CHEM1033 - Week 9 Lecture - Analysis of univariate functions

Chapter 21 of Monk and Munro, "Maths for Chemistry", 2nd edition.

Minima, maxima and inflection points

A stationary point of a function $f(x)$ is defined as a point in which the rate of change of that function is zero, meaning that its first derivative is zero. Solving the corresponding equation

$$f'(x)=0 \tag{1}$$

would produce a list of all stationary points. For univariate functions, stationary points come in three general categories: minima, maxima and inflection points.

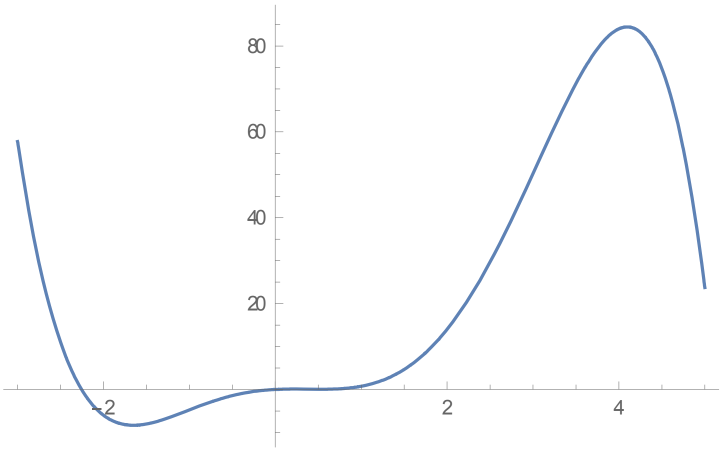
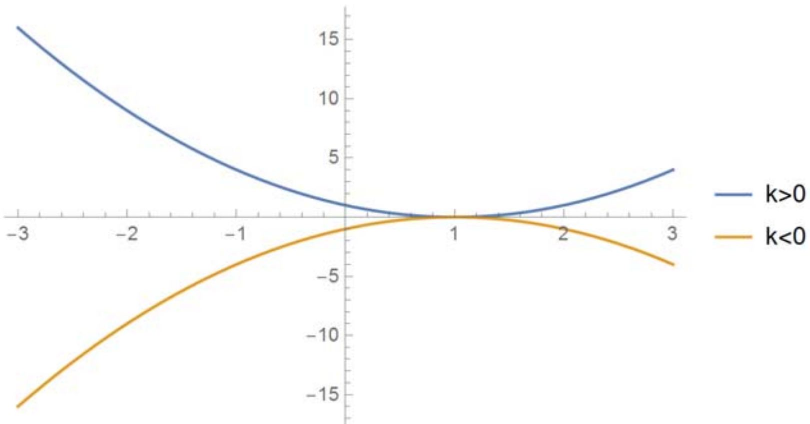


***Figure 1.** An example of a function featuring a minimum, a maximum and an inflection point.*

The nature of the stationary point may be determined by looking at the second and higher derivatives of the function. The best illustration is provided by a quadratic function. In the case of a parabola:

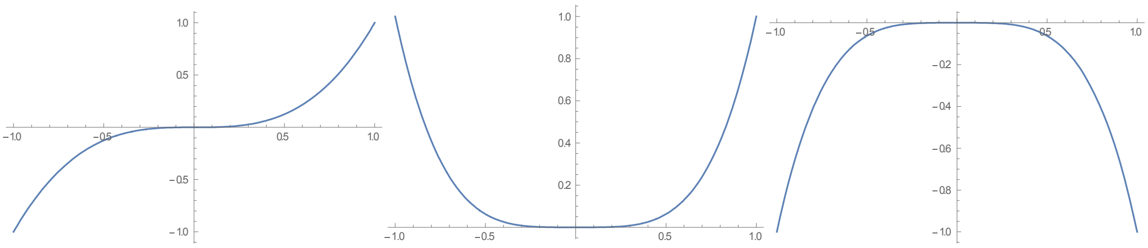
$$f(x)=k(x-1)^2 \quad \Rightarrow \quad f'(x)=2k(x-1) \quad \Rightarrow \quad f''(x)=2k \tag{2}$$

The derivative becomes zero at $x=1$, so that is a stationary point. If the second derivative is positive ($k>0$), then the stationary point is a minimum. If the second derivative is negative, then the stationary point is a maximum:



If the second derivative is zero, the point may still be a minimum, a maximum or an inflection point. Good examples are provided by cubic and quartic polynomials:

$$f(x) = x^3 \qquad g(x) = x^4 \qquad h(x) = -x^4 \tag{3}$$



In practice this means that the situation when the second derivative is zero requires further investigation and, quite frequently, detailed plotting in order to understand the nature of the stationary point.

