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 standard notation used in thermodynamics

for concepts that you already know: In Analysis II, we wrote vector fields like

$$f(x,y) = \begin{pmatrix} x^2 + 3y \\ x + 5y \end{pmatrix}$$

In thermodynamics, we write this vector field as

$$\delta f = (x^2 + 3y)dx + (x + 5y)dy$$

And call this object a **differential form**. The symbol δ in front of δf indicates that this is a differential form.

If we have a function $f\colon \mathbb{R}^2 \to \mathbb{R}$, like $f(x,y) = 3x^2 + 4xy - 3y^2$, we can generate a vector field by taking the gradient

$$\nabla f(x,y) = \begin{pmatrix} 6x + 4y \\ 4x - 6y \end{pmatrix}$$

In thermodynamics, we say that we compute the **differential of** f , also called the **total derivative** of f , written as

$$df = (6x + 4y)dx + (4x - 6y)dy$$

We can compute the integral of a differential form along a curve $\gamma\colon I \to \mathbb{R}^n$ in the same way as for vector fields along curves since we are only changing the notation. Answer the following questions:

a. Let $f(x,y) = x^3 - y$ and consider the integral of its total derivative along two different curves

$$I_1 = \int_{\gamma_1} df\,, \qquad I_2 = \int_{\gamma_2} df,$$

Where $\gamma_1\colon [0,1] \to \mathbb{R}^2$, $\gamma_1(s) = (s, 0)$ is the straight-line segment from $A = (0,0)$ to $B = (1,0)$ and $\gamma_2\colon [0,\ 1] \to \mathbb{R}^2$, $\gamma_2(s) = (s,\ s - s^2)$ is a parabolic curve with the **same endpoints**.

Try to answer this question without doing any calculations: Is $I_1 = I_2$?

According to our notation, df is an exact differential. Hence, its integral over a path depends only on its beginning and end. Since γ_1 and γ_2 have the same endpoints, the two integrals give the same result.

NOTE: if you are unsure whether a 2-dimensional differential $dg = m(x,y)\,dx + n(x,y)\,dy$ is exact or not, you can verify if the following relation holds

$$\frac{\partial m(x,y)}{\partial y} = \frac{\partial n(x,y)}{\partial x}$$

in which case the differential is exact. The relation is a result of the symmetry of second derivatives

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$$

b. Can you explain why? (you will need a theorem about line integrals)

The previous statement follows from the (second) fundamental theorem of calculus. Remember that for a function $F(x)$ with derivative $F'(x)$, the integral

$$\int_a^b F'(x)dx \; = \; F(b) \; - \; F(a)$$

depends only on the value of the function at the endpoints. This fundamental result can be generalized to curve integrals as follows

$$\int_\gamma df \; = \; f(B) \; - f(A).$$

Note: The state functions in thermodynamics always have exact differential hence they are path-independent.

c. Let $\delta g \; = \; xy\,dx \; + \; y^2\,dy$ be a differential form that cannot be written as a total derivative of a function and consider the two integrals

$$I_3 \; = \; \int_{\gamma_1} \delta g\,, \quad I_4 \; = \; \int_{\gamma_2} \delta g.$$

Again, without doing any calculations: what can you say about the relation between I_3 and I_4?

Since δg is not an exact differential, the fundamental theorem of calculus does not apply, and we cannot infer anything about the relation between the two integrals without explicitly performing the calculation.

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 =?)

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