Physics 129a
Calculus of Variations
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1 Introduction

Many problems in physics have to do with extrema. When the problem involves finding a function that satisfies some extremum criterion, we may attack it with various methods under the rubric of "calculus of variations". The basic approach is analogous with that of finding the extremum of a function in ordinary calculus.

2 The Brachistochrone Problem

Historically and pedagogically, the prototype problem introducing the calculus of variations is the "brachistochrone", from the Greek for "shortest time". We suppose that a particle of mass m moves along some curve under the influence of gravity. We'll assume motion in two dimensions here, and that the particle moves, starting at rest, from fixed point a to fixed point b. We could imagine that the particle is a bead that moves along a rigid wire without friction [Fig. 1(a)]. The question is: what is the shape of the wire for which the time to get from a to b is minimized?

First, it seems that such a path must exist – the two outer paths in Fig. 2(b) presumably bracket the correct path, or at least can be made to bracket the path. For example, the upper path can be adjusted to take an arbitrarily long time by making the first part more and more horizontal. The lower path can also be adjusted to take an arbitrarily long time by making the dip deeper and deeper. The straight-line path from a to b must take a shorter time than both of these alternatives, though it may not be the shortest.

It is also readily observed that the optimal path must be single-valued in x, see Fig. 1(c). A path that wiggles back and forth in x can be shortened in time simply by dropping a vertical path through the wiggles. Thus, we can describe path C as a function $y(x)$.

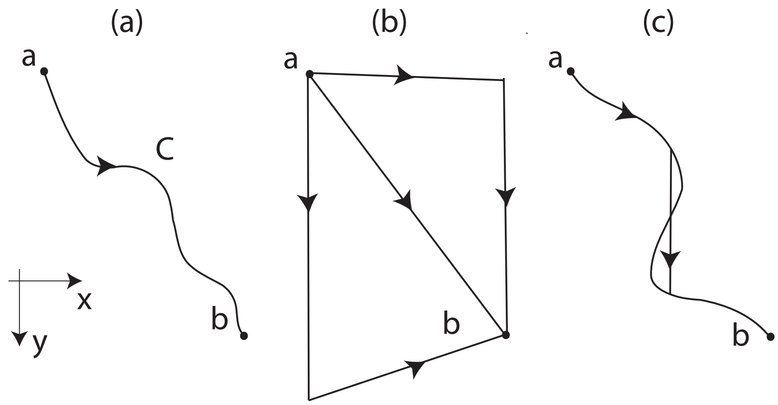

Figure 1: The Brachistochrone Problem: (a) Illustration of the problem; (b) Schematic to argue that a shortest-time path must exist; (c) Schematic to argue that we needn't worry about paths folding back on themselves.

We'll choose a coordinate system with the origin at point a and the y axis directed downward (Fig. 1). We choose the zero of potential energy so that it is given by:

$$V(y) = -mgy.$$

The kinetic energy is

$$T(y) = -V(y) = \frac{1}{2}mv^2,$$

for zero total energy. Thus, the speed of the particle is

$$v(y) = \sqrt{2gy}.$$

An element of distance traversed is:

$$ds = \sqrt{(dx)^2 + (dy)^2} = \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\, dx.$$

Thus, the element of time to traverse ds is:

$$dt = \frac{ds}{v} = \frac{\sqrt{1 + \left(\frac{dy}{dx}\right)^2}}{\sqrt{2gy}} dx,$$

and the total time of descent is:

$$T = \int_0^{x_b} \frac{\sqrt{1 + \left(\frac{dy}{dx}\right)^2}}{\sqrt{2gy}} dx.$$

Different functions $y(x)$ will typically yield different values for T; we call T a "functional" of y. Our problem is to find the minimum of this functional with respect to possible functions y. Note that y must be continuous – it would require an infinite speed to generate a discontinuity. Also, the acceleration must exist and hence the second derivative d^2y/dx^2. We'll proceed to formulate this problem as an example of a more general class of problems in "variational calculus".

Consider all functions, $y(x)$, with fixed values at two endpoints; $y(x_0) = y_0$ and $y(x_1) = y_1$. We wish to find that $y(x)$ which gives an extremum for the integral:

$$I(y) = \int_{x_0}^{x_1} F(y, y', x)\, dx,$$

where $F(y, y', x)$ is some given function of its arguments. We'll assume "good behavior" as needed.

In ordinary calculus, when we want to find the extrema of a function $f(x, y, \ldots)$ we proceed as follows: Start with some candidate point $(x_0, y_0, \ldots)$, Compute the total differential, df, with respect to arbitrary infinitesimal changes in the variables, $(dx, dy, \ldots)$:

$$df = \left(\frac{\partial f}{\partial x}\right)_{x_0, y_0, \ldots} dx \quad + \quad \left(\frac{\partial f}{\partial y}\right)_{x_0, y_0, \ldots} dy \quad + \ldots$$

Now, df must vanish at an extremum, independent of which direction we choose with our infinitesimal $(dx, dy, \ldots)$. If $(x_0, y_0, \ldots)$ are the coordinates of an extremal point, then

$$\left(\frac{\partial f}{\partial x}\right)_{x_0, y_0, \ldots} = \left(\frac{\partial f}{\partial y}\right)_{x_0, y_0, \ldots} = \quad \ldots \quad = \quad 0.$$

Solving these equations thus gives the coordinates of an extremum point.

