Methods in Applied Mathematics

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September 3, 2013

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Chapter 1

Dimensional Analysis

1.1 The program of applied mathematics

The program of applied mathematics consists of the following procedures.

- Observe a phenomenon, determine variables (quantities) that we are concerned with. Physical quantities have *dimension* such as "length"L, "time"T, "mass"M, "charge"e. Quantify the variables by choosing "UNIT". Many physical quantities are derivatives of certain fundamental dimensions. For instance, the dimension of energy is ML^2T^{-2}. The dimension of a variable is denoted by $[\,\cdot\,]$.

- Modeling: Find relations among quantities

    1. determine dependent / independent variables
    2. determine parameters
    3. The relation can be found based on basic physical laws and/or dimensional analysis
    4. Relations are in the forms of algebraic relations, ordinary/partial differential equations, integral equations, ...
    5. The key is "In a relation, each term has to be of the same dimension."

- Simplification and Reduction

    1. Reduce numbers of parameters by dimensional analysis
    2. Reduce numbers of unknowns (dependent variables) by perturbation methods
    3. Sensitivity analysis to find important quantities

- Find solutions by analytic, computational methods

- Perform experiments to check solutions, modify models if needed.

1.2 Dimensional Analysis

Population model

$$\frac{dP}{dt} = rP - bP^2.$$

Here, r is the growth rate, b is the competition rate per each individual. It means that the species compete for the same resource and causes the reduction of population. Thus, this is an environmental constraint. The initial population is P_0. In this model, the quanities are P, t, P_0, r and b. t is the independent variable, P the depedent variable, P_0, r and b are parameters. The dimensions of them are

$$[t] = T, [P] = P, [P_0] = P, [r] = \frac{1}{T}, [b] = \frac{1}{TP}.$$

We see that there are only two fundamental dimensions T and P. We can rescale this equation by a proper scaling as the follows. We write the equation by

$$\frac{dP}{d(rt)} = P - \frac{b}{r}P^2 = P\left(1 - \frac{P}{K}\right), K = \frac{r}{b}.$$

Thus, we can introduce the following dimensionless variables

$$t' = rt, P' = \frac{P}{K}, P_0' = \frac{P_0}{K},$$

then the equation is equivalent

$$\frac{dP'}{dt'} = P'(1 - P'),\ P'(0) = P_0'.$$

This equivalent equation depends only on 3 *dimensionless* quantities P', t' and P_0', instead of 5 quantities.

A falling object

1. Quantities
   (a) independent variables: t.
   (b) dependent variables: x
   (c) parameters: g, V, m, h
2. Relations Newton's law:

$$m\ddot{x} = -mg,\ x(0) = h,\ \dot{x}(0) = V,$$

3. Dimensional Analysis
   (a) $[x] = [h] = L$

(b) $[t] = T$,

(c) $[g] = L/T^2$.

(d) $[V] = L/T$

We will find a relation between x, t, g, h, V. Notice that there are only two fundamental dimensions, namely, L and T.

4. Scaling: A natural way is to introduce h and V as our fundamental dimensions, which are the observed (or controlled) parameters. Then we rescale $x' = x/h$, $v' = v/V$, $t' = t/T = t/(h/V)$. With these, the equation becomes

$$\frac{d^2x'}{dt'^2} = -gh^{-1}T^2 = -ghV^{-2} = -\frac{1}{\text{Fr}^2}.$$

The initial conditions are

$$x'(0) = 1, \frac{dx'}{dt'}(0) = 1.$$

Here, we introduce a dimensionless parameter

$$\text{Fr} = \frac{V}{\sqrt{gh}} = \frac{\text{inertial force}}{\text{gravitational force}},$$

called Froude number, which also appears in water wave theory. Then the dimensionless variables are (x', t') and the Froude number Fr. Thus, the number of variables and parameters are reduced.

The solution of the above dimensionless equation is

$$x'(t') = 1 + t' - \frac{1}{2}\frac{t'^2}{\text{Fr}^2}.$$

The critical time that the particle starts to fall is

$$\frac{dx'}{dt'}(t') = 0.$$

That is,

$$t' = \text{Fr}^2.$$

Thus, the larger the Froude number is (i.e. inertia force $>>$ gravitation force), the longer time the particle starts to fall. Notice that if we drop an object from height h. The speed it touches the ground is $\sqrt{2gh}$.

Notice that h can be the length we are interested in, needs not be the initial height. Further, the dimensionless parameters are not uniquely chosen. For instance, another way is to choose $v' = VT/h = V/\sqrt{gh}$. Then the rescaled system becomes

$$\frac{d^2x'}{dt'^2} = -1$$

with the initial conditions

$$x'(0) = 1,\ \frac{dx'}{dt'}(0) = v',$$

a relation involve the three dimensionless quantities x', t', v'.

People usually use the first scaling because (1) the initial velocity V is something we can control, it is natural to scale velocity in terms of V; (2)the parameter Fr appears in the equation, we can study solution property (bifurcation, for instance) in terms of the parameter without solving it directly, whereas the solution property in terms of initial condition usually requires solving the equation first.

Body mass index (BMI) The BMI is defined to be

$$\text{BMI} = \frac{w}{h^2},$$

where w is the weight in kilogram and h is the height in meter. What is the dimension of BMI? Why it measures the amount of fat of your body?

Rain droplet Why the viscous force of an object is propotional with the its area? With a fixed density, why the body force of the object is propotional to its volume? Can you answer what size of the raindrop will fall?

Projectile

1. Quantities:
   - independent variable t
   - Dependent variables: z,
   - Parameters: m, g, R (earth radius), V initial velocity
2. The relation:

   $$m\frac{d^2z}{dt^2} = -G\frac{Mm}{(z+R)^2}$$

   This implies

   $$\frac{d^2z}{dt^2} = -\frac{R^2g}{(R+z)^2}$$

   where $g = \frac{GM}{R^2}$.

   $$z(0) = 0, \frac{dz}{dt}(0) = V.$$

3. Dimensional Analysis: the dimensions of the quantities are

$$[t] = T, [V] = LT^{-1}, [z] = L, [g] = LT^{-2}, [R] = L.$$

There are 5 quantities, but only 2 fundamental dimensions involved. Thus, we expect that there are 3 dimensionless quantities. Let us suppose the dimensionless quantity π is a combination of the 5 quantities in the following form:

$$\begin{aligned} [\pi] &= [t^{\alpha_1} z^{\alpha_2} R^{\alpha_3} V^{\alpha_4} g^{\alpha_5}] \\ &= T^{\alpha_1 - \alpha_4 - 2\alpha_5} L^{\alpha_2 + \alpha_3 + \alpha_4 + \alpha_5} \end{aligned}$$

In order to have π to be dimensionless, i.e. $[\pi] = 1$, the admissible exponents leading to the following equations:

$$\begin{aligned} \alpha_1 - \alpha_4 - 2\alpha_5 &= 0 \\ \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 &= 0. \end{aligned}$$

Let us use α_3, α_4 and α_5 as free parameters. We then obtain three sets of solutions:

- $\alpha_3 = -1$, $\alpha_4 = \alpha_5 = 0$. This gives $\alpha_2 = 1$ and $\alpha_1 = 0$. We then get $\pi_1 = z/R$.
- $\alpha_4 = 1$, $\alpha_3 = \alpha_5 = 0$. This gives $\alpha_1 = -\alpha_2 = \alpha_4 = 1$. We get $\pi_2 = tz^{-1}V$.
- $\alpha_5 = 1$, $\alpha_3 = \alpha_4 = 0$. This gives $\alpha_1 = 2$, $\alpha_2 = -1$. We get $\pi_3 = t^2 z^{-1} g$.

Alternatively, we can use

$$\pi_x = z/R, \pi_t = tV/R, \ \pi = \frac{gR}{V^2}.$$

Then the differential equation can be written as

$$\frac{d^2\pi_x}{d\pi_t^2} = \frac{R}{V^2}\frac{d^2 z}{dt^2} = -\frac{gR}{V^2}\frac{1}{(1+\pi_x)^2} = -\frac{\pi}{(1+\pi_x)^2}.$$

with $\pi_x(0) = 0$ and $\frac{d\pi_x}{d\pi_t}(0) = 1$. This is the dimensionless relation, which is a relation among π_x, π_t and π. So, numbers of variables are reduced from 5 to 3.

The general strategy to select dimensionless variables are

- rescale the spatial variable z by z/R
- rescale the temporal variable t by $t/(R/V)$.
- Select the rest dimensionless parameters from the equations so that its form is simple.

Diffusion process Consider an explosion process in the space. We are interested in the heat propagation of this exploration. The variables and parameters of this process are:

- independent variables: x and t;
- dependent variables: u (temperature), q heat flux;
- parameters: energy released at the exploration center, k (conductivity),c (heat capacity at constant volume).

