3 Exponential Model

The exponential model is widely used in ecology and environmental science, for example, in population growth, mass loss, depuration of a toxicant from an organism, and decay of pollutants in water. In addition, the exponential model is a common building block of many models. In this chapter, we explain the fundamentals of the exponential model and expand on two simple applications in environmental modeling. The first is in population dynamics, for example, the growth or decline of populations (Hallam, 1986b). The second is in chemical fate, for example, the decay of chemicals (Hemond and Fechner, 1994).

3.1 FUNDAMENTALS

The simplest and most common ecological and environmental model is the **exponential model.** An exponential law of change of a variable $X(t)$ with time t is obtained by raising the number e to an exponent related to elapsed time:

$$X(t) = X(0)e^{kt} \tag{3.1}$$

Equation 3.1 is often written using the function exp(·) as

$$X(t) = X(0)\exp(kt) \tag{3.2}$$

Equation 3.1, or equivalently Equation 3.2, describes the changes of a variable X with time t, beginning at the initial value $X(0)$ at time zero ($t = 0$).

This law results from solving an ordinary differential equation (ODE) or **model** stating that the **rate of change** of X at any given time t is proportional to the value of X at that time t. In other words, the rate of change of a variable = coefficient × variable. Using the derivative of X with respect to time t for the rate of change of X, we have

$$\frac{dX(t)}{dt} = kX(t) \tag{3.3}$$

where the coefficient k is a **per unit** rate of change or **rate coefficient.** When X multiplies this rate, we get the **net or total** rate of change, which will vary according to the value of X at any particular time t.

When the coefficient k does not depend on X, the model is **linear.** This occurs when k is either dependent only on time t or a constant. In this case, the exponential model is very simple and easy to work with. Figure 3.1 illustrates the linear rate for three values of the rate coefficient: one negative, another one positive, and the other equal to 0.

Why is Equation 3.2 the solution to Equation 3.3? To see this, we use the method described in the previous chapter to integrate Equation 3.3. Move X to the left-hand side (divide both sides by X) to obtain the per unit rate of change:

$$\frac{1}{X}\frac{dX}{dt} = k \tag{3.4}$$

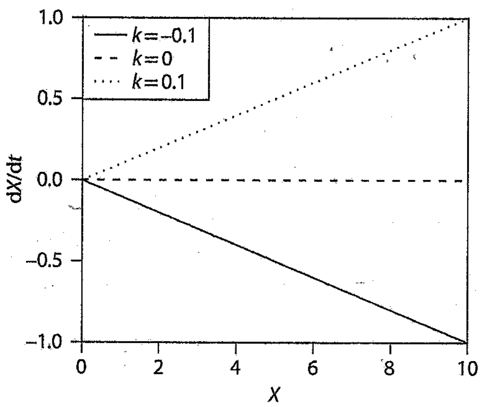

FIGURE 3.1 Exponential model for different values of the constant k. The slope of the line is the coefficient k.

Then, move dt to the right-hand side (multiply both sides by dt) and integrate both sides between the initial time, t_0, and the final time, t_f:

$$\int_{x(t_0)}^{x(t_f)} \frac{1}{X} dX = \int_{t_0}^{t_f} k dt \tag{3.5}$$

Recall that the integral on the left is the natural log to get

$$\ln[X(t_f)] - \ln[X(t_0)] = \ln\left[\frac{X(t_f)}{X(t_0)}\right] = k(t_f - t_0) \tag{3.6}$$

and now invert the log to obtain the exponential function for X at the final time, t_f,

$$X(t_f) = X(t_0)\exp\left[k(t_f - t_0)\right] \tag{3.7}$$

which can be calculated once we have the initial condition $X(t_0)$. It is common practice to let $t_0 = 0$ and t_f as variable t. In this manner, we get $X(t) = X(0)\exp(kt)$, which is precisely the solution given by Equation 3.1 or 3.2.

