

Higher order functionals or a challenge to mathematical notation and type setting system!

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Functionals is the name given to functions of a higher order i.e. functions that take other functions as arguments and whose values are numbers (typically real or complex), and the square bracket notation is often used with capital letters for the functional, for example a functional of a function $f(\cdot)$ and the numbers (assumed complex) a and b can be defined by

$$F[f(\cdot), a, b] = \int_a^b f(x)dx \quad (1)$$

(though if in doubt the path of integration would have to be specified). Note that the parentheses and dot notation to indicate the number of arguments of the function argument to the functional. This may be omitted if it is clear from the context. Also note that the functional argument should not be written as $f(x)$ unless just the value of $f(\cdot)$ at the single argument x was intended, and is clearly not the case here. Operators that map functions to functions e.g.

$$G[f(\cdot)] = f'(\cdot) \quad (2)$$

are clearly also functionals, for example this can be expressed as

$$G[f(\cdot), x] = f'(x). \quad (3)$$

So in general a functional is a function with any number of function and number arguments, and with a number as its value, and operators can be expressed like this by including appropriate extra number arguments. Now it is possible to extend this concept by considering functionals as arguments, and clearly an infinite hierarchy is possible. I will here not go beyond higher order functionals that have functionals (as defined above) as arguments and call these second order functionals.

The general analogue of a Taylor series for a functional is an expression of the form

$$\begin{aligned} F[f(\cdot)] = & a_0 + \int dx f(x) a_1(x) + \int dx_1 \int dx_2 f(x_1) f(x_2) a_2(x_1, x_2) \quad (4) \\ & + \int dx_1 \int dx_2 \int dx_3 f(x_1) f(x_2) f(x_3) a_3(x_1, x_2, x_3) + \dots \end{aligned}$$

where the range of integration is the same in each case and is given by the range of the function values that are involved in F typically $[0, \infty)$ or $(-\infty, \infty)$. Equation (4) can be written compactly as

$$F[f(\cdot)] = \sum_{N=0}^{\infty} \int dx_1 \dots \int dx_N \prod_{i=1}^N f(x_i) a_N(x_1, \dots, x_N), \quad (5)$$

or avoiding the use of the ellipsis as

$$F[f(\cdot)] = \sum_{N=0}^{\infty} \prod_{i=1}^N \left(\int dx_i f(x_i) \right) a_N(\{x_i\}_{i=1}^N) \quad (6)$$

In these equations note that the number of factors is N in term N , and when $N = 0$ this indicates a factor of 1 or the identity operator. Now suppose we wish to find the general expansion of a functional of two functions $F[f_1(\cdot), f_2(\cdot)]$ then in the above formula replace f by f_1 , the dummy index N by N_1 and the dummy variables x_i by x_{1i} , also a_{N_1} for each N_1 is now a functional of f_2 so write

$$a_{N_1}(\{x_{1i}\}_{i=1}^{N_1}) = \sum_{N_2=0}^{\infty} \prod_{j=1}^{N_2} \left(\int dx_{2j} f_2(x_{2j}) \right) a_{N_1 N_2}(\{x_{1i}\}_{i=1}^{N_1}, \{x_{2j}\}_{j=1}^{N_2}) \quad (7)$$

and putting it all together gives

$$F[f_1(\cdot), f_2(\cdot)] = \sum_{N_1=0}^{\infty} \sum_{N_2=0}^{\infty} \prod_{i=1}^{N_1} \left(\int dx_{1i} f_1(x_{1i}) \right) \prod_{j=1}^{N_2} \left(\int dx_{2j} f_2(x_{2j}) \right) a_{N_1, N_2}(\{x_{1i}\}_{i=1}^{N_1}, \{x_{2j}\}_{j=1}^{N_2}) \quad (8)$$

Extending this formally to L functions, the x 's are indexed thus: x_{ki} with $1 \leq i_k \leq N_k$ for $1 \leq k \leq L$

