A General Approach to the Modelling of Trophic Chains

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Abstract

Based on the law of mass action (and its microscopic foundation) and mass conservation, we present here a method to derive consistent dynamic models for the time evolution of systems with an arbitrary number of species. Equations are derived through a mechanistic description, ensuring that all parameters have ecological meaning. After discussing the biological mechanisms associated to the logistic and Lotka-Volterra equations, we show how to derive general models for trophic chains, including the effects of internal states at fast time scales. We show that conformity with the mass action law leads to different functional forms for the Lotka-Volterra and trophic chain models. We use mass conservation to recover the concept of carrying capacity for an arbitrary food chain.

Keywords: Trophic chains, logistic equation, mass action, mass conservation.

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1. Introduction

There exists a multitude of models for trophic interactions. For example, Royama (1971) and May (1974) describe different alternatives to model the same interactions, and Berryman et al. (1995a) give a table of twenty-five alternatives to model predator-prey systems. However, the calibration and validation of these models with experimental and observational data is systematically lacking, and most ecologists prefer to adjust time series data with empirical models that have no connection to the specific ecological processes (Solow, 1995).

For single-species population dynamics, the logistic equation is the basic paradigm, introduced in almost any ecology textbook. It accurately predicts population densities in systems such as bacterial batch cultures (Schlegel, 1992) and human populations (Banks, 1994) and, when generalized, describes the dynamics of many single species populations in both laboratory and field (Gause, 1934; Allee et al., 1949; Thomas et al., 1980; Berryman and Millstein, 1990). It is applicable to multiple situations in ecology and biology (Banks, 1994) and bioeconomics (Clark, 1990). However, the logistic equation has been criticized with the argument that the underlying carrying capacity concept has no mechanistic meaning, being simply a fitting parameter (Kooi et al., 1998), and obscuring the relation between population growth and resource availability (Getz, 1984).

For multi-species population dynamics, the basic model is the Lotka-Volterra equations. They are the basis of almost all the theory of trophic interactions. A further development of these equations was the recognition that there exist limits to the capacity for consumption, leading to the introduction of the Holling functional response, commonly called Type II (Holling, 1959). It was later verified that the functional form of this curve coincides with the Monod function used in microbiology and the Michaelis-Menten mechanism in enzyme kinetics. The Holling Type II functional response lies at the heart of current trophic chain dynamics theory (Oksanen et al., 1981).

In 1928 Volterra adopted the mass action principle of chemical kinetics to write the dynamic equations for the densities of a prey-predator system (Berryman, 1992). In 1977, Nicolis and Prigogine showed that the logistic equation could be derived in analogy with chemical kinetics, using the mass action law and a mass conservation principle. The mass action law lies at the heart of most population dynamics theory, as in epidemiology (Anderson and May, 1991) and in structured population models (Metz and Diekmann, 1986; Metz and de Roos, 1992).

Mass conservation is a controversial issue in population dynamics. Some authors have argued that population dynamics models do not have to conform to
mass conservation (e.g. Berryman et al., 1995b). However, the effect of mass conservation on the dynamics of communities has been ascertained (De Angelis et al., 1989).

On the other hand, one of the problems with the complexity of ecological systems is that there may exist internal states of the systems which we cannot measure (Arditi and Ginzburg, 1989). There is a systematic way of eliminating these variables from the system description, if their dynamics occur at faster time scales than the time scale of population dynamics. In physics this is called the adiabatic approximation (Haken, 1983), and in chemistry it is called the quasi-steady state assumption (Segel, 1988; Segel and Slemrod, 1989; Borghans et al., 1996; Stiefenhofer, 1998). This approach has been used in ecology to distinguish between different time scales (O’Neill et al., 1986; Michalski et al., 1997).

In this paper, we take the chemical kinetics analogy to its full consequences, showing how to derive the population dynamic equations of an arbitrary food web from the ecological mechanisms of interaction. This approach is based on the fact that both organisms and molecules are discrete entities that interact with each other. The advantage of this analogy is that we can bring from physics to ecology the knowledge of statistical mechanics about the transition from individual motions to macroscopic behavior, deriving the precise limits of validity of the deterministic population dynamics description (Maurer, 1998). This program unifies the deterministic with the stochastic approach to population dynamics, as far as local densities of individuals do not fluctuate too much around the average density of the whole population.

This paper is organized as follows. In the next section we review the main techniques for deriving evolution equations of chemical kinetics, with the necessary modifications for ecological systems. The general evolution equations are taken in accordance to the mass action law. We then impose a conservation law which is equivalent to the assumption of closedness of the ecological system. This mass conservation law makes it possible to model a renewable resource, leading to the concept of carrying capacity. To account for internal states occurring at fast time scales, we introduce the mechanism that leads to a Michaelis-Menten resource uptake, which can be compared with logistic type mechanisms. In section 5, we show that the correct application of the mass action law leads to a new Lotka-Volterra type system of equations, for two-species and $n$-species interactions. In section 6, we derive the general form of the evolution equations for a trophic chain where species can have internal states. Taking limits of ecologically significant parameters, more complicated models are reduced exactly to simpler ones.
2. From chemical kinetics to ecological mechanisms: the mass action law

In order to construct population dynamics models with clear and ecologically significant mechanisms and precise conditions of validity and applicability, we now introduce the analytical technique that will be used in this paper.