An easy way to check that Equation 3.1 is indeed the solution of Equation 3.3 is to take the derivative of Equation 3.1 with respect to t and plug it into the left-hand side of Equation 3.3 (Davis, 2002).

Exercise 3.1

Demonstrate that the derivative of Equation 3.1 satisfies the ODE given in Equation 3.3.

3.2 UNITS

Units are very important in modeling because variables represent physical, chemical, and biological properties and quantities, and therefore, to specify the amount of each variable we need to provide the units. The units of both sides of an equation must match. For example, the units of the left-hand side of Equation 3.3 are $dX(t)/dt$ = [units of X][units of t]$^{-1}$ and the units of the right-hand side are $kX(t)$ = [units of k][units of X]. For the units of both sides to match, it follows that the units of the coefficient k must be the inverse of the unit of time; that is to say, [units of k] = [units of t]$^{-1}$.

Recall that abbreviations to denote powers of ten are very useful for shorthand. Some common ones are **k** of kilo for 10^3 (e.g., kg, read as kilogram), **m** of milli for 10^{-3} (e.g., mg, read as milligram), μ of micro for 10^{-6} (e.g., μg read as microgram), and **p** of pico for 10^{-12} (e.g., pg read as picogram).

The **concentration** is given as a ratio of solute to solvent or of solute to solution. There are different ways of expressing this ratio. Two basic ones are per volume of solution or by weight of solution. Take, for example, percent by volume, milligrams per liter (mg/liter), and parts per million (ppm).

A useful convention to specify units is to give **dimensions** of length, mass, and time with the letters L, M, and T, regardless of the actual units. For example, mass in g or kg will both be specified with M; concentration in g/liter or mg/liter by $M \cdot L^{-3}$. This type of unit notation is very useful to perform a check on units without all the details of the actual units. For example, for Equation 3.3, when X is the concentration of a chemical $[M \cdot L^{-3}][T^{-1}] = [\text{units of } k][M \cdot L^{-3}]$, then we can see that $[\text{units of } k] = T^{-1}$.

Exercise 3.2

Suppose we are using an exponential model to describe the changes of light intensity as a function of the depth, z, in a water column. What are the units of coefficient k? Use the dimensional notation and then specify the units if z is given in meters.

Molar mass is the sum of all the atomic masses in a chemical formula. It is the mass corresponding to one mole. For example, the molar mass of silver chloride (AgCl) is 143.32 g/mole. Another important concentration unit is **molarity**, which is the ratio of moles of solute to the volume of solution in liters. That is to say,

$$M = \frac{\text{moles of solute}}{\text{liter of solution}}$$

Therefore, 1 M (read as one **molar**) is 1 mole per liter. Do not confuse M used here for molarity with the M used for mass in the dimensional notation L, M, and T explained earlier. Converting from mass of solute to moles of solute requires knowing the molar mass. For example, if you have 0.14332 g = 143.32 mg of AgCl in 1 liter, then the molarity is 1 milliM (one millimolar) or 1 mM because

$$\frac{143.32\,\text{mg/liter}}{143.32\,\text{g/mol}} = 1 \times 10^{-3}\,\text{mol/liter} = 1\,\text{mM}$$

Exercise 3.3

What would be the molarity if you have 1.4332 ng = 1433.2 pg of AgCl in 1 liter?

3.3 POPULATION DYNAMICS

A population could be defined as a collection of organisms of the same species in a given region (Ford, 1999; Hallam, 1986b; Keen and Spain, 1992). The exponential model applies to nonstructured, spatially homogeneous populations and assumes **density-independent** growth, which is, to say the per capita rate is independent of population density.

By population density we mean the number of individuals per unit area or per unit volume, depending on what type of population we are considering. For example, for trees we may use individuals per unit area, and for zooplankton we may use individuals per unit volume (of water). Therefore, units of population density are expressed in $[\text{individuals}] \cdot L^{-2}$ or L^{-3}. For simplicity we will use [ind] or [indiv] to denote population density regardless of whether we are dealing with area or volume.

