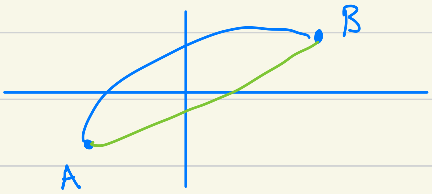
$f'(x) = 0.$ Stationary point

local min / max sign of $f''(x)$.

functional : $D(f(x))$. $D(f)$. Distance function: from A to B. along f.



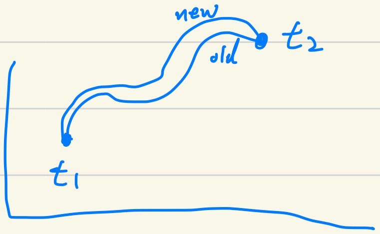
Traditional Calculus : $\mathbb{R} \to f \to \mathbb{R}$. → Stationary point

variational Calculus: $f(x) \to f \to \mathbb{R}$. → Stationary function.

$$D(f) = \int_{x_1}^{x_2} \overset{\text{curve}}{ds} = \int_{x_1}^{x_2} \sqrt{1+f'(x)^2}\, dx$$ minimize this integral.

Variational Calculus: Find some function f s.t.

$$I[f] = \int_{x_1}^{x_2} \overset{\text{Lagrangian.}}{\underline{F(x, f(x), f'(x))}}\, dx$$ is stationary.



$$I[q] = \int_{t_1}^{t_2} \mathcal{L}(t, q(t), q'(t))\, dt.$$

$$I[q + s\cdot\delta q] = \int_{t_1}^{t_2} \mathcal{L}[t, \hat{q}(t), \hat{q}'(t)]\, dt.$$

$$\Rightarrow \frac{d\, I[\hat{q}]}{ds} = \int_{t_1}^{t_2} \partial_s \mathcal{L}[t, \hat{q}(t), \hat{q}'(t)]\, dt.$$

old: q ⤳ new $q + s\cdot\delta q$

$$\underbrace{q(x) + s\cdot\delta q(x).}_{= \hat{q}}$$

for $s \downarrow 0$: $\hat{q} = q$.

boundary: $\delta q(t_1) = \delta q(t_2) = 0$.

$$\begin{array}{lll} & 0 & 1 \\ + & \partial_{\hat q'}\mathcal{L} & \delta\dot q \\ - & \frac{d}{dt}\partial_{\hat q'}\mathcal{L} & \delta q \end{array}$$

$$\partial_t f(x(t), y(t)) = \partial_x f \cdot \partial_t x + \partial_y f \cdot \partial_t y.$$

$$I[q+s\cdot\delta q] = \int_{t_1}^{t_2} \mathcal{L}[t, \hat q(t), \hat q'(t)]\, dt.$$

$$\Rightarrow \quad \frac{d\, I[\hat q]}{ds} = \int_{t_1}^{t_2} \partial_s \mathcal{L}[t, \hat q(t), \hat q'(t)]\, dt.$$

$$= \int_{t_1}^{t_2} \partial_{\hat q}\mathcal{L} \cdot \underbrace{\partial_s \hat q}_{\delta q} + \partial_{\hat q'}\mathcal{L} \cdot \underbrace{\partial_s \hat q'}_{\delta q'} \quad dt.$$

← variation →

$\delta\hat q'$ vanish at t_2, t_1

$$I' = \int_{t_1}^{t_2} \delta q\, \partial_{\hat q}\mathcal{L}\, dt + \delta q\, \partial_{\hat q'}\mathcal{L}\Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \delta q\, \frac{d}{dt}\partial_{\hat q'}\mathcal{L}\, dt.$$

$$= \int_{t_1}^{t_2} \delta q \left[\partial_{\hat q}\mathcal{L} - \frac{d}{dt}\partial_{\hat q'}\mathcal{L}\right] dt$$ seeking minimization.

since q is the optimal.

$$\Rightarrow I'\Big|_{s=0} = 0. = \int_{t_1}^{t_2} \delta q \left[\overbrace{\partial_q \mathcal{L} - \frac{d}{dt}\partial_{q'}\mathcal{L}}\right] dt \longrightarrow$$ Euler-Lagrange equation.

for $s=0$. for $s=0$.

