Calculus of Variation and its Application

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Outline

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Calculus

- Calculus was developed in the late 17th century by Newton and Leibniz individually.
- It is a mathematical discipline focus on limit, derivative, integral and infinite series.
- **Derivative** of a function at the point $x_0$:

  \[ f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}. \]

  We also denote by $\frac{df}{dx}(x_0)$ as well.

- **Integral** of a function:

  \[ \int_a^b f(x) \, dx = \lim_{n \to \infty, \Delta x_i \to 0} \sum_{i=0}^{n-1} f(x_i) \Delta x_i \]

  where $\Delta x_i = x_{i+1} - x_i$.

- Fundamental theorem of calculus

  \[ \int_a^b f'(x) \, dx = f(b) - f(a). \]
Finding the Maximum and Minimum

Finding maximums and minimums for a giving a smooth function $f(x)$:
Considerer the Taylor expansion of the smooth function $f(x)$:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + \text{higher order terms}$$

- $f'(x_0) > 0$ implies the function $f(x)$ is increasing around $x_0$.
- $f'(x_0) < 0$ implies the function $f(x)$ is decreasing around $x_0$.
- $f'(x_0) = 0$ and $f''(x_0) > 0$ implies $x_0$ is the local minimum.
- $f'(x_0) = 0$ and $f''(x_0) < 0$ implies $x_0$ is the local maximum.
Suppose $f$ is a $C^2$-function on $\mathbb{R}^2$.

- The **directional derivative** of the function $f$ at $\vec{x}$ along the direction $\vec{v}$ is defined as

$$D_{\vec{v}} f(\vec{x}) \equiv \lim_{t \to 0} \frac{f(\vec{x} + t \vec{v}) - f(\vec{x})}{t} = \nabla f(\vec{x}) \cdot \vec{v}$$

- Direction derivative can also be denoted by

$$\nabla_{\vec{v}} f(\vec{x}), \quad \partial \frac{f(\vec{x})}{\partial \vec{v}}, \quad f'_{\vec{v}}(\vec{x}), \quad D_{\vec{v}} f(\vec{x}).$$

- The derivative of $f$ at $\vec{x} \in \mathbb{R}^2$ along the direction $\vec{v}$:

$$D^2_{\vec{v}} f(\vec{x}) \equiv \lim_{t \to 0} \frac{f(\vec{x} + t\vec{v}) - f(\vec{x}) - t\vec{v} \cdot \nabla f(\vec{x})}{t^2}$$

$$= f_{x_1x_1}(\vec{x}) v_1^2 + 2f_{x_1x_2}(\vec{x}) v_1 v_2 + f_{x_2x_2}(\vec{x}) v_2^2$$

Here $\vec{x} = (x_1, x_2)$ and $\vec{v} = (v_1, v_2)$. 
Taylor expansion of a multi-dimensional function

\[
f(x + tv) = f(x) + t D_v f(x) + \frac{t^2}{2} D^2_v f(x) + \text{higher order terms}
\]

\[
= f(x) + t \left( f_{x_1} (x) v_1 + f_{x_2} (x) v_2 \right)
\]

\[
+ \frac{t^2}{2} \left( f_{x_1x_1} (x) v_1^2 + 2 f_{x_1x_2} (x) v_1 v_2 + f_{x_2x_2} (x) v_2^2 \right)
\]

\[
+ \text{higher order terms}
\]
Johann Bernoulli’s Challenge

The calculus of variations as a recognizable as a part of mathematics had its origins in Johann Bernoulli’s challenge in 1696 to the mathematicians of Europe to find the curve of quickest descent, or brachistochrone. The brachistochrone means the ”shortest time” in Greek.

Start the two balls at the top at the same time. The one rolling along the curved path travels further, but reaches the bottom first.
Brachistochrone Curve

- Newton was challenged to solve the problem, and did so the very next day.
- In fact, the solution, which is a segment of a cycloid, was found by Leibniz, L’Hospital, Newton, and the Johann Bernoullis and Jakob Bernoullis.
Formulation of the brachistochrone problem

The time of travel from a point $P_1$ to a point $P_2$ is given by

$$\text{Time} = \int_{P_1}^{P_2} \frac{ds}{v}$$

where $s$ is the arclength and $v$ is the speed.

$$\frac{1}{2}mv^2 = mgy \Rightarrow v = \sqrt{2gy}$$

$$ds = \sqrt{dx^2 + dy^2} = \sqrt{1 + \left(\frac{dy}{dx}\right)^2} \, dx$$

Therefore we obtain the following functional

$$F(y) := \int_{P_1}^{P_2} \frac{\sqrt{1 + y'^2}}{\sqrt{2gy}} \, dx$$

You may think functional $F$ as a function defined on a class of paths $(x, y(x))$ which connect two points $P_1$ and $P_2$. 
Geodesic Problems

**Problem:** Find a curve, joining points $A$ and $B$, with a shortest distance.

- Geodesic problem on a plane.
  
