

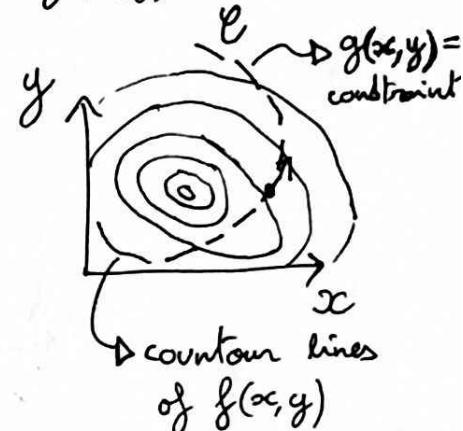
III] Extrema under constraint - Lagrange multipliers

① Reminder on the principle of Lagrange multiplier

let $f(x, y)$ be a function of two variables. Let a constraint between x and y written in the form $g(x, y) = 0 \rightsquigarrow$ curve " $y(x)$ " in the xy -plane.

x and y are not independent.

Goal: find the extrema of f under the constraint g .



1st option: solve $g(x, y) = 0$ to get $y(x)$ one several solutions.

introduce $h(x) = f(x, y(x))$ and look for extrema of h as a function of x . This can get quite cumbersome, in particular when the number of variables is large.

Yet this approach helps understand the strategy.

- First, let C be the curve $g(x, y) = 0$ and (dx, dy) an elementary displacement along that curve: then

$$dg = \left(\frac{\partial g}{\partial x}\right)_y dx + \left(\frac{\partial g}{\partial y}\right)_x dy = 0$$

Close to an extremum of f along that curve, we have also

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy = 0 \quad (N.B.: \vec{\nabla} f \neq 0 \text{ in general at this point})$$

By simplification $\begin{pmatrix} \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \\ \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ since $(dx, dy) \neq \vec{0}$

this means that the determinant is null or in other words that the two column vectors are \parallel .

$$\begin{vmatrix} \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \\ \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \end{vmatrix} = 0 \Leftrightarrow \left(\frac{\partial g}{\partial x} \right)_y \left(\frac{\partial f}{\partial y} \right)_x = \left(\frac{\partial g}{\partial y} \right)_x \left(\frac{\partial f}{\partial x} \right)_y \text{ at } (x^*, y^*)$$

↳ extremum

or

$$\vec{\nabla} f(x^*, y^*) = \lambda^* \vec{\nabla} g(x^*, y^*)$$

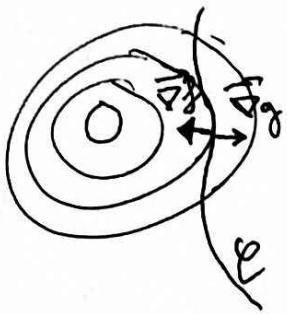
↳ proportionality coefficient

geometrical interpretation:

balance of two forces $\overset{\text{pointed to } \lambda^*}{\rightarrow}$

$$\vec{\nabla} f - \lambda \vec{\nabla} g = \vec{0}$$

λ takes you down the potential \rightarrow compensates to keep the point on the curve



when the balance of force is zero, then the particle does not move, it is either maximum/minimum.

You have to look for points such that $\vec{\nabla} f \parallel \vec{\nabla} g$ and then adjust λ to make the forces vanish.

From the balance of forces, we guess that it is the quantity $f - \lambda g$ to be minimized. Otherwise, let's consider the extremalisation of $h(x) = f(x, y(x))$

$$\frac{dh}{dx} = \left(\frac{\partial f}{\partial x} \right)_y + \left(\frac{dy}{dx} \right)_y \left(\frac{\partial f}{\partial y} \right)_x = 0$$

Then, $\left(\frac{dy}{dx} \right)_y = - \left(\frac{\partial f}{\partial y} \right)_x / \left(\frac{\partial f}{\partial x} \right)_y$

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[we assumed $\left(\frac{\partial g}{\partial y}\right)_x \neq 0$]

$$\Rightarrow \frac{dh}{dx} = \left(\frac{\partial f}{\partial x}\right)_y - \frac{\left(\frac{\partial f}{\partial y}\right)_{xc}}{\left(\frac{\partial g}{\partial y}\right)_x} \left(\frac{\partial g}{\partial x}\right)_y = 0$$

we define $\lambda^* = \frac{\left(\frac{\partial f}{\partial y}\right)_{xc}(x^*, y^*)}{\left(\frac{\partial g}{\partial y}\right)_{xc}(x^*, y^*)}$

now, if we introduce $\tilde{h}(y) = f(x(y), y)$

$$\frac{d\tilde{h}}{dy} = \left(\frac{\partial f}{\partial y}\right)_x - \frac{\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial g}{\partial y}\right)_x}{\left(\frac{\partial g}{\partial x}\right)_y} = 0$$

but from the main equality $\frac{\left(\frac{\partial f}{\partial x}\right)_y}{\left(\frac{\partial g}{\partial x}\right)_y} = \frac{\left(\frac{\partial f}{\partial y}\right)_x}{\left(\frac{\partial g}{\partial y}\right)_x} = \lambda^*$ (a number)

(2) The recipe

Thus, consider $\tilde{f}(x, y, \lambda) = f(x, y) - \lambda g(x, y)$ and treat x, y, λ as independent variables to extremalize \tilde{f} :

$$\left(\frac{\partial \tilde{f}}{\partial x}\right)_{y, \lambda} = \left(\frac{\partial f}{\partial x}\right)_y - \lambda \left(\frac{\partial g}{\partial x}\right)_y = 0$$

three equations
for three unknowns

x^*, y^*, λ^*

$$\left(\frac{\partial \tilde{f}}{\partial y}\right)_{x, \lambda} = \left(\frac{\partial f}{\partial y}\right)_x - \lambda \left(\frac{\partial g}{\partial y}\right)_x = 0$$

$$\left(\frac{\partial \tilde{f}}{\partial \lambda}\right)_{x, y} = g(x, y) = 0 \Rightarrow \text{ensures the constraint is satisfied}$$

Combining the first two gives back the main equality and sets $\lambda^* \Rightarrow$ same solutions of the same equations.

