1.3. Functionals

A real-valued function maps a point in its domain to a real number.
A functional maps a function (or a point in a function space) into a number.

Functionals are usually represented in terms of integrals.

Let

$$\mathcal{F}[g(x)] = \mathcal{F}[g]$$

be the functional of the function $g(x)$. The functional derivative of $\mathcal{F}$ with respect to $g(y)$ is defined as

$$\frac{\delta \mathcal{F}}{\delta g(y)} = \lim_{\varepsilon \to 0} \frac{\mathcal{F}[\,g(x) + \varepsilon\, \delta(x-y)\,] - \mathcal{F}[g(x)]}{\varepsilon} \qquad (1.25)$$

For example, if

$$\mathcal{F}[g(x)] = \int_a^b dx\, [g(x)]^n$$

then

$$\mathcal{F}[g(x) + \varepsilon\, \delta(x-y)] = \int_a^b dx \left[\, g(x) + \varepsilon\, \delta(x-y)\,\right]^n$$

$$= \int_a^b dx \left\{ [g(x)]^n + \varepsilon\, n\, \delta(x-y) [g(x)]^{n-1} + O\!\left(\varepsilon^2\right) \right\}$$

$$\rightarrow \qquad \frac{\delta \mathcal{F}}{\delta g(y)} = \int_a^b dx\, n\, \delta\,(x-y)\, g^{n-1}\,(x)$$

$$= \begin{cases} n\,[g(y)]^{n-1} & \text{if } \; y \in (a,\, b) \\ 0 & \text{otherwise} \end{cases} \qquad (1.26)$$

In fact, the fore-going proof can be easily adapted to show that if

$$\mathcal{F}[g(x)] = \int_a^b dx\, F(g(x))$$

then

$$\frac{\delta \mathcal{F}}{\delta g(y)} = \left.\frac{\partial F(g)}{\partial g}\right|_{g = g(y)} \qquad \forall\; y \in (a,\, b) \qquad (1.26a)$$

Since eq(1.25) has the form of the ordinary derivative of functions, it also leads to the Leibniz rule

$$\frac{\delta \mathcal{F}\mathcal{G}}{\delta g(x)} = \frac{\delta \mathcal{F}}{\delta g(x)}\, g + \mathcal{F}\, \frac{\delta\, \mathcal{G}}{\delta g(x)} \qquad (1.27)$$

The Taylor expansion of a well behaved functional is

$$\mathcal{F}[g] = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \ldots dx_n\, [g(x_1) - f(x_1)] \ldots [g(x_n) - f(x_n)] \qquad (1.29)$$

$$\times \left.\frac{\delta^n \mathcal{F}}{\delta g(x_1) \ldots \delta g(x_n)}\right|_{g = f}$$

while the MacClauren formula is

$$\mathcal{F}[g] = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \ldots dx_n\, g(x_1) \ldots g(x_n) \left.\frac{\delta^n \mathcal{F}}{\delta g(x_1) \ldots \delta g(x_n)}\right|_{g=0} \qquad (1.28)$$

For small $\delta g(x)$, eq(1.29) becomes

$$\mathcal{F}[g + \delta g] = \mathcal{F}[g] + \int dx\, \delta g(x) \left.\frac{\delta \mathcal{F}}{\delta g(x)}\right|_{\delta g = 0} + O(\delta g)^2 \qquad (1.30)$$

We thus define the infinitesimal variation of $\mathcal{F}$ as

$$\begin{aligned}\delta\mathcal{F}[g] &\equiv \mathcal{F}[g+\delta g]-\mathcal{F}[g]\\ &= \int dx\,\delta g(x)\,\frac{\delta\mathcal{F}}{\delta g(x)} \\ &= \left\langle \delta g \,\middle|\, \frac{\delta\mathcal{F}}{\delta g}\right\rangle\end{aligned} \tag{1.31}$$

which is the functional analog of the differential of an ordinary multi-variable function

$$\begin{aligned}d f(\boldsymbol{x}) &= f(\boldsymbol{x}+d\,\boldsymbol{x})-f(\boldsymbol{x})\\ &= \nabla f(\boldsymbol{x})\cdot d\,\boldsymbol{x}\end{aligned} \tag{1.32}$$

From

$$\begin{aligned}\delta\mathcal{F} &= \int dx\,\delta g(x)\,\frac{\delta\mathcal{F}}{\delta g(x)}\\ &= \int dx\,dy\,\frac{\delta g(x)}{\delta f(y)}\,\delta f(y)\,\frac{\delta\mathcal{F}}{\delta g(x)}\end{aligned}$$

we get the chain rule

$$\frac{\delta\mathcal{F}}{\delta f(y)} = \int dx\,\frac{\delta g(x)}{\delta f(y)}\,\frac{\delta\mathcal{F}}{\delta g(x)} \tag{1.34}$$

Extension to the multi-function case is straight-forward:

$$\delta\mathcal{F}[g_1\ldots g_n] = \int dx\,\delta g_j(x)\,\frac{\delta\mathcal{F}}{\delta g_j(x)} \tag{1.36}$$

where rule of implicit summation over repeated indices is observed.