  Answer: a **straight line** joining the points $A$ and $B$.

- Geodesic problem on a sphere.
  
  Answer: a **great circle** joining the points $A$ and $B$. 
Geodesic problem on a sphere

Using spherical coordinate,

\[ Y = (R \cos \theta \sin \varphi, R \sin \theta \sin \varphi, R \cos \varphi) \]

A given the curve joining \( A \) to \( B \) could be represented by a pair of function \((\theta(t), \varphi(t))\) for \( t \in [0, 1] \) with \( \varphi(0) = \theta(1) = 0; \varphi(1) = \varphi_1 \)

The resulting curve defined by

\[ Y(t) = (R \cos \theta(t) \sin \varphi(t), R \sin \theta(t) \sin \varphi(t), R \cos \varphi(t)) \]

and its derivative is

\[ Y'(t) = R (-\sin \theta(\sin \varphi)\theta' + \cos \theta(\cos \varphi)\varphi', \cos \theta(\sin \varphi)\theta' + \sin \theta(\cos \varphi)\varphi', -\sin \varphi \varphi') (t). \]
Geodesic problem on a sphere

The length of the curve is

\[ L(Y) := \int_0^1 |Y'(t)| \, dt = R \int_0^1 \sqrt{\sin^2 \varphi(t) \theta'(t)^2 + \varphi'(t)^2} \, dt \]

The Problem

Find a minimum of the functional \( L \) among a curve \( Y(t) \), represented by \((\theta(t), \varphi(t))\), satisfying \( \varphi(0) = \theta(1) = 0; \varphi(1) = \varphi_1 \)

\[ \min L(Y) = \min R \int_0^1 \sqrt{\sin^2 \varphi(t) \theta'(t)^2 + \varphi'(t)^2} \, dt \]

\[ L(Y) \geq R \int_0^1 \varphi'(t) \, dt = R\varphi(t) \bigg|_0^1 = R\varphi_1 \]

Let \( Y_1(t) \) is a curve represented by \( \theta(t) = 0, \varphi(t) = t\varphi_1 \). Then

\[ L(Y_1) = R \int_0^1 \sqrt{\sin^2(t\varphi_1) 0^2 + \varphi_1^2} \, dt = R\varphi_1 \]
Minimal Area Problem

Find a least-area surface among all smooth surface which can be represented as a graph of a smooth function \( u = u(x, y) \) on a planar domain \( D \) and satisfies the boundary condition \( u|_{\partial D} = \gamma \) for some given function defined on the boundary \( \partial D \).

Let \( S(u) \) be the associated surface area. The problem is formulated in the following form:

\[
\min_{u \in \mathcal{A}} S(u) = \min_{u \in \mathcal{A}} \int_D \sqrt{1 + u_x^2 + u_y^2} \, dx \, dy
\]

where \( \mathcal{A} \) is a collection of continuous differentiable functions

\[
\mathcal{A} = \{ u \in C^1(D) : u = g \text{ on } \partial D \}.
\]
Plateau’s Problem

Suppose $C$ is a closed curve in space. What is the surface $S$ of smallest area having boundary $C$?

- This problem is called **Plateau’s problem** in honor of the physicist, J. Plateau (1801-1883), who experimentally determined a number of the geometric properties of soap films and soap bubbles through interesting experiments with soap films.

- In mathematics, Plateau’s problem is to show the existence of a minimal surface with a given boundary.
The simplest One-dimensional Example:

The variational problem is

$$\min_{y \in A} E(y) = \min_{y \in A} \int_{0}^{1} \left| \frac{dy}{dx} \right|^2 \, dx$$

where the collection $A$ of functions is given by

$$A = \{ y \in C^1(0, 1) : y(0) = 0, \, y(1) = 2 \}.$$ 

Suppose $y \in A$ is a minimizer of the functional $E(y)$. Let $\varphi(x)$ be any continuous differentiable function with $\varphi(0) = \varphi(1) = 0$.

$$E(y + t\varphi) = \int_{0}^{1} \left| \frac{dy}{dx} + t \frac{d\varphi}{dx} \right|^2 \, dx$$
The first variation

\[ \delta E(y, \varphi) \equiv \left. \frac{dE(y + t\varphi)}{dt} \right|_{t=0} \]

Since \( y \) is a minimizer of the functional \( E \), the following derivative is zero.

\[ \delta E(y, \varphi) = 2 \int_0^1 \left( \frac{dy}{dx} + t \frac{d\varphi}{dx} \right) \frac{d\varphi}{dx} \bigg|_{t=0} \, dx = 2 \int_0^1 \frac{dy}{dx} \frac{d\varphi}{dx} \, dx = 0 \]

For any \( \varphi \in C^1[0, 1] \) with \( \varphi(0) = \varphi(1) = 0 \), the following it true

\[ \int_0^1 \frac{dy}{dx} \frac{d\varphi}{dx} \, dx = 0. \]

