Lecture 11. Integral principles and variational calculus

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Integral principles and variational calculus

- Second Newton's law
- Lagrange equations
- Lagrangian of a second kind
- Hamilton principle
- Lebesgue integral
- Sobolev space

Second Newton's law for conservative system

Three Newton's laws made possible a sunrise of mathematical analysis at consequence centuries.
As system of equations for moving particles can be wrote as follows:

$$
\begin{aligned}
m_i x_i'' &= X_i, \\
m_i y_i'' &= Y_i, \\
m_i z_i'' &= Z_i.
\end{aligned} \tag{1}
$$

Here $i = 1, \ldots, N$, m_i is a mass of i-th particle, (x_i, y_i, z_i) are their coordinates and (X_i, Y_i, Z_i) is coordinates of a force for i-th particle. A dimension of the system is equal $3N$.

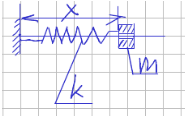
Constrains

In general the particles have *geometric constrains* like ropes, joints and etc.. Such constrains can be written as equations:

$$\phi_s(x_1, y_1, z_1, \ldots, z_n, t) = 0, \quad s = 1, \ldots, m. \tag{2}$$

Every geometric constrain decreases a degree of freedom. A s a result *number of the degrees of freedom* is equal to *dimension of a configuration space* of the system (1) with additional constrains (2) is equal to $3N - m$.
For simplicity we will consider only the geometric constrains and *kinematic constrains* became out of our attention.

Examples

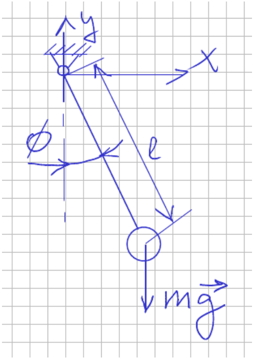


The bead with mass m on
a rod with spring stiffness coefficient k looks like

$$mx'' = -k(x - x_0), \quad y = 0, \quad z = 0.$$

It is important to say a form of this equation *depends on coordinate system*.

Examples



A pendulum with mass m on a rod length l which is jointed l in a gravitational field g can be defined by a system of equations:

$$mx'' = mg\cos(\phi)\sin(\phi),$$
$$my'' = mg - mg\cos^2(\phi)$$

with geometrical constrain:

$$x^2 + y^2 = l^2, \quad z = 0.$$

More convenient
form of this equation looks like follows:

$$\phi'' + \frac{g}{l}\sin(\phi) = 0.$$

This shows *the Newton's equations are non-universal for defining of motion for certain mechanical systems*.

Kinetic and potential energy

Let us multiply by x_i', y_i' and z_i' consequently both parts of the Newton's equations and sum all equations for any particles. As a result we get:

$$\frac{d}{dt}\sum_{i=1}^{n}\left(\frac{m_i}{2}\left[(x_i')^2+(y_i')^2+(z_i')^2\right]\right)=\sum_{i=1}^{n}\left(X_i x_i'+Y_i y_i'+Z_i z_i'\right).$$

The left-hand side of the formula contains a derivative of kinetic energy T on independent variable t.
In the right-hand side we will consider the forces $\mathrm{P}_i=(X_i,Y_i,Z_i)$, which depend on coordinates only. In this case the right-hand side is a derivative of a potential energy with respect to t.

$$\frac{dU}{dt}=\sum_{i=1}^{n}\left(\frac{\partial U}{\partial x_i}x_i'+\frac{\partial U}{\partial y_i}y_i'+\frac{\partial U}{\partial z_i}z_i'\right).$$

Here $U=U(x_1,y_1,z_1,\ldots,z_n)$ is *potential energy* .

Lagrangian

Define

$$L(x, y, z, x', y', z') = T - U.$$

The function L is called *Lagrangian*. This definition can be used for getting the equation for motion:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial x_i'}\right) - \frac{\partial L}{\partial x_i} = 0,$$
$$\frac{d}{dt}\left(\frac{\partial L}{\partial y_i'}\right) - \frac{\partial L}{\partial y_i} = 0,$$
$$\frac{d}{dt}\left(\frac{\partial L}{\partial z_i'}\right) - \frac{\partial L}{\partial z_i} = 0.$$

This form of equations for motion were obtained by Lagrange at 1788 year. This equations are called *the Lagrange equations of first kind*.

