AN ANALYTICAL FORMALISM OF DYNAMICAL SYSTEMS

Symposium 11: Mathematical modeling of complex systems

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1. Dynamical systems: mechanical approach versus teleological approach.
2. The Lagrangian approach: the Havas approach.
3. The Hamiltonian approach: the Dirac approach.
4. Application to the one-dimensional autonomous systems.
5. Thermodynamics interpretation of the analytical formalism.

1. Dynamical systems: mechanical approach versus teleological approach.

Dynamical system: a system of coupled first order differential equations

$$\dot{q}_i(t) = f_i(t, \boldsymbol{q}) \quad i=1, 2, \ldots, n.$$

Mechanical approach: mathematical representation of the causal relations among the system variables.

Teleological approach: can the system follow a trajectory given by an objective? → Yes: the system trajectory is that one that minimizes the **Action S(t)**:

$$S(t) = \int_{t_1}^{t_2} L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})\, dt$$

$L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$: **Lagrangian function**

2. The Lagrangian approach: the Havas approach.

$$S(t) = \int_{t_1}^{t_2} L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})\, dt \quad \overset{¿?}{\Longleftrightarrow} \quad \dot{q}_i(t) = f_i(t, \boldsymbol{q}) \quad i=1, 2, \ldots, n.$$

How to become equivalent both formulations?

If $S(t)$ must be minimum $\Rightarrow$ $\delta S(t) = 0$

$$\Downarrow$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0 \quad j=1, 2, \ldots, n.$$

Lagrange Equations

¿?

$$\dot{q}_i(t) = f_i(t, \boldsymbol{q}) \quad j=1, 2, \ldots, n.$$

This is the so-called as:
Lagrange inverse problem

2. The Lagrangian approach: the Havas approach.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0$$

Lagrange Equations

Lagrange inverse problem

$$\dot{q}_i(t) = f_i(t, \boldsymbol{q})$$

Differential system

P. Havas solution (1973)

(convention of the repeated subscripts assumed as a sum from now onwards)

$$L(t, \boldsymbol{q}, \dot{\boldsymbol{q}}) = g_k(t, \boldsymbol{q})\, \dot{q}_k - V(t, \boldsymbol{q})$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0$$

$$F_{ij}(t, \boldsymbol{q})\, \dot{q}_j = -\frac{\partial g_i(t, \boldsymbol{q})}{\partial t} - \frac{\partial V(t, \boldsymbol{q})}{\partial q_i}$$

Vector field equations

such that:

$$F_{ij}(t, \boldsymbol{q}) = \frac{\partial g_i(t, \boldsymbol{q})}{\partial q_j} - \frac{\partial g_i(t, \boldsymbol{q})}{\partial q_j}$$

F_{ij} antisymetric matrix

2. The Lagrangian approach: the Havas approach.

Lagrange inverse problem

$$F_{ij}(t,\boldsymbol{q})\,\dot{q}_j = -\frac{\partial g_i(t,\boldsymbol{q})}{\partial t} - \frac{\partial V(t,\boldsymbol{q})}{\partial q_i} \Longrightarrow \dot{q}_i(t) = f_i(t,\boldsymbol{q})$$

Vector field equations

Differential system

(Even n or regular case)

(Odd n or singular case)

$$det\big(F_{ij}(t,\boldsymbol{q})\big) \neq 0$$

$$det\big(F_{ij}(t,\boldsymbol{q})\big) = 0$$

(add one equation and variable)

$$\left.\begin{aligned} \dot{q}_i(t) &= f_i(t,\boldsymbol{q}) \\ \dot{q}_{n+1}(t) &= f_{n+1}(t,\boldsymbol{q}) \end{aligned}\right\}$$

$$F_{ij}(t,\boldsymbol{q})\, f_j(t,\boldsymbol{q}) = -\frac{\partial g_i(t,\boldsymbol{q})}{\partial t} - \frac{\partial V(t,\boldsymbol{q})}{\partial q_i}$$

$$\frac{\partial F_{ki}(t,\boldsymbol{q})}{\partial t} = \frac{\partial}{\partial q_k}\Big(F_{ij}(t,\boldsymbol{q})\, f_j(t,\boldsymbol{q})\Big) - \frac{\partial}{\partial q_i}\Big(F_{kj}(t,\boldsymbol{q})\, f_j(t,\boldsymbol{q})\Big)$$

