Graduate Course – Term 1, Sept-Dec 2018
30.502: Research Methods

SINGAPORE UNIVERSITY OF TECHNOLOGY AND DESIGN
Established in collaboration with MIT

Problem Set 2

Due: Friday 19^{th} Oct, 17:00
Delivery method: E-dimension
Format: Portable Document Format (PDF)

Python problems: For all the python based questions in this problem set, please copy and past the code that you used for each function/operation and the result of the calculation.

Problem 1

The consumption of resources is modelled as:

$$Q(t) = \int_0^t P_0 e^{rt} dt = \frac{P_0}{r}(e^{rt} - 1) \tag{1}$$

Where P_0 is the initial consumption rate, and r is the exponential rate of growth. The world coal consumption in 1986 was equal to 5.0 billion tonnes per a year and the estimated recoverable reserves of coal were estimated at 1000 billion tonnes. The consumption rate, r, is 2.7%

Calculate the standard deviation in the estimated time before the coal reserves are depleted, σ_t using:

(a) An analytical approach

(b) The Monte Carlo method

You may assume that the growth rate, r, and the recoverable reserves, Q, are subject to random uncertainty with $\sigma_r = 0.2$ % (absolute) and $\sigma_Q = 10\%$ (relative) respectively.

Problem 2

The latest generation of Intel memory solid state memory devices (Optane Memory) rely on phase change materials. Data is stored by changing the *phase* of a thin film between disordered (amorphous) and ordered (crystalline) structures. Importantly, the amorphous state is stable (will not lose data) provided that its atoms have insufficient energy to crystallise. An important quantity when studying the crystallisation of phase change materials is the activation energy for crystallisation, E_a. It is essentially a barrier that prevents atoms from rearranging into the ordered structure. If the thermal energy of the atoms is greater than, or some substantial fraction of the the activation energy, then the material will crystallise easily.

The activation energy can be obtained using Kissinger Analysis [1]. Essentially, the crystallisation temperature, T_c, is measured at different heating rates, ϕ. The crystallisation temperature changes with heating rate because crystallisation is an *activated* process. Then, E_a is obtained by fitting a strait line to $\ln \frac{\phi}{T_c^2}$ vs $\frac{1}{T}$ and analysing its gradient according to equation 2, where $k_B = 8.6173303 \times 10^{-5}$ eV.K^{-1} is Boltzmann's constant and C is a constant.

$$\ln\left(\frac{\phi}{T_c^2}\right) = -\frac{E_a}{k_B}\frac{1}{T_c} + C \tag{2}$$

The measured crystallisation temperatures of the phase change material AgInSbTe for different heating rates are given in Table 1. Based on this data please answer the following questions and give your answers in electron volts (eV).

(a) If the crystallisation temperature measurement standard deviation is σ_t =0.2 °C, and the heating rate standard deviation is σ_ϕ =0.1 °C.min^{-1}, use the Monte Carlo propagation of error method to generate simulate 10,000 experiments.

mean

T_c (K)	ϕ (K/min)
440.6	4.5
440.3	3.4
439.7	3.2
438.2	2.7
437.3	2.1
434.4	1.0
431.7	0.8
429.7	0.5

variance

Table 1: Crystallisation temperature of AgInSbTe for different heating rates, as reported in [2]

(b) Plot a histogram of the 10,000 simulations

(c) What is the standard deviation in the activation energy dataset?

(d) What is the standard error in the activation energy dataset?

(e) State the 95% confidence bounds in E_a within which we would expect the true vale of E_a to exist when stating the value of E_a.

References

[1] H. Kissinger. Variation of peak temperature with heating rate in differential thermal analysis. *J. Res. Nat. Bur. Stand*, 57(4):217–21, 1956.

[2] W. K. Njoroge and M. Wuttig. Crystallization kinetics of sputter-deposited amorphous AgInSbTe films. *J. Appl. Phys.*, 90(8):3816–3821, 10 2001.