The main assumption of the exponential population model is (Hallam, 1986b) that the net rate of change is proportional to the density, X:

$$\text{rate of change} = r \times \text{density}$$

Mathematically, the ODE is given by

$$\frac{dX}{dt} = rX \tag{3.8}$$

The constant r is the **per capita rate of change** or the rate coefficient. The letter r commonly denotes the rate coefficient in population dynamics. The net rate of change, rX, will vary according to the value of X at any particular time, t.

The units are: for density [ind] and for rate [ind] $\cdot$ T^{-1}. For example, if the unit of t is [days] then the unit of r is [days^{-1}] and the unit of dX/dt is [ind days^{-1}].

Exercise 3.4

A population has a density of $X(t) = 1$ [ind] at time $t = 2$ [years]. This population grows with a rate coefficient of $r = 0.5$ [year^{-1}]. What is the net rate of change of the population at time $t = 2$ [years]? What are the units?

The solution of the exponential model is

$$X(t) = X_0 \exp(rt) \tag{3.9}$$

where $X_0 = X(0)$, that is, the initial density. This solution is the same as Equation 3.2. It is a simple, "closed form" solution. We do not really need a computer simulation for this model.

The exponential model can generate three main outcomes (Figure 3.2) according to the value of the coefficient r as follows:

- When $r > 0$, the net rate of change is positive, X increases, and the population grows.
- When $r < 0$, the net rate of change is negative, X decreases, and the population declines.
- When $r = 0$, the net rate of change is zero and the population does not change.

This simple exponential model and its solution can help answer questions like this: How long does it take for a population to double if the intrinsic rate of growth is known? That is to say, how long does it take for X to double if r is known? To answer this question, denote t_d for the unknown doubling time and substitute in the solution (Equation 3.9) for the exponential model

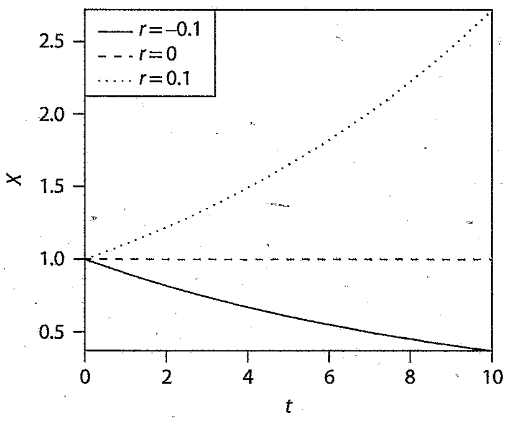

FIGURE 3.2 Exponential solution for the three ranges of r.

$$X(t_d) = X_0 \exp(rt_d) \tag{3.10}$$

Now, when the density doubles, we must have $X(t_d) = 2X_0$. Therefore, substitute $2X_0$ for $X(t_d)$ in the left-hand side to obtain

$$2X_0 = X_0 \exp(rt_d) \tag{3.11}$$

and after eliminating X_0 on both sides, we have

$$2 = \exp(rt_d) \tag{3.12}$$

we need to solve for t_d. Recall that the natural logarithm function ln(.), or log with base e, is the inverse of the exponential function. Take the natural log of both sides to obtain

$$\ln(2) = \ln(\exp(rt_d)) = rt_d \tag{3.13}$$

Now solve for t_d to obtain

$$t_d = \frac{\ln(2)}{r} = \frac{0.693}{r} \tag{3.14}$$

This is the final expression for the doubling time.

