Sketching functions with free parameters

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This is a tutorial for learning to sketch non-linear functions with free parameters, and we will focus on the type of functions one typically encounters in biological modeling. First note that working with free parameters instead of numbers mathematically makes no difference because the same rules apply, e.g.,

$$a + b + c = (a + b) + c = a + (b + c) \ , \quad a(b + c) = ab + bc \ , \quad \text{and}$$

$$\frac{a}{b} + \frac{c}{d} = \frac{ad}{bd} + \frac{bc}{bd} = \frac{ad + cb}{bd} \ , \quad \frac{a}{b} \times \frac{c}{d} = \frac{ac}{bd} \quad \text{and} \quad \frac{a}{b} : \frac{c}{d} = \frac{a}{b} \times \frac{d}{c} = \frac{ad}{bc} \ ,$$

with the only difference that one should not divide by zero (just fill in integer numbers for a, b, c and d to check these expressions).

Second, sketching linear functions like $y = a + bx$ is straightforward because one basically fills in $x = 0$ to find that a is the intercept with the vertical y-axis, solving $0 = a + bx$ gives that $x = -a/b$ is the intercept with the horizontal x-axis, and finally one draws a straight line (with slope a) through these points. Sketching non-linear functions like $y = a + bx + cx^2$ or $y = \frac{ax}{b+x}$ is more difficult as these may have asymptotes, minima, maxima, and inflection points. The general approach is to find:
1. intersections with the horizontal and vertical axis (like one does for linear functions),
2. to check for horizontal and vertical asymptotes,
3. to check for minima and maxima, i.e., x-values where the derivative, y', equals zero, and
4. to finally consider special points and the slope of the function in these points.

One can sketch any function using the function `plot` in WolframAlpha or the function `curve()` in R, but this can only be done for numerical examples, i.e., one has to fill in arbitrary values for the free parameters. Since the shape of the function may depend on these values, numerical examples need not be general. Therefore, we here provide a general procedure for sketching non-linear functions with free parameters.

1 Quadratic functions

For instance, lets us consider the general quadratic function,

$$y = f(x) = ax^2 + bx + c \ ,$$

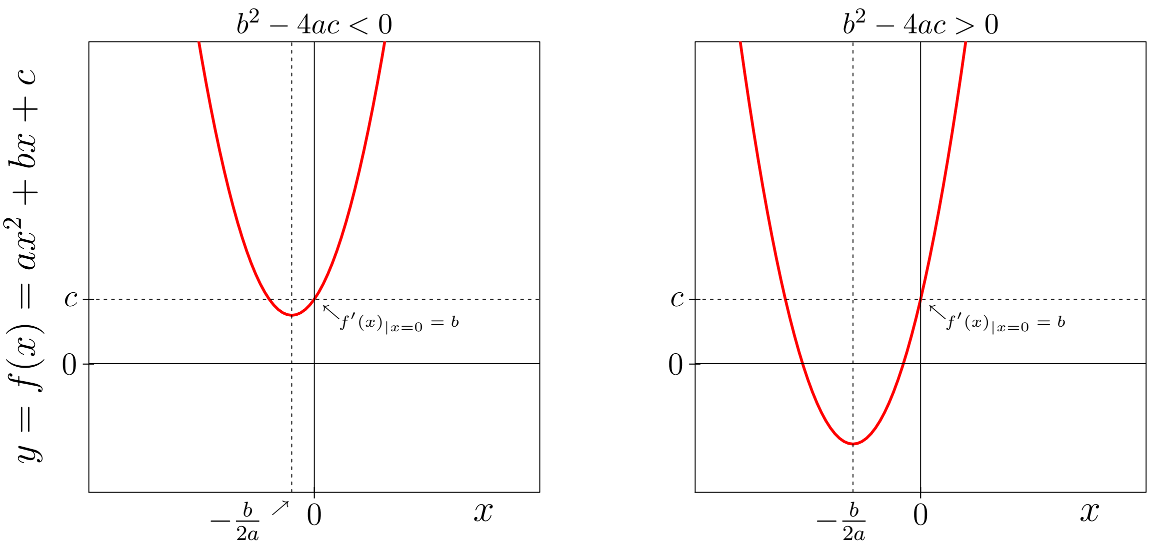
where $f(x)$ is a function, a, b and c are parameters, and x and y are variables. Our aim is to sketch $f(x)$ as a function of x for all values of x, and for positive values of the parameters. Let us agree that we explicitly write the sign of our parameters when defining a function. Because a is positive, you will probably see that this is a parabola opening upwards. Now, consider our general approach:

1. For the intersection with the axes
   a. One substitutes $x = 0$ to find that $y = c$ is the intercept with the vertical y-axis. This makes sense because the curve $y = ax^2 + bx$ is shifted upwards over a distance c.

b. One solves $y = 0 = ax^2 + bx + c$ to find that $x_{\pm} = \frac{-b \pm \sqrt{b^2-4ac}}{2a}$ form two intercepts with the horizontal x-axis (which are only present when the Discriminant $b^2 - 4ac > 0$). Since $\sqrt{b^2 - 4ac} < b$, both intercepts, $x_{\pm}$, will be less than zero, and they are located at the same distance $\frac{\sqrt{b^2-4ac}}{2a}$ from their midpoint $x = -\frac{b}{2a}$.

