Sample questions

1. The \( C_\alpha \) coordinates of four protein structures are \( X_1, X_2, X_3, X_4 \). The lengths of all four proteins are the same. All the geometric centers are at \((0,0,0)\). The task is to find a single rotation matrix \( U \) that will minimize the sum of the six distances\(^2\)

\[
D_{ij}^2 = \text{norm}\left(X_i - UX_j\right)^2 \quad \text{minimize} \quad \sum_{i<j} D_{ij}^2(U) \quad \text{as a function of the rotation matrix } U.
\]

a. Write the target function to be minimized, and its derivatives with respect to \( u_{ij} \), the matrix element of the rotation matrix.

b. Discuss the similarities and differences of the present problem compared to the problem of overlapping only two structures. Based on the similarities, suggests a solution to the rotation matrix

2. Starting with random numbers sampled uniformly between 0 and 1 generate random numbers from the probability density \( p(x) = \sqrt{x} \) (the probability of observing \( x \) between \( x \) and \( x + dx \) is \( p(x)dx \)).

3. Starting with random numbers sampled uniformly between 0 and 1 suggest an algorithm that produces random numbers sampled from the probability density

\[
p(x) = \left(\frac{2}{b^3}\right)x, \quad x \in [0, b]
\]

4. Outline how can you use the accept/reject sampling procedure to estimate the number \( \pi \)

5. Derive a lower bound to the number of possible alignments of the sequence \( A \) length \( n \) and the sequence \( B \) length \( m \).

6. In the class we plotted the protein chain using a cubic spline interpolation that kept the second derivative continuous. Suppose, we care only on first derivative. How would you change the interpolation?

7. You attempt to overlap two protein chains \( (X_A, X_B) \) of equal length. The determinant of the rotation matrix that was determined using the procedure described in the class is \(-1\). What (if) steps are you going to take to compute a new rotation matrix and a new distance

8. We wish to sample random numbers from the probability density \( p(x) \propto x^2 \) for \( x \in [1, 2] \) based on uniform random numbers distributed between 0 and 1. Suggests how the desired random number could be generated with (a) coordinate transformation, and (b) reject/accept algorithm.
9. We sample random numbers from a uniform distribution between 0 and 1. We need to generate random numbers distributed between 0 and 1 according to \( p(x) = ax^2 \). Determine the coefficient \( a \). Explain how will you use the uniformly distributed random numbers to obtain a sample from the desired distribution.

10. Consider the linear equation \( Ax = b \) where \( A \) is a symmetric \( N \times N \) positive definite matrix. The task is to solve for \( x \). Estimate the number of floating-point operations and its dependence on \( N \) using the Gaussian elimination algorithm and the Conjugate gradient procedure.