Relations: based on conservation of energy, we have

$$\frac{d}{dt}\int_\Omega cu\,dx = \int_{\partial\Omega} q\cdot(-n)\,dS$$

This yields

$$\int_\Omega cu_t\,dx = -\int_\Omega \nabla\cdot q\,dx$$

This is valid for any arbitrary Ω. Thus, we get

$$cu_t + \nabla\cdot q = 0.$$

The heat flux is related to the gradient of the temperature. This is the Fourier law:

$$q = -k\nabla u.$$

Plug this into trhe above equation, The heat equation becomes

$$u_t = \nabla\cdot\frac{k}{c}\nabla u = D\triangle u.$$

Here, the notation $\triangle = \nabla^2$ is the Laplacian. The dimensions of these quantities are

$$[u] = \Theta, [c] = E\Theta^{-1}L^{-3}, [q] = ET^{-1}L^{-2}, [k] = ET^{-1}L^{-1}\Theta^{-1}, [D] = L^2T^{-1}.$$

In the diffusion equation, the only quantities are x, t, u and D. There are three fundamental dimensions: L, T and Θ. Thus, there is only one dimensionless quantity left. Suppose it is $\pi = t^{\alpha_1}x^{\alpha_2}u^{\alpha_3}D^{\alpha_4}$. In order to be dimensionless, we get

$$\pi_1 = \frac{x}{\sqrt{Dt}}$$

Another one is

$$\pi_2 = \frac{uc}{e}x^3 = \frac{uc}{e}\pi_1^3(Dt)^{3/2}$$

Suppose we have a relation: $\pi_2 = g(\pi_1)$. This leads to a relation which can express the unknown u in terms of the independent variable x, t and the parameter D:

$$u = \frac{e}{c}(Dt)^{-3/2}g(\frac{x}{\sqrt{Dt}}). \tag{1.1}$$

Using dimensional analysis, we can find possible relation such as (1.1), which says that (1) the diffusion length scale x is $\sqrt{Dt}$; (2) the maximum of the heat decays like $(Dt)^{-3/2}$ in three space dimensions. We obtain this without solving the PDE at all, simply a guess from dimensional analysis.

There is another technique that used commonly. We can plug this ansatz into equation. Then we will get an ODE for g. Eventually we will get $g(\pi_1) = e^{-\pi_1^2}$.

Fluid Mechanics The incompressible flows are governed by the following Navier-Stokes equations:

$$\nabla \cdot u = 0,$$

$$\rho(u_t + u \cdot \nabla u) + \nabla p = \mu \triangle u.$$

Here, u is the velocity, ρ the density, p the pressure, μ the viscosity. We consider the domain has length scale L and time scale T, or equivalent the velocity has scale $U = L/T$. Notice that what we usually measures are the typical spatial scale L and the velocity U. The time scale T is a derived dimension. The dimension of $[\rho] = M/L^{-3}$. It is equivalent to use $[\rho]$ or M. It is more natural to use $[\rho]$ for fluids. The dimension of pressure is

$$[p] = \frac{MU}{TL^2} = \frac{\rho L^3 U}{(L/U)L^2} = \rho U^2.$$

By matching the dimensions of the Navier-Stokes equation, we see that the dimension of the viscosity μ should be

$$[\mu] = \rho U^2 L^{-1} U^{-1} L^2 = \rho U L.$$

Now, we rescale $x = Lx'$, $u = Uu'$. Hence the time scale $T = L/U$ and time is rescaled by $t = t'T = t'L/U$. The pressure p is rescaled as $p = p'\rho U^2$.

With these, the momentum equation becomes

$$\frac{\rho U^2}{L}\left(u'_{t'} + u' \cdot \nabla' u' + \nabla' p'\right) = \mu \frac{U}{L^2} \triangle' u'.$$

Or

$$u'_{t'} + u' \cdot \nabla' u' + \nabla' p' = \frac{1}{Re} \triangle' u'$$

Here, the dimensionless quantity

$$Re = \frac{\text{inertia force}}{\text{viscous force}} = \frac{\rho U^2 L^{-1}}{\mu U L^{-2}} = \frac{\rho U L}{\mu} = \frac{UL}{\nu},$$

called Renold's number. The independent variables are (x', t'), the dependent variables are (u', p'). The parameter is Re. The parameters (ρ, L, U) are scaled out. The advantages of these scaling is that the typical length and vlocity are scaled out. Thus, we can perform experiments for small size vehicles at low speed, yet we can get the same results for large size vehicles at high speed.

1.3 The Buckingham Pi Theorem

Suppose we have a physical relation

$$f(q_1, \cdots, q_m) = 0.$$

A physical relation is called *unit free* if it is independent of the particular set of units we choose for $q_1, \cdots, q_m$. "Time" is a dimension, while "year", "month", "second" are units of the dimension "time. There are some fundamental dimensions such as *length, time, mass, charge*. Suppose there are n fundamental dimensions $L_1, \cdots, L_n$, $n < m$ involved in the quantities $q_1, \cdots, q_m$. Each qnatity q_i has dimension

$$[q_i] = L_1^{a_{1i}} \cdots L_n^{a_{ni}}$$

The matrix $(a_{ij})_{n\times m}$ is called the *dimension matrix*. Suppose the matrix (a_{ij}) has rank r. Then we can determine $m - r$ dimensionless quantities

$$\pi_k = \prod_i q_i^{\alpha_{ik}}, k = 1, \cdots, m - r,$$

and a relateion

$$g(\pi_1, \cdots, \pi_{m-r}) = 0$$

such that $f = 0$ if and only if $g = 0$. This is called the Buckingham's π theorem.

Proof. Let us first look for a dimensionless quantity π:

$$\pi = \prod_i q_i^{\alpha_i}.$$

The dimension of π is

$$[\pi] = \prod_i \left(\prod_j L_j^{a_{ji}} \right)^{\alpha_i} = \prod_j L_j^{\sum_i a_{ji}\alpha_i}$$

In order to have π to be dimensionless , we should require

$$\sum_{i=1}^{m} a_{ji}\alpha_i = 0, \text{ for all } j = 1, \cdots, n$$

Since the rank of the dimension matrix A is r, the kernel space of A has dimension $m - r$. Indeed, let $A = V\Sigma U^T$ be the singular value decomposition of A, where U,V are orthogonal matrices and Σ has the form

$$\Sigma = \begin{pmatrix} (\Sigma_1)_{r\times r} & 0_{r\times(m-r)} \\ 0_{(n-r)\times r} & 0_{(n-r)\times(m-r)} \end{pmatrix}$$

where Σ_1 is a diagonal and invertible matrix. Suppose $U = (\alpha_1, \cdots, \alpha_m)$, then the null space of A is span$\{\alpha_{r+1}, \cdots, \alpha_m\}$. That is, $A\alpha_k = 0$ for $k = r + 1, \cdots, m$. Now, we can choose $\pi_k =$

$\prod_i q_i^{\alpha_{k,i}}$, $k = 1, \cdots, m$. Here, $\alpha_k = (\alpha_{k,1}, \cdots, \alpha_{k,n})^T$. From $A\alpha_k = 0$ for $k = r+1, \cdots, m$, we get π_k with $k = r+1, \cdots, m$ are dimensionless.

To find a relation in terms of the dimensionless variables $\pi_{r+1}, \cdots, \pi_m$, which is also equivalent to $f = 0$, we first notice that there is an 1-1 corresponding between $(q_1, \cdots, q_m)$ and $(\pi_1, \cdots, \pi_m)$ because U is non-singular. Thus, for any $(\pi_1, \cdots, \pi_m)$, we define

$$g(\pi_1, \cdots, \pi_m) = f(q_1, \cdots, q_m).$$

To show that g depends only on $(\pi_{r+1}, \cdots, \pi_m)$, we will use the unit free property of $f = 0$. Let us rescale the fundamental dimensions by

$$\bar{L}_j = \lambda_j L_j, j = 1, \cdots, n.$$

Then q_i is scaled to

$$\bar{q_i} = \prod_j \lambda_j^{a_{ji}} q_i$$

The property *unit free* of $f = 0$ means that

$$f(\bar{q}_1, \cdots, \bar{q}_m) = 0 \Leftrightarrow f(q_1, \cdots, q_m) = 0 \text{ for any } \lambda_j > 0., j = 1, ..., n$$

As translated to g, we get

$$\begin{aligned} & f(\bar{q}_1, \cdots, \bar{q}_m) = 0 \Leftrightarrow f(q_1, \cdots, q_m) = 0 \\ \Leftrightarrow \quad & g(\pi_1, \cdots, \pi_m) = 0 \Leftrightarrow g(\bar{\pi}_1, \cdots, \bar{\pi}_m) = 0. \end{aligned}$$

Because $\pi_{r+1}, \cdots, \pi_m$ are dimensionless, we have $\bar{\pi}_{r+1} = \pi_{r+1}, \cdots, \bar{\pi}_m = \pi_m$ for any choices of $\lambda_j > 0$, $j = 1, ..., n$. We will choose λ_j such that the dimensions

$$\bar{\pi}_1 = \cdots = \bar{\pi}_r = 1.$$

To see these λ_j can be found, we derive the conditions for λ_j as the follows.

$$\begin{aligned} \bar{\pi}_k &= \prod_i \bar{q}_i^{\alpha_{k,i}} \\ &= \prod_i \prod_j \lambda_j^{a_{ji}\alpha_{k,i}} \left(\prod_i q_i^{\alpha_{k,i}} \right) \\ &= \prod_j \lambda_j^{\sum_i a_{ji}\alpha_{k,i}} \left(\prod_i q_i^{\alpha_{k,i}} \right) \\ &= \exp\left(\sum_j (\sum_i a_{ji}\alpha_{k,i})\mu_j \right) \pi_k \end{aligned}$$

Recall that $AU = V\Sigma$, let us write $A\alpha_k = \sigma_k\beta_k$, $k = 1, \cdots, r$, $\sigma_k \neq 0$. Then taking log of the above equations, we get

$$0 = \sum_{j=1}^{n} \beta_{k,j}\mu_j + \ln \pi_k, k = 1, \cdots, r.$$

This set of equations is always solvable because $(\beta_1, \cdots, \beta_r)$ are orthogonal. Once we determine μ, hence λ, then

$$g(\bar{\pi}_1, \cdots, \bar{\pi}_m) = g(1, \cdots, 1, \bar{\pi}_{r+1}, \cdots, \bar{\pi}_m).$$

□

1.4 Applications of dimensional analysis

1.4.1 Use dimensional analysis for finding possible relation

Gauss-Bonnet Theorem In geometry, the principal curvature κ_i has dimension L^{-1}. For two dimensional surfaces, the Gaussian curvature $K = \kappa_1\kappa_2$ has dimension L^{-2}. Thus, consider a closed surface Σ, the quantity

$$\int_\Sigma K\, dS$$

is dimensionless, because the surface element dS has dimension L^2. Thus, $\int_\Sigma K\, dS$ is scale independent. A more ambitious guess is that this quantity is independent of a continuous variation of Σ. That is, $\int_\Sigma K\, dS$ is a topological quantity. We can then compute this quantity for sphere, torus, etc and get the following conjecture:

$$\int_\Sigma K\, dS = 2\pi\chi(\Sigma),$$

where $\chi(\Sigma)$ is the Euler characteristic of Σ. For orientable compact closed surfaces, $\chi(\Sigma) = 2-2g$, where g is the *genus* of the surface. Any such a surface is topologically equivalent to a sphere with some handles attached, and g is the number of the handles.