2. For the asymptotes we observe that:
   a. $f(x) \to \infty$ when $x \to \infty$ and when $x \to -\infty$, meaning that there are no horizontal asymptotes,
   b. This not a rational function, i.e., none of the x-values would lead to a division by zero, and hence there are no vertical asymptotes.
3. The derivative of $f(x)$ is $f'(x) = 2ax + b$ which will be zero when $x = -\frac{b}{2a}$. Since the slope $f'(x)$ is negative when $x < -\frac{b}{2a}$ and positive when $x > -\frac{b}{2a}$, this extreme point corresponds to the minimum of the parabola.
4. For special points
   a. One could substitute $x = \frac{-b}{2a}$ into $y = ax^2 + bx + c$ to find the y-value of the minimum $y = c - \frac{b^2}{4a}$.
   b. One could substitute $x = 0$ into $f'(x) = 2ax + b$ to find that b is the slope of the line in the y-intercept.

This allows us the sketch the following pictures,



where the exact shape and location indeed depends on the parameter values.

We can generalize this analysis somewhat because $f(x) = ax^2 + bx - c$ will just be shifted in the vertical direction, and have $y = -c$ as the intercept with the vertical axis. The function $f(x) = ax^2 - bx + c$ will be the mirror image of the figure sketched above, with the minimum located at $x = \frac{b}{2a}$, and the function $f(x) = -ax^2 + bx + c$ will be a parabola opening downwards (see the exercises).

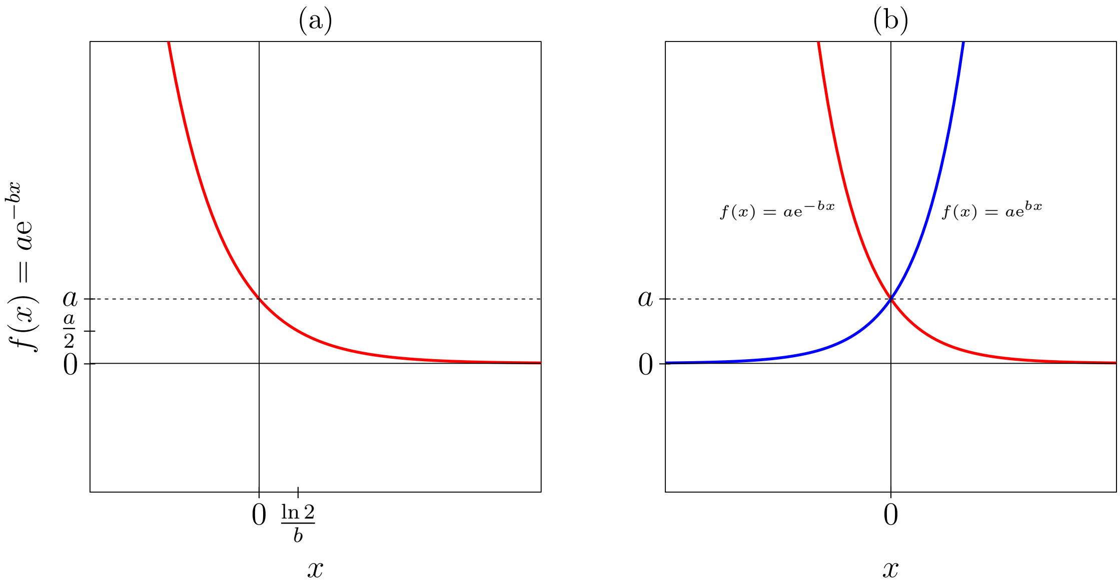
Finally, to sketch a function like $y = a\sqrt{x}$, one could start by squaring both sides, $y^2 = a^2 x$, and interchange x and y to define $x^2 = a^2 y$ or $y = bx^2$ where b is a new arbitrary constant. Thus the shape of $y = a\sqrt{x}$ can be inferred by rotating the parabola, $y = bx^2$, while noting that the function is only defined for $x \geq 0$. Following our procedure we indeed see that the origin (0,0) is the one and only intercept with the axes, that there are no asymptotes, and that the derivative $f'(x) = \frac{a}{2\sqrt{x}}$ is always positive, i.e., the function always increases with an ever decreasing slope. In the origin the derivative approaches infinity, i.e., the slope approaches the vertical y-axis, and in the special point $x = 1$ one obtains $y = a$ and a slope $f'(x) = a/2$.

