1 Intro

A quantity commonly needed is the signed angle θ between two vectors v_1, v_2. The naive approach to calculating this angle is to use the dot product identity

$$\theta = \cos^{-1} \frac{v_1 \cdot v_2}{\|v_1\|\|v_2\|}.$$

There are at least three problems with this formula:

- The formula is valid for $0 \leq \theta < 2\pi$, whereas for many applications $-\pi < \theta < \pi$ is required instead.
- In the most important case where θ is small, numerical error can cause the argument of $\cos^{-1}$ to exceed 1, which will lead to NaNs in programming languages like Matlab, C, etc.
- When θ is small, even when the formula above does not encounter the previous problem, $\cos^{-1}$ is flat near 0 and so the derivatives of θ (needed when calcuating forces, etc.) will be numerically ill-conditioned.

2 Robust θ Calculation

The usual solution to the above three problems is to use a formula based on the tangent half-angle identity instead:

$$\theta = 2\tan^{-1} \frac{\sin\theta}{1+\cos\theta} = 2\tan^{-1} \frac{(v_1 \times v_2)\cdot \hat{z}}{\|v_1\|\|v_2\| + v_1 \cdot v_2}.$$

Notice that in code it is most robust to use the atan2 function rather than $\tan^{-1}$, which has special handling to give the right sign and handle robustly the case where the denominator is small:

$$\theta = 2\,\mathrm{atan2}((v_1 \times v_2)\cdot \hat{z}, \|v_1\|\|v_2\| + v_1 \cdot v_2).$$

(**Important**: The above assumes $\mathrm{atan2}(y, x) = \tan^{-1} \frac{y}{x}$. In some languages the order is reversed.)

3 Derivative of θ

From the above we can calculate the robust derivatives of θ:

$$\begin{aligned}
\nabla_{v_1}\theta &= \frac{2}{1+\left(\frac{(v_1\times v_2)\cdot\hat{z}}{\|v_1\|\|v_2\|+v_1\cdot v_2}\right)^2} \nabla_{v_1} \frac{(v_1 \times v_2)\cdot \hat{z}}{\|v_1\|\|v_2\| + v_1 \cdot v_2} \\
&= \frac{2}{1+\left(\frac{(v_1\times v_2)\cdot\hat{z}}{\|v_1\|\|v_2\|+v_1\cdot v_2}\right)^2} \left[\frac{v_2 \times \hat{z}}{\|v_1\|\|v_2\| + v_1 \cdot v_2} - (v_1 \times v_2)\cdot\hat{z} \frac{\hat{v_1}\|v_2\| + v_2}{(\|v_1\|\|v_2\| + v_1 \cdot v_2)^2}\right] \\
&= \frac{(\|v_1\|\|v_2\| + v_1\cdot v_2)(v_2 \times \hat{z}) - [(v_1\times v_2)\cdot\hat{z}](\hat{v_1}\|v_2\| + v_2)}{\|v_1\|^2\|v_2\|^2 + \|v_1\|\|v_2\| v_1 \cdot v_2} \\
&= \frac{1}{\|v_1\|}\left[\hat{v_2}\times\hat{z} - \frac{[(\hat{v_1}\times\hat{v_2})\cdot\hat{z}](\hat{v_1}+\hat{v_2})}{1+\hat{v_1}\cdot\hat{v_2}}\right] \\
&= \frac{\hat{v_1}\times\hat{z}}{\|v_1\|},
\end{aligned}$$

and of course by symmetry

$$\nabla_{v_2}\theta = -\frac{\hat{v_2}\times\hat{z}}{\|v_2\|}.$$

4 Example: Bending Energy

Suppose your bending energy per node is

$$E_i = \frac{k_{\theta_i}}{2}(\theta_i - \theta_i^0)^2$$

where θ_i is the angle between $x_{i+1} - x_i$ and $x_i - x_{i-1}$ and k_{θ_i}, θ_i^0 are scalar constants (NB: this energy is almost certainly not correct unless k_{θ_i} takes into account the nodal area of x_i). Then

$$\begin{aligned}
\theta_i &= 2\,\mathrm{atan2}\left([(x_i - x_{i-1}) \times (x_{i+1} - x_i)] \cdot \hat{z}\ ,\ \|x_i - x_{i-1}\|\|x_{i+1} - x_i\| + (x_i - x_{i-1}) \cdot (x_{i+1} - x_i)\right) \\
E_i &= \frac{k_{\theta_i}}{2}(\theta_i - \theta_i^0)^2 \\
F_i^{i-1} &= -\nabla_{x_{i-1}} E_i = k_{\theta_i}(\theta_i - \theta_i^0)\frac{(x_i - x_{i-1}) \times \hat{z}}{\|x_i - x_{i-1}\|^2} \\
F_i^{i+1} &= k_{\theta_i}(\theta_i - \theta_i^0)\frac{(x_{i+1} - x_i) \times \hat{z}}{\|x_{i+1} - x_i\|^2} \\
F_i^i &= -F_i^{i+1} - F_i^{i-1}.
\end{aligned}$$