1.4.2 *Other Applications of Dimensional Analysis in the estimates of PDEs

Poincarè inequality In PDEs, we usually need to estimate the L^p norm of our variables. The estimates are usually in the forms of inequalities, which should be *scale invariant*. To find such inequalities, an important technique is the dimensional analysis. We define the dimension of $\|u\|_{L^p}\|$ in a small region in $\mathbb{R}^n$ by [1]

$$[\|u\|_{L^p}] = (U^p L^n)^{1/p} = UL^{n/p}$$

The dimension of $\|Du\|_{L^p}$ is

$$[\|\nabla u\|_{L^p}] = \left(\left(\frac{U}{L}\right)^p L^n\right)^{1/p} = UL^{n/p-1}.$$

[1] This means that a ball in $\mathbb{R}^n$. It also means that the estimates here are interior estimates in a compact domain.

An important inequality is the Poincarè's inequality. It relates $\|u\|_{L^2}$ and $\|\nabla u\|_{L^2}$ in a bounded domain with zero boundary condition:

$$\|u\|_{L^2} \leq C\|\nabla u\|_{L^2}$$

By comparing the dimension, we see that

$$UL^{n/2} = [C]UL^{n/2-1}$$

This shows that $[C] = L$, which is indeed the diameter of the domain.

Sobolev's inequality We want to know the relation between $\|u\|_{L^{p^*}}$ and $\|Du\|_{L^p}$.

Theorem 1.1. *Assume $1 \leq p < n$, there exists a constant C such that*

$$\|u\|_{L^{p^*}(\Omega)} \leq C\|Du\|_{L^p(\Omega)}$$

where $p^* = np/(n-p)$.

Remark.

- From dimension analysis, we have

  $$[\|u\|_{L^{p^*}}] = UL^{n/p^*}$$

  $$[\|Du\|_{L^p}] = UL^{-1+n/p}$$

  The inequality can hold only when the dimensions on both sides match. This leads to

  $$\frac{n}{p^*} = \frac{n}{p} - 1.$$

  This gives the formula p^*.

- The above formula says that u can gain some integrability (i.e. $p^* > p$) if its derivative Du is already p-integrable. From $[Du] = [u] - 1$, we see that if $Du \in L^p$, which means that $[Du]L^{n/p} = [u]L^{-1+n/p}$ is finite as $L \to 0$. Thus, there is some more room of integrability of u.

- If $p > n$, the constraint is even stronger, we should have $p = \infty$. In fact, we have

  $$\|u\|_{C^{0,1-n/p}} \leq C\|Du\|_{L^p}$$

  for all $u \in C_c^\infty$.

- When $p = n$, it is the BMO case, see **??**.

Interpolation Formula In nonlinear PDEs, it is commonly to estimate the norm of a medium derivatives in terms of high derivatives and low derivatives. This is the interpolation formula.

Theorem 1.2. *Let $0 \le j < m$ and $1 \le q, r \le \infty$. Then for smooth function u in a bounded domain in $\mathbb{R}^n$, we have*

$$\|D^j u\|_{L^p} \le C\|D^m u\|_{L^r}^{\alpha}\|u\|_{L^q}^{1-\alpha},$$

where

$$\frac{1}{p} = \frac{j}{n} + \alpha\left(\frac{1}{r} - \frac{m}{n}\right) + (1-\alpha)\frac{1}{q},$$

for α satisfying $j/m \le \alpha \le 1$.

We can find the relation by matching the dimensions of the above inequatity.

$$UL^{n/p-j} = \left(UL^{n/r-m}\right)^{\alpha}\left(UL^{n/q}\right)^{1-\alpha} = UL^{(n/r-m)\alpha+(1-\alpha)(n/q)}$$

This gives

$$\frac{n}{p} - j = \alpha\left(\frac{n}{r} - m\right) + (1-\alpha)\frac{n}{q}.$$

1.5 Scaling

In the differential equations, we usually have some small parameters (or large parameters) after performing scaling. Roughly speaking, the high order derivative terms are important in a small spatial region or short time, while low order terms are important in large domain or long time. For instance, consider the following second order equation

$$y'' + ay' + by = 0.$$

If we perform the scaling $x^* = x/\epsilon$. This means that in a small region of $O(\epsilon)$ width, x is blowup to x/ϵ. The equation in terms of x^* is

$$\frac{1}{\epsilon^2}\frac{d^2y}{dx^{*2}} + \frac{1}{\epsilon}\frac{dy}{dx^*} + by = 0.$$

In this equation, the highest order term is the most important term. On the other hand, if we rescale $x = \lambda x'$ with $\lambda >> 1$, then the lowest order term is the most important term.

1.6 Homework

- pp. 17: 1, 2, 3
- pp. 19: 12, 15.
  - –
  - – The dimension of mass concentration is $[C] = ML^{-3}$.
- pp. 30: 3, 6, 7, 13

1.7 Projects

Choose one of the following subject for your project. This should be turned in near the end of this semester.

1. Study Benard Flow and its dimensional analysis. Ref.
2. Study atmospherical flows and the corresponding dimensional analysis
3. Study Komogorov's turbulence theory.
4. Study water wave theory and its dimensional analysis
5. Study phase field model for multiphase flows
6. Study Schrödinger equation and its semi-classical scaling.
7. Study the Ginzburg-Landau theory for superconductivity, perform dimensional analysis and derive a dimensionless form.

Chapter 2

Perturbation Methods

2.1 Perturbation methods for algebraic equations

Let us suppose our algebraic equations depend on a parameter ϵ. Suppose the root can be found for $\epsilon = 0$. We look for roots for small ϵ. The procedure of regular perturbation are the follows:

- Express $x = x_0 + \epsilon x_1 + \epsilon^2 x_2 + \cdots$;
- Plug this expression into equation, make Taylor expansion of coefficients of the equation.
- Equating the coefficients with like power of ϵ;
- Solve x_0, x_1 successively.

Example 1 Consider $x(x-1) = \epsilon$.

- Let $x = x_0 + \epsilon x_1 + \cdots$. Plug this into equation, we get

$$(x_0 + \epsilon x_1 + \cdots)(x_0 + \epsilon x_1 + \cdots - 1) = \epsilon.$$

- Equating the coefficients of like powers:

$$\begin{array}{rcl} \epsilon^0 & : & x_0(x_0-1) = 0, \\ \epsilon^1 & : & 2x_0x_1 - x_1 = 1, \\ \vdots & : & \vdots \end{array}$$

  This leads to two sets of solutions:

$$x_a^{(1)} = 0 - \epsilon;\ x_a^{(2)} = 1 + \epsilon$$

The true solution is

$$x = \frac{1 \pm \sqrt{1+4\epsilon}}{2} \approx \frac{1}{2}(1 \pm (1+2\epsilon)).$$

which are consistent to the regular perturbation solutions.

Example 2 Let us consider the equation $x^2 = \epsilon$. You will see that

- The expansion $x = x_0 + \epsilon x_1 + \cdots$ does not work. You should try $x = \sqrt{\epsilon}$.
- For $\epsilon < 0$, the solution becomes imaginary.

So, we should try $x = x_0 + \delta(\epsilon)x_1 + \delta(\epsilon)^2 x_2 + \cdots$.

- Plug this ansatz, we get

$$x_0^2 + 2x_0\delta x_1 + \delta^2 x_1^2 + 2\delta^2 x_0 x_2 + \cdots = \epsilon.$$

  By comparing both sides, we see that we should have $x_0 = 0$. Then this gives

$$\delta^2 x_1^2 + \cdots = \epsilon$$

  To equate both sides, we need to choose $\delta^2 = \epsilon$. This give $\delta = \sqrt{\epsilon}$ and $x_1 = 1$.

Example 3. Let us consider

$$\epsilon x^2 + ax + b = 0.$$

As $\epsilon \to 0$, there is only one root. Thus, the perturbation method can not recover the other root, which goes to ∞ as $\epsilon \to 0$. If $a = 0$, there is no root as $\epsilon \to 0$, the reduced equation is even inconsistent at all. Thus, the above perturbation method does not work for such case.

