FUNCTIONALS AND FUNCTIONAL DERIVATIVES

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References: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014) - Problem 1.2

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

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

If $f(x)=x^2$

$$F\left[x^2\right] = \int_{-1}^{1}x^2dx \tag{2}$$

$$= \frac{2}{3} \tag{3}$$

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.

Obviously, 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

$$\delta f(x)=\varepsilon\delta(x-x_0) \tag{4}$$

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

$$\boxed{\frac{\delta F[f]}{\delta f(x_0)} \equiv \lim_{\varepsilon\to 0}\frac{F[f(x)+\varepsilon\delta(x-x_0)]-F[f(x)]}{\varepsilon}} \tag{5}$$

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. For example, with $F[f]$ defined as in 1, we get

$$\frac{\delta F[f]}{\delta f(x_0)} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left[\int_{-1}^{1}(f(x)+\varepsilon\delta(x-x_0))\,dx-\int_{-1}^{1}f(x)\,dx\right] \tag{6}$$

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

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

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

Example 2. Define the functional

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

Then

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

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

$$= G(x,z) \tag{12}$$

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

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

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

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

$$=3f^2\left(x_0\right) \tag{15}$$

where in going from line 1 to line 2, we kept only the term first order in ε since higher order terms vanish in the limit $\varepsilon\to 0$. The result assumes $-1<x_0<1$ (the answer is 0 otherwise). Now we can take a second derivative by just applying the definition again.

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

$$=6f\left(x_0\right)\delta\left(x_0-x_1\right) \tag{17}$$

Example 4. Now suppose we have the functional

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

The derivative is

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

$$=2\int_a^b f'\left(y\right)\delta'\left(y-x\right)dy \tag{20}$$

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

$$\int_a^b f'\left(y\right)\delta'\left(y-x\right)dy=f'\left(y\right)\delta\left(y-x\right)\Big|_a^b-\int_a^b f''\left(y\right)\delta\left(y-x\right)dy \tag{21}$$

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

$$\int_a^b f'(y)\,\delta'(y-x)\,dy = -f''(x) \tag{22}$$

so

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

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

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

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

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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