Exercise 02
Molecular Dynamics 2019

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Problem 02.1 *Energy minimisation of force fields*

a Gradient and Hessian are defined as

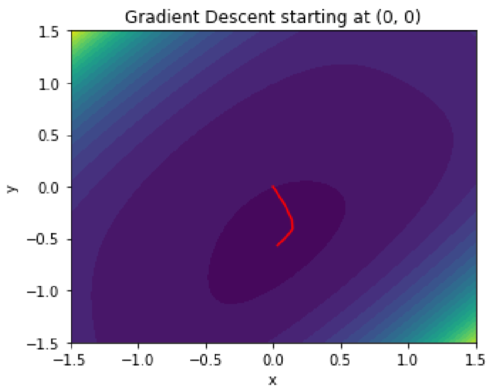
$$\nabla f_i = \frac{\partial f}{\partial x_i}$$
$$\mathbf{H}_{i,j}(f) = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

respectively. Given our function $U(x, y)$, the function, gradient, and hessian matrix are defined

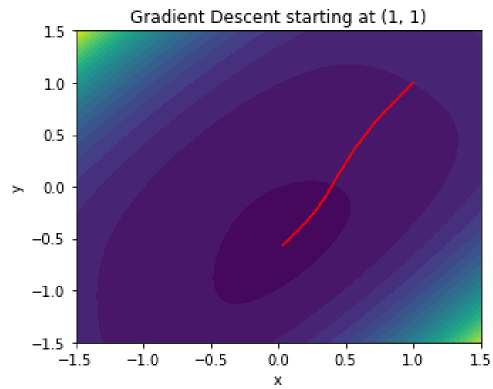
$$U(x, y) = (x - y)^4 + 2x^2 + y^2 - x + 2y \tag{1}$$
$$\nabla U(x, y) = \begin{pmatrix} 4(x - y)^3 + 4x - 1 & -4(x - y)^3 + 2y + 2 \end{pmatrix}^T \tag{2}$$
$$\mathbf{H}(U(x, y)) = \begin{pmatrix} 12(x - y)^2 + 4 & -12(x - y)^2 \\ -12(x - y)^2 & 12(x - y)^2 + 2 \end{pmatrix}. \tag{3}$$

b

Col1	Col2	Col2	Col3
1	6	87837	787
2	7	78	5415
3	545	778	7507
4	545	18744	7560
5	88	788	6344



(a) 1a



(b) 1b

Figure 1: plots of....