$F_{ij}(t,\boldsymbol{q})$ matrix field equations

2. The Lagrangian approach: the Havas approach.

Summarizing the **Havas approach**:

1. Add a new equation $\dot{q}_{n+1}(t) = f_{n+1}(t, \boldsymbol{q}, q_{n+1})$ to (1) if the dimension *n* is odd.

2. Solve the $F_{ij}(t, \boldsymbol{q})$ functions by:

$$\frac{\partial F_{ki}(t,\boldsymbol{q})}{\partial t} = \frac{\partial}{\partial q_k}\left(F_{ij}(t, \boldsymbol{q})\, f_j(t, \boldsymbol{q})\right) - \frac{\partial}{\partial q_i}\left(F_{kj}(t, \boldsymbol{q})\, f_j(t, \boldsymbol{q})\right)$$

3. Solve the $g_i(t, \boldsymbol{q})$ functions by: $F_{ij}(t, \boldsymbol{q}) = \frac{\partial g_i(t,\boldsymbol{q})}{\partial q_j} - \frac{\partial g_i(t,\boldsymbol{q})}{\partial q_j}$

4. Solve the $V(t, \boldsymbol{q})$ function by: $F_{ij}(t, \boldsymbol{q})\, \dot{q}_j = -\frac{\partial g_i(t,\boldsymbol{q})}{\partial t} - \frac{\partial V(t,\boldsymbol{q})}{\partial q_i}$

5. The Lagrangian is given by: $L(t, \boldsymbol{q}, \dot{\boldsymbol{q}}) = g_k(t, \boldsymbol{q})\, \dot{q}_k - V(t, \boldsymbol{q})$

Note: in those cases where the F_{ij}, g_i and V functions do not depend explicitly on the time, the steps 3 and 4 can be exchanged.

3. The Hamiltonian approach: the Dirac approach.

Momenta

$$p_j = \frac{\partial L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}_j} \Longrightarrow H(t, \boldsymbol{q}, \boldsymbol{p}) = p_j \dot{q}_j - L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$$

Hamiltonian function

Hamilton equations:
equivalent to Lagrange equations

$$\left.\begin{aligned} \dot{q}_j &= \frac{\partial H(t, \boldsymbol{q}, \boldsymbol{p})}{\partial p_j} \\ \dot{p}_j &= -\frac{\partial H(t, \boldsymbol{q}, \boldsymbol{p})}{\partial q_j} \end{aligned}\right\}$$

Present case: $L(t, \boldsymbol{q}, \dot{\boldsymbol{q}}) = g_k(t, \boldsymbol{q})\, \dot{q}_k - V(t, \boldsymbol{q})$

$p_j = g_j(t, \boldsymbol{q})$

$$H(t, \boldsymbol{q}, \boldsymbol{p}) = V(t, \boldsymbol{q})$$

Problem!! $\Longrightarrow$ The Hamiltonian do not depend on momenta

3. The Hamiltonian approach: the Dirac approach.

The **Dirac approach** (Paul A. M. Dirac,1964):

1. Define the **primary constraints**: $\phi_m(t,\boldsymbol{q},\boldsymbol{p}) = p_m - g_m(t,\boldsymbol{q}) = 0$

2. Insert them in the Hamiltonian:

$$H_T(t,\boldsymbol{q},\boldsymbol{p}) = V(t,\boldsymbol{q}) + \lambda_m(t,\boldsymbol{q},\boldsymbol{p})\,\phi_m(t,\boldsymbol{q},\boldsymbol{p})$$

$\lambda_m(t,\boldsymbol{q},\boldsymbol{p}) \Longrightarrow$ unknown multiplying functions to be found

