Calculus of Variations & Lagrange Multipliers

Dr. Sasan Mahmoodi
The objective: Find $f$ to minimise functional $E$

Lagrangian $L$ is a function of $f$ and $f'$ such as $\sqrt{1+f'^2}$, $(f^2 + \alpha f'^2)$ and so on.

The objective: Find $f$ to minimise functional $E$
$$f_v(s) = f(s) + \alpha y(s)$$

$$a \leq s \leq b$$

$y(s)$ is differentiable

and $y(a) = y(b) = 0$

$\alpha$ is a small quantity

$$f'_v = f' + \alpha y'$$

where $$f' = \frac{df}{ds}$$

$$E_v(\alpha) = \int_a^b L(f'_v, f'_v, s) \, ds$$

The condition for $E_v$ to have extremum (maximum or minimum) is: $$\frac{dE_v}{d\alpha} = 0$$
\[
\frac{dE_v}{d\alpha} = \int_a^b \left[ \frac{\partial L}{\partial f_v} \frac{\partial f_v}{\partial \alpha} + \frac{\partial L}{\partial f'_v} \frac{\partial f'_v}{\partial \alpha} \right] ds = 0
\]

\[
f_v(s) = f(s) + \alpha y(s) \quad \Rightarrow \quad \frac{\partial f_v}{\partial \alpha} = y(s)
\]

\[
f'_v(s) = f'(s) + \alpha y'(s) \quad \Rightarrow \quad \frac{\partial f'_v}{\partial \alpha} = y'(s)
\]

\[
\frac{dE_v}{d\alpha} = \int_a^b \left[ \frac{\partial L}{\partial f_v} y(s) + \frac{\partial L}{\partial f'_v} y'(s) \right] ds = 0
\]

\[
\frac{\partial L}{\partial f'_v} y'(s) = \frac{\partial L}{\partial f'_v} \frac{dy(s)}{ds} = \frac{d}{ds} \left( \frac{\partial L}{\partial f'_v} y(s) \right) - y(s) \frac{d}{ds} \left( \frac{\partial L}{\partial f'_v} \right)
\]
\[
\frac{dE_v}{d\alpha} = \int_a^b \left[ \frac{\partial L}{\partial f_v} y(s) + \frac{d}{ds} \left( \frac{\partial L}{\partial f_v} y(s) \right) - y(s) \frac{d}{ds} \left( \frac{\partial L}{\partial f_v} \right) \right] ds = 0
\]

\[
\frac{dE_v}{d\alpha} = \left[ \frac{\partial L}{\partial f_v} y(s) \right]_a^b + \int_a^b \left[ \frac{\partial L}{\partial f_v} - \frac{d}{ds} \left( \frac{\partial L}{\partial f_v} \right) \right] y(s) ds = 0
\]

\[
\frac{dE_v}{d\alpha} = \int_a^b \left[ \frac{\partial L}{\partial f_v} - \frac{d}{ds} \left( \frac{\partial L}{\partial f_v} \right) \right] y(s) ds = 0
\]

\[
f_v(s) - f(s) = \alpha y(s)
\]

\[
y(s) \neq 0 \quad a \leq s \leq b
\]

\[
\frac{\partial L}{\partial f_v} - \frac{d}{ds} \left( \frac{\partial L}{\partial f_v} \right) = 0
\]

\[
\frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) = 0
\]
Summary:

The function $f(s)$ minimising or maximising functional $E = \int_{a}^{b} L(f, f', s)ds$, is the solution of Euler-Lagrange equation:

$$\frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) = 0$$

Example

$$E = \int (f^2 + \alpha f'^2) ds \quad \Rightarrow \quad L = f^2 + \alpha f'^2$$

$$\frac{\partial L}{\partial f} = 2f \quad \text{and} \quad \frac{\partial L}{\partial f'} = 2\alpha f' \quad \Rightarrow \quad \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) = 2\alpha f''$$

$$\frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) = 0 \quad \Rightarrow \quad 2f - 2\alpha f'' = 0 \quad \Rightarrow \quad f(s) = Ae^{\sqrt{\alpha s}} + Be^{-\sqrt{\alpha s}}$$

$A, B = \text{constant}$
Example 1: Let us now consider the following problem:

What is the shortest path between two points in a plane?