2 Exponential functions

Next, consider the classical declining exponential function $y = f(x) = a\mathrm{e}^{-bx}$. According to our general procedure:

1. For the intersection with the axes
   a. One substitutes $x = 0$ to find that $y = a$ is the intercept with the vertical y-axis.
   b. Since $0 = a\mathrm{e}^{-bx}$ has no solutions there is no intercept with the horizontal x-axis.
2. For the potential asymptotes we observe that
   a. when $x \to \infty$ the function $f(x)$ approaches zero, meaning that the horizontal axis is an asymptote. When $x \to -\infty$ the function approaches infinity.
   b. none of the x-values would lead to a division by zero, and hence there is no vertical asymptote.
3. The derivative is $-ab\mathrm{e}^{-bx}$ which is negative and never zero.
4. For the other special points, we could solve that $f(x) = \frac{a}{2}$ when $x = \frac{\ln 2}{b}$.

This allows us the sketch the following two pictures:



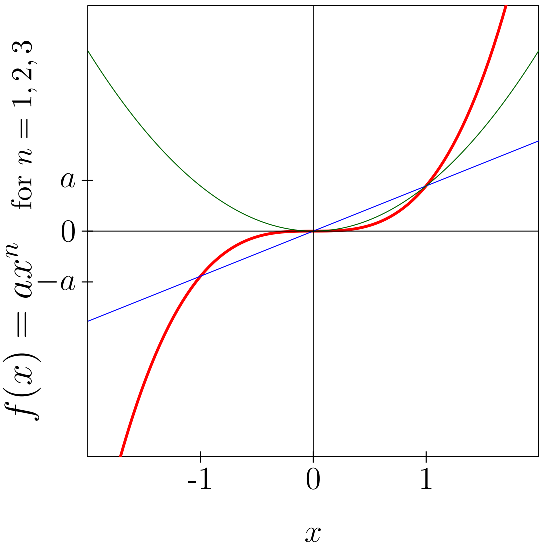
where we plot $f(x) = a\mathrm{e}^{-bx}$ in Panel (a), and add on $f(x) = a\mathrm{e}^{bx}$ in blue in Panel (b) by just inverting the horizontal axis.

3 Third order functions

Polynomial functions of the form $y = ax^3 + bx^2 + cx + d$ are typically hard to sketch because one has to solve third order functions. Sometime they are written in a simpler form, $y =$

$(x-a)(x-b)(x-c)d$, which conveniently reveals that $y = 0$ when $x = a, b$ or c.

To get an idea we could start with considering $y = ax^3$. Following our procedure we see that the origin (0,0) is the one and only intercept with the axes, that there are no asymptotes, and that the derivative $f'(x) = 3ax^2$ is always positive, i.e., the function always increases. In the origin the derivative is zero, i.e., the slope approaches the horizontal x-axis. In the special point $x = 1$ one obtains $y = a$ and a slope $f'(x) = 3a$, and when $x = -1$ one obtains $y = -a$ and the same slope $f'(x) = 3a$. This allows us the sketch the following picture:



where we have added $y = ax^2$ (green) and $y = ax$ (blue) for comparison.

Returning to the full third order polynomial written as $y = f(x) = (x-a)(x-b)(x-c)d$, we first note that d just scales the amplitude of the function (i.e., the y-axis), and that since a, b and c are free, we can place them in an arbitrary order and consider the special case where $a < b < c$ without loss of generality (note that we agreed that all parameters are positive, here we add on that they are not identical).

1. For the intersection with the axes
   a. One substitutes $x = 0$ to find that $y = -abcd$ is the intercept with the vertical y-axis.
   b. Solving $y = 0$ one immediately sees that $x = a$, $x = b$ and $x = c$ form three intercepts with the horizontal x-axis.
2. For the potential asymptotes:
   a. We first study what happens when $x \to \infty$. Since for large values of x the function simplifies to $y \simeq dx^3$ (because $x - e \to x$ when $x \to \infty$), there is no horizontal asymptote, and we observe that $f(x) \to \infty$ when $x \to \infty$. This also implies that $f(x) > 0$ when $x > c$. Likewise when $x \to -\infty$ the function $f(x) \to -\infty$, implying that there is no horizontal asymptote, and that $f(x) < 0$ when $x < a$. Note that because the function approaches $f(x) \simeq dx^3$ for large and small values of x, it is also not approaching another linear asymptote, $\alpha x + \beta$ (i.e., a slant asymptote; see below).
   b. Second, since this not a rational function, i.e., none of the x-values would lead to a division by zero, we conclude that there is no vertical asymptote.
3. Using the product rule one sees that the derivative,

$$f'(x) = [(x-a)(x-b) + (x-a)(x-c) + (x-b)(x-c)]d \ ,$$

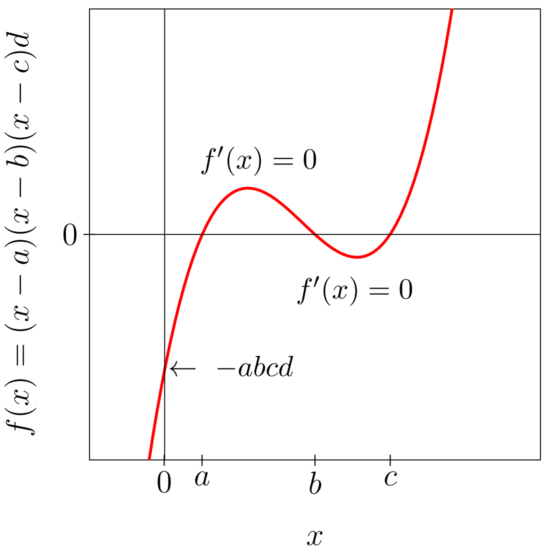
is a quadratic equation that will be zero when

$$x_\pm = \frac{1}{3}\left(a+b+c \pm \sqrt{a^2+b^2+c^2-ab-ac-bc}\right) ,$$

which are both positive (because $(a+b+c)^2 > a^2+b^2+c^2-ab-ac-bc$). Thus, we find a minimum or maximum for two positive values of x.