Nevertheless, we can try the following thing. We know the other solution goes to infinity as $\epsilon \to 0$, we try $x = \frac{x^*}{\epsilon}$. Plug this into equation, we obtain

$$\frac{x^{*2}}{\epsilon} + a\frac{x^*}{\epsilon} + b = 0.$$

We see that x^* satisfies an equation where the regular perturbation method can handle. We write

$$x^* = x_0^* + \epsilon x_1^* + \cdots,$$

Plug this into the above rescaled equation, we get

$$\begin{aligned} x_0^{*2} + ax^* &= 0 \\ 2x_0^* x_1^* + ax_1^* + b &= 0 \end{aligned}$$

These equations give the $x_0^* = -a$ and $x_1^* = b/a$, lead to the second solution of the orginal equation

$$x^{(2)} = -\frac{a}{\epsilon} + \frac{b}{a} + \cdots.$$

You may think how to handle the case when $a = 0$.

Homework

1. Find the asymptotic behaviors of the equations
   (a) $\epsilon x^3 + x - 2 = 0$;
   (b) $\epsilon^2 x^4 + \epsilon x^3 + x - 1 = 0$
   (c) $\epsilon x^5 + x^3 - 1 = 0$;
2. There are infinite roots of $\tan x = x$. Find their asymptotic fomula.

2.1.1 Justification of regular perturbation method for algebraic equations

Implicit Function Theorem

Theorem 2.3. *Let $F : \mathbb{R}^{n+1} \to \mathbb{R}^n$ be smooth. Suppose x_0 is a solution of $F(x_0, 0) = 0$ and suppose $\partial F/\partial x(x_0, 0)$ is non-singular. Then there is a smooth solution set $x(\epsilon)$ satisfying $F(x(\epsilon), \epsilon) = 0$ for small ϵ.*

The proof of this theorem is based on method of contraction map. We rewrite the above equation as a perturbtion equation: let us write $x(\epsilon) = x_0 + y(\epsilon)$, then $y(\epsilon)$ satisfies

$$\frac{\partial F}{\partial x}(x_0, 0)y + \frac{\partial F}{\partial \epsilon}(x_0, 0)\epsilon + r(y) = 0.$$

Here,

$$r(y) = F(x_0 + y, \epsilon) - F(x_0, 0) - \frac{\partial F}{\partial x}(x_0, 0)y - \frac{\partial F}{\partial \epsilon}(x_0, 0)\epsilon = O(|y|^2 + \epsilon^2).$$

Since $J := \partial F/\partial x(x_0, 0)$ is non-singular, we take its inversion and get

$$y = Ty := J^{-1}\left(-\frac{\partial F}{\partial \epsilon}(x_0, 0)\epsilon - r(y)\right).$$

We want to find a small number ϵ_0 and another number η such that for any $|\epsilon| \le \epsilon_0$, the mapping T is a strict contraction map from $|y| \le \eta$ to itself. Then by the fixed point theorem, we can obtain a fixed point $y(\epsilon)$.

This process also tell us the construction of the perturbed solution. The method breaks down when the Jacobian $J := \frac{\partial F}{\partial x}(x_0, 0)$ is singular, or when it has very small eigenvalue.

Extended study

1. A short note on regular perturbation method by Eric Vanden-Eijnden.

2.2 Regular perturbation method for differential equations

We start from some examples.

A falling object with resistivity The model reads

$$m\frac{dv}{dt} = -av + bv^2, v(0) = V_0.$$

We introduce the dimensionless variables $y = v/V_0$, $\tau = at/m$, then the equation becomes

$$\frac{dy}{d\tau} = -y + \epsilon y^2,$$

where

$$\epsilon = \frac{bV_0}{a} << 1.$$

It means the resistivity (damping) is very large, as compared with V_0 and b. This equation has exact solution

$$y(\tau) = \frac{e^{-\tau}}{1 + \epsilon(e^{-\tau} - 1)}.$$

which has the following Taylor expansion in ϵ:

$$y = e^{-\tau} + \epsilon(e^{-\tau} - e^{-2\tau}) + \epsilon^2(e^{-\tau}2e^{-2\tau} + e^{-3\tau}) + \cdots .$$

The regular perturbation method introduces a Taylor expansion of y in terms of ϵ:

$$y(\tau, \epsilon) = y_0(\tau) + \epsilon y_1(\tau) + \epsilon^2 y_2(\tau) + \cdots .$$

We plug this ansatz into the equation, equating the coefficients of like powers of ϵ. We get

$$\begin{aligned} y_0' &= -y_0, \\ y_1' &= -y_1 + y_0^2 \\ y_2' &= -y_2 + 2y_0y_1, \\ &\vdots \end{aligned}$$

Equating the initial conditions, we get

$$y_0(0) = 1, y_1(0) = y_2(0) = \cdots = 0.$$

Solving these equations, we get

$$y_a = e^{-\tau} + \epsilon(e^{-\tau} - e^{-2\tau}) + \epsilon^2(e^{-\tau}2e^{-2\tau} + e^{-3\tau}) + \cdots ,$$

We find this approach does work for this example.

The logistic model We consider the logistic model for population dynamics:

$$\frac{dP}{dt} = P(1 - \frac{P}{K})$$

with $P(0) = 1$. We assume the $K >> 1$. Can the above approach work? What is the limitation?

Nonlinear oscillator Consider a nonlinear oscillator

$$m\frac{d^2y}{d\tau^2} = -ky - ay^3, y(0) = A, \frac{dy}{d\tau}(0) = 0.$$

This is so-called hard spring. We rescale it by

$$t = \frac{\tau}{m/k}, u = \frac{y}{A}.$$

Then we get the Duffing equation:

$$\frac{d^2u}{dt^2} + u + \epsilon u^3 = 0$$
$$u(0) = 1, u'(0) = 0.$$

We perform regular perturbation method

$$u(t,\epsilon) = u_0(t) + \epsilon u_1(t) + \epsilon^2 u_2(t) + \cdots,$$

Plugging this into equation and the initial conditions, we get

$$\begin{aligned} \ddot{u}_0 + u_0 &= 0, u_0(0) = 1, \dot{u}_0(0) = 0, \\ \ddot{u}_1 + u_1 &= -u_0^3, u_1(0) = 0, \dot{u}_1(0) = 0, \end{aligned}$$

From the fisrt equationm, we obtain

$$u_0(t) = \cos t.$$

The second equation becomes

$$\ddot{u}_1 + u_1 = -\cos^3 t = -\frac{1}{4}(3\cos t + \cos 3t)$$

Solving this equation with initial condition, we get

$$u_1(t) = \frac{1}{32}(\cos 3t - \cos t) - \frac{3}{8}t\sin t.$$

The term $t\sin t$ is a resonant term from $\cos t$. Such a term is called a secular term. It will grow linearly and eventually to infinite as $t \to \infty$. However, by energy method, one can show that the solution is bounded. What wrong is that the expansion is only good for finite time. The estimate $|y_a(t,\epsilon) - y_e(t,\epsilon)| = O(\epsilon^2)$ is only valid for $t \in [0,T]$ for a finite T.

Asymptotic Expansion First, we give some definitions of some notations.

- The notation $f(\epsilon) = o(g(\epsilon))$ means that $f/g \to 0$ as $\epsilon \to 0$.
- If f and g are also function of t in an interval I, the notation

  $$f(t,\epsilon) = o(g(t,\epsilon)) \text{ as } \epsilon \to 0, t \in I$$

  means that for every $t \in I$, we have $f(t,\epsilon)/g(t,\epsilon) \to 0$ as $\epsilon \to 0$.

- If the above limit is uniform for $t \in I$, we say that $f(t,\epsilon) = o(g(t,\epsilon))$ as $\epsilon \to 0$ uniformly on $t \in I$.

Definition 2.1.

- *A sequence of gauge functions $\{g_n(t,\epsilon)\}$ is an asymptotic sequence on $t \in I$ as $\epsilon \to 0$ if*

$$g_{n+1}(t,\epsilon) = o(g_n(t,\epsilon)) \text{ for every } t \in I.$$

- *Given a function $y(t,\epsilon)$ and an asymptotic sequence $\{g_n(t,\epsilon)$ on $t \in I$, the formal expansion $\sum_{n=0}^{\infty} a_n g_n(t,\epsilon)$ is said to be an asymptotic expansion of $y(t,\epsilon)$ as $\epsilon \to 0$ if*

$$y(t,\epsilon) - \sum_{n=0}^{N} a_n g_n(t,\epsilon) = o(g_N(t,\epsilon)), \text{ as } \epsilon \to 0,$$

for any N. If the limits are uniform for $t \in I$, we say it is a uniform asymptotic expansion on I.

The expansion sequences are usually seperable such as

- $\epsilon^n u_n(t)$
- $\epsilon^{\alpha_n} u_n(x)$, where α_n is a strictly increasing sequence.
- $\epsilon^n \ln \epsilon u_n(x)$.

A rigorous proof for regular perturbation method has been done. Basically, the highest order term is elliptic operator on finite domain, the perturbation should be in the low orders and can be controlled by the elliptic operator. For instance, consider

$$\triangle u = f(u, Du, \epsilon) \text{in } \Omega,$$

$$u = 0 \text{ on } \partial\Omega.$$

We assume the equation is solvable for $\epsilon = 0$. We also assume $f(u, Du, \epsilon)$ can be controlled by $\triangle u$. This means that $\triangle^{-1} f(u, Du, \epsilon)$ is a compact smooth map from, say H^1 to H^1. Then we can apply implicit function theorem to get the solution for small ϵ. In general, the term Du is harder to control, it relies on Sobolev embedding theorem.

If the underlying operator is wave opertor, or Schrödinger, then it is even harder. There is no such compactness property. Nash-Moser technique is introduced.

