Z-Matrix Derivatives

We do so much work with Z-matrices and Cartesians that we should really have an analytic representation of the Jacobian. So let's get on that. We'll start by going from Z-matrix to Cartesian. To do that we note that we need 3 pieces of info

- The origin x_0, can be assumed to be $(0, 0, 0)$ by default
- The axis system $(e_1,\ e_2,\ e_3)$, can be assumed to be I_3
- The Z-matrix

For every atom, our Z-matrix tells us 6 things

- What are the reference positions, x_{i-1}, x_{i-2}, x_{i-3}
- What are the reference values, $z_{i,1}$, $z_{i,2}$, $z_{i,3}$

Derivation

We define our coordinates recursively as

$$\begin{aligned}
v_i &= x_{i-2} - x_{i-1} \\
n_i &= (x_{i-2} - x_{i-1}) \times (x_{i-3} - x_{i-1}) \\
x_i &= x_{i-1} + R\,(z_{i,3},\ v_i) \cdot R\,(z_{i,2},\ n_i) \cdot v_i
\end{aligned}$$

where $R(\theta,\ v)$ is a rotation of θ radians about axis v, given by

$$R(\theta,\ v) = \begin{pmatrix} \cos\theta & -v_z \sin\theta & v_y \sin\theta \\ v_z \sin\theta & \cos\theta & -v_x \sin\theta \\ -v_y \sin\theta & v_x \sin\theta & \cos\theta \end{pmatrix} + \begin{pmatrix} {v_x}^2 & v_x\, v_y & v_x\, v_z \\ v_x\, v_y & {v_y}^2 & v_y\, v_z \\ v_x\, v_z & v_y\, v_z & {v_z}^2 \end{pmatrix} (1 - \cos\theta)$$

This means we get

$$\frac{dx_i}{dq} = \frac{dx_{i-1}}{dq} + \frac{d}{dq}\,(R(z_{i,3},\ v_i) \cdot R(z_{i,2},\ n_i) \cdot v_i)$$

Assuming q is the x, y, or z axes, this isn't terrible to get.

We'll condense the rotation matrices into a single rotation

$$\Theta = R(z_{i,3},\ v_i) \cdot R(z_{i,2},\ n_i)$$

which means that we get

$$\begin{aligned}
\frac{dx_i}{dq} &= \frac{dx_{i-1}}{dq} + \left(\frac{d}{dq}\,\Theta\right) \cdot v_i + \Theta \cdot \frac{d}{dq}\,v_i \\
&= \frac{dx_{i-1}}{dq} + \left(\frac{d}{dq}\,\Theta\right) \cdot v_i + \Theta \cdot \left(\frac{dx_{i-2}}{dq} - \frac{dx_{i-1}}{dq}\right)
\end{aligned}$$

Then we can note that the product rule for matrices also applies as usual, since q is scalar, so we get

$$\frac{d}{dq}\Theta=\left(\frac{d}{dq}R(z_{i,3},\ v_i)\right)\cdot R(z_{i,2},\ n_i)+R(z_{i,3},\ v_i)\cdot\frac{d}{dq}R(z_{i,2},\ n_i)$$

and applying this to our general analytic forms we get

$$\begin{aligned}\frac{d}{dq}R(\theta,\ v)&=\frac{d}{dq}\begin{pmatrix}\cos\theta & -v_z\sin\theta & v_y\sin\theta\\ v_z\sin\theta & \cos\theta & -v_x\sin\theta\\ -v_y\sin\theta & v_x\sin\theta & \cos\theta\end{pmatrix}+(1-\cos\theta)\frac{d}{dq}\begin{pmatrix}{v_x}^2 & v_x\,v_y & v_x\,v_z\\ v_x\,v_y & {v_y}^2 & v_y\,v_z\\ v_x\,v_z & v_y\,v_z & {v_z}^2\end{pmatrix}\\ &=\sin\theta\begin{pmatrix}0 & -\frac{dv_z}{dq} & \frac{dv_y}{dq}\\ \frac{dv_z}{dq} & 0 & -\frac{dv_x}{dq}\\ -\frac{dv_y}{dq} & \frac{dv_x}{dq} & 0\end{pmatrix}+(1-\cos\theta)\frac{d}{dq}\begin{pmatrix}2\frac{dv_x}{dq} & \frac{dv_x}{dq}v_y+v_x\frac{dv_y}{dq} & \frac{dv_x}{dq}v_z+v_x\frac{dv_z}{dq}\\ \frac{dv_x}{dq}v_y+v_x\frac{dv_y}{dq} & 2\frac{dv_x}{dy} & \frac{dv_y}{dq}v_z+v_y\frac{dv_z}{dq}\\ \frac{dv_x}{dq}v_z+v_x\frac{dv_z}{dq} & \frac{dv_y}{dq}v_z+v_y\frac{dv_z}{dq} & 2\frac{dv_x}{dz}\end{pmatrix}\end{aligned}$$

