On the Derivatives of the Area of a Triangle in \mathbb{R}^3 with Respect to the Coordinates of the Vertices

by Charles S. Peskin, June 29, 2014

Let a triangle in \mathbb{R}^3 have vertices \mathbf{X}^1 , \mathbf{X}^2 , and \mathbf{X}^3 . Although we shall be concerned with the scalar area and its derivatives, it is useful first to consider the area vector, which points normal to the plane of the triangle and is given by

$$\mathbf{A} = \frac{1}{2} \left(\mathbf{X}^{1} - \mathbf{X}^{3} \right) \times \left(\mathbf{X}^{2} - \mathbf{X}^{3} \right)$$

$$= \frac{1}{2} \left[\left(\mathbf{X}^{1} \times \mathbf{X}^{2} \right) + \left(\mathbf{X}^{2} \times \mathbf{X}^{3} \right) + \left(\mathbf{X}^{3} \times \mathbf{X}^{1} \right) \right]$$

$$= \frac{1}{4} \sum_{p=1}^{3} \epsilon_{pqr} \left(\mathbf{X}^{q} \times \mathbf{X}^{r} \right)$$
(1)

where ϵ_{pqr} has the value +1 if (p,q,r) is an even permutation of (1,2,3), has the value -1 if (p,q,r) is an odd permutation of (1,2,3), and has the value 0 if there are any repeats among the indices (p,q,r).

Throughout this note (until further notice) we are using the summation convention, so summation over q, r = 1, 2, 3 in understood in (1), but the summation over p needs to be written out explicitly since p is not a repeated index.

In components,

$$A_i = \frac{1}{4} \sum_{p=1}^{3} \epsilon_{pqr} \epsilon_{ijk} X_j^q X_k^r \tag{2}$$

Now we differentiate with respect to X_l^s and then with respect to X_m^t . In doing so we make use of

$$\frac{\partial X_j^q}{\partial X_l^s} = \delta_{qs} \delta_{jl} \tag{3}$$

and similarly for other instances of the derivative of a coordinate with respect to a coordinate. Equation (3) simply expresses the fact that we are treating all coordinates of the triangle's vertices as independent variables.

It follows from (2) with the help of (3) that

$$\frac{\partial A_i}{\partial X_l^s} = \frac{1}{4} \sum_{p=1}^3 \left(\epsilon_{psr} \epsilon_{ilk} X_k^r + \epsilon_{pqs} \epsilon_{ijl} X_j^q \right)
= \frac{1}{2} \sum_{p=1}^3 \epsilon_{psr} \epsilon_{ilk} X_k^r$$
(4)

where, in the last step of the foregoing, we have simply noted that the two terms obtained by differentiating A_i are, in fact, equal. To show this, one need only replace q by r and j by k in the second term, and then note that $\epsilon_{prs}\epsilon_{ikl}=\epsilon_{psr}\epsilon_{ilk}$, since both factors have changed sign.

Differentiating both sides of (4) with respect to X_m^t , we find

$$\frac{\partial^2 A_i}{\partial X_l^s \partial X_m^t} = \frac{1}{2} \sum_{p=1}^3 \epsilon_{pst} \epsilon_{ilm} \tag{5}$$

Equations (2), (4), and (5) are all that we need in order to evaluate $\|\mathbf{A}\|$ and also the first and second derivatives of $\|\mathbf{A}\|$ with respect to the coordinates of the vertices of the triangle. To see this, note that

$$\|\mathbf{A}\|^2 = A_i^2 \tag{6}$$

$$\|\mathbf{A}\| \frac{\partial \|\mathbf{A}\|}{\partial X_l^s} = A_i \frac{\partial A_i}{\partial X_l^s} \tag{7}$$

$$\frac{\partial \|\mathbf{A}\|}{\partial X_m^t} \frac{\partial \|\mathbf{A}\|}{\partial X_l^s} + \|\mathbf{A}\| \frac{\partial^2 \|\mathbf{A}\|}{\partial X_l^s \partial X_m^t} = \frac{\partial A_i}{\partial X_m^t} \frac{\partial A_i}{\partial X_l^s} + A_i \frac{\partial^2 A_i}{\partial X_l^s \partial X_m^t}$$
(8)