4. Remembering that $a < b < c$, we observe for the other special points:
   a. $x = a$ that $f'(x) = (a-b)(a-c)d > 0$, i.e., the slope of $f(a)$ is positive.
   b. $x = b$ that $f'(x) = (b-a)(b-c)d < 0$, i.e., the slope of $f(b)$ is negative.
   c. $x = c$ that $f'(x) = (c-a)(c-b)d > 0$, i.e., the slope of $f(c)$ is positive.

This allows us the sketch the following picture:



4 Rational functions

In biology we often use saturation functions having a horizontal asymptote to define a maximum effect. For instance consider

$$y = f(x) = \frac{ax^n}{b^n + x^n} ,$$

where n is a positive integer ($n = 1, 2, 3, \ldots$). It may seems strange to define an arbitrary constant as b^n, but we will see this helps to sketch the function for several values of n. We again see that a just scales the amplitude of the function:

1. For the intersection with the axes
   a. One substitutes $x = 0$ into $f(x)$, i.e., $y = \frac{a \cdot 0}{b^n+0} = 0$, to find that $y = 0$ is the intercept with the vertical y-axis.
   b. Solving $y = 0 = \frac{ax^n}{b^n+x^n}$ one finds that $x = 0$ is the only intercept with the horizontal x-axis.

   Thus, we find the origin (0,0) as the only intersection with the two axes (independent of the value of n).
2. For the potential asymptotes

a. We first rewrite the function by dividing the numerator and denominator by the highest power of x. Dividing numerator and denominator by x^n we obtain $f(x) = \frac{a}{(b/x)^n+1}$. Next we send $x \to \infty$ to observe that $y \to a$, and when we send $x \to -\infty$ we see that y again approaches a. Thus we find a single horizontal asymptote $y = a$, independent of the value of n.

b. To find vertical asymptotes we solve $b^n + x^n = 0$ and find that $x = -b$ will be a vertical asymptote when n is an odd number (there is no vertical asymptote when n is even). When n is an odd number and x approaches $-b$ from above, i.e., when $x \downarrow -b$, the numerator $(ax^n)_{|x=-b}$ will be negative and the denominator $(b^5 + x^n)_{|x\downarrow -b}$ will be positive, implying that $y \to -\infty$. When x approaches $-b$ from below, i.e., when $x \uparrow -b$, both the numerator and the denominator will be negative, implying that $y \to \infty$. Thus, when $n = 1, 3, \ldots$ there is a vertical asymptote at $x = -b$ with $f(x)$ approaching ∞ at its left side and $-\infty$ at its right side.

3. For the derivative, we need to remember the quotient rule of differentiation, i.e.,

$$f(x) = \frac{T}{N} \qquad \to \qquad f'(x) = \frac{T'}{N} - \frac{TN'}{N^2} = \frac{NT' - TN'}{N^2} \; .$$

- Let us first apply this to our function $f(x)$ for $n = 1$, i.e., for $f(x) = \frac{ax}{b+x}$:

$$f'(x) = \frac{a}{b+x} - \frac{ax}{(b+x)^2} \; ,$$

which readily reveals that the slope in the origin is $f'(x)_{|x=0} = \frac{a}{b}$. To test for extrema we have to solve $f'(x) = 0$, i.e.,

$$\frac{a}{b+x} = \frac{ax}{(b+x)^2} \qquad \leftrightarrow \qquad 1 = \frac{x}{b+x} \; ,$$

which has no solutions for $b \neq 0$. Thus, for $n = 1$ there are no extreme points and we obtain the hyperbolic function sketched below.

- Next consider $n = 2$, i.e., $f(x) = \frac{ax^2}{b^2+x^2}$, and compute the derivative

$$f'(x) = \frac{2ax}{b^2+x^2} - \frac{ax^2 \cdot 2x}{(b^2+x^2)^2} \; ,$$

which readily delivers that the slope in the origin is zero, i.e., $f'(x)_{|x=0} = 0$. To test if there are any additional extrema we divide by x and solve $f'(x)/x = 0$:

$$\frac{2a}{b^2+x^2} = \frac{2ax^2}{(b^2+x^2)^2} \qquad \leftrightarrow \qquad 1 = \frac{x^2}{b^2+x^2} \; ,$$

which has no solutions for $b \neq 0$. Thus, for $n = 2$ the origin is the only extreme point. Close to the origin $f'(x) \simeq \frac{2ax}{b^2}$ which is negative when $x < 0$ and positive when $x > 0$. The origin is therefore a minimum, giving us enough information to sketch the sigmoid function depicted below.