2.3 The Poincaré-Lindstedt Method

In the Duffin's equation:

$$\ddot{u} + u + \epsilon u^3 = 0, u(0) = 1, \dot{u}(0) = 0,$$

the regular perturbation method leds to a secular term, which is incorrect for large time. One way to solve this problem is to introduce a change of time scale. Let

$$u(\tau) = u_0(\tau) + \epsilon u_1(\tau) + \cdots,$$

$$\tau = \omega(\epsilon)t, \omega = 1 + \epsilon\omega_1 + \epsilon^2\omega_2 + \cdots,$$

Then

$$\omega^2 u'' + u + \epsilon u^3 = 0, u(0) = 1, u'(0) = 0,$$

where $' = d/d\tau$. We plug the expansion above for u and ω into this equation, equating the coefficients of likely powers of ϵ, we get

$$(1 + 2\epsilon\omega_0\omega_1 + \cdots)(u_0'' + \epsilon u_1'' + \cdots) + (u_0 + \epsilon u_1 + \cdots) + \epsilon(u_0^3 + 3\epsilon u_0^2 u_1 + \cdots) = 0,$$

$$u_0(0) + \epsilon u_1(0) + \cdots = 1,\ u_0'(0) + \epsilon u_1'(0) + \cdots = 0,$$

$$u_0'' + u_0 = 0, u_0(0) = 1, u_0'(0) = 0, \cdots,$$

$$u_1'' + u_1 = -2\omega_1 u_0'' - u_0^3, u_1(0) = u_1'(0) = 0,$$

This gives

$$u_0(\tau) = \cos\tau.$$

$$u_1'' + u_1 = 2\omega_1 \cos\tau - \cos^3\tau = (2\omega_1 - \frac{3}{4})\cos\tau - \frac{1}{4}\cos 3\tau.$$

If we choose $\omega_1 = 3/8$, then the secular term can be avoided. This leads

$$u_1(\tau) = \frac{1}{32}(\cos 3\tau - \cos\tau).$$

Thus, we get the expansion

$$u(\tau) = \cos\tau + \frac{\epsilon}{32}(\cos 3\tau - \cos\tau) + \cdots,$$

$$\tau = t + \frac{3}{8}\epsilon t + \cdots.$$

Homework.

- pp. 101: 8(a),
- pp. 102: 11, 13. 15.

2.4 Singular perturbation methods

2.4.1 Outer solutions, inner solutions and matched asymptotics

If the small parameter ϵ appears in the highest order term, then this term is unimportant in most of the region except in a small region where the high order derivatives are important. Let us see the following example:

$$au_x = \epsilon u_{xx}, x \in (0, 1),$$

$$u(0) = 0, u(1) = 1.$$

Here, we assume $a < 0$. Physically, ϵ is the viscosity, a the advection velocity. In our present situation, the advection direction is toward left. This equation can be solved easily. We integrate it once to get

$$-au + \epsilon u_x = C_1,$$

where C_1 is a constant to be determined. Using method of separation of variable,

$$\frac{du}{C_1 + au} = \frac{dx}{\epsilon}.$$

Integrate this again, we get

$$\frac{1}{a}\ln(au + C_1) = \frac{x}{\epsilon} + C_2.$$

This gives

$$u = C_3 \exp\left(\frac{ax}{\epsilon}\right) + C_4.$$

Putting the boundary conditions, we get

$$C_3 + C_4 = 0, C_3 e^{a/\epsilon} + C_4 = 1.$$

These gives

$$C_3 = \frac{1}{e^{a/\epsilon} - 1}, \quad C_4 = -\frac{1}{e^{a/\epsilon} - 1}.$$

Hence, the exact solution is

$$u_e(x) = \frac{1 - e^{ax/\epsilon}}{1 - e^{a/\epsilon}}.$$

Next, we shall use perturbation method to find approximate solution. It consists of three steps: (1) finding outer solution, (2) finding inner solution, (3) matching the outer and inner solution.

Finding Outer solution Let us first solve this equation with $\epsilon = 0$:

$$au_x = 0.$$

This leads to $u = constant$. From boundary conditions, they are two possible solutions, $u = 0$ or $u = 1$. As we shall see later that the condition $a < 0$ leads to the flows move toward left and hence we should use the boundary condition $u(1) = 1$. This implies $u(x) \equiv 1$ for the unperturbed equation. This also means that $u(x) \equiv 1$ in the region where u is smooth (hence ϵu_{xx} is small. The solution

$$u_o(x) = 1$$

is called *outer solution*.

Finding inner solution However, u cannot be smooth through out the whole region $(0,1)$ because $u(0)=0$. Therefore, we expect there is an abrupt change of u near $x=0$. This region is called *boundary layer*. Let us suppose its thickness is $\delta(\epsilon)$. We rescale $\xi = x/\delta$. The rescaled equation becomes

$$\frac{\epsilon}{\delta^2}\frac{d^2u}{d\xi^2} - \frac{a}{\delta}\frac{du}{d\xi} = 0.$$

If we want to have these two terms to be equally important, then we should take

$$\frac{\epsilon}{\delta^2} = \frac{1}{\delta}.$$

In this case, $\delta = \epsilon$. The resulting equation is

$$u_{\xi\xi} = a u_\xi$$

with boundary condition $u(0)=0$. Now, we get the same equation without ϵ. This gives

$$u_\xi = au + C_1.$$

The solution is

$$u(\xi) = C\left(e^{a\xi} - 1\right).$$

where C is to be determined. The solution

$$u_i(x) = C\left(e^{ax/\epsilon} - 1\right)$$

is called inner solution. This inner solution is an approximate in the region $(0,\epsilon)$. To determine C, we need to match $u_i(x)$ and $u_o(x)$ for x in some overlapping zone. A natural overlapping zone is when $\eta = x/\sqrt{\epsilon}$ with $\eta = O(1)$. In this case, let us fix η and we expect $u_o(\sqrt{\epsilon}\eta) - u_i(\sqrt{\epsilon}\eta) \to 0$ as $\epsilon \to 0$. This implies

$$\lim_{\epsilon\to 0} C\left(e^{a\eta/\sqrt{\epsilon}} - 1\right) = 1.$$

Since $a<0$, we get from the above limit that $C=-1$. Thus,

$$u_i(x) = 1 - e^{ax/\epsilon}.$$

Match inner and outer solutions We can define an approximate solution to be the sum of the inner solution and outer solution minus the overlapping value. The overlapping value is 1. Thus, we define

$$u_a(x) = u_o(x) + u_i(x) - 1 = 1 - e^{ax/\epsilon}.$$

We see that $u_a(0)=0$, $u_a(1) = 1 - e^{a/\epsilon}$. In fact,

$$\begin{aligned} u_e(x) - u_a(x) &= \left(1 - e^{ax/\epsilon}\right)\left(\frac{1}{1-e^{a/\epsilon}} - 1\right) \\ &= \left(1 - e^{ax/\epsilon}\right)\frac{e^{a/\epsilon}}{1-e^{a/\epsilon}} \end{aligned}$$

Remark. Notice that the above approximate solution $u_a(x)$ does not satisfy the boundary condition at $x = 1$, but has a small error. It does satisfy the equation and the boundary condition at $x = 0$. Alternatively, we can choose different approximate solution. For instance, let $\omega(x)$ be a weighted function which is 1 for $0 \le x \le 1/3$ and 0 for $2/3 \le x \le 1$ and smoothly and monotonely connect 1 and 0 for $1/3 \le x \le 2/3$. Using this weighted function, we define

$$u_a(x) = \omega\left(\frac{x}{\epsilon^\beta}\right) u_i(x) + \left(1 - \omega\left(\frac{x}{\epsilon^\beta}\right)\right) u_o(x).$$

Here, β is any number between 0 and 1. This approximate solution satisfies the boundary condition, but does not satisfy the equation, with a small residual.

Example This example is taken from J. Cole's book, Singular Perturbation, pp. 21. Consider

$$\epsilon u_{xx} + \sqrt{x} u_x - u = 0, x \in (0, 1),$$
$$u(0) = 0, u(1) = e^2.$$

1. **Finding outer solution:** just like regular perturbation method, we assume

   $$u(x) = u_0(x) + \epsilon u_1(x) + \cdots .$$

   Plugging this into equation and the boundary conditions, equating the coefficients of the like power terms of ϵ, we get

   $$\sqrt{x} u_{0,x} = u_0,\ u_0(1) = e^2,$$
   $$\sqrt{x} u_{1,x} = u_0 - u_{0,xx},\ u_1(1) = 0.$$

   This leads to the outer expansion:

   $$u_o(x) = e^{2\sqrt{x}} \left(1 - \epsilon \left(\frac{1}{2x} - \frac{2}{\sqrt{x}} + \frac{3}{2}\right) + O\left(\frac{\epsilon^2}{x^{5/2}}\right)\right)$$

   The reason why we only use the boundary condition at $x = 1$ is because the advection velocity is negative ($-\sqrt{x}$), which means that the upwind direction is right. By the method of characteristics, the solution is determined by its upwind data, thus, from the right. Hence the boundary condition for the outer solution is from $x = 1$.