Finding the extremum of a functional in variational calculus follows the same basic approach. Instead of a point $(x_0, y_0, \ldots)$, we consider a candidate function $y(x) = Y(x)$. This candidate must satisfy our specified behavior at the endpoints:

$$\begin{aligned} Y(x_0) &= y_0 \\ Y(x_1) &= y_1. \end{aligned} \tag{1}$$

We consider a small change in this function by adding some multiple of another function, $h(x)$:

$$Y(x) \to Y(x) + \epsilon h(x).$$

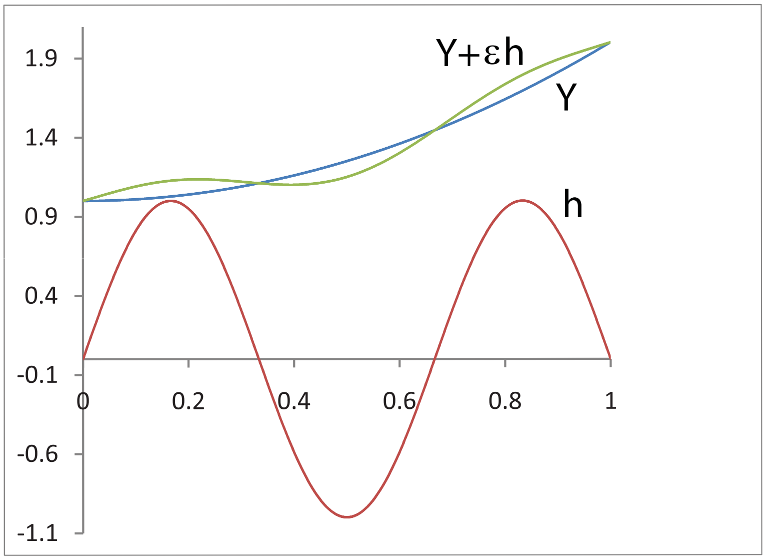

Figure 2: Variation on function Y by function ϵh.

To maintain the endpoint condition, we must have $h(x_0) = h(x_1) = 0$. The notation δY is often used for $\epsilon h(x)$.

A change in functional form of $Y(x)$ yields a change in the integral I. The integrand changes at each point x according to changes in y and y':

$$\begin{aligned} y(x) &= Y(x) + \epsilon h(x), \\ y'(x) &= Y'(x) + \epsilon h'(x). \end{aligned} \tag{2}$$

To first order in ϵ, the new value of F is:

$$F(Y+\epsilon h, Y'+\epsilon h') \approx F(Y, Y', x) + \left(\frac{\partial F}{\partial y}\right)_{\substack{y=Y \\ y'=Y'}} \epsilon h(x) + \left(\frac{\partial F}{\partial y'}\right)_{\substack{y=Y \\ y'=Y'}} \epsilon h'(x). \tag{3}$$

We'll use "δI" to denote the change in I due to this change in functional form:

$$\begin{aligned} \delta I &= \int_{x_0}^{x_1} F(Y + \epsilon h, Y' + \epsilon h', x)\, dx - \int_{x_0}^{x_1} F(Y, Y', x)\, dx, \\ &\approx \epsilon \int_{x_0}^{x_1} \left[\left(\frac{\partial F}{\partial y}\right)_{\substack{y=Y \\ y'=Y'}} h + \left(\frac{\partial F}{\partial y'}\right)_{\substack{y=Y \\ y'=Y'}} h' \right] dx. \end{aligned} \tag{4}$$

We may apply integration by parts to the second term:

$$\int_{x_0}^{x_1} \frac{\partial F}{\partial y'} h'\, dx = - \int_{x_0}^{x_1} h \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) dx, \tag{5}$$

where we have used $h(x_0) = h(x_1) = 0$. Thus,

$$\delta I = \epsilon \int_{x_0}^{x_1} \left[\frac{\partial F}{\partial y} + \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\right]_{\substack{y=Y \\ y'=Y'}} h\, dx. \tag{6}$$

When I is at a minimum, δI must vanish, since, if $\delta I > 0$ for some ϵ, then changing the sign of ϵ gives $\delta I < 0$, corresponding to a smaller value of I. A similar argument applies for $\delta I < 0$, hence $\delta I = 0$ at a minimum. This must be true for arbitrary h and ϵ small but finite. It seems that a necessary condition for I to be extremal is:

$$\left[\frac{\partial F}{\partial y} + \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\right]_{\substack{y=Y \\ y'=Y'}} = 0. \tag{7}$$

This follows from the fundamental theorem:

Theorem: If $f(x)$ is continuous in $[x_0, x_1]$ and

$$\int_{x_0}^{x_1} f(x)h(x)\, dx = 0 \tag{8}$$

for every continuously differentiable $h(x)$ in $[x_0, x_1]$, where $h(x_0) = h(x_1) = 0$, then $f(x) = 0$ for $x \in [x_0, x_1]$.

Proof: Imagine that $f(\chi) > 0$ for some $x_0 < \chi < x_1$. Since f is continuous, there exists $\epsilon > 0$ such that $f(x) > 0$ for all $x \in (\chi - \epsilon, \chi + \epsilon)$. Let

$$h(x) = \begin{cases} (x-\chi+\epsilon)^2(x-\chi-\epsilon)^2, & \chi - \epsilon \leq x \leq \chi + \epsilon \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

Note that $h(x)$ is continuously differentiable in $[x_0, x_1]$ and vanishes at x_0 and x_1. We have that

$$\begin{aligned} \int_{x_0}^{x_1} f(x)h(x)\, dx &= \int_{\chi-\epsilon}^{\chi+\epsilon} f(x)(x-\chi+\epsilon)^2(x-\chi-\epsilon)^2\, dx && (10) \\ &> 0, && (11) \end{aligned}$$

since $f(x)$ is larger than zero everywhere in this interval. Thus, $f(x)$ cannot be larger than zero anywhere in the interval. The parallel argument follows for $f(x) < 0$.