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\frac{\partial F}{\partial y'} = 0.$$

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\frac{\partial F}{\partial y'} = 0. \qquad \frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'} = 0.$$

$$F(f(x)) : f \to \mathbb{R}.$$

$$F = D(y) = \int_{x_1}^{x_2} \sqrt{1+y'(x)^2}\, dx.$$

$$\frac{\partial F}{\partial y} = 0, \qquad \frac{d}{dx}\left[\frac{d\sqrt{1+y'(x)^2}}{d\, y'(x)}\right] = \frac{y''(x)}{\sqrt{1+y'(x)^2}\ \ y'(x)^2} = 0.$$

$$\Rightarrow y''(x) = 0 \quad \Rightarrow \quad f(x) = C_0 + C_1 x.$$

First Variation.

The first variation of a functional $J(y)$ is defined as the linear functional $\delta J(y)$ mapping the function h to $\delta J(y,h) = \lim_{\varepsilon \to 0} \frac{J(y+\varepsilon h) - J(y)}{\varepsilon} = \frac{d}{d\varepsilon} J(y+\varepsilon h)\Big|_{\varepsilon=0}$,

where y and h are functions, and ε is a scalar.

- e.g. Compute the first variation of $J(y) = \int_a^b y y' dx$, $y = y(x)$, $y' = y'(x)$.

From the definition above,

$$\delta J(y,h) = \frac{d}{d\varepsilon} J(y+\varepsilon h)\Big|_{\varepsilon=0}$$

$$= \frac{d}{d\varepsilon} \int_a^b (y+\varepsilon h)(y'+\varepsilon h')\, dx \Big|_{\varepsilon=0}$$

$$= \frac{d}{d\varepsilon} \int_a^b yy' + y\varepsilon h' + y'\varepsilon h + \varepsilon^2 hh' \;\; dx \Big|_{\varepsilon=0}$$

$$= \int_a^b \frac{d}{d\varepsilon} \left\{ yy' + y\varepsilon h' + y'\varepsilon h + \varepsilon^2 hh' \right\} dx \Big|_{\varepsilon=0}$$

$$= \int_a^b \; yh' + y'h + 2\varepsilon hh' \;\; dx \Big|_{\varepsilon=0}$$

$$= \int_a^b (yh' + y'h)\, dx.$$

calculus of variations
Functional derivatives.

Functionals and functional derivative

In an integral L of a functional, if a function f is varied by adding to it another function δf that is arbitrarily small, and the resulting integrand is expanded in powers of δf, the coefficient of δf in the first order term is called functional derivative.

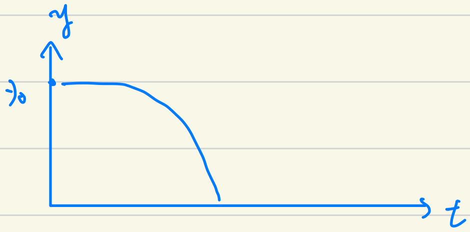
consider functional $J[f] = \int_a^b L(x, f(x), f'(x))\, dx$.

where $f'(x) = \frac{df}{dx}(x)$. If f is varied by adding to it a function δf, and the resulting integrand $L(x, f+\delta f, f'+\delta f')$ is expanded in powers of δf, then the change in the value to J to first order in δf can be:

$$\delta J = \int_a^b \left(\frac{\partial L}{\partial f} \delta f(x) + \frac{\partial L}{\partial f'} \frac{d}{dx} \delta f(x) \right) dx$$

$$= \int_a^b \left(\frac{\partial L}{\partial f} - \frac{d}{dx} \frac{\partial L}{\partial f'} \right) \delta f(x)\, dx + \frac{\partial L}{\partial f'}(b)\, \delta f(b) - \frac{\partial L}{\partial f'}(a)\, \delta f(a) .$$

physics.



