Calculus of Variations

The ultimate objective in the variational calculus is to determine the solution function that minimizes an integral. The integral, which involves the function, is called a functional. However, as an introduction, rather consider the familiar multi-variable function $F(\mathbf{q})$, where $\mathbf{q}$ is the vector of variables, not functions. Moreover, consider the second-order Taylor expansion of this function in the vicinity of the point $\mathbf{q}$, specifically at a small variation $\delta\mathbf{q}$ from $\mathbf{q}$:

$$F(\mathbf{q}+\delta\mathbf{q}) \approx F(\mathbf{q}) + \nabla F(\mathbf{q})^T \delta\mathbf{q} + \frac{1}{2}\cdot\delta\mathbf{q}^T \mathbf{H}\delta\mathbf{q} \quad (1)$$

where $\mathbf{H}$ is the Hessian matrix of double-derivatives. To investigate whether $\mathbf{q}$ is a stationary point, i.e., either a minimum or maximum point, the second-order term is omitted and the first variation, δF, is defined as the variation in function value due to the variation $\delta\mathbf{q}$ of the variables:

$$\delta F = F(\mathbf{q}+\delta\mathbf{q}) - F(\mathbf{q}) = \nabla F(\mathbf{q})^T \delta\mathbf{q} \quad (2)$$

In other words, the first variation is defined as the linear term in the Taylor expansion. For F to attain a stationary value it is necessary that the linear term, i.e., the first variation, δF, is zero:

$$\delta F = \nabla F(\mathbf{q})^T \delta\mathbf{q} = \frac{\partial F}{\partial q_i}\cdot\delta q_i = 0 \quad (3)$$

where summation over equal indices is implied in the index notation. This equation is central in the application of calculus of variations in structural mechanics. Because the variable variations are arbitrary the requirement for stationarity is:

$$\frac{\partial F}{\partial q_i} = 0 \quad (4)$$

Next, having identified a stationary point, to identify whether the point is a maximum, minimum, or saddle point it is necessary to study the second-order term. For this purpose the second variation, $\delta^2 F$, is defined as the second term in the Taylor expansion, without the ½ factor for brevity:

$$\delta^2 F = \delta\mathbf{q}^T \mathbf{H}\delta\mathbf{q} = \frac{\partial^2 F}{\partial q_i \partial q_j}\delta q_i \delta q_j \quad (5)$$

If the second variation $\delta^2 F$ is positive for arbitrary parameter variations then $\mathbf{q}$ is a minimum point. Now, consider the functional

$$I = \int_a^b F(x, w, w', w'', \cdots)\, dx \quad (6)$$

where the objective is to determine the function $w=w(x)$ that yields a stationary value of I. Let δw denote an arbitrary variation of w. Notice the difference between δw, which is an infinitesimal, virtual, arbitrary new function, and dw, which is the change in function value over an infinitesimal length dx. The variation operator has the following properties:

$$\frac{d}{dx}\delta w = \delta w' \tag{7}$$

$$\delta \int_a^b F\,dx = \int_a^b \delta F\,dx \tag{8}$$

For the functional I to be stationary, its variation, δI, must be zero:

$$\delta I = \delta \int_a^b F\,dx = \int_a^b \delta F\,dx = \int_a^b \left(\frac{\partial F}{\partial w}\delta w + \frac{\partial F}{\partial w'}\delta w' + \frac{\partial F}{\partial w''}\delta w'' + \cdots \right) dx = 0 \tag{9}$$

Furthermore, integration by parts is applied to pull the variation δw outside the parenthesis:

$$\begin{aligned} \delta I &= \int_a^b \left(\frac{\partial F}{\partial w} - \frac{d}{dx}\frac{\partial F}{\partial w'} + \frac{d^2}{dx^2}\frac{\partial F}{\partial w''} + \cdots \right) \delta w\,dx \\ &+ \left[\frac{\partial F}{\partial w'}\delta w \right]_a^b + \left[\frac{\partial F}{\partial w''}\delta w' \right]_a^b - \left[\frac{d}{dx}\frac{\partial F}{\partial w'}\delta w \right]_a^b + \cdots \\ &= 0 \end{aligned} \tag{10}$$

Because δw is an arbitrary variation the parenthesis must be zero:

$$\frac{\partial F}{\partial w} - \frac{d}{dx}\frac{\partial F}{\partial w'} + \frac{d^2}{dx^2}\frac{\partial F}{\partial w''} + \cdots = 0 \tag{11}$$

which is called the Euler equation; when it is satisfied then the functional attains a stationary value. Furthermore, the boundary terms must vanish. They may do so because values of w or its derivatives are prescribed as kinematic boundary conditions at a and/or b, called essential boundary conditions, in which case the corresponding variation vanish. Alternatively, the variations in the boundary terms in Eq. (10) are non-zero, which produce the natural boundary conditions:

$$\left.\begin{aligned} \frac{\partial F}{\partial w'} &= 0 \\ \frac{\partial F}{\partial w''} &= 0 \\ \frac{d}{dx}\frac{\partial F}{\partial w'} &= 0 \end{aligned}\right. \qquad \text{at } a \text{ and/or } b \tag{12}$$

which are here force-based, i.e., mechanical, boundary conditions. In other words, the natural boundary conditions are part of the variational formulation. Instead of aiming for the Euler equation it is often of greater practical interest to study the discretized version of the functional. Suppose the unknown function is discretized by generalized displacements with amplitudes collected in the vector **q** the first variation is

$$\delta I = \frac{\partial I}{\partial \mathbf{q}} \cdot \delta \mathbf{q} \tag{13}$$

and arbitrary variations implies that a zero variation requires

$$\frac{\partial I}{\partial \mathbf{q}} = \mathbf{0} \tag{14}$$