Homework 2

Question 1. The entropy of dipoles in a field.

You have a solution of dipolar molecules with a positive charge at the head and a negative charge at the tail. When there is no electric field applied to the solutions, the dipoles point north (n), east (e), west (w), or south (s) with equal probabilities. However, when you apply a field to the solution, you now observe a different distribution with more heads pointing north: (n,e,w,s) = (7/16, 1/4, 1/4, 1/16).

1. What is the polarity of the applied field?
2. Calculate the entropy of the system in the absence of the field.
3. Calculate the entropy of the system in the presence of the field.
4. Does the system become more ordered or disordered when the field is applied?

Answer.

1. The field has its most positive pole facing south, because the (positive) heads are facing north.
2. The formula for the entropy of the system is:
$$S = -k \sum_i p_i \ln p_i.$$
In absence of the field,
$$S_{\text{no}} = -k \cdot 4 \ln\left(\frac{1}{4}\right) = 8k \ln 2.$$
3. In presence of the field,
$$S_{\text{yes}} = -k\left(\frac{7}{16}\ln\frac{7}{16} + \frac{2}{4}\ln\frac{1}{4} + \frac{1}{16}\ln\frac{1}{16}\right).$$
4. The system becomes less disordered when the field is applied, because the field limits the degrees of freedom of the system—orientation in space. Moreover, $\Delta S < 0$.

Question 2. Finding extrema subject to constraints.

Find the point $(x^\star, y^\star, z^\star)$ that is at the minimum of the function.

$$f(x,y,z) = 2x^2 + 8y^2 + z^2$$

subject to the constraint equation

$$g(x,y,z) = 6x + 4y + 4z - 72 = 0$$

using Lagrange multipliers.

Answer. Set of equations to solve the problem using Lagrange multipliers method:

$$\left(\frac{\partial f}{\partial x}\right) = \lambda\left(\frac{\partial g}{\partial x}\right),$$
$$\left(\frac{\partial f}{\partial y}\right) = \lambda\left(\frac{\partial g}{\partial y}\right),$$
$$\left(\frac{\partial f}{\partial z}\right) = \lambda\left(\frac{\partial g}{\partial z}\right).$$

Calculate partial derivatives.

$$\nabla f = (4\,x, 16\,y, 2\,z), \quad \nabla g = (6, 4, 4).$$

So:

$$\begin{aligned} 4\,x^\star &= 6\lambda \quad \Longrightarrow \quad x^\star = 1.5\,\lambda, \\ 16\,y^\star &= 4\lambda \quad \Longrightarrow \quad y^\star = 0.25\,\lambda, \\ 2\,z^\star &= 4\lambda \quad \Longrightarrow \quad z^\star = 2\,\lambda. \end{aligned}$$

Insert above equalities into the constraint equation to find λ.

$$9\lambda + \lambda + 8\lambda = 72 \quad \Longrightarrow \quad \lambda = 4.$$

In conclusion, $(x^\star, y^\star, z^\star) = (6, 1, 8)$.

Question 3. Maximum entropy in Las Vegas.

You play a slot machine in Las Vegas. For every \$1 coin you insert, there are three outcomes:

1. you loose \$1.
2. you win \$1 (so profit is \$0)
3. you win \$5 (so profit is \$4).

Suppose that your average profit over many trials is \$0. Find the maximum entropy distribution for the probabilities p_1, p_2, p_3 of observing each of these three outcomes.

Answer. Maximum entropy solution in case of average observable constraint is:

$$p_i^\star = \frac{\mathrm{e}^{-\beta\varepsilon_i}}{\sum_{i=1}^{t} \mathrm{e}^{-\beta\varepsilon_i}},$$

where β is a Lagrange multiplier. Defie $x \equiv \mathrm{e}^{-\beta\varepsilon_i}$. Then,

$$p_i^\star = \frac{x^{\varepsilon_i}}{x^{\varepsilon_1} + x^{\varepsilon_2} + x^{\varepsilon_3}} = \frac{x^{\varepsilon_i}}{x^{-1} + 1 + x^4}.$$