Then

$$F[f_1(\cdot), f_2(\cdot), \dots, f_L(\cdot)] = \sum_{N_1=0}^{\infty} \dots \sum_{N_L=0}^{\infty} \left(\prod_{i_1=1}^{N_1} \int dx_{1i_1} f_1(x_{1i_1}) \right) \dots \left(\prod_{i_L=1}^{N_L} \int dx_{Li_L} f_L(x_{Li_L}) \right) \times a_{N_1, \dots, N_L}(\{x_{1i_1}\}_{i_1=1}^{N_1}, \dots, \{x_{Li_L}\}_{i_L=1}^{N_L}) \quad (9)$$

Note the placement of the parentheses is different here. The choice of where they should go is somewhat arbitrary. Here I have chosen to put them round

the integral operators rather than the range of the product (which of course here indicates composition of integral operators).

Now the point has been reached where the formula for the expansion of the general second order functional is derivable. Because a (first order) functional is characterised by (4) i.e. by a hierarchy of functions a_N with arity $N = 0, 1, 2, 3, \dots$ a second order functional is a functional with an infinite number of function arguments, one for each arity $N \geq 0$. The general formula for such a functional can be obtained from (9). Let f_i have arity i (i.e. has i arguments), then (9) can be written as

$$\begin{aligned}
F[f_0, f_1(\cdot), f_2(\cdot), \dots, f_L(\cdot)] = & \tag{10} \\
& \sum_{N_0=0}^{\infty} \sum_{N_1=0}^{\infty} \dots \sum_{N_L=0}^{\infty} f_0^{N_0} \left(\prod_{i_1=1}^{N_1} \int dx_{1i_1} f_1(x_{1i_1}) \right) \left(\prod_{i_2=1}^{N_2} \prod_{j=1}^2 \int dx_{2i_2j} f_2(x_{2i_21}, x_{2i_22}) \right) \\
& \dots \left(\prod_{i_L=1}^{N_L} \prod_{j=1}^L \int dx_{Li_Lj} f_L(x_{Li_L1}, \dots, x_{Li_LL}) \right) \times \\
& a_{N_0, N_1, \dots, N_L} \left(\{x_{1i_11}\}_{i_1=1}^{N_1}, \{\{x_{2i_2j}\}_{i_2=1}^{N_2}\}_{j=1}^2 \dots \{\{x_{Li_Lj}\}_{i_L=1}^{N_L}\}_{j=1}^L \right).
\end{aligned}$$

The treatment of the factor involving N_0 is not quite obvious from (9) but becomes clear if the extra f_0 dependence of a is introduced in (9), then replaced by a maclaurin series in powers of f_0 .

This can be expressed more succinctly without the ellipses as

$$\prod_{s=0}^{\infty} \left(\sum_{N_s=0}^{\infty} \prod_{i_s=1}^{N_s} \prod_{j=1}^s \int dx_{si_sj} f_s(\{x_{si_sj}\}_{j=1}^s) \right) a_{\{N_s\}_{s=0}^{\infty}} \left(\{\{\{x_{si_sj}\}_{i_s=1}^{N_s}\}_{j=1}^s\}_{s=1}^{\infty} \right) \tag{11}$$

after pushing the sums as far to the right as possible when the whole expression becomes a product over the index s running from 0 to L . Then the limit $L \rightarrow \infty$ is taken. Note that the $s = 0$ case contributes no x variables, justifying starting s at 1 inside the variable list for the function a .

This then is the general formula for the functional expansion of a second order functional subject to a kind of differentiability, where the functional argument is represented by the functions f_i , and the coefficients are the a functions. The number of variables in a typical a function is $N = N_1 + 2N_2 + \dots = \sum_{i=1}^{\infty} iN_i$.

N	N_1	N_2	N_3	N_4
1	1			
2	2			
	0	1		
3	3			
	1	1		
	0	0	1	
4	4			
	0	2		
	2	1		
	1	0	1	
	0	0	0	1