- Next consider $n = 3$ and compute the derivative

$$f'(x) = \frac{3ax^2}{b^3+x^3} - \frac{ax^3 \cdot 3x^2}{(b^3+x^3)^2} \; ,$$

which again reveals that the slope in the origin is zero, i.e., $f'(x)_{|x=0} = 0$. To test if there are any other extrema we solve $f'(x)/x = 0$:

$$\frac{3ax}{b^3+x^3} = \frac{3ax^4}{(b^3+x^3)^2} \qquad \leftrightarrow \qquad 1 = \frac{x^3}{b^3+x^3} \; ,$$

which again has no solutions for $b > 0$. Thus, also for $n = 3$ the origin is the only extreme point. Close to the origin $f'(x) \simeq \frac{3ax^2}{b^3}$ which is always positive. The origin is therefore an inflection point, giving us enough information to sketch the function depicted below. Note that around the origin this function is similar to the $y = ax^3$ sketched above, which is natural because $f(x) = \frac{ax^3}{b^3+x^3} \simeq \frac{ax^3}{b^3}$ when $x \to 0$.

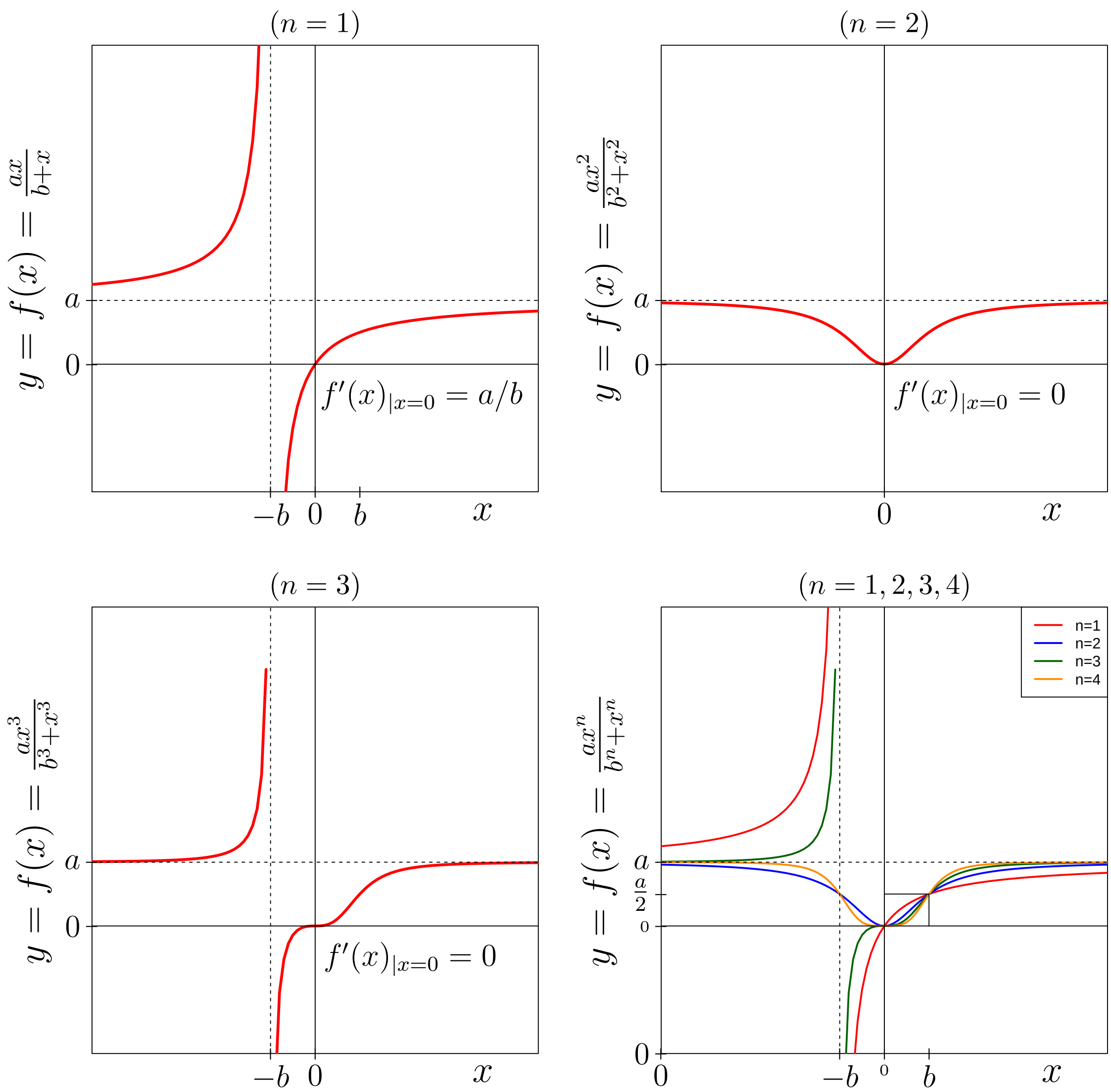
- Finally, we could have used the general form, $f(x) = \frac{ax^n}{b^n+x^n}$, and have written

$$f'(x) = \frac{anx^{n-1}(b^n + x^n)}{(b^n + x^n)^2} - \frac{ax^n nx^{n-1}}{(b^n + x^n)^2} = \frac{ab^n nx^{n-1} + anx^{2n-1} - anx^{2n-1}}{(b^n + x^n)^2} = \frac{ab^n nx^{n-1}}{(b^n + x^n)^2},$$

