

6 February 2020

Note : Please get your own laptops to the class, pre-installed with compilers/interpreters corresponding to your coding language.

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**Question 1: Using a coin toss process to create an Uniform Random Number Generator**

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Assume that you have an unbiased coin with two outcomes. Use this coin to create a Uniform Random Number (URN) generator. Simulate the process using your favourite coding language. Note : Almost all the scripting and statistical languages have a command to simulate a coin toss. For example in Python:

```
import numpy as np
np.random.choice(['H', 'T'])
np.random.choice([0,1])
```

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**Question 2: Uniform Distribution**

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Generate atleast 1000 URNs and prove that the numbers indeed obey a uniform distribution. Use the URN generator in your coding language and check the distribution obtained from it with that of yours.

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**Question 3: Calculating  $\pi$  value using Monte-Carlo scheme**

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Using Monte-Carlo scheme discussed in the class and your URN generator, estimate the value of  $\pi$ .

- Plot the estimate obtained with increasing number of random points used in the scheme.
- Plot the error observed (assuming the real value of  $\pi$  to be 3.14159) with increasing number of random points used in the scheme. Overlay the plot  $1/\sqrt{N}$  on the obtained plot.

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**Question 4: Sampling from a different distribution**

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Transform the URN generator to sample random numbers from the following probability distribution in the interval  $[0, \infty)$

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

Generate atleast 1000 such random numbers and show that they indeed obey the above distribution.

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**Question 5: A Boy and His Atom**

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In 2013, IBM Research division released a 1.5 minute stop-motion animated short film depicting the story of a boy and a wayward atom who meet and become friends. The individual frames of the movie were created by carefully placing carbon monoxide molecules on a copper surface and then visualizing them under a scanning tunneling microscope.

More details of the experiment: [here](#)

Check it out: [www.youtube.com/watch?v=oSCX78-8-q0](http://www.youtube.com/watch?v=oSCX78-8-q0)

Consider the surface of copper to be composed of  $N$  sites and the chamber filled with  $M$  CO molecules where  $N \gg M$ .

Calculate the possible number of configurations possible in each of the following scenarios:

- a) Each site can accommodate only one molecule of CO.
- b) Each site can accommodate more than one molecule of CO.

Now fill the chamber with  $M$  different gas molecules each having different chemical identities

- a) Each site can accommodate only one molecule.
- b) Each site can accommodate more than one molecule .

**This question does not require coding.**

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### Question 6: Making a Transition Matrix

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A researcher performed a single molecule FRET experiment on protein-211 and noticed significant jumps in FRET efficiencies with time. He got interested and performed an all-atom molecular simulation to look at the conformational changes. From his long trajectory of simulation he noticed that the protein takes 2 states (A and B) and all the conformations fall into either of these 2 states. From the trajectory, he made a long sequence of the changes observed in the simulation which can be found [here](#). Help him to make a transition matrix.