By using the integration by part,

\[ 0 = \int_0^1 \frac{dy}{dx} \frac{d\varphi}{dx} \, dx = \frac{dy}{dx} \varphi \bigg|_0^1 - \int_0^1 \frac{d^2y}{dx^2} \varphi \, dx = - \int_0^1 \frac{d^2y}{dx^2} \varphi \, dx. \]

The Euler-Lagrange equation:

\[ \left\{ \begin{array}{l} \frac{d^2y}{dx^2} = 0 \text{ in } (0, 1) \\ y(0) = 0, \ y(1) = 2 \Rightarrow y(x) = 2x. \end{array} \right. \]
The second variation

- The above discussion only guarantee the solution $y = 2x$ is a critical point for the functional $E$ among all possible variation $\varphi$.

- Consider the second variation

$$
\delta^2 E(y, \varphi) \equiv \frac{d^2E(y + t\varphi)}{dt^2} \Big|_{t=0} = 2 \int_0^1 \left(\frac{d\varphi}{dx}\right)^2 dx > 0
$$

Suppose we set $\Phi(t) = E(y + t\varphi)$. According to the Taylor expansion of the function $\Phi(t)$ at $t = 0$, we find

$$
\Phi(t) = \Phi(0) + \Phi'(0) t + \frac{1}{2} \Phi''(0) t^2 + \text{high order terms,}
$$

that is

$$
E(y + t\varphi) = E(y) + \delta E(y, \varphi) t + \frac{1}{2} \delta^2 E(y, \varphi) t^2 + \text{high order terms}
$$

- We could conclude that

$$
y = 2x
$$

is a minimizer.
Typical One-dimensional Variational Problems

Let $L(x, y, z)$ a function with continuous first and second (partial) derivatives in $x, y, z$. Let $E(y)$ be a functional defined by

$$E(y) = \int_0^1 L(x, y(x), y'(x)) \, dx$$

on the class $\mathcal{A}$ of functions

$$\mathcal{A} = \{ y \in C^1[0, 1] : y(0) = a, y(1) = b \}.$$

Then the extreme $y(x)$ of the functional $E(y)$ satisfies the Euler-Lagrange equation:

$$\frac{\partial L}{\partial y} - \frac{d}{dx} \frac{\partial L}{\partial y'} = 0 \quad \text{in} \quad (0, 1).$$

with the boundary condition $y(0) = a, \ y(1) = b$. 

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The simplest 2-dimensional problem

Let $D$ be some smooth bounded domain and $g$ is a function defined on the boundary $\partial D$. Set

$$A = \{ u \in C^1(D) : u(x, y) = g(x, y) \text{ for } (x, y) \in \partial D \}.$$

The following is one of the simplest 2-d minimization problem

$$\min_{u \in A} E(u) = \min_{u \in A} \int_D u_x^2 + u_y^2 \, dx \, dy$$

The Euler-Lagrange equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial x^2} = 0 \quad \text{in } D$$

with the boundary condition

$$u(x, y) = g(x, y) \quad \text{on } (x, y) \in \partial D.$$
The typical 2-dimensional variational problem

Let $D$ be some smooth bounded domain and $g$ is a function defined on the boundary $\partial D$. Set

$$\mathcal{A} = \{ u \in C^1(D) : u(x, y) = g(x, y) \text{ for } (x, y) \in \partial D \}.$$

Let $L(x, y, z, p_1, p_2)$ be a $C^2$ function in all arguments. Let $E(y)$ be a functional defined by

$$E(u) = \int_D L(x, y, u, u_x, u_y) \, dx dy$$

Then the extreme $u(x, y) \in \mathcal{A}$ of the functional $E(u)$ satisfies the Euler-Lagrange equation:

$$\frac{\partial L}{\partial y} - \frac{d}{dx} \left( \frac{\partial L}{\partial u_x} \right) - \frac{d}{dy} \left( \frac{\partial L}{\partial u_y} \right) = 0 \quad \text{in } D$$

with the boundary condition $u(x, y) = g(x, y)$ on $(x, y) \in \partial D$. 

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The Area Minimizing Problem

Let $S(u)$ be the associated surface area.

$$\min_{u \in \mathcal{A}} S(u) = \min_{u \in \mathcal{A}} \int_D \sqrt{1 + u_x^2 + u_y^2} \, dx \, dy$$

where $\mathcal{A}$ is a collection of continuous differentiable functions

$$\mathcal{A} = \{u \in C^1(D) : u = g \text{ on } \partial D\}.$$

The Euler-Lagrange equation

$$\nabla \cdot \frac{(u_x, u_y)}{\sqrt{1 + u_x^2 + u_y^2}} = 0$$

with the boundary condition

$$u(x, y) = g(x, y) \quad \text{for } (x, y) \in \partial D.$$
Ideas from Calculus

