

On Certain Functional Derivatives¹

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Abstract. The functional derivative $\nabla J_y = F_y - (d/dx)F_{y'}$ of the functional $J[y] = \int_a^b F(x, y, y') dx$ may be computed by the limit $\nabla J_y(x) = \lim_{\Delta\sigma \rightarrow 0} (\Delta J / \Delta\sigma)$, where $\Delta\sigma$ is the area under a positive local variation at x , provided the height of the variation vanishes faster than the square of its width. This justifies the use of this limit by Gelfand and Fomin (Ref. 1).

Key Words. Calculus of variations, functional derivatives, local variations, functional extrema.

1. Introduction

We consider functionals $J: Y \rightarrow X$ of the form

$$J[y] = \int_a^b F(x, y, y') dx, \tag{1}$$

where Y is the set of real, twice continuously differentiable functions on $[a, b]$, X is the real line, and $F: R^3 \rightarrow R$ has second-order partial derivatives all continuous. The difference

$$\Delta J[y; h] = J[y + h] - J[y]$$

has the following unique representation (Ref. 1):

$$\Delta J[y; h] = dJ[y; h] + R[y; h], \tag{2}$$

where the *differential* dJ is continuous and linear in h and

$$\lim_{h \rightarrow 0} [R[y; h] / \|h\|] = 0. \tag{3}$$

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The norm $\|\cdot\|$ on Y is given by

$$\|y\| = \max|y(x)| + \max|y'(x)|,$$

where the maximum is taken over $[a, b]$. We note that the Gâteaux and Fréchet differentials coincide for the class of functionals considered here (Ref. 3).

The *functional derivative* (or *functional gradient*) ∇J_y of J is defined by the following expression (Ref. 2, p. 117):

$$dJ[y; h] = (\nabla J_y, h), \quad (4)$$

where the inner product on Y is given by

$$(f, g) = \int_a^b f(x)g(x) dx.$$

For the class of functionals (1), we have

$$\nabla J_y(x) = F_y(x, y, y') - (d/dx)F_{y'}(x, y, y').$$

We consider the following statement:

$$\nabla J_y(x) = \lim_{\Delta\sigma \rightarrow 0} (\Delta J / \Delta\sigma), \quad (5)$$

where $\Delta\sigma$ is the area under a positive variation h which is localized at x . Gelfand and Fomin (Ref. 1) in their text on the Calculus of Variations use Eq. (5) to discuss the invariance of functional extrema under coordinate transformations and also to treat extrema with functional side conditions. In this paper, we make more precise the limit process under which $\Delta\sigma \rightarrow 0$ and establish the conditions for which Eq. (5) is correct.

2. Local Variations

We choose a real, twice continuously differentiable function g with the following properties:

$$g(x) = 0, \quad |x| \geq 1,$$

$$g(x) \geq 0, \quad |x| < 1,$$

$$0 < \max[g(x)] \leq 1,$$

$$0 < \max|g'(x)| \leq 1,$$

$$\exists c > 0 \text{ and } x_0 \in (-1, 1) \text{ such that } g(x_0) > c.$$

It follows that positive, nonzero numbers A, B, C exist such that

$$\int_{-1}^1 g(x) dx = A, \quad \int_{-1}^1 g^2(x) dx = B, \quad \int_{-1}^1 (g'(x))^2 dx = C.$$

Also,

$$0 < \|g\| \leq 2.$$

We use g to construct a *local variation* h_{st} at x_0 . Thus,

$$h_{st}(x) = tg((x - x_0)/s);$$

and, setting

$$I = [x_0 - s, x_0 + s],$$

we have

$$\Delta\sigma = \int_I h_{st}(x) dx = stA, \quad \int_I h_{st}^2(x) dx = st^2B, \quad \int_I (h'_{st}(x))^2 dx = t^2C/s.$$

Also,

$$0 < \|h_{st}\| \leq t(s + 1)/s.$$

3. Example

Consider the functional

$$J[y] = \int_a^b \{y^2(x) + (y'(x))^2\} dx.$$

For variations $h \in Y$ satisfying $h(a) = h(b) = 0$, we find that

$$\Delta J[y; h] = \int_a^b 2(y - y'')h dx + \int_a^b \{h^2 + (h')^2\} dx.$$

From Eq. (4), the functional derivative becomes

$$\nabla J_y(x) = 2\{y(x) - y''(x)\},$$

which is a continuous function of x . Hence,

$$\begin{aligned} \Delta J/\Delta\sigma = \nabla J_y(x_0) + (1/\Delta\sigma) \int_a^b \{\nabla J_y(x) - \nabla J_y(x_0)\}h(x) dx \\ + (1/\Delta\sigma) \int_a^b \{h^2 + (h')^2\} dx. \end{aligned}$$

Choosing the local variation h_{st} at x_0 , we find that

$$|\Delta J/\Delta\sigma - \nabla J_y(x_0)| \leq s \sup_{x \in I} |\nabla J_y(x) - \nabla J_y(x_0)| + (B + C/s^2)t/A.$$

It is clearly necessary in this case to require that $t/s^2 \rightarrow 0$, in order to have

$$\lim_{\Delta\sigma \rightarrow 0} (\Delta J/\Delta\sigma) = \nabla J_y(x_0).$$

4. General Case

Consider functionals of the form

$$J[y] = \int_a^b F(x, y, y') dx,$$

where $F(x, y, z)$ has continuous partial derivatives up to second order in all three variables.