At the scale of interatomic distances, the motion of molecules in a solution is random. When two eventually binding chemical species collide, a new molecule appears, decreasing the mole number of the initial chemical species and increasing the mole number of the newly formed chemical species. Analogously, in population dynamics, if we assume randomness in the motion of individuals, the interaction of individuals with a resource is a collision. At collision, the individual can consume the resource — binding — or simply ignore it. Therefore, both systems can be considered similar and, at the macroscopic level, the mean densities (mole number per unit volume, in chemical kinetics; number of individuals per unit area or volume, in population dynamics) are described by the same evolution laws.

So, we consider a closed area (or volume) $S$ with several species or resources, $A_j$, $j = 1, \ldots, m$, with number of individuals given by $n_j$. Interactions in $S$ are described by the collision diagrams

$$
\nu_{i1} A_1 + \cdots + \nu_{im} A_m \rightarrow^{r_i} \mu_{i1} A_1 + \cdots + \mu_{im} A_m, \quad i = 1, \ldots, n
$$

(2.1)

where $\nu_{ij}$ and $\mu_{ij}$ are positive parameters measuring the number of individuals that are consumed and produced, with $\nu_{ij}$ being integers, and the constants $r_i$ measure the rate of the interaction.

Suppose further that the species $A_j$ is well distributed in $S$ with mean density $a_j = n_j/S$. It follows from a master equation approach (van Kampen, 1992, pp. 166-172) that

$$
\frac{d a_j}{dt} = \sum_{i=1}^{n} r_i (\mu_{ij} - \nu_{ij}) a_1^{\nu_{i1}} \cdots a_m^{\nu_{im}}, \quad j = 1, \ldots, m
$$

(2.2)

Equation (2.2) expresses the mass action law and is derived using the following assumptions, establishing its limits of validity.

i) At each instant of time, the densities of each species are approximately constant over the finite territory $S$.

ii) The densities are low.

iii) Individual motions are independent of each other, in such a way that the collision frequency is proportional to the product of the probability densities of finding the different individuals in a small region.
iv) Interaction probabilities are independent of the past history of organisms.

v) The motion of individuals is random and is due to some form of collision with the environment, as in Brownian motion (Haken, 1983).

Adopting this analogy between ecological and chemical interactions, it is possible to derive the usual interaction laws found in the ecological literature, with the advantage that now these evolution laws have a precise mechanistic meaning given by the collision diagrams (2.1).

In the following, we will make an additional simplification. Defining the order of a reaction as \( \sum_{i=1}^{n} \nu_{ij} \), we will only consider second or lower order reactions, i.e., \( \sum_{i=1}^{n} \nu_{ij} \leq 2 \), since higher order reactions have comparatively negligible probabilities of occurrence.

In the following and to simplify the notation, we will represent species and species densities in diagram (2.1) and equations (2.2) by the same symbol \( A_j \).

### 3. Logistic autotrophs

Let us represent by \( N \) the density of individuals of a species per unit of area or volume. Let us represent resources by \( A \). Schematically we can represent the ecological interaction — species consuming resources and reproducing — by the following diagram

\[
A + N \rightarrow r_0 (1 + e)N
\]

where \( e > 0 \) is a constant expressing the increase in species density, and \( r_0 \) is a rate constant expressing the velocity of the transformation, at the population dynamics time scale.

Based on the mass action law of \( \S 2 \), the time evolution associated to the transformation (3.1) is

\[
\frac{dN}{dt} = r_0 eAN
\]

\[
\frac{dA}{dt} = -r_0 AN
\]

Multiplying by \( e \) the second equation in (3.2) and adding to the first one, it follows that the time variation of \( N(t) + eA(t) \) is zero, and, therefore, \( N(t) + eA(t) = \text{constant} \). With \( K = N(0) + eA(0) \), and eliminating \( A \) from equations (3.2), we obtain

\[
\frac{dN}{dt} = r_0 N(K - N) := rN \left( 1 - \frac{N}{K} \right)
\]

where \( K \) is the carrying capacity, and \( r = r_0 K \) is the intrinsic growth rate of the population. The species dynamics (3.3) has the solution

\[
N(t) = KN(0)e^{rt}/(K + N(0) - r_0 N(0))
\]
predictions about the values of the density of a population can be obtained by fitting a time series with the explicit solution \( N(t) \). In the limit \( t \to \infty \), \( N(t) \to K \).

In order to make the mechanism (3.1) more realistic, we introduce death rate occurring at the ecological time scale:

\[
\begin{align*}
A + N & \rightarrow^{r_0} (1 + e)N \\
N & \rightarrow^d \beta A
\end{align*}
\] (3.4)

where the second diagram represents the death of individual with death rate \( d \), and \( \beta \) is a recycling constant determined below. The time evolution of the transformation (3.4) is now

\[
\begin{align*}
\frac{dN}{dt} &= r_0 eAN - dN \\
\frac{dA}{dt} &= -r_0 AN + d\beta N
\end{align*}
\] (3.5)

Imposing a conservation law of the form, \( \gamma A + N = \text{constant} \), and introducing (3.5) into the equation \( \gamma \dot{A} + \dot{N} = 0 \), we obtain, \( \gamma = e \) and \( \beta = 1/e \). Therefore, with \( K = N(0) + eA(0) \), and eliminating \( A \) from equations (3.5), we obtain

\[
\frac{dN}{dt} = r_0 N(K - N) - dN := rN \left( 1 - \frac{N}{K} \right) - dN
\] (3.6)

where \( K \) is the carrying capacity, \( r = r_0 K \) is the intrinsic growth rate of the population, and \( d \) is the death rate. If \( r > d \), (3.6) has a stable equilibrium solution for \( N = K(r - d)/r \). If \( r < d \), the only (stable) nonnegative solution is \( N = 0 \). But now, the carrying capacity parameter \( K \) is not the equilibrium value attained by the population in the limit \( t \to \infty \), instead it is the value of the conservation law associated to (3.5). In this case, the solution of (3.6) is \( N(t) = e^{rt} K(d - r)/(Ce^{dt} - re^{rt}) \), where \( C = r + K(d - r)/N(0) \), and time series fitting of observational data is straightforward.