From the constraint equation, we have

$$0 = \langle\varepsilon\rangle = \sum_{i=1}^{3} \varepsilon_i p_i^\star = (-1)\,p_1^\star + 0 \cdot p_2^\star + 4\,p_3^\star = \frac{-x^{-1} + 4\,x^4}{x^{-1} + 1 + x^4}.$$

Therefore,

$$\frac{1}{x} = 4\,x^4 \quad \Longrightarrow \quad \frac{1}{4} = x^5 \quad \Longrightarrow \quad x = \left(\frac{1}{4}\right)^{1/5}.$$

The maximum entropy distribution is:

$$(p_1^\star, p_2^\star, p_3^\star) = \left(\frac{\left(\frac{1}{4}\right)^{-\frac{1}{5}}}{\left(\frac{1}{4}\right)^{-\frac{1}{5}} + 1 + \left(\frac{1}{4}\right)^{\frac{4}{5}}}, \frac{1}{\left(\frac{1}{4}\right)^{-\frac{1}{5}} + 1 + \left(\frac{1}{4}\right)^{\frac{4}{5}}}, \frac{\left(\frac{1}{4}\right)^{\frac{4}{5}}}{\left(\frac{1}{4}\right)^{-\frac{1}{5}} + 1 + \left(\frac{1}{4}\right)^{\frac{4}{5}}} \right).$$

Question 4. The maximum entropy distribution is Gaussian when the second moment is given.

Prove that the probability distribution p_i that maximizes the entropy for die rolls subject to a constant value of the second moment $\langle i^2 \rangle$ is a Gaussian function. Use $\varepsilon_i = i$.

The second moment for the possible outcomes of a t-sided die is:

$$\langle \varepsilon^2 \rangle = \sum_{i=1}^{t} p_i \varepsilon_i^2. \tag{1}$$

The constraint equations are:

$$g(p_1, \ldots, p_t) = \sum_{i=1}^{t} p_i = 1 \quad \Rightarrow \quad \sum_{i=1}^{t} \mathrm{d}p_i = 0 \tag{2}$$

$$h(p_1, \ldots, p_t) = \langle \varepsilon^2 \rangle = \sum_{i=1}^{t} p_i \varepsilon_i^2 \quad \Rightarrow \quad \sum_{i=1}^{t} \varepsilon_i^2 \,\mathrm{d}p_i = 0 \tag{3}$$

The maximum entropy solution is given by the method of Lagrange multipliers:

$$\left(\frac{\partial S}{\partial p_i}\right) - \alpha \left(\frac{\partial g}{\partial p_i}\right) - \beta \left(\frac{\partial h}{\partial p_i}\right) = 0 \quad \text{for} \quad i = 1, \ldots, t, \tag{4}$$

where α and β are unknown multiplers. The partial derivatives are evaluated for each p_i:

$$\left(\frac{\partial S}{\partial p_i}\right) = -1 - \ln p_i, \quad \left(\frac{\partial g}{\partial p_i}\right) = 1, \quad \left(\frac{\partial h}{\partial p_i}\right) = \varepsilon_i^2 \tag{5}$$

Substitute eq. (5) into eq. (4) to get t equations of the form

$$-1 - \ln p_i^\star - \alpha - \beta \varepsilon_i^2 = 0, \tag{6}$$

where the $p_i^\star$'s the values of p_i that maximize the entropy. For each $p_i^\star$:

$$p_i^\star = \mathrm{e}^{-1-\alpha-\beta\varepsilon_i^2}. \tag{7}$$

To eliminate α in eq. (7), use eq. (2) to divide both sides by one.

$$p_i^\star = \frac{p_i^\star}{\sum_{i=1}^{t} p_i^\star} = \frac{\mathrm{e}^{-1-\alpha-\beta\varepsilon_i^2}}{\sum_{i=1}^{t} \mathrm{e}^{(-1-\alpha)}\,\mathrm{e}^{-\beta\varepsilon_i^2}} = \frac{\mathrm{e}^{-\beta\varepsilon_i^2}}{\sum_{i=1}^{t} \mathrm{e}^{-\beta\varepsilon_i^2}}. \tag{8}$$

Input $\varepsilon_i = i$ to get a Gaussian in i

$$p_i^\star = \frac{\mathrm{e}^{-\beta i^2}}{\sum_{i=1}^{t} \mathrm{e}^{-\beta i^2}}. \tag{9}$$