CHEM1047 – Week 4 Lecture 1 – Optimisation

☐ *Sections 4.10 and 9.4 of Steiner, "The Chemistry Maths Book", 2nd edition.*

☐ *Section 4.4 of Cockett and Doggett, "Maths for Chemists", Vol 1.*

A common task in physical sciences, engineering and economics is to find a set of parameters of a physical system, device or arrangement of assets that maximises or minimises a certain function. For example, the yield of a chemical reaction chain might depend on concentrations, pressures, temperatures and other parameters, and we are interested in maximising the yield and minimising the amount of unproductive reagent loss. Yield and loss are functions of all those concentrations, temperatures and pressures:

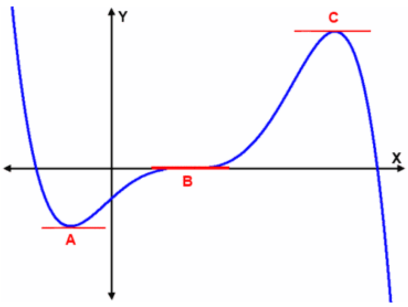


Figure 1. *A local minimum (A), an inflection point (B) and a local maximum (C) of a univariate function.*

$$\text{yield} = f(x, y, z, ...) \qquad \text{loss} = g(x, y, z, ...) \qquad (1)$$

We need find the values of the parameters that would maximise the yield-to-loss ratio:

$$\{x_{\text{opt}}, y_{\text{opt}}, z_{\text{opt}}, ...\} = \underset{x,y,z,...}{\arg\max} \frac{f(x, y, z, ...)}{g(x, y, z, ...)} \qquad (2)$$

Such problems are called *optimisation problems*. Chemical systems requiring optimisation are normally modelled with some physical, chemical and financial equations. Within the resulting model, a *figure of merit* is identified and optimised. In Equation (2), the figure of merit is the yield-to-loss ratio f/g.

1. Univariate optimisation

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

$$f'(x) = 0 \qquad (3)$$

for x would produce a list of all stationary points. For univariate functions, stationary points come in three types: *minima, maxima* and *inflection points* (Figure 1).

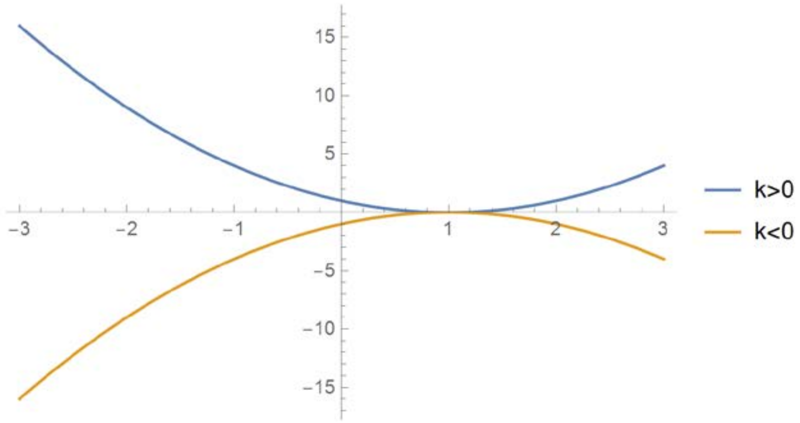


Figure 2. *Parabolas y=k(x-1)² with a minimum (blue) and a maximum (orange) depending on the sign of k.*

The nature of the stationary point may be determined by looking at the second and higher derivatives of the function. A good illustration is provided by a quadratic function (Figure 2):

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

The first derivative is zero at $x=1$. That is a stationary point. If the second derivative is positive ($k>0$), then the point is a minimum. If the second derivative is negative, then the 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 (Figure 3).

