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 $u(\boldsymbol{x})$ 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 $H^1_0(\Omega)$. Then we consider the functional

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

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 $u \in H^1_0(\Omega)$, since these functions are assumed to have square-integrable derivatives. One physical interpretation of (43) is that $u(\boldsymbol{x})$ describes the transverse deflection of a membrane at a point $\boldsymbol{x} \in \Omega$, 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, where f is the force (per unit area) in the transverse direction. The last term in (43) describes the loss of potential due to transverse forces (per unit length) σ_0 on Γ_N. Finally, the strictly positive function $k = k(\boldsymbol{x})$, which is assumed to be bounded, describes the tension in the membrane.

We are interested in finding solutions $u^\star$ to the minimization problem

$$\min_{u \in H^1_0(\Omega)} \Pi(u). \tag{44}$$

A minimum $u^\star$ is characterized by $\Pi(u^\star + \varepsilon\hat{u}) \geq \Pi(u^\star)$ for all $\hat{u}$ and $\varepsilon > 0$, with $u^\star + \varepsilon\hat{u} \in H^1_0(\Omega)$. Thus, a minimum $u^\star$ must satisfy the *Euler-Lagrange* condition for stationarity, namely

$$\frac{\partial \Pi(u^\star + \varepsilon\hat{u})}{\partial \varepsilon}|_{\varepsilon=0} = 0 \text{ for all } \hat{u} \in H^1_0(\Omega). \tag{45}$$

Note that the condition (45) is a necessary, but not sufficient, condition for a minimum of (43). Here, variations $\hat{u}$ are allowed such that for sufficiently small ε, the function $u^\star + \varepsilon\hat{u}$ is admissible for (44). Substituting $u^\star + \varepsilon\hat{u}$ in (43) and differentiating with respect to ε we obtain

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

Setting $\varepsilon = 0$, we obtain the *weak* (or *variational*) *form*: Find $u^\star \in H_0^1(\Omega)$ such that

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

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

$$\int_\Omega k\nabla u \cdot \nabla v\, dx = -\int_\Omega u\nabla \cdot (k\nabla v)\, dx + \int_{\partial\Omega} uk\nabla v \cdot \boldsymbol{n}\, ds \tag{47}$$

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

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

for all $\hat{u} \in H_0^1(\Omega)$. In the last step, we split the boundary integral into portions corresponding to Γ_N and Γ_D, and used the fact that $\hat{u} = 0$ on Γ_D. Next, we will argue that, since $\hat{u}$ is arbitrary, the only way the above expression can vanish is if the factors multiplying $\hat{u}$ are zero. This is a common argument in variational calculus. Since $\hat{u} \in H_0^1(\Omega)$ is arbitrary on Γ_N, the Neumann boundary condition

$$k\nabla u^\star \cdot \boldsymbol{n} = \sigma_0 \text{ on } \Gamma_N \tag{48a}$$

must hold. An analogous argument also holds for the domain integral: since $\hat{u}$ is arbitrary in Ω, it must satisfy the differential equation

$$-\nabla \cdot (k\nabla u^\star) = f \text{ in } \Omega. \tag{48b}$$

Finally, since $u^\star$ belongs to $H_0^1(\Omega)$, it also satisfies the Dirichlet boundary condition

$$u^\star = 0 \text{ on } \Gamma_D. \tag{48c}$$

The equations (48) are the *strong form* of the variational problem (46). To summarize, the Euler-Lagrange necessary condition for (44) leads to a weak form that must be satisfied by a solution $u^\star$. Integration by parts leads to the strong form of the boundary value problem that must be satisfied by $u^\star$.

Note that in (44) we have assumed that $u^\star$ vanishes on Γ_D; variations $\hat{u}$ also have to satisfy a homogeneous Dirichlet boundary condition Γ_D in order for $u^\star + \varepsilon\hat{u}$ to vanish on Γ_D. If instead we had imposed a non-homogeneous Dirichlet boundary condition on $u^\star$ (i.e., $u^\star = g$ on Γ_D), we would still have to consider variations $\hat{u}$ that vanish on Γ_D, since with these variations $u^\star + \varepsilon\hat{u} = g$ is satisfied on Γ_D. To put it another way, $\hat{u} \in H_0^1(\Omega)$ even when $u^\star \in H^1(\Omega)$.