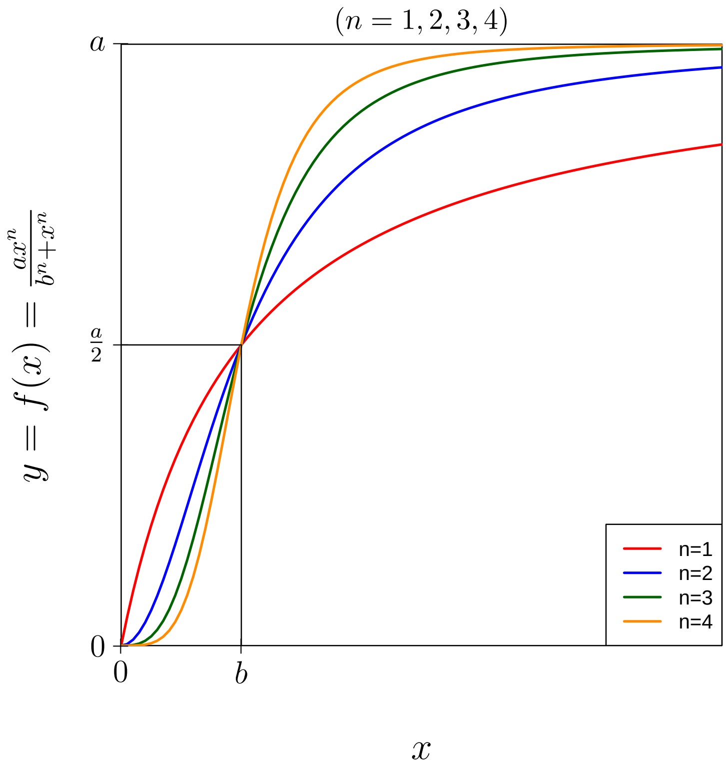
and obtain the same results as above.

4. For the other special points we see that $x = b$ is an interesting point because $y = \frac{ab^n}{b^n+b^n} = a/2$. Thus, at $x = b$ the y-values is half way the horizontal asymptote $y = a$, which is independent of n. Finally, the slope in the special point, $f'(x)_{|x=b} = \frac{an}{4b}$, which reveals that n determines the steepness of $f(x)$.

This allows us the sketch the following picture for $n = 1, 2, 3$ and $n = 4$:



Since, this function forms a convenient family of graphs in the positive quadrant that approach a maximum value a at high values of x, are half-maximal at $x = b$, are sigmoid when $n > 1$, and become steeper when n becomes larger, it is often used for modeling saturation effects in biology (where it is known as a Hill function). Indeed, plotting the function in its positive domain gives the classical family of saturation functions:



5 Slant asymptotes

Instead of approaching a horizontal asymptote, some functions $f(x)$ approach a straight line with a non-zero slope for large and/or small values of x. These are called slant asymptotes, and such an asymptote would be defined as a line, $y = \alpha x + \beta$, where α is this slope and β is the intersect with the vertical axis. Thus, slant asymptotes arise when a function, $f(x)$, approaches a slope α for large values of x. For example the function $f(x) = (a + x)(b + c/x)$ will approach $f(x) \simeq bx$ when x is sufficiently large, because $a + x \simeq x$ and $b + c/x \simeq b$ when x is much larger than a and c.

The general procedure for finding slant asymptotes is to first check if $f(x)$ approaches a line with a slope α for large positive and/or small negative values of x. This is done by taking the limit of $f(x)/x$ for $x \to \infty$ and $x \to -\infty$. For example,

$$\frac{(a + x)(b + c/x)}{x} = \left(\frac{a}{x} + 1\right)\left(b + \frac{c}{x}\right)$$

approaches b when $x \to \infty$, and when $x \to -\infty$, which identifies the presence of a slant asymptote with a slope $\alpha = b$. This also implies that the function does not have any horizontal asymptotes. To find the intercept, β, we use the definition of the asymptote, $y = \alpha x + \beta$, and write

$$\lim_{x\to\infty} [f(x) - (\alpha x + \beta)] = 0 \quad \leftrightarrow \beta = \lim_{x\to\infty} [f(x) - \alpha x] \ ,$$

