THE SYMPLECTIC CONDITION FOR N-PARTICLES AND D-DIMENSIONS

In the last class (on Dec 1st) we focused on the system comprised by 1 particle and 1 dimension which represents a simplified case. Here, we tackle the explanation of the symplectic condition for N-particles and d-dimensions.

The pair $\vec{\Gamma}$ of generalized positions q_i and momenta p_i is defined as,

$$\vec{\Gamma} = \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix}, \tag{1}$$

where both $\vec{q}$ and $\vec{p}$ have $d \times N$ elements, namely $\vec{q} = (q_1, q_2, \cdots, q_{dN})^T$ and $\vec{p} = (p_1, p_2, \cdots, p_{dN})^T$.

The time evolution of q_i and p_i are defined by Hamilton's equation,

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \tag{2}$$

In terms of $\vec{\Gamma}$, Eq. 2 can be rewritten as,

$$\frac{d\vec{\Gamma}}{dt} = \hat{J}\frac{\partial H}{\partial \vec{\Gamma}}, \quad \hat{J} = \begin{pmatrix} 0 & \hat{1} \\ -\hat{1} & 0 \end{pmatrix}, \tag{3}$$

where $\hat{1}$ is an $(d \times N) \times (d \times N)$ identity matrix, $\hat{J}$ is a $2(d \times N) \times 2(d \times N)$ matrix and the operator $\partial/\partial\vec{\Gamma} \equiv (\partial/\partial\Gamma_1, \partial/\partial\Gamma_2, \cdots, \partial/\partial\Gamma_{2dN})^T = (\partial/\partial q_1, \partial/\partial q_2, \cdots, \partial/\partial q_{dN}, \partial/\partial p_1, \partial/\partial p_2, \cdots, \partial/\partial p_{dN})^T$.

Moreover, a second pair of generalized positions and momenta $\vec{\Gamma}'$ can be derived from the canonical transformation $\vec{\Gamma}$ to $\vec{\Gamma}'$. Hence $\vec{\Gamma}'$ satisfies the Hamilton's equation

$$\frac{d\vec{\Gamma}'}{dt} = \hat{J}\frac{\partial H}{\partial \vec{\Gamma}'}. \tag{4}$$

Since $\vec{\Gamma}'$ is a function as $\vec{\Gamma}$, the time evolution of Γ'_i, which is a i-element of $\vec{\Gamma}'$, can be described as,

$$\frac{d\Gamma'_i}{dt} = \sum_{j=1}^{2dN} \frac{\partial\Gamma'_i}{\partial\Gamma_j}\frac{d\Gamma_j}{dt} = \sum_{j,k=1}^{2dN} \frac{\partial\Gamma'_i}{\partial\Gamma_j} J_{jk} \frac{\partial H}{\partial\Gamma_k} = \sum_{j,k,l=1}^{2dN} \frac{\partial\Gamma'_i}{\partial\Gamma_j} J_{jk} \frac{\partial\Gamma'_l}{\partial\Gamma_k}\frac{\partial H}{\partial\Gamma'_l}. \tag{5}$$

After introducing the Jacobian matrix $\hat{M}$ of the transformation from $\vec{\Gamma}$ to $\vec{\Gamma}'$, Eq. 5 can be rewritten as,

$$\frac{d\vec{\Gamma}'}{dt} = \hat{M}\hat{J}\hat{M}^T\frac{\partial H}{\partial \vec{\Gamma}'}, \quad M_{ij} = \frac{\partial\Gamma'_i}{\partial\Gamma_j}. \tag{6}$$

If the transformation from $\vec{\Gamma}$ to $\vec{\Gamma'}$ is the canonical transformation, $\hat{M}$ satisfied

$$\hat{M}\hat{J}\hat{M}^T = \hat{J}. \tag{7}$$

Eq. 7 is called the symplectic condition. From partitioning the matrix $\hat{M}$ into 4 $(d \times N) \times (d \times N)$ block matrix, namely:

$$\hat{M} = \begin{pmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{pmatrix}, \tag{8}$$

Eq. 7 can be written as,

$$\hat{A}\hat{D}^T - \hat{B}\hat{C}^T = \hat{1}, \tag{9}$$

$$\hat{A}\hat{B}^T = \hat{B}\hat{A}^T, \tag{10}$$

$$\hat{C}\hat{D}^T = \hat{D}\hat{C}^T. \tag{11}$$

Only when $d \times N = 1$, namely in the system for 1 particle and 1 dimension, these condition reduce to 1 condition $det(\hat{M}) = 1$ that is equivalence as Liouville's theorem. In general, the symplectic condition is a strong condition in comparison with $det(\hat{M}) = 1$.

The time evolution $\vec{\Gamma}(t)$ to $\vec{\Gamma}(t + \Delta t)$ based on Hamilton's equation is also the canonical transformation. Hence, Eq. 7 is automatically satisfied in this transformation. However, the symplectic condition may be violated by the numerical integration of discrete Hamilton's equation due to discrete time.

Here, we consider the time evolution $\vec{\Gamma}^n$ to $\vec{\Gamma}^{n+1}$, where index n indicates the time. The elements of matrix $\hat{A}, \hat{B}, \hat{C}$ and $\hat{D}$ are represented as

$$A_{ij} = \frac{\partial q_i^{n+1}}{\partial q_j^n}, \quad B_{ij} = \frac{\partial q_i^{n+1}}{\partial p_j^n}, \quad C_{ij} = \frac{\partial p_i^{n+1}}{\partial q_j^n}, \quad D_{ij} = \frac{\partial p_i^{n+1}}{\partial p_i^n}. \tag{12}$$

The symplectic condition is equivalent as

$$\sum_k A_{ik}D_{jk} + \sum_k B_{ik}C_{jk} = \delta_{ij}, \tag{13}$$

$$\sum_k A_{ik}B_{jk} = \sum_k B_{ik}A_{jk}, \tag{14}$$

$$\sum_k C_{ik}D_{jk} + \sum_k D_{ik}C_{jk}. \tag{15}$$

Example problem

Demonstrate that the Euler algorithm defined as

$$q_i^{n+1} = q_i^n + \frac{p_i^n}{m}h \tag{16}$$

$$p_i^{n+1} = p_i^n - \frac{\partial V}{\partial q_i^n}h \tag{17}$$

don't satisfied the symplectic condition for N particles and d dimensions.

Answer

From Eq. 12, the elements of matrix $\hat{A}, \hat{B}, \hat{C}$ and $\hat{D}$ are represented as

$$A_{ij} = \delta_{ij}, \quad B_{ij} = \frac{h}{m}\delta_{ij}, \quad C_{ij} = -\frac{\partial^2 V}{\partial q_i^n \partial q_j^n}, \quad D_{ij} = \delta_{ij}. \tag{18}$$

Substituting these into Eq. 13, one obtain the following equation

$$\sum_k A_{ik}D_{jk} + \sum_k B_{ik}C_{jk} = \delta_{ij} - \frac{\partial^2 V}{\partial q_i^n \partial q_j^n}\frac{h^2}{m}. \tag{19}$$

Thus, the Euler algorithm don't satisfied the symplectic condition.

Additional exercise

Demonstrate that the leap frog algorithm defined as

$$q_i^{n+1} = q_i^n + \frac{p_i^{n+1}}{m}h \tag{20}$$

$$p_i^{n+1} = p_i^n - \frac{\partial V}{\partial q_i^n}h \tag{21}$$

satisfied the symplectic condition for N particles and d dimensions.