site within the whole system is calculated as ω_r/Ω . With these considerations, we are able to arrive at an expression for the transition

rates from first principles in dynamical terms:

$$W_r(\mathbf{n}) = \left(\frac{k_r^0 \omega_r^{s_r-1}}{\prod_i s_{ir}!} \right) \Omega \prod_i \frac{n_i!}{(n_i - s_{ir})! \Omega^{s_{ir}}}. \quad (6)$$

The quantity inside the parenthesis is what we usually call interaction rates when dealing with the infinite limit, so it is important to define it now:

$$k_r = k_r^0 \frac{\omega_r^{s_r-1}}{\prod_i s_{ir}!}. \quad (7)$$

This parameter carries all information about the domain-specific conversion rate of encounters k_r^0 and the effective interaction volume ω_r . It is also commonly defined in the representation of interactions as their standard rate, for example:



with $k_r = \alpha$.

Above is the whole specification of a system that can be used as a model in the context of population dynamics. By adding different kinds of interactions over different sets of populations, we can specify a broad range of dynamical situations (just as an example, models of evolutionary game theory and replicator dynamics are a subset of these).

4 Deterministic limit

Following from this probabilistic approach where a finite number of individuals reside in a space of a finite size Ω , we can devise a limit of infinite system, where we consider the system to become larger and larger while it maintains its local properties. By averaging over the whole system, we can reformulate this same dynamical law (described mathematically by the master equation) now in terms

of population densities following a set of differential equations. We now show the steps for performing this limit.

The deterministic or continuous limit is the thermodynamics of the infinite system, where the stochastic dynamics is replaced by precise trajectories of population densities. If we infinitely replicate the system and ask about its finite properties, we get the deterministic equations. The change of state from the stochastic number of elements to the deterministic densities of populations is done through a specific limit:

$$\eta_i = \lim_{(n_i, \Omega) \rightarrow \infty} \frac{n_i}{\Omega} \quad (9)$$

valid for every population i . The pair (n_i, Ω) is not going to infinity in any way, this is the same system of size Ω just being infinitely extended, keeping its local configuration the same. By doing this, all uncertainties about the jumps become insignificant and the law of motion for population densities outputs exact smooth trajectories. It is in this domain that the differential equations are exactly valid.

The analogous quantity of the transition rates, which ultimately changes densities as a consequence of local reactions occurring, is given by:

$$W_r^d = \lim_{(n_i, \Omega) \rightarrow \infty} \frac{W_r}{\Omega} = k_r \prod_i \eta_i^{s_{ir}}. \quad (10)$$

By applying the limit to the ME, it then becomes the widespread set of differential equations that we call the dynamical law of mass action:

$$\frac{d\eta_i}{dt} = \sum_r k_r S_{ir} \prod_j \eta_j^{s_{jr}}. \quad (11)$$

Note that this is a function of the compound interaction rates k_r , the jump

sizes S_{ir} , and the densities themselves. This equation also coincides with the equation for the time-evolution of the average $E(\mathbf{n})$, but only in the limit of infinite system anyway.

5 Examples

Now, with these results in hand, we discuss some examples. If we have a population X that only can grow by reproducing at a rate $k_r = \omega$, we represent it as:

$$X \xrightarrow{\omega} 2X. \quad (12)$$

From this, it follows that the exact dynamics of this population is a stochastic growth governed by the master equation with a simple reproduction transition rate equal to $W_r(n_x) = \omega n_x$, so the ME becomes:

$$\frac{dP(n_x, t)}{dt} = \omega(n_x - 1)P(n_x - 1, t) - \omega n_x P(n_x, t). \quad (13)$$

This is how we read it: the system can be in state $(n_x - 1)$ and jump into state n_x with probability $\omega(n_x - 1)$ (thus increasing the probability distribution of state n_x), or it can be in state n_x and jump out of it with probability ωn_x (thus decreasing the probability distribution of state n_x). The deterministic differential equation for this system is simply:

$$\frac{d\eta_x}{dt} = \omega \eta_x. \quad (14)$$

This equation results in an exponential growth $\eta_x(t) = \eta_x(0)e^{\omega t}$. Thus, the master equation above pictures a stochastic exponential growth.

