Math 6008 Numerical PDEs–Lecture 12

Calculus of variation for mathematical physical equations

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1 Introduction to calculus of variation

Many physical models described by differential equations can be viewed as critical points of certain functionals.

In many problems arising from applications, a functional (泛函) is a mapping $J : K \to \mathbb{R}$ where K is a certain subspace of the space of functions defined on $\Omega \subset \mathbb{R}^d$ (in mathematics, often one chooses $K \subset L^2(\Omega)$ for $\Omega \subset \mathbb{R}^d$). Hence, J is a function of functions in these applications. (Of course, in mathematics, a functional means a mapping defined on a general Banach space.)

Definition 1. *The variational problem is to optimize J over K:*

$$\min_{u \in K} J(u).$$

For functions in $\mathbb{R}^d$, at the minimum (or similarly maximum), the derivative (gradient) equals zero. Hence, for functionals, we expect the same thing. The derivative of J can be taken similarly as that for functions defined in $\mathbb{R}^d$. In fact, for any "direction" v (which is a function), consider $u + \epsilon v$, where ϵ is small and can be both positive and negative, then the "directional derivative" (方向导数) can be given by

$$D_v J[u] := \lim_{\epsilon \to 0} \frac{J(u + \epsilon v) - J(u)}{\epsilon}.$$

If u is a local minimizer, $J(u+\epsilon v) \geq J(u)$ for any ϵ small enough. If this limit exists, then it must be zero since ϵ can be both positive and negative.

It can be shown in mathematics that $D_v J[u]$ is linear in v so that the Riesz theorem in functional analysis tells us that there exists $J'(u)$ such that

$$D_v J[u] = \langle J'(u), v \rangle.$$

Clearly, $J'(u)$ is an analogue of the gradient (梯度). Hence, a necessary condition is

$$J'(u) = 0.$$

The above argument seems abstract. Let us try to understand it in some concrete setting below. Often, the inner product is given by (of course, there are many other choices)

$$\langle f, g \rangle := \int_\Omega f g \, dx.$$

For example, for 1D problems, this is

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

To see why $\langle G, v \rangle = 0$ for all suitable v implies $G = 0$, we have the following (as a side note, a more general version for functions in the so-called Sobolev spaces can also be shown)

Lemma 1. *Suppose that $u \in C[a,b]$ which is continuous. If for all $v \in C_c(a,b)$ (continuous functions that are only nonzero on a closed subinterval of (a,b)), one has*

$$\int_a^b u(x) v(x) \, dx = 0,$$

then $u \equiv 0$.

Remark 1. *The condition $v \in C_c(a,b)$ implies that there exists a small number ϵ (depending on v), such that v is zero on $[a, a+\epsilon]$ and $[b-\epsilon, b]$. Hence, any derivative of v is zero at the endpoints.*

The proof is easy: suppose u is not zero, then there exists $\xi \in (a,b)$ such that $u(\xi) = 0$ (it is impossible that u is zero in the interior but nonzero on the boundary by the continuity). Without loss of generality, we assume

$u(\xi) > 0$ (otherwise, we replace u with $-u$ to perform the argument). By continuity, there is a neighborhood of ξ on which $u(x) > 0$. Then, we take a smooth function v that is zero outside this neighborhood and positive at ξ. This will then give a contradiction.

1.1 Examples

In this subsection, we will take some examples to illustrate the calculus of variation and the condition above

$$J'(u) = 0.$$

Brachistochrone problem(最速降线问题)

Consider a point mass released at $A(0,0)$ and moves to a target point $B(x_1, y_1)$ along a smooth curve connecting A and B under the gravity. Here, the positive direction of the y-axis is downward so that the the gravity is positive and $y_1 > 0$, $x_1 > 0$. The problem is to find the optimal curve ℓ among such a class so that the total time needed is the least.

The class of curves is set to be the class of functions defined on $[0, x_1]$, subject to $y(x_1) = y_1$, or

$$K := \{y \in C^1[0, x_1] : y(0) = 0, \quad y(x_1) = y_1\}.$$

Now, for a curve $y \in K$ given, the speed of the mass at x can be given by the conservation of energy:

$$v = \sqrt{2gy}.$$

Hence,

$$dt = \frac{ds}{v} = \sqrt{\frac{1 + (y'(x))^2}{2gy}}dx,$$

so that the total time is

$$T = J(y) = \int_0^{x_1} \sqrt{\frac{1 + (y'(x))^2}{2gy}}dx.$$

The problem is thus given by:

$$\min_{y\in K} J(y).$$

If $y \leq 0$ somewhere, $T = \infty$.

Below, we assume that the minimizer $y_0 \in K$ exists and try to find it.