The recycling condition \( N \rightarrow \beta A \) has been introduced in (3.4) in order to have a conservation law, which leads to the decoupling of system (3.6), and the determination of an explicit solution. But, for example, in bacterial batch cultures, where the logistic equation is tested, the recycling condition is not verified. In these systems, after the bacterial population has exhausted the resources, the population density decreases, a feature that can not be obtained with the recycling condition in the logistic equation.

Dropping the recycling condition in (3.4), we obtain the mechanism

\[
\begin{align*}
A + N & \rightarrow^{r_0} (1 + e)N \\
N & \rightarrow^d B
\end{align*}
\] (3.7)
where $B$ is some nonrecycling resource. In this case, the evolution equations associated to $A$ and $N$ are

$$\frac{dN}{dt} = r_0 eAN - dN$$
$$\frac{dA}{dt} = -r_0 AN$$

(3.8)

but no conservation law exists enabling its integration. Therefore, the fitting parameters are more difficult to estimate. Clearly, the system $\{A, N\}$ is open, but the system $\{A, N, B\}$ is closed and has a conservation law ($eA + N + B = constant$).

In Fig. 1 we show the graph of the solution $N(t)$ of the logistic type models (3.3), (3.6) and (3.8). Comparing the qualitative behavior of the three systems, we take the following conclusions.

i) For large values of available resources $A$, the solutions of the three systems are quantitatively similar.

ii) The carrying capacity parameter $K$ only coincides with the equilibrium value of the population if there are no deaths and populations remain constant after exhausting the resources.

iii) In the exponential growth phase, the three models give qualitatively and quantitatively similar results.

iv) If the death rate is small compared with the rate constant $r_0$, the maximum density of populations calculated by the three logistic models is approximated by the carrying capacity $K$, and the population densities in the exponential phase of growth are similar.

In the following, we will always keep the biomass recycling hypothesis, leading to a conservation law and, therefore, to a carrying capacity.

Specifying intermediate internal states in the life cycle of a species, we now show that, under a steady state approximation, we also obtain a logistic equation.

Suppose that the species $N$ has $n$ behavioral internal states, $N_1, \ldots, N_n$, and that reproduction occurs according to the mechanism

$$A + N_1 \xrightarrow{r_1} N_2 \quad N_1 \xrightarrow{d} \beta_1 A$$
$$A + N_2 \xrightarrow{r_2} N_3 \quad N_2 \xrightarrow{d} \beta_2 A$$
$$\vdots$$
$$A + N_n \xrightarrow{r_n} (1 + e)N_1 \quad N_n \xrightarrow{d} \beta_n A$$

(3.9)
where the $\beta_i$ are constants to be determined later, in order to introduce a conservation law. The dynamical equations of mechanism (3.9) are

$$\frac{dA}{dt} = -\sum_{i=1}^{n} r_i A N_i + d \sum_{i=1}^{n} \beta_i N_i$$

$$\frac{dN_1}{dt} = -r_1 A N_1 + r_n (1+e) A N_n - d N_1$$

$$\frac{dN_i}{dt} = r_{i-1} A N_{i-1} - r_i A N_i - d N_i, \quad i = 2, \ldots, n \quad (3.10)$$

We now impose the conservation law,

$$\frac{dA}{dt} + \gamma_1 \frac{dN_1}{dt} + \cdots + \gamma_n \frac{dN_n}{dt} = 0 \quad (3.11)$$

Introducing (3.10) into (3.11), and solving this equation for any $A$ and $N_i$, we obtain the parameter values

$$\gamma_i = \frac{n}{e} + i - 1, \quad \beta_i = \gamma_i, \quad i = 1, \ldots, n \quad (3.12)$$

and, from (3.11), the conservation law is

$$A + \gamma_1 N_1 + \cdots + \gamma_n N_n = K \quad (3.13)$$

We now introduce a steady state assumption, over the internal states,

$$\frac{dN_i}{dt} = 0, \quad i = 2, \ldots, n \quad (3.14)$$

Solving equations (3.14), we obtain,

$$N_i = \frac{r_{i-1} A}{r_i A + d} N_{i-1} = \frac{r_{i-1}}{r_i + d/A} N_{i-1}, \quad i = 2, \ldots, n \quad (3.15)$$

where, by (3.13), $A$ is a function of the $N_i'$. But, taking the limit, $d \to 0$, we obtain, $N_i = r_{i-1} N_{i-1}/r_i$, which, by induction, gives,

$$N_i = \frac{r_1}{r_i} N_1, \quad i = 2, \ldots, n \quad (3.16)$$

and, with $N = N_1 + \cdots + N_n$, by (3.10), (3.11), (3.13) and (3.16),

$$\frac{dN}{dt} = er_n A N_n - dN = \frac{e}{r_1} + \cdots + \frac{1}{r_n} N \left( K - N \sum_{i=1}^{n} \frac{\gamma_i}{r_i} \left( \frac{1}{r_1} + \cdots + \frac{1}{r_n} \right) \right) - dN$$

$$\quad (3.17)$$
which is the logistic equation.