From Euclidean geometry, we know that the shortest path between two points is a straight line.
Now we would like to show this by employing the calculus of variations.

Let us initially calculate the element of distance:

\[ ds = \sqrt{(dx)^2 + (dy)^2} = \sqrt{1 + y_x^2} \, dx \]

The distance \( J \) between two points A and B can be written as:

\[ J_{AB} = \int_{x_A,y_A}^{x_B,y_B} ds = \int_{x_A}^{x_B} \sqrt{1 + y_x^2} \, dx \]

Lagrangian is therefore written as:

\[ L(y, y_x, x) = \sqrt{1 + y_x^2} \]
Euler-Lagrange equations can therefore be written as:

\[- \frac{d}{dx} \left[ \frac{1}{(1 + y_x^2)^{\frac{1}{2}}} \right] = 0 \quad \Rightarrow \quad \left[ \frac{1}{(1 + y_x^2)^{\frac{1}{2}}} \right] = C\]

Therefore \( y_x \) is a constant, i.e.:

\[ y_x = a \quad \Rightarrow \quad y = ax + b \]

\[ E = \int L(f, f', s) ds \quad \Rightarrow \quad \frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) = 0 \]

-Euler-Lagrange equation with higher order derivatives:

\[ E = \int L(f, f', f'', s) ds \quad \Rightarrow \quad \frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) + \frac{d^2}{ds^2} \left( \frac{\partial L}{\partial f''} \right) = 0 \]
- Euler-Lagrange equations with several dependent variables:

\[ E = \int L(f, f', g, g', s) ds \quad \Rightarrow \quad \begin{cases}
\frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) = 0 \\
\frac{\partial L}{\partial g} - \frac{d}{ds} \left( \frac{\partial L}{\partial g'} \right) = 0
\end{cases} \]

- Example: Particle Trajectory

- Finding the exterma of the following functional leads to the equation of the particle motion (trajectory) \((m \text{ and } g \text{ are constant})\):

\[ E = \int \left[ \frac{m}{2} \left( x'^2 + y'^2 \right) - mg \right] dt \]

- Euler-Lagrange equations lead to:

\[
\begin{align*}
x''(t) &= 0 \quad \Rightarrow \quad x(t) = at + b \\
y''(t) &= -g \quad \Rightarrow \quad y(t) = -\frac{1}{2} gt^2 + ct + d
\end{align*}
\]
- Euler-Lagrange equations with several dependent variables and higher orders of derivative:

\[
E = \int L(f, f', f'', g, g', g'', s) ds \Rightarrow \begin{cases} \\
\frac{\partial L}{\partial f} - \frac{d}{ds} \left( \frac{\partial L}{\partial f'} \right) + \frac{d^2}{ds^2} \left( \frac{\partial L}{\partial f''} \right) = 0 \\
\frac{\partial L}{\partial g} - \frac{d}{ds} \left( \frac{\partial L}{\partial g'} \right) + \frac{d^2}{ds^2} \left( \frac{\partial L}{\partial g''} \right) = 0 
\end{cases}
\]

-Euler-Lagrange equations with several independent variables:

\[
E = \iiint L(f, f_x, f_y, f_z, x, y, z) dx dy dz \Rightarrow \frac{\partial L}{\partial f} - \frac{\partial}{\partial x} \frac{\partial L}{\partial f_x} - \frac{\partial}{\partial y} \frac{\partial L}{\partial f_y} - \frac{\partial}{\partial z} \frac{\partial L}{\partial f_z} = 0
\]

- Example 1: Laplace Equation

- In Physics, energy density of an Electric field is defined as:

\[
\text{Energy Density} = \frac{1}{2} \varepsilon E^2
\]
So that: $E = -\nabla \phi$ where $\phi(x, y, z)$ is known as potential function

We want to find $\phi(x, y, z)$ so that the total energy in a volume is minimised:

$$E = \iiint \varepsilon (\nabla \phi)^2 \, dx dy dz = \iiint \varepsilon (\phi_x^2 + \phi_y^2 + \phi_z^2) \, dx dy dz$$

Euler-Lagrange equation leads to the Laplace equation:

$$\nabla^2 \phi = \phi_{xx} + \phi_{yy} + \phi_{zz} = 0$$

- Example 2: Vibrating String

- A function $u(x,t)$ describing small amplitude string vibrations is required so that the following functional is minimal.