This theorem then permits the assertion that

$$\left[\frac{\partial F}{\partial y} + \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\right]_{\substack{y=Y \\ y'=Y'}} = 0. \tag{12}$$

whenever $y = Y$ such that I is an extremum, at least if the expression on the right is continuous. We call the expression on the right the "Lagrangian derivative" of $F(y, y', x)$ with respect to $y(x)$, and denote it by $\frac{\delta F}{\delta y}$.

The extremum condition, relabeling $Y \to y$, is then:

$$\frac{\delta F}{\delta y} \equiv \frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = 0. \tag{13}$$

This is called the Euler-Lagrange equation.

Note that $\delta I = 0$ is a necessary condition for I to be an extremum, but not sufficient. By definition, the Euler-Lagrange equation determines points for which I is "stationary". Further consideration is required to establish whether I is an extremum or not.

We may write the Euler-Lagrange equation in another form. Let

$$F_a(y, y', x) \equiv \frac{\partial F}{\partial y'}. \tag{14}$$

Then

$$\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = \frac{dF_a}{dx} = \frac{\partial F_a}{\partial x} + \frac{\partial F_a}{\partial y}y' + \frac{\partial F_a}{\partial y'}y'' \tag{15}$$

$$= \frac{\partial^2 F}{\partial x \partial y'} + \frac{\partial^2 F}{\partial y \partial y'}y' + \frac{\partial^2 F}{\partial y'^2}y''. \tag{16}$$

Hence the Euler-Lagrange equation may be written:

$$\frac{\partial^2 F}{\partial y'^2}y'' + \frac{\partial^2 F}{\partial y \partial y'}y' + \frac{\partial^2 F}{\partial x \partial y'} - \frac{\partial F}{\partial y} = 0. \tag{17}$$

Let us now apply this to the brachistochrone problem, finding the extremum of:

$$\sqrt{2g}T = \int_0^{x_b} \sqrt{\frac{1 + y'^2}{y}}dx. \tag{18}$$

That is:

$$F(y, y', x) = \sqrt{\frac{1 + y'^2}{y}}. \tag{19}$$

Notice that, in this case, F has no explicit dependence on x, and we can take a short-cut. Starting with the Euler-Lagrange equation, if F has no explicit x-dependence we find:

$$0 = \left[\frac{\partial F}{\partial y} - \frac{d}{dx}\frac{\partial F}{\partial y'}\right]y' \tag{20}$$

$$= \frac{\partial F}{\partial y}y' - y'\frac{d}{dx}\frac{\partial F}{\partial y'} \tag{21}$$

$$= \frac{dF}{dx} - \frac{\partial F}{\partial y'}y'' - y'\frac{d}{dx}\frac{\partial F}{\partial y'} \tag{22}$$

$$= \frac{d}{dx}\left(F - y'\frac{\partial F}{\partial y'}\right). \tag{23}$$

Hence,

$$F - y'\frac{\partial F}{\partial y'} = \text{constant} = C. \tag{24}$$

In this case,

$$y'\frac{\partial F}{\partial y'} = (y')^2 / \sqrt{y\,(1+y'^2)}. \tag{25}$$

Thus,

$$\sqrt{\frac{1+y'^2}{y}} - (y')^2 / \sqrt{y\,(1+y'^2)} = C, \tag{26}$$

or

$$y\left(1+y'^2\right) = \frac{1}{C^2} \equiv A. \tag{27}$$

Solving for x, we find

$$x = \int\sqrt{\frac{y}{A-y}}dy. \tag{28}$$

We may perform this integration with the trigonometric substitution: $y = \frac{A}{2}(1-\cos\theta) = A\sin^2\frac{\theta}{2}$. Then,

$$x = \int\sqrt{\frac{\sin^2\frac{\theta}{2}}{1-\sin^2\frac{\theta}{2}}}A\sin\frac{\theta}{2}\cos\frac{\theta}{2}d\theta \tag{29}$$

$$= A\int\sin^2\frac{\theta}{2}d\theta \tag{30}$$

$$= \frac{A}{2}(\theta - \sin\theta) + B. \tag{31}$$

We determine integration constant B by letting $\theta = 0$ at $y = 0$. We chose our coordinates so that $x_a = y_a = 0$, and thus $B = 0$. Constant A is determined by requiring that the curve pass through (x_b, y_b):

$$x_b = \frac{A}{2}(\theta_b - \sin\theta_b), \tag{32}$$

$$y_b = \frac{A}{2}(1 - \cos\theta_b). \tag{33}$$

This pair of equations determines A and θ_b. The brachistochrone is given parametrically by:

$$x = \frac{A}{2}(\theta - \sin\theta), \quad (34)$$

$$y = \frac{A}{2}(1 - \cos\theta). \quad (35)$$

In classical mechanics, Hamilton's principle for conservative systems that the action is stationary gives the familiar Euler-Lagrange equations of classical mechanics. For a system with generalized coordinates $q_1, q_2, \ldots, q_n$, the action is

$$S = \int_{t_0}^{t} L\left(\{q_i\}, \{\dot{q}_i\}, t'\right) dt, \quad (36)$$

where L is the Lagrangian. Requiring S to be stationary yields:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \quad i = 1, 2, \ldots, n. \quad (37)$$

3 Relation to the Sturm-Liouville Problem

Suppose we have the Sturm-Liouville operator:

$$L = \frac{d}{dx}p(x)\frac{d}{dx} - q(x), \quad (38)$$

with $p(x) \geq 0$, $q(x) \geq 0$, and $x \in (0, U)$. We are interested in solving the inhomogeneous equation $Lf = g$, where g is a given function.

