Homework Set 1
Chemistry 553, Spring 2021
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Due Friday, April 9th

Problem 1. In this problem we will explore some basic concepts of random numbers.

(a) Consider a random variable $\hat{X}$ that us uniformly distributed on the interval $[0, 1]$, i.e., its probability distribution is

$$p(x) = \begin{cases} 1 & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise.} \end{cases}$$

Calculate the mean and the variance of $\hat{X}$.

$$p(x) = P(\{x \in \Omega : \hat{X}(x) = x\}) = \begin{cases} 1 & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise.} \end{cases}$$

This says that when $0 \le x \le 1$, $\hat{X}(\omega) = \omega$, so we can solve for the mean and variance by the following:

$$\begin{aligned} \text{mean} = \left\langle \hat{X} \right\rangle &= \int_{\Omega} \hat{X}(x) p(x)\, dx \\ &= \int_{o}^{1} x p(x)\, dx = \left. \frac{x^2}{2} \right|_0^1 = \frac{1}{2} \end{aligned}$$

$$\begin{aligned} \text{Variance} = var(\hat{X}) &= \left\langle \hat{X}^2 \right\rangle - \left\langle \hat{X} \right\rangle^2 \\ &= \int_0^1 \hat{X}(x)^2 p(x)\, dx - \left\langle \hat{X} \right\rangle^2 \\ &= \int_0^1 x^2 p(x)\, dx - \left\langle \hat{X} \right\rangle^2 \\ &= \left. \frac{x^3}{3} \right|_0^1 - \frac{1}{4} = \frac{1}{12} \end{aligned}$$

(b) Now consider two such random variable, $\hat{X}_1$ and $\hat{X}_2$, each distributed uniformly on $[0, 1]$. Assume these random variables are independent. We can calculate the average of $\hat{X}_1$ and $\hat{X}_2$:

$$\hat{S} = \frac{1}{2}\left(\hat{X}_1 + \hat{X}_2\right),$$

which is itself a random variable. Calculate the probability distribution, the mean, and the variance of $\hat{S}$.

Probability distribution: ?

$$\text{mean} = \left\langle \hat{S} \right\rangle = \frac{1}{2}\left(\left\langle \hat{X}_1 \right\rangle + \left\langle \hat{X}_2 \right\rangle\right) = \frac{1}{2}$$

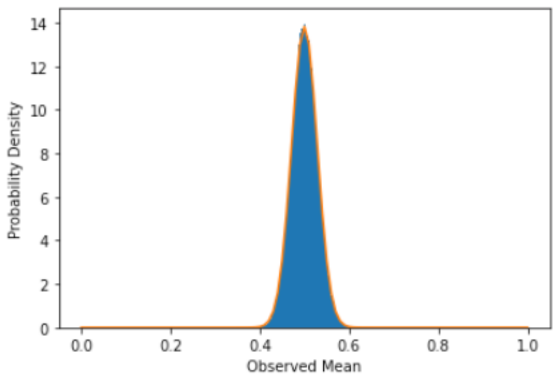
$$\begin{aligned}
var(\hat{S}) &= \left\langle \hat{S}^2 \right\rangle - \left\langle \hat{S} \right\rangle^2 \\
&= \left\langle \left(\frac{1}{2} \left(\hat{X}_1 + \hat{X}_2 \right) \right)^2 \right\rangle - \left\langle \hat{S} \right\rangle^2 \\
&= \frac{1}{4} \left(\left\langle \hat{X}_1^2 \right\rangle + \left\langle \hat{X}_2^2 \right\rangle + 2 \left\langle \hat{X}_1 \right\rangle \left\langle \hat{X}_2 \right\rangle \right) - \left\langle \hat{S} \right\rangle^2 \\
&= \frac{1}{24}
\end{aligned}$$

(c) We can also take the average of N independent, uniformly distributed random variables,

$$\hat{S} = \frac{1}{N} \sum_{i=1}^{N} \hat{X}_i.$$

Based on what you found in part (a), what would you expect the probability distribution of $\hat{S}$ to be if N is large? What about its expectation value and its variance? If N is large, by the Central Limit Theorem, the probability density of $\hat{S}$ will be the Gaussian distribution that has parameters μ and σ^2 for the mean and variance, respectively. The mean will be equal to the mean of each individual $\hat{X}_i$ and the variance will be $\frac{1}{N}$ times the variance of each individual $\hat{X}_i$