- In calculus, suppose \( f(x) \) is a \( C^2 \)-continuous function.
  \[
  f'(x_0) = 0 \implies x_0 \text{ is a critical point.}
  \]

- In order to check whether \( x_0 \) is a maximal point or a minimal point we need to check the sign of the second derivative.
  \[
  f''(x_0) > 0 \implies f(x_0) \text{ is a local minimal.}
  \]
  \[
  f''(x_0) < 0 \implies f(x_0) \text{ is a local maximum.}
  \]

- Suppose \( f(x, y) \) is a \( C^2 \)-continuous function. The Taylor expansion of the function \( f(x, y) \) at \((x_0, y_0)\) is
  \[
  f(x_0 + tu, y_0 + tv) = f(x_0, y_0) + [f_x(x_0, y_0)u + f_y(x_0, y_0)v]t \\
  + \frac{1}{2}[f_{xx}(x_0, y_0)u^2 + 2f_{xy}(x_0, y_0)uv + f_{yy}(x_0, y_0)v^2]t^2 \\
  + \text{higher order terms}
  \]
Suppose $E(y) \equiv \int_0^1 L(x, y(x), y'(x)) \, dx$ and $A = \{ y \in C^1[0, 1] : y(0) = a, y(1) = b \}$.

- The same issue happen in the calculus of variation.

\[ \delta E(u, \varphi) = 0 \text{ for all possible variation } \varphi \]

i.e.

\[ \frac{\partial L}{\partial y} - \frac{d}{dx} \frac{\partial L}{\partial y'} = 0 \text{ in on } (0, 1). \]

only implies

\[ y \text{ is a local extreme point in } A. \]

- In order to tell whether the extreme $y$ of the functional $E(y)$ is a local minimum or a local maximum, we need check the second variation of $E(y)$. 

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The Second Variation of $E(y)$

\[
\delta^2 E(y, \varphi) = \left. \frac{d^2 E(y + t\varphi)}{dt^2} \right|_{t=0}
= \int_0^1 \left. \frac{d^2}{dt^2} L(x, y + t\varphi, y' + t\varphi') \right|_{t=0} dx
= \int_0^1 \left( L_{yy} \varphi^2 + 2L_{yy'} \varphi \varphi' + L_{y'y'} \varphi'^2 \right) dx
\]

Suppose $y(x)$ is a local extreme, i.e. $\delta E(y, \varphi) = 0$ for all $\varphi \in C^1_0[0, 1]$. We have the following conclusion:

- If $L_{y'y'}(x, y(x), y'(x)) > 0$ for all $\varphi \in C^1_0[0, 1]$ and $\delta^2 E(y, \varphi) > 0$ for all $\varphi \in C^1_0[0, 1]$, then $y(x)$ is a weak minimum.
- If $L_{y'y'}(x, y(x), y'(x)) < 0$ for all $\varphi \in C^1_0[0, 1]$ and $\delta^2 E(y, \varphi) < 0$ for all $\varphi \in C^1_0[0, 1]$, then $y(x)$ is a weak maximum.
The classical indirect method of variational problems is based on the optimistic idea that every minimum problem has a solution. In order to determine this solution, one looks for conditions which have to satisfy by a minimizer. An analysis of the necessary conditions often permits one to eliminate many candidates and eventually identifies a unique solution. For example, we only have one solution of the Euler-Lagrange equation satisfying all prescribed conditions. We tempted to infer that this solution is also be a solution to the original minimum problem.

The above approach is false. We have to prove the existence of minimizer before we could conclude the uniqueness of solutions to the Euler-Lagrange equation.

Usually, in higher dimension solving the Euler-Lagrange equation is more difficult than finding a minimizer of a functional.
The Direct Method for area minimizing problem

Let $F$ be the a functional defined on an unit disk.

$$ F(u) = \int_D \sqrt{1 + u_x^2 + u_y^2} \, dx \, dy $$

We can find an area minimizing sequence $\{u_n\}$ such that

$$ \lim_{n \to \infty} F(u_n) = \min_u F(u) = \pi. $$

If the area minimizing sequence is "nice enough", we could see the sequence $\{u_n\}$ is getting closer and closer to the unit disk.

**Guess**: The minimal surface is the unit disk.
The Main Idea of Direct Method

Consider a minimization problem on some class $\mathcal{A}$ of functions:

$$\min_{u \in \mathcal{A}} E(u)$$

- Suppose there exist a minimizing sequence $\{u_n\}$ in $\mathcal{A}$. i.e.

$$\lim_{n \to \infty} E(u_n) = \min_{u \in \mathcal{A}} E(u) < +\infty.$$ 

- Suppose we could find an element $v_0$ in $\mathcal{A}$ such that

"$u_n \to v_0$" as $n \to \infty$.