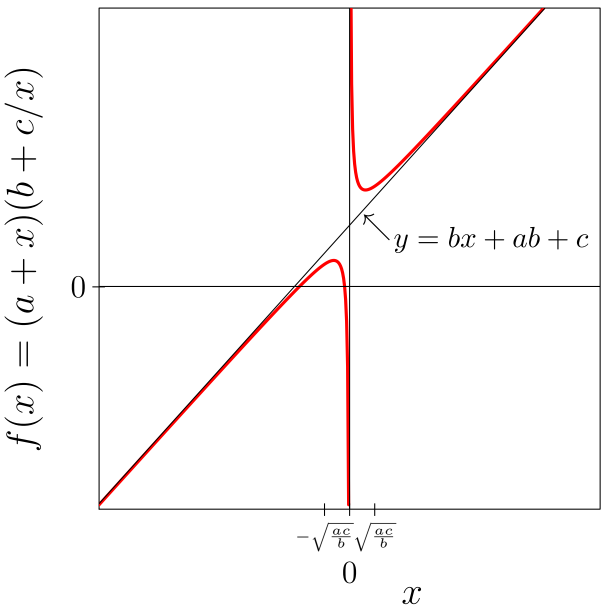
which for our example corresponds to

$$\beta = \lim_{x\to\infty} [(a+x)(b+c/x) - bx] = \lim_{x\to\infty} \left[ab + \frac{ac}{x} + bx + c - bx\right] = ab + c \ ,$$

revealing that the function approaches the line $y = bx + ab + c$ when $x \to \infty$ and $x \to -\infty$.

To sketch the function $f(x) = (a + x)(b + c/x)$ we next follow our general procedure:
1. The intersections with the axes:
   a. Substituting $x = 0$ leads to division by zero, i.e., a vertical asymptote at $x = 0$.
   b. Solving $f(x) = 0$ leads to two intersections with the horizontal axis at $x = -a$ and $x = -c/b$.
2. For the asymptotes:
   a. There is a slant asymptote $y = bx + ab + c$.
   b. There is a vertical asymptote at $x = 0$. When $x \downarrow 0$ the function approaches ∞, and when $x \uparrow 0$ the function approaches $-\infty$.
3. Using the product rule, the derivative is $f'(x) = b + \frac{c}{x} - (a+x)\frac{c}{x^2}$, and we solve $f'(x) = 0$ by first multiplying with x^2, i.e., $0 = bx^2 + cx - c(a+x) = bx^2 - ac$, giving $x_\pm = \pm\sqrt{\frac{ac}{b}}$. Thus, the function $f(x)$ has slope zero at a distance $\sqrt{\frac{ac}{b}}$ left and right from the origin. Since in the positive quadrant $f(x) \to \infty$ at $x = 0$ and $f(x) \to bx + ab + c$ when $x \to \infty$, the x_+ solution is a minimum of $f(x)$. Because for negative values of x the function $f(x) \to -\infty$ at $x = 0$ and $f(x) \to bx + ab + c$ when $x \to \infty$, the x_- solution is a maximum of $f(x)$.

This allows us to sketch the following:



The function $f(x) = (a+x)(b+c/x)$ in red, with its slant asymptote $y = bx+ab+c$ in black.

6 Optimum functions

In biology we often need functions that exert their maximum affect at some intermediate value of x. Convenient optimum functions arise when increasing and decreasing Hill functions (each representing a particular biological process) are multiplied with each other. For instance, consider $y = f(x) = \frac{ax}{b+x}\,\frac{c}{c+x}$ for positive values of x.

Following our general approach:

1. We find for the intersection with the axes that $x = 0$ gives $y = 0$ and that $y = 0$ can only occur when $x = 0$. The origin is therefore the one and only intercept with the axes.
2. For the asymptotes we observe:
   a. That rewriting $f(x)$ into $y = \frac{a}{b/x+1}\,\frac{c}{c+x}$ reveals that $x \to \infty$ leads to $y \to 0$. The horizontal axis therefore corresponds to the one and only horizontal asymptote (in the positive domain).
   b. That $x = -b$ and $x = -c$ define vertical asymptotes that appear in the negative domain only.
3. The derivative of $f(x) = \frac{ax}{b+x}\,\frac{c}{c+x} = \frac{acx}{(b+x)(c+x)}$ can be written as

$$f'(x) = \frac{ac(b+x)(c+x)}{(b+x)^2(c+x)^2} - \frac{acx(2x+b+c)}{(b+x)^2(c+x)^2} \;.$$