Consider the functional

$$J = \int_0^U \left(pf'^2 + qf^2 + 2gf\right) dx. \quad (39)$$

The Euler-Lagrange equation for J to be an extremum is:

$$\frac{\partial F}{\partial f} - \frac{d}{dx}\left(\frac{\partial F}{\partial f'}\right) = 0, \quad (40)$$

where $F = pf'^2 + qf^2 + 2gf$. We have

$$\frac{\partial F}{\partial f} = 2qy + 2g \quad (41)$$

$$\frac{d}{dx}\left(\frac{\partial F}{\partial f'}\right) = 2p'f' + 2pf''. \quad (42)$$

Substituting into the Euler-Lagrange equation gives

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right] - q(x)f(x) = 0. \tag{43}$$

This is the Sturm-Liouville equation! That is, the Sturm-Liouville differential equation is just the Euler-Lagrange equation for the functional J.

We have the following theorem:

Theorem: The solution to

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right] - q(x)f(x) = g(x), \tag{44}$$

where $p(x) > 0$, $q(x) \geq 0$, and boundary conditions $f(0) = a$ and $f(U) = b$, exists and is unique.

Proof: First, suppose there exist two solutions, f_1 and f_2. Then $d = f_1 - f_2$ must satisfy the homogeneous equation:

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}d(x)\right] - q(x)d(x) = 0, \tag{45}$$

with homogeneous boundary conditions $d(0) = d(U) = 0$. Now multiply Equation 45 by $d(x)$ and integrate:

$$\begin{aligned}\int_0^U d(x)\frac{d}{dx}\left(p(x)\frac{d}{dx}d(x)\right)dx \quad - \quad \int_0^U q(x)d(x)^2\,dx = 0 \\ = d(x)p(x)\frac{dd(x)}{dx}\Big|_0^U - \int_0^U \left(\frac{dd(x)}{dx}\right)^2 p(x)\,dx \\ = -\int_0^U pd'^2\,dx. \end{aligned} \tag{46}$$

Thus,

$$\int_0^U \left(pd'^2(x) + q(x)d(x)^2\right)\,dx = 0. \tag{47}$$

Since $pd'^2 \geq 0$ and $qd^2 \geq 0$, we must thus have $pd'^2 = 0$ and $qd^2 = 0$ in order for the integral to vanish. Since $p > 0$ and $pd'^2 = 0$ it must be true that $d' = 0$, that is d is a constant. But $d(0) = 0$, therefore $d(x) = 0$. The solution, if it exists, is unique.

The issue for existence is the boundary conditions. We presume that a solution to the differential equation exists for some boundary conditions, and must show that a solution exists for the given boundary condition. From elementary calculus we know that two linearly independent solutions to the homogeneous differential equation exist. Let $h_1(x)$ be a non-trivial solution to the homogeneous differential equation with $h_1(0) = 0$. This must be possible because we can take a suitable linear combination of our two solutions. Because the solution to the inhomogeneous equation is unique, it must be true that $h_1(U) \neq 0$. Likewise, let $h_2(x)$ be a solution to the homogeneous equation with $h_2(U) = 0$ (and therefore $h_2(0) \neq 0$). Suppose $f_0(x)$ is a solution to the inhomogeneous equation satisfying some boundary condition. Form the function:

$$f(x) = f_0(x) + k_1 h_1(x) + k_2 h_2(x). \tag{48}$$

We adjust constants k_1 and k_2 in order to satisfy the desired boundary condition

$$\begin{aligned} a &= f_0(0) + k_2 h_2(0), & (49) \\ b &= f_0(U) + k_1 h_1(U). & (50) \end{aligned}$$

That is,

$$\begin{aligned} k_1 &= \frac{b - f_0(U)}{h_1(U)}, & (51) \\ k_2 &= \frac{a - f_0(0)}{h_2(U)}. & (52) \end{aligned}$$

We have demonstrated existence of a solution.

This discussion leads us to the variational calculus theorem:

Theorem: For continuously differentiable functions in $(0, U)$ satisfying $f(0) = a$ and $f(U) = b$, the functional

$$J = \int_0^U \left(p f'^2 + q f^2 + 2 g f \right) dx, \tag{53}$$

with $p(x) > 0$ and $q(x) \geq 0$, attains its minimum if and only if $f(x)$ is the solution of the corresponding Sturm-Liouville equation.

Proof: Let $s(x)$ be the unique solution to the Sturm-Liouville equation satisfying the given boundary conditions. Let $f(x)$ be any other continuously differentiable function satisfying the boundary conditions. Then $d(x) \equiv f(x) - s(x)$ is continuously differentiable and $d(0) = d(U) = 0$.

Solving for f, squaring, and doing the same for the dervative equation, yields

$$
\begin{aligned}
f^2 &= d^2 + s^2 + 2sd, \qquad (54)\\
f'^2 &= d'^2 + s'^2 + 2s'd'. \qquad (55)
\end{aligned}
$$

Let

$$
\begin{aligned}
\Delta J &\equiv J(f) - J(s) \qquad (56)\\
&= \int_0^U \left(pf'^2 + qf^2 + 2gf - ps'^2 - qs^2 - 2gs\right)\, dx \qquad (57)\\
&= \int_0^U \left[p\left(d'^2 + 2s'd'\right) + q\left(d^2 + 2ds\right) + 2gf\right]\, dx \qquad (58)\\
&= 2\int_0^U (pd's' + qds + gd)\, dx + \int_0^U \left(pd'^2 + qd^2\right)\, dx. \qquad (59)
\end{aligned}
$$

But

$$
\begin{aligned}
\int_0^U (pd's' + qds + gd)\, dx &= dps'\Big|_0^U + \int_0^U \left[-d(x)\frac{d}{dx}(ps') + qds + gd\right] dx\\
&= \int_0^U d(x)\left[-\frac{d}{dx}(ps') + qs + g\right] dx, \quad \text{since } d(0) = d(U) = 0\\
&= 0; \quad \text{integrand is zero by the differential equation.} \qquad (60)
\end{aligned}
$$

Thus, we have that

$$
\Delta J = \int_0^U \left(pd' + qd^2\right)\, dx \geq 0. \qquad (61)
$$

In other words, f does no better than s, hence s corresponds to a minimum. Furthermore, if $\Delta J = 0$, then $d = 0$, since $p > 0$ implies d' must be zero, and therefore d is constant, but we know $d(0) = 0$, hence $d = 0$. Thus, $f = s$ at the minimum.

