Deterministic functions for ecological modeling

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1 Summary

This chapter first covers the mathematical tools and R functions that you need in order to figure out the shape and properties of a mathematical function from its formula. It then presents a broad range of commonly used functions and explains their general properties and ecological uses.

2 Introduction

You've now learned how to start exploring the patterns in your data. The methods introduced in Chapter 2 provide only *qualitative* descriptions of patterns: when you explore your data, you don't want to commit yourself too soon to any particular description of those patterns. In order to tie the patterns to ecological theory, however, we often want to use particular mathematical functions to describe the deterministic patterns in the data. Sometimes phenomenological descriptions, intended to describe the pattern as simply and accurately as possible, are sufficient. Whenever possible, however, it's better to use mechanistic descriptions with meaningful parameters, derived from a theoretical model that you or someone else has invented to describe the underlying processes driving the pattern. (Remember from Chapter ?? that the same function can be either phenomenological or mechanistic depending on context.) In any case, you need to know something about a wide range of possible functions, and even more to learn (or remember) how to discover the properties of a new mathematical function. This chapter first presents a variety of analytical and computational methods for finding out about functions, and then goes through a "bestiary" of useful functions for ecological modeling. The chapter uses differential calculus heavily. If you're rusty, it would be a good idea to look at the Appendix for some reminders.

For example, look again at the data introduced in Chapter 2 on predation rate of tadpoles as a function of tadpole size (Figure 1). We need to know what kinds of functions might be suitable for describing these data. The data which are humped in the middle and slightly skewed to the right, which probably reflects the balance between small tadpoles' ability to hide from (or be ignored by) predators large tadpoles' ability to escape them or be too big to swallow.
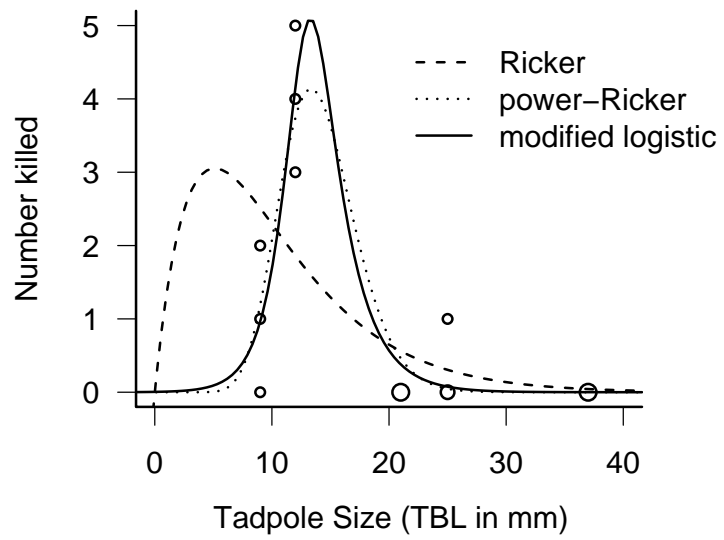
Figure 1: Tadpole predation as a function of size, with some possible functions fitted to the data.

What functions could fit this pattern? What do their parameters mean in terms of the shapes of the curves? In terms of ecology? How do we "eyeball" the data to obtain approximate parameter values, which we will need as a starting point for more precise estimation and as a check on our results?

The Ricker function, $y = axe^{-bx}$, is a standard choice for hump-shaped ecological patterns that are skewed to the right, but Figure 1 shows that it doesn't fit well. Two other choices, the power-Ricker (Persson et al., 1998) and a modified logistic equation (Vonesh and Bolker, 2005) and fit pretty well: later in the chapter we will explore some strategies for modifying standard functions to make them more flexible.

3 Finding out about functions numerically

3.1 Calculating and plotting curves

You can use R to experiment numerically with different functions. It's better to experiment numerically *after* you've got some idea of the mathematical and ecological meanings of the parameters: otherwise you may end up using the computer as an expensive guessing tool. It really helps to have some idea what the parameters of a function mean, so you can eyeball your data first and get a rough idea of the appropriate values (and know more about what to tweak, so you can do it intelligently). Nevertheless, I'll show you first some of the ways that you can use R to compute and draw pictures of functions so that you can sharpen your intuition as we go along.

As examples, I'll use the (negative) exponential function, ae^{-bx} (R uses `exp(x)` for the exponential function e^x) and the Ricker function, axe^{-bx}. Both are very common in ecological modeling.

As a first step, you can simply use R as a calculator to plug values into functions: e.g. `2.3*exp(1.7*2.4)`. Since most functions in R operate on vectors (or "are vectorized", ugly as the expression is), you can calculate values for a range of inputs or parameters with a single command.

Next simplest, you can use the `curve` function to have R compute and plot values for a range of inputs: use `add=TRUE` to add curves to an existing plot (Figure 2). (Remember the differences between mathematical and R notation: the exponential is ae^{-bx} or $a\exp(-bx)$ in math notation, but it's `a*exp(-b*x)` in R. Using math notation in a computer context will give you an error. Using computer notation in a math context is just ugly.)

If you want to keep the values of the function and do other things with them, you may want to define your own vector of x values (with `seq`: call it something like `xvec`) and then use R to compute the values (e.g., `xvec = seq(0,7,length=100)`).

If the function you want to compute *does not* work on a whole vector at once, then you can't use either of the above recipes. The easiest shortcut in this case, and a worthwhile thing to do for other reasons, is to write your own small R function that computes the value of the function for a given input value, then
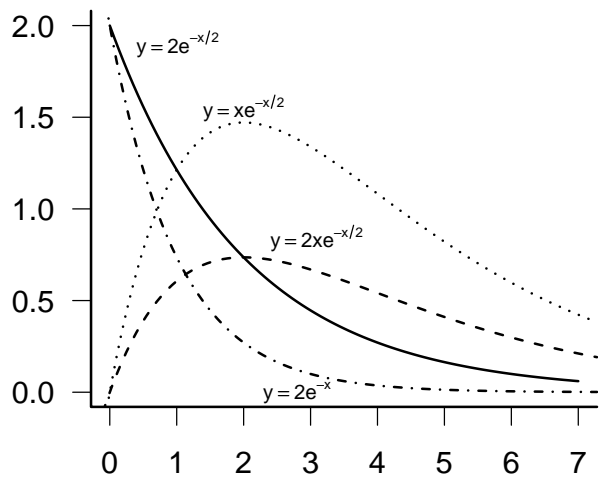
Figure 2: Negative exponential ($y = ae^{-bx}$) and Ricker ($y = axe^{-bx}$) functions: `curve`

use `sapply` to run the function on all of the values in your x vector. When you write such an R function, you would typically make the input value (x) be the first argument, followed by all of the other parameters. It often saves time if you assign *default values* to the other parameters: in the following example, the default values of both a and b are 1.

```
> ricker = function(x, a = 1, b = 1) {
+     a * x * exp(-b * x)
+ }
> yvals = sapply(xvec, ricker)
```

(in this case, since `ricker` only uses vectorized operations, `ricker(xvec)` would work just as well).[*]

3.2   Plotting surfaces

Things get a bit more complicated when you consider a function of two (or more) variables: R's range of 3D graphics is more limited, it is harder to vectorize operations over two different parameters, and you may want to compute the value of the function so many times that you start to have to worry about computational efficiency (this is our first hint of the so-called *curse of dimensionality*, which will come back to haunt us later).

Base R doesn't have exact multidimensional analogues of `curve` and `sapply`, but I've supplied some in the `emdbook` package: `curve3d` and `apply2d`. The `apply2d` function takes an x vector and a y vector and computes the value of a function for all of the combinations, while `curve3d` does the same thing for surfaces that `curve` does for curves: it computes the function value for a range of values and plots it[†]. The basic function for plotting surfaces in R is `persp`. You can also use `image` or `contour` to plot 2D graphics, or `wireframe` [`lattice` package], or `persp3d` [`rgl` package] as alternatives to `persp`. With `persp` and `wireframe`, you may want to play with the viewing point for the 3D perspective (modify `theta` and `phi` for `persp` and `screen` for `wireframe`); the `rgl` package lets you use the mouse to move the viewpoint.

For example, Vonesh and Bolker (2005) suggested a way to combine size- and density-dependent tadpole mortality risk by using a variant logistic function of size as in Figure 1 to compute an attack rate $\alpha(s)$, then assuming that *per capita* mortality risk declines with density N as $\alpha(s)/(1 + \alpha(s)HN)$, where H is the handling time (Holling type II functional response). Supposing we already have a function `attackrate` that computes the attack rate as a function of size, our mortality risk function would be:

```
> mortrisk = function(N, size, H = 0.84) {
+     a <- attackrate(size)
```

---

[*]The definition of "input values" and "parameters" is flexible. You can also compute the values of the function for a fixed value of x and a range of one of the parameters, e.g. `ricker(1,a=c(1.1,2.5,3.7))`.