Asymptotes

An *asymptote* is a line that a function approaches infinitely closely in some limit. For example, $f(x) = 1/x$ has a horizontal asymptote $f = 0$ for $x \to \pm\infty$ and a vertical asymptote $x = 0$ for small values of the argument.

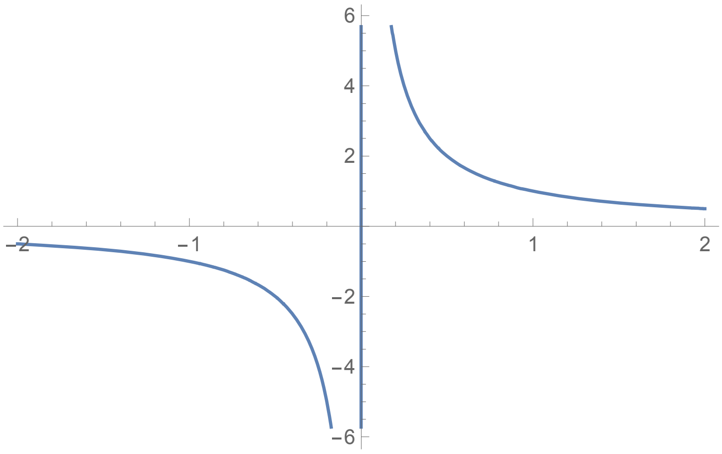


Figure 2. *A plot of f(x)=1/x, illustrating the fact that the function approaches the X axis at infinity and the Y axis at zero.*

Some functions have oblique asymptotes that do not coincide with horizontal or vertical curves. Asymptotes also need not be approached monotonically. Some examples are given below.

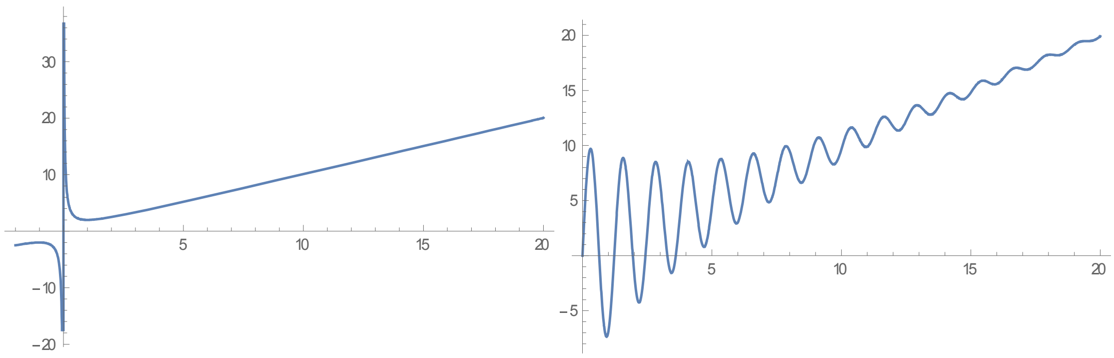


Figure 3. *Examples of functions with oblique asymptotes. Left: f(x)=x+1/x. Right: f(x)=x+10sin(5x)exp(-x/5).*

Looking at asymptotic behaviour of functions is often useful for sketching their graphs and for designing approximations that are valid in the limit of very large or very small values of the argument.

Analytical optimisation

A situation frequently arises in physical sciences and engineering when the value of a particular function $f(x)$ needs to be maximised (in the case of desired parameters, such as chemical yield or efficiency) or minimised (in the case of undesired parameters, such as acoustic noise or nitrogen oxide emissions) as a function of some variable x (pressure, temperature, concentration, *etc.*). Some model is usually provided that gives the dependence of the quantity in question on that variable.

