Problem set Cyclic Coord Descent

Note Title 5/2/2007

Given 1COA residues 34-46 form loop

1. extract bond length, bond angle, & dihedral angle parameters from given coordinates
2. Choose random ϕ, ψ dihedrals for loop,
3. Construct coords from parameters – note this breaks the loop at C_{46}
4. Use Cyclic Coord Descent on loop ϕ, ψs to bring C_{46} back to correct position
   - adjust each angle in turn $\phi_{34}, \psi_{34}, \phi_{35}, \psi_{35} \ldots \phi_{46}, \psi_{46}$
   - bring C_{46} as close to position as possible by changing ϕ_i (or ψ_i).
5. Repeat from 2 to get 10 loop conformations.

Coordinates to parameters

Bond length ab $\|a-b\| = \sqrt{(a.x-b.x)^2 + (a.y-b.y)^2 + (a.z-b.z)^2}$

MATLAB `norm(a-b) = sqrt(sum((a-b).^2, 2))`

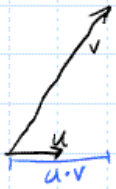
↗ works if a, b are nx3 vectors.

Math review for 3-d vector geometry:

dot product $u \cdot v = u_x \cdot v_x + u_y \cdot v_y + u_z \cdot v_z$

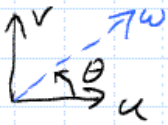
when u is a unit vector, i.e $\|u\| = \sqrt{u \cdot u} = 1$

$u \cdot v$ = the length of the projection of v onto u.



Thus if v is perpendicular to u, $u \cdot v = 0$.

We can use perpendicular unit vectors u, v to give coordinates on the uv plane.

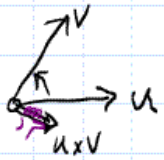


E.g. here is the angle to the projection of w:

$\theta = \text{atan2}(w \cdot v, w \cdot u)$

cross product $u \times v = (u_y v_z - u_z v_y, u_z v_x - u_x v_z, u_x v_y - u_y v_x)$

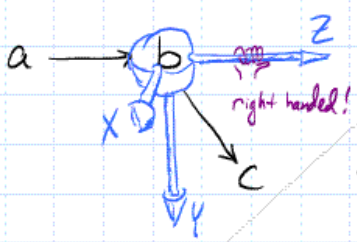
gives perpendicular vector in 3d. (0 if u, v colinear!)



order matters – curl fingers of right hand from u to v

Don't forget to divide by length if you want to use for coordinates.

Bond angles & dihedrals will be most easily constructed if we agree on a standard coordinate frame:

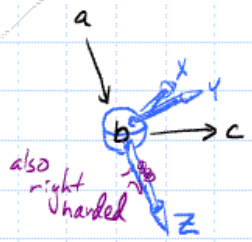


For atom b in the sequence $a \to b \to c$,

let $Z = \frac{b-a}{\|b-a\|}$, the unit vector $a \to b$

$X = \frac{(a-b)\times(c-b)}{\|(a-b)\times(c-b)\|}$, the unit vector $\perp$ to plane abc

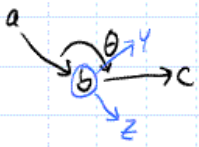
Note: choose any $\perp$ to Z if a,b,c colinear.



$Y = \frac{Z \times X}{\|Z \times X\|}$ ← should already be 1.

Result of this choice:

Bond angle: angle to rotate a around X to match c.



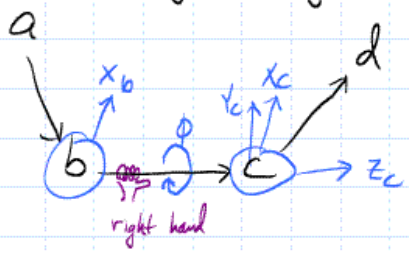
Since c is in the YZ plane,

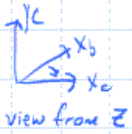
$\theta = \pi - \text{atan2}((c-b)\cdot Y, (c-b)\cdot Z)$

Dihedral angle: angle to rotate abc plane around bc to match bcd plane.

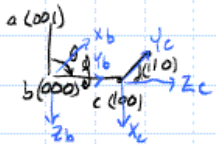
≡ Rotate X_b to X_c, since both are $\perp$ to bc

$\phi = -\text{atan2}(X_b \cdot Y_c, X_b \cdot X_c)$





Check signs for a small example.



$\theta = \pi - \text{atan}(1,0) = \frac{\pi}{2}$ ✓

$\phi = -\text{atan}(1,0) = -\frac{\pi}{2}$ ✓

Let's write our coordinate frame (p, X, Y, Z) as four 4-element vectors.

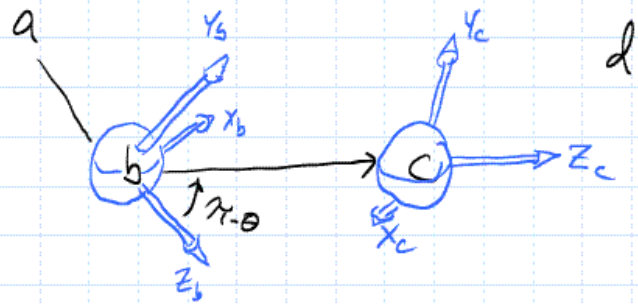
$$\text{frame} = \begin{bmatrix} X_x & Y_x & Z_x & p_x \\ X_y & Y_y & Z_y & p_y \\ X_z & Y_z & Z_z & p_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

vectors; atom coordinates

Doing this lets us write both rotations & translations as 4x4 matrices.

R · frame T · frame

To get coordinates from parameters we can transform coordinate frames. Assume b is (0,0,0), the origin



See also Kavraki's http://cnx.org/content/m11621/latest/

R_x first Rotate around X by $\theta-\pi$ to move Z_b to Z_c

R_z second Rotate around Z by ϕ to move X_b onto X_c

T_z finally Translate along Z by -length(bc) to move c to origin.

$$R_x = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta-\pi & -\sin\theta-\pi & 0 \\ 0 & \sin\theta-\pi & \cos\theta-\pi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R_z = \begin{bmatrix} \cos\phi & -\sin\phi & 0 & 0 \\ \sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$T_z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -\text{length(bc)} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

note order

$$\therefore \text{new frame} = T_z \cdot R_z \cdot R_x \cdot \text{frame}$$

this is a single 4x4 matrix, since matrix multiplication is associative.

Each bond gives us a transformation defined by its parameters.
12 residue loop ⇒ 36 backbone bonds ⇒ 36 4x4 matrices.