[†]For simple functions you can use the built-in `outer` function, but `outer` requires vectorized functions: `apply2d` works around this limitation.
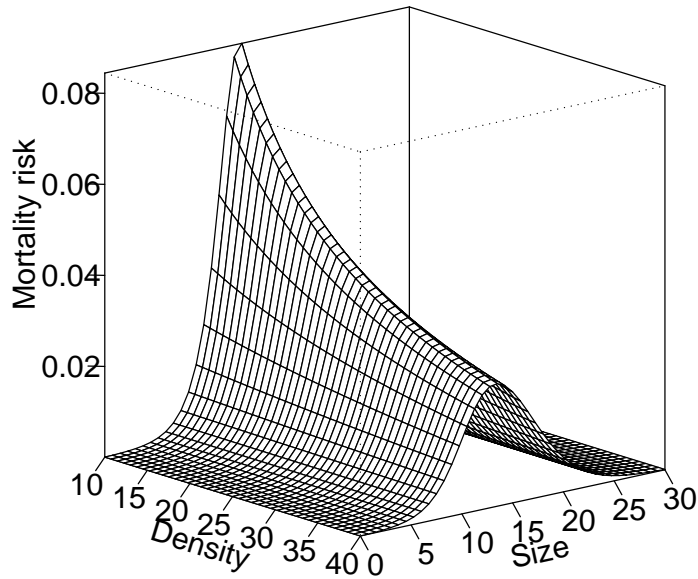
Figure 3: Perspective plot for the mortality risk function used in Vonesh and Bolker (2005): `curve3d(mortrisk(N=x,size=y),to=c(40,30),theta=50)`.

```
+       a/(1 + a * N * H)
+ }
```

The `H=0.84` in the function definition sets the *default* value of the handling time parameter: if I leave `H` out (e.g. `mortrisk(N=10,size=20)`) then R will fill in the default values for any missing parameters. Specifying reasonable defaults can save a lot of typing.

4   Finding out about functions analytically

Exploring functions numerically is quick and easy, but limited. In order to really understand a function's properties, you must explore it analytically — i.e., you have to analyze its equation mathematically. To do that and then translate your mathematical intuition into ecological intuition, you must remember some algebra and calculus. In particular, this section will explain how to take limits at the ends of the range of the function; understand the behavior in the middle of the range; find critical points; understand what the parameters mean and how they affect the shape of the curve; and approximate the function near an

arbitrary point (Taylor expansion). These tools will probably tell you everything you need to know about a function.

4.1 Taking limits: what happens at either end?

Function values   You can take the limit of a function as x gets large ($x \to \infty$) or small ($x \to 0$, or $x \to -\infty$ for a function that makes sense for negative x values). The basic principle is to throw out lower-order terms. As x grows, it will eventually grow much larger than the largest constant term in the equation. Terms with larger powers of x will dwarf smaller powers, and exponentials will dwarf any power. If x is very small then you apply the same logic in reverse; constants are bigger than (positive) powers of x, and negative powers ($x^{-1} = 1/x$, $x^{-2} = 1/x^2$, etc.) are bigger than any constants. (Negative exponentials go to 1 as x approaches zero, and 0 as x approaches ∞.) Exponentials are stronger than powers: $x^{-n}e^x$ eventually gets big and $x^n e^{-x}$ eventually gets small as x increases, no matter how big n is.

Our examples of the exponential and the Ricker function are almost too simple: we already know that the negative exponential function approaches 1 (or a, if we are thinking about the form ae^{-bx}) as x approaches 0 and 0 as x becomes large. The Ricker is slightly more interesting: for $x = 0$ we can calculate the value of the function directly (to get $a \cdot 0 \cdot e^{-b \cdot 0} = 0 \cdot 1 = 0$) or argue qualitatively that the e^{-bx} part approaches 1 and the ax part approaches zero (and hence the whole function approaches zero). For large x we have a concrete example of the $x^n e^{-x}$ example given above (with $n = 1$) and use our knowledge that exponentials always win to say that the e^{-bx} part should dominate the ax part to bring the function down to zero in the limit. (When you are doing this kind of qualitative reasoning you can almost always ignore the constants in the equation.)

As another example, consider the Michaelis-Menten function ($f(x) = ax/(b+x)$). We see that as x gets large we can say that $x \gg b$, no matter what b is ($\gg$ means "is much greater than"), so $b + x \approx x$, so

$$\frac{ax}{b+x} \approx \frac{ax}{x} = a : \tag{1}$$

the curve reaches a constant value of a. As x gets small, $b \gg x$ so

$$\frac{ax}{b+x} \approx \frac{ax}{b} : \tag{2}$$

the curve approaches a straight line through the origin, with slope a/b. As x goes to zero you can see that the value of the function is exactly zero $(a \times 0)/(b+0) = 0/b = 0$).

For more difficult functions that contain a fraction whose numerator and denominator both approach zero or infinity in some limit (and thus make it hard to find the limiting value), you can try *L'Hôpital's Rule*, which says that the limit of the function equals the limit of the ratio of the derivatives of the

numerator and the denominator:

$$\lim \frac{a(x)}{b(x)} = \lim \frac{a'(x)}{b'(x)}. \tag{3}$$

(a'(x) is an alternative notation for $\frac{da}{dx}$).

Derivatives   As well as knowing the limits of the function, we also want to know how the function increases or decreases toward them: the limiting slope. Does the function shoot up or down (a derivative that "blows up" to positive or negative infinity), change linearly (a derivative that reaches a positive or negative constant limiting value), or flatten out (a derivative with limit 0)? To figure this out, we need to take the derivative with respect to x and then find its limit at the edges of the range.

The derivative of the exponential function $f(x) = ae^{-bx}$ is easy (if it isn't, review the Appendix): $f'(x) = -abe^{-bx}$. When $x = 0$ this becomes ab, and when x gets large the e^{-bx} part goes to zero, so the answer is zero. Thus (as you may already have known), the slope of the (negative) exponential is negative at the origin $(x = 0)$ and the curve flattens out as x gets large.

The derivative of the Ricker is only a little harder (use the product rule):

$$\frac{daxe^{-bx}}{dx} = (a \cdot e^{-bx} + ax \cdot -be^{-bx}) = (a - abx) \cdot e^{-bx} = a(1 - bx)e^{-bx}. \tag{4}$$

At zero, this is easy to compute: $a(1 - b \cdot 0)e^{-b \cdot 0} = a \cdot 1 \cdot 1 = a$. As x goes to infinity, the $(1 - bx)$ term becomes negative (and large in magnitude) and the e^{-bx} term goes toward zero, and we again use the fact that exponentials dominate linear and polynomial functions to see that the curve flattens out, rather than becoming more and more negative and crashing toward negative infinity. (In fact, we already know that the curve approaches zero, so we could also have deduced that the curve must flatten out and the derivative must approach zero.)

In the case of the Michaelis-Menten function it's easy to figure out the slope at zero (because the curve becomes approximately $(a/b)x$ for small x), but in some cases you might have to take the derivative first and then set x to 0. The derivative of $ax/(b + x)$ is (using the quotient rule)

$$\frac{(b + x) \cdot a - ax \cdot 1}{(b + x)^2} = \frac{ab + ax - ax}{(b + x)^2} = \frac{ab}{(b + x)^2} \tag{5}$$

which (as promised) is approximately a/b when $x \approx 0$ (following the rule that $(b + x) \approx b$ for $x \approx 0$). Using the quotient rule often gives you a complicated denominator, but when you are only looking for points where the derivative is zero, you can calculate when the numerator is zero and ignore the derivative.

4.2   What happens in the middle? Scale parameters and half-maxima

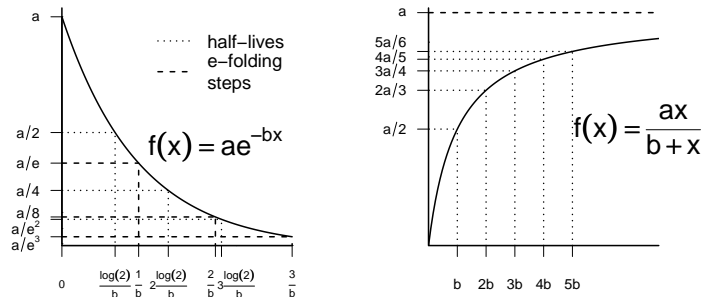It's also useful to know what happens in the middle of a function's range.

Figure 4: (Left) Half-lives and e-folding times for a negative exponential function. (Right) Half-maximum and characteristic scales for a Michaelis-Menten function.

For *unbounded* functions (functions that increase to ∞ or decrease to $-\infty$ at the ends of their range), such as the exponential, we may not be able to find special points in the middle of the range, although it's worth trying out special cases such as $x = 1$ (or $x = 0$ for functions that range over negative and positive values) just to see if they have simple and interpretable answers.

In the exponential function ae^{-bx}, b is a *scale parameter*. In general, if a parameter appears in a function in the form of bx or x/c, its effect is to scale the curve along the x-axis — stretching it or shrinking it, but keeping the qualitative shape the same. If the scale parameter is in the form bx then b has inverse-x units (if x is a time measured in hours, then b is a rate per hour with units hour^{-1}). If it's in the form x/c then c has the same units as x, and we can call c a "characteristic scale". Mathematicians often choose the form bx because it looks cleaner, while ecologists may prefer x/c because it's easier to interpret the parameter when it has the same units as x. Mathematically, the two forms are equivalent, with $b = 1/c$; this is an example of changing the *parameterization* of a function (see p. 11).

For the negative exponential function ae^{-bx}, the characteristic scale $1/b$ is also sometimes called the *e-folding time* (or e-folding distance if x measures distance rather than time). The value of the function drops from a at $x = 0$ to $a/e = ae^{-1}$ when $x = 1/b$, and drops a further factor of $e = 2.718\ldots \approx 3$ every time x increases by $1/b$ (Figure 4). Exponential-based functions can also be described in terms of the *half-life* (for decreasing functions) or *doubling time* (for increasing functions), which is $T_{1/2} = \ln 2/b$. When $x = T_{1/2}$, $y = a/2$, and every time x increases by $T_{1/2}$ the function drops by another factor of 2.)

