

CHAPTER 3

Calculus of variations and weak forms

The theory of calculus of variations concerns the minimization of functionals, where a functional refers to a mapping from a set of functions to the real numbers. These optimization problems can be seen as the infinite-dimensional version of the finite-dimensional optimization problem (28). In this section, we will use examples to demonstrate basic principles in variational calculus using prototype model problems.

1. Linear elliptic model problem

We assume a two-dimensional domain $\Omega \subset \mathbb{R}^2$, for which the boundary $\partial\Omega$ is split into disjoint parts Γ_N and Γ_D . We consider functions $u(\mathbf{x})$ defined on Ω with square integrable derivatives, i.e., functions in $H^1(\Omega)$. We further restrict ourselves to functions which are zero on Γ_D , and we denote this set of functions by $H_0^1(\Omega)$. Then we consider the functional

$$(43) \quad \Pi(u) := \frac{1}{2} \int_{\Omega} k \nabla u \cdot \nabla u \, dx - \int_{\Omega} f u \, dx - \int_{\Gamma_N} \sigma_0 u \, ds,$$

where $f \in L^2(\Omega)$ and $\sigma_0 \in L^2(\Gamma_N)$ are given. Note that $\Pi(u)$ is well-defined for functions $u \in H_0^1(\Omega)$, since these functions are assumed to have square-integrable derivatives. One physical interpretation of (43) is that $u(\mathbf{x})$ describes the transverse deflection of a membrane at a point $\mathbf{x} \in \Omega$, in which case $\Pi(u)$ is the total potential energy in the membrane. The first term in (43) describes the potential of internal forces and the second term the loss of potential of applied distributed forces f (given in force per unit area), where f the force in the transverse direction. The last term in (43) describes the loss of potential due to transverse forces σ_0 (given in force per unit length) on Γ_N . Finally, the strictly positive function $k = k(\mathbf{x})$, which is assumed to be bounded, describes the tension in the membrane.

We are interested in finding solutions u^* to the minimization problem

$$(44) \quad \min_{u \in H_0^1(\Omega)} \Pi(u).$$

A minimum u^* is characterized by $\Pi(u^* + \varepsilon \hat{u}) \geq \Pi(u^*)$ for all \hat{u} and $\varepsilon > 0$ with $u^* + \varepsilon \hat{u} \in H_0^1(\Omega)$. Thus, a minimum must u^* satisfies the *Euler-Lagrange* conditions for stationarity, namely

$$(45) \quad \left. \frac{\partial \Pi(u^* + \varepsilon \hat{u})}{\partial \varepsilon} \right|_{\varepsilon=0} = 0 \text{ for all } \hat{u} \in H_0^1(\Omega).$$

Here, variations \hat{u} are allowed such that for sufficiently small ε , the function $u^* + \varepsilon\hat{u}$ is admissible for (44). Substituting $u^* + \varepsilon\hat{u}$ in (43) and differentiating with respect to ε we obtain

$$\frac{\partial \Pi(u^* + \varepsilon\hat{u})}{\partial \varepsilon} = \int_{\Omega} k \nabla(u^* + \varepsilon\hat{u}) \cdot \nabla \hat{u} \, dx - \int_{\Omega} f \hat{u} \, dx - \int_{\Gamma_N} \sigma_0 \hat{u} \, dx$$

Setting $\varepsilon = 0$, we obtain the *weak* or *variational form*

$$(46) \quad \int_{\Omega} k \nabla u^* \cdot \nabla \hat{u} \, dx - \int_{\Omega} f \hat{u} \, dx - \int_{\Gamma_N} \sigma_0 \hat{u} \, dx = 0 \quad \text{for all } \hat{u} \in H_0^1(\Omega).$$

We now employ Green's identity, which is a multidimensional version of integration-by-parts. The identity states that for all $u, v \in H^1(\Omega)$ holds

$$(47) \quad \int_{\Omega} k \nabla u \nabla v \, dx = - \int_{\Omega} \hat{u} \nabla \cdot (k \nabla v) \, dx + \int_{\partial \Omega} \hat{u} k \nabla v \cdot \mathbf{n} \, ds$$