(d) Work through the posted "Random Numbers" Jupyter Notebook on random numbers. Do you find your expectations confirmed? Modify the last command block in that notebook to obtain the distribution of $\hat{S}$ for N=100. On the same plot, graph the Gaussian normal distribution with the mean and variance that you would expect for that value of N, and compare the two. Yes everything is what I expect. Please excuse the pixelated plot below.



Problem 2. Consider a quantum-mechanical harmonic oscillator, which has states enumerated by a quantum number $n = 0, 1, 2, \ldots$. As we will see later, the probability that the oscillator is in the n-th state is

$$P(n) = \frac{1}{Z} \mathrm{e}^{-\beta E_n}$$

where β is a positive number, $E_n = \hbar\omega(n + 1/2)$ is the energy of the n-th state, and Z is a normalization constant. Find this normalization constant, i.e., find the expression of Z such that

$$\sum_{n=0}^{\infty} P(n) = 1.$$

You can use the the following result for the *geometric series*:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$$

for all $|x| < 1$.

$$\begin{aligned}
\sum_{n=0}^{\infty} P(n) &= \sum_{n=0}^{\infty} \frac{1}{Z} \mathrm{e}^{-\beta\hbar\omega(n+1/2)} = 1 \\
&= \frac{1}{Z} \sum_{n=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega n} \mathrm{e}^{-\frac{1}{2}\beta\hbar\omega} = 1 \\
&= \frac{\mathrm{e}^{-\frac{1}{2}\beta\hbar\omega}}{Z} \sum_{n=0}^{\infty} \left(\mathrm{e}^{-\beta\hbar\omega}\right)^n = 1 \\
&= \frac{\mathrm{e}^{-\frac{1}{2}\beta\hbar\omega}}{Z} \frac{1}{1-\mathrm{e}^{\beta\hbar\omega}} = 1 \\
Z &= \frac{\mathrm{e}^{-\frac{1}{2}\beta\hbar\omega}}{1-\mathrm{e}^{\beta\hbar\omega}}
\end{aligned}$$

Problem 3. Show that the Gaussian normal distribution

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-\dfrac{(x-\mu)^2}{2\sigma^2}},$$

where μ and σ are two parameters, is normalized. In other words, show that

$$\int_{-\infty}^{\infty} p(x) \mathrm{d}x = 1.$$

It might help to first show that

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\dfrac{x^2}{2}} \mathrm{d}x = 1$$

by calculating

$$\left(\int_{-\infty}^{\infty} \mathrm{e}^{-\dfrac{x^2}{2}} \mathrm{d}x \right)^2,$$

which you can do by solving a two-dimensional integral in polar coordinates.

$$\left(\int_{-\infty}^{\infty} \mathrm{e}^{-\dfrac{x^2}{2\sigma^2}} \mathrm{d}x \right)^2 = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}\, dx \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma^2}}\, dy$$

we then use u-substitution to get x' and y':

$$\begin{aligned}
&= 2\sigma^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x'^2+y'^2)}\, dx'\, dy' \\
&= 2\sigma^2 \int_0^{2\pi} \int_0^{\infty} e^{-r^2} r\, dr\, d\Theta \\
&= 4\pi\sigma^2 \int_0^{\infty} re^{-r^2}\, dr \text{ we use u-substitution again} \\
&= 2\pi\sigma^2 \int_o^{\infty} e^s\, ds = 2\pi\sigma^2
\end{aligned}$$

Now we can say that $\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \mathrm{e}^{-\dfrac{x^2}{2\sigma^2}} \mathrm{d}x = 1$ The only difference between this and the gaussian distribution is the μ term in the exponent of the gaussian. This does not change the integral. We are integrating over all real numbers so a translational shift in the position of the curve along the x-axis has no impact on the integral. Therefore, we can say that $\int_{-\infty}^{\infty} p(x)\mathrm{d}x = 1$