Lemma 4.1. Given $y \in Y$, suppose that $h \in Y$ with $h(a) = h(b) = 0$. Then, for each $\delta > 0$, there exists M_δ such that, for all $h, \|h\| < \delta$, we have

$$|\Delta J[y; h] - dJ[y; h]| \leq M_\delta(b - a)\|h\|^2.$$

Proof. By Taylor's theorem, we have

$$F(x, x + h, y' + h') - F(x, y, y') = F_y(x, y, y')h + F_{y'}(x, y, y')h' + r_1,$$

where

$$r_1 = \frac{1}{2}\{F_{yy}(x, y + \theta h, y' + \theta h')h^2 + 2F_{yy'}(x, y + \theta h, y' + \theta h')h'h + F_{y'y'}(x, y + \theta h, y' + \theta h')(h')^2\},$$

and $0 < \theta < 1$. Therefore,

$$\Delta J[y; h] = \int_a^b (F_y h + F_{y'} h') dx + R[y; h],$$

where

$$R[y; h] = \int_a^b r_1 dx.$$

We consider the set $S \subset R^3$ given by

$$S = \{(x, y + \theta h, y' + \theta h') : \text{given } y, \|h\| < \delta, 0 \leq \theta \leq 1, a \leq x \leq b\}.$$

Since $y \in Y$ and $h \in Y$, S is bounded and the closure \bar{S} of S is compact. $F_{yy}, F_{yy'}, F_{y'y'}$ are continuous; therefore, there exist $M_1^\delta, M_2^\delta, M_3^\delta < \infty$ such that

$$\sup_{\bar{S}} |F_{yy}| < M_1^\delta, \quad \sup_{\bar{S}} |F_{yy'}| < M_2^\delta, \quad \sup_{\bar{S}} |F_{y'y'}| < M_3^\delta.$$

We write

$$M_\delta = \frac{1}{2}(M_1^\delta + 2M_2^\delta + M_3^\delta),$$

and we find that

$$|R[y; h]| = \left| \int_a^b r_1 dx \right| \leq \int_a^b |r_1| dx \leq M_\delta(b-a)\|h\|^2.$$

Thus, the lemma is established.

Let h be a local variation at x_0 with $\|h\| < \delta$ and $a < x_0 < b$; then, by the above lemma, we have

$$\left| \Delta J[y; h] - \int_I (F_y - (d/dx)F_{y'}) h dx \right| \leq M_\delta 2s \|h\|^2.$$

We note that $2s$ has replaced $b - a$ on the right-hand side of this inequality, because the local variation vanishes outside the interval $I = [x_0 - s, x_0 + s]$. Hence,

$$\left| \Delta J/\Delta\sigma - \nabla J_y(x_0) - (1/\Delta\sigma) \int_I \{\nabla J_y(x) - \nabla J_y(x_0)\} h(x) dx \right| \leq M_\delta 2s \|h\|^2/\Delta\sigma,$$

that is,

$$|\Delta J/\Delta\sigma - \nabla J_y(x_0)| \leq 2s \sup_I |\nabla J_y(x) - \nabla J_y(x_0)| + 4M_\delta t(s+1)^2/A s^2.$$

Thus, provided $t/s^2 \rightarrow 0$, we have

$$\lim_{\Delta\sigma \rightarrow 0} (\Delta J/\Delta\sigma) = \nabla J_y(x_0). \tag{6}$$

We conclude that the necessary and sufficient condition on the limit process for computing the functional derivative ∇J_y of any functional of the form (1) from the quantity $\Delta J/\Delta\sigma$ is that $t/s^2 \rightarrow 0$ as $\Delta\sigma \rightarrow 0$, where the shape $g(x)$ of the local variation is arbitrary subject to the given constraints.

Another way of writing (6) is the following:

$$\Delta J[y; h] = (\nabla J_y(x_0) + \varepsilon)\Delta\sigma, \tag{7}$$

where $\varepsilon \rightarrow 0$ as $\Delta\sigma \rightarrow 0$. Eq. (7) expresses the change in $J[y]$ due to a local variation at x_0 in terms of the variations derivative ∇J_y at x_0 and the area $\Delta\sigma$ under the variation.

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