- Suppose the functional $E$ has some kind of continuity. Therefore

$$\lim_{n \to \infty} E(u_n) = E(v_0).$$

- We conclude that $v_0$ is a minimizer of the functional $E$ because

$$E(v_0) = \lim_{n \to \infty} E(u_n) = \min_{u \in \mathcal{A}} E(u).$$
The Difficulty of Direct Method

A surface with area $\pi + 1$

A surface with area $\pi + \frac{1}{4}$

A surface with area $\pi + \frac{1}{16}$

A surface with area $\pi + \frac{1}{64}$
The Setting of the Direct Method

Consider a minimization problem on some class $\mathcal{A}$ of functions:

$$\min_{u \in \mathcal{A}} E(u)$$

Suppose we have following properties on $E$ and $\mathcal{A}$.

1. **(Lower-semi-continuity)** For every sequence $u_n \to u_0$, we have

   $$E(u_0) \leq \liminf_{n \to \infty} E(u_n).$$

2. **(Compactness)** For a bounded sequence $\{u_n\}$ in $\mathcal{A}$, there exist a convergent subsequence $\{u_{n_k}\}$ to some $u_0 \in \mathcal{A}$. 
Existence of a Minimizer by the Direct method

Suppose \( \{v_n\} \) is a minimizing sequence.

\[
\lim_{n \to \infty} E(v_n) = \inf_{v \in A} E(v) < +\infty
\]

If we are possible to show \( \{v_n\} \) is bounded in \( A \), there exist a subsequence \( \{v_{n_k}\} \) and \( v_0 \in A \) such that

\[
v_{n_k} \to v_0 \quad \text{as} \quad k \to \infty.
\]

By the lower-semi-continuity of the functional \( E \), we have

\[
E(v_0) \leq \liminf_{k \to \infty} E(v_{n_k}) = \lim_{n \to \infty} E(v_n) = \inf_{v \in A} E(v)
\]

This implies \( v_0 \) is a minimizer.
A minimum problem without a minimizer

\[
\min_{u \in A} \int_0^1 (u_x^2 - 1)^2 + u^2 \, dx
\]

where

\[ A = \{ u \in C^1[0, 1] : u(0) = u(1) = 0 \} \]

Choose a minimizing sequence \( \{ u_n \} \) which are zigzag functions with slope \( \pm 1 \) and \( u_n \to 0 \) as \( n \to \infty \).

We have

\[
\lim_{n \to \infty} E(u_n) = 0
\]

but

\[
E(0) = 1.
\]

Therefore the minimum is not attained.
Variational principles in physics

There are many laws of physics which are written as variational principles.

- **The Fermat’s principle** in optics
- **The principle of least action** This principle is equivalent to the Newton second law of motion in a mechanical system.
- **The law of maximum entropy**: Thermal equilibrium will reach the maximum entropy of the system.
Fermat’s Principle

- In optics, the **Fermat’s principle**, also called the **principle of the least time**, states that a path taken by a ray of light between two points is the least-time path among all "possible" paths.
- The law of reflection and the law of refraction could be derived from the Fermat’s principle.

Reflection

Refraction

- The Fermat’s principle motivate the principle of least action in mechanic systems.
The Principle of Least Action

- In Physics, the **principle of least action** states that the motion of a mechanical system will follow the trajectory which minimize the action of the system.

- In classical mechanics, the action is defined as an integral along an actual or virtual space-time trajectory $q(t)$ connecting two space-time events, initial event $A \equiv (q_A, t_A = 0)$ and final event $B \equiv (q_B, t_B = T)$. The action is defined as

$$S(q) = \int_{0}^{T} L(q(t), \dot{q}(t)) \, dt$$

where $L(q, \dot{q})$ is the Lagrangian, and $\dot{q} = \frac{dq}{dt}$. The Lagrangian is given as the difference of kinetic energy $K$ and potential energy $V$ along the trajectory $q(t)$:

$$L(q, \dot{q}) = K - V.$$
Classical Mechanics

Let’s consider the one-particle system in a conservative field. The relation between the potential energy of the particle and the force acting on the particle is given by \( \mathbf{F} = (F_1, F_2, F_3) = -\nabla V = -(V_x, V_y, V_z) \) or

\[
\text{Work} = V(A) - V(B) = \int_A^B \mathbf{F} \cdot d\mathbf{s}.
\]

The kinetic energy of the particle is

\[
K = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2).
\]

The associated Lagrangian is

\[
L(x, y, z, \dot{x}, \dot{y}, \dot{z}) = K - V = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V(x, y, z).
\]
Consider the variational problem

$$\min S(x(t), y(t), z(t)) = \min \int_0^T \frac{1}{2} m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V(x, y, z) \, dt$$

$$\delta S = \int_0^T m(\dot{x}\delta\dot{x} + \dot{y}\delta\dot{y} + \dot{z}\delta\dot{z}) - (V_x\delta x + V_y\delta y + V_z\delta z) \, dt$$

$$\delta S = \int_0^T -m(\ddot{x}\delta x + \ddot{y}\delta y + \ddot{z}\delta z) + (F_1\delta x + F_2\delta y + F_3\delta z) \, dt$$

$$\delta S = \int_0^T (F_1 - m\dddot{x})\delta x + (F_2 - m\dddot{y})\delta y + (F_3 - m\dddot{z})\delta z \, dt$$

