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Statistical Methods in Physics (14P058)

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Exercise VI – Maximum likelihood principle

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In this exercise, we will use the maximum likelihood principle to perform parameter estimation. We will first generate the energy for a large number of atoms which follows the Boltzmann distribution. Then, we assume this to be the experimental data from an actual measurement and estimate the temperature of the system based on this data.

Similar to the previous exercise, we consider a box system containing a large number of 85 Rb atoms with mass $m = 85 m_0$ at room temperature T, where m_0 is the atomic mass unit. The kinetic energy of the system E follows the probability density function

$$f(E) = 2\left(\frac{1}{k_B T}\right)^{3/2} \sqrt{\frac{E_k}{\pi}} e^{-\frac{E_k}{k_B T}} \tag{1}$$

As a reminder: the expectation value of this distribution is $1.5 k_B T$.

- 1. Write a Monte Carlo process which generates the energy distribution for $N_{par} = 400$ particles at temperature $T = 300 \,\mathrm{K}$. In the following, we will assume this is the data from a single measurement in an actual thermal gas experiment.
- 2. Write a function which computes the likelihood $L(E_1, E_2, ..., E_{N_{par}} | T)$ of your data at a given temperature T. As a reminder: the definition of the likelihood follows

$$L(\vec{X}|\theta) = \prod_{i} f(x_i|\theta). \tag{2}$$

- 3. In actual experiment, we may know in advance a wide range of temperatures where the system's temperature locates. In our case, assume that we know the system has a temperature in the range [250 K, 350 K]. Taking a list of T in the range [250 K, 350 K] with a distance of 1 K, plot $-\ln L$ as a function of T and locate the minimum of $-\ln L$. This will be your estimation of T_e .
- 4. Now, we would like to perform two different methods to estimate the uncertainty of the obtained T_e . We start with repeating the same estimation process and study the distribution of T_e . To do so, you should repeat the same process of question 1-3 with $N_{exp} = 200$. (In an actual experiment, this means you perform the same measurement 200 times on the same system.) Then, check that the distribution of T_e follows a Gaussian. Find the standard variance σ_{T_e} of this Gaussian.
- 5. Another estimation of the uncertainty focuses only on a single set of measurement. Taking your data from question 3, find the two values T_1 and T_2 which satisfy: (a) the difference between its corresponding $-\ln L$ and the one of T_e is less than 0.5, (b) the value $T_2 T_1$

- is maximized. Then, the obtained value $(T_2 T_1)/2$ is the estimation of the uncertainty. Compare it with the result from question 4.
- 6. Fix $N_{exp}=200$, estimate the Fisher information $I(\hat{T})$ with particle numbers $N_{par}=100,200,400$. Comment on your results.
- 7. Fix $N_{par}=200$, estimate the Fisher information $I(\hat{T})$ with experiment numbers $N_{exp}=100,200,400$. Comment on your results.