

Chapter 1

Calculus of variation and Functionals

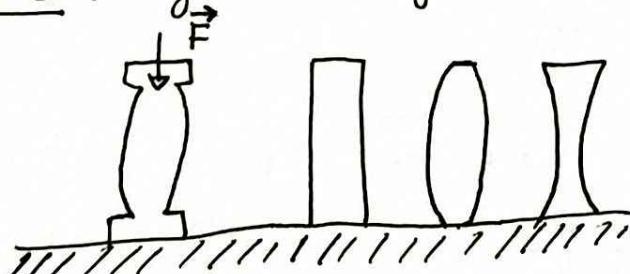
Goals: what for?

- an essential tool in theoretical physics, mainly for formalism and to model and derive equations from general principles.

fields: classical mechanics, field theory (classical and quantum), statistical physics, elasticity, electromagnetism, general relativity, ...

- a practical tool for applied mathematics, engineering and control/optimization theory.

For instance: given a fixed volume and height, what is the shape of the strongest column?
(the one for which buckling appears for the largest force)



I) Functionals

In most situations, an optimization problem or minimization principle corresponds to finding the optimal function that extremizes a cost function among possible functions (function space).

① Notations and definition

- let $\vec{x} \in \Omega$ a vector in d-dimensional space, belonging to domain Ω and $y: \vec{x} \in \Omega \mapsto y(\vec{x}) \in \mathbb{R}$ a real function (easy to generalize to complex variables/functions)
- a functional F is an application from a given function space \mathcal{Y} (functions satisfying to given properties, like continuity, differentiability, domain of definition, ...) to a scalar quantity (the cost).

$$F: y \in \mathcal{Y} \mapsto F[y] \in \mathbb{R}$$

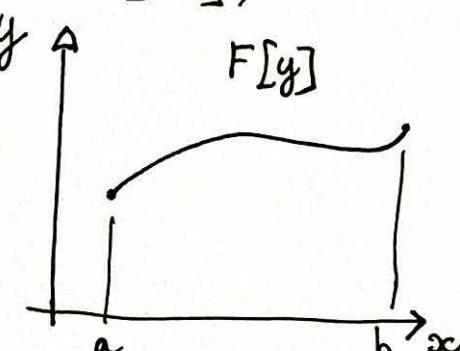
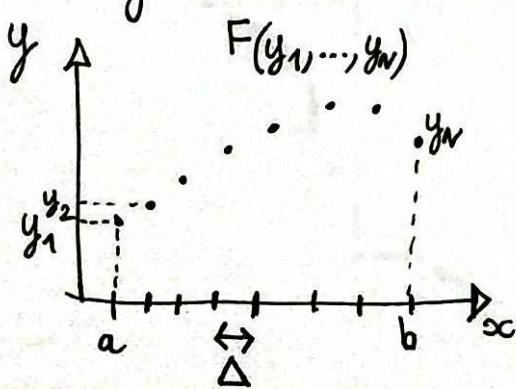
The bracket notation is used not to confuse with usual variables. An heavier possible notation is $F[y(\vec{x})]$.

basic examples:

- $F[y] = \max_{\vec{x} \in \Omega} (y(\vec{x}))$
- $F[y] = y(\vec{x}_0)$ where \vec{x}_0 is a point of Ω
- $F[y] = \int_{\Omega} y(\vec{x}) d\vec{x}$

② The discrete point of view

It is most of the time very instructive and intuitive to understand functionals as the limit of infinite number of variables functions. Here, $d=1$, $\Omega = [a, b]$,



Then,

(2)

$$"F[\vec{y}] = \lim_{\substack{\Delta \rightarrow 0 \\ N \rightarrow \infty}} F(y_1, \dots, y_N)" \text{ not a mathematical definition}$$

Example: using Riemann sums, $\vec{y} = (y_1, \dots, y_i, \dots, y_N)$

$$F(\vec{y}) = \Delta^d \sum_{i=1}^N y_i^2 = \Delta^d \vec{y}^2 \mapsto F[y] = \int_{\Omega} y(\vec{x}) d\vec{x}$$