For the Ricker function, we already know that the function is zero at the origin and approaches zero as x gets large. We also know that the derivative is

positive at zero and negative (but the curve is flattening out, so the derivative is increasing toward zero), as x gets large. We can deduce* that the derivative must be zero and the function must reach a peak somewhere in the middle; we will calculate the location and height of this peak in the next section.

For functions that reach an asymptote, like the Michaelis-Menten, it's useful to know when the function gets "halfway up"—the *half-maximum* is a point on the x-axis, not the y-axis. We figure this out by figuring out the asymptote ($=a$ for this parameterization of the Michaelis-Menten function) and solving $f(x_{1/2}) = \text{asymptote}/2$. In this case

$$\frac{ax_{1/2}}{b + x_{1/2}} = \frac{a}{2}$$
$$ax_{1/2} = \frac{a}{2} \cdot (b + x_{1/2})$$
$$\left(a - \frac{a}{2}\right) x_{1/2} = \frac{ab}{2}$$
$$x_{1/2} = \frac{2}{a} \cdot \frac{ab}{2} = b.$$

The half-maximum b is the characteristic scale parameter for the Michaelis-Menten: we can see this by dividing the numerator and denominator by b to get $f(x) = a \cdot (x/b)/(1 + x/b)$. As x increases by half-maximum units (from $x_{1/2}$ to $2x_{1/2}$ to $3x_{1/2}$), the function first reaches $1/2$ its asymptote, then $2/3$ of its asymptote, then $3/4$ … (Figure 4).

We can calculate the half-maximum for any function that starts from zero and reaches an asymptote, although it may not be a simple expression.

4.3 Critical points and inflection points

We might also be interested in the *critical points*—maxima and minima — of a function. To find the critical points of f, remember from calculus that they occur where $f'(x) = 0$; calculate the derivative, solve it for x, and plug that value for x into $f(x)$ to determine the value (peak height/trough depth) at that point*. The exponential function is *monotonic*: it is always either increasing or decreasing depending on the sign of b (its slope is always either positive or negative for all values of x) — so it never has any critical points.

The Michaelis-Menten curve is also monotonic: we figured out above that its derivative is $ab/(b + x)^2$. Since the denominator is squared, the derivative is always positive. (Strictly speaking, this is only true if $a > 0$. Ecologists are usually sloppier than mathematicians, who are careful to point out all the assumptions behind a formula (like $a > 0$, $b > 0$, $x \geq 0$). I'm acting like an ecologist rather than a mathematician, assuming parameters and x values are positive unless otherwise stated.) While remaining positive, the derivative

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*Because the Ricker function has continuous derivatives

*The derivative is also zero at *saddle points*, where the function temporarily flattens on its way up or down.

decreases to zero as $x \to \infty$ (because $a/(1 + bx)^2 \approx a/(bx)^2 \propto 1/x^2$); such a function is called *saturating*.

We already noted that the Ricker function, axe^{-bx}, has a peak in the middle somewhere: where is it? Using the product rule:

$$\frac{d(axe^{-bx})}{dx} = 0$$
$$ae^{-bx} + ax(-be^{-bx}) = 0$$
$$(1 - bx)ae^{-bx} = 0$$

The left-hand side can only be zero if $1 - bx = 0$, $a = 0$ (a case we're ignoring as ecologists), or $e^{-bx} = 0$. The exponential part e^{-bx} is never equal to 0, so we simply solve $(1 - bx) = 0$ to get $x = 1/b$. Plugging this value of x back into the equation tells us that the height of the peak is $(a/b)e^{-1}$. (You may have noticed that the peak location, $1/b$, is the same as the characteristic scale for the Ricker equation.)

4.4   Understanding and changing parameters

Once you know something about a function (its value at zero or other special points, value at ∞, half-maximum, slope at certain points, and the relationship of these values to the parameters), you can get a rough idea of the meanings of the parameters. You will find, alas, that scientists rarely stick to one parameterization. Reparameterization seems like an awful nuisance — why can't everyone just pick one set of parameters and stick to it? — but, even setting aside historical accidents that make different fields adopt different parameterizations, different parameterizations are useful in different contexts. Different parameterizations have different mechanistic interpretations. For example, we'll see in a minute that the Michaelis-Menten function can be interpreted (among other possibilities) in terms of enzyme reaction rates and half-saturation constants or in terms of predator attack rates and handling times. Some parameterizations make it easier to estimate parameters by eye. For example, half-lives are easier to see than e-folding times, and peak heights are easier to see than slopes. Finally, some sets of parameters are strongly correlated, making them harder to estimate from data. For example, if you write the equation of a line in the form $y = ax + b$, the estimates of the slope a and the intercept b are negatively correlated, but if you instead say $y = a(x - \bar{x}) + \bar{y}$, estimating the mean value of y rather than the intercept, the estimates are uncorrelated. You just have to brush up your algebra and learn to switch among parameterizations.

We know the following things about the Michaelis-Menten function $f(x) = ax/(b + x)$: the value at zero $f(0) = 0$; the asymptote $f(\infty) = a$; the initial slope $f'(0) = a/b$; and the half-maximum (the characteristic scale) is b.

You can use these characteristics crudely estimate the parameters from the data. Find the asymptote and the x value at which y reaches half of its maximum value, and you have a and b. (You can approximate these values by eye, or use a more objective procedure such as taking the mean of the last 10% of the data

to find the asymptote.) Or you can estimate the asymptote and the initial slope ($\Delta y/\Delta x$), perhaps by linear regression on the first 20% of the data, and then use the algebra $b = a/(a/b) = $ asymptote/(initial slope) to find b.

Equally important, you can use this knowledge of the curve to translate among algebraic, geometric, and mechanistic meanings. When we use the Michaelis-Menten in community ecology as the Holling type II functional response, its formula is $P(N) = \alpha N/(1 + \alpha H N)$, where P is the predation rate, N is the density of prey, α is the attack rate, and H is the handling time. In this context, the initial slope is α and the asymptote is $1/H$. Ecologically, this makes sense because at low densities the predators will consume prey at a rate proportional to the attack rate ($P(N) \approx \alpha N$) while at high densities the predation rate is entirely limited by handling time ($P(N) \approx 1/H$). It makes sense that the predation *rate* is the inverse of the handling *time*: if it takes half an hour to handle (capture, swallow, digest, etc.) a prey, and essentially no time to locate a new one (since the prey density is very high), then the predation rate is $1/(0.5 \text{ hour}) = 2/\text{hour}$. The half-maximum in this parameterization is $1/(\alpha H)$.

On the other hand, biochemists usually parameterize the function more as we did above, with a maximum rate $v_{\max}$ and a half-maximum K_m: as a function of concentration C, $f(C) = v_{\max}C/(K_m + C)$.

As another example, recall the following facts about the Ricker function $f(x) = axe^{-bx}$: the value at zero $f(0) = 0$; the initial slope $f'(0) = a$; the horizontal location of the peak is at $x = 1/b$; and the peak height is $a/(be)$. The form we wrote above is algebraically simplest, but it might be more convenient to parameterize the curve in terms of its peak location (let's say $p = 1/b$): $y = axe^{-x/p}$. Fisheries biologists often use another parameterization, $R = Se^{-a_3 - bS}$, where $a_3 = \ln a$ (Quinn and Deriso, 1999).

4.5   Transformations

Beyond changing the parameterization, you can also change the scales of the x and y axes, or in other words *transform* the data. For example, in the Ricker example just given ($R = Se^{-a_3 - bS}$), if we plot $-\ln(R/S)$ against S, we get the line $-\ln(R/S) = a_3 + bS$, which makes it easy to see that a_3 is the intercept and b is the slope.

Log transformations of x or y or both are common because they make exponential relationships into straight lines. If $y = ae^{-bx}$ and we log-transform y we get $\ln y = \ln a - bx$ (a *semi-log* plot). If $y = ax^b$ and we log-transform both x and y we get $\ln y = \ln a + b\ln x$ (a *log-log* plot).

Another example: if we have a Michaelis-Menten curve and plot x/y against y, the relationship is

$$x/y = \frac{x}{ax/(b+x)} = \frac{b+x}{a} = \frac{1}{a} \cdot x + \frac{b}{a},$$

which represents a straight line with slope $1/a$ and intercept b/a.

All of these transformations are called *linearizing transformations*. Researchers often used them in the past to fit straight lines to data when when

computers were slower. Linearizing is not recommended when there is another alternative such as nonlinear regression, but transformations are still useful. Linearized data are easier to eyeball, so you can get rough estimates of slopes and intercepts by eye, and it is easier to see deviations from linearity than from (e.g.) an exponential curve. Log-transforming data on geometric growth of a population lets you look at *proportional* changes in the population size (a doubling of the population is always represented by the distance on the y axis). Square-root-transforming data on variances lets you look at standard deviations, which are measured in the same units as the original data and may thus be easier to understand.