Thus, we can successively evaluate

$$\|\mathbf{A}\| = \sqrt{A_i^2} \tag{9}$$

$$\frac{\partial \|\mathbf{A}\|}{\partial X_i^s} = \frac{A_i}{\|\mathbf{A}\|} \frac{\partial A_i}{\partial X_i^s} \tag{10}$$

$$\frac{\partial \|\mathbf{A}\|}{\partial X_m^t} = \frac{A_i}{\|\mathbf{A}\|} \frac{\partial A_i}{\partial X_m^t} \tag{11}$$

$$\frac{\partial^2 \|\mathbf{A}\|}{\partial X_l^s \partial X_m^t} = \frac{1}{\|\mathbf{A}\|} \left[-\frac{\partial \|\mathbf{A}\|}{\partial X_m^t} \frac{\partial \|\mathbf{A}\|}{\partial X_l^s} + \frac{\partial A_i}{\partial X_m^t} \frac{\partial A_i}{\partial X_l^s} + A_i \frac{\partial^2 A_i}{\partial X_l^s \partial X_m^t} \right]$$
(12)

Of course (11) is just another instance of (10), but we write it out because it is needed in (12).

As an application, consider the discrete Helfrich bending energy and its derivatives. Instead of a single triangle, we now have a triangulated surface, with triangles numbered $l=1,\ldots,n_t$ and vertices denoted $\mathbf{X}^k, k=1,\ldots,n_v$. Let $\mathcal{T}(k)$ be the set of indices of the triangles that touch vertex k.

To be consistent with our previous notation, we let A(l) be the vector area of triangle l. The scalar area is then the Euclidean norm of this vector, which is

denoted $\|\mathbf{A}(l)\|$. The discrete total curvature times area vector at vertex k of the triangulated surface is defined as

$$\mathbf{H}^{k} = -\frac{\partial}{\partial \mathbf{X}^{k}} \sum_{l=1}^{n_{t}} \|\mathbf{A}(l)\|$$

$$= -\sum_{l=1}^{n_{t}} \frac{\partial}{\partial \mathbf{X}^{k}} \|\mathbf{A}(l)\|$$

$$= -\sum_{l \in \mathcal{T}(k)} \frac{\partial}{\partial \mathbf{X}^{k}} \|\mathbf{A}(l)\|$$
(13)

Note that \mathbf{H}^k conceptually includes the amount of area associated with vertex k, which we denote by a^k and define as follows:

$$a^{k} = \frac{1}{3} \sum_{l \in \mathcal{I}(k)} \|\mathbf{A}(l)\| \tag{14}$$

The discrete Helfrich bending energy of the whole triangulated surface is defined as

$$E_{b} = \frac{K_{b}}{2} \sum_{k=1}^{n_{v}} \frac{\|\mathbf{H}^{k}\|^{2}}{a^{k}}$$
 (15)

At this point, we stop using the summation convention, and we denote the component indices of vectors by Greek subscripts. The α component of the force on vertex j that results from the Helfrich bending energy is

$$(\mathbf{F}_{b})_{\alpha}^{j} = -\frac{\partial}{\partial X_{\alpha}^{j}} E_{b}$$

$$= -\frac{K_{b}}{2} \sum_{k=1}^{n_{v}} \frac{\partial}{\partial X_{\alpha}^{j}} \frac{\|\mathbf{H}^{k}\|^{2}}{a^{k}}$$

$$= -\frac{K_{b}}{2} \sum_{k=1}^{n_{v}} \frac{a^{k} \frac{\partial (\|\mathbf{H}^{k}\|^{2})}{\partial X_{\alpha}^{j}} - \|\mathbf{H}^{k}\|^{2} \frac{\partial (a^{k})}{\partial X_{\alpha}^{j}}}{(a^{k})^{2}}$$

$$(16)$$

The derivatives that appear in the above equation are

$$\frac{\partial \left(\|\mathbf{H}^{k}\|^{2}\right)}{\partial X_{\alpha}^{j}} = \frac{\partial \left(\mathbf{H}^{k} \cdot \mathbf{H}^{k}\right)}{\partial X_{\alpha}^{j}}$$

$$= 2 \sum_{\beta=1}^{3} \sum_{l \in \mathcal{T}(k)} \frac{\partial \|\mathbf{A}(l)\|}{\partial X_{\beta}^{k}} \sum_{m \in (\mathcal{T}(k) \cap \mathcal{T}(j))} \frac{\partial^{2} \|\mathbf{A}(m)\|}{\partial X_{\beta}^{k} \partial X_{\alpha}^{j}} \qquad (17)$$

and

$$\frac{\partial \left(a^{k}\right)}{\partial X_{\alpha}^{j}} = \frac{1}{3} \sum_{l \in (\mathcal{T}(k) \cap \mathcal{T}(j))} \frac{\partial \|\mathbf{A}(l)\|}{\partial X_{\alpha}^{j}} \tag{18}$$

Thus the computation of \mathbf{F}_b involves only the (scalar) areas of the triangles that comprise the triangulated surface together with the first and second derivatives of those areas. These can all be evaluated by the methodology outlined in the first part of this note.