Now, a standard way to define the logistic growth from first principles (dynamically speaking) is to consider the events of reproduction with rate ω , death

with rate μ , and competition for limited resources with rate γ :



The last interaction, the competition, happens whenever two individuals share the same space (defined by the effective interaction range), this space has a source of renewable resources, but the resources are finite. With a rate γ the resources will not be enough for both, then one of them will perish. This system will result in a ME that has as a limit the equation

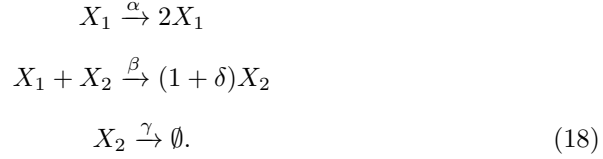
$$\frac{d\eta_x}{dt} = \eta_x(\omega - \mu - \gamma\eta_x). \tag{16}$$

From this, we can make a correspondence to the reproduction rate and carrying capacity of the logistic equation:

$$\begin{aligned}
r &= \omega - \mu, \\
K &= \frac{(\omega - \mu)}{\gamma}.
\end{aligned} \tag{17}$$

The reproduction rate is actually the effective growth of the combined birth and death interactions, and the carrying capacity is a balance between the effective growth and the limitedness of resources that has an intraspecific conflict as a consequence. These are the parameters r and K of the logistic equation derived from local individual interactions. Remember that ω , μ , and γ can in turn be decomposed as functions of domain-specific parameters and the effective ranges of interactions.

As a last example and also an illustration of the passage from stochastic to deterministic dynamics, we consider the Lotka-Volterra competition model:



The prey X_1 can reproduce on its own, the predator X_2 can consume prey and, by doing that, give rise to a batch of δ new predator individuals, and also the predators can die on their own.

This is the ME derived from the model (stochastic Lotka-Volterra):

$$\begin{aligned}
\frac{dP(n_1, n_2)}{dt} &= \alpha \left((n_1 - 1)P(n_1 - 1, n_2) - n_1 P(n_1, n_2) \right) \\
&+ \frac{\beta}{\Omega} \left((n_1 + 1)(n_2 - \delta)P(n_1 + 1, n_2 - \delta) - n_1 n_2 P(n_1, n_2) \right) \\
&+ \gamma \left((n_2 + 1)P(n_1, n_2 + 1) - n_2 P(n_1, n_2) \right).
\end{aligned} \tag{19}$$

This is the deterministic system of Lotka-Volterra differential equations:

$$\begin{aligned}
\frac{d\eta_1}{dt} &= \omega\eta_1 - \beta\eta_1\eta_2 \\
\frac{d\eta_2}{dt} &= \delta\beta\eta_1\eta_2 - \mu\eta_2.
\end{aligned} \tag{20}$$

Finally, we can sample the ME using the Gillespie algorithm and also perform a numerical integration of the deterministic system.

In figure 1, we show a sample of the stochastic system together with the trajectories of the correspondent deterministic system, for a system size of $\Omega = 1$. We see the contrast between both dynamics with such a low system size. Figure 2 shows the connection between them as the system gets bigger, for the

prey trajectory. We maintain the same initial deterministic concentration and other parameter values through all four scenarios. Note how, at size $\Omega = 100$, both dynamics already are hardly distinguishable.

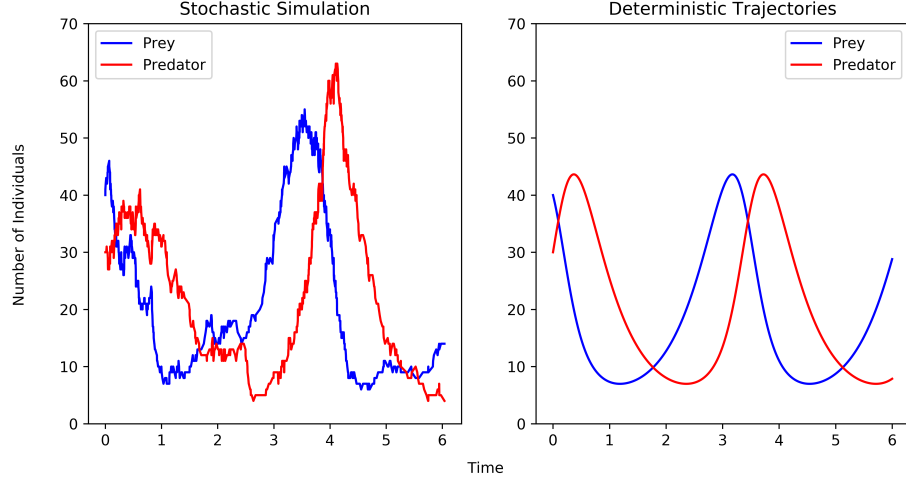


Figure 1: Predator-Prey reaction network. Left: a sample of the master equation from the SSA (Gillespie). Right: a numeric solution of the deterministic equation. The system size is $\Omega = 1$, so both scales coincide. Initial values are $n_1 = \eta_1 = 40$ and $n_2 = \eta_2 = 30$. With arbitrary time-scale, we have $\alpha = \gamma = 2$, $\beta = 0.1$, and $\delta = 1$.