then we have a relation for v_i as

$$\frac{dv_i}{dq}=\frac{dx_{i-2}}{dq}-\frac{dx_{i-2}}{dq}$$

which is pretty easy to build out, but the n_i term is much nastier

$$\frac{dn_i}{dq}=\frac{d}{dq}((x_{i-2}-x_{i-1})\times(x_{i-3}-x_{i-1}))$$

and then we'll want to look at the expression for a cross-product

$$v_1\times v_2=(x_1\quad y_1\quad z_1)\times(x_2\quad y_2\quad z_2)=(-y_2\,z_1+y_1\,z_2\quad x_2\,z_1-x_1\,z_2\quad -x_2\,y_1+x_1\,y_2)$$

then we can get the derivative of this

$$\begin{aligned}\frac{d(v_1\times v_2)}{dq}&=\left(\frac{d}{dq}(-y_2\,z_1+y_1\,z_2)\quad \frac{d}{dq}(x_2\,z_1-x_1\,z_2)\quad \frac{d}{dq}(-x_2\,y_1+x_1\,y_2)\right)\\ &=\begin{pmatrix}-\frac{d}{dq}y_2\,z_1+\frac{d}{dq}y_1\,z_2\\ \frac{d}{dq}x_2\,z_1-\frac{d}{dq}x_1\,z_2\\ -\frac{d}{dq}x_2\,y_1+\frac{d}{dq}x_1\,y_2\end{pmatrix}\\ &=\begin{pmatrix}-\left(\frac{d}{dq}y_2\right)z_1-y_2\frac{d}{dq}z_1+\left(\frac{d}{dq}y_1\right)z_2+y_1\frac{d}{dq}z_2\\ \left(\frac{d}{dq}x_2\right)z_1+x_2\frac{d}{dq}z_1-\left(\frac{d}{dq}x_1\right)z_2-x_1\frac{d}{dq}z_2\\ -\left(\frac{d}{dq}x_2\right)y_1-x_2\frac{d}{dq}y_1+\left(\frac{d}{dq}x_1\right)y_2+x_1\frac{d}{dq}y_2\end{pmatrix}\end{aligned}$$

and for n_i we have

$$\frac{dx_1}{dq}=\frac{d}{dq}\,x_{i-2,x}-\frac{d}{dq}\,x_{i-1,x} \quad \frac{dy_1}{dq}=\frac{d}{dq}\,x_{i-2,y}-\frac{d}{dq}\,x_{i-1,y} \quad \frac{dz_1}{dq}=\frac{dx_{i-2,z}}{dq}-\frac{dx_{i-1,z}}{dq}$$

$$\frac{dx_2}{dq}=\frac{d}{dq}\,x_{i-3,x}-\frac{d}{dq}\,x_{i-1,x} \quad \frac{dy_2}{dq}=\frac{d}{dq}\,x_{i-3,y}-\frac{d}{dq}\,x_{i-1,y} \quad \frac{dz_2}{dq}=\frac{dx_{i-3,z}}{dq}-\frac{dx_{i-1,z}}{dq}$$

so now we have all of our components, and can nicely write out

$$\begin{aligned}\frac{dx_i}{dq}&=\frac{d}{dq}\,(x_{i-1}+R(z_{i,3},\ v_i)\cdot R(z_{i,2},\ n_i)\cdot v_i)\\&=\frac{dx_{i-1}}{dq}+\frac{d}{dq}\,R(z_{i,3},\ v_i)\cdot R(z_{i,2},\ n_i)\cdot v_i+R(z_{i,3},\ v_i)\cdot\frac{d}{dq}\,R(z_{i,2},\ n_i)\cdot v_i+R(z_{i,3},\ v_i)\cdot R(z_{i,2},\ n_i)\cdot\frac{d}{dq}\,v_i\end{aligned}$$

and we know how to write out every one of these components