4 The Rayleigh-Ritz Method

Consider the Sturm-Liouville problem:

$$
\frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right] - q(x)f(x) = g(x), \qquad (62)
$$

with $p > 0$, $q \geq 0$, and specified boundary conditions. For simplicity here, let's assume $f(0) = f(U) = 0$. Imagine expanding the solution in some set of complete functions, $\{\beta_n(x)\}$ (not necessarily eignefunctions):

$$f(x) = \sum_{n=1}^{\infty} A_n \beta_n(x).$$

We have just shown that our problem is equivalent to minimizing

$$J = \int_0^U \left(pf'^2 + qf^2 + 2gf \right) dx. \tag{63}$$

Substitute in our expansion, noting that

$$pf'^2 = \sum_m \sum_n A_m A_n p(x) \beta'_m(x) \beta'_n(x). \tag{64}$$

Let

$$C_{mn} \equiv \int_0^U p\beta'_m \beta'_n \, dx, \tag{65}$$

$$B_{mn} \equiv \int_0^U p\beta_m \beta_n \, dx, \tag{66}$$

$$G_n \equiv \int_0^U g\beta_n \, dx. \tag{67}$$

Assume that we can interchange the sum and integral, obtaining, for example,

$$\int_0^U pf'^2 \, dx = \sum_m \sum_n C_{mn} A_m A_n. \tag{68}$$

Then

$$J = \sum_m \sum_n \left(C_{mn} + B_{mn} \right) A_m A_n + 2 \sum_n G_n A_n. \tag{69}$$

Let $D_{mn} \equiv C_{mn} + B_{mn} = D_{nm}$. The D_{mn} and G_n are known, at least in principle. We wish to solve for the expansion coefficients $\{A_n\}$. To accomplish this, use the condition that J is a minimum, that is,

$$\frac{\partial J}{\partial A_n} = 0, \quad \forall n. \tag{70}$$

Thus,

$$0 = \frac{\partial J}{\partial A_n} = \sum_{m=1}^{\infty} D_{nm} A_m + G_n, \quad n = 1, 2, \ldots \tag{71}$$

This is an infinite system of coupled inhomogeneous equations. If D_{nm} is diagonal, the solution is simple:

$$A_n = -G_n / D_{nn}. \tag{72}$$

The reader is encouraged to demonstrate that this occurs if the β_n are the eigenfunctions of the Sturm-Liouville operator.

It may be too difficult to solve the eigenvalue problem. In this case, we can look for an approximate solution via the "Rayleigh-Ritz" approach: Choose some finite number of linearly independent functions $\{\alpha_1(x), \alpha_2(x), \ldots, \alpha_N(x)\}$. In order to find a function

$$\bar{f}(x) = \sum_{n=1}^{N} \bar{A}_n \alpha(n)(x) \tag{73}$$

that approximates closely $f(x)$, we find the values for $\bar{A}_n$ that minimize

$$J(\bar{f}) = \sum_{n,m=1}^{N} \bar{D}_{nm} \bar{A}_m \bar{A}_n + 2 \sum_{n=1}^{N} \bar{G}_n \bar{A}_n, \tag{74}$$

where now

$$\bar{D}_{nm} \equiv \int_0^U \left(p\alpha_n' \alpha_m' + q\alpha_n \alpha_m\right) dx \tag{75}$$

$$\bar{G}_n \equiv \int_0^U g\alpha_n \, dx. \tag{76}$$

The minimum of $J(\bar{f})$ is at:

$$\sum_{m=1}^{N} \bar{D}_{nm} \bar{A}_m + \bar{G}_n = 0, \quad n = 1, 2, \ldots \tag{77}$$

In this method, it is important to make a good guess for the set of functions $\{\alpha_n\}$.

It may be remarked that the Rayleigh-Ritz method is similar in spirit but different from the variational method we typically introduce in quantum mechanics, for example when attempting to compute the ground state energy of the helium atom. In that case, we adjust parameters in a non-linear function, while in the Rayleigh-Ritz method we adjust the linear coefficients in an expansion.

5 Adding Constraints

As in ordinary extremum problems, constraints introduce correlations, now in the possible variations of the function at different points. As with the ordinary problem, we may employ the method of Lagrange multipliers to impose the constraints.

We consider the case of the "isoperimetric problem", to find the stationary points of the functional:

$$J = \int_a^b F(f, f', x)\, dx, \tag{78}$$

in variations δf vanishing at $x = a, b$, with the constraint that

$$C \equiv \int_a^b G(f, f', x)\, dx \tag{79}$$

is constant under variations.

We have the following theorem:

Theorem: (Euler) The function f that solves this problem also makes the functional $I = J + \lambda C$ stationary for some λ, as long as $\frac{\delta C}{\delta f} \neq 0$ (i.e., f does not satisfy the Euler-Lagrange equation for C).