The *logit* or *log-odds* function, $\text{logit}(x) = \log(x/(1-x))^*$ (`qlogis(x)` in R) is another common linearizing transformation. If x is a probability then $x/(1-x)$ is the ratio of the probability of occurrence (x) to the probability of non-occurrence $1-x$, which is called the odds (for example, a probability of 0.1 or 10% corresponds to odds of $0.1/0.9 = 1/9$). The logit transformation makes a logistic curve, $y = e^{a+bx}/(1+e^{a+bx})$, into a straight line:

$$
\begin{aligned}
y &= e^{a+bx}/(1+e^{a+bx}) \\
\left(1 + e^{a+bx}\right) y &= e^{a+bx} \\
y &= e^{a+bx}(1-y) \\
\frac{y}{1-y} &= e^{a+bx} \\
\log\left(\frac{y}{1-y}\right) &= a + bx
\end{aligned}
\tag{6}
$$

4.6   Shifting and scaling

Another way to change or extend functions is to shift or scale them. For example, let's start with the simplest form of the Michaelis-Menten function, and then see how we can manipulate it (Figure 5). The function $y = x/(1+x)$ starts at 0, increases to 1 as x gets large, and has a half-maximum at $x = 1$.

- We can stretch, or scale, the x axis by dividing x by a constant — this means you have to go farther on the x axis to get the same increase in y. If we substitute x/b for x everywhere in the function, we get $y = (x/b)/(1 + x/b)$. Multiplying the numerator and denominator by b shows us that $y = x/(b+x)$, so b is just the half-maximum, which we identified before as the characteristic scale. In general a parameter that we multiply or divide x by is called a *scale parameter* because it changes the horizontal scale of the function.

- We can stretch or scale the y axis by multiplying the whole right-hand side by a constant. If we use a, we have $y = ax/(b+x)$, which as we have seen above moves the asymptote from 1 to a.

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*Throughout this book I use $\log(x)$ to mean the natural logarithm of x, also called $\ln(x)$ or $\log_e(x)$. If you need a refresher on logarithms, see the Appendix.
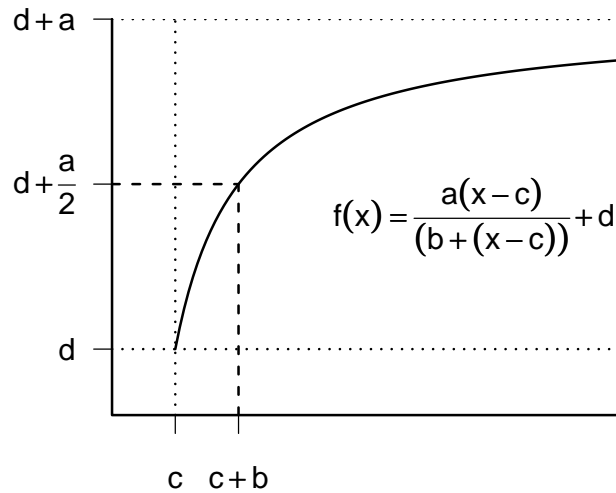
$$f(x) = \frac{a(x-c)}{(b+(x-c))} + d$$

Figure 5: Scaled, shifted Michaelis-Menten function $y = a(x-c)/((x-c)+b)+d$.

- We can shift the whole curve to the right or the left by subtracting or adding a constant *location parameter* from x throughout; subtracting a (positive) constant from x shifts the curve to the right. Thus, $y = a(x - c)/(b + (x - c))$ hits $y = 0$ at c rather than zero. (You may want in this case to specify that $y = 0$ if $y < c$ — otherwise the function may behave badly [try `curve(x/(x-1),from=0,to=3)` to see what might happen].)

- We can shift the whole curve up or down by adding or subtracting a constant to the right-hand side: $y = a(x - c)/(b + (x - c)) + d$ would start from $y = d$, rather than zero, when $x = c$ (the asymptote also moves up to $a + d$).

These recipes can be used with any function. For example, Emlen (1996) wanted to describe a relationship between the prothorax and the horn length of horned beetles where the smallest beetles in his sample had a constant, but non-zero, horn length. He added a constant to a generalized logistic function to shift the curve up from its usual zero baseline.

4.7   Taylor series approximation

The *Taylor series* or *Taylor approximation* is the single most useful, and used, application of calculus for an ecologist. Two particularly useful applications of Taylor approximation are understanding the shapes of goodness-of-fit surfaces (Chapter **??**) and the delta method for estimating errors in estimation (Chapter **??**).

The Taylor series allows us to approximate a complicated function near a point we care about, using a simple function — a polynomial with a few terms, say a line or a quadratic curve. All we have to do is figure out the slope (first derivative) and curvature (second derivative) at that point. Then we can construct a parabola that matches the complicated curve in the neighborhood of the point we are interested in. (In reality the Taylor series goes on forever — we can approximate the curve more precisely with a cubic, then a 4th-order polynomial, and so forth — but in practice ecologists never go beyond a quadratic expansion.)

Mathematically, the Taylor series says that, near a given point x_0,

$$f(x) \approx f(x_0) + \frac{df}{dx}\bigg|_{x_0} \cdot (x - x_0) + \frac{d^2 f}{dx^2}\bigg|_{x_0} \cdot \frac{(x - x_0)^2}{2} + \ldots + \frac{d^n f}{dx^n}\bigg|_{x_0} \cdot \frac{(x - x_0)^n}{n!} + \ldots$$

(7)

(the notation $\frac{df}{dx}\big|_{x_0}$ means "the derivative evaluated at the point $x = x_0$"). Taylor *approximation* just means dropping terms past the second or third.

Figure 6 shows a function and the constant, linear, quadratic, and cubic approximations (Taylor expansion using 1, 2, or 3 terms). The linear approximation is bad but the quadratic fit is good very near the center point, and the cubic accounts for some of the asymmetry in the function. In this case one more term would match the function exactly, since it is actually a 4th-degree polynomial.

the exponential function   The Taylor expansion of the exponential, e^{rx}, around $x = 0$ is $1 + rx + (rx)^2/2 + (rx)^3/(2 \cdot 3) \ldots$. Remembering this fact rather than working it out every time may save you time in the long run — for example, to understand how the Ricker function works for small x we can substitute $(1 - bx)$ for e^{-bx} (dropping all but the first two terms!) to get $y \approx ax - abx^2$: this tells us immediately that the function starts out linear, but starts to curve downward right away.

the logistic curve   Calculating Taylor approximations is often tedious (all those derivatives), but we usually try to do it at some special point where a lot of the complexity goes away (such as $x = 0$ for a logistic curve).

The general form of the logistic (p. 26) is $e^{a+bx}/(1 + e^{a+bx})$, but doing the algebra will be simpler if we set $a = 0$ and divide numerator and denominator by e^{bx} to get $f(x) = 1/(1 + e^{-bx})$. Taking the Taylor expansion around $x = 0$:
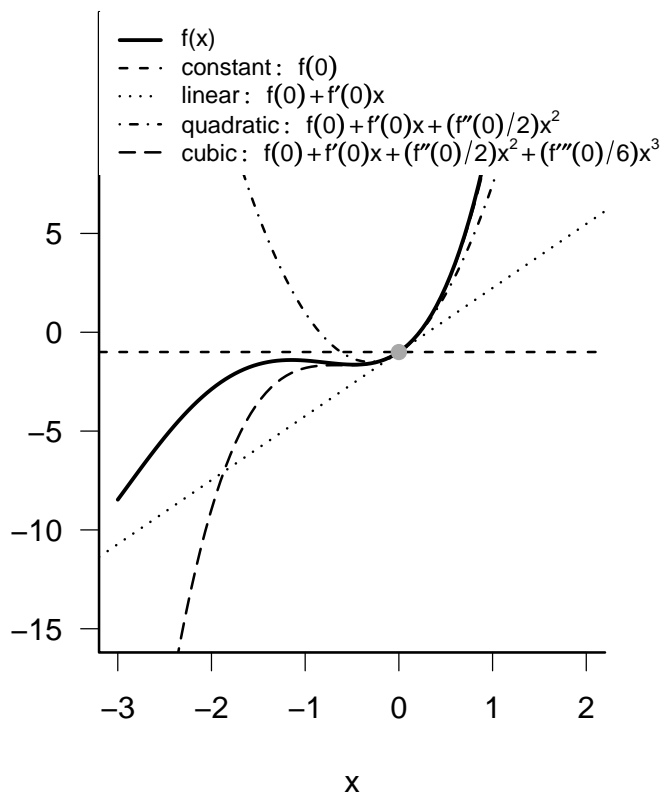
- $f(0) = 1/2$

Figure 6: Taylor series expansion of a 4th-order polynomial.

- $f'(x) = \frac{be^{-bx}}{(1+e^{-bx})^2}$ (writing the formula as $(1+e^{-bx})^{-1}$ and using the power rule and the chain rule twice) so $f'(0) = (b \cdot 1)/((1+1)^2) = b/4^*$

- Using the quotient rule and the chain rule:

$$
\begin{aligned}
f''(0) &= \left. \frac{(1 + e^{-bx})^2(-b^2 e^{-bx}) - (be^{-bx})(2(1 + e^{-bx})(-be^{-bx}))}{(1 + e^{-bx})^4} \right|_{x=0} \\
&= \frac{(1+1)^2(-b^2) - (b)(2(1+1)(-b))}{(1+1)^4} \\
&= \frac{(-4b^2) + (4b^2)}{16} \\
&= 0
\end{aligned}
\tag{8}
$$

R will actually compute simple derivatives for you (using D: see p. 33), but it won't simplify them at all. If you just need to compute the numerical value of the derivative for a particular b and x, it may be useful, but there are often general answers you'll miss by doing it this way (for example, in the above case that $f''(0)$ is zero for any value of b).