2. **Finding inner solution:** The boundary layer occurs near $x = 0$. We rescale x by introducing the layer variable

   $$\xi = \frac{x}{\delta(\epsilon)}.$$

   The boundary layer expansion is

   $$u = w_0(\xi)\nu_0(\epsilon) + w_1(\xi)\nu_1(\epsilon) + \cdots ,$$

   Plug this into the equation, we get

   $$\frac{\epsilon}{\delta^2}\left(\nu_0 w_{0,\xi\xi} + \nu_1 w_{1,\xi\xi} + \cdots\right) + \frac{\sqrt{\delta}}{\delta}\sqrt{\xi}\left(\nu_0 w_{0,\xi} + \nu_1 w_{1,\xi} + \cdots\right) \quad -\nu_0 w_0 - \nu_1 w_1 - \cdots = 0.$$

We choose $\delta(\epsilon)$ so that

$$\frac{\epsilon}{\delta^2} = \frac{\sqrt{\delta}}{\delta}.$$

This gives

$$\delta(\epsilon) = \epsilon^{2/3}.$$

The dominant boundary equation becomes

$$w_{0,\xi\xi} + \sqrt{\xi} w_{0,\xi} = 0, w_0(0) = 0.$$

Its solution is

$$w_0(\xi) = C_0 \int_0^\xi \exp\left(-\frac{2}{3}\zeta^{3/2}\right) d\zeta.$$

Thus, the inner solution has the form:

$$u_i(x) = w_0\left(\frac{x}{\epsilon^{2/3}}\right) + \cdots.$$

3. **Matching:** Let the matching scale is

$$x_\eta = \frac{x}{\eta}$$

$\eta(\epsilon)$ is chosen so that, with fixed x_η, as $\epsilon \to 0$,

- the outer variable $x = \eta x_\eta \to 0$;
- the inner variable: $\xi = x/\delta = x_\eta \eta/\delta \to \infty$.

For instance, we can choose $\eta = \epsilon^\beta$ with $0 < \beta < 2/3$. The outer and inner solution should match in the overlapping zone where x_η is fixed. As $\epsilon \to 0$,

- The outer solution $u_0(x) \to 1,$ as $x \to 0$.
- The inner solution

$$w_0(\xi) \to C_0 \int_0^\infty \exp\left(-\frac{2}{3}\zeta^{3/2}\right) d\zeta, \text{ as } \xi \to \infty.$$

To match these two limits, we should require

$$C_0 = \left(\int_0^\infty \exp\left(-\frac{2}{3}\zeta^{3/2}\right) d\zeta\right)^{-1}.$$

This gives the complete description of inner solution. The approximate solution is then defined to be

$$\text{outer solution } + \text{ inner solution } - \text{ overlapped value}$$

That is,

$$u_a(x) = u_o(x) + w_0\left(\frac{x}{\epsilon^{2/3}}\right) - 1.$$

Remark. The next term is $\nu_1(\epsilon) = \epsilon^{1/3}$. Check by yourself.

2.4.2 The boundary layers, initial layers and interior layers

Initial layer Let us consider a damped spring-mass system:

$$m\ddot{y} + a\dot{y} + ky = 0,$$

with $y(0) = 0$ and $m\dot{y}(0) = I$. This means that we apply an impulse at the mass at $t = 0$. The dimensions of these variables are

$$[m] = M, [a] = MT^{-1}, [k] = MT^{-2}, [I] = MLT^{-1}.$$

Three possible time scales are

$$\frac{m}{a}, \sqrt{\frac{m}{k}}, \frac{a}{k},$$

corresponding to balancing inertia and damping, inertia and spring stiffness, damping and spring stiffness. Possible length scales are

$$\frac{I}{a}, \frac{I}{\sqrt{mk}}, \frac{aI}{mk}$$

We expect that the impulse will cause an abrupt change of the mass position in short time, then relax to its equilibrium. The first time period is called an initial phase, the second is called an relaxation phase. In the initial phase, the dominated terms should be the inertia term and the damping terms. In the relaxation phase, it should be a balancing between damping and spring stiffness. Thus, for the realxation phase, we introduce the time scale

$$\bar{t} = \frac{t}{a/k}.$$

The equation becomes

$$\frac{ma^2}{k^2}\frac{d^2y}{d\bar{t}^2} + \frac{a^2}{k}\frac{dy}{d\bar{t}} + ky = 0,$$

In the initial phase, the amptitude of the mass is related to I and the damping, and the mass too. However, from dimensional analysis, the mass M appears in both I and a. Thus, the amptitude should be related only to I/a. Thus, in the relaxation phase, we rescale the length by

$$\bar{y} = \frac{y}{I/a}.$$

The rescaled equation becomes

$$\epsilon\bar{y}'' + \bar{y}' + \bar{y} = 0,$$
$$\bar{y}(0) = 0, \epsilon\bar{y}'(0) = 1.$$

Here, the dimensionless parameter

$$\epsilon = \frac{mk}{a^2} << 1.$$

The outer solution is a solution of $\bar{y}' + \bar{y} = 0$, this gives the outer solution

$$\bar{y}_o(\bar{t}) = Ce^{-\bar{t}}.$$

During the initial phase, we rescale $\tau = \bar{t}/\epsilon$ and $Y = \bar{y}$. Then

$$\frac{d^2Y}{d\tau^2} + \frac{dY}{d\tau} + \epsilon Y = 0.$$

The conditions $\bar{y}(0) = 0$, $\epsilon\bar{y}'(0) = 1$ gives the inner solution

$$\bar{y}_i(\bar{t}) = Y(\frac{\bar{t}}{\epsilon}) = 1 - e^{-\bar{t}/\epsilon}.$$

Matching the outer solution and inner slution in an overlapping zone, (i.e. $\bar{t}_\eta = \bar{t}\sqrt{\epsilon}$ is fixed), we should require

$$\lim_{\epsilon\to 0} \bar{y}_0(\bar{t}) = \lim_{\epsilon\to 0} \bar{y}_i(\bar{t}).$$

This leads to $C = 1$ in the outer solution. Thus, the final approximate solution is

$$\begin{aligned} \bar{y}_a(\bar{t}) &= \bar{y}_o(\bar{t}) + \bar{y}_i(\bar{t}) - \lim_{\epsilon\to 0} \bar{y}_i(\bar{t}) \\ &= e^{-\bar{t}} - e^{-\bar{t}/\epsilon}. \end{aligned}$$

In terms of the original variables, it reads

$$y_a(t) = \frac{I}{a}\left(e^{-kt/a} - e^{-at/m}\right).$$

Enzyme Kinetics Consider the following chemical reaction:

$$\mathbf{A} + \mathbf{B} \rightleftharpoons \mathbf{C} \to \mathbf{P} + \mathbf{B}$$

Here, $\mathbf{A}$ (a substrate) and $\mathbf{B}$ (an enzyme) combine to form a molecule $\mathbf{C}$. $\mathbf{C}$ breaks into a product $\mathbf{P}$ and an orginal enzyme $\mathbf{B}$. Let a, b, etc represent their concentration. The equations for the kinetics are

$$\begin{aligned} \dot{a} &= -k_1ab + k_2c \\ \dot{b} &= -k_1ab + k_2c + k_3c \\ \dot{c} &= k_1ab - k_2c - k_3c \\ \dot{p} &= k_3c. \end{aligned}$$

The initial concentrations are

$$a(0) = \hat{a}, b(0) = \hat{b}, c(0) = 0, p(0) = 0.$$

It is easy to see that $b+c=\hat{b}$. The first three equations do not involve p. Thus, we have the reduced equations

$$\begin{aligned}\dot{a} &= -k_1 a(\hat{b}-c)+k_2 c,\\ \dot{c} &= k_1 a(\hat{b}-c)-(k_2+k_3)c.\end{aligned}$$

The dimensions of each quantities are

$$[a]=C,[c]=C,[k_1]=T^{-1}C^{-1},[k_2]=[k_3]=T^{-1}.$$

Here, C is the dimension of concentration. We can rescale a and c by $\bar{a}=a/\hat{a}$ and $\bar{c}=c/\hat{b}$. We also rescale time by $\bar{t}=t/T$. The dimensionless equation becomes

$$\frac{\hat{a}}{T}\frac{d\bar{a}}{d\bar{t}}=-k_1\hat{a}\hat{b}\bar{a}(1-\bar{c})+k_2\hat{b}\bar{c},$$

$$\frac{\hat{b}}{T}\frac{d\bar{c}}{d\bar{t}}=k_1\hat{a}\hat{b}\bar{a}(1-\bar{c})-(k_2+k_3)\hat{b}\bar{c},$$

To determine the time scale T, we notice that our interest is to study how $\mathbf{A}$ is converted to $\mathbf{P}$ through the enzyme $\mathbf{B}$. Thus, the decreasing time scale should be the time scale we should concern. Thus, we should balance $\frac{\hat{a}}{T}$ and $k_1\hat{a}\hat{b}$ in the equation for $\bar{a}$. Thus, T is taken to be

$$T=\frac{1}{k_1\hat{b}}.$$

With this time scale, we obtain the dimensionless equations:

$$\begin{aligned}\frac{d\bar{a}}{d\bar{t}} &= -\bar{a}+(\bar{a}+\lambda)\bar{c},\\ \epsilon\frac{d\bar{c}}{d\bar{t}} &= \bar{a}-(\bar{a}+\mu)\bar{c}.\end{aligned}$$

Here,

$$\epsilon=\frac{\hat{b}}{\hat{a}}<<1,\lambda=\frac{k_2}{\hat{a}k_1},\mu=\frac{k_2+k_3}{\hat{a}k_1}.$$

The initial conditions are

$$\bar{a}(0)=1,\bar{c}(0)=0.$$

The outer solution is obtained by setting $\epsilon=0$. From this, we obtain $\bar{a}-(\bar{a}+\mu)\bar{c}=0$, which gives

$$\bar{c}=\frac{\bar{a}}{\bar{a}+\mu},$$

and the first equation becomes

$$\frac{d\bar{a}}{d\bar{t}}=-\frac{\mu-\lambda}{1+\frac{\mu}{\bar{a}}}$$

By separation of variable and integrating it, we get

$$\bar{a} + \mu \ln \bar{a} = -(\mu + \lambda)\bar{t} + K.$$

Here, the constant K will be determined from matiching with the inner solution. These two solutions a and c are our outer solutions. We denote them by a_o and c_o respectively.