Therefore, at the ecological scale, internal intermediate states do not introduce further dynamical changes in population dynamics equations, as far as the death rate \( d \) is small.

For general systems with several basic nutrients, one conservation law for each resource should be introduced.

### 4. Monod autotrophs

In order to derive the mechanisms for Monod type population dynamics models, we consider a system with an autotroph \( N \), which can be found in two states: searching for nutrient, \( N_s \), and processing (handling) nutrient \( N_h \), with \( N = N_s + N_h \). When the autotrophs find nutrient, they switch from searching to handling, increasing their biomass. At a behavioral time scale, handling autotrophs decay to searching autotrophs, and reproduce. The death rate is the same for both handling and searching autotrophs. The kinetic mechanism is thus:

\[
\begin{align*}
A + N_s & \xrightarrow{r_1} (1 + e)N_h & N_h & \xrightarrow{d} \beta A \\
N_h & \xrightarrow{r_2} N_s & N_s & \xrightarrow{d} \beta A 
\end{align*}
\]  

(4.1)

where \( e > 0 \) is the conversion constant accounting for the increase in species density, \( r_1 \) and \( r_2 \) are the rates at which processes occur, and \( \beta \) is a recycling constant that will be calculated later under the assumptions of a conservation law. The resource density is \( A \).

Let us now apply the formalism of \$2 to the interaction given by diagram (4.1). By (2.1) and (2.2), we obtain

\[
\begin{align*}
\frac{dA}{dt} &= -r_1 AN_s + d\beta(N_s + N_h) \\
\frac{dN_s}{dt} &= -r_1 AN_s + r_2 N_h - dN_s \\
\frac{dN_h}{dt} &= r_1 (1 + e)AN_s - r_2 N_h - dN_h 
\end{align*}
\]  

(4.2)

as evolution equations of resources and individuals.

From the point of view of population dynamics, we can count species numbers but resources are difficult to estimate. Therefore, in order to apply and compare the predictions of system (4.2) with a real system, we must be able to rewrite (4.2) without modelling explicitly the resource density \( A \). As in the logistic equation, the only way to do this is to impose a conservation law,

\[
\gamma \frac{dA}{dt} + \frac{dN_s}{dt} + \frac{dN_h}{dt} = 0 
\]  

(4.3)
Introducing (4.3) into (4.2), and solving for the parameters, we obtain,

$$\gamma = e, \beta = \frac{1}{e}$$  \hspace{1cm} (4.4)

and the conservation law, \( eA + N_s + N_h = constant = K \). Under these conditions, the system described by the mechanism (4.1) with \( \beta \) given by (4.4) is,

$$\frac{dN_s}{dt} = -\frac{r_1}{e}N_s(K - N_s - N_h) + r_2N_h - dN_s$$

$$\frac{dN_h}{dt} = \frac{r_1(1 + e)}{e}N_s(K - N_s - N_h) - r_2N_h - dN_h$$  \hspace{1cm} (4.5)

where \( K = eA + N_s + N_h \) is the carrying capacity.

But, at the ecological time scale, our goal is to follow the time evolution of the total density of a population, \( N = N_s + N_h \), without knowledge of behavioral states of the population. Therefore, with \( N = N_s + N_h \), system (4.5) is rewritten as,

$$\frac{dN}{dt} = r_1(N - N_h)(K - N) - dN$$

$$\frac{dN_h}{dt} = \frac{r_1(1 + e)}{e}(N - N_h)(K - N) - r_2N_h - dN_h$$  \hspace{1cm} (4.6)

It is natural to assume that there are two time scales in this problem: at the ecological time scale the dynamics of \( N_h \) is so fast that \( N_h \) is constant. This allows us to apply the steady state assumption,

$$\frac{dN_h}{dt} = 0$$  \hspace{1cm} (4.7)

implying that, at the ecological scale,

$$\frac{dN}{dt} = r_1N(K - N)\frac{1}{1 + \frac{r_1(1 + e)}{e(d + r_2)}(K - N)} - dN := r_1N(K - N)\frac{1}{1 + \delta(K - N)} - dN$$  \hspace{1cm} (4.8)

where \( \delta = r_1(1 + e)/e(d + r_2) \). System (4.8) has an equilibrium state for \( N = (Kr_1 - d(1 + \delta K))/(r_1 - \delta d) \). This equilibrium state equals the value of the carrying capacity \( K \) when \( d \to 0 \).

If we take the behavioral dynamics in (4.1) infinitely fast when compared with the ecological time scale, \( r_2 \to \infty, \delta \to 0 \) and (4.8) reduces to the logistic equation (3.6). For the steady state assumption (4.7) to be valid, the dynamics of \( N_h \) must be much faster than the dynamics of \( N \), which is simply obtained for large \( r_2 \).

In Fig. 2, we compare density growth curves of the one species model (4.8) with the logistic model (3.6), for the same parameters values. The effect of the
introduction of an intermediate state, delays the growth and slightly changes the steady state. This contrasts with model (3.9), where the introduction of intermediate behavioral states corresponding to the different states of the life cycle of an individual do not change the overall time behavior of the population at the ecological time scale.

5. Modified Lotka-Volterra trophic chains

We now consider a kinetic mechanism in accordance with the assumptions underlying the Lotka-Volterra prey-predator equations. We represent resources by $A$, prey by $N_1$ and predators by $N_2$. In order to be able to derive a conservation law we introduce a recycling mechanism depending upon two unknown parameters, $\beta_1$ and $\beta_2$. Under these conditions, the prey-predator mechanism is:

$$A + N_1 \xrightarrow{r_1} (1 + e_1)N_1 \quad N_1 \xrightarrow{d_1} \beta_1 A$$
$$N_1 + N_2 \xrightarrow{r_2} (1 + e_2)N_2 \quad N_2 \xrightarrow{d_2} \beta_2 A$$

where $e_1$ and $e_2$ are conversion factors, and $d_1$ and $d_2$ are death rates.