Proof: (partial) We make stationary the integral:

$$I = J + \lambda C = \int_a^b (F + \lambda G) dx. \tag{80}$$

That is, f must satisfy

$$\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'} + \lambda \left(\frac{\partial G}{\partial f} - \frac{d}{dx}\frac{\partial G}{\partial f'} \right) = 0. \tag{81}$$

Multiply by the variation $\delta f(x)$ and integrate:

$$\int_a^b \left(\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'} \right) \delta f(x)\, dx + \lambda \int_a^b \left(\frac{\partial G}{\partial f} - \frac{d}{dx}\frac{\partial G}{\partial f'} \right) \delta f(x)\, dx = 0. \tag{82}$$

Here, $\delta f(x)$ is arbitrary. However, only those variations that keep C invariant are allowed (e.g., take partial derivative with respect to λ and require it to be zero):

$$\delta C = \int_a^b \left(\frac{\partial G}{\partial f} - \frac{d}{dx}\frac{\partial G}{\partial f'} \right) \delta f(x)\, dx = 0. \tag{83}$$

5.1 Example: Catenary

A heavy chain is suspended from endpoints at (x_1, y_1) and (x_2, y_2). What curve describes its equilibrium position, under a uniform gravitational field?

The solution must minimize the potential energy:

$$V = g\int_1^2 y dm \tag{84}$$

$$= \rho g\int_1^2 y ds \tag{85}$$

$$= \rho g\int_{x_1}^{x_2} y\sqrt{1+y'^2}dy, \tag{86}$$

where ρ is the linear density of the chain, and the distance element along the chain is $ds = dx\sqrt{1+y'^2}$.

We wish to minimize V, under the constraint that the length of the chain is L, a constant. We have,

$$L = \int_1^2 ds = \int_{x_1}^{x_2} \sqrt{1+y'^2}dx. \tag{87}$$

To solve, let (we multiply L by ρg and divide out of the problem)

$$F(y, y', x) = y\sqrt{1+y'^2} + \lambda\sqrt{1+y'^2}, \tag{88}$$

and solve the Euler-Lagrange equation for F.

Notice that F does not depend explicitly on x, so we again use our short cut that

$$F - y'\frac{\partial F}{\partial y'} = \text{constant} = C. \tag{89}$$

Thus,

$$C = F - y'\frac{\partial F}{\partial y'} \tag{90}$$

$$= (y+\lambda)\left(\sqrt{1+y'^2} - \frac{y'^2}{\sqrt{1+y'^2}}\right) \tag{91}$$

$$= \frac{(y+\lambda)}{(\sqrt{1+y'^2}.} \tag{92}$$

Some manipulation yields

$$\frac{dy}{\sqrt{(y+\lambda)^2 - C^2}} = \frac{dx}{C}. \tag{93}$$

With the substitution $y + \lambda = C\cosh\theta$, we obtain $\theta = \frac{x+k}{C}$, where k is an integraton constant, and thus

$$y + \lambda = C\cosh\left(\frac{x+k}{C}\right). \tag{94}$$

There are three unknown constants to determine in this expression, C, k, and λ. We have three equations to use for this:

$$y_1 + \lambda = C \cosh\left(\frac{x_1 + k}{C}\right), \tag{95}$$

$$y_2 + \lambda = C \cosh\left(\frac{x_2 + k}{C}\right), \quad \text{and} \tag{96}$$

$$L = \int_{x_1}^{x_2} \sqrt{1 + y'^2} dx. \tag{97}$$

6 Eigenvalue Problems

We may treat the eigenvalue problem as a variational problem. As an example, consider again the Sturm-Liouville eigenvalue equation:

$$\frac{d}{dx}\left[p(x)\frac{df(x)}{dx}\right] - q(x)f(x) = -\lambda w(x)f(x), \tag{98}$$

with boundary conditions $f(0) = f(U) = 0$. This is of the form

$$Lf = -\lambda w f. \tag{99}$$

Earlier, we found the desired functional to make stationary was, for $Lf = 0$,

$$I = \int_0^U \left(pf'^2 + qf^2\right) dx. \tag{100}$$

We modify this to the eigenvalue problem with $q \to q - \lambda w$, obtaining

$$I = \int_0^U \left(pf'^2 + qf^2 - \lambda w f^2\right) dx, \tag{101}$$

which possesses the Euler-Lagrange equation giving the desired Sturm-Liouville equation. Note that λ is an unknown parameter - we want to determine it.

It is natural to regard the eigenvalue problem as a variational problem with constraints. Thus, we wish to vary $f(x)$ so that

$$J = \int_0^U \left(pf'^2 + qf^2\right) dx \tag{102}$$

is stationary, with the constraint

$$C = \int_0^U w f^2 dx = \text{constant}. \tag{103}$$

Notice here that we may take $C = 1$, corresponding to normalized eigenfunctions f, with respect to weight w.