The Lagrangian equations with forces of constrains

If the system have additional constrains:

$$f_i(x_1, \dots, z_N) = 0, \quad i = 1, \dots, k,$$

then one should add an additional terms which are reactions of the constrains on i-th particle X_i', Y_i', Z_i'.
The Lagrangian equations look like:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial x_i'}\right) - \frac{\partial L}{\partial x_i} = X_i',$$
$$\frac{d}{dt}\left(\frac{\partial L}{\partial y_i'}\right) - \frac{\partial L}{\partial y_i} = Y_i',$$
$$\frac{d}{dt}\left(\frac{\partial L}{\partial z_i'}\right) - \frac{\partial L}{\partial z_i} = Z_i', \qquad i = 1, \dots, N.$$

The forces of constrains

The force connected with the j-th constrain defined by a gradient: $(\partial f_i/\partial x, \partial f_i/\partial y, \partial f_i/\partial z)$.
Then a sum of forces on i-th particle:

$$X_i' = \left(\lambda_1 \frac{\partial f_1}{\partial x} + \cdots + \lambda_k \frac{\partial f_k}{\partial x}\right)\Bigg|_{x_i, y_i, z_i},$$

$$Y_i' = \left(\lambda_1 \frac{\partial f_1}{\partial y} + \cdots + \lambda_k \frac{\partial f_k}{\partial y}\right)\Bigg|_{x_i, y_i, z_i},$$

$$Z_i' = \left(\lambda_1 \frac{\partial f_1}{\partial z} + \cdots + \lambda_k \frac{\partial f_k}{\partial z}\right)\Bigg|_{x_i, y_i, z_i}.$$

$$f_j(x_1, \ldots, z_N) = 0, \qquad j = 1, \ldots, k.$$

Here λ_j are *Lagrange multipliers*.

The Lagrangian with constrains

$$L = T - U - \sum_{j=1}^{k} l_j f_j.$$

The number of independent variables is $3N + k$.
The invariant form of the equations:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial q_i'}\right) - \frac{\partial L}{\partial q_i} = 0,$$

where new independent variables q_i are $q_i = x_i$, $q_{i+1} = y_i$, $q_{i+2} = z_i$, $i = 1, \ldots, N$, $\quad q_{3N+j} = l_j$, $j = 1, \ldots, k$.

- To construct the Lagrangian of first kind one should find the kinetic energy, potential energy and constrains.
- The equations of motion are defined in invariant form.

Example

The first kind Lagrangian for a pendulum looks like:

$$L = \frac{m}{2}(x'^2 + y'^2) + mgly + \lambda(x^2 + y^2 - 1).$$

The equations of motion are:

$$\begin{aligned} mx'' - 2\lambda x &= 0, \\ my'' - mgl - 2ly &= 0, \\ x^2 + y^2 - 1 &= 0. \end{aligned}$$

Lagrangian of the second kind

Let us define curvilinear coordinates $\mathrm{q} = (q_1, q_2, \ldots, q_n)$. The coordinates of i-th particle q:

$$x_i = f_i(\mathrm{q}, t), \quad y_i = g_i(\mathrm{q}, t), \quad z_i = h_i(\mathrm{q}, t). \tag{3}$$

Notice

$$\frac{\partial x_i'}{\partial q_r'} = \frac{\partial}{\partial q_r'}\left(\frac{\partial f_i}{\partial q_1}q_1' + \cdots + \frac{\partial f_i}{\partial q_n}q_n' + \frac{\partial f_i}{\partial t}\right) = \frac{\partial f_i}{\partial q_r}. \tag{4}$$