In general, we don't care about the last equation and the actual value of the Lagrange multiplier, just there to ensure the main equality.

② Generalizations:

. if $f(\vec{y})$ is to be optimized under $M \leq \dim(\vec{y})$ constraints

$g_m(\vec{y})$ one introduces M Lagrange multipliers as:

$$\tilde{f}(\vec{y}, \lambda_1, \dots, \lambda_M) = f(\vec{y}) - \sum_{m=1}^M \lambda_m g_m(\vec{y})$$

and extremalize \tilde{f} w.r.t. \vec{y} and λ_m .

. for a functional \rightarrow same strategy. Introduce

$$\tilde{F}[y](\lambda) = F[y] - \lambda G[y]$$

and compute $\frac{\delta \tilde{F}}{\delta y(x)} = 0$, $\frac{\partial \tilde{F}}{\partial \lambda} = 0$

Functional integrals - Path integral

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We do not introduce them physically nor mathematically and we take the picture of the discrete point of view to understand.

Starting from the multiple integral

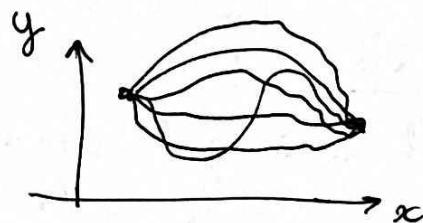
$$I = \int \dots \int dy_1 \dots dy_N F(y_1, \dots, y_N)$$

We try to understand the limit $N \rightarrow \infty$. Mathematically, defining the integration measure in this limit is ill defined in general. Formally, we write

$$\text{``Dy}(\vec{y}) = \lim_{N \rightarrow \infty} dy_1 \dots dy_N \text{''}$$

The elementary volume in the space of function. It formally means "summing contributions of all functions"

$$I = \int \text{Dy}(\vec{y}) F[y]$$



Examples:

* let M_{ij} be a positive definite matrix and

$$I = \int \dots \int dy_1 \dots dy_N e^{-\sum_{i,j} y_i M_{ij} y_j}$$

$$\xrightarrow[N \rightarrow \infty]{} I = \int \text{Dy}(\vec{x}) e^{-\iint d\vec{x} d\vec{x}' y(\vec{x}) M(\vec{x}, \vec{x}') y(\vec{x}')}}$$

we will formally extend Gaussian integrals to path integrals (see later).

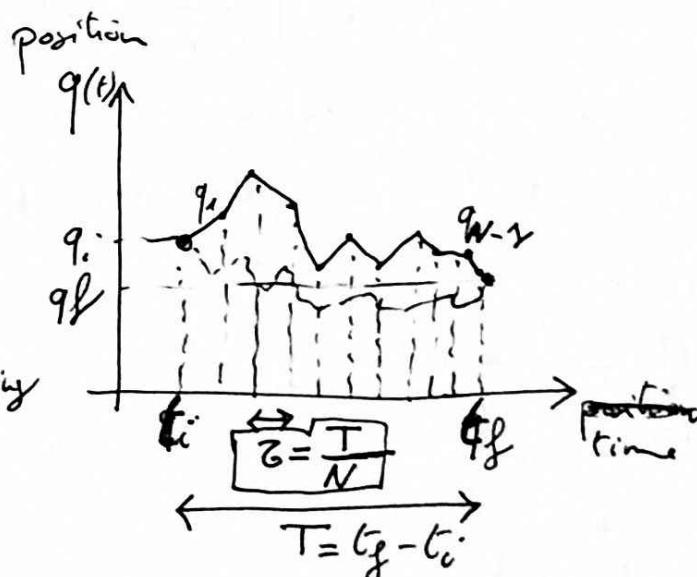
* most of the time, path integral are used to formally compute correlators or averages. Somehow, the issue coming from the definition of the measure cancels out when it appears in numerator/denominator.

$$\langle A(\vec{y}) \rangle = \frac{\int \mathcal{D}y(\vec{y}) A(\vec{y}) e^{-\beta E[y]}}{\int \mathcal{D}y(\vec{y}) e^{-\beta E[y]}}$$

(see exercise)

* in quantum mechanics (see option in quantum field theory)
single particle, Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{q})$

One can reformulate quantum mechanics as follow: the probability amplitude that the particle is at q_f at t_f knowing it was at q_i at t_i , reads



$$\langle q_f | U(t_f, t_i) | q_i \rangle$$

// explicit calculation from Schrödinger equation.

$$\lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar i\beta} \right)^{\frac{N}{2}} \int \dots \int dq_1 \dots dq_{N-1} e^{\frac{i}{\hbar} S(q_0, q_1, \dots, q_{N-1}, q_f)}$$

with $S = \beta \sum_{i=0}^{N-1} \frac{m}{2} \left(\frac{q_{i+1} - q_i}{\hbar} \right)^2$

$$= \int \mathcal{D}q(t) e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \left(\frac{m}{2} \dot{q}(t)^2 - V(q(t)) \right)}$$

to action $-V(q_{i+1})$

The path $q(t)$ with smallest action contribute more. $\mathcal{D}q = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar i\beta} \right)^{\frac{N}{2}} dq_1 \dots dq_N$