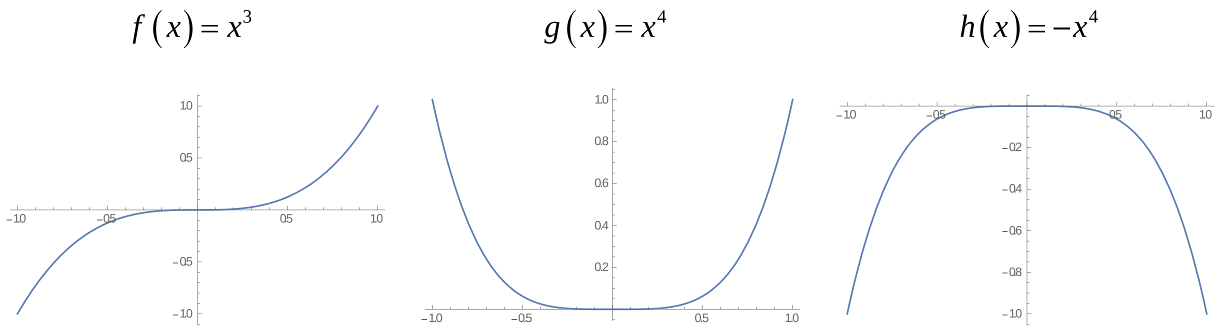


Figure 3. *Higher order stationary points.* ***Left:*** *cubic inflection point.* ***Middle:*** *quartic minimum.* ***Right:*** *quartic maximum.*

In practice this means that situations when the second derivative is zero require further investigation. Detailed plotting may be necessary to determine the nature of the stationary point.

Example 1: a cylindrical 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 required and calculate the minimum steel cost.

Solution: the area of a cylindrical surface is $A=2\pi r^2+2\pi rh$. The volume enclosed by that surface is $V=\pi r^2 h$. Because the volume is fixed, the height of the cylinder is necessarily related to its radius: $h=V/\pi r^2$. After substituting this into the expression for the area, we get:

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

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:

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

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

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

Cosmetic simplifications may be applied to these equations if necessary.

Some optimisation problems can have constraints: certain variables may be limited to specific ranges, and other variables may be linked by mathematical relations. *Constrained optimisation problems* are outside the scope of this course – look up *Lagrange multipliers* if you are interested.

2. Multivariate optimisation

The multivariate case is richer in possibilities – stationary points can be maxima (Figure 4a), minima (Figure 4b), but also *both* (Figure 4c): a point can be a minimum along one coordinate and a maximum along another. Such stationary points are called *saddle points*.

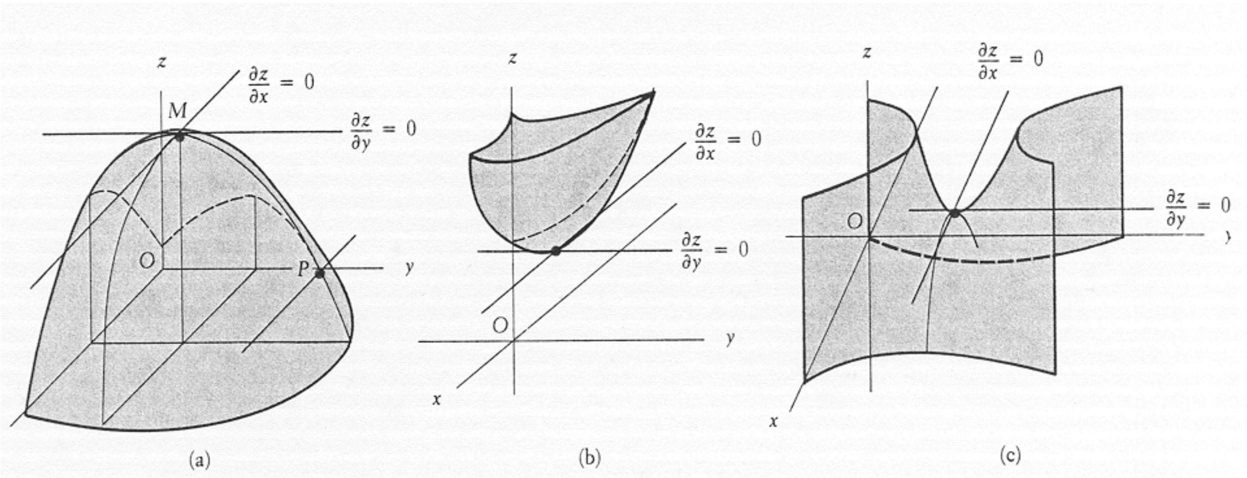


Figure 4. *Schematic drawings of a maximum (a), a minimum (b) and a saddle point (c) for a function of two variables.*