3. Hamilton equations for H_T:

$$\left.\begin{aligned} \dot{q}_j &= \frac{\partial H_T(t,\boldsymbol{q},\boldsymbol{p})}{\partial p_j} = \lambda_j(t,\boldsymbol{q},\boldsymbol{p}) \\ \dot{p}_j &= -\frac{\partial H_T(t,\boldsymbol{q},\boldsymbol{p})}{\partial q_j} = -\frac{\partial V(t,\boldsymbol{q})}{\partial q_j} + \lambda_m(t,\boldsymbol{q},\boldsymbol{p})\frac{\partial g_m(t,\boldsymbol{q})}{\partial q_j} \end{aligned}\right\}$$

3. The Hamiltonian approach: the Dirac approach.

4. State the **consistency conditions** for the primary constants ϕ_m :

$$\dot{\phi}_l(t,\boldsymbol{q},\boldsymbol{p}) = \frac{\partial \phi_l(t,\boldsymbol{q},\boldsymbol{p})}{\partial t} + \frac{\partial \phi_l(t,\boldsymbol{q},\boldsymbol{p})}{\partial q_k}\dot{q}_k + \frac{\partial \phi_l(t,\boldsymbol{q},\boldsymbol{p})}{\partial p_k}\dot{p}_k = 0$$

Hamilton equations

$$F_{lm}(t,\boldsymbol{q})\,\lambda_m(t,\boldsymbol{q},\boldsymbol{p}) = -\frac{\partial g_l(t,\boldsymbol{q})}{\partial t} - \frac{\partial V(t,\boldsymbol{q})}{\partial q_l}$$

Follow Havas approach

No approach followed

Even n

Odd n

$$det\left(F_{ij}(t,\boldsymbol{q})\right) \neq 0$$

$$\lambda_m(t,\boldsymbol{q},\boldsymbol{p}) = f_m(t,\boldsymbol{q})$$

$$\lambda_m(t,\boldsymbol{q},\boldsymbol{p}) = f_m(t,\boldsymbol{q})$$

But some either some $g_l(t,\boldsymbol{q})$ functions or $V(t,\boldsymbol{q})$ function are undetermined

3. The Hamiltonian approach: the Dirac approach.

5. Hamiltonian: $H_T(t,\boldsymbol{q},\boldsymbol{p})$
$= V(t,\boldsymbol{q}) + f_m(t,\boldsymbol{q})(p_m - g_m(t,\boldsymbol{q}))$

6. If $g_l(\boldsymbol{q})$ and $V(\boldsymbol{q})$ independent on time and the system is autonomous, i.e., $f_m(\boldsymbol{q})$, the system **Energy E** can be stated as a motion constant:

$$E = V(\boldsymbol{q}) + f_m(\boldsymbol{q})(p_m - g_m(\boldsymbol{q}))$$

7. Hamilton-Jacobi equation: $S(t,\boldsymbol{q}) \longrightarrow$ Action

$$\frac{\partial S(t,\boldsymbol{q})}{\partial t} + f_m(t,\boldsymbol{q})\left(\frac{\partial S(t,\boldsymbol{q})}{\partial q_m} - g_m(t,\boldsymbol{q})\right) + V(t,\boldsymbol{q}) = 0$$

This equation is very important to interpret the quantum approach

4. Application to the one-dimensional autonomous systems.

$$\dot{q}(t) = f(t, q) \xrightarrow[\text{Autonomous}]{} \dot{q}(t) = f(q)$$

Havas approach: $\left.\begin{array}{l} \dot{q}_1(t) = f_1(q_1) \\ \dot{q}_2(t) = f_2(q_1) \end{array}\right\}$ $\begin{array}{l} \Rightarrow \dot{q}(t) = f(q) \\ \Rightarrow \text{Arbitrary } f_2 \end{array}$