$$\frac{\partial \Pi(x)}{\partial t} = -\frac{\partial}{\partial x}[A(x)\Pi(x)] + \frac{\partial^2}{\partial x^2}[B(x)\Pi(x)] \quad (21)$$

$$\frac{\partial \Pi(x)}{\partial t} = -\frac{\partial}{\partial x}[(\omega x - \mu x - \gamma x^2)\Pi(x)] + \frac{1}{2} \frac{\partial^2}{\partial x^2}[(\omega x + \mu x + \gamma x^2)\Pi(x)] \quad (22)$$

$$\frac{n}{\Omega} = \eta + \frac{\xi}{\sqrt{\Omega}} \quad (23)$$

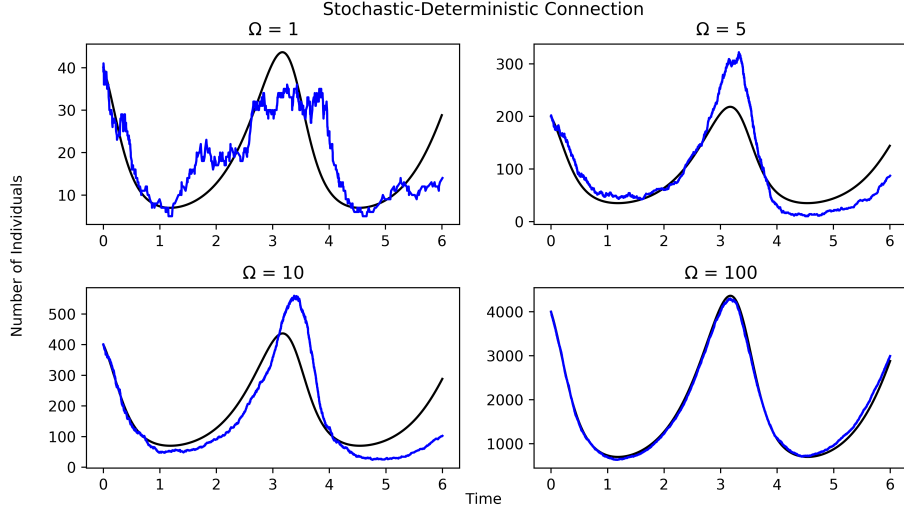


Figure 2: Number of preys compared for the four system sizes $\Omega = 1, 5, 10, 100$. The deterministic solution ($\Omega\eta_1$) is shown in black and the stochastic samples from the SSA (n_1) are shown in blue. Initial values of concentrations are kept at $\eta_1 = 40$ and $\eta_2 = 30$, and the initial number of individuals are scaled accordingly, $n_1 = 40\Omega$ and $n_2 = 30\Omega$. With arbitrary time-scale, we have $\alpha = \gamma = 2$, $\beta = 0.1$, and $\delta = 1$.

$$\frac{\partial \Pi(\xi)}{\partial t} = -\frac{\partial}{\partial \xi}[(\omega - \mu - 2\gamma\eta)\xi\Pi(x)] + \frac{1}{2}\frac{\partial^2}{\partial \xi^2}[(\omega\eta + \mu\eta + \gamma\eta^2)\Pi(x)] + \mathcal{O}(\Omega^{-1/2}) \quad (24)$$

$$dx = A(x)dt + C(x)dW \quad (25)$$

$$dx = (\omega x - \mu x - \gamma x^2)dt + \sqrt{\omega x}dW_1 + \sqrt{\mu x}dW_2 + \sqrt{\gamma x^2}dW_3 \quad (26)$$

$$dW = \mathcal{N}(0, 1)\sqrt{dt} \quad (27)$$

$$dx = (\omega x - \mu x - \gamma x^2)dt + \sqrt{(\omega x + \mu x + \gamma x^2)}dW \quad (28)$$