A stationary point of a multivariate function must be a stationary point *in every direction*. This means that every partial derivative must be put to zero to obtain the list of stationary points of $f(x,y,...)$:

$$\begin{cases} \partial f(x,y,...)/\partial x = 0 \\ \partial f(x,y,...)/\partial y = 0 \\ ... \end{cases} \tag{4}$$

The solutions of this system of equations are stationary points. Their classification is a complicated matter (we do not have sufficient time to cover it fully in this course), but for a function of two variables, solutions to the following quadratic equation with respect to λ determine the type:

$$\left(f''_{xx}-\lambda\right)\left(f''_{yy}-\lambda\right)-\left(f''_{xy}\right)^2=0 \tag{5}$$

Two positive solutions indicate a minimum, two negative solutions a maximum. One positive and one negative solution indicates a saddle point.

Example 3: by considering its partial derivatives with respect to both coordinates, find and classify the stationary points of $f(x,y)=(x-1)^2-(y-2)^2$.

Solution: computing the derivatives

$$\frac{\partial f}{\partial x}=2(x-1), \qquad \frac{\partial f}{\partial y}=-2(y-2),$$

setting them to zero, and solving the resulting system of equations yields:

$$\begin{cases} 2(x-1)=0 \\ -2(y-2)=0 \end{cases} \Rightarrow \begin{cases} x=1 \\ y=2 \end{cases}$$

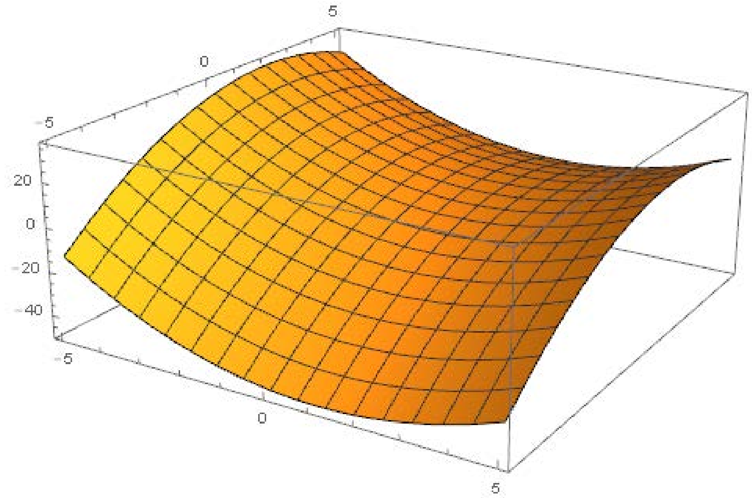
Computing second derivatives at this point produces:

$$f''_{xx} = \frac{\partial^2 f}{\partial x^2} = 2, \qquad f''_{yy} = \frac{\partial^2 f}{\partial y^2} = -2, \qquad f''_{xy} = \frac{\partial^2 f}{\partial x \partial y} = 0$$

Plugging this into the diagnostic equation given above and solving it for λ yields:

$$(2-\lambda)(2+\lambda) = 0 \quad \Rightarrow \quad \lambda = \pm 2$$

and therefore the stationary point in question is a saddle point. Plotting the function in *Mathematica* confirms this conclusion.



3. Setting up optimisation problems

The following is an approximate plan for setting up and solving optimisation problems.

1. Create a system model and identify the figure of merit. This may be the total cost, total fuel consumption, the accuracy of some mechanical process, *etc.* The figure of merit must be a function of the parameters you can control.
2. Identify penalties and constraints. Penalties may be maintenance costs, personnel costs and other matters that reduce the merit of the proposal. Constraints are hard boundaries (physical, legal, moral, *etc.*) that the solution is not allowed to cross.
3. Write down the equation for the figure of merit, and subtract penalty terms. The result is the total quantity that must be maximised or minimised.
4. Calculate first partial derivatives, make them equal to zero and find the solutions for the resulting system of algebraic equations.
5. Calculate the Hessian and make sure the stationary point(s) you have found are of the type that you want – minima or maxima, probably not saddle points.
6. Make sure the stationary points satisfy the constraints.
7. ???
8. PROFIT.

Note that the method will diligently optimise whatever it is given. Like the proverbial jinn, it would simply grant your wishes even when they are poorly thought out. The choice of reasonable figures of merit, penalties, and constraints is your responsibility.