Let us multiply left-hand side of the Newton equations (1) by $\partial x_i'/\partial q_r'$, $\partial y_i'/\partial q_r'$ and $\partial z_i'/\partial q_r'$, and the right-hand side multiply by $\partial f_i/\partial q_r$, $\partial g_i/\partial q_r$ and $\partial h_i/\partial q_r$ then add these equations as i:

$$\sum_i m_i\left(x_i''\frac{\partial x_i'}{\partial q_r'} + y_i''\frac{\partial y_i'}{\partial q_r'} + z_i''\frac{\partial z_i'}{\partial q_r'}\right) = \sum_i\left(X_i\frac{\partial f_i}{\partial q_r} + Y_i\frac{\partial g_i}{\partial q_r} + Z_i\frac{\partial h_i}{\partial q_r}\right). \tag{5}$$

Kinetic energy

The left-hand side can be considered as:

$$x_i'' \frac{\partial x_i'}{\partial q_r'} = \frac{d}{dt}\left(x_i' \frac{\partial x_i'}{\partial q_r'}\right) - x_i' \frac{d}{dt}\left(\frac{\partial x_i}{\partial q_r}\right) =$$

$$\frac{d}{dt}\left[\frac{\partial}{\partial q_r}\left(\frac{1}{2}(x_i')^2\right)\right] - \frac{\partial}{\partial q_r}\left(\frac{1}{2}(x_i')^2\right).$$

The same formulas can be obtained for projections on Oy and Oz:

$$\sum_i m_i \left(x_i'' \frac{\partial x_i'}{\partial q_r'} + y_i'' \frac{\partial y_i'}{\partial q_r'} + z_i'' \frac{\partial z_i'}{\partial q_r'}\right) =$$

$$= \frac{1}{2} \sum_i m_i \frac{d}{dt}\left[\frac{\partial}{\partial q_r'}\left((x_i')^2 + (y_i')^2 + (z_i')^2\right)\right] -$$

$$\frac{1}{2} \sum_i m_i \frac{\partial}{\partial q_r}\left((x_i')^2 + (y_i')^2 + (z_i')^2\right).$$

The formula for *kinetic energy* is:

$$T = \frac{1}{2} \sum_i m_i \left((x_i')^2 + (y_i')^2 + (z_i')^2\right) \tag{6}$$

Kinetic energy

Obviously that due to (3) *kinetic energy depends on* q, and using (6) and

$$x_i' = \sum_{r=1}^{n} \frac{\partial f_i}{\partial q_r} q_r' + \frac{\partial f_i}{\partial t}, \quad y_i' = \sum_{r=1}^{n} \frac{\partial g_i}{\partial q_r} q_r' + \frac{\partial g_i}{\partial t}, \quad z_i' = \sum_{r=1}^{n} \frac{\partial h_i}{\partial q_r} q_r' + \frac{\partial h_i}{\partial t} \tag{7}$$

kinetic energy depends on q$'$ *as quadratic*. Also we assume that T *does not depend on time*.
Define the right-hand side of (5) as Q_r, then

$$\frac{d}{dt}\left[\frac{\partial T}{\partial q_r'}\right] - \frac{\partial T}{\partial q_r} = Q_r, \quad r = 1, \ldots, n. \tag{8}$$

$$X = \frac{\partial V}{\partial x}, \quad Y = \frac{\partial V}{\partial y}, \quad Z = \frac{\partial V}{\partial z}.$$

In this case

$$Q_r = \frac{\partial V}{\partial q_r}.$$

Lagrangian of second kind

The function Lagrange looks like:

$$L = T - V.$$

Then the Lagrangian equations can be written as

$$\frac{d}{dt}\left[\frac{\partial L}{\partial q'_r}\right] - \frac{\partial L}{\partial q_r} = 0, \quad r = 1, \ldots, n.$$

These equations are called the Euler-Lagrange equation.

Hamilton principle

The functional

$$S = \int_{t_0}^{t_1} dt\, L(\mathrm{q}, \mathrm{q}', t)$$

is called as action.