$$E = \iint \left( \frac{1}{2} \rho u_t^2 - \frac{1}{2} \pi u_x^2 \right) \, dx dt$$

- Euler-Lagrange equation leads to the wave equation for vibrations

$$\frac{\partial^2 u}{\partial x^2} = \frac{\rho}{\tau} \frac{\partial^2 u}{\partial t^2}$$
Lagrange Multipliers

- Let us consider a differentiable function $f(x,y,z)$, we would like to extermise $f(x,y,z)$ with constraint $\phi(x, y, z) = 0$:

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz$$

To extermise $f$, $df$ should vanish, i.e.:

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz = 0 \quad (1)$$

On the other hand,

$$\phi(x, y, z) = 0 \quad \text{lead to} \quad d\phi = \frac{\partial \phi}{\partial x} dx + \frac{\partial \phi}{\partial y} dy + \frac{\partial \phi}{\partial z} dz = 0 \quad (2)$$

From (1) and (2), we can write: $df + \lambda d\phi = 0$ ( $\lambda$ is constant)
Or

\[ df + \lambda d\phi = \left( \frac{\partial f}{\partial x} + \lambda \frac{\partial \phi}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial \phi}{\partial y} \right) dy + \left( \frac{\partial f}{\partial z} + \lambda \frac{\partial \phi}{\partial z} \right) dz = 0 \quad (3) \]

We choose \( \lambda \) so that \( \left( \frac{\partial f}{\partial z} + \lambda \frac{\partial \phi}{\partial z} \right) = 0 \) \quad (4)

Equation (3) can then be written as:

\[ \left( \frac{\partial f}{\partial x} + \lambda \frac{\partial \phi}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial \phi}{\partial y} \right) dy = 0 \quad (5) \]

In order for (5) to be zero, the following terms need to be zero.

\[ \left( \frac{\partial f}{\partial x} + \lambda \frac{\partial \phi}{\partial x} \right) = 0 \quad (6) \]

\[ \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial \phi}{\partial y} \right) = 0 \quad (7) \]
If we have a set of constraints so that

\[ \phi_k(x, y, z) = 0 \quad k = 1, 2, \ldots, N \]

Then equations (4), (6) and (7) become:

\[
\left( \frac{\partial f}{\partial x_i} + \sum_k \lambda_k \frac{\partial \phi_k}{\partial x_i} \right) = 0
\]

Example 1: In quantum mechanics, we want to find \( a, b \) and \( c \) to minimise the energy (\( E \)) of a particle in a box with sides \( a, b \) and \( c \) so that the volume of the box is constant, i.e.:

\[
\text{minimise } E(a, b, c) = \frac{\hbar^2}{8m} \left( \frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right)
\]

with constraint \( V(a, b, c) = abc = k = \text{constant} \)
\[ f(a, b, c) = E(a, b, c) \]
\[ \phi(a, b, c) = abc - k = 0 \]

Using Lagrange multipliers, we can write:

\[ \frac{\partial E}{\partial a} + \lambda \frac{\partial \phi}{\partial a} = \frac{-h^2}{4ma^3} + \lambda bc = 0 \]
\[ \frac{\partial E}{\partial b} + \lambda \frac{\partial \phi}{\partial b} = \frac{-h^2}{4mb^3} + \lambda ac = 0 \]
\[ \frac{\partial E}{\partial c} + \lambda \frac{\partial \phi}{\partial c} = \frac{-h^2}{4mc^3} + \lambda ab = 0 \]

\[ \left\{ \begin{array}{c}
\frac{\partial E}{\partial a} + \lambda \frac{\partial \phi}{\partial a} = \frac{-h^2}{4ma^3} + \lambda bc = 0 \\
\frac{\partial E}{\partial b} + \lambda \frac{\partial \phi}{\partial b} = \frac{-h^2}{4mb^3} + \lambda ac = 0 \\
\frac{\partial E}{\partial c} + \lambda \frac{\partial \phi}{\partial c} = \frac{-h^2}{4mc^3} + \lambda ab = 0
\end{array} \right\} \rightarrow a = b = c \]

Example 2: In a nuclear reactor, we want to minimise the volume of a reactor vessel (with the shape of circular cylinder of radius \( R \) and height \( H \)) with the following constraint. How should we choose \( R \) and \( H \)?