(Also solvable by Newtonian Mechanics : $F = m a$).

$E_{pot} = m \cdot g \cdot h . = m \cdot g \cdot y$ $\qquad m$ = mass

g = acceleration due to gravity.

$E_K = \frac{1}{2} m v^2 = \frac{1}{2} m \dot{y}^2$ $\qquad h = y$, $v = \dot{y} = \frac{dy}{dt}$.

if $m = 2$ kg, $g = 2$ m/s². , then if $H = 1$m , then $T = 1$s.

$\Rightarrow E_K = \dot{y}^2$, $E_{pot} = 4y$

$$\int_0^1 E_K - E_{pot} \qquad dt$$

Lagrangian Mechanics.

$$I(y) = \int_0^1 \dot{y}^2_{(t)} - 4y_{(t)} \, dt$$

$$\begin{cases} y(0) = 1 \\ y(1) = 0. \end{cases}$$

"function of function"

I : takes in a function y and outputs a scalar ⇒ called functional

$$I(y = 1 - t) = \int_0^1 \dot{\overline{(1-t)}}^2 - 4 \cdot (1-t) \, dt$$

$$= \int_0^1 (-1)^2 - 4 + 4t \, dt = \int_0^1 -3 + 4t \, dt = -3t + 2t^2 \Big|_0^1 = -1.$$

$$I(y = 1 - t^2) = \int_0^1 \dot{\overline{(1-t^2)}}^2 - 4 \cdot (1 - t^2) \, dt$$

$$= \int_0^1 (-2t)^2 - 4 + 4t^2 \, dt$$

$$= \int_0^1 8t^2 - 4 \, dt$$

$$= \left[\frac{8}{3} t^2 - 4t \right]_0^1 = \frac{8}{3} - 4 = -\frac{4}{3} \approx -1.333.$$

$$I(y = 1 - t^3) = \int_0^1 \dot{\overline{(1-t^3)}}^2 - 4(1-t^3)\,dt$$

$$= \int_0^1 (-3t^2)^2 - 4 + 4t^3\,dt$$

$$= \int_0^1 9t^4 - 4 + 4t^3\,dt$$

$$= \left[\frac{9}{5} t^5 - 4t + t^4 \right]_0^1 = \frac{9}{5} - 4 + 1 = -\frac{6}{5} = -1.2.$$

$I(y = 1 - t) = -1$

$I(y = 1 - t^2) = -1.33 \leftarrow$ Min Min Energy principle.

$I(y = 1 - t^3) = -1.2$

- Functional ? $y : \mathbb{R} \to \mathbb{R}$

$I : (\ldots.) \longrightarrow \mathbb{R}.$

function space

↳ e.g: • infinitely often cont diff functions: $C^\infty[\mathbb{R}, \mathbb{R}]$ $\mathbb{R} \to \mathbb{R}.$

• square - integrable function $L_2[\mathbb{R}, \mathbb{R}]$

• Space of p-polynomial.

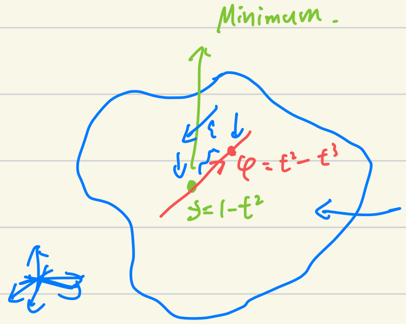
The true solution is attrive at Minimum energy.

How to minimize a functional?

build derivative and set to 0

Functional derivative

$$\frac{\delta I}{\delta y}$$



function space

infinite-dimensional vector space.

$$\frac{\delta I}{\delta y} = \frac{d\, I(y+\varepsilon\varphi)}{d\varepsilon}\Big|_{\varepsilon=0}$$

→ directional derivative in function space.