The dynamic equations for mechanism (5.1) become,

$$\frac{dA}{dt} = -r_1 AN_1 + d_1 \beta_1 N_1 + d_2 \beta_2 N_2$$
$$\frac{dN_1}{dt} = e_1 r_1 AN_1 - r_2 N_1 N_2 - d_1 N_1$$
$$\frac{dN_2}{dt} = r_2 e_2 N_1 N_2 - d_2 N_2$$

(5.2)

Imposing the conservation law,

$$A + \gamma_1 N_1 + \gamma_2 N_2 = K$$

(5.3a)

and after derivation, by (5.2), we obtain

$$\beta_1 = \gamma_1 = 1/e_1 \quad \beta_2 = \gamma_2 = 1/(e_1 e_2)$$

(5.3b)

Using the conservation law (5.3) to eliminate $A$ from (5.2), the equations for the prey-predator mechanism become

$$\frac{dN_1}{dt} = e_1 r_1 \left( \frac{K}{e_1} - \frac{N_1}{e_1} - \frac{N_2}{e_1 e_2} \right) N_1 - r_2 N_1 N_2 - d_1 N_1$$
$$\frac{dN_2}{dt} = r_2 e_2 N_1 N_2 - d_2 N_2$$

(5.4)
These equations are functionally equivalent to the usual Lotka-Volterra equations. However, due to mass conservation, the parameters no longer have exactly the same meaning. In fact, prey growth is not only controlled by predation but also by the fact that predators retain nutrient within them.

We can generalize the preceding mechanism to trophic chains of arbitrary length:

\[ A + N_1 \xrightarrow{r_1} (1 + e_1)N_1 \quad N_1 \xrightarrow{d_1} \frac{1}{e_1} A \]

\[ N_1 + N_2 \xrightarrow{r_2} (1 + e_2)N_2 \quad N_2 \xrightarrow{d_2} \frac{1}{e_1e_2} A \]

\[ \vdots \]

\[ N_{n-1} + N_n \xrightarrow{r_n} (1 + e_n)N_n \quad N_n \xrightarrow{d_n} \frac{1}{e_1...e_n} A \]

This system has the conservation law:

\[ A + \frac{N_1}{e_1} + \frac{N_2}{e_1e_2} + \ldots + \frac{N_n}{e_1e_2...e_n} = K \]  

(5.6)

Using the conservation law to eliminate \( A \), the dynamical equations become

\[ \frac{dN_1}{dt} = e_1r_1\left( K - \frac{N_1}{e_1} - \frac{N_2}{e_1e_2} - \ldots - \frac{N_n}{e_1e_2...e_n} \right) N_1 - r_2N_1N_2 - d_1N_1 \]

(5.7)

\[ \frac{dN_i}{dt} = r_i e_i N_{i-1}N_i - d_i N_i, \quad i = 2, \ldots, n \]

For trophic chains of length greater than two, the equation for the basal species is functionally different from the Lotka-Volterra food chain. The basal species is controlled by all the other species, since they are all retaining nutrient (this effect increases with the increase in nutrient retained in the nonbasal trophic levels).

6. Trophic chains with internal states

We now derive the basic population dynamics equations for the time evolution of \( n \) species in a food chain, assuming that all the species involved have some refractory time, during which they are not able to consume resources.

Consider a food chain with \( n \) species, \( N_1, \ldots, N_n \) and a primary resource \( A \). Suppose in addition that each species has two states \( N_{is} \) and \( N_{ih} \), where subscripts \( s \) and \( h \) stand, respectively, for "searching for prey" and "handling for
prey”. Introducing this distinction we have \( N_i = N_{is} + N_{ih} \). With a characteristic time \( t_{ih} \), handling predators finish handling their prey and return to the searching state. Reproduction transforms searching into handling predators. Under these conditions, the mechanism for the trophic chain is

\[
A + N_{1s} \xrightarrow{r_1} (1 + e_1)N_{1h} \quad N_{1s} \xrightarrow{d_{1s}} \beta_1 A \\
N_{1h} \xrightarrow{t_{1h}^{-1}} N_{1s} \quad N_{1h} \xrightarrow{d_{1h}} \beta_1 A \\
N_{1s} + N_{2s} \xrightarrow{r_2} (1 + e_2)N_{2h} \quad N_{2h} \xrightarrow{d_2} \beta_2 A \\
N_{1h} + N_{2s} \xrightarrow{r_2} (1 + e_2)N_{2h} \\
N_{2h} \xrightarrow{t_{2h}^{-1}} N_{2s} \quad N_{2s} \xrightarrow{d_2} \beta_2 A \\
\vdots \\
N_{n-1s} + N_{ns} \xrightarrow{r_n} (1 + e_n)N_{nh} \quad N_{nh} \xrightarrow{d_n} \beta_n A \\
N_{n-1h} + N_{ns} \xrightarrow{r_n} (1 + e_n)N_{nh} \\
N_{nh} \xrightarrow{t_{nh}^{-1}} N_{ns} \quad N_{ns} \xrightarrow{d_n} \beta_n A
\]