Stopping to interpret the answer we got from all that tedious algebra: we find out that the slope of a logistic function around its midpoint is $b/2$, and its curvature (second derivative) is zero: that means that the midpoint is an *inflection point* (where there is no curvature, or where the curve switches from being concave to convex), which you might have known already. It also means that near the inflection point, the logistic can be closely approximated by a straight line. (For y near zero, exponential growth is a good approximation; for y near the asymptote, exponential approach to the asymptote is a good approximation.)

5 Bestiary of functions

The remainder of the chapter describes different families of functions that are useful in ecological modeling: Table 1 gives an overview of their qualitative properties. This section includes little R code, although the formulas should be easy to translate into R. You should skim through this section on the first reading to get an idea of what functions are available. If you begin to feel bogged down you can skip ahead and use the section for reference as needed.

5.1 Functions based on polynomials

A polynomial is a function of the form $y = \sum_{i=0}^{n} a_i x^i$.

---

*We calculate $f'(x)$ and evaluate it at $x = 0$. We *don't* calculate the derivative of $f(0)$, because $f(0)$ is a constant value ($1/2$ in this case) and its derivative is zero.

Function	Range	Left end	Right end	Middle
Polynomials				
Line	$\{-\infty,\infty\}$	$y \to \pm\infty$, constant slope	$y \to \pm\infty$, constant slope	monotonic
Quadratic	$\{-\infty,\infty\}$	$y \to \pm\infty$, accelerating	$y \to \pm\infty$, accelerating	single max/min
Cubic	$\{-\infty,\infty\}$	$y \to \pm\infty$, accelerating	$y \to \pm\infty$, accelerating	up to 2 max/min
Piecewise polynomials				
Threshold	$\{-\infty,\infty\}$	flat	flat	breakpoint
Hockey stick	$\{-\infty,\infty\}$	flat or linear	flat or linear	breakpoint
Piecewise linear	$\{-\infty,\infty\}$	linear	linear	breakpoint
Rational				
Hyperbolic	$\{0,\infty\}$	$y \to \infty$ or finite	$y \to 0$	decreasing
Michaelis-Menten	$\{0,\infty\}$	$y = 0$, linear	asymptote	saturating
Holling type III	$\{0,\infty\}$	$y = 0$, accelerating	asymptote	sigmoid
Holling type IV ($c < 0$)	$\{0,\infty\}$	$y = 0$, accelerating	asymptote	hump-shaped
Exponential-based				
Neg. exponential	$\{0,\infty\}$	y finite	$y \to 0$	decreasing
Monomolecular	$\{0,\infty\}$	$y = 0$, linear	$y \to 0$	saturating
Ricker	$\{0,\infty\}$	$y = 0$, linear	$y \to 0$	hump-shaped
logistic	$\{0,\infty\}$	y small, accelerating	asymptote	sigmoid
Power-based				
Power law	$\{0,\infty\}$	$y \to 0$ or $\to \infty$	$y \to 0$ or $\to \infty$	monotonic
von Bertalanffy	like logistic			
Gompertz	ditto			
Shepherd	like Ricker			
Hassell	ditto			
Non-rectangular hyperbola	like Michaelis-Menten			

Table 1: Qualitative properties of bestiary functions.

Examples

- linear: $f(x) = a + bx$, where a is the intercept (value when $x = 0$) and b is the slope. (You know this, right?)

- quadratic: $f(x) = a + bx + cx^2$. The simplest nonlinear model.

- cubics and higher-order polynomials: $f(x) = \sum_i^n a_i x_i$. The *order* or *degree* of a polynomial is the highest power that appears in it (so e.g. $f(x) = x^5 + 4x^2 + 1$ is 5th-order).

Advantages   Polynomials are easy to understand. They are easy to reduce to simpler functions (*nested* functions) by setting some of the parameters to zero. High-order polynomials can fit arbitrarily complex data.

Disadvantages   On the other hand, polynomials are often hard to justify mechanistically (can you think of a reason an ecological relationship should be a cubic polynomial?). They don't level off as x goes to $\pm\infty$ — they always go to $-\infty$ or ∞ as x gets large. Extrapolating polynomials often leads to nonsensically large or negative values. High-order polynomials can be unstable: following Forsythe et al. (1977) you can show that extrapolating a high-order polynomial from a fit to US census data from 1900–2000 predicts a population crash to zero around 2015!

It is sometimes convenient to parameterize polynomials differently. For example, we could reparameterize the quadratic function $y = a_1 + a_2 x + a_3 x^2$ as $y = a + c(x - b)^2$ (where $a_1 = a + cb^2$, $a_2 = 2cb$, $a_3 = c$). It's now clear that the curve has its minimum at $x = b$ (because $(x - b)^2$ is zero there and positive everywhere else), that $y = a$ at the minimum, and that c governs how fast the curve increases away from its minimum. Sometimes polynomials can be particularly simple if some of their coefficients are zero: $y = bx$ (a line through the origin, or *direct proportionality*, for example, or $y = cx^2$. Where a polynomial actually represents proportionality or area, rather than being an arbitrary fit to data, you can often simplify in this way.

The advantages and disadvantages listed above all concern the mathematical and phenomenological properties of polynomials. Sometimes linear and quadratic polynomials do actually make sense in ecological settings. For example, a population or resource that accumulates at a constant rate from outside the system will grow linearly with time. The rates of ecological or physiological processes (e.g. metabolic cost or resource availability) that depend on an organism's skin surface or mouth area will be a quadratic function of its size (e.g. snout-to-vent length or height).

5.1.1   Piecewise polynomial functions

You can make polynomials (and other functions) more flexible by using them as components of *piecewise* functions. In this case, different functions apply over

different ranges of the predictor variable. (See p. 32 for information on using R's `ifelse` function to build piecewise functions.)

Examples

- Threshold models: the simplest piecewise function is a simple threshold model — $y = a_1$ if x is less than some threshold T, and $y = a_2$ if x is greater. Hilborn and Mangel (1997) use a threshold function in an example of the number of eggs a parasitoid lays in a host as a function of how many she has left (her "egg complement"), although the original researchers used a logistic function instead (Rosenheim and Rosen, 1991).

- The *hockey stick* function (Bacon and Watts, 1971, 1974) is a combination of a constant and a linear piece: typically either flat and then increasing linearly, or linear and then suddenly hitting a plateau. Hockey-stick functions have a fairly long history in ecology, at least as far back as the definition of the Holling type I functional response, which is supposed to represent foragers like filter feeders that can continually increase their uptake rate until they suddenly hit a maximum. Hockey-stick models have recently become more popular in fisheries modeling, for modeling stock-recruitment curves (Barrowman and Myers, 2000), and in ecology, for detecting edges in landscapes (Toms and Lesperance, 2003)*. Under the name of *self-excitable threshold autoregressive* (SETAR) models, such functions have been used to model density-dependence in population dynamic models of lemmings (Framstad et al., 1997), feral sheep (Grenfell et al., 1998), and moose (Post et al., 2002); in another population dynamic context, Brännström and Sumpter (2005) call them *ramp* functions.

- Threshold functions are flat (i.e., the slope is zero) on both sides of the breakpoint, and hockey sticks are flat on one side. More general piecewise linear functions have non-zero slope on both sides of the breakpoint s_1:

$$y = a_1 + b_1 x$$

for $x < s_1$ and

$$y = (a_1 + b_1 s_1) + b_2(x - s_1)$$

for $x > s_1$. (The extra complications in the formula for $x > s_1$ ensure that the function is continuous.)

- *Cubic splines* are a general-purpose tool for fitting curves to data. They are *piecewise cubic* functions that join together smoothly at transition points called *knots*. They are typically used as purely phenomenological curve-fitting tools, when you want to fit a smooth curve to data but don't particularly care about interpreting its ecological meaning Wood (2001, 2006). Splines have many of the useful properties of polynomials

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*It is surely only a coincidence that so much significant work on hockey-stick functions has been done by Canadians.
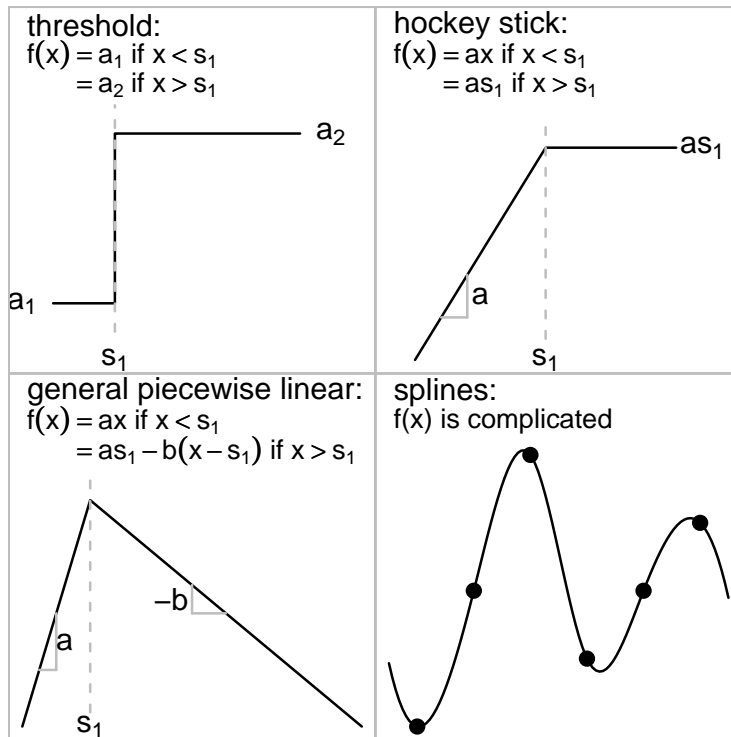
Figure 7: Piecewise polynomial functions: the first three (threshold, hockey stick, general piecewise linear) are all piecewise linear. Splines are piecewise cubic; the equations are complicated and usually handled by software (see `?spline` and `?smooth.spline`).