In the initial layer, we use the non-dimensional variables

$$\tau = \frac{t}{\epsilon}, A = a, C = c.$$

The resulting equations

$$\begin{aligned} \frac{dA}{d\tau} &= \epsilon(-A + (A + \lambda)C) \\ \frac{dC}{d\tau} &= A - (A + \mu)C \end{aligned}$$

Setting $\epsilon = 0$, we obtain $dA/d\tau = 0$. From the initial condition $\bar{a} = 1$, we should take $A = 1$. Plug this into the second equation, we get

$$\frac{dC}{d\tau} = 1 - (1 + \mu)C.$$

With the initial condition $c(0) = 0$, we obtain

$$C = \frac{1 - e^{-(\mu+1)\tau}}{\mu + 1}.$$

For matching, we should have the outer solution $a_o(0) = A(\infty)$ and $c_o(0) = C(\infty)$. After some calculation, we get $K = 1$ from matching condition. Thus, the final approximate solution is

$$\begin{aligned} a_a(t) &= a_o(\bar{t}) \\ c_a(t) &= c_o(\bar{t}) + C(\tau) - \frac{1}{\mu + 1}. \end{aligned}$$

Boundary layers and internal layers We have seen that the Sturm-Liouville system

$$\epsilon u_{xx} - a(x)u_x - b(x)u = 0 \, x \in (0, 1),$$

$$u(0) = u_0, \; u(1) = u_1,$$

may have boundary layer. We will show that

- if $a(x) > 0$ for $x \in (0, 1)$, then the boundary layer appears at $x = 1$;
- if $a(x) < 0$ for $x \in (0, 1)$, then the boundary layer appears at $x = 0$;
- if $a(x)$ changes sign once in $(0, 1)$ with $a(0) > 0$ and $a(1) < 0$, then an internal layer is formed.

Shock wave Consider the Burgers' equation

$$uu_x = \epsilon u_{xx}, x \in (-1, 1)$$

with $u(-1) = 1$ and $u(1) = -1$. We can see that the outer solution is

$$u_o(x) = \begin{cases} 1 & -1 \le x < x_0 \\ -1 & x_0 < x \le 1 \end{cases}$$

The constant x_0 will be determined later.

For inner solution, we rescale it by $\bar{x} = (x - x_0)/\epsilon$. The equation becomes

$$\left(\frac{u^2}{2}\right)_{\bar{x}} = u_{\bar{x}\bar{x}}.$$

We integrate it once to get

$$\frac{u^2}{2} - u_{\bar{x}} = C.$$

Applying matching condition ($u(\pm\infty) = \mp 1$), we obtain $C = 1/2$. Using separation of variable, we get

$$\frac{2du}{u^2 - 1} = d\bar{x}.$$

Integrating

$$\ln\left(\frac{u+1}{u-1}\right) = \bar{x} - \bar{x}_0$$

Here, $\bar{x}_0$ is a constant. We can absorb $\bar{x}_0$ into x_0. Thus, we take $\bar{x}_0 = 0$. Then

$$\frac{u+1}{u-1} = e^{\bar{x}}.$$

This yields

$$u(\bar{x}) = \frac{1 + e^{\bar{x}}}{1 - e^{\bar{x}}} = -\tanh(\bar{x}).$$

The parameter x_0 is not unique. Any such interior layer solution with the outer solution forms an approximate solution unless we impose an extra condition. Usually, we impose an excess mass based on conservation of mass. This means that

$$\int_{-1}^{1} u(x) - u_o(x)\, dx = m$$

where m is called the excess mass. With this, $\bar{x}_0$ is determined by

$$\int_{-1}^{x_0} -\tanh\left(\frac{x - x_0}{\epsilon}\right) - 1, dx + \int_{x_0}^{1} -\tanh\left(\frac{x - x_0}{\epsilon}\right) + 1, dx = m$$

By taking $\epsilon \to 0$, we can obtain an approximation for x_0.

$$x_0 = \frac{m}{2} + O(\epsilon).$$

Homework The Burgers equation:

$$u_t + uu_x = \epsilon u_{xx}$$

is a prototype in continuum mechanics, turbulence theory, etc. Here we consider the steady Burgers' equation

$$uu_x = \epsilon u_{xx},\ x \in (0,1),$$

with the boundary condition

$$u(0) = u_0, u(1) = u_1$$

Find its asymptotic solutions. You need to classify different cases according to the signs of u_0 and u_1.

2.5 WKB method

The WKB method is a perturbation method for solving problems of the followng form

$$-\epsilon^2 u'' + q(x)u = 0$$

When $q < 0$, we expect exponential decay solution. When $q > 0$, we expect oscillatory solution. In both cases, we look solution of the form $e^{w(x)}$.

Nonoscillatory Case Consider

$$\epsilon^2 u'' - k(x)^2 u = 0, x \in (0, \infty)$$

Let us try regular perturbation for large x. We write

$$u = u_0 + \epsilon u_1 + \epsilon^2 u_2 + O(\epsilon^3),$$

Plug into the equation, we get

$$-k^2 u_0 - \epsilon k^2 u_1 + \epsilon^2 (u_0'' - k^2 u_2) + \cdots = 0,$$

This leads to $u_0 = u_1 = u_2 = \cdots = 0$. We get no information from regular perturbation for large x. If we observe the equation more carefully, suppose $k > 0$, then we expect the solution decays for large x. Thus, let us figure how it decays by trying the ansatz $u = e^{w(x)}$. Then

$$u' = w' e^w, u'' = (w'' + w'^2) e^w,$$

and the equation becomes

$$\left(\epsilon^2 (w'' + w'^2) - k^2\right) e^w = 0.$$

Thus, as long as $w \neq -\infty$, we get

$$\epsilon^2 (w'' + w'^2) - k(x)^2 = 0.$$

Let us introduce $v = \epsilon w'$ We have

$$\epsilon v' + v^2 - k(x)^2 = 0.$$

Apply the regular perturbation method

$$v = v_0 + \epsilon v_1 + \cdots$$

We get

$$v_0(x) = \pm k(x), v_1(x) = -\frac{k'}{2k}.$$

This gives

$$\epsilon w' = \pm k(x) - \epsilon \frac{k'}{2k} + O(\epsilon^2)$$

Or

$$w(x) = \frac{1}{\epsilon}\left(\pm \int_a^x k(\xi)\, d\xi - \frac{\epsilon}{2} \ln k(x) + O(\epsilon^2) \right).$$

Thus, we get an expansion

$$\begin{aligned} u(x) &= \frac{1}{\sqrt{k(x)}} \exp\left(\pm \frac{1}{\epsilon} \int_a^x k(\xi)\, d\xi + O(\epsilon) \right) \\ &= \frac{1}{\sqrt{k(x)}} \exp\left(\pm \frac{1}{\epsilon} \int_a^x k(\xi)\, d\xi \right) (1 + O(\epsilon)). \end{aligned}$$

If we require $u(\infty)$ to be bounded, then we can only accept the exponential term. Suppose $k > 0$, for instance, then

$$u(x) = C \frac{1}{\sqrt{k(x)}} \exp\left(-\frac{1}{\epsilon} \int_a^x k(\xi)\, d\xi \right) (1 + O(\epsilon))$$

is admissible.

For $x \sim 0$, we can rescale x by $x' = x/\epsilon$. Expand $u(x')$ in Taylor series near $x' = 0$. We get

$$-2u_2 - 6u_3 x' + (k_0 + k_1 x' + ...)(u_0 + u_1 x + ...) = 0.$$

This leads to

$$\begin{aligned} k_0 u_0 - 2u_2 &= 0 \\ -6u_3 + k_0 u_1 + k_1 u_0 &= 0, \end{aligned}$$

We can determine u_0 from the boundary condition. We can determine u_1 from the matching with the outer solution. In doing so, we find that the outer solution $u = e^w$ is also suitable for $x \sim 0$.

Oscillatory cases For the Schrödinger equation

$$\epsilon^2 u'' + k(x)^2 u = 0,$$

where $k > 0$, we can approximate u by $e^{iw(x)}$. Then

$$u' = iw'e^{iw}, u'' = (iw'' - w'^2)e^{iw},$$

and equation becomes

$$\epsilon^2(iw'' - w'^2) + k^2 = 0.$$

If we introduce $v = \epsilon w'$, then

$$i\epsilon v' - v^2 + k^2 = 0.$$

The ansatz for the regular perturbation $v = v_0 + \epsilon v_1 + \cdots$ gives

$$v_0 = \pm k, v_1 = \frac{iv_0'}{2v_0} = i(\ln\sqrt{v_0})'.$$

$$w(x) = \pm\frac{1}{\epsilon}\int_a^x k(\xi)\,d\xi + i\ln\sqrt{\pm k(x)} + O(\epsilon).$$

$$u(x) = \exp\left(\pm i\int_a^x k(\xi)\,d\xi\right)\exp\left(-\ln\sqrt{\pm k(x)}\right)(1 + O(\epsilon)).$$

Thus,

$$u(x) = \frac{c_1}{\sqrt{k(x)}}\exp\left(\frac{i}{\epsilon}\int_a^x k(\xi)\,d\xi\right) + \frac{c_2}{\sqrt{k(x)}}\exp\left(-\frac{i}{\epsilon}\int_a^x k(\xi)\,d\xi\right).$$

2.5.1 Method of geometric optics

In optics, the governing equation is

$$u_{tt} = c(x)^2 \triangle u.$$

For waves with a fixed frequency ω, the solution has the form: $u(x,t) = e^{-i\omega t}u(x)$ and $u(x)$ satisfies the Helmholtz equation

$$\triangle u + \frac{\omega^2}{c(x)^2}u = 0.$$

We are interested in the high frequency approximation of its solution.