Applying the mass action law of §2, we obtain the evolution equations,

\[
\frac{dA}{dt} = -r_1AN_{1s} + \sum_{i=1}^{n} \beta_id_i(N_{is} + N_{ih}) \\
\frac{dN_{1s}}{dt} = -r_1AN_{1s} + t_{1h}^{-1}N_{1h} - d_1N_{1s} - r_2N_{1s}N_{2s} \\
\frac{dN_{1h}}{dt} = r_1(1 + e_1)AN_{1s} - t_{1h}^{-1}N_{1h} - d_1N_{1h} - r_2N_{1h}N_{2s} \\
\vdots \\
\frac{dN_{is}}{dt} = -r_i(N_{i-1s} + N_{i-1h})N_{is} + t_{ih}^{-1}N_{ih} - d_iN_{is} - r_{i+1}N_{is}N_{i+1s} \\
\frac{dN_{ih}}{dt} = r_i(1 + e_i)(N_{i-1s} + N_{i-1h})N_{is} - t_{ih}^{-1}N_{ih} - d_iN_{ih} - r_{i+1}N_{ih}N_{i+1s} \\
\vdots \\
\frac{dN_{ns}}{dt} = -r_n(N_{n-1s} + N_{n-1h})N_{ns} + t_{nh}^{-1}N_{nh} - d_nN_{ns} \\
\frac{dN_{nh}}{dt} = r_n(1 + e_n)(N_{n-1s} + N_{n-1h})N_{ns} - t_{nh}^{-1}N_{nh} - d_nN_{nh}
\]

where, \( i = 2, \ldots, n - 1 \). We now impose a conservation law of the form,

\[
\frac{dA}{dt} + \gamma_1 \left( \frac{dN_{1s}}{dt} + \frac{dN_{1h}}{dt} \right) + \cdots + \gamma_n \left( \frac{dN_{ns}}{dt} + \frac{dN_{nh}}{dt} \right) = 0 
\]
where $\gamma_i$ are unknown parameters. Introducing (6.2) into (6.3), and solving for $\gamma_i$ and $\beta_i$, we obtain

$$\gamma_i = \frac{1}{e_1 \ldots e_i}, \beta_i = \gamma_i, i = 1, \ldots, n$$

(6.4)

Hence, the conservation law is

$$A + \frac{1}{e_1}N_1 + \ldots + \frac{1}{e_1 \ldots e_n}N_n = K$$

(6.5)

where $K$ is the carrying capacity, and $N_i = N_{is} + N_{ih}$.

Let us now introduce a steady state assumption over the behavioral states $N_{ih}$:

$$\frac{dN_{ih}}{dt} = 0, i = 1, \ldots, n$$

(6.6)

With, $N_i = N_{is} + N_{ih}$, and writing the system of equations (6.2) as a function of $N_n$ and $N_{ns}$, we obtain the dynamic equations for species densities,

$$\frac{dN_1}{dt} = e_1 r_1 (K - \frac{1}{e_1}N_1 - \ldots - \frac{1}{e_1 \ldots e_n}N_n)N_{1s} - r_2 N_1 N_{2s} - d_1 N_1$$

$$\vdots$$

$$\frac{dN_i}{dt} = e_i r_i N_{is} N_{i-1} - r_{i+1} N_i N_{i+1s} - d_i N_i$$

(6.7)

$$\vdots$$

$$\frac{dN_n}{dt} = e_n r_n N_{ns} N_{n-1} - d_n N_n$$

In order to eliminate $N_{is}$ from (6.7), we solve the system of equations (6.6) together with the relation $N_i = N_{is} + N_{ih}$. Therefore, (6.7) together with (6.6) are the general equations for a trophic chain.

Let us now analyze the case $n = 2$. In this case, (6.7) and (6.6) simplify to

$$\frac{dN_1}{dt} = e_1 r_1 (K - \frac{1}{e_1}N_1 - \frac{1}{e_1 e_2}N_2)N_{1s} - r_2 N_1 N_{2s} - d_1 N_1$$

$$\frac{dN_2}{dt} = e_2 r_2 N_1 N_{2s} - d_2 N_2$$

$$\frac{dN_{1h}}{dt} = r_1 (1 + e_1) AN_{1s} - t_{1h}^{-1}(N_1 - N_{1s}) - d_1 (N_1 - N_{1s}) - r_2 (N_1 - N_{1s}) N_{2s} = 0$$

$$\frac{dN_{2h}}{dt} = r_2 (1 + e_2) N_1 N_{2s} - t_{2h}^{-1}(N_2 - N_{2s}) - d_2 (N_2 - N_{2s}) = 0$$

(6.8)
Solving the two last equations in (6.8) for $N_{1s}$ and $N_{2s}$, we obtain,

$$N_{2s} = N_2 \frac{t_{1h}^{-1} + d_2}{t_{2h}^{-1} + d_2 + r_2(1 + e_2)N_1}$$

$$N_{1s} = N_1 \frac{t_{1h}^{-1} + d_1 + r_2 N_2}{t_{1h}^{-1} + d_1 + r_1(1 + e_1)(K - \frac{1}{e_1}N_1 - \frac{1}{e_1 e_2}N_2) + r_2 N_2} \frac{t_{2h}^{-1} + d_2}{t_{2h}^{-1} + d_2 + r_2(1 + e_2)N_1}$$

Therefore, system (6.8) simplifies to

$$\frac{dN_1}{dt} = e_1 r_1 (K - \frac{1}{e_1}N_1 - \frac{1}{e_1 e_2}N_2) N_{1s} - r_2 N_1 N_{2s} - d_1 N_1$$

$$\frac{dN_2}{dt} = e_2 r_2 N_2 N_1 - d_2 N_2$$

(6.10)

where $N_{1s}$ and $N_{2s}$ are given by (6.9).