Remark 2. *For rigorous mathematical analysis that ensures the existence of the curve, the class K should be enlarged that is closed under a certain topology imposed on the space of functions.*

First of all, we determine the "direction" or perturbation v allowed. Clearly, we require

$$y_0 + \epsilon v \in K,$$

for ϵ small. This requires that $v(0) = v(x_1) = 0$ and $v \in C^1$. In particular, we can choose $v \in C_c(0, x_1)$.

Now, we need

$$\langle J'(y_0), v\rangle := \frac{d}{d\epsilon} J(y_0 + \epsilon v)|_{\epsilon=0} = 0.$$

The right hand can be computed to be

$$\begin{aligned}\frac{d}{d\epsilon} J(y_0 + \epsilon v)|_{\epsilon=0} &= \int_0^{x_1} \frac{1}{2\sqrt{2g}} \left(\frac{1+(y_0')^2}{y_0}\right)^{-1/2} \frac{2y_0'v'y_0 - (1+(y_0')^2)v}{y_0^2}\, dx \\ &= \frac{1}{2\sqrt{2g}} \int_0^{x_1} \left[-\left(\frac{2y_0'}{\sqrt{(1+(y_0')^2)y_0}}\right)' - \sqrt{\frac{1+(y_0')^2}{y_0^3}}\right] v dx.\end{aligned}$$

This implies that

$$\frac{\delta J}{\delta y}(y) := J'(y) = \frac{1}{2\sqrt{2g}} \left[-\left(\frac{2y'}{\sqrt{(1+(y')^2)y}}\right)' - \sqrt{\frac{1+(y')^2}{y^3}}\right],$$

and we need this to be zero at the minimizer y_0. Simplifying this, one has

$$\frac{2y_0''((y')^2 - (1+(y')^2))}{1+(y_0')^2} + \frac{(y')^2 - (1+(y')^2)}{y_0} = 0.$$

This condition is reduced to

$$\frac{2y_0''}{1+(y_0')^2} = -\frac{1}{y_0} \Rightarrow y_0(1+(y_0')^2) = C > 0.$$

This gives (it is clear that we need to pick the positive sign in the square root)

$$\sqrt{\frac{y_0}{C-y_0}}dy_0 = dx_0$$

The integral of the left hand side can be evaluated by the trigonometric substitution, for example setting $y_0 = C\sin^2\theta$, which yields

$$x_0 = C_2 + C\frac{\sin\theta}{\cos\theta}2\sin\theta\cos\theta d\theta = C_2 + 2C\int \sin^2\theta d\theta = C_2 + \frac{C}{2}(2\theta - \sin(2\theta)).$$

The condition $y(0) = 0$ gives $C_2 = 0$ and $y(x_1) = y_1$ determines C. Setting $\alpha = 2\theta$, one has

$$y = a(1-\cos\alpha), \quad x = a(\alpha - \sin\alpha), \quad a = C/2.$$

Minimal surface

The problem is to impose a boundary curve in 3D. Then, to determine the surface that has the smallest area with the given boundary.

In particular, let $\Omega \subset \mathbb{R}^2$ be the region enclosed by the projection of the boundary in xy plane. The boundary is thus

$$u|_{\partial\Omega} = \varphi(x,y)$$

given. The surface we seek may be written as $u = u(x,y)$. The position vector is thus $\vec{r}(x,y) = (x,y,u(x,y))$. Hence, the area is

$$S = \int_\Omega |\vec{r}_x \times \vec{r}_y| dxdy = \int_\Omega \sqrt{1+u_x^2+u_y^2}dxdy.$$

Hence, one can formulate the space

$$K = \{u \in C^1(\bar{\Omega}) : u|_{\partial\Omega} = \varphi(x,y)\}.$$

The problem is

$$\min_{u\in K} J(u) := \min_{u\in K} \int_\Omega \sqrt{1+u_x^2+u_y^2}dxdy.$$

This problem is not easy to solve. If one assumes $u \ll 1$ so that

$$\sqrt{1+u_x^2+u_y^2} \approx \frac{1}{2}|\nabla u|^2,$$

the simplified problem

$$\min_{u\in K} \frac{1}{2}\int_\Omega |\nabla u|^2 dxdy =: \min_{u\in K} \hat{J}(u)$$

is simpler.

Assume that the minimizer exists (again to ensure existence theoretically, a larger space need to be considered in mathematics, which we shall see later), then we may derive the equation for the minimizer. Take $v \in C^1$ that is zero on $\partial\Omega$ (or one can take $v \in C_c^1$). Then,

$$\frac{d}{d\epsilon}\frac{1}{2}\int |\nabla u + \epsilon v|^2 dxdy|_{\epsilon=0} = 0.$$

This gives

$$\int_\Omega \nabla u \cdot \nabla v \, dxdy = 0 \Rightarrow \frac{\delta \hat{J}}{\delta u} = -\Delta u = 0.$$

This is the Laplace equation.