Let's attempt to find approximate solutions using the Rayleigh-Ritz method. Expand

$$f(x) = \sum_{n=1}^{\infty} A_n u_n(x), \tag{104}$$

where $u(0) = u(U) = 0$. The u_n are some set of expansion functions, not the eigenfunctions – if they are the eigenfunctions, then the problem is already solved! Substitute this into I, giving

$$I = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} (C_{mn} - \lambda D_{mn}) A_m A_n, \tag{105}$$

where

$$C_{mn} \equiv \int_0^U (p u'_m u'_n + q u_m u_n)\, dx \tag{106}$$

$$D_{mn} \equiv \int_0^U w u_m u_n dx. \tag{107}$$

Requiring I to be stationary,

$$\frac{\partial I}{\partial A_m} = 0, \quad m = 1, 2, \ldots, \tag{108}$$

yields the infinite set of coupled homogeneous equations:

$$\sum_{n=1}^{\infty} (C_{mn} - \lambda D_{mn}) A_n = 0, \quad m = 1, 2, \ldots \tag{109}$$

This is perhaps no simpler to solve than the original differential equation. However, we may make approximate solutions for $f(x)$ by selecting a finite set of linearly independent functions $\alpha_1, \ldots, \alpha_N$ and letting

$$\bar{f}(x) = \sum_{n=1}^{N} \bar{A}_n \alpha_n(x). \tag{110}$$

Solve for the "best" approximation of this form by finding those $\{\bar{A}_n\}$ that satisfy

$$\sum_{n=1}^{N} \left(\bar{C}_{mn} - \bar{\lambda} \bar{D}_{mn}\right) \bar{A}_n = 0, \quad m = 1, 2, \ldots, N, \tag{111}$$

where

$$\bar{C}_{mn} \equiv \int_0^U (p \alpha'_m \alpha'_n + q \alpha_m \alpha_n)\, dx \tag{112}$$

$$\bar{D}_{mn} \equiv \int_0^U w \alpha_m \alpha_n dx. \tag{113}$$

This looks like N equations in the $N+1$ unknowns $\bar{\lambda}$, $\{\bar{A}_n\}$, but the overall normalization of the A_n's is arbitrary. Hence there are enough equations in principle, and we obtain

$$\bar{\lambda} = \frac{\sum_{m,n=1}^{N} \bar{C}_{mn}\bar{A}_m\bar{A}_n}{\sum_{m,n=1}^{N} \bar{D}_{mn}\bar{A}_m\bar{A}_n}. \tag{114}$$

Notice the similarity of Eqn. 114 with

$$\lambda = \frac{\int_0^U (pf'^2 + qf^2)\,dx}{\int_0^U wf^2 dx} = \frac{J(f)}{C(f)}. \tag{115}$$

This follows since $I = 0$ for f a solution to the Sturm-Liouville equation:

$$\begin{aligned} I &= \int_0^U \left(pf'^2 + qf^2 - \lambda w f^2\right) dx \\ &= pff'\Big|_0^U + \int_0^U \left[-f\frac{d}{dx}(pf') + qf^2 - \lambda w f^2\right] dx \\ &= 0 + \int_0^U \left(-qf^2 + \lambda w f^2 + qf^2 - \lambda w f^2\right) dx \\ &= 0, \end{aligned} \tag{116}$$

where we have used the both the boundary condition $f(0) = f(U) = 0$ and Sturm-Liouville equation $\frac{d}{dx}(pf') = qf - \lambda w f$ to obtain the third line. Also,

$$\bar{\lambda} = \frac{J(\bar{f})}{C(\bar{f})}, \tag{117}$$

since, for example,

$$\begin{aligned} J(\bar{f}) &= \int_0^U \left(p\bar{f}'^2 + q\bar{f}^2\right) dx \\ &= \int_0^U \left(p\sum_{m,n} \bar{A}_n\bar{A}_m\alpha'_m\alpha'_n + q\sum_{m,n} \bar{A}_n\bar{A}_m\alpha_m\alpha_n\right) dx \\ &= \sum_{m,n} \bar{C}_{mn}\bar{A}_n\bar{A}_m. \end{aligned} \tag{118}$$

That is, if $\bar{f}$ is "close" to an eigenfunction f, then $\bar{\lambda}$ should be "close" to an eigenvalue λ.

Let's try an example: Find the lowest eigenvalue of $f'' = -\lambda f$, with boundary conditions $f(\pm 1) = 0$. We of course readily see that the first eigenfunction is $\cos(\pi x/2)$ with $\lambda_1 = \pi^2/4$, but let's try our method to see how we do. For simplicity, we'll try a Rayleigh-Ritx approximation with only one term in the sum.

As we noted earlier, it is a good idea to pick the functions with some care. In this case, we know that the lowest eigenfunction won't wiggle much, and a good guess is that it will be symmetric with no zeros in the interval $(-1, 1)$. Such a function, which satisfies the boundary conditions, is:

$$\bar{f}(x) = \bar{A}\left(1 - x^2\right), \tag{119}$$

and we'll try it. With $N = 1$, we have $\alpha_1 = \alpha = 1 - x^2$, and

$$C \equiv \bar{C}_{11} = \int_{-1}^{1} \left(p\alpha'^2 + q\alpha^2\right) dx. \tag{120}$$

In the Sturm-Liouville form, we have $p(x) = 1$, $q(x) = 0$, $w(x) = 1$.

With $N = 1$, we have $\alpha_1 = \alpha = 1 - x^2$, and

$$C = \int_{-1}^{1} 4x^2 dx = \frac{8}{3}. \tag{121}$$

Also,

$$D \equiv \bar{D}_{11} = \int_{-1}^{1} w\alpha^2 dx = \int_{-1}^{1} \left(1 - x^2\right)^2 dx = \frac{16}{15}. \tag{122}$$

The equation

$$\sum_{n=1}^{N} \left(\bar{C}_{mn} - \bar{\lambda}\bar{D}_{mn}\right) \bar{A}_n = 0, \quad m = 1, 2, \ldots, N, \tag{123}$$

becomes

$$(C - \bar{\lambda}D)\bar{A} = 0. \tag{124}$$

If $\bar{A} \neq 0$, then

$$\bar{\lambda} = \frac{C}{D} = \frac{5}{2}. \tag{125}$$

We are within 2% of the actual lowest eigenvalue of $\lambda_1 = \pi^2/4 = 2.467$. Of course this rather good result is partly due to our good fortune at picking a close approximation to the actual eigenfunction, as may be seen in Fig. 6.