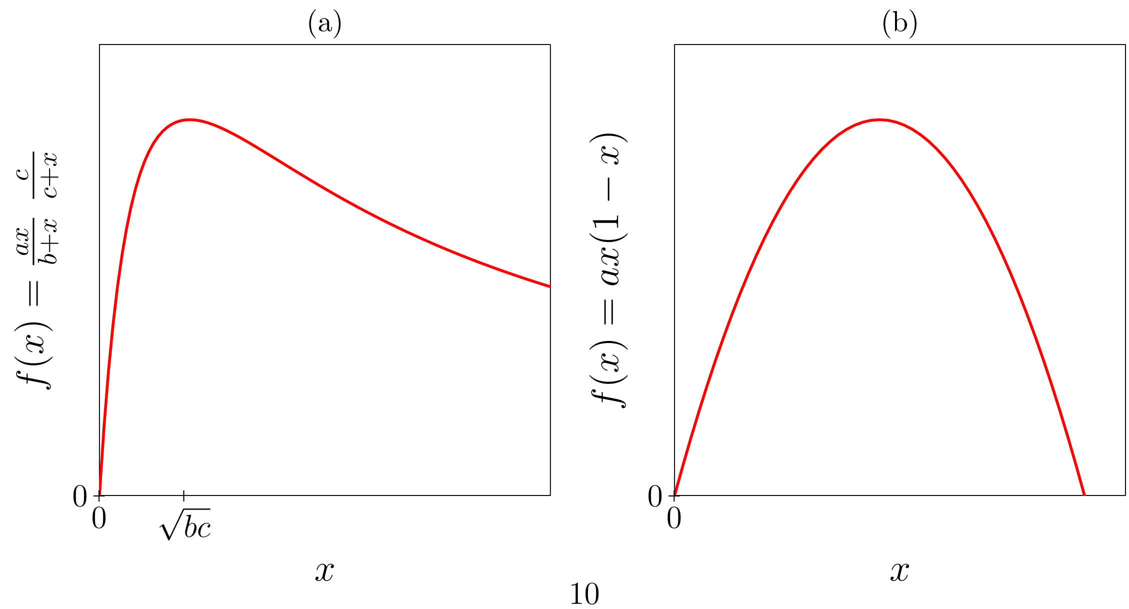
   For $x = 0$ this delivers $f'(x) = \frac{a}{b}$ which is positive, while for large x the positive term and the negative term go to zero. For solving $f'(x) = 0$ we consider the two numerators of the second expression, i.e.,

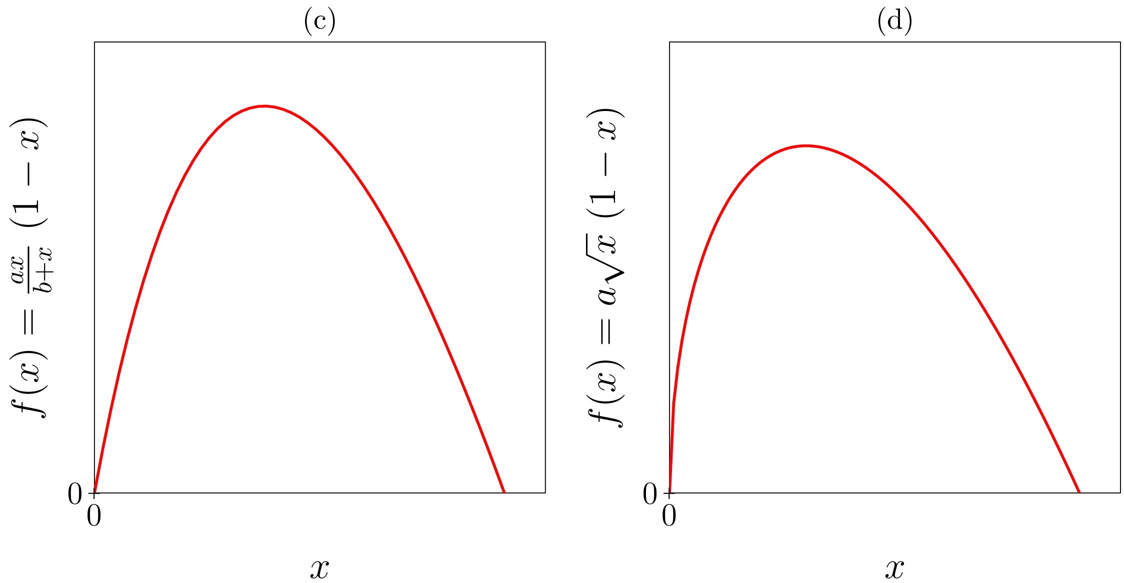
$$ac(b+x)(c+x) = acx(2x+b+c) \leftrightarrow x^2 + bx + cx + bc = 2x^2 + bx + cx \leftrightarrow bc = x^2 \;,$$

   to find that $x = \pm\sqrt{bc}$. Considering the positive root only, we see that when $x < \sqrt{bc}$ the first term is larger than the second term, implying that $f'(x) > 0$. When $x > \sqrt{bc}$ this is the other way around, and we find that $f'(x) < 0$. Hence, $x = \sqrt{bc}$ corresponds to a maximum, which is located in between $x = b$ and $x = c$ (or at $x = b = c$ when $b = c$).
4. For the special points we note that a just scales the amplitude of the function, and that the function value at the maximum remains a complicated expression of all parameters.

Note that this function has a maximum for all (positive) values of a, b, and c.

This allows us to sketch the graph in Panel (a). The three other panels provide other simple examples of functions with an optimum.





Several simple functions with a maximum.

7 Exercises

Sketch $y = -a^2 + bx + c$.

Sketch $y = a\mathrm{e}^{-bx^2}$.

Sketch $y = \frac{a}{1+(x/b)^n}$ for $n = 1$ and $n = 2$.

Determine the maxima in Panels (b) to (d) in the last figure.