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 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

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

Then, by using the chain rule we have the value of the gradient, $\vec{f_x} := \nabla_{\vec{x}} E(\vec{x})$

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

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

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

$$\frac{\partial}{\partial \phi_r} = \cos \sin \frac{\partial}{\partial \theta_r} = \cos \sin \tag{5}$$