→ called Gateaux Derivative.

just $\frac{\delta I}{\delta y} \overset{set}{=} 0$ solve for y.

$$I(y) = \int_0^1 \dot{y}(t)^2 - 4y(t)\, dt.$$

$$I(y+\varepsilon\varphi) = \int_0^1 (\dot{\overline{y+\varepsilon\varphi}})^2 - 4(y+\varepsilon\varphi)\, dt$$

ε does not depend on t

$$= \int_0^1 (\dot{y}+\varepsilon\dot{\varphi})^2 - 4y - 4\varepsilon\varphi\, dt$$

$$= \int_0^1 \dot{y}^2 + 2\dot{y}\varepsilon\dot{\varphi} + \varepsilon^2\dot{\varphi}^2 - 4y - 4\varepsilon\varphi\, dt$$

$$\frac{d\, I(y+\varepsilon\varphi)}{d\varepsilon} = \int_0^1 0 + 2\dot{y}\dot{\varphi} + 2\varepsilon\dot{\varphi}^2 - 0 - 4\varphi\, dt$$

$$= \int_0^1 2\dot{y}\dot{\varphi} + 2\varepsilon\dot{\varphi}^2 - 4\varphi\, dt$$

$$\left.\frac{dI(y+\varepsilon\varphi)}{d\varepsilon}\right|_{\varepsilon=0} = \underbrace{\int_0^1 2\dot{y}\dot{\varphi} - 4\varphi \, dt.}_{\text{How to rearrange for } y} = \frac{\delta I}{\delta y}$$

$$\int_0^1 2\dot{y}\dot{\varphi} - 4\varphi \, dt = \int_0^1 2\dot{y}\dot{\varphi} \, dt - \int_0^1 4\varphi \, dt$$

int by parts $$= \underset{=0}{2\dot{y}\cancel{\varphi}\Big|_0^1} - \int_0^1 2\ddot{y}\varphi \, dt - \int_0^1 4\varphi \, dt$$

φ is test function. vanish at boundary. $\forall \varphi \in V$

$$= -\int_0^1 (2\ddot{y}+4)\varphi \, dt = \frac{\delta I}{\delta y} \overset{\text{set to}}{=} 0.$$

$\downarrow$ Fundamental Lemma of Calculus of variations.

$$\Rightarrow \frac{\delta I}{\delta y} = -2\ddot{y} - 4. \quad \Rightarrow$$

$$-(2\ddot{y}+4) = 0.$$

$$2\ddot{y} + 4 = 0$$

$$\ddot{y} = -2$$ condition for optimal solution.

$\ddot{y} = -2$ because $g=2$ we rediscover Newtonian

$$\dot{y} = -2t + \underset{=0}{\cancel{\dot{y}_0}}$$

$$y = -t^2 + y_0 \qquad y_0 = 1.$$

$y(t) = 1 - t^2.$ is indeed the correct solution as it minimize the energy function

↳ Minimize Energy principle.

Functional Derivative

- Def : [Functional] : is a rule which associates a number with a set of function

$$f_1, f_2, \dots \quad \longrightarrow \quad \mathcal{F}[f_1, \dots,] = \mathbb{R}.$$

- Variation of the Functional : $\delta F = F[f + \delta f] - F[f].$

$$\downarrow$$

$$\delta f = \overset{\substack{\text{Infinitesimal}\\ \downarrow}}{\varepsilon} \cdot \eta \longrightarrow \text{arbitrary function}$$

- $F[\eta] = A \int \eta(r)^{5/3} \, d\vec{r}^{\,3}$ [The Thomas-Fermi Kinetic energy function]