Example 1: a cylindrical chemical reactor is required with a volume of V cubic metres. The price of corrosion-resistant steel is P pounds per square metre. Find the dimensions of the cylinder that minimise the amount of steel that is required and calculate the minimum steel cost.

Solution: the area of the cylinder surface is $A=2\pi r^2+2\pi rh$, the volume of the cylinder is $V=\pi r^2 h$. Because the volume is fixed, the height of the cylinder is necessarily related to its radius: $h=V/\pi r^2$. Substituting this relationship into the expression for the area, we get:

$$A(r)=2\pi r^2+2V/r, \qquad V>0 \tag{4}$$

We now need to find the minimum of this quantity with respect to the radius of the cylinder. The first and the second derivatives are:

$$A'(r)=4\pi r-2V/r^2, \qquad A''(r)=4\pi+4V/r^3 \tag{5}$$

The first derivative has a zero at $r_0=\sqrt[3]{2V/4\pi}$ and the second derivative is positive at that point. This means that the minimum is found and the steel price at that minimum is:

$$PA(r_0)=2\pi P(2V/4\pi)^{2/3}+2VP/\sqrt[3]{2V/4\pi} \tag{6}$$

where some cosmetic simplifications may be applied if necessary.

Example 2: find the inflection point of $y=x^3-6x^2+12x-5$.

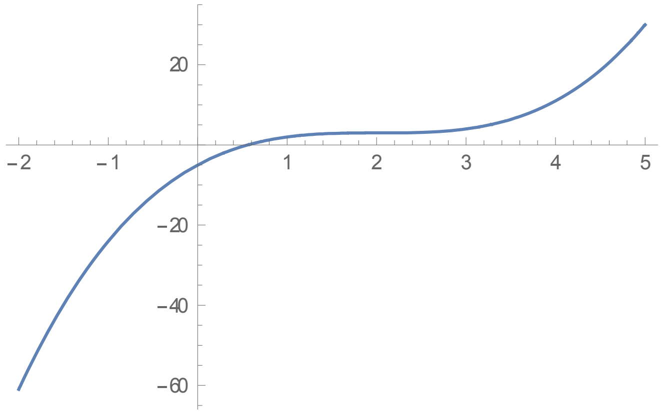
Solution: setting the first derivative to zero and solving the resulting quadratic equation yields

$$y'(x)=3x^2-12x+12=0 \quad \Rightarrow \quad x=2 \tag{7}$$

The second derivative of the function is zero at that point:

$$y''(x)=6x-12 \qquad y''(2)=0 \tag{8}$$

Plotting the function around $x=2$ confirms that it is indeed an inflection point:



Numerical optimisation

Numerical optimisation of univariate functions is an instance of the numerical root-finding problem that we already considered in the previos lectures. The task, however, is now to find numerically a point at which *the derivative* of the function turns to zero:

$$f'(x)=0 \tag{9}$$

This may be accomplished, for example, using Newton-Raphson iteration, in which the derivative of the function is now featured in the numerator and the second derivative in the denominator:

$$x_{n+1}=x_n-\frac{f'(x_n)}{f''(x_n)} \tag{10}$$

Note that the Newton-Raphson method would converge to the *nearest stationary point*. It is still your responsibility to find out what the nature of that point is.

Example: find the nearest stationary point of $f(x)=x^3-e^x$ to $x=1$ and show that it is a minimum.

Solution: the Newton-Raphson iteration for this problem is

$$x_{n+1}=x_n-\frac{3x_n^2-e^{x_n}}{6x_n-e^{x_n}} \tag{11}$$

Starting from $x_0=1.0000$, the iterations are $x_1=0.9142$, $x_2=0.9100$ and $x_3=0.9100$. The second derivative if the function at this point is positive, $f''(0.9100)=2.9757$, and therefore the point is a minimum.

Week 10 workshop exercises

Monk and Munro, 2nd edition: self-tests 21.1, 21.2, 21.3.

Steiner, 2nd edition: section 4.13, problems 78-83.

Extra difficulty exercises for the brave

Steiner, 2nd edition: section 4.13, problems 84, 85, 86.

N.B. Monk and Munro incorrectly refer to first and second *derivative*s as first and second *differentials*.