Equation (6.10) describes a trophic chain with a prey, a predator and a renewable resource. The carrying capacity of the system is the constant $K$. The introduction of the intermediate states $N_{ih}$, specifying the existence of a refractory time where species are not consuming resources, implies a functional response of Holling type II, with ecologically meaningful parameters. If we consider that the basal species in $N_1$ has negligible handling time, $t_{1h}^{-1} \to \infty$, then, by (6.9), $N_{1s} \to N_1$, and (6.10) reduces to

$$\frac{dN_1}{dt} = e_1 r_1 (K - \frac{1}{e_1}N_1 - \frac{1}{e_1 e_2}N_2) N_1 - r_2 N_1 N_2 \frac{t_{2h}^{-1} + d_2}{t_{2h}^{-1} + d_2 + r_2(1 + e_2)N_1} - d_1 N_1$$

$$\frac{dN_2}{dt} = e_2 r_2 N_1 N_2 \frac{t_{2h}^{-1} + d_2}{t_{2h}^{-1} + d_2 + r_2(1 + e_2)N_1} - d_2 N_2$$

(6.11)

which is a modified Rosenzweig-MacArthur (1963) predation model.

In the case the handling times $t_{1h}^{-1}$ and $t_{2h}^{-1}$ go to infinity, by (6.9), $N_{is}$ converges to $N_i$, and (6.10) reduces to the modified Lotka-Volterra equation (5.4).

We now compare the time evolution of system (6.10) with the modified prey-predator Lotka-Volterra system (5.4). We take the parameter values: $r_1 = 1.0$, $r_2 = 0.2$, $e_1 = 1$, $e_2 = 1$, $d_1 = 0.1$, $d_2 = 0.2$, $t_{1h}^{-1} = 1.0$, $t_{2h}^{-1} = 2.0$, $K = 8$, $N_1(0) = 1.0$ and $N_2(0) = 0.1$. In Fig. 3, we depict the time evolution of the two models, for prey and predators. In the case of model equations (5.4), the system attains an equilibrium value given by $N_1 = d_2/e_2 r_2$ and $N_2 = (r_2(K e_1 r_1 - d_1) - d_2 r_1)/(r_2(r_1 + e_2 r_2))$. However, for system (6.10), we obtain stable oscillations corresponding to a limit cycle in phase space.
For the general case of an arbitrary trophic chain we have equation (6.2) together with the carrying capacity relation (6.5), and, eventually, the steady state conditions (6.6).

7. Conclusions

We have developed a systematic formalism, based on chemical kinetics, for the derivation of equations in population dynamics based on the mechanisms of interaction between individuals. We have started from the simplest equation, the logistic, and then introduced successive levels in a trophic chain. The dynamical equations are derived using the laws of mass action and mass conservation, and, when necessary, a steady state assumption. Our approach includes any kind of trophic interaction between species and resources and internal states. This approach gives a consistent mechanistic basis for the derivation of the trophic chain equations of population biology, making it possible to settle several controversies in Ecology. Moreover, this formalism allows the precise development of more complicated models, with the introduction of more mechanisms and interactions, allowing the development of extensions of the logistic equation with precise applicability conditions.

This approach has the advantage that all the parameters have an \textit{a priori} biological meaning. Moreover, we show the necessity of the introduction of a conservation law relating populations and primary resource densities. In this context, the carrying capacity parameter is the value assumed by the conservation law, and appears in all population dynamics models, from one species to arbitrary food webs. However, the numerical equilibrium value attained by the populations only equals the carrying capacity in the case of the logistic equation.

The use of the mass action law, together with its microscopic foundation, allows the development of models with stochastic fluctuation around a mean value (Bailey, 1964; Haken, 1983), as well as the development of equations with different growth forms and the introduction of individual variability.

Finally, one of the consequences of the systematic use of the mass action law is the proof of the empirical observation that the growth rate \(r\), and the carrying capacity \(K\) in the logistic equation, both increase proportionally to enrichment.
References

Allee, W. C., Emerson, A. E., Park, O., Park, T. and Schmidt, K. P., 1949. Principles of Animal Ecology. Saunders, Philadelphia, Pennsylvania.

Anderson, R. M. and May, R. M., 1991. Infectious Diseases of Humans: Dynamics and Control. Oxford University Press, Oxford.

Arditi, R. and Ginzburg, L. R., 1989. Coupling in predator-prey dynamics: ratio-dependence. J. Theor. Biol., 139: 311-326.

Bailey, N. T. J., 1964. The Elements of Stochastic Processes: With Applications to the Natural Sciences. J. Wiley and Sons, New York.

Banks, R. B., 1994. Growth and Diffusion Phenomena: Mathematical Frameworks and Applications. Texts in Applied Mathematics Vol. 14. Springer-Verlag, Berlin, 19+455 pp.

Berryman, A. A., 1992. The origins and evolution of predator-prey theory. Ecology, 73: 1530-1535.

Berryman, A. A. and Millstein, J. A., 1990. Population Analysis System: POPSYS Series 1, One-Species Analysis (Version 2.5). Ecological Systems Analysis, Pullman, Washington.

Berryman, A. A., Gutierrez, A. P. and Arditi, R., 1995a. Credible, parsimonious and useful predator-prey models: a reply to Abrams, Gleeson, and Sarnelle. Ecology, 76: 1980-1985.