Example: A bacterial population has a density of $X(t) = 10^3$ ind or cells · liter^{-1} at time $t = 0$ days. In this case [ind] is a density in per volume basis. This population grows with a rate coefficient of $r = 1\ \text{d}^{-1}$. The doubling time is given by

$$t_d = \frac{\ln(2)}{r} = \frac{0.693}{r} = 0.693\ \text{d}$$

What is the net rate of change of the population after 2 days? To answer this question, we calculate the rate coefficient × density after 2 days

$$\frac{dX(2)}{dt} = rX(2)$$

First, calculate density after 2 days using the exponential model solution at $t = 2$ d with $r = 1\ \text{d}^{-1}$:

$$X(2) = X(0)\exp(rt) = 10^3 \exp(1 \times 2) = 7.39 \times 10^3\ \text{cells} \cdot \text{liter}^{-1}$$

Therefore, the rate after 2 days is given by

$$\frac{dX(2)}{dt} = rX(2) = 1 \times 7.39 \times 10^3 = 7.39 \times 10^3\ \text{cells} \cdot \text{liter}^{-1} \cdot \text{d}^{-1}$$

Exercise 3.5

A population has a density of $X(t) = 100$ ind at time $t = 0$ days. This population grows with a rate coefficient of $r = 0.1\ \text{d}^{-1}$. What is the doubling time? What is the net rate of change of the population after 4 days?

Exercise 3.6

We know that the doubling time is 2 days. What is the rate coefficient? Include the units for the rate coefficient in your answer.

Let us make a linkage to a **difference equation** often used in population modeling. Go back to Equation 3.9 and define T as the duration of a cycle or season of reproduction. Using the population at a cycle, k, as the initial condition for the next cycle, $k + 1$, we can write

$$X((k+1)T) = \exp(rT)X(kT) \qquad k = 0, 1, 2, \ldots \tag{3.15}$$

Now define $\lambda = \exp(rT)$ as a net rate of growth and drop the T for brevity, then we have

$$X(k+1) = \lambda X(k) \qquad k = 0, 1, 2, \ldots \tag{3.16}$$

Equation 3.16 is a commonly used model of population growth in discrete time.

Exercise 3.7

Calculate λ for $r = 0.02$ year^{-1}, and $T = 1$ year is a reproductive season. For a population $X(k) = 100$, calculate the population at the end of the next season, that is to say $X(k + 1)$.

The solution of Equation 3.16 is found by iterating for $k = 1, 2, 3, \ldots$

$$\begin{aligned} X(1) &= \lambda X(0) \\ X(2) &= \lambda X(1) = \lambda^2 X(0) \\ X(3) &= \lambda X(2) = \lambda^3 X(0) \end{aligned} \tag{3.17}$$

which can be generalized as

$$X(k) = \lambda^k X(0) \tag{3.18}$$

The sequence of the population values $X(k)$ grows without bound when $\lambda > 1$, declines to 0 when $\lambda < 1$, and remains constant when $\lambda = 1$; see Figure 3.3.

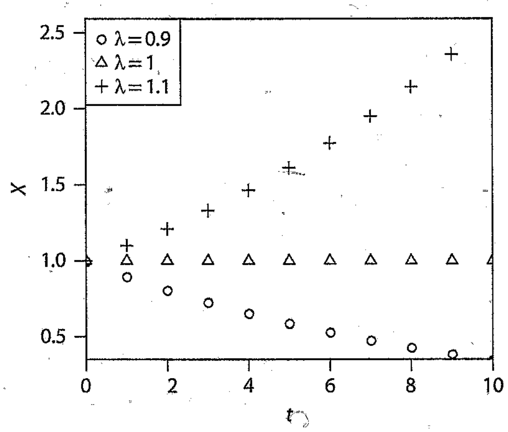

FIGURE 3.3 Discrete-time solution of the difference equation for the three ranges of λ.

Exercise 3.8

Does the population described in the previous exercise grow or decline?

3.4 CHEMICAL FATE

In this case, the dependent variable X denotes the concentration of a compound in some environmental medium, for example, in water, sediments of a stream, or soil (Ford, 1999, pp. 29–30; Keen and Spain, 1992, pp. 17–22).