(adjustable complexity or smoothness; simple basic components) without their instability.

Advantages   Piecewise functions make sense if you believe there could be a biological switch point. For example, in optimal behavior problems theory often predicts sharp transitions among different behavioral strategies (Hilborn and Mangel, 1997, ch. 4). Organisms might decide to switch from growth to reproduction, or to migrate between locations, when they reach a certain size or when resource supply drops below a threshold. Phenomenologically, using piecewise functions is a simple way to stop functions from dropping below zero or increasing indefinitely when such behavior would be unrealistic.

Disadvantages   Piecewise functions present some special technical challenges for parameter fitting, which probably explains why they have only gained attention more recently. Using a piecewise function means that the rate of change
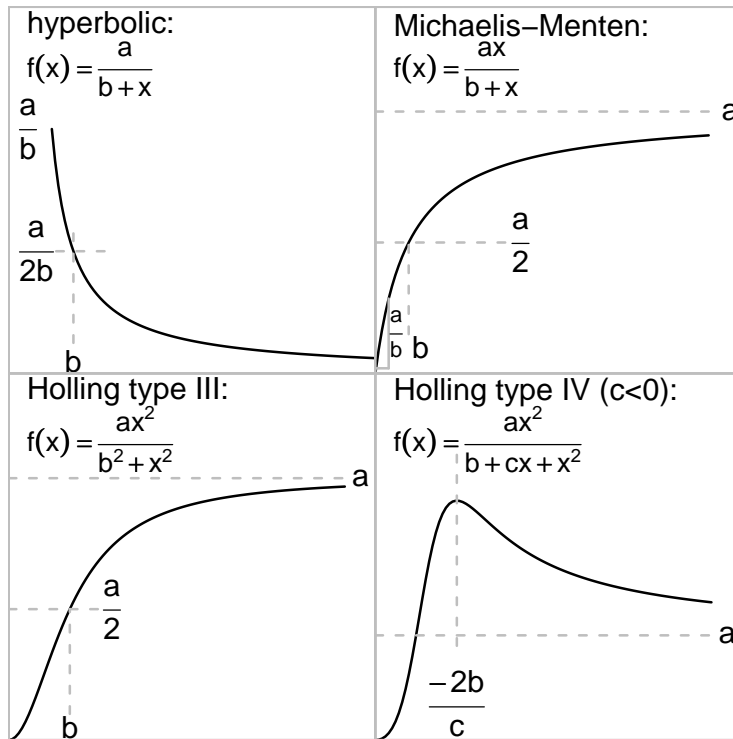
Figure 8: Rational functions.

(the derivative) changes suddenly at some point. Such a discontinuous change may make sense, for example, if the last prey refuge in a reef is filled, but transitions in ecological systems usually happen more smoothly. When thresholds are imposed phenomenologically to prevent unrealistic behavior, it may be better to go back to the original biological system and try to understand what properties of the system would actually stop (e.g.) population densities from becoming negative: would they hit zero suddenly, or would a gradual approach to zero (perhaps represented by an exponential function) be more realistic?

5.1.2 Rational functions: polynomials in fractions

Rational functions are ratios of polynomials, $(\sum a_i x^i)/(\sum b_j x^j)$.

Examples

- The simplest rational function is the *hyperbolic* function, a/x; this is often used (e.g.) in models of plant competition, to fit seed production as a function of plant density. A mechanistic explanation might be that if resources per unit area are constant, the area available to a plant for resource exploitation might be proportional to 1/density, which would

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translate (assuming uptake, allocation etc. all stay the same) into a hyperbolically decreasing amount of resource available for seed production. A better-behaved variant of the hyperbolic function is $a/(b + x)$, which doesn't go to infinity when $x = 0$ (Pacala and Silander, 1987, 1990).

- The next most complicated, and probably the most famous, rational function is the *Michaelis-Menten* function: $f(x) = ax/(b + x)$. Michaelis and Menten introduced it in the context of enzyme kinetics: it is also known, by other names, in resource competition theory (as the Monod function), predator-prey dynamics (Holling type II functional response), and fisheries biology (Beverton-Holt model). It starts at 0 when $x = 0$ and approaches an asymptote at a as x gets large. The only major caveat with this function is that it takes surprisingly long to approach its asymptote: $x/(1 + x)$, which is halfway to its asymptote when $x = 1$, still reaches 90% of its asymptote when $x = 9$. The Michaelis-Menten function can be parameterized in terms of any two of the asymptote, half-maximum, initial slope, or their inverses.

  The mechanism behind the Michaelis-Menten function in biochemistry and ecology (Holling type II) is similar; as substrate (or prey) become more common, enzymes (or predators) have to take a larger and larger fraction of their time handling rather than searching for new items. In fisheries, the Beverton-Holt stock-recruitment function comes from assuming that over the course of the season the mortality rate of young-of-the-year is a linear function of their density (Quinn and Deriso, 1999).

- We can go one more step, going from a linear to a quadratic function in the denominator, and define a function sometimes known as the *Holling type III* functional response: $f(x) = ax^2/(b^2 + x^2)$. This function is *sigmoid*, or S-shaped. The asymptote is at a; its shape is quadratic near the origin, starting from zero with slope zero and curvature a/b^2; and its half-maximum is at $x = b$. It can occur mechanistically in predator-prey systems because of predator switching from rare to common prey, predator aggregation, and spatial and other forms of heterogeneity (Morris, 1997).

- Some ecologists have extended this family still further to the *Holling type IV* functional response: $f(x) = ax^2/(b + cx + x^2)$. Turchin (2003) derives this function (which he calls a "mechanistic sigmoidal functional response") by assuming that the predator attack rate in the Holling type II functional response is itself an increasing, Michaelis-Menten function of prey density – that is, predators prefer to pursue more abundant prey. In this case, $c > 0$. If $c < 0$, then the Holling type IV function is *unimodal* or "hump-shaped", with a maximum at intermediate prey density. Ecologists have used this version of the Holling type IV phenomenologically to describe situations where predator interference or induced prey defenses lead to decreased predator success at high predator density (Holt, 1983; Collings, 1997; Wilmshust et al., 1999; Chen, 2004). Whether c is negative or posi-

tive, the Holling type IV reaches an asymptote at a as $x \to \infty$. If $c < 0$, then it has a maximum that occurs at $x = -2b/c$.

- More complicated rational functions are potentially useful but rarely used in ecology. The (unnamed) function $y = (a + bx)/(1 + cx)$ has been used to describe species-area curves (Flather, 1996; Tjørve, 2003).

Advantages Like polynomials, rational functions are very flexible (you can always add more terms in the numerator or denominator) and simple to compute; unlike polynomials, they can reach finite asymptotes at the ends of their range. In many cases, rational functions make mechanistic sense, arising naturally from simple models of biological processes such as competition or predation.

Disadvantages Rational functions can be complicated to analyze because the quotient rule makes their derivatives complicated. Like the Michaelis-Menten function they approach their asymptotes very slowly, which makes estimating the asymptote difficult — although this problem really says more about the difficulty of getting enough data rather than about the appropriateness of rational functions as models for ecological systems. Section 5.3 shows how to make rational functions even more flexible by raising some of their terms to a power, at the cost of making them even harder to analyze.

5.2 Functions based on exponential functions

5.2.1 Simple exponentials

The simplest examples of functions based on exponentials are the exponential growth (ae^{bx}) or decay (ae^{-bx}) and saturating exponential growth (*monomolecular*, $a(1-e^{-bx})$). The monomolecular function (so named because it represents the buildup over time of the product of a single-molecule chemical reaction) is also

- the *catalytic curve* in infectious disease epidemiology, where it represents the change over time in the fraction of a cohort that has been exposed to disease (Anderson and May, 1991);

- the simplest form of the *von Bertalanffy* growth curve in organismal biology and fisheries, where it arises from the competing effects of changes in catabolic and metabolic rates with changes in size (Essington et al., 2001);

- the *Skellam model* in population ecology, giving the number of offspring in the next year as a function of the adult population size this year when competition has a particularly simple form (Skellam, 1951; Brännström and Sumpter, 2005).

