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BIO-4371
Structure-Based Drug Design
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Institute for Bioinformatics
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Assignment Sheet 7

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A.7.1: Gradient Calculation

Calculation of the gradient of the following function:
$f(x, y, z) = \sqrt{x^2 + y^2 + z^2} = (x^2 + y^2 + z^2)^{\frac{1}{2}}$

$\frac{\partial f}{\partial x} = \frac{1}{2}(x^2 + y^2 + z^2)^{-1/2} \cdot 2x = \frac{x}{\sqrt{x^2+y^2+z^2}}$
$\frac{\partial f}{\partial y} = \frac{1}{2}(x^2 + y^2 + z^2)^{-1/2} \cdot 2y = \frac{y}{\sqrt{x^2+y^2+z^2}}$
$\frac{\partial f}{\partial z} = \frac{1}{2}(x^2 + y^2 + z^2)^{-1/2} \cdot 2z = \frac{z}{\sqrt{x^2+y^2+z^2}}$

$\nabla f(x, y, z) = (\frac{x}{\sqrt{x^2+y^2+z^2}}, \frac{y}{\sqrt{x^2+y^2+z^2}}, \frac{z}{\sqrt{x^2+y^2+z^2}})$

Calculation of the gradient of the distance r_{ij}:
$r_{ij} = |r_i - r_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} = \sqrt{(r_i - r_j)^2}$
since $r_i = (x_i, y_i, z_i)$ and $r_j = (x_j, y_j, z_j)$

$\nabla_{r_i} r_{ij} = \frac{1}{2} \cdot \frac{1}{\sqrt{(r_i - r_j)^2}} \cdot 2 \cdot (2_i - r_j) = \frac{r_i - r_j}{\sqrt{(r_i - r_j)^2}} = \frac{r_i - r_j}{|r_i - r_j|} = \frac{r_i - r_j}{r_{ij}}$

Geometric Point of View:
The gradient of the length $r_{ij} = |r_i - r_j|$ with respect to r_i is a unit vector pointing from r_j to r_i. So in other words, it is the normalized direction vector from atom j to atom i.

Calculate the gradient of the full harmonic stretch term with respect to atom position r_i:
$E(r_i, r_j) = k_s \times (r_{ij} - r_0)^2$
Use the chain rule to solve this:
$\nabla_{r_i} E(r_i, r_j) = 2 \cdot k_s(r_{ij} - r_0) \cdot \nabla_{r_i} r_{ij} = 2 \cdot k_s(r_{ij} - r_0) \cdot \frac{r_i - r_j}{r_{ij}}$