Digital Chemistry, Problem set 2

Due March 20, 2024

1. What is the probability of the coin turning face up in the second throw if it turned tails up in the first throw?

2. There are two apples and two oranges in a box. Somebody took a fruit from that box at random. What is the probability that we get an orange when taking another fruit at random?

3. The following is the probability distribution function ($f(\theta)$)of the angles between three consecutive α-carbon atoms in proteins (θ), excluding proline and glycine residues, extracted from the Protein Data Bank.

θ [deg]	$f(\theta)$
65.0	0.000230
75.0	0.002860
85.0	0.020190
95.0	0.017760
105.0	0.017335
115.0	0.016505
125.0	0.012970
135.0	0.009675
145.0	0.002340
155.0	0.000135

   (a) Check if the distribution is normalized to 1 (total probability) and correct the values if necessary.

   (b) Make a plot of the distribution and of the respective cumulative distribution function ($F(\theta)$).

   (c) Determine the most probable value of θ and the average value of θ. Comment the result.

   (d) Compute the variance, skewness, and kurtosis and draw conclusions about the character of the distribution.

   Hint: When computing the average and central moments keep in mind that the value of the distribution assigned to a given θ value is an average over the $[\theta, x + \Delta\theta]$ interval and does not correspond ONLY to θ.