These functions have two parameters, the multiplier a which expresses the starting or final size depending on the function, and the exponential rate b or "e-folding time" $1/b$ (the time it takes to reach e times the initial value, or the
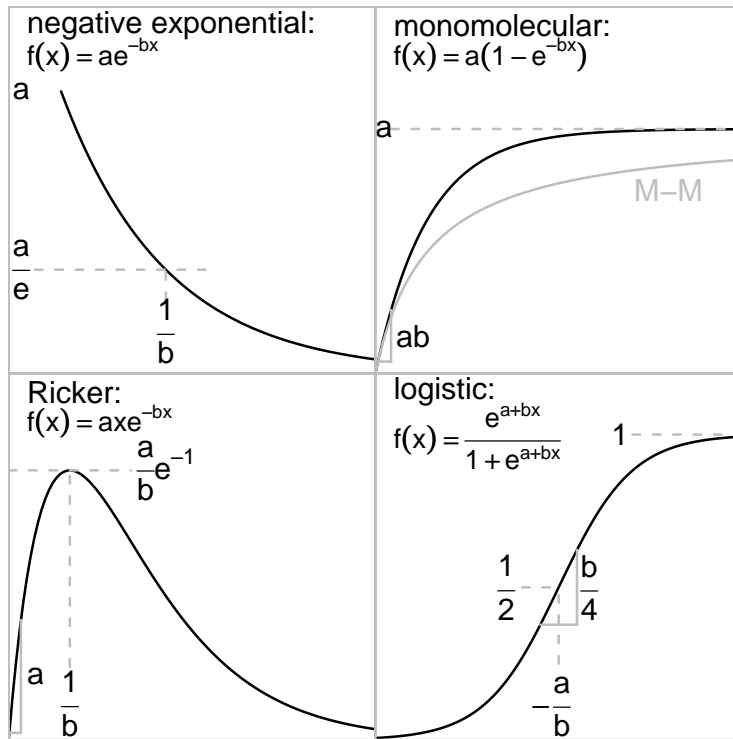
Figure 9: Exponential-based functions. "M-M" in the monomolecular figure is the Michaelis-Menten function with the same asymptote and initial slope.

initial value divided by e, depending whether b is positive or negative). The e-folding time can be expressed as a half-life or doubling time $(\ln(2)/b)$ as well. Such exponential functions arise naturally from any compounding process where the population loses or gains a constant proportion per unit time; one example is *Beers' Law* for the decrease in light availability with depth in a vegetation canopy (Teh, 2006).

The differences in shape between an exponential-based function and its rational-function analogue (e.g. the monomolecular curve and the Michaelis-Menten function) are usually subtle. Unless you have a lot of data you're unlikely to be able to distinguish from the data which fits better, and will instead have to choose on the basis of which one makes more sense mechanistically, or possibly which is more convenient to compute or analyze (Figure 9).

5.2.2 Combinations of exponentials with other functions

Ricker function The Ricker function, $ax \exp(-bx)$, is a common model for density-dependent population growth; if *per capita* fecundity decreases exponentially with density, then overall population growth will follow the Ricker

function. It starts off growing linearly with slope a and has its maximum at $x = 1/r$; it's similar in shape to the generalized Michaelis-Menten function $(RN/(1 + (aN)^b))$. It is used very widely as a phenomenological model for ecological variables that start at zero, increase to a peak, and decrease gradually back to zero.

Several authors (Hassell, 1975; Royama, 1992; Brännström and Sumpter, 2005) have derived Ricker equations for the dependence of offspring number on density, assuming that adults compete with each other to reduce fecundity; Quinn and Deriso (1999, p. 89) derive the Ricker equation in a fisheries context, assuming that young-of-year compete with each other and increase mortality (e.g. via cannibalism).

Logistic function   There are two widely used parameterizations of the logistic function. The first,

$$y = \frac{e^{a+bx}}{1 + e^{a+bx}} \tag{9}$$

(or equivalently $y = 1/(1 + e^{-(a+bx)})$) comes from a statistical or phenomenological framework. The function goes from 0 at $-\infty$ to 1 at $+\infty$. The location parameter a shifts the curve left or right: the half-maximum ($y = 0.5$), which is also the inflection point, occurs at $x = -a/b$ when the term in the exponent is 0. The scale parameter b controls the steepness of the curve*.

The second parameterization comes from population ecology:

$$n(t) = \frac{K}{1 + \left(\frac{K}{n_0} - 1\right) e^{-rt}} \tag{10}$$

where K is the carrying capacity, n_0 the value at $t = 0$, and r the initial *per capita* growth rate. (The statistical parameterization is less flexible, with only two parameters: it has $K = 1$, $n_0 = e^a/(1 + e^a)$, and $r = b$.)

The logistic is popular because it's a simple sigmoid function (although its rational analogue the Holling type III functional response is also simple) and because it's the solution to one of the simplest population-dynamic models, the *logistic equation*:

$$\frac{dn}{dt} = rn\left(1 - \frac{n}{K}\right), \tag{11}$$

which says that *per capita* growth rate ($(dn/dt)/n$) decreases linearly from a maximum of r when n is much less than K to zero when $n = K$. Getting from the logistic equation (11) to the logistic function (10) involves solving the differential equation by integrating by parts, which is tedious but straightforward (see any calculus book, e.g. Adler (2004)).

In R you can write out the logistic function yourself, using the `exp` function, as `exp(x)/(1+exp(x))`, or you can also use the `plogis` function. The *hyperbolic*

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*If we reparameterized the function as $\exp(b(x-c))/(1+\exp(b(x-c)))$, the half-maximum would be at c. Since b is still the steepness parameter, we could then shift and steepen the curve independently.

tangent (`tanh`) function is another form of the logistic. Its range extends from -1 as $x \to -\infty$ to 1 as $x \to \infty$ instead of from 0 to 1.

Gompertz function   The *Gompertz* function, $f(x) = e^{-ae^{-bx}}$, is an alternative to the logistic function. Similar to the logistic, it is accelerating at $x = 0$ and exponentially approaches 1 as x gets large, but it is asymmetric — the inflection point or change in curvature occurs $1/e \approx 1/3$ of the way up to the asymptote, rather than halfway up. In this parameterization the inflection point occurs at $x = 0$; you may want to shift the curve c units to the right by using $f(x) = e^{-ae^{b(x-c)}}$. If we derive the curves from models of organismal or population growth, the logistic assumes that growth decreases linearly with size or density while the Gompertz assumes that growth decreases exponentially.

5.3   Functions involving power laws

So far the polynomials involved in our rational functions have been simple linear or quadratic functions. Ecological modelers sometimes introduce an arbitrary (fractional) power as a parameter (x^b) instead of having all powers as fixed integer values (e.g. x, x^2 x^3); using power laws in this way is often a phenomenological way to vary the shape of a curve, although these functions can also be derived mechanistically.

Here are some categories of power-law functions.

- Simple power laws $f(x) = ax^b$ (for non-integer b; otherwise the function is just a polynomial: Figure 10a) often describe allometric growth (e.g. reproductive biomass as a function of diameter at breast height (Niklas, 1993), or mass as a function of tarsus length in birds); or quantities related to metabolic rates (Etienne et al., 2006); or properties of landscapes with fractal geometry (Halley et al., 2004); or species-area curves (Tjørve, 2003).

- The generalized form of the von Bertalanffy growth curve, $f(x) = a(1 - \exp(-k(a - d)t))^{1/(1-d)}$, (Figure 10b) allows for energy assimilation to change as a function of mass (assimilation = mass^d). The parameter d is often taken to be 2/3, assuming that energy assimilation is proportional to length^2 and mass is proportional to length^3 (Quinn and Deriso, 1999).

- A generalized form of the Michaelis-Menten function, $f(x) = ax/(b + x^c)$ (Figure 10c), describes ecological competition (Maynard-Smith and Slatkin, 1973; Brännström and Sumpter, 2005). This model reduces to the standard Michaelis-Menten curve when $c = 1$; $0 < c < 1$ corresponds to "contest" (undercompensating) competition, while $c > 1$ corresponds to "scramble" (overcompensating) competition (the function has an intermediate maximum for finite densities if $c > 1$). In fisheries, this model is called the *Shepherd function*. Quinn and Deriso (1999) show how the Shepherd function emerges as a generalization of the Beverton-Holt function

when the density-dependent mortality coefficient is related to the initial size of the cohort.

- A related function, $f(x) = ax/(b + x)^c$, is known in ecology as the *Hassell* competition function (Hassell, 1975; Brännström and Sumpter, 2005); it is similar to the Shepherd/Maynard-Smith/Slatkin model in allowing Michaelis-Menten ($c = 1$), undercompensating ($c < 1$) or overcompensating ($c > 1$) dynamics.

- Persson et al. (1998) used a generalized Ricker equation, $y = A(\frac{x}{x_0} \exp(1 - \frac{x}{x_0}))^\alpha$, to describe the dependence of attack rate y on predator body mass x (Figure 1 shows the same curve, but as a function of *prey* body mass). In fisheries, Ludwig and Walters proposed this function as a stock-recruitment curve (Quinn and Deriso, 1999). Bellows (1981) suggested a slightly different form of the generalized Ricker, $y = x \exp(r(1 - (a/x)^\alpha))$ (note the power is inside the exponent instead of outside), to model density-dependent population growth.

- Emlen (1996) used a generalized form of the logistic, $y = a + b/(1 + c \exp(-dx^e))$ extended both to allow a non-zero intercept (via the a parameter, discussed above under "Scaling and shifting") and also to allow more flexibility in the shape of the curve via the power exponent e.