Using this identity for the first term in (46), we obtain

$$\begin{aligned} 0 &= \int_{\Omega} -\nabla \cdot (k \nabla u^*) \hat{u} \, dx + \int_{\partial \Omega} (k \nabla u^* \cdot \mathbf{n}) \hat{u} \, ds \\ &\quad - \int_{\Omega} f \hat{u} \, dx - \int_{\Gamma_N} \sigma_0 \hat{u} \, dx \\ &= \int_{\Omega} -[f + \nabla \cdot (k \nabla u^*)] \hat{u} \, dx + \int_{\Gamma_N} [(k \nabla u^* \cdot \mathbf{n}) - \sigma_0] \hat{u} \, ds \end{aligned}$$

for all $\hat{u} \in H_0^1(\Omega)$. In the last step, we split the boundary integral into parts corresponding to Γ_N and to Γ_D , and used the fact that $\hat{u} = 0$ on Γ_D . Next, we will argue that, since \hat{u} is arbitrary, this implies that the factors multiplying \hat{u} must vanish. This is a very common argument in variational calculus. Since $\hat{u} \in H_0^1(\Omega)$ is arbitrary on Γ_N , the condition

$$(48a) \quad k \nabla u^* \cdot \mathbf{n} = \sigma_0 \text{ on } \Gamma_N$$

must hold. The analogous argument also holds for the domain integral, since \hat{u} is arbitrary in Ω , and thus

$$(48b) \quad -\nabla \cdot (k \nabla u^*) = f \text{ on } \Omega.$$

Since u^* is in $H_0^1(\Omega)$, it also satisfies the Dirichlet boundary condition

$$(48c) \quad u^* = 0 \text{ on } \Gamma_D.$$

The equations (48) are the *strong form* of the variational problem (46). To summarize, the Euler-Lagrange equations lead to variational (or weak) conditions for a solution u^* of (44). The strong form of these conditions result in a linear boundary value problem, which has to be satisfied by the solution u^* .

Note that in (44) we have assumed vanishing boundary conditions for u^* on Γ_D ; variations \hat{u} also have to satisfy homogeneous Dirichlet boundary conditions in order for $u^* + \varepsilon\hat{u}$ to be feasible for (44). If the solution u^* is sought in a space with nonzero boundary conditions such as $u^* = g$

on Γ_D , we again have to consider variations \hat{u} in $H_0^1(\Omega)$ since with these variations $u^* + \varepsilon \hat{u} = g$ is satisfied on Γ_D . Thus, the space of variations has to satisfy vanishing Dirichlet boundary conditions even if the space of feasible minimizers satisfies inhomogeneous Dirichlet conditions.

2. Nonlinear elliptic model problem

Next we consider a non-quadratic, and thus more complicated, energy functional. We again assume a domain Ω with boundary Γ and consider

$$\Pi(u) = \frac{1}{2} \int_{\Omega} k(u) \nabla u \cdot \nabla u \, dx - \int_{\Omega} f u \, dx,$$

where the coefficient k depends on u through $k(u) = k_1 + k_2 u^2$, with $k_1, k_2 > 0$. We are interested in finding a function u^* that satisfies the Dirichlet boundary condition $u = g$ on Γ and minimizes Π :

$$(49) \quad \min_{\substack{u \in H^1(\Omega) \\ u=g \text{ on } \Gamma}} \Pi(u).$$

To characterize a solution u^* for (49), we again use the Euler-Lagrange equations. We allow variations \hat{u} with $\hat{u} = 0$ on Γ , i.e., $\hat{u} \in H_0^1$. From the Euler-Lagrange equations we obtain a condition that a solution u^* to (49) must satisfy the variational form

$$(50) \quad 0 = \int_{\Omega} \left[k(u) \nabla u^* \cdot \nabla \hat{u} + \frac{\partial k(u^*)}{\partial u} \hat{u} \nabla u^* \cdot \nabla u^* \right] dx - \int_{\Omega} f \hat{u} \, dx \\ = \int_{\Omega} \hat{u} [-\nabla \cdot (k(u) \nabla u^*) + 2k_2 u^* \nabla u^* \cdot \nabla u^* - f] \, dx$$

for all $\hat{u} \in H_0^1$. Here, we used Green's identity and the fact that $\hat{u} = 0$ on Γ , which causes the boundary term to drop out. Thus, the strong form corresponding to the variational form (50) is

$$(51) \quad \begin{aligned} -\nabla \cdot (k(u) \nabla u^*) + 2k_2 u^* \nabla u^* \cdot \nabla u^* &= f \text{ on } \Omega, \\ u^* &= g \text{ on } \Gamma. \end{aligned}$$

