Due: Workshop-3d

Physical Chemistry II

Exercises Set 1

1. Random Numbers

Use the MS-Excel utility with its random-number generator and data analysis functions RAND, AVERAGE, STDEV, FREQUENCY for the following tasks:

- **a)** Populate 2 columns of a blank XLS worksheet with sets "Datax" and "Datay," each with 300 random integer numbers between 5 and 20. Generate a scatter plot for each set.
- **b)** Calculate mean, variance, and standard deviation for the "Datax" and "Datay" arrays.
- **c)** Plot the two-dimensional (2D) scatter plot of "Datay" vs. "Datax."
- **d)** Generate a trend line (mouse right click) for the 2D data. Discuss the presence or absence of x-y correlations in the 2D data.

2. Central Limit Theorem

Test experimentally the validity of the Central Limit Theorem. This theorem states that the sums $S(N) = \sum_{i=1}^{N} x_i$ of large numbers of uniformly distributed random numbers $\{x_i,\ i = 1 - N\}$ approach a Gaussian "Normal" distribution for large *N*.

- **a)** Use MS-Excel to generate several (*5*) instances of the mean expectation value $E_N(x) = \frac{1}{N}\sum_{i=1}^{N} x_i$ of random-number sets $\{0 \le x_i \le 1\}$ for *N=10*.
- **b)** Generate and record additional data sets $\{E_N^{(n)}(x),\ n = 1,\ldots,5\}$ for *N= 50, 100,200*.
- **c)** Compare the average values $\left\langle E_N^{(n)}(x)\right\rangle_n$ and the spreads in the sets $\{E_N^{(n)}(x)\}$ for *N = 10, 50, 100,200*. Consider the ratio of variance to mean value.

3. <u>Functions of Statistical Variables</u>

Assume a set of real random numbers $\{x\}$ with a finite average $\langle x\rangle$ and finite variance $\sigma^2 = \langle x^2\rangle - \langle x\rangle^2$. Are the functional values $\{y\} = \{f(x), x \in \{x\}\}$ also statistically distributed with $f(\langle x\rangle) = \langle f(x)\rangle$? Do you know why, or why not? Consider the following functions:

a) $f(x) = 3 + 2 \cdot x^2$

b) $f(x) = 2 - 3 \cdot x$

c) $f(x) = 3 + 2 \cdot \exp\{-x^2\}$

4. <u>Probability Generators</u> (AC*)

Consider the Laplace transformation $\Lambda(s) := \int_0^\infty e^{s \cdot x} P(x)\,dx$ of a properly normalized probability distribution, with $\int_0^\infty P(x)dx = 1$.

a) Devise a differential operation on $\Lambda(s)$ producing the mean value (first moment) $\langle x\rangle = \int_0^\infty x \cdot P(x)\,dx$

b) Expand the method to obtain higher moments $\langle x^n\rangle$ of the probability distribution.

c) Apply the method to the function $\Lambda(s) = a \cdot (s-a)^{-1}$, which is Laplace transform of a function describing the exponential decay of a pharmaceutical in time (t), and determine its mean lifetime $\langle t\rangle$.

*AC= augmented credit for graduate students