Algorithms in Structural Bioinformatics

Assignment 3 (I. Emiris)

version 6/3/13. Deadline: Tue. 12/3/13, start of class

Structure alignment

You may find useful to use an algebra package like Matlab (or its free equivalent, Scilab), Maple (available from my Lab), Mathematica or another. Future assignments may require such a tool.

a) Compute the (coordinate) c-RMSD of the following labeled pointsets in $\mathbb{R}^3$:

$$x_1 = (0,0,0), x_2 = (2,0,0), x_3 = (1,1,0), x_4 = (0,0,1),$$

$$y_1 = (2,0,0), y_2 = (2,-2,0), y_3 = (3,-1,0), y_4 = (2,0,1).$$

b) Compute their centroids and translate both sets to the origin: compute their new c-RMSD.
c) Find the optimal rotation for alignment. Apply it to one pointset. Compute the new c-RMSD.

Questions (d) to (f) are for Grads only:
d) For the input sets, compute their (distance) d-RMSD. Can you now guess the d-RMSD for the final sets in (c) without computing any d-RMSD?
e) We wish to align set x with: $z_1 = (0,0,0), z_2 = (4,0,0), z_3 = (2,2,0), z_4 = (0,0,2)$.
Would you repeat (a) to (c) or would you apply another transform?
f) Repeat (a) to (c) for $x_1, \ldots, x_4, x_5 = (-1,1,-1)$, and $y_1, \ldots, y_4, y_5 = (0,1,1)$.

C-space

The "molecule" is a straight-line segment (antenna) of length $\sqrt{5}$. Its base-point moves on the x-axis and its "antenna" defines angle θ with it: $\theta = 0$ (respectively π) when the molecule lies on the axis with the antenna to the right (resp. left). In Figure 1, integer points $x = -2, -1, 0, 1, 2, 3$ are marked, and two polygonal obstacles with corners at $(-1,1), (1,1)$, extending upwards ($y \to \infty$), and to the left ($x \to -\infty$) or right ($x \to \infty$), respectively.

I propose using cotangent $\cot\theta \in (-\infty, \infty)$ to parameterize the angle (but you may use θ). Three configurations are shown: (i) $x = -1, \cot\theta = 2$, (ii) $x = 3, \cot\theta = -2$ and (iii) $x = 3, \cot\theta = 2$.

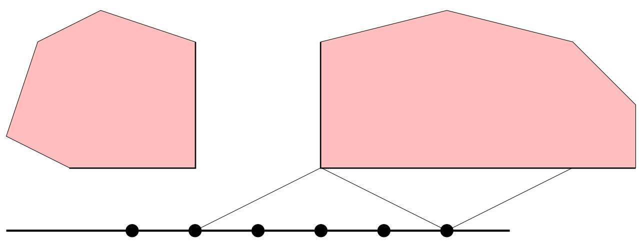

Figure 1: Physical space of molecule with 2 degrees of freedom.

a) Plot the Configuration space in x and $\cot\theta$ (or θ). Show the obstacles in C-space.

Take starting configuration A at $x = 5, \cot\theta = 4$, target configuration B at $x = -5, \cot\theta = -4$.
b) Show a min-length path A to B in C-space maximizing minimum distance from the obstacles.

c) Show a path from A to B in C-space comprised of a minimum number of straight-line segments.