2. Nonlinear elliptic model problem

In the previous model problem, we began with a quadratic (in u and its derivatives) energy functional and showed, using variational calculus, that the minimizer $u^\star$ must satisfy a linear boundary value problem. Next we consider a non-quadratic 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 $u^\star$ that satisfies the Dirichlet boundary condition $u = g$ on Γ and minimizes Π:

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

To characterize a solution $u^\star$ for (49), we again invoke the Euler-Lagrange condition. We allow variations $\hat{u}$ with $\hat{u} = 0$ on Γ, i.e., $\hat{u} \in H_0^1$. The resulting necessary condition is that a solution $u^\star$ to (49) must satisfy the weak form

$$\begin{aligned} 0 &= \int_\Omega \left[k(u^\star)\nabla u^\star \cdot \nabla \hat{u} + \frac{\partial k(u^\star)}{\partial u}\hat{u}\,\nabla u^\star \cdot \nabla u^\star \right] dx - \int_\Omega f\hat{u}\, dx \\ &= \int_\Omega \hat{u}\left[-\nabla \cdot (k(u^\star)\nabla u^\star) + 2k_2 u^\star \nabla u^\star \cdot \nabla u^\star - f \right] dx \end{aligned} \tag{50}$$

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 weak form (50) is

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

Note that the weak form (50) and the corresponding strong from (51) are nonlinear in $u^\star$. Thus the necessary condition corresponding to the minimization problem (49) is a nonlinear boundary value problem.

This nonlinear BVP can be solved for $u^\star$ using an *infinite-dimensional* Newton method. The Hessian operator required by Newton's method is

found by taking a second variation of Π with respect to u, denoted by $\delta_u^2\Pi$. This is defined in terms of the first variation $\delta_u\Pi$ as follows:

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

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

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

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

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

$$u \leftarrow u + \tilde{u}. \tag{55}$$

As with the finite dimensional Newton's method, the above iteration is globalized via a line search.

3. Discretization and minimization

Usually, variational minimization problems such 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 following question arises: at what stage of the minimization should discretization be introduced? Should the energy functional $\Pi(u)$ be directly discretized, after which finite dimensional optimization is carried out? Or should the weak form of the necessary condition for minimization of $\Pi(u)$ first be derived, after which discretization is introduced? An advantage of discretizing the problem at the stage of the energy functional Π is that this results in a finite dimensional nonlinear optimization problem, for which Newton's method (or other descent algorithm) can be employed. On the other hand, deriving the Euler-Lagrange equation(s), and then discretizing the resulting weak form, is usually cleaner and more concise and avoids differentiating through numerical artifacts. However, in general it is unclear if the resulting discrete necessary condition still corresponds to 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 called *discretize-then-optimize*, or DTO. The second approach, which first takes variations in infinite dimensions and then discretizes the resulting Euler-Lagrange equation, is 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.

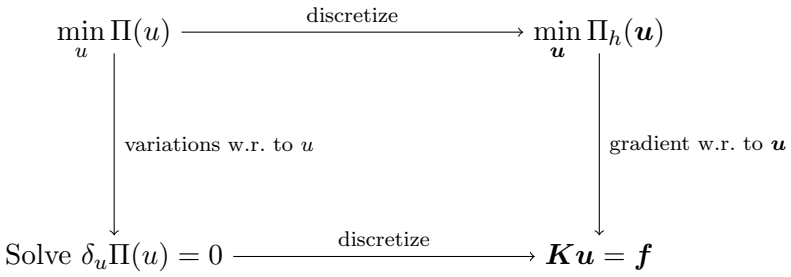

FIGURE 1. Illustration of the optimize-then-discretize and discretize-then-optimize approaches to solving a (quadratic) variational minimization problem. The two approaches can be equivalent when the appropriate weak form and discretization scheme are chosen.