Homework 1 Solution

Exercise 1

In thermodynamics a function in the form of $y = x \ln x$ is used extensively. Calculate the first and second derivatives of the function.

Using the product rule, we get

$$y' = lnx + 1 \quad y'' = \frac{1}{x}$$

Exercise 2

You are given the function $y = \frac{1}{6}x^3 - x^2 - 6x + 2$

a) Calculate the local minimum and maximum of the function.

$$y = \frac{1}{6}x^3 - x^2 - 6x + 2$$

$$\frac{dy}{dx} = \frac{1}{2}x^2 - 2x - 6 \ ; \quad \frac{dy}{dx} = 0 \quad \rightarrow \quad \frac{1}{2}x^2 - 2x - 6 = 0 \quad x = -2 \ or \ 6$$

$$y(-2) = \frac{26}{3} \quad ; \quad y(6) = -34$$

b) Calculate the inflection point of the function.

$$y'' = x - 2 \quad y'' = 0 \quad \rightarrow \quad x = 2 \quad y(2) = -\frac{28}{3}$$

Exercise 3

In this exercise, we introduce some mathematical notation and concepts that are used in thermodynamics:

If we have a function like $f(x, y) = 3x^2 + 4xy - 7y^2$, we can compute the partial derivatives

$$\left(\frac{\partial f}{\partial x}\right)_y = 6x + 4y, \qquad \left(\frac{\partial f}{\partial y}\right)_x = 4x - 14y$$

Using these, the **(total) differential of** f, also called the **total derivative** of f, is defined as

$$\mathrm{d}f = (6x + 4y)\mathrm{d}x + (4x - 14y)\mathrm{d}y$$

In general

$$\mathrm{d}f = \left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y$$

Please note that in Analysis III, you will learn about gradients of vector fields which are very closely related but have a different notation.

a) Compute the total derivative of $f(x, y) = x^3 y$.

   The partial derivatives are $\left(\frac{\partial f}{\partial x}\right)_y = 3x^2 y$ and $\left(\frac{\partial f}{\partial y}\right)_x = x^3$. So the total derivative becomes $df = 3x^2 y\, dx + x^3 dy$.

b) Compute the total derivative of $f(x, y, z) = x^2 y + y^2 z + z^4$.
   Also with three variables, we can use the same method as before.
   The partial derivatives are $\left(\frac{\partial f}{\partial x}\right)_{y,z} = 2xy$, $\left(\frac{\partial f}{\partial y}\right)_{x,z} = x^2 + 2yz$ and $\left(\frac{\partial f}{\partial z}\right)_{x,y} = y^2 + 4z^3$.
   The total derivative therefore is $df = 2xy\, dx + (x^2 + 2yz)dy + (y^2 + 4z^3)dz$.

c) At the intuitive level, df represents how much f (for example, the energy of a material) changes if we change the inputs x and y (for example, x and y could be the temperature and pressure) by very tiny amounts dx and dy. How can we interpret the two terms in $df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy$?
   The function $f(x, y)$ depends on two variables. Therefore, f can change either because x changes or because y changes. The partial derivative $\left(\frac{\partial f}{\partial x}\right)_y$ measures how sensitive f is with respect to changes in x. Thus, $\left(\frac{\partial f}{\partial x}\right)_y dx$ represents how much f changes due to a tiny change dx of the first input x. Similarly, the second term represents how much f changes due to a tiny change dy of the second input y.

Exercise 4

The ideal gas law states: $pV = nRT$

a) Calculate the following partial derivatives:

$$\left(\frac{\partial p}{\partial T}\right)_V ; \left(\frac{\partial T}{\partial V}\right)_p ; \left(\frac{\partial V}{\partial p}\right)_T$$

$$pV = nRT$$

$$p = \frac{nRT}{V} \quad \rightarrow \quad \left(\frac{\partial p}{\partial T}\right)_V = \frac{nR}{V}$$

$$T = \frac{pV}{nR} \quad \rightarrow \quad \left(\frac{\partial T}{\partial V}\right)_p = \frac{p}{nR}$$

$$V = \frac{nRT}{p} \quad \rightarrow \quad \left(\frac{\partial V}{\partial p}\right)_T = -\frac{nRT}{p^2}$$

b) What does the following equation equal to?

$$\left(\frac{\partial p}{\partial T}\right)_V \cdot \left(\frac{\partial T}{\partial V}\right)_p \cdot \left(\frac{\partial V}{\partial p}\right)_T = ?$$

$$\left(\frac{\partial p}{\partial T}\right)_V \cdot \left(\frac{\partial T}{\partial V}\right)_p \cdot \left(\frac{\partial V}{\partial p}\right)_T = \frac{nR}{V} \cdot \frac{p}{nR} \cdot \left(-\frac{nRT}{p^2}\right) = -1$$

This is the famous triple product rule or Euler's chain rule!

c) Calculate the total derivative of pressure as a function of T and V.(dp =?)

$$dp = \left(\frac{\partial p}{\partial T}\right)_V dT + \left(\frac{\partial p}{\partial V}\right)_T dV = \left(\frac{nR}{V}\right) dT + \left(-\frac{nRT}{V^2}\right) dV$$