Note that the weak form (50) and the corresponding strong form (51) are nonlinear in the solution u^* . Thus we obtain a nonlinear boundary value problem.

This nonlinear BVP can be solved for u^* using an *infinite-dimensional* Newton method by taking a second variation of Π with respect to u , denoted by $\delta_u^2 \Pi$, which is defined in terms of the first variation $\delta_u \Pi$ as follows:

$$(52) \quad \delta_u \Pi(u, \hat{u}) := \frac{\partial \Pi(u + \varepsilon \hat{u})}{\partial \varepsilon} \Big|_{\varepsilon=0},$$

$$(53) \quad \delta_u^2 \Pi(u, \hat{u}, \tilde{u}) := \frac{\partial \delta_u \Pi(u + \varepsilon \tilde{u}, \hat{u})}{\partial \varepsilon} \Big|_{\varepsilon=0},$$

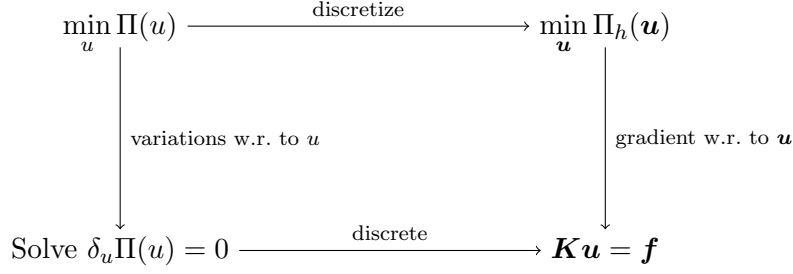


FIGURE 1. Optimize-then-discretize vs. discretize-then-optimize. The two approaches can be equivalent when the appropriate weak form and discretization scheme are chosen.

where \tilde{u} , the second variation of u , is the Newton step. We start with an initial guess for u which must satisfy $u = g$ on Γ ; then, at each iteration of Newton's method, we find $\tilde{u} \in H_0^1$ such that

$$(54) \quad \delta_u^2 \Pi(u, \hat{u}, \tilde{u}) = -\delta_u \Pi(u, \hat{u})$$

for all $\hat{u} \in H_0^1$, and then update the solution as

$$(55) \quad u \leftarrow u + \tilde{u}.$$

3. Discretization and minimization

Usually, energy minimization problems as those discussed above cannot be solved analytically, and their solution has to be approximated numerically, i.e., a corresponding discretized problem is solved. The question arises at what stage the problem should be discretized. Should it be discretized at the stage of the energy functional $\Pi(u)$, or at the stage of the the variational (or the strong) form? An advantage of discretizing the problem at the stage of the energy functional Π is that this results in a discrete nonlinear optimization problem (as discussed in Section ??), and a finite-dimensional iterative descent algorithm can be used for the minimization. On the other hand, deriving the Euler-Lagrange equation(s), and then discretizing the resulting (variational) form is usually cleaner and more concise. However, in general it is unclear if the resulting discrete problem still has an underlying discrete energy functional and thus originates from an optimization problem. The first approach in which the optimization problem is discretized before variations are taken is usually called *discretize-then-optimize*, or DTO, in the literature. The second approach, which first takes variations in infinite dimensions and then discretizes the resulting Euler-Lagrange equation, is generally referred to as *optimize-then-discretize*, or OTD. The two alternatives are sketched in Figure 1. Fortunately, for an important class of problems (such as those above) and discretizations (such as Galerkin), the two approaches are equivalent.