DRP - 2025

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0.1 Some preminilary definitions

Take N particles $X_i \in \mathbb{R}^3$ $i = 1, \ldots, N$. We introduce the following notation: the ith particle $X_i \in \mathbb{R}^3$ has coordinates (x_i, y_i, z_i) We denote the vector of N particles by:

$$P = (x_1, x_2, \ldots, x_n, y_1, y_2, \ldots, y_n, z_1, z_2, \ldots, z_n)$$

Definition: A dynamical system is an equation of the form $\frac{dx}{dt} = f(x)$ where $f : \mathbb{R}^n \to \mathbb{R}^m$.

A **steady state** of a dynamical system is a point x such that $\frac{dx}{dt} = f(x) = 0$ This can also be denoted by $\dot{x} = f(x) = 0$

A **gradient system** is a dynamical system that can be written in the form $\frac{dx}{dt} = f(x) = -\nabla E(x)$ where $E : \mathbb{R}^n \to \mathbb{R}$.

∇E is called the **gradient** of E, i.e. if E takes as input $X = (x_1, x_2, ..., x_n)$, then $\nabla E = (\frac{\partial E}{\partial x_1}, \frac{\partial E}{\partial x_2}, ..., \frac{\partial E}{\partial x_n})$.

The **Hessian** H of $E(x)$ is defined by the following matrix:

$$H(\mathbf{x}) = \begin{pmatrix} \frac{\partial^2 E}{\partial x_1^2} & \frac{\partial^2 E}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 E}{\partial x_1 \partial x_n} \\ \frac{\partial^2 E}{\partial x_2 \partial x_1} & \frac{\partial^2 E}{\partial x_2^2} & \cdots & \frac{\partial^2 E}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 E}{\partial x_n \partial x_1} & \frac{\partial^2 E}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 E}{\partial x_n^2} \end{pmatrix}$$

Definition: The finite difference method is a method used to numerically compute the derivative of a function at a specific point. It uses the usual definition of the derivative, but it computes it using a finite rate of change h:

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h} \qquad \frac{\partial f(x,y)}{\partial x} \approx \frac{f(x+h,y) - f(x,y)}{2h}$$

0.2 Particular Dynamical System

Take N particles $X_i \in \mathbb{R}^3$ $i = 1, \ldots, N$. The energy function is given by

$$E(X_1, \ldots, X_N) = \frac{1}{2N} \sum_{i \neq j} K_{\alpha,\lambda}(|X_i - X_j|)$$

where the interaction kernel is

$$K_{\alpha,\lambda}(r) := \frac{1}{\alpha} r^{\alpha} + \frac{1}{\lambda} r^{-\lambda} \tag{1}$$

The kernel came from this paper [1].

Given two particles $X_1 = (x_1, y_1, z_1)$ and $X_2 = (x_2, y_2, z_2)$ in $\mathbf{R}^3$. The distance between them $|X_1 - X_2|$ is given by

$$|X_1 - X_2| = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}.$$

When finding steady states: Each particle $i = 1, \ldots, N$ is tracked via the system of ODEs :

$$\frac{dX_i}{dt} = -\nabla_{X_i} E(X) = -\frac{1}{N} \sum_{j=1}^{N} \nabla K_{\alpha,\lambda}(|X_i - X_j|)$$

0.3 Example $N = 3$

Suppose we have the particles X_1, X_2, X_3. Let's look at $\frac{dX_1}{dt}$

$$\frac{dX_1}{dt} = \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \frac{\partial E}{\partial y_1} \\ \frac{\partial E}{\partial z_1} \end{bmatrix} = -\frac{1}{3} \begin{bmatrix} \frac{\partial K_{\alpha,\lambda}(|X_1 - X_2|)}{\partial x_1} \\ \frac{\partial K_{\alpha,\lambda}(|X_1 - X_2|)}{\partial y_1} \\ \frac{\partial K_{\alpha,\lambda}(|X_1 - X_2|)}{\partial z_1} \end{bmatrix} - \frac{1}{3} \begin{bmatrix} \frac{\partial K_{\alpha,\lambda}(|X_1 - X_3|)}{\partial x_1} \\ \frac{\partial K_{\alpha,\lambda}(|X_1 - X_3|)}{\partial y_1} \\ \frac{\partial K_{\alpha,\lambda}(|X_1 - X_3|)}{\partial z_1} \end{bmatrix}$$

A computation show that :

$$\frac{\partial K_{\alpha,\lambda}(|X_1 - X_j|)}{\partial x_1} = (x_1 - x_j)(r_{1j}^{\alpha-2} - r_{1j}^{-(\lambda+2)})$$

$$\frac{\partial K_{\alpha,\lambda}(|X_1 - X_j|)}{\partial y_1} = (y_1 - y_j)(r_{1j}^{\alpha-2} - r_{1j}^{-(\lambda+2)})$$

$$\frac{\partial K_{\alpha,\lambda}(|X_1 - X_j|)}{\partial z_1} = (z_1 - z_j)(r_{1j}^{\alpha-2} - r_{1j}^{-(\lambda+2)})$$

Similarly:

$$\frac{\partial K_{\alpha,\lambda}(|X_2 - X_j|)}{\partial x_2} = (x_2 - x_j)(r_{2j}^{\alpha-2} - r_{2j}^{-(\lambda+2)})$$

$$\frac{\partial K_{\alpha,\lambda}(|X_2 - X_j|)}{\partial y_2} = (y_2 - y_j)(r_{2j}^{\alpha-2} - r_{2j}^{-(\lambda+2)})$$

$$\frac{\partial K_{\alpha,\lambda}(|X_2 - X_j|)}{\partial z_2} = (z_2 - z_j)(r_{2j}^{\alpha-2} - r_{2j}^{-(\lambda+2)})$$

