

MAP 5485, Maple Tutorial, Discrete curves

First open the worksheet for the Maple tutorial on discrete curves.

Exercises

- (1) Using the procedures for stacking matrices found in the worksheet and using the construction `IdentityMatrix`, construct the matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

- (2) Use the procedure `plotcurve` in the worksheet to plot the discrete curve

$$\left[\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ 2 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 3 \\ -1 \end{bmatrix}, \begin{bmatrix} 0 \\ 2 \\ -2 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \right].$$

This is the chair form of cyclohexane. Can you see why it is called the chair form?

- (3) Use the torsion angle and bond angle procedures to find the torsion angles and bond angles for cyclohexane. What are the distances between consecutive atoms?
- (4) Look at the drawing by Pauling of the alpha helix. Verify that there are 13 atoms in the cycle of atoms formed by the hydrogen bond and that the exterior bond angles are (approximately)

$$[0, 60, 60, 70, 60, 60, 70, 60, 60, 70, 60, 60, 0]$$

and the torsion angles are (approximately)

$$[0, 0, \phi, \psi, 180, \phi, \psi, 180, \phi, \psi, 0, 0, 0].$$

For simplicity, take all bond lengths equal to 1. For simplicity we are assuming all ϕ torsion angles are the same and all ψ torsion angles are the same.

Using the procedures in the worksheet construct an expression distance of the oxygen from the hydrogen as a function of ϕ and ψ . Do a 3D plot of this function and try to determine ϕ and ψ for which the function is a minimum.