Computational Laboratory in Statistical Mechanics: Project 1
PHYS 31453 Spring 2021

Assigned: February 15, 2021; Due: TBD

USEFUL INFORMATION

Central Limit Theorem

A simple version of the central limit theorem (CLT) states that for large N, the sum of N independent identically distributed variables is approximately a Gaussian distribution. Let $X_1, ..., X_N$ be N independent random variables with the same probability distribution $P(x)$. The probability distribution satisfies:

$$\int P(x)dx = 1 \quad \text{(normalization)}, \quad \int xP(x)dx = \langle X \rangle = \mu \quad \text{(mean)}, \tag{1}$$

$$\int (x-\mu)^2 P(x)dx = \langle X^2 \rangle - \mu^2 = \sigma^2 \quad \text{(variance)}. \tag{2}$$

Let Y be a random variable defined as $Y = \sum_i^N X_i$. The central limit theorem states that:

$$P(y) = \text{Prob}\{Y = y\} = \frac{1}{\sigma\sqrt{2\pi N}} \exp\left\{-\frac{(y-N\mu)^2}{2N\sigma^2}\right\}. \tag{3}$$

The theorem can be generalized to vector-valued random variables, random variables that do not necessarily have the same probability distributions, or are not independent.

Maxwell-Boltzmann distribution

Consider an ideal gas in a box (in three dimensions). The probability distribution of the velocity of particles is given by the Maxwell-Boltzmann distribution,

$$f(v)\ \mathrm{d}^3v = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left\{-\frac{mv^2}{2kT}\right\} \mathrm{d}^3v. \tag{4}$$

We can integrate over all possible directions of the velocity to obtain the probability distribution of the **speeds** of the molecules,

$$f(v)\ \mathrm{d}v = \left(\frac{m}{2\pi kT}\right)^{3/2} 4\pi v^2 \exp\left\{-\frac{mv^2}{2kT}\right\} \mathrm{d}v. \tag{5}$$

We can also change variables and obtain the energy distribution of particles:

$$f_E(E) = 2\sqrt{\frac{E}{\pi}} \left(\frac{1}{kT}\right)^{3/2} \exp\left(\frac{-E}{kT}\right). \tag{6}$$

PROBLEM STATEMENT

Start with the simpler problem of an ideal gas in a two-dimensional box. The probability distribution of the energy (E) of a single gas particle is

$$P_1(E) = A \exp\left\{-\frac{E}{k_B T}\right\}, \tag{7}$$

where A is the normalization constant, k_B is the Boltzmann constant and T is the temperature.

1. (a) I randomly draw one particle from the 2-D box at room temperature. Plot the probability distributions of its energy and velocity.

   (b) Plot the average, variance and standard deviation of energy against the temperature. How does this compare with what you already know about the energy of an ideal gas?

   (c) Plot the (i) most likely, (ii) average and (iii) root mean square (rms) speed against temperature. How do your results compare with the known (theoretically obtained) values?

   (d) Now we randomly draw N particles from the box at room temperature. $\bar{E}$ is the average energy of the drawn particles (in other words, the energy per particle). Plot the probability distribution of $\bar{E}$ for $N = 2,\ 4,\ 8$ and 16. What is the average energy per particle?

   (e) Superimpose these probability distributions on the Gaussian distribution (Eq. 3) using the appropriate means and variances.

   (f) Comment on your result.

2. Now solve the more realistic case of an ideal gas in a three-dimensional box.

   (a) Write a program that generates random numbers according to the Maxwell-Boltzmann distribution (Eq. 5).

   (b) Repeat parts (b) to (f) of problem 1 for the three-dimensional ideal gas.

COMPUTATIONAL LABORATORY IN STATISTICAL MECHANICS
GRADING POLICY FOR SPRING 2021

Grade composition: 20%: Participation in class discussions. 80%: Project reports (20% each).

Each report will be worth 50 points, broken down as follows:

Preparation and methods (5)

Completion of readings for the physical problem; participation in relevant in-class planning discussions during the project; derivation of any further mathematical relations needed for the calculation; reading about the numerical implementation and any likely concerns; communicating with course instructors about obstacles and pitfalls encountered during code development; numerical methods chosen appropriately for the problem at hand (explain why they are appropriate, in comparison to other methods) and correctly implemented.

Analysis of correctness (10)

Verification of the validity of the numerical code and the program as a whole (*e.g.*, by testing against known cases); assessment of the accuracy of the numerical calculations (e.g., you may need to verify that your solution doesn't depend on step size or other numerical parameters of the solution method).

Results (10)

Physical results ("the solution") are obtained and presented; the dependence of the solution on variations on the physical parameters (or initial conditions, input data, *etc.*) is explored.

Coding practices (10)

The code is cleanly structured and clearly documented. *Following are some specific points which it may be helpful to keep in mind:*

Code structure: Code is factored into logical sub-units (modules and functions); excessive cut-and-paste duplication of code is avoided (*e.g.*, by refactoring); flow control (loops and conditionals) is structured cleanly and logically; functions communicate with their caller through parameters and return values (not global variables); tools to optimize performance and minimize floating-point operations are employed where practicable.

Code documentation/style: Code is laid out for logical clarity and readability (lines of code are arranged into logical groupings of statements, with each block headed by a comment line and separated by blank lines); module files are identified with an initial docstring; function interfaces are documented with docstrings delineating function input and output, each with variable types; remaining code is documented with comments as appropriate; variable meanings are clearly defined, and variable and function names are meaningful; run parameters and constants are represented clearly as named variables (rather than as cryptic "magic numbers" appearing buried in expressions).

Note: The emphasis here is on *appropriate* documentation, not excessively verbose documentation.

Visualization (10)

Graphical output is used to effectively present the results; the form of output is conducive to communicating the content (plots and axes adequately labeled, plot range chosen appropriately, *etc.*).

Note: The emphasis here is on competence and clarity of communication, not fanciness.

Overall quality of report (10)

Report introduces the problem, provides any necessary background (*e.g.*, how this problem is formulated mathematically) ***with appropriate references***, explains the technical aspects of the project (methods used, the general structure of the code, and its validation), clearly and insightfully presents the results, and ***reflects on the physical interpretation, computational challenges, and potential methods of improvement and generalizations of the code to further problems.***