According to the principle of least action $\delta S = 0$, we obtain

$$\begin{cases} 
m \dddot{x} = F_1 \\
m \dddot{y} = F_2 \\
m \dddot{z} = F_3.
\end{cases}$$

This is the Newton second law of motion,

$$\mathbf{F} = m\mathbf{a}.$$
Lagrangian Mechanics

The Lagrangian is given by

\[ L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) = K(\dot{q}_1, \ldots, \dot{q}_n) - V(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) \]

where \( K \) is the kinetic energy and \( V \) is the potential energy of the system and \((q_1, \ldots, q_n)\) is a generalized coordinate. The action \( S \) is defined by

\[ S(q_1, \ldots, q_n) = \int_0^T L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) \, dt. \]

According to the principle of least action, the Euler-Lagrange equations are

\[
\begin{align*}
\frac{\partial L}{\partial q_1} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_1} &= 0 \\
&\vdots \\
\frac{\partial L}{\partial q_n} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_n} &= 0
\end{align*}
\]

We usually called \( F \equiv (\frac{\partial L}{\partial q_1}, \ldots, \frac{\partial L}{\partial q_n}) \) a generalized force and \( P \equiv (\frac{\partial L}{\partial \dot{q}_1}, \ldots, \frac{\partial L}{\partial \dot{q}_n}) \) a generalized momentum. Therefore, we derive a Newton second law, \( \dot{P} = F \), in the general coordinate.
The principle of least action

\[ \min S(q_1, \ldots, q_n) = \min \int_0^T L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) \, dt \]

provide us a way to find a "suitable" coordinate system for the mechanical system.

The principle of least action could also be applied in the theory of relativity, quantum mechanics and quantum field theory.
A Legendre transformation of a convex function $f$ is defined by

$$f^*(p) = \max_x (px - f(x)).$$

- If $f$ is differentiable, then $f^*(p)$ can be interpreted as the negative of the $y$-intercept of the tangent line to the graph of $f$ that has slope $p$. The value of $x$ attains the maximum has the property

$$f'(x) = p.$$

$$f^*(f'(x)) = x f'(x) - f(x).$$

- Another definition: Set $p = f'(x)$. The inverse function theorem implies $x = x(p)$. Thus we define

$$f^*(p) = p x(p) - f(x(p)).$$
Properties of Legendre Transformation

Set $p = f'(x)$. The inverse function theorem implies $x = x(p)$. Thus we define

$$f^*(p) = px(p) - f(x(p)).$$

- We have following relations:

$$p = \frac{df}{dx}(x),$$

$$x = \frac{df^*}{dp}(p).$$

- Also we have

$$f(x) + f^*(p) = xp.$$  

- And also

$$f = f^{**}.$$
Hamiltonian Mechanics

The Lagrangian of a system is given by \( L(q, \dot{q}) \). We introduce the Hamiltonian function

\[
H(q, p) = \max_{\dot{q}} (p \dot{q} - L(q, \dot{q})).
\]

This is equivalent to

\[
H(q, p) = p \dot{q} - L(q, \dot{q}) \quad \text{and} \quad p = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}),
\]

where the second equation gives us the relation \( \dot{q} = \dot{q}(q, p) \).

Since the double Legendre transformation is itself, we have

\[
L(q, \dot{q}) = p \dot{q} - H(q, p) \quad \text{and} \quad \dot{q} = \frac{\partial H}{\partial p}(q, p).
\]

Example: A system of a single particle

\[
L(q, \dot{q}) = \frac{m}{2} \dot{q}^2 - V(q), \quad p = \frac{\partial L}{\partial \dot{q}} = m \dot{q} \quad \Rightarrow \quad \dot{q} = \frac{p}{m}
\]

\[
H(q, p) = p \dot{q} - L(q, \dot{q}) = \frac{p^2}{m} - (\frac{p^2}{2m} - V(q)) = \frac{p^2}{2m} + V(q) = \text{Total energy}
\]
Hamilton’s equations

Applying the principle of least action to \( L(q, \dot{q}) = p \dot{q} - H(q, p) \), we have

\[
\delta \int_{t_1}^{t_2} L \, dt = \delta \int_{t_1}^{t_2} [p \dot{q} - H(q, p)] \, dt.
\]

We will find

\[
\int_{t_1}^{t_2} \left[ \dot{q} \delta p + p \delta \dot{q} - \frac{\partial H}{\partial p} \delta p - \frac{\partial H}{\partial q} \delta q \right] dt = 0,
\]

\[
\int_{t_1}^{t_2} \left( \dot{q} - \frac{\partial H}{\partial p} \right) \delta p + \left( -\dot{p} - \frac{\partial H}{\partial q} \right) \delta q \, dt = 0.
\]

This leads us to Hamilton’s equations

\[
\begin{cases}
\dot{q} &= \frac{\partial H}{\partial p}, \\
\dot{p} &= -\frac{\partial H}{\partial q}.
\end{cases}
\]
Thermodynamics

- **Thermodynamics** is a branch of physics which study physical systems through **macroscopic** quantities, such as temperature, volume, pressure, etc.