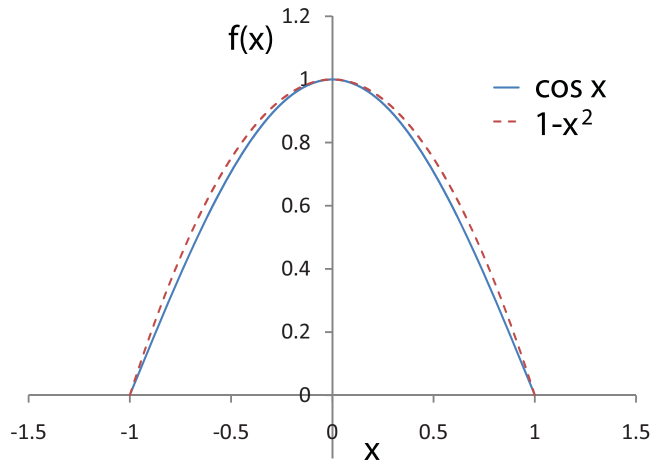

Figure 3: Rayleigh-Ritz eigenvalue estimation example, comparing exact solution with the guessed approximation.

7 Extending to Multiple Dimensions

It is possible to generalize our variational problem to multiple independent variables, e.g.,

$$I(u) = \iint_D F\left(u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, x, y\right) dxdy, \tag{126}$$

where $u = u(x, y)$, and bounded region D has $u(x, y)$ specified on its boundary S. We wish to find u such that I is stationary with respect to variation of u.

We proceed along the same lines as before, letting

$$u(x, y) = u(x, y) + \epsilon h(x, y), \tag{127}$$

where $h(x, y)|_S = 0$. Look for stationary I: $\left.\frac{dI}{d\epsilon}\right|_{\epsilon=0} = 0$. Let

$$u_x \equiv \frac{\partial u}{\partial x}, \;\; u_y \equiv \frac{\partial u}{\partial y}, \;\; h_x \equiv \frac{\partial h}{\partial x}, \text{ etc.} \tag{128}$$

Then

$$\frac{dI}{d\epsilon} = \iint_D \left(\frac{\partial F}{\partial u} h + \frac{\partial F}{\partial u_x} h_x + \frac{\partial F}{\partial u_y} h_y\right) dxdy. \tag{129}$$

We want to "integrate by parts" the last two terms, in analogy with the single-variable case. Recall Green's theorem:

$$\oint_S (Pdx + Qdy) = \iint_D \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dxdy, \tag{130}$$

and let

$$P = h\frac{\partial F}{\partial u_x}, \quad Q = -h\frac{\partial F}{\partial u_y}. \tag{131}$$

With some algrbra, we find that

$$\frac{dI}{d\epsilon} = \oint_S h \left(\frac{\partial F}{\partial u_x} dx - \frac{\partial F}{\partial u_y} dy \right) + \iint_D h \left[\frac{\partial F}{\partial u} - \frac{D}{Dx}\left(\frac{\partial F}{\partial u_x}\right) - \frac{D}{Dy}\left(\frac{\partial F}{\partial u_y}\right) \right] dxdy, \tag{132}$$

where

$$\frac{Df}{Dx} \equiv \frac{\partial f}{\partial x} + \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial u_x}\frac{\partial^2 u}{\partial x^2} + \frac{\partial f}{\partial u_y}\frac{\partial^2 u}{\partial x \partial y} \tag{133}$$

is the "total partial derivative" with respect to x.

The boundary integral over S is zero, since $h(x \in \{S\}) = 0$. The remaining double integral over D must be zero for arbitrary functions h, and hence,

$$\frac{\partial F}{\partial u} - \frac{D}{Dx}\left(\frac{\partial F}{\partial u_x}\right) - \frac{D}{Dy}\left(\frac{\partial F}{\partial u_y}\right) = 0. \tag{134}$$

This result is once again called the Euler-Lagrange equation.

8 Exercises

1. Suppose you have a string of length L. Pin one end at $(x, y) = (0, 0)$ and the other end at $(x, y) = (b, 0)$. Form the string into a curve such that the area between the string and the x axis is maximal. Assume that b and L are fixed, with $L > b$. What is the curve formed by the string?

2. We considered the application of the Rayleigh-Ritz method to finding approximate eigenvalues satisfying

$$y'' = -\lambda y, \tag{135}$$

with boundary conditions $y(-1) = y(1) = 0$. Repeat the method, now with two functions:

$$\begin{aligned} \alpha_1(x) &= 1 - x^2, & (136)\\ \alpha_2(x) &= x^2(1 - x^2). & (137) \end{aligned}$$

You should get estimates for two eigenvalues. Compare with the exact eigenvalues, including a discussion of which eigenvalues you have managed to approximate and why. If the eigenvalues you obtain are not the two lowest, suggest another function you might have used to get the lowest two.

3. The Bessel differential equation is

$$\frac{d^2y}{dx^2} + \frac{1}{x}\frac{dy}{dx} + \left(k^2 - \frac{m^2}{x^2}\right) y = 0. \tag{138}$$

A solution is $y(x) = J_m(kx)$, the mth order Bessel function. Assume a boundary condition $y(1) = 0$. That is, k is a root of $J_m(x)$. Use the Rayleigh-Ritz method to estimate the first non-zero root of $J_3(x)$. I suggest you try to do this with one test function, rather than a sum of multiple functions. But you must choose the function with some care. In particular, note that J_3 has a third-order root at $x = 0$. You should compare your result with the actual value of 6.379. If you get within, say, 15% of this, declare victory.