2 The Euler-Lagrange equations for necessary conditions and the boundary conditions

In this subsection, we focus on a specific class of functionals that is very common in applications. Namely,

$$J(u) = \int_a^b F(x, u, u')dx.$$

2.1 The Euler-Lagrange equation

Consider here the space

$$K = \{y \in C^1[a,b] : y(a) = y_a, \quad y(b) = y_b\}.$$

We optimize J over this space. Our goal is to derive a differential equation for the minimizer. The equation will be called the "Euler-Lagrange equation".

As above, we consider a perturbation direction v. Clearly, we require

$$v(a) = v(b) = 0.$$

Moreover,

$$\frac{dJ}{d\epsilon}|_{\epsilon=0} = \int_a^b [\frac{\partial F}{\partial y} v + \frac{\partial F}{\partial y'} v'] dx = \int_a^b [\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)] v dx$$

Here, $\frac{\partial F}{\partial y'}$ means that we take partial derivative of F on the third argument and then plug in y' into the position for that argument.

Remark 3. *Informally, we often write $\delta y := v$ and then think it as small perturbation (the rigorous definition in mathematics is a tangent vector in the tangent sapce), then one can write*

$$\delta J = \int_a^b [\frac{\partial F}{\partial y}\delta y + \frac{\partial F}{\partial y'}\delta y'] dx = \int_a^b [\frac{\partial F}{\partial y}\delta y - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\delta y] dx$$

It follows that

$$\frac{\delta J}{\delta y} = \frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right).$$

Hence, the minimizer satisfies the following differential equation

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = 0.$$

$$y(a) = y_a, \quad y(b) = y_b.$$

This is called the **Euler-Lagrange equation**. Clearly, the equation for the Brachistochrone problem is obtained this way.

2.2 The issue of the natural boundary condition

We just considered the variational problems for functions with boundary values fixed. For example, finding minimizer of the functional

$$J(u) = \frac{1}{2}\int_0^1 |u'(x)|^2 dx - \int_0^1 f(x)u(x)dx,$$

subject to $u(0) = u(1) = 0$.

The corresponding Euler-Lagrange equation is

$$-u''(x) = f(x), \quad u(0) = u(1) = 0.$$

Now, suppose we throw away the boundary condition $u(1) = 0$. Then, the equation

$$-u''(x) = f(x), \quad u(0) = 0$$

is not well-posed because the solution is not unique. However, the variational problem is well-defined: we can happily talk about the minimizer of $J(u)$ over

$$H = \{u : \int u^2 + |u'|^2 dx < \infty, \quad u(0) = 0\}.$$

Well, what is the equation for this minimizer? We take variation and have

$$\int_0^1 u'\delta u' dx - \int f\delta u dx = 0.$$

Integrating by parts,

$$u'\delta u'|_0^1 - \int u''\delta u\, dx - \int f\delta u\, dx = 0.$$

Since the functions in H must have the value at $x = 0$ to be 0, then

$$\delta u(0) = 0,$$

but $\delta u(1)$ is arbitrary. Hence,

$$-u'(1)\delta u(1) - \int (u'' + f)\delta u\, dx = 0.$$

This means that the minimizer should satisfy

$$u'(1) = 0, \quad -u'' = f.$$

Hence, the minimizer in fact satisfies the equation

$$-u''(x) = f(x), \quad u(0) = 0, \quad u'(1) = 0.$$

The boundary condition $u(0) = 0$ is called the essential boundary conditons (本质边界条件), which is imposed in the solution class, so it is a geometric boundary condition. The condition $u'(1) = 0$ is called the natural boundary condition (自然边界条件), which is not imposed in the solution class, but implied by the variational formulation.

3 The variaitonal formulations for typical mathematical physics equations; the weak solutions

Previously, we are given a functional and then derive the ODE or PDE for the minimizer, with either essential boundary conditions or the natural boundary conditions.

Often, we are given a PDE, we will try to find the functional and variaitonal problem for the PDE, or find the corresponding weak formulation so that we can define the so-called "weak solutions".

3.1 Basic concepts by a simple example

Consider the equation

$$-Tu'' = f(x).$$

To find the corresponding energy functional, one may

- Use the physical meaning and then construct the energy behind. Here, there are kinetical energy and the potential energy corresponding to f.

- Secondly, play around with the terms (by multiplying u and integrating etc).

By doing this, one may construct an energy functional:

$$J = \frac{1}{2}\int T|u'|^2 - fu\,dx.$$

As soon as we have the functional, we may solve the ODE or PDE by minimizing the energy functional.

$$\min_{u\in K} J(u). \tag{1}$$

This is the variational approach.

Moreover, as we have seen already, if we take the variation (the directional derivative), we will have an equation like

$$\langle J'(u), v\rangle = D_v J[u] = 0, \tag{2}$$

for any perturbational direction v. The perturbation v is the so-called virtual displacement in physics. The equation here indicates that the virtual work with the virtual displacement is zero. In other words, $J'(u) = 0$ is in fact the force balance equation.