The Hamilton principle claims that the mechanical system should get an extrema for the functional (1834):

$$S(q, q') = \int_{t_0}^{t_1} dt\, L(\mathrm{q}, \mathrm{q}', t) \to \text{extr.}$$

Variation of the functional

Let us consider $\delta q = \delta q(t)$ and $\delta q(t_0) - \delta q(t_1) = 0$ as a small smooth function which is called as infinitesimal variation.
A linear part of a difference with respect to δq is called variation of the functional:

$$\delta S = S(q + \delta q, q' + \delta q') - S(q, q').$$

The variation is follows:

$$\delta S = \int_{t_0}^{t_1} dt\, L(\mathrm{q} + \delta q, \mathrm{q}' + \delta q, t) - L(\mathrm{q}, \mathrm{q}', t) =$$

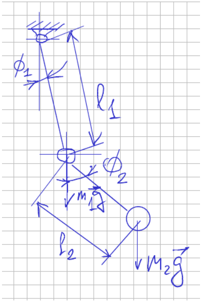
$$\int_{t_0}^{t_1} dt \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial q'}\delta q' = \frac{\partial L}{\partial q'}\delta q'|_{t=t_0}^{t=t_1} +$$

$$\int_{t_0}^{t_1} dt \left(-\frac{d}{dt}\left(\frac{\partial L}{\partial q'}\right) + \frac{\partial L}{\partial q}\right)\delta q.$$

The extremal value of S the functional reaches for the $q = q(t)$ such that:

$$-\frac{d}{dt}\left(\frac{\partial L}{\partial q'}\right) + \frac{\partial L}{\partial q} = 0.$$

Example. Double pendulum



Kinetic energy of the pendulum is:

$$T = \frac{1}{2} m_1 (l_1 \phi_1')^2 \; + \; \frac{1}{2} m_2 \big((l_1 \phi_1')^2 + (l_2 \phi_2')^2 + 2 l_1 l_2 \phi_1' \phi_2' \cos(\phi_1 - \phi_2) \big);$$

potential energy can be written as follows:

$$V = -m_1 l_1 \cos(\phi_1) - m_2 (l_1 \cos(\phi_1) l_2 \cos(\phi_2)).$$

System of equations
for the double pendulum is follows:

$$m_1 l_1^2 \phi_1'' + m_2 l_2^2 \phi_1'' + m_2 l_1 l_2 \phi_2'' \cos(\phi_1 - \phi_2) - m_2 l_1 l_2 \phi_2' (\phi_1' - \phi_2') \sin(\phi_1 - \phi_2) - \big(- m_1 l_1 \sin(\phi_1) - m_2 l_1 \sin(\phi_1) l_2 \cos(\phi_2) \big) = 0,$$

$$m_2 l_2^2 \phi_2'' + m_2 l_1 l_2 \phi_1'' \cos(\phi_1 - \phi_2) - m_2 l_1 l_2 \phi_1' (\phi_1' - \phi_2') \sin(\phi_1 - \phi_2) - - m_2 l_1 \cos(\phi_1) \sin(\phi_2) = 0.$$

Lebesgue integral

Let us consider a function $f(x)$ and a measure μ of set x where $a < f(x) < b$ as $\mu(a < f(x) < b)$.
Slice an interval of values of $f(x)$ on N pieces.
Define a sum:

$$S = \sum_{i=1}^{N} \mu(y_i < f(x) < y_{i+1}).$$

The limit for such sum as $N \to \infty$:

$$\lim_{N\to\infty} \sum_{i=1}^{N} \mu(y_i < f(x) < y_{i+1}) = \int_a^b f(x)dx.$$

is called Lebesgue integral.

Examples of the Lebesgue integrals

- Let us consider a Dirichlet function:

$$f(x) = \begin{cases} 1, & x \in [0,1] \cap \mathbb{Q}; \\ 0 & x \in [0,1] \setminus \mathbb{Q}. \end{cases}$$

This function does not integrabe in a Riemann sense but their Lebesgue integral is equal zero:

$$\int_0^1 f(x) dx = 0.$$

Spaces of distributions

A solution of a Schroedinger equation is a distribution for which only a squared module has a physical sense. Namely a probability of a location for a quantum particle is equals:

$$P(a < x < b) = \int_a^b |\Psi(x,t)|^2 dx.$$

This means that the Ψ should be integrated with squared of the module.