Berryman, A. A., Michalski, J., Gutierrez, A. P. and Arditi, R., 1995b. Logistic theory of food web dynamics. Ecology, 76: 336-343.

Borghans, J. A. M., De Boer, R. J. and Segel, L. A., 1996. Extending the quasi-steady state approximation by changing variables, Bull. Math. Biol., 58: 43-63.

Clark, C. W., 1990. Mathematical Bioeconomics. John Wiley and Sons, New York, New York.

DeAngelis, D. L., Bartell, S. M. and Brenkert, A. L., 1989. Effects of nutrient recycling and food-chain length on resilience. Am. Nat., 134: 778-805.

Gause, G. F., 1934. The Struggle for Existence. Williams and Wilkins, New York, New York.

Getz, W. M., 1984. Population dynamics: a per capita resource approach. J. Theor. Biol., 108: 623-643.
Haken, H., 1983. Synergetics (3rd edition). Springer-Verlag, Berlin.

Holling, C. S., 1959. The components of predation as revealed by a study of small mammal predation of the European pine sawfly. The Canadian Entomologist, 91: 293-320.

Kooi, B. W., Boer, M. P. and Kooijman, S. A. L. M., 1998. On the use of the logistic equation in models of food chains. Bull. Math. Biol., 60: 231-246.

Maurer, B. A., 1998. Ecological Science and Statistical Paradigms: At the Threshold. Science, 279: 502-503.

May, R. M., 1974. Stability and Complexity in Model Ecosystems (2nd Ed.). Monographs in Population Biology Vol. 6. Princeton University Press, Princeton, New Jersey.

Metz, J. A. J. and de Roos, A. M., 1992. The role of physiologically structured population models within a general individual-based modelling perspective. In: D. L. DeAngelis and L. J. Gross (Editors), Individual-Based Models and Approaches in Ecology: Populations, Individuals and Ecosystems, Chapman and Hall, New York, New York, pp. 88-111.

Metz, J. A. J. and Diekmann, O. (Editors), 1986. The Dynamics of Physiologically Structured Populations. Lecture Notes in Biomathematics 68. Springer-Verlag, Berlin.

Michalski, J., Poggiale, J.-Ch., Arditi, R. and Auger, P. M., 1997. Macroscopic dynamic effects of migrations in patchy predator-prey systems. J. Theor. Biol., 185: 459-474.

Nicolis, G. and Prigogine, I., 1997. Self-Organization in Nonequilibrium Systems. J. Wiley and Sons, New York.

Oksanen, L., Fretwell, S. D., Arruda, J. and Niemela, P., 1981. Exploitation ecosystems in gradients of primary productivity. Am. Nat., 140: 938-960.

O’Neill, R. V., DeAngelis, D. L., Waide, J. B. and Allen, T. F. H., 1986. A Hierarchical Concept of Ecosystems. Monographs in Population Biology Vol. 23. Princeton University Press, Princeton, New Jersey, 7+253 pp.

Rosenzweig, M. and MacArthur, R. H. 1963. Graphical representation and stability conditions of predator-prey interactions. Am. Nat., 107: 275-294.

Royama, T., 1971. A comparative study of models for predation and parasitism. Res. Popul. Ecol. Supp. 1.
Schlegel, H. G., 1992. General Microbiology (7th edition). Cambridge University Press, Cambridge.

Segel, L. A., 1988. On the validity of the steady state assumption of enzyme kinetics. Bull. Math. Biol., 6: 579-593.

Segel, L. A. and Slemrod, M., 1989. The quasi steady state assumption: a case study in perturbation. SIAM Rev., 31: 466-477.

Solow, A. R., 1995. Fitting population models to time series data. In: T. M. Powell and J. H. Steele (Editors), Ecological Time Series, Chapman and Hall, New York, New York, pp. 20-27.

Stiefenhofer, M. 1998. Quasi-steady-state approximation for chemical reaction networks. J. Math. Biol. 36, 593-609.

Thomas, W. R., Pomerantz, M. J. and Gilpin, M. E., 1980. Chaos, assymetric growth and group selection for dynamical stability. Ecology, 61: 1312-1320.

Van Kampen, N. G., 1992. Stochastic Processes in Physics and Chemistry, Elsevier, Amsterdam, 1992.
Figure Captions

**Figure 1:** Solution $N(t)$ of the logistic type models (3.3), (3.6) and (3.8). The parameter values are: $e = 1$, $r_0 = 1$, $d = 0.2$, $K = 20$, $N(0) = 0.1$ and $A(0) = (K - N(0))/e = 19.9$.

**Figure 2:** Solution $N(t)$ for the logistic and Monod type model (4.8). The parameter values are: $e = 1$, $r_1 = 1$, $r_2 = 10$, $d = 0.2$, $K = 20$, $N(0) = 0.1$, $A(0) = (K - N(0))/e = 19.9$ and $\delta = 0.196$. In the limit $\delta \to 0$ (or $r_2 \to \infty$) the solution of the Monod type model approaches the solution of the logistic equation.

**Figure 3:** Solutions $N(t)$ of the modified Lotka-Volterra model (5.4) and trophic model (6.10). The parameter values are: $r_1 = 1.0$, $r_2 = 0.2$, $e_1 = 1$, $e_2 = 1$, $d_1 = 0.1$, $d_2 = 0.2$, $t_{1h}^{-1} = 1.0$, $t_{2h}^{-1} = 2.0$, $K = 8$, $N_1(0) = 1.0$ and $N_2(0) = 0.1$. 
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