- Thermodynamics concerns phenomena that are in **thermal equilibrium**. Studies of non-equilibrium physical processes are out of the scope of the classical thermodynamics.

- The results of thermodynamics are essential for other fields of physics and chemistry, chemical engineering, aerospace engineering, mechanical engineering, cell biology, biomedical engineering, materials science, and economics.
Laws of Thermodynamics

- **Zeroth law of thermodynamics**: states that if two systems are in thermal equilibrium with a third system, they are also in thermal equilibrium with each other.

- **First law of thermodynamics**: states that heat is a form of energy. The law is no more than a statement of the principle of conservation of energy. Energy can be transformed from one to another.

\[ \Delta U = \Delta Q - W \]

\[ \Delta Q = Q_H - Q_C \]

- **Second law of thermodynamics**: is also called the law of increase of entropy. It states that if a closed system is in a configuration that is not the equilibrium configuration, the most probable consequence will be that the entropy of the system will increase monotonically in successive of time.

- **Third law of thermodynamics**: states that the entropy of a system approaches to a constant value as the temperature approaches zero.
Entropy

- There are two definitions of entropy. One is the thermodynamic definition and the other is the statistic mechanics definition.

- **Thermodynamic entropy** is a non-conserved state function of physical systems. Thermodynamic entropy is more generally defined from the statistical viewpoint, in which the molecular nature of matter is explicitly considered.

- In statistical mechanics, **statistical entropy** is a measure of ways which a system could be arranged. The entropy $S$ is defined as

$$S = k_B \ln \Omega$$

where $\Omega$ is a number of ways and $k_B$ is the Boltzmann constant.

- Boltzmann showed the statistical entropy is equivalent to the thermodynamic one.

- The first law of thermodynamics tells us that energy is conserved in a thermodynamic system. The second law tells us natural processes have a preferred direction of progresses.
Thermal Equilibrium

- A system that is in equilibrium experience no change when isolated from its surroundings.
- In thermodynamics, a system is in thermal equilibrium when it is in thermal equilibrium, mechanical equilibrium, radiative equilibrium, and chemical equilibrium.

One of important questions in thermodynamics is what is the equilibrium state after we remove the boundary between a isolated thermal system and its surrounding.

![Diagram of system and surroundings](image-url)
Callen’s Postulates of Thermodynamics

I. There exist particular states (called equilibrium states) that, macroscopically, are characterized completely by the specification of the internal energy $U$ and a set of extensive parameters $X_1, X_2, \ldots, X_t$ later to be specifically enumerated.

II. There exists a function (called the entropy) of the extensive parameters, defined for all equilibrium states, and having the following property. The values assumed by the extensive parameters in the absence of a constraint are those that maximize the entropy over the manifold of constrained equilibrium states.

III. The entropy of a composite system is additive over the constituent subsystems (whence the entropy of each constituent system is a homogeneous first-order function of the extensive parameters). The entropy is continuous and differentiable and is a monotonically increasing function of the energy.

IV. The entropy of any system vanishes in the state for which
$$T \equiv \left( \frac{\partial U}{\partial S} \right)_{X_1, X_2, \ldots} = 0.$$
The Internal Energy of a system

\[ U = U(X_0, X_1, X_2, X_3, \ldots, X_t) = U(S, V, X_2, \ldots, X_t) \]

where \( X_0 \) denote the entropy \( S \), \( X_1 \) the volume, and the remaining \( X_j \) are the mole numbers. For non-simple systems, the \( X_j \) may represent magnetic, electric, elastic extensive parameters to the system considered.

\[ dU = TdS + \sum_{k=1}^{t} P_k dX_k = \sum_{k=0}^{t} P_k dX_k \]

\[ T = \frac{\partial U}{\partial S} \]

\[ P = \frac{\partial U}{\partial V} \]

\[ P_k = \frac{\partial U}{\partial X_k} \quad \text{for} \ k = 0, \ldots t \]

\( TdS \) is the flux of heat and \( \sum_{k=1}^{t} P_k dX_k \) is the work.
Entropy Maximum Principle and Energy Minimum Principle

\[ S = S(U, X_1, X_2, \ldots, X_t) \iff U = U(S, X_1, X_2, \ldots, X_t) \]

\[
\max_{X_1, \ldots, X_t} S(U_0, X_1, \ldots, X_t) \quad \text{Entropy Maximum Principle}
\]

\[
\min_{X_1, \ldots, X_t} U(S_0, X_1, \ldots, X_t) \quad \text{Energy Minimum Principle}
\]
Legendre Transformations of the Internal Energy

- Experimenters frequently find that the intensive parameters are the more easily measured and controlled and therefore is likely to think of the intensive parameters as operationally independent variables and of the extensive parameters as operationally derived quantities.