Δ better
way
to treat
 Δ ?

$$F(\vec{y}) = \Delta^d \sum_{i=1}^N \frac{(y_{i+1} - y_i)^2}{\Delta^2} \rightarrow F[y] = \int_{\Omega} (\nabla y(\vec{x}))^2 d\vec{x}$$

$$F(\vec{y}) = \Delta^d \vec{h} \cdot \vec{y} \rightarrow F[y] = \int_{\Omega} h(\vec{x}) y(\vec{x}) d\vec{x}$$

(3) Examples of optimization problems

* Lagrangian mechanics and principle of least action:

trajectory $q(t)$: $S[q] = \int_{t_i}^{t_f} dt L(q, \dot{q}, t)$; $\dot{q} = \frac{dq}{dt}$

action \leftarrow \hookrightarrow Lagrangian

* Field theory: let $\varphi(\vec{x}, t)$ be a classical field

$$S[\varphi] = \int dt \int d\vec{x} \mathcal{L}(\varphi, \dot{\varphi}, \vec{\nabla} \varphi)$$

\hookrightarrow Lagrangian density

* Ginzburg-Landau theory: $\phi(\vec{r})$ an order parameter

$$F[\phi] = \int d\vec{r} \left\{ g(\vec{\nabla} \phi)^2 + a \phi^2 + b \phi^4 \right\}$$

* Shortest path kind of problems:

- . Fermat principle: finding path of light in inhomogeneous refractive index to minimize time

$$T = \frac{1}{c} \int_A^B n(s) ds \quad \text{where } s \text{ is the curvilinear abscissa}$$

- . Geodesics: path of light on curved spaces : shortest path between two points in curved space



applications to general relativity.

- . minimal surface: minimize surface tension energy

$$F = \gamma \int dA$$

Soap films

\Rightarrow no boundaries



* In physics most functionals are local or additive i.e. they can be written as

$$F[y] = \int_{\Omega} d\vec{x} f(y(\vec{x}), \vec{\nabla}y(\vec{x}), \vec{x}, \dots)$$

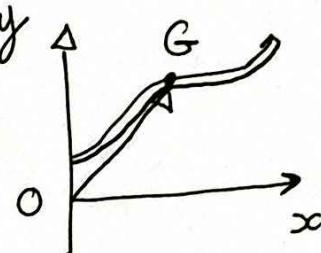
\rightarrow "density"

a counter example for non-local functionals is

$$\vec{F}[y] = \vec{OG} = \frac{\int \vec{OM} ds}{\int ds}$$

$\hookrightarrow x_G = \int_{\Gamma} \vec{x} \cdot \frac{\sqrt{ds^2 + dy^2}}{\int ds}$ (Simplify!)

center of mass of the rod



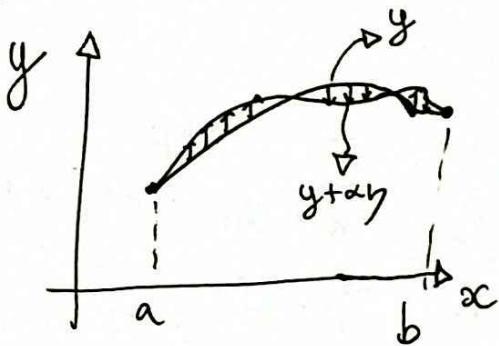
IV Functional derivative.

(3)

(1) Definition

We are looking for stationary "points/functions" of $F[y]$ so we need to determine how F varies when y varies.

We consider a set of functions with same boundary conditions $\partial\Omega$ (frontier of Ω). [This is not the most general situation].



a variation of y can be written

$$y(\vec{x}) \rightarrow y(\vec{x}) + \alpha y(\vec{x})$$

with α a scaling factor meant to be small enough and $y(\vec{x})$

a function with the same

properties (continuity, differentiability, ...) as y but such that $y(x)|_{\partial\Omega} = 0$ so that $y+\alpha y$ belongs to the same space as y .