From the simplifying hypotheses that $g_l(\boldsymbol{q})$ and $V(\boldsymbol{q})$ are independent on time :

$$L(\boldsymbol{q}) = \frac{\mathrm{e}^{q_2 - \int \frac{f_2(q_1)}{f_1(q_1)} dq_1}}{f_1(q_1)} \dot{q}_1 + \mathrm{e}^{q_2} \dot{q}_2 - \mathrm{e}^{q_2 - \int \frac{f_2(q_1)}{f_1(q_1)} dq_1}$$

$$E = H(\boldsymbol{q}, \boldsymbol{p}) = f_1(q_1)\, p_1 + f_2(q_1)\, p_2 - f_2(q_1)\, \mathrm{e}^{q_2}$$

$\Downarrow \longleftarrow$ $\dot{q}_2(t) = f_2(q_1) = 1$, i.e., $q_2 = t$

$$E = H(\boldsymbol{q}, \boldsymbol{p}) = f_1(q_1)\, p_1 + p_2 - \mathrm{e}^{q_2}$$

4. Application to the one-dimensional autonomous systems.

Dirac approach to: $\dot{q}(t) = f(t,q)$

$$H_T(t,q,p) = V(t,q) + \lambda(t,q,p)\,\phi(t,q,p) \quad \phi(t,q,p) = p - g(t,q)$$

Consistency condition: $\dot{\phi} = \dfrac{\partial g(t,q)}{\partial t} + \dfrac{\partial V(t,q)}{\partial q} = 0$ Problem: $\lambda(t,q,p)$ is not present

$$\Downarrow$$

Secondary constraint: $\chi(t,q,p) = \dfrac{\partial g(t,q)}{\partial t} + \dfrac{\partial V(t,q)}{\partial q} = 0$

$$\Downarrow$$

Consistency condition: $\dot{\chi}(t,q,p) = 0$

$$\Downarrow$$

$$\frac{\partial^2 g(t,q)}{\partial t^2} + \frac{\partial^2 V(t,q)}{\partial t\,\partial q} + f(t,q)\left(\frac{\partial^2 g(t,q)}{\partial q\,\partial t} + \frac{\partial^2 V(t,q)}{\partial q^2}\right) = 0$$

4. Application to the one-dimensional autonomous systems.

$$\dot{q}(t) = f(t,q) \xrightarrow[\text{Autonomous}]{} \dot{q}(t) = f(q)$$

From the simplifying hypotheses that $g_l(\boldsymbol{q})$ and $V(\boldsymbol{q})$
are independent on time, the consistency condition becomes:

$$f(q)\,V''(q) = 0$$

$$\Downarrow$$

$$E = H_T(q,p) = f(q)\,p + k\,q - f(q)\,g(q)$$

The **system energy** is undetermined by the $g(q)$ function

5. Thermodynamics interpretation of the analytical formalism.

Consider the autonomous system: $\dot{q}_i(t) = f_i(\boldsymbol{q})$

The Hamiltonian is:

$$H_T(t,q,p) = \sum_k f_k(q)\, p_k + V(t,q) - \sum_k f_k(q)\, g_k(t,q)$$

Develop $f_k(\boldsymbol{q})$ about an atractor $\boldsymbol{q_a}$ $\qquad f_k(\boldsymbol{q}) = \sum_i A_{ki}(q_i - q_{ia}) + F_k(q)$

$$H_T(t,q,p) = \sum_k A_{kk} q_k\, p_k + \sum_{k\neq i} A_{ki} q_i\, p_k - \sum_{ki} A_{ki} q_{ia}\, p_k + \sum_k F_k(q)\, p_k + V(t,q) - \sum_k f_k(q)\, g_k(t,q)$$

Identify H_T with the thermodynamic Euler equation:

$$U = T\,\Omega + Y_k\, X_k$$

T the temperature and *Ω* the entropy

Y_k as extensive variables and X_k as intensive variables

Identification: $Y_k \rightarrow A_{kk}\, p_k$ and $X_k \rightarrow q_k$

Identification: $\mathrm{T}\Omega = \sum_{k\neq i} A_{ki}\, p_k q_i - \sum_{ki} A_{ki} q_{ia}\, p_k + \sum_k F_k(q)\, p_k + V(t,q) - \sum_k f_k(q)\, g_k(t,q)$