\[ \phi(R, H) = \left( \frac{2.4048}{R} \right)^2 + \left( \frac{\pi}{H} \right)^2 = \text{constant} \]

minimise \( f(R, H) = \pi R^2 H \)
\[
\begin{align*}
\frac{\partial f}{\partial R} + \lambda \frac{\partial \phi}{\partial R} &= 2\pi RH - 2\lambda \frac{(2.4048)^2}{R^3} = 0 \\
\frac{\partial f}{\partial H} + \lambda \frac{\partial \phi}{\partial H} &= \pi R^2 - 2\lambda \frac{(\pi)^2}{H^3} = 0
\end{align*}
\]

\[
H = \frac{\sqrt{2\pi} R}{2.4048} = 1.847 R
\]

Variation with Constraints

We would like to find the exterma of the following functional with some constraints.

\[
E = \int L \left( y_i, \frac{\partial y_i}{\partial x_j}, x_j \right) dx_j
\]

a) A constraint might be described as:

\[
\phi_k (y_i, x_j) = 0
\]

In this case, we can multiply by a function \( \lambda_k (x_j) \) and integrate over the same range as in the functional to obtain:

\[
\int \lambda_k (x_j) \phi_k (y_i, x_j) dx_j = 0
\]
or

b) A constraint may appear in the form of an integral, i.e.:

\[ \int \phi_k (y_i, \frac{\partial y_i}{\partial x_j}, x_j) dx_j = \text{constant} \]

In both cases, we can form a new functional \( J \) as follows:

\[
J = \int \left( L \left( y_i, \frac{\partial y_i}{\partial x_j}, x_j \right) + \sum_k \lambda_k \phi_k (y_i, x_j) \right) dx_j
\]

For case (a), \( \lambda_k \) are a function of \( x_j \), whereas for case (b), \( \lambda_k \) are simple coefficients.

Functional \( J \) can then be extermsed to find the required solutions. The Lagrangian of functional \( J \) is described as:

\[
\Sigma = L \left( y_i, \frac{\partial y_i}{\partial x_j}, x_j \right) + \sum_k \lambda_k \phi_k (y_i, x_j)
\]

This Lagrangian must satisfy the usual Euler-Lagrange equations, i.e.:

\[
\frac{\partial \Sigma}{\partial y_i} - \sum_j \frac{\partial}{\partial x_j} \left( \frac{\partial \Sigma}{\partial \left( \frac{\partial y_i}{\partial x_j} \right)} \right) = 0
\]
- Example 1: Simple Pendulum

- We need to extremise the following functional:

\[
E = \int \left[ \frac{m}{2} \left( \left( \frac{dr}{dt} \right)^2 + r^2 \left( \frac{d\theta}{dt} \right)^2 \right) + mgr \cos(\theta) \right] dt
\]

with constraint: \( \phi = r - l = 0 \)

\[
\Sigma = \frac{m}{2} \left( r_i^2 + r^2 \theta_i^2 \right) + mgr \cos(\theta) + \lambda (r - l)
\]

\[
\frac{\partial \Sigma}{\partial r} - \frac{d}{dt} \left( \frac{\partial \Sigma}{\partial r_i} \right) = 0 \quad \rightarrow \quad \frac{d}{dt} (mr_i) - mr_i \theta_i^2 - mg \cos(\theta) - \lambda = 0 \quad (1)
\]

\[
\frac{\partial \Sigma}{\partial \theta} - \frac{d}{dt} \left( \frac{\partial \Sigma}{\partial \theta_i} \right) = 0 \quad \rightarrow \quad \frac{d}{dt} (mr_i \theta_i^2) + mgs \sin(\theta) = 0 \quad (2)
\]
Due to the constraint: \[ r = l \quad \rightarrow \quad \frac{dr}{dt} = 0 \]

\[ ml \left( \frac{d\theta}{dt} \right)^2 + mg \cos(\theta) + \lambda = 0 \quad (3) \]

\[ ml^2 \frac{d^2 \theta}{dt^2} + mgl \sin(\theta) = 0 \quad (4) \]

For small values of \( \theta \), equation (4) yields simple harmonic motion and \( \lambda \) can be calculated from equation (3).