Taylor Expansion :

$$F[f + \varepsilon\eta] = F[f] + \left.\frac{dF[f+\varepsilon\eta]}{d\varepsilon}\right|_{\varepsilon=0} \cdot \varepsilon + \frac{1}{2} \left.\frac{d^2F[f+\varepsilon\eta]}{d\varepsilon^2}\right|_{\varepsilon=0} \cdot \varepsilon^2$$

first order : $$\left.\frac{dF[f+\varepsilon\eta]}{d\varepsilon}\right|_{\varepsilon=0} \overset{\text{def}}{=} \int \frac{\boxed{\delta F[f]}\,\eta(x_1)}{\boxed{\delta f(x_1)}} \, dx_1$$

second order : $$\left.\frac{d^2F[f+\varepsilon\eta]}{d\varepsilon^2}\right|_{\varepsilon=0} \overset{\text{def}}{=} \int \frac{\boxed{\delta^2 F[f]}\,\eta(x_1)\,\eta(x_2)}{\boxed{\delta f(x_1)\,\delta f(x_2)}} \, dx_1 \, dx_2$$

$$\delta F = \int \frac{\delta F(x_1)}{\delta f(x_1)} \cdot \delta f(x_1) \, dx_1 + \frac{1}{2} \int \frac{\delta^2 F(x_1)}{\delta f(x_1)\,\delta f(x_2)} \cdot \delta f(x_1) \cdot \delta f(x_2) \, dx_1 \, dx_2 + \dots$$

$$\delta F = A\int \left[\left(n(\vec r) + \varepsilon\eta(\vec r)\right)^{5/3} - n(\vec r)^{5/3} \right] d\vec r$$

Taylor $$= A\int n(\vec r)^{5/3} \sum_{k=1}^{\infty} \binom{5/3}{k} \left(\frac{\varepsilon\eta(\vec r)}{n(\vec r)}\right)^{k} d\vec r$$

first order: $\frac{\delta F}{\delta n(\vec r)} = \frac{5}{3} A\, n(\vec r)^{2/3}$, second order: $\frac{\delta^2 F}{\delta n(\vec r)\,\delta n(\vec r\,')} = \frac{10}{9} A\, n(\vec r)^{-1/3}\,\delta(\vec r - \vec r\,')$.

- Given $F[\rho] = \int f(\vec r, \rho(\vec r), \vec\nabla\rho(\vec r))\, d\vec r \rightarrow \frac{\delta F}{\delta\rho(\vec r)}$? general expression?

From definition:

$$\int \frac{\delta F}{\delta\rho(\vec r)}\,\eta(\vec r)\, d\vec r = \frac{d}{d\varepsilon}\int f(\vec r, \rho+\varepsilon\eta, \vec\nabla\rho+\varepsilon\vec\nabla\eta)\, d\vec r \Big|_{\varepsilon=0}$$

$$= \int \left(\frac{\partial f}{\partial\rho}\eta + \underbrace{\frac{\partial f}{\partial\vec\nabla\rho}}\cdot\vec\nabla\eta \right) d\vec r$$

derivative of a scalar w.r.t. a vector.

product rule for divergence: $\vec\nabla\cdot\left(\frac{\partial f}{\partial\vec\nabla\rho}\eta\right) = \frac{\partial f}{\partial\vec\nabla\rho}\cdot\vec\nabla\eta + \eta\cdot\vec\nabla\cdot\frac{\partial f}{\partial\vec\nabla\rho}$.

$$= \int [\frac{\partial f}{\partial\rho}\eta + \vec\nabla\cdot(\frac{\partial f}{\partial\vec\nabla\rho}\eta)) - \eta\cdot\vec\nabla\cdot\frac{\partial f}{\partial\vec\nabla\rho} \quad d\vec r$$

Divergence Thm + condition $\eta=0$ at the boundary: $\int\vec\nabla\cdot\left(\frac{\partial f}{\partial\vec\nabla\rho}\eta\right) d\vec r = 0$

$$= \int \left(\frac{\partial f}{\partial\rho} - \vec\nabla\cdot\frac{\partial f}{\partial\vec\nabla\rho}\right)\eta\, d\vec r$$

$$\Rightarrow \boxed{\frac{\delta F}{\delta\rho(\vec r)} = \frac{\partial f}{\partial\rho} - \vec\nabla\frac{\partial f}{\partial\vec\nabla\rho}}$$ given $F[\rho] = \int f(\vec r, \rho(\vec r), \vec\nabla\rho(\vec r))\, d\vec r$.