Definition

A space of functions which can be integrated with squared module is called L^2. A function $u(x) \in L^2[a,b]$ if

$$\int_a^b |u(x)|^2 < \infty.$$

Examples

Let us define $\phi(x)$ as a smooth and finite function of x.
Let us find a derivative of $|x|$:

$$\int \frac{d|x|}{dx}\phi(x)dx = |x|\frac{d\phi}{dx}\bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} |x|\frac{d\phi}{dx}dx =$$

$$\int_{-\infty}^{0} x\frac{d\phi}{dx}dx - \int_{0}^{\infty} x\frac{d\phi}{dx}dx =$$

$$-\int_{-\infty}^{0} \phi(x)dx + \int_{0}^{\infty} \phi(x)dx =$$

$$\int_{-\infty}^{\infty} \mathrm{sgn}(x)\phi(x)dx.$$

Therefore:

$$\frac{d|x|}{dx} = \mathrm{sgn}(x).$$

Examples

Let us find a derivative of $\operatorname{sgn}(x)$:

$$\int \frac{d\,\operatorname{sgn}(x)}{dx}\phi(x)dx = \operatorname{sgn}(x)\frac{d\phi}{dx}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \operatorname{sgn}(x)\frac{d\phi}{dx}dx =$$
$$\int_{-\infty}^{0} \frac{d\phi}{dx}dx - \int_{0}^{\infty} \frac{d\phi}{dx}dx =$$
$$\phi(0) - \phi(-\infty) - \phi(\infty) + \phi(0) = 2\phi(0).$$

Therefore:

$$\frac{d\,\operatorname{sgn}(x)}{dx} = 2\delta(x),$$

where

$$\int_{-\infty}^{\infty} \delta(x)\phi(x)dx = 2\phi(0).$$

Extrema of a functional

Let us consider solution of Schroedinger equation in the form:

$$\Psi(x,t) = e^{-iEt/\hbar}\psi(y), \quad y = x/\hbar.$$

The Schroedinger equation can be written as:

$$\frac{1}{2}\frac{\partial^2\psi}{\partial y} - E\psi(y) = 0$$

This equation is a condition for an extrema of a functional:

$$F(\psi) = \frac{1}{2}\int\left|\frac{\partial\psi}{\partial y}\right|^2 dy + E\int|\psi(y)|^2 dy.$$

Variation of a functional

Let us assume for a simplicity that $\psi(y)$ is a real and find a variation:

$$\delta F = F(\psi + \delta\psi) - F(\psi) = \frac{1}{2}\int \left(\frac{\partial(\psi + \delta\psi)}{\partial y}\right)^2 dy +$$

$$E\int (\psi(y) + \delta\psi)^2 dy - \frac{1}{2}\int \left(\frac{\partial \psi}{\partial y}\right)^2 dy + E\int \psi^2(y) dy =$$

$$\int \frac{\partial\psi}{\partial y}\frac{\partial\delta\psi}{\partial y} dy + 2E\int \psi(y)\delta\psi dy = 2\int \left(-\frac{1}{2}\frac{\partial^2\psi}{\partial y^2} + E\psi\right)\delta\psi dy.$$

Therefore $\delta F(\psi) = 0$ if ψ is a solution of the equation:

$$\frac{1}{2}\frac{\partial^2\psi}{\partial y} - E\psi(y) = 0.$$

Distributions and Sobolev space

A functional space of distributions u such that:

$$\int_a^b \left(\frac{\partial u}{\partial x}\right)^2 dx + \int_a^b u^2(x) dx < \infty$$

is called Sobolev space $H_2^1(a, b)$.
More general Sobolev spaces like H_2^k are defined as

$$\sum_{j=0}^{k} \int_a^b \left(\frac{\partial^j u}{\partial x^j}\right)^2 dx < \infty.$$

The norm of Sobolev space define functional like a generalized function which can be undefined at a countable set of points $x \in \{x_i\}$.