Gradient-based minimisation on surfaces: the Thomson problem as example

César L. Pastrana

Here I show how to use a gradient-based minimisation to find the optimal distribution of particles on a spherical shell. We express the coordinates in the spherical coordinate system with azimuth angle ϕ and polar angle θ. We consider a unit sphere, where each particle is repelled via a coulombic-like potential:

$$E = \sum_{\langle i,j \rangle} \frac{1}{s_{ij}} = \frac{1}{\alpha_{ij}} \tag{1}$$

Given a pair of particles $\vec{r} = \vec{r}(\phi, \theta)$ and $\vec{u} = \vec{u}(\phi, \theta)$, the angle between them is then

$$\alpha = acos(\vec{r} \cdot \vec{u}) \tag{2}$$

By using the chain rule we determine the the gradient $\vec{f_x} := \nabla_{\vec{x}} E(\vec{x})$:

$$\vec{f_r} = \frac{1}{\alpha^2 \sqrt{1 - \vec{r} \cdot \vec{u}}} \left[\frac{\partial(\vec{r} \cdot \vec{u})}{\partial \phi_r} \hat{\phi} + \frac{\partial(\vec{r} \cdot \vec{u})}{\partial \theta_r} \hat{\theta} \right] \tag{3}$$

$$\vec{f_u} = \frac{1}{\alpha^2 \sqrt{1 - \vec{r} \cdot \vec{u}}} \left[\frac{\partial(\vec{r} \cdot \vec{u})}{\partial \phi_u} \hat{\phi} + \frac{\partial(\vec{r} \cdot \vec{u})}{\partial \theta_u} \hat{\theta} \right] \tag{4}$$

Is important to note that the coordinates are expressed in the spherical coordinate system. Thus, the dot product cannot be used directly as $\vec{r} \cdot u \neq \phi_r \phi_u + \theta_r \theta_u$[1]. We have to consider the expression for the dot product in spherical coordinates. Then, the derivatives are given by:

$$\frac{\partial(\vec{r} \cdot \vec{u})}{\partial \phi_r} = \cos\theta_r \sin\theta_r \sin\theta_u \cos\phi_u + \cos\theta_r \sin\phi_r \sin\theta_u \sin\phi_u - \sin\theta_r \cos\theta_u \tag{5}$$

$$\frac{\partial(\vec{r} \cdot \vec{u})}{\partial \theta_r} = -\sin\theta_r \sin\phi_r \sin\theta_u \cos\phi_u + \sin\theta_u \sin\phi_u \tag{6}$$

The approach here shown could be used to find the optimal distribution of particles in other parametric surfaces after appropriate modification of s_{ij} to specific geodesic distance between points on the surface.

[1] The general expresion for the dot product (inner product) in non-Euclidean systems is $\langle \vec{r}, \vec{u} \rangle = g_{ij} u^i v^j \equiv u^i v_j \equiv u_i v^j$, where $\vec{u}$ and $\vec{v}$ are contravariant vectors and g_{ij} is the metric tensor. In summary, one first converts one of the vectors the the complementary type and then takes the inner product. See Tensor Calculus, D.C Kay (Schaum's Outlines).