The simplest assumption is linearity or first-order **kinetics** that leads to an exponential model stating that the rate of decay or degradation or breakdown is proportional to the concentration:

$$dX/dt = -kX \tag{3.19}$$

where k is the degradation or decay rate. Usually there are different chemical, physical, or biological mechanisms and agents to drive the reaction, for example, oxidation by chemicals, photolysis by light, and biodegradation by bacteria.

The model and its solution are the same as in the population example, except that we always assume a negative sign. In addition, we use a different letter, k, for the coefficient because k commonly denotes rate coefficient in kinetics.

The concentration unit for X is $\mathrm{M \cdot liter^{-3}}$, and therefore, the left-hand side has unit $\mathrm{M \cdot liter^{-3} \cdot T^{-1}}$ and the right-hand side has [units of k] $\mathrm{M \cdot liter^{-3}}$. Therefore [units of k] = $\mathrm{T^{-1}}$ as explained earlier. For example, X could be in $\mathrm{mg \cdot liter^{-1}}$ and k in $\mathrm{hour^{-1}}$ or $\mathrm{h^{-1}}$.

We can answer questions like how long does it take for the concentration, X, of a compound to reduce to one-half? The calculation process is the same as in Equations 3.10 through 3.14 but by using ½ instead of 2. Use t_h to denote the half-life (time that it takes for the concentration to degrade to one-half of the initial concentration) and therefore we have

$$\frac{1}{2}X_0 = X_0 \exp(-kt_h) \tag{3.20}$$

that is,

$$1/2 = \exp(-kt_h) \tag{3.21}$$

Take the natural log of both sides as before, and recall that the log of a ratio is the log of the numerator minus the log of the denominator to obtain

$$\ln(1) - \ln(2) = \ln(\exp(-kt_h)) \tag{3.22}$$

and that the log of 1 is zero,

$$-\ln(2) = -kt_h \tag{3.23}$$

The negative sign cancels on both sides and solves for the half-life,

$$t_h = \frac{\ln(2)}{k} = \frac{0.693}{k} \tag{3.24}$$

as a function of the degradation rate coefficient, k.

As an example, assume that a fungicide degrades at a rate of $k = 0.0693\ \mathrm{d}^{-1}$. What is the half-life? The half-life is given by

$$t_h = \frac{\ln(2)}{k} = \frac{0.693}{0.0693} = 10\ \mathrm{d}$$

Exercise 3.9

Assume that the decay rate coefficient is $0.5\ \mathrm{h}^{-1}$; what is the half-life?

Assume that a chemical has $k = 0.0693\ \mathrm{d}^{-1}$. How long does it take to degrade to 1% of the initial value? Use the solution of the exponential model:

$$\frac{1}{100} X(0) = X(0)\exp(kt_{1\%})$$

Cancel $X(0)$ on both sides, take logarithms of both sides, and simplify to obtain

$$t_{1\%} = \frac{\ln(100)}{k} = \frac{4.60}{0.0693} = 66.45\ \mathrm{d}$$

Therefore, it takes 66.45 days to degrade to 1% of the initial value.

Exercise 3.10

A pesticide degrades with a rate coefficient of $k = 0.693\ \mathrm{d}^{-1}$. What is the half-life? How long does it take to degrade to 5% of the initial value?

R can be used for quick calculations. For example, if the doubling time is 4 days, then what is r?

```
> 0.693/4
[1] 0.17325
```

If the decay rate is $2\ \mathrm{d}^{-1}$, what is the half-life?

```
> 0.693/2
[1] 0.3465
```

3.5 MODEL TERMS

It is important to reiterate the terminology used in modeling. We can do this at this stage by recognizing how some of the terms apply to the exponential model as follows:

- $dX/dt = rX$ is a dynamic **model**. In this case, it is given by an **ODE**.
- $X(t)$ is the **state variable** at time t. In the simple exponential model that we are considering in this chapter, the state is also the **output**. In other cases, the output is a function of the state.
- r is a parameter.
- X_0 is the **initial condition** or **initial state** (technically it is also a parameter).