

**Digital Chemistry, Problem set 2****Due March 19, 2025**

1. What is the probability of getting a total of 6 dots in two consecutive rolls of a regular non-biased dice?
2. There are 4 faulty and 6 good batteries in a box. Somebody took a battery from the box at random. What is the probability of getting a good battery in the second draw? Can we increase our chances of getting at least one good battery when doing two consecutive draws?
3. The following is the probability distribution function,  $f(d)$ , of the difference of structures of a small protein simulated by Molecular Dynamics from its experimental structure. This difference is commonly referred to as the Root Mean Square Deviation (RMSD).

$d$ [Å]	$f(d)$
1.5	0.011
2.0	0.122
2.5	0.312
3.0	0.401
3.5	0.344
4.0	0.275
4.5	0.235
5.0	0.169
5.5	0.069
6.0	0.038
6.5	0.015
7.0	0.006
7.5	0.002
8.0	0.001

- (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 ( $F(d)$ ).
- (c) Determine the most probable value of  $d$  and the average value of  $d$ . 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  $d$  value is an average over the  $[d, d + \Delta d]$  interval.