- The *non-rectangular hyperbola* (Figure 10, lower right), based on first principles of plant physiology, describes the photosynthetic rate P as a function of light availability I:

$$P(I) = \frac{1}{2\theta} \left(\alpha I + p_{\max} - \sqrt{(\alpha I + p_{\max})^2 - 4\theta \alpha I p_{\max}} \right),$$

where α is photosynthetic efficiency (and initial slope); $p_{\max}$ is the maximum photosynthetic rate (asymptote); and θ is a sharpness parameter. In the limit as $\theta \to 0$, the function becomes a Michaelis-Menten function: in the limit as $\theta \to 1$, it becomes piecewise linear (a hockey stick: Thornley, 2002).

Advantages Functions incorporating power laws are flexible, especially since the power parameter is usually added to an existing model that already allows for changes in location, scale, and curvature. In many mechanistically derived power-law functions the value of the exponent comes from intrinsic geometric or allometric properties of the system and hence does not have to be estimated from data.

Disadvantages Many different mechanisms can lead to power-law behavior (Mitzenmacher, 2003). It can be tempting but is often misguided to reason backward from an observed pattern to infer something about the meaning of a particular estimated parameter.

power laws:
$f(x) = ax^b$
$0 < b < 1$
$b > 1$
$b < 0$

von Bertalanffy:
$f(x) = a(1 - e^{-k(a-d)x})^{(1/(1-d))}$
a

Shepherd, Hassell:
$f(x) = \dfrac{ax}{b + x^c}, f(x) = \dfrac{ax}{(b + x)^c}$
H
S
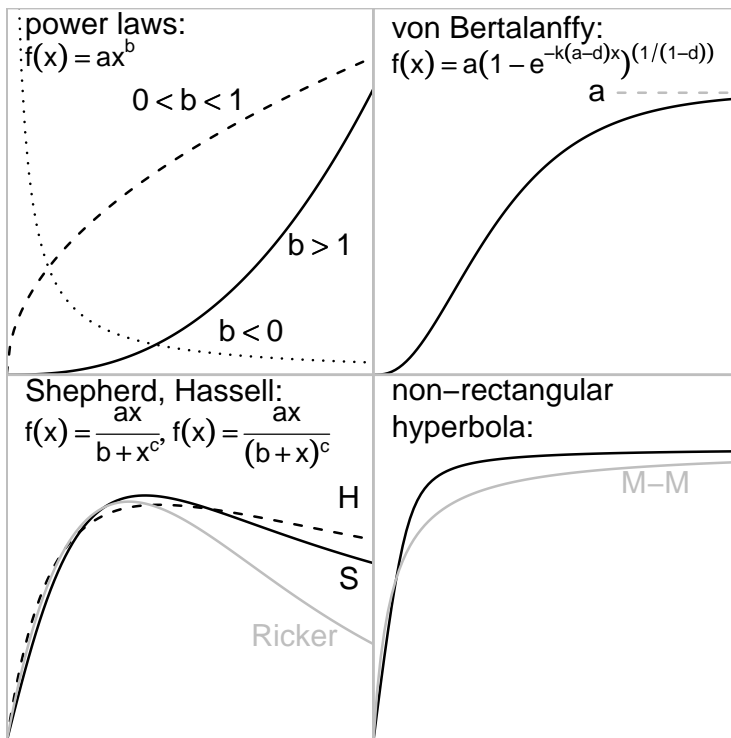Ricker

non–rectangular hyperbola:
M–M

Figure 10: Power-based functions. The lower left panel shows the Ricker function for comparison with the Shepherd and Hassell functions. The lower right shows the Michaelis-Menten function for comparison with the non-rectangular hyperbola.

Despite the apparent simplicity of the formulas, estimating exponents from data can be numerically challenging — leading to poorly constrained or unstable estimates. The exponent of the non-rectangular hyperbola, for example, is notoriously difficult to estimate from reasonable-size data sets (Thornley, 2002). (We will see another example when we try to fit the Shepherd model to data in Chapter 5.)

5.4   Other possibilities

Of course, there is no way I can enumerate all the functions used even within traditional population ecology, let alone fisheries, forestry, ecosystem, and physiological ecology. Haefner (1996, pp. 90-96) gives an alternative list of function types, focusing on functions used in physiological and ecosystem ecology, while Turchin (2003, Table 4.1, p. 81) presents a variety of predator functional response models. Some other occasionally useful categories are:

- *curves based on other simple mathematical functions*: for example, trigonometric functions like sines and cosines (useful for fitting diurnal or seasonal patterns), and functions based on logarithms.

- *generalized or "portmanteau" functions*: these are complex, highly flexible functions that reduce to various simpler functions for particular parameter values. For example, the four-parameter Richards growth model

$$y = \frac{k_1}{\left(1 + \left(\frac{k_1}{k_2} - 1\right) e^{-k_3 k_4 x}\right)^{1/k_4}} \tag{12}$$

includes the monomolecular, Gompertz, von Bertalanffy, and logistic equation as special cases (Haefner, 1996; Damgaard et al., 2002). Schnute (1981) defines a still more generalized growth model.

- *Functions not in closed form*: sometimes it's possible to define the dynamics of a population, but not to find an analytical formula (what mathematicians would call a "closed-form solution") that describes the resulting population density.

  - The *theta-logistic* or *generalized logistic* model (Nelder, 1961; Richards, 1959; Thomas et al., 1980; Sibly et al., 2005) generalizes the logistic equation by adding a power (θ) to the logistic growth equation given above (11):
    $$\frac{dn}{dt} = rn \left(1 - \left(\frac{n}{K}\right)^\theta\right). \tag{13}$$
    When $\theta = 1$ this equation reduces to the logistic equation, but when $\theta \neq 1$ there is no closed-form solution for $n(t)$ — i.e., no solution we can write down in mathematical notation. You can use the `odesolve` library in R to solve the differential equation numerically and get a value for a particular set of parameters.

- the *Rogers random-predator equation* (Rogers, 1972; Juliano, 1993) describes the numbers of prey eaten by predators, or the numbers of prey remaining after a certain amount of time in situations where the prey population becomes depleted. Like the theta-logistic, the Rogers equation has no closed-form solution, but it can be written in terms of a mathematical function called the *Lambert W function* (Corless et al., 1996). (See `?lambertW` in the `emdbook` package.)

6   Conclusion

The first part of this chapter has shown you (or reminded you of) some basic tools for understanding the mathematical functions used in ecological modeling — slopes, critical points, derivatives, and limits — and how to use them to figure out the basic properties of functions you come across in your work. The second part of the chapter briefly reviewed some common functions. You will certainly run across others, but the tools from the first part should help you figure out how they work.

7 R supplement

7.1 Plotting functions in various ways

Using `curve`:

Plot a Michaelis-Menten curve:

```
> curve(2 * x/(1 + x))
```

You do need to specify the parameters: if you haven't defined `a` and `b` previously `curve(a*x/(b+x))` will give you an error. But if you're going to use a function a lot it can be helpful to define a function:

```
> micmen <- function(x, a = 2, b = 1) {
+     a * x/(b + x)
+ }
```

Now plot several curves (being more specific about the desired x and y ranges; changing colors; and adding a horizontal line (`abline(h=...)`) to show the asymptote).

```
> curve(micmen(x), from = 0, to = 8, ylim = c(0, 10))
> curve(micmen(x, b = 3), add = TRUE, col = 2)
> curve(micmen(x, a = 8), add = TRUE, col = 3)
> abline(h = 8)
```

Sometimes you may want to do things more manually. Use `seq` to define x values:

```
> xvec <- seq(0, 10, by = 0.1)
```

Then use vectorization (`yvec=micmen(xvec)`) or `sapply` (`yvec=sapply(xvec,micmen)`) or a `for` loop (`for i in (1:length(xvec)) { yvec[i]=micmen(xvec[i])}`) to calculate the y values. Use `plot(xvec,yvec,...)`, `lines(xvec,yvec,...)`, etc. (with options you learned Chapter 2) to produce the graphics.

7.2 Piecewise functions using `ifelse`

The `ifelse` function picks one of two numbers (or values from one of two vectors) depending on a logical condition. For example, a simple threshold function:

```
> curve(ifelse(x < 5, 1, 2), from = 0, to = 10)
```

or a piecewise linear function:

```
> curve(ifelse(x < 5, 1 + x, 6 - 3 * (x - 5)), from = 0,
+     to = 10)
```

You can also nest `ifelse` functions to get more than one switching point:

```
> curve(ifelse(x < 5, 1 + x, ifelse(x < 8, 6 - 3 *
+     (x - 5), -3 + 2 * (x - 8))), from = 0, to = 10)
```

7.3 Derivatives

You can use D or `deriv` to calculate derivatives (although R will not simplify the results at all): D gives you a relatively simple answer, while `deriv` gives you a function that will compute the function and its derivative for specified values of x (you need to use `attr(...,"grad")` to retrieve the derivative — see below). To use either of these functions, you need to use `expression` to stop R from trying to interpret the formula.

```
> D(expression(log(x)), "x")

1/x

> D(expression(x^2), "x")

2 * x

> logist <- expression(exp(x)/(1 + exp(x)))
> dfun <- deriv(logist, "x", function.arg = TRUE)
> xvec <- seq(-4, 4, length = 40)
> y <- dfun(xvec)
> plot(xvec, y)
> lines(xvec, attr(y, "grad"))
```

Use `eval` to fill in parameter values:

```
> d1 <- D(expression(a * x/(b + x)), "x")
> d1

a/(b + x) - a * x/(b + x)^2

> eval(d1, list(a = 2, b = 1, x = 3))

[1] 0.125
```

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