Week 4 workshop exercises

1. Find the maximum and minimum values and the points of inflection of the following functions. In each case, sketch a graph and show the positions of these points.

   (a) $y = x^3 - 7x^2 + 15x - 9$ (b) $y = xe^{-x}$ (c) $y = 2x^5 - 5x^4 + 3$

2. Confirm that the cubic function $y = x^3 - 7x^2 + 16x - 10$ has local maximum and minimum values at $x = 2$ and $x = 8/3$.

3. The Lennard-Jones potential for the interaction of atoms of inert gases at a distance r is:

$$U(r) = \frac{a}{r^{12}} - \frac{b}{r^6}$$

   where a and b are constants. The equilibrium separation r_e is the value of r at which the potential has a minimum. The energy at that point is called the binding energy $U_\mathrm{b} = U(r_\mathrm{e})$.

   (a) Find the equilibrium separation as a function of a and b.

   (b) Express a and b in terms of r_e and U_b.

   (c) Express $U(r)$ in terms of r, r_e, and U_b.

4. The probability density of a molecule of mass m in a gas at temperature T having velocity v is given by the Maxwell-Boltzmann distribution:

$$p(v) = 4\pi \left[\frac{m}{2\pi kT}\right]^{3/2} v^2 \exp\left[-\frac{mv^2}{2kT}\right]$$

   where k is Boltzmann's constant. Find the most probable velocity for a nitrogen molecule at room temperature. This function has a single maximum – do not compute the second derivative.

5. Find the stationary points of the following functions and determine their type:

   (a) $f(x, y) = 3 - x^2 - xy - y^2 + 2y$ (b) $f(x, y) = x^3 + y^2 - 3x - 4y + 2$

6. Obtain least squares fitting parameters from the calibration set in Table 1 of W4L2 for the following linear functions:

   (a) $A = aC + b$ (b) $C = aA + b$

   where A is absorbance and C is concentration.

7. Using the parameters from the previous problem, determine protein concentrations in samples M1, M2, C1 and C2.

8. Using the least squares method, find the straight line fit for the following data points:

x	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0	11.0	12.0
y	4.4	4.9	6.4	7.3	8.8	10.3	11.7	13.2	14.8	15.3	16.5	17.2