Computer Simulations
1^{st} problem set

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Submission deadline:
Schedule A: week of March 31
Schedule B: week of April 7
Please upload your files in the Teach Center before the assessment discussion with your tutor.

Density and velocity distribution of an ideal gas

To simulate an ideal gas of N particles in a volume $V = 1 \times 1 \times 1$, you will sample their density and velocity distribution.

1. **Density fluctuations**

   (a) Distribute the particles in one dimension between 0 and 1 by generating N uniformly distributed random numbers.[1] Plot a histogram, normalized as a probability density function (pdf). This means that the count of each bin has to be normalized by Nb, where b is the bin width.

   (b) Add error bars to the histogram of part 1a. Estimate the size of the error of each bar in the histogram from the frequentist expression (see lecture notes). Plot the histogram with error bars.[2] Vary N and verify, using two examples, that the size of the error bars corresponds to the magnitude of the fluctuations in the histograms (around 68% of the values should lie within one standard deviation from the mean).

   (c) Examine the fluctuations of the height of an individual bar, denoted i. Generate $M = 1000$ samples of N random numbers each. For each sample, calculate (but do not plot) a histogram, normalized as a pdf. Consider the height of the bar corresponding to random numbers $0.5 < x < 0.6$ (*i.e.* the sixth of 10 bars). What is the expectation value of this height? Collect the M heights and plot a histogram of these values. How should the width of this histogram depend on N? Verify the expected behavior with a few examples, *e.g.* with $N = 10^m$, $m = 3$ and 5 (m between 2 and 6 should work well).[3]

   (d) Consider the N_i particles in the volume V_i corresponding to bar i in your histogram. Calculate the isothermal compressibility in units k_BT from

   $$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T \approx \frac{V_i}{k_BT}\frac{\langle N_i^2\rangle - \langle N_i\rangle^2}{\langle N_i\rangle^2} \quad \text{if } V_i \ll V.$$

   Compare to the ideal gas prediction $\kappa_T = (\rho k_BT)^{-1}$, with $\rho = N/V$.

2. **Inverse transformation sampling**

   Write a program which generates random numbers according to the exponential distribution

   $$g(x) = \exp(-x)$$

   using the inverse transformation method. You first need to find the corresponding cumulative distribution function.

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[1] Matlab: *rand(N,1)*, Python: *random.rand(N)*.

[2] Matlab: *errorbar*, which needs the coordinates of the bin-centers, the heights of the bars, and the (normalized) size of the errors as input. These numbers can be obtained using *h=histogram(...)*; *w=h.BinWidth*, *etc*. Python: *yerr=...* in *bar* from *matplotlib.pyplot*.

[3] Matlab: consider using *histcounts* and *histogram*.

3. **Rejection sampling**

To generate the velocity in one dimension, you need to sample from the Gaussian distribution with standard deviation $\sigma = \sqrt{k_B T/m}$, with m being the mass, and zero mean. These numbers can be generated using $Y = \sigma X$ where X has been drawn from the Gaussian distribution with $\sigma = 1$, which is symmetric and has the half-sided pdf

$$f(x) = \sqrt{\frac{2}{\pi}} \exp\left(-\frac{x^2}{2}\right) \quad \text{for } x \geq 0.$$

Use the function $c\,g(x)$ as an envelope of $f(x)$, where c has been chosen such that $c\,g(x) \geq f(x)$ for all $x \geq 0$.

(a) Calculate c by maximizing the function $h(x) = f(x)/g(x)$.

(b) Use the set of numbers X generated according to the exponential pdf $g(x)$ of part 2. Now generate numbers u from the uniform distribution. When $u > f(x)/(c\,g(x))$, reject the number x, otherwise accept it as part of the set X'. Plot a histogram of the set X', normalized as a pdf, and verify that it follows the pdf $f(x')$.

(c) Choose an alternative enveloping function for the rejection method and repeat the calculation of part 3b. The envelope needs to have an invertable cumulative distribution function. Note that your enveloping function does not need to be optimal; the envelope can be noticeably larger than the desired distribution and still perform well. Evaluate the acceptance rates of the two rejection methods.

4. **Velocity distribution**

(a) Construct independent velocity distributions in three dimensions, labeled 1, 2 and 3, and calculate the magnitude of the velocity $v = \sqrt{v_1^2 + v_2^2 + v_3^2}$. Plot a pdf of the distribution of v and show that it equals the Maxwell-Boltzmann pdf

$$p(v) = \sqrt{\frac{2}{\pi}}\, v^2 \exp\left(-\frac{v^2}{2}\right).$$

(b) Repeat the generation of $p(v)$ with all three generators from part 3. For all generators, perform a frequentist analysis to calculate histograms with error bars.

(c) For the first generator (exponential distribution), also perform a Bayesian analysis (see lecture notes) to calculate the histogram and error estimates.

(d) In all cases, plot the histograms together with the error bars and the desired pdf. Are the sizes of the error bars reasonable? What size should you (roughly) expect? Do the sizes scale correctly with the number of entries in the sample? Are the histograms compatible with the desired distributions, given the uncertainties? When do the differences between the frequentist and the Bayesian analysis become visible ?