

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

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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:

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

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

$$\alpha = \arccos(\vec{r} \cdot \vec{u}) \quad (2)$$

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

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

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

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

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

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

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.