For the third particle we have

$$\frac{\partial K_{\alpha,\lambda}(|X_3 - X_j|)}{\partial x_3} = (x_3 - x_j)(r_{3j}^{\alpha-2} - r_{3j}^{-(\lambda+2)})$$

$$\frac{\partial K_{\alpha,\lambda}(|X_3 - X_j|)}{\partial y_3} = (y_3 - y_j)(r_{3j}^{\alpha-2} - r_{3j}^{-(\lambda+2)})$$

$$\frac{\partial K_{\alpha,\lambda}(|X_3 - X_j|)}{\partial z_3} = (z_3 - z_j)(r_{3j}^{\alpha-2} - r_{3j}^{-(\lambda+2)})$$

We introduce the following notation: the ith particle $X_i \in \mathbb{R}^3$ has coordinates (x_i, y_i, z_i) We denote the vector of N particles by:

$$P = (x_1, x_2, \dots, x_n, y_1, y_2, \dots, y_n, z_1, z_2, \dots, z_n)$$

Consider the case N = 3. $\frac{dP}{dt} = -\nabla_p E$ and this is given by:

$$\nabla_p E = \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \frac{\partial E}{\partial x_2} \\ \frac{\partial E}{\partial x_3} \\ \frac{\partial E}{\partial y_1} \\ \frac{\partial E}{\partial y_2} \\ \frac{\partial E}{\partial y_3} \\ \frac{\partial E}{\partial z_1} \\ \frac{\partial E}{\partial z_2} \\ \frac{\partial E}{\partial z_3} \end{bmatrix} = -\frac{1}{3} \begin{bmatrix} \frac{\partial(K_{\alpha,\lambda}(|X_1-X_2|)+K_{\alpha,\lambda}(|X_1-X_3|))}{\partial x_1} \\ \frac{\partial(K_{\alpha,\lambda}(|X_1-X_2|)+K_{\alpha,\lambda}(|X_1-X_3|))}{\partial y_1} \\ \frac{\partial(K_{\alpha,\lambda}(|X_1-X_2|)+K_{\alpha,\lambda}(|X_1-X_3|))}{\partial z_1} \\ \frac{\partial(K_{\alpha,\lambda}(|X_2-X_1|)+K_{\alpha,\lambda}(|X_2-X_3|))}{\partial x_2} \\ \frac{\partial(K_{\alpha,\lambda}(|X_2-X_1|)+K_{\alpha,\lambda}(|X_2-X_3|))}{\partial y_2} \\ \frac{\partial(K_{\alpha,\lambda}(|X_2-X_1|)+K_{\alpha,\lambda}(|X_2-X_3|))}{\partial z_2} \\ \frac{\partial(K_{\alpha,\lambda}(|X_3-X_1|)+K_{\alpha,\lambda}(|X_3-X_2|))}{\partial x_3} \\ \frac{\partial(K_{\alpha,\lambda}(|X_3-X_1|)+K_{\alpha,\lambda}(|X_3-X_2|))}{\partial y_3} \\ \frac{\partial(K_{\alpha,\lambda}(|X_3-X_1|)+K_{\alpha,\lambda}(|X_3-X_2|))}{\partial z_3} \end{bmatrix}$$

$$= -\frac{1}{3}\begin{bmatrix} (x_1 - x_2)(r_{12}^{\alpha-2} - r_{12}^{-(\lambda+2)}) + (x_1 - x_3)(r_{13}^{\alpha-2} - r_{13}^{-(\lambda+2)}) \\ (y_1 - y_2)(r_{12}^{\alpha-2} - r_{12}^{-(\lambda+2)}) + (y_1 - y_3)(r_{13}^{\alpha-2} - r_{13}^{-(\lambda+2)}) \\ (z_1 - z_2)(r_{12}^{\alpha-2} - r_{12}^{-(\lambda+2)}) + (z_1 - z_3)(r_{13}^{\alpha-2} - r_{13}^{-(\lambda+2)}) \\ (x_2 - x_1)(r_{21}^{\alpha-2} - r_{21}^{-(\lambda+2)}) + (x_2 - x_3)(r_{23}^{\alpha-2} - r_{23}^{-(\lambda+2)}) \\ (y_2 - y_1)(r_{21}^{\alpha-2} - r_{21}^{-(\lambda+2)}) + (y_2 - y_3)(r_{23}^{\alpha-2} - r_{23}^{-(\lambda+2)}) \\ (z_2 - z_1)(r_{21}^{\alpha-2} - r_{21}^{-(\lambda+2)}) + (z_2 - z_3)(r_{23}^{\alpha-2} - r_{23}^{-(\lambda+2)}) \\ (x_3 - x_1)(r_{31}^{\alpha-2} - r_{31}^{-(\lambda+2)}) + (x_3 - x_1)(r_{31}^{\alpha-2} - r_{31}^{-(\lambda+2)}) \\ (y_3 - y_1)(r_{31}^{\alpha-2} - r_{31}^{-(\lambda+2)}) + (y_3 - y_1)(r_{31}^{\alpha-2} - r_{31}^{-(\lambda+2)}) \\ (z_3 - z_1)(r_{31}^{\alpha-2} - r_{31}^{-(\lambda+2)}) + (z_3 - z_1)(r_{31}^{\alpha-2} - r_{31}^{-(\lambda+2)}) \end{bmatrix}$$

References

[1] Almut Burchard, Rustum Choksi, and Elias Hess-Childs. “On the strong attraction limit for a class of nonlocal interaction energies”. In: *Nonlinear Analysis* 198 (2020), p. 111844. ISSN: 0362-546X. DOI: `https://doi.org/10.1016/j.na.2020.111844`. URL: `https://www.sciencedirect.com/science/article/pii/S0362546X20301036`.