One of the earliest application of functional methods to physics is the Lagrangian formulism of Newtonian mechanics. In particular, Newton's law

$$m\ddot{x} = F(x) = -\frac{dV}{dx} \tag{1.37}$$

is just the condition on $x(t)$ for which the action functional

$$\begin{aligned}S[x(t)\,;\,t_a,t_b] &= \int_{t_a}^{t_b} dt\,\mathcal{L}(x,\dot{x})\\ &= \int_{t_a}^{t_b} dt\left[\frac{1}{2}m\ddot{x}-V(x)\right]\end{aligned} \tag{1.38}$$

is stationary (or extremized), i.e.,

$$\delta S = 0$$

From eq(1.31), we have

$$\delta S = \int_{t_a}^{t_b} dt\left[\frac{\delta S}{\delta x(t)}\,\delta x(t)+\frac{\delta S}{\delta\,\dot{x}(t)}\,\delta\dot{x}(t)\right]$$

Note that

$$\frac{\delta\dot{x}(t')}{\delta x(t)} = \frac{d}{dt'}\,\frac{\delta x(t')}{\delta x(t)} = \frac{d}{dt'}\,\delta(t-t') \tag{1.39}$$

Using

$$\delta\dot{x}(t) = \frac{d}{dt}\,\delta x(t)$$

& setting the B.C.

$$\delta x(t_b) = \delta x(t_a) = 0 \tag{1.39a}$$

we can integrate by part to get

$$\delta S = \int_{t_a}^{t_b} dt \left[\frac{\delta S}{\delta x(t)} - \frac{d}{dt} \frac{\delta S}{\delta \dot{x}(t)} \right] \delta x(t) = 0 \qquad (1.40)$$

Since $\delta x(t)$ is arbitrary aside from the B.C. eq(1.39a), eq(1.40) can be satisfied only if

$$\frac{\delta S}{\delta x(t)} - \frac{d}{dt} \frac{\delta S}{\delta \dot{x}(t)} = 0 \qquad (1.41a)$$

Using eq(1.26a), we have

$$\frac{\delta S}{\delta x(t)} = \frac{\partial \mathcal{L}}{\partial x}(t) \qquad \qquad \frac{\delta S}{\delta \dot{x}(t)} = \frac{\partial \mathcal{L}}{\partial \dot{x}}(t)$$

where $\frac{\partial \mathcal{L}}{\partial x}(t)$ means doing the partial treating the arguments of $\mathcal{L}$ as simple variables & then setting these variables as functions of t.

Eq(1.41a) is therefore just the Euler-Lagrange eq.

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0 \qquad (1.41)$$

The generalized momentum conjugate to the generalized coordinate $q_i(t)$ is defined as

$$p_i(t) = \frac{\delta S}{\delta \dot{q}_i(t)} \qquad \to \qquad p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \qquad (1.42)$$

The hamiltonian is obtained by a Legendre transform

$$H(p, q) = p_i \dot{q}_i - \mathcal{L}(q, \dot{q}) \qquad (1.43)$$

where $\dot{q}$ is assumed to be in the form $\dot{q} = \dot{q}(p, q)$.

$$\frac{dH}{dt} = \dot{p}_i \dot{q}_i + p_i \ddot{q}_i - \dot{q}_i \frac{\partial \mathcal{L}}{\partial q_i} - \ddot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial t}$$

$$= -\frac{\partial \mathcal{L}}{\partial t} \qquad [\text{ Eqs(1.41-2) used }] \qquad (1.44)$$

Hence, H is conserved if $\mathcal{L}$ is not explicitly dependent on t.

The Hamiltonian formulism starts by using eq(1.43) to rewrite the action as

$$S[p, q; t_a, t_b] = \int_{t_a}^{t_b} dt \left[p_i \dot{q}_i - H(p, q) \right] \qquad (1.45)$$

$$\to \qquad \delta S = \int_{t_a}^{t_b} dt \left(\frac{\delta S}{\delta q_i(t)} \delta q_i(t) + \frac{\delta S}{\delta p_i(t)} \delta p_i(t) \right) = 0$$

$$\frac{\delta S}{\delta q_i(t)} = \int_{t_a}^{t_b} dt' \, p_i(t') \frac{d}{dt'} \delta(t - t') - \frac{\partial H}{\partial q_i}(t)$$

$$= -\dot{p}_i(t) - \frac{\partial H}{\partial q_i}(t)$$

$$\frac{\delta S}{\delta p_i(t)} = \dot{q}_i(t) - \frac{\partial H}{\partial p_i}(t)$$

Since δq_i & δp_i are arbitrary, we obtain the Hamiltonian eqs. of motion

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \qquad \dot{q}_i = \frac{\partial H}{\partial p_i} \qquad (1.47)$$

A canonical transformation can be defined as any transformation on p & q such that the jacobian is 1.

An alternative definition is that it keeps the Poisson bracket invariant.

The Poisson bracket of 2 phase space functions $A(p, q)$ & $B(p, q)$ is defined as

$$\{A, B\}_{p,q} \equiv \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \tag{1.48}$$

$$\frac{dA}{dt} = \frac{\partial A}{\partial q_i} \dot{q}_i + \frac{\partial A}{\partial p_i} \dot{p}_i + \frac{\partial A}{\partial t}$$

$$= \frac{\partial A}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial A}{\partial t} \qquad \text{[Eq(1.47) used.]}$$

$$= \{A, H\}_{p,q} + \frac{\partial A}{\partial t} \tag{1.49}$$

$$\{q_j, p_k\}_{p,q} = \frac{\partial q_j}{\partial q_i} \frac{\partial p_k}{\partial p_i} - \frac{\partial p_k}{\partial q_i} \frac{\partial q_j}{\partial p_i}$$

$$= \delta_{ij} \delta_{ki}$$

$$= \delta_{jk} \tag{1.50}$$