In the variational formulation (1), u does not have to be twice differentiable. In fact, as long as

$$\int u^2 + (u')^2 dx < \infty,$$

(1) makes sense. Hence, (1) in fact gives a solution to

$$-Tu'' = f$$

in a weaker sense, called the weak solution.

Similarly, the virtual work formulation (2) also gives a definition of solution in a weaker sense if we move some derivatives onto v. In fact,

$$\int Tu'v' - fv\,dx = 0. \tag{3}$$

Clearly, in this formulation, u does not need to have second order derivatives either. This is a way as well to define the weak solution (弱解).

The formulation (1) is called the Ritz's variational formulation (corresponding to least potential principle). The formulation (3) is called the Galerkin's variational formulation (corresponding to virtual work principle), or the **weak formulation**.

Below, we explore these formulations for some typical problems, especially some elliptic problems.

3.2 1D elliptic problems

Consider

$$
\begin{aligned}
&-(p(x)u')' + q(x)u = f(x), \\
&u(a) = \alpha, \quad u'(b) = 0,
\end{aligned}
$$

where $p(x) \ge p_0 > 0$.

We start with the Galerkin's formulation, or the weak formulation. To do this, we **do not** start with the energy functional. Instead, we multiply the test function v (试探函数). Then, integration by parts:

$$
-\int_a^b (pu')'v\,dx + \int_a^b quv\,dx = \int_a^b fv\,dx.
$$

For the first term, do integration by parts, one has

$$
-pu'v|_a^b + \int_a^b pu'v'\,dx + \int_a^b quv\,dx = \int_a^b fv\,dx.
$$

Now, in the second term, there is no high order derivatives and the order is kind of balanced for u and v, so we stop doing further integration by parts.

The first term by $u'(b) = 0$, one has $p(a)u'(a)v(a)$. **Now, if we choose** $v(a) = 0$**, this term will vanish as well.** Note that choosing $v(a) = 0$ means that we restrict the test functions to a special class of functions. This will not lose information.

Remark 4. *If you leave $v(a)$ arbitrary, then you need the boundary value of $u'(a)$ to make this weak formulation to be defined. In mathematics, if you would like the boundary value $u'(a)$ to be defined, you need higher regularity than requiring $\int (u')^2 dx < \infty$. Hence, we do not desire $u'(a)$.*

Hence, we need to define the space for the test function

$$H = \{v : \int_a^b v^2 + (v')^2 \, dx < \infty, \quad v(a) = 0\}.$$

The set for u is

$$E = \{u : \int_a^b v^2 + (v')^2 \, dx < \infty, \quad u(a) = \alpha\}.$$

Clearly, $E = u_0 + H$ where u_0 is a particular function satisfying $u_0(a) = \alpha$. If $\alpha = 0$, then $E = H$.

Definition 2. *The Galerkin's formulation, or the weak formulation is: find $u \in E$ such that*

$$D(u, v) := \int_a^b pu'v' \, dx + \int_a^b quv \, dx = \int_a^b fv \, dx =: F(v), \quad \forall v \in H.$$

The solution is the weak solution (弱解).

Here, $D : H^1 \times H^1 \to \mathbb{R}$ is a bilinear form (where H^1 is the space without requirements on the boundary conditions, larger than H and E), and F is a linear funcional.

Reversely, if the minimizer of the weak formulation is twice continuously differentiable, it is easy to see that

$$-(p(x)u')' + q(x)u = f(x), \quad u(a) = \alpha, \quad u'(b) = 0.$$

As we have discussed already, $u(a) = \alpha$ is the essential boundary condition, which is imposed in the weak formulation. The condition $u'(b) = 0$ is implied by the variational formulation, or the natural boundary condition. We now know that the natural boundary conditions are for the *force*, implied by the minimizer of the variational problem. The essential boundary conditions are given by the constraints, or conditions for the geometry.

The problem here also has a Ritz variational formulation. In fact,

Definition 3.

$$J(u) = \frac{1}{2}\int_a^b (p(u')^2 + qu^2)dx - \int_a^b f(x)u\,dx = \frac{1}{2}D(u,u) - F(u), \quad u \in E.$$

The Ritz formulation is given by

$$\min_{u\in E} J(u).$$

It can be shown that the minimizer of J is the solution of the differential equaiton. Reversely, the solution of the differential equation is also the minimizer of this problem. Again, the natural boundary condition does not appear explicitly.

We remark that some elliptic equations like

$$-(pu')' + qu' + cu = f$$

does not have a corresponding energy functional J as u' is antisymmetric, but it allows a weak formulation (or the virtual work principle).

Exercise: think about how to treat the mixed boundary condition, or the third type boundary conditions