- A partial Legendre transformation can be made by replacing the variables $X_0, X_1, \ldots, X_s$ by $P_0, P_1, \ldots, P_s$.

\[
U^*(P_0, P_1, \ldots, P_s, X_{s+1}, \ldots, X_t) = \min_{X_0, \ldots, X_s} \left( U(X_0, X_1, \ldots, X_t) - \sum_{k=0}^{s} P_k X_k \right).
\]

The equilibrium values of any unconstrained extensive parameters $(X_{s+1}, \ldots, X_t)$ in a system in contact with reservoirs of constant $P_0, P_1, \ldots, P_s$ minimize the thermodynamic free energy (potential) $U^*$.

\[
\min_{X_0, \ldots, X_t} \left( U(X_0, X_1, \ldots, X_t) - \sum_{k=0}^{s} P_k X_k \right) = \min_{X_{s+1}, \ldots, X_t} U^*(P_0, P_1, \ldots, P_s, X_{s+1}, \ldots, X_t).
\]
Some Classical Thermodynamic Free Energies

Suppose the internal energy take the form

\[ U = U(S, V, N). \]

- **Helmholtz Free Energy**

\[
A(T, V, N) = \min_S [U(S, V, N) - TS]
\]

\[
\min_{V, N} A(T, V, N)
\]

- **Gibbs Free Energy**

\[
G(T, p, N) = \min_{S, V} [U(S, V, N) + pV - TS]
\]

\[
\min_{N} G(T, p, N)
\]

- **Enthaply**

\[
H(S, p, N) = \min_V [U(S, V, N) + pV]
\]

\[
\min_{S, N} H(S, p, N)
\]

**Remark:** Here \( pV \) related to the work done to the surrounding. It could be replaced by other kinds of work in other system.
Nonuniform Binary Systems

Consider a binary system of $A$ component and $B$ component. The Gibbs energy of the system take the form

$$G(c) = \int_{\Omega} \kappa |\nabla c|^2 + \omega c(1 - c) + kT[c \ln c + (1 - c) \ln(1 - c)] \, dx$$

where $c$ is the mole fraction of the $A$ component and $(1 - c)$ is the mole fraction of the $B$ component.

$T$ temperature
$k$ Boltzmann constant
$\omega$ interaction constant between two components
$\kappa$ some constant

We will see that sufficient cooling may lead to phase separation. (Phase transition)
Equilibrium state

The equilibrium state $c$ of the binary system will minimize the Gibbs energy

$$\min_c G(c) = \min_c \int_\Omega \kappa |\nabla c|^2 + f(c) \, dx.$$  

Here we set

$$f(c) = (1 - c^2)^2.$$  

The Euler-Lagrange equation is

$$-2\kappa \nabla c + \frac{\partial f}{\partial c} = 0 \quad \text{in } \Omega$$

and the boundary condition

$$\mathbf{n} \cdot \nabla c = 0 \quad \text{on } \partial \Omega.$$
One-dimensional Interface

Suppose interface is one-dimensional. We have to consider the problem

$$\min_c \int_{-\infty}^{\infty} \kappa |\frac{dc}{dx}|^2 + f(c) \, dx$$

and $c(x) \to -1$ as $x \to -\infty$ and $c(x) \to 1$ as $x \to \infty$.

$$-2\kappa \frac{d^2 c}{dx^2} + \frac{df}{dc} = 0$$

$$\left(-2\kappa \frac{d^2 c}{dx^2} + \frac{df}{dc}\right) \frac{dc}{dx} = 0$$

$$\frac{d}{dx} \left(-\kappa \left(\frac{dc}{dx}\right)^2 + f(c)\right) = 0$$

$$-\kappa \left(\frac{dc}{dx}\right)^2 + f(c) = \text{constant} = 0$$
\[ \kappa^{1/2} \frac{dc}{dx} = \sqrt{f(c)} = 1 - c^2 \]

\[ \frac{\kappa^{1/2}}{1 - c^2} \frac{dc}{dx} = 1 \]

\[ c(x) = \frac{\exp\left(\frac{x}{\sqrt{\kappa}}\right) - \exp\left(-\frac{x}{\sqrt{\kappa}}\right)}{\exp\left(\frac{x}{\sqrt{\kappa}}\right) + \exp\left(-\frac{x}{\sqrt{\kappa}}\right)} = \tanh\left(\frac{x}{\sqrt{\kappa}}\right) \]

- This tells us the thickness of the interface is \( \sqrt{\kappa} \).
- The energy concentrate near the interface.
- We may guess

\[ G(c) \rightarrow \text{Area functional of the interface} \]

as \( \kappa \rightarrow 0 \). It is true but the rigorous proof requires more mathematics.
Thank you for your attention!