Let us rewrite $\omega = 1/\epsilon$. The ansatz is

$$u(x) = A(x,\epsilon)e^{i\phi(x)/\epsilon} = (A_0(x) + A_1(x)\epsilon + \cdots)e^{i\phi(x)/\epsilon}$$

where ϕ is a phase function, A the amptitude. We plug u into the Helmholtz equation to get

$$u_{x_i} = A_{x_i}e^{i\phi/\epsilon} + \frac{iA}{\epsilon}\phi_{x_i}e^{i\phi/\epsilon},$$

$$\triangle u = \left(\triangle A + \frac{2i}{\epsilon} \nabla A \cdot \nabla \phi + \frac{iA}{\epsilon} \triangle \phi - \frac{A}{\epsilon^2} |\nabla \phi|^2 \right) e^{i\phi/\epsilon}$$

$$\left(-\frac{A}{\epsilon^2} |\nabla \phi|^2 + \frac{i}{\epsilon} (A \triangle \phi + 2 \nabla A \cdot \phi) + \triangle A \right) + \frac{A}{\epsilon^2 c(x)^2} = 0.$$

Expanding A in $A_0 + \epsilon A_1 + \cdots$ and equating the coefficients of ϵ, we get

$$|\nabla \phi|^2 = \frac{1}{c(x)^2},$$

$$A_0 \triangle \phi + 2 \nabla A_0 \cdot \nabla \phi = 0.$$

The first equation is called the eikonal equation. The second equation is called the transport equation. In the second equation, if we rename $A_0 = \sqrt{\rho_0}$, then the transport equation becomes

$$\sqrt{\rho_0} \triangle \phi + 2 \nabla \sqrt{\rho_0} \cdot \nabla \phi = \sqrt{\rho_0} \triangle \phi + \frac{1}{\sqrt{\rho_0}} \nabla \rho_0 \cdot \nabla \phi = 0.$$

Thus, this is equivalent to

$$\nabla \cdot (\rho_0 \nabla \phi) = 0.$$

WKB method for Schrödinger equation Consider the Schrödinger equation

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x) \psi.$$

We look solution of the form: $\psi = e^{w/\hbar}$. We have

$$\begin{aligned} \partial_t \psi &= \frac{1}{\hbar} \partial_t w e^{w/\hbar}, \\ \nabla \psi &= \frac{1}{\hbar} \nabla w e^{w/\hbar}, \\ \nabla^2 \psi &= \left(\frac{1}{\hbar} \nabla^2 w + \frac{1}{\hbar^2} \sum_k (\partial_{x_k} w)^2 \right) e^{w/\hbar}. \end{aligned}$$

Thus, we get

$$i \partial_t w = -\frac{1}{2m} \left(\hbar \nabla^2 w + \sum_k (\partial_{x_k} w)^2 \right) + V.$$

We write $w = R + iS$, real part and imaginary part. Then

$$i \partial_t (R + iS) = -\frac{1}{2m} \left(\hbar \nabla^2 (R + iS) + |\nabla R|^2 - |\nabla S|^2 + 2i \nabla R \cdot \nabla S \right) + V.$$

Equating the real part and imaginary part, we get

$$\partial_t R = -\frac{1}{2m} \left(\hbar \nabla^2 S + 2 \nabla R \cdot \nabla S \right),$$

$$-\partial_t S = -\frac{1}{2m}\left(\hbar\nabla^2 R + |\nabla R|^2 - |\nabla S|^2\right) + V.$$

[1] Since $[S] = ET = ML^2T^{-1}$, $[\nabla S] = MLT^{-1}$, we can define $p = \nabla S$, $v = (\nabla S)/m$. Multiplying the first equation by $e^{2R/\hbar}$, we get

$$\begin{aligned} e^{2R/\hbar}\partial_t R &= -\frac{1}{2m}\left(\hbar e^{2R/\hbar}\nabla^2 S + 2e^{2R/\hbar}\nabla R\cdot\nabla S\right) \\ &= -\frac{\hbar}{2m}\nabla\cdot\left(e^{2R/\hbar}\nabla S\right) \end{aligned}$$

Next, we define $\rho = e^{2R/\hbar}$, use $v = \nabla S/m$, then the first equation can be written as

$$\partial_t\rho + \nabla\cdot(\rho v) = 0.$$

This is the continuity equation.

For the second equation

$$S_t + \frac{1}{2m}|\nabla S|^2 + V = \frac{1}{2m}(|\nabla R|^2 + \hbar\nabla^2 R)$$

We express the RHS in terms of ρ. We get

$$S_t + \frac{1}{2m}|\nabla S|^2 + V = \frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho}.$$

We take gradient of this equation to get

$$mv_t + m\nabla\left(\frac{|v|^2}{2}\right) + \nabla V = \frac{\hbar^2}{4m}\nabla\left(\frac{\nabla^2\rho}{\rho}\right)$$

$$v_t + v\cdot\nabla v + \frac{1}{m}\nabla V = \frac{\hbar^2}{4m^2}\nabla\left(\frac{\nabla^2\rho}{\rho}\right)$$

Multiplying ρ to this equation, we get

$$\rho(v_t + v\cdot\nabla v) + \frac{\rho}{m}\nabla V = \frac{\rho\hbar^2}{4m^2}\nabla\left(\frac{\nabla^2\rho}{\rho}\right)$$

The left-hand side is the pressureless momentum equation for the gas dynamics. The right-hand side is a dispersion term. It regularizes the solution.

Thus, solving the outer solution based on the WKB approach for the Schrödinger equation is equivalent to solve a pressureless Euler equation. Although it is also not an easy job, the WKB approach provides us an insight of the macroscopic structure of the Schrödinger equationm. It also make a link between qnautum mechanics and classical mechanics.

[1] The dimension of w and $\hbar$ are action, which energy times time ET. The dimension of the first equation is $[R]MT^{-1} = [\hbar][S]L^{-2} = [R][S]L^{-2}$, Thus, this is consistent to $E = T^{-2}L^2M$.

Reference

1. Bender-Orszag's book has a complete description of WKB method for Sturm-Liouville equation (in one dimension). In particular, it contains the descriptio of turning point.

2. Griffith's book on Quantum mechanics has a good description on application of WKB for Schrödinger in one dimension.

Homework

- pp. 141: 2, 3, 5, 6,8.

2.6 Asymptotic expansion of integrals

2.6.1 Laplace method for approximation of integrals

In applied mathematics, many solution or approximate solution has integral representation. For instance, using WKB method, we can have approximate Green's function formula (See Bender-Orszag). Using this formulation, we can have an integral representation of the solution. In particular, the following Laplace integral appears quite often in one dimensional problem:

$$I(\lambda) = \int_a^b f(t)e^{-\lambda g(t)}\, dt, \lambda >> 1. \tag{2.1}$$

And we are interested in its behavior for large λ. A generalization is when t is in the complex plane:

$$I(\lambda) = \int_C f(z)e^{\lambda g(z)}\, dz,\ \lambda >> 1,$$

where C is a contour on complex plane. This leads to method of stationary phase and method of saddle point.

Laplace integrals We will study the asymptotic behavior of the integral of the form (2.1). The first observation is that the integrand $e^{-\lambda g(t)}$ is important at those minima of g. So, let us first consider the case where g is monotonic in $[a, b]$. We may assume g is monotonic increasing in $[a, b]$ without loss of generality. In this case, we can normalize the integral by the change of variable: $s = g(t) - g(a)$. Then the integral becomes

$$I(\lambda) = e^{-\lambda g(a)} \int_0^{g(b)-g(a)} \frac{f(t(s))}{g'(t(s))} e^{-\lambda s}\, ds.$$

This is a standard form of the Laplace integral. The important part of the integral is near s 0. So, we decompose the integral into two regions: $[0, T]$ and $[T, g(b) - g(a)]$. In the latter region, the term $e^{-\lambda s}$ will be exponential small (i.e. $e^{-\lambda T}$. For the former region, we make Taylor expansion of $f(t(s))/g'(t(s))$ near s 0, then integrate term by term to get expansion. We illustrate this approach by the following examples.

1. Example 1. Consider the integral

$$I(\lambda) = \int_0^\infty \frac{\sin t}{t} e^{-\lambda t}\, dt, \lambda >> 1.$$

We decompose $\int_0^\infty = \int_0^T + \int_T^\infty$. For the latter integral, we have

$$\left| \int_T^\infty \frac{\sin t}{t} e^{-\lambda t}\, dt \right| \leq \int_T^\infty e^{-\lambda t}\, dt = \frac{1}{\lambda} e^{-\lambda T}$$

For any fixed T, this term is always $O(\lambda^{-N})$ for any N. We call it exponential small term (EST).

For the first integral, we make Taylor expansion of $\sin t$ near $t = 0$, we get

$$\begin{aligned}
I(\lambda) &= \int_0^T \frac{\sin t}{t} e^{-\lambda t}\, dt + EST \\
&= \int_0^T \left(\sum_{n=0}^N (-1)^n \