The functional derivative exists if one can write the induced variation in F as a finite quantity to first order in α :

$$F[y+\alpha y] - F[y] = \alpha \int_{\Omega} y(\vec{x}) \frac{\delta F}{\delta y(\vec{x})} d\vec{x} + O(\alpha^2)$$

$\underbrace{\frac{\delta F}{\delta y(\vec{x})}}$ identified as the functional derivative.

By consequence: $\frac{\delta F}{\delta y} : \vec{x} \rightarrow \mathbb{R}$ is a function of \vec{x} .

A more concise notation is:

$$\delta F[y] = \int_{\Omega} d\vec{x} \frac{\delta F}{\delta y(\vec{x})} \delta y(\vec{x})$$

where $\delta y = \alpha y$ and $\delta F = F[y+\alpha y] - F[y]$

② Discrete point of view and higher orders

Taylor expansion of a multi-variable function:

$$F(y_1 + \alpha y_1, \dots, y_N + \alpha y_N) = F(y_1, \dots, y_N) + \alpha \sum_{i=1}^N \left(\frac{\partial F}{\partial y_i} \right) y_i + O(\alpha^2)$$

not a well defined limit $\xrightarrow{N \rightarrow \infty}$

$$\xrightarrow{i \mapsto \vec{x} \text{ "continuous index" }} F[y] + \alpha \int_{\Omega} \frac{\delta F}{\delta y}(\vec{x}) y(\vec{x}) d\vec{x} + O(\alpha^2)$$

higher order Taylor expansion:

$$F(\vec{y} + \alpha \vec{y}) = F(\vec{y}) + \sum_{n=1}^{\infty} \frac{\alpha^n}{n!} \sum_{i_1} \dots \sum_{i_n} \frac{\partial^n F}{\partial y_{i_1} \dots \partial y_{i_n}} y_{i_1} \dots y_{i_n}$$

$$\rightarrow F[y] + \sum_{n=1}^{\infty} \frac{\alpha^n}{n!} \int_{\Omega} \dots \int d\vec{x}_1 \dots d\vec{x}_n \frac{\delta^n F}{\delta y(\vec{x}_1) \dots \delta y(\vec{x}_n)} y(\vec{x}_1) \dots y(\vec{x}_n)$$

\Rightarrow the n^{th} derivative is a function of n variables $(\vec{x}_1, \dots, \vec{x}_n)$

③ Some properties and examples

$$F[y] = \int d\vec{x} f(y(\vec{x})) \rightarrow \frac{\delta F}{\delta y(\vec{x})} = f'(y(\vec{x}))$$

$$F[y](\vec{x}') = \int d\vec{x} K(\vec{x}, \vec{x}') y(\vec{x}) \rightarrow \frac{\delta F}{\delta y(\vec{x})} = K(\vec{x}, \vec{x}')$$

$$F[y](\vec{x}') = f(y(\vec{x}')) \rightarrow \frac{\delta F}{\delta y(\vec{x})} = f'(y(\vec{x})) \delta(\vec{x} - \vec{x}')$$

$$F[y] = \int d\vec{x} (\vec{\nabla} y(\vec{x}))^2 \rightarrow \frac{\delta F}{\delta y(\vec{x})} = -2 \vec{\nabla}^2 y(\vec{x}) = -2 \Delta y(\vec{x})$$

Laplacian \downarrow

chain rule: for usual functions:

$$\frac{d}{dh} F(y(h)) = \frac{dF}{dy}(y(h)) \frac{dy}{dh}(h)$$

for multi-variable functions: and functional $F[y[h]]$

$$\frac{\partial F}{\partial h_i}(\vec{y}(h)) = \sum_j \frac{\partial F}{\partial y_j}(\vec{y}(h)) \times \frac{\partial y_j}{\partial h_i}(h) \rightarrow$$

$$\boxed{\frac{\delta F}{\delta h(\vec{x})} = \int d\vec{x}' \frac{\delta F}{\delta y(\vec{x}')} \frac{\delta y(\vec{x}')}{\delta h(\vec{x})}}$$