

FUNCTIONALS AND FUNCTIONAL DERIVATIVES

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One of the mathematical tools used in quantum field theory is the *functional* and its derivative, known as a *functional derivative*. Just as an ordinary function takes a number as input and produces a number as output, a functional takes an entire function as input and produces a number. Many functionals are defined as integrals over the input function. The notation for a functional F with input function f is $F[f]$. For example

$$F[f] = \int_{-1}^1 f(x) dx \quad (1)$$

If $f(x) = x^2$

$$F[x^2] = \int_{-1}^1 x^2 dx \quad (2)$$

$$= \frac{2}{3} \quad (3)$$

Just as a regular function has a derivative with respect to its argument, a functional can have a functional derivative with respect to its input function. In a regular derivative, the idea is to change the independent variable (x for a function $f(x)$) a little bit (dx) and see how the function changes in response. A functional derivative changes the entire input function by a small amount $\delta f(x)$ and observes how the functional changes in response.

There are an infinite number of ways we could change $f(x)$ in the functional; in the functional above, we might increase $f(x)$ a bit between -1 and 0 and decrease it a bit between 0 and $+1$, or we might increase or decrease it a bit over the entire range and so on. We clearly need something a bit more definite if we're to get a consistent definition of a functional derivative.

The definition used in Lancaster & Blundell is

$$\delta f(x) = \epsilon \delta(x - x_0) \quad (4)$$

where $\delta(x - x_0)$ is the Dirac delta function and ϵ is some small number. The quantity x_0 is some value of x within the domain of $f(x)$. The idea is

that the small change in $f(x)$ occurs at one point only (at $x = x_0$). With this definition, we can now define the functional derivative as

$$\boxed{\frac{\delta F[f]}{\delta f(x_0)} \equiv \lim_{\epsilon \rightarrow 0} \frac{F[f(x) + \epsilon \delta(x - x_0)] - F[f(x)]}{\epsilon}} \quad (5)$$

Note that δ is used in the notation $\frac{\delta F[f]}{\delta f(x_0)}$ for a functional derivative, replacing d in an ordinary derivative $\frac{df}{dx}$.

Example 1. With $F[f]$ defined as in 1, we get

$$\frac{\delta F[f]}{\delta f(x_0)} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[\int_{-1}^1 (f(x) + \epsilon \delta(x - x_0)) dx - \int_{-1}^1 f(x) dx \right] \quad (6)$$

$$= \int_{-1}^1 \delta(x - x_0) dx \quad (7)$$

The value of the derivative depends on whether x_0 is within the range of integration, so we get

$$\frac{\delta F[f]}{\delta f(x_0)} = \begin{cases} 1 & \text{if } -1 < x_0 < 1 \\ 0 & \text{otherwise} \end{cases} \quad (8)$$

Example 2. Define the functional

$$H[f] = \int_a^b G(x, y) f(y) dy \quad (9)$$

Then

$$\frac{\delta H[f]}{\delta f(z)} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[\int_a^b G(x, y) (f(y) + \epsilon \delta(y - z)) dy - \int_a^b G(x, y) f(y) dy \right] \quad (10)$$

$$= \int_a^b G(x, y) \delta(y - z) dy \quad (11)$$

$$= G(x, z) \quad (12)$$

assuming $a < z < b$, zero otherwise.

Example 3. Returning to 1, we can now find a second derivative of $F[f^3]$. We start with the first derivative:

$$\frac{\delta F [f^3]}{\delta f (x_0)} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[\int_{-1}^1 (f(x) + \epsilon \delta(x - x_0))^3 dx - \int_{-1}^1 f^3(x) dx \right] \quad (13)$$

$$= 3 \int_{-1}^1 f^2(x) \delta(x - x_0) dx \quad (14)$$

$$= 3f^2(x_0) \quad (15)$$

where in going from line 1 to line 2, we kept only the term first order in ϵ in the expansion of the cube, since higher order terms vanish in the limit $\epsilon \rightarrow 0$. The result assumes $-1 < x_0 < 1$ (the answer is 0 otherwise). Now we can take a second derivative by applying the definition again. This time, however, the object being differentiated is a function rather than an integral.

$$\frac{\delta F [f^3]}{\delta f (x_0) \delta f (x_1)} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[3(f(x_0) + \epsilon \delta(x_0 - x_1))^2 - 3f^2(x_0) \right] \quad (16)$$

$$= 6f(x_0) \delta(x_0 - x_1) \quad (17)$$

Note that the second derivative is non-zero only if both derivatives are taken at the same point, that is, only if $x_0 = x_1$.

Example 4. Now suppose we have the functional

$$J[f] = \int_a^b \left(\frac{\partial f}{\partial y} \right)^2 dy \quad (18)$$

The derivative is

$$\frac{\delta J[f]}{\delta f (x)} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[\int_a^b \left(\frac{\partial (f + \epsilon \delta(y - x))}{\partial y} \right)^2 dy - \int_a^b \left(\frac{\partial f}{\partial y} \right)^2 dy \right] \quad (19)$$

$$= 2 \int_a^b f'(y) \delta'(y - x) dy \quad (20)$$

where a prime indicates a derivative with respect to y . We can solve this using integration by parts:

$$\int_a^b f'(y) \delta'(y - x) dy = f'(y) \delta(y - x) \Big|_a^b - \int_a^b f''(y) \delta(y - x) dy \quad (21)$$

Provided that neither a nor b coincides with x , the delta function in the integrated term is zero at both limits so the first term vanishes and we're left with

$$\int_a^b f'(y) \delta'(y-x) dy = -f''(x) \quad (22)$$

so

$$\frac{\delta J[f]}{\delta f(x)} = -2 \frac{\partial^2 f}{\partial x^2} \quad (23)$$

if $a < x < b$, zero otherwise.

[Incidentally, if you're worried about switching the derivative from y to x in

$$\int_a^b f''(y) \delta(y-x) dy = \int_a^b \frac{\partial^2 f}{\partial y^2} \delta(y-x) dy = \frac{\partial^2 f}{\partial x^2} \quad (24)$$

it doesn't matter whether we take the derivative with respect to y and then set $y = x$ or whether we set $y = x$ first and then take the derivative with respect to x . All we're doing is using a different variable name for the same derivative operation, so the two orders of doing things are equivalent.]

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