Exercise 4 – Algebraic Curve, Surface Splines - IV: Molecular Models

CS384R, CAM 395T, BME 385J: Fall 2007

October 6, Due: October 24

Question 1. Describe the LEG (Labelled Embedded Graph) atomic representations as per class notes, of the twenty protein amino acids (or protein residues), and the two common protein secondary structures (i.e., α-helices and β-sheets) .

Question 2. Given a LEG representation of a protein (created from the PDB), describe an algorithm to detect and output the LEG representations of all α-helices and β-sheets in that protein. Your algorithm should be able to distinguish between *parallel* and *anti-parallel* β-sheets.

Question 3. Given a LEG representation of a protein P,

- (a) Describe an algorithm to compute the vDW (union-of-spheres) surface of P.
- (b) Describe an algorithm to detect all solvent exposed atoms of P.
- (c) Augment the algorithm of part (b) to detect where two or three of these exposed atoms intersect.
- (d) Describe how to construct the L-R molecular surface (also called a sphere solvent contact surface) of the protein P, using the information generated in parts (b) and (c).
- (e) Describe a method to detect where if at all, the L-R surface of part (d), self intersects.
- (f) Can you solve parts (b) and (c) in $\mathcal{O}(n \log n)$ time, where n is the number of atoms in the protein? You can assume for simplicity that all atoms have the same radius.

Question 4. Knowing how to generate the L-R molecular surface representations of a protein P (as per Question 3.),

- (a) Describe C^0 continuous A-patch representations of the L-R molecular surface of a typical α-helix, typical parallel and anti-parallel β-sheets, and of the protein P.
- (b) Sketch a method of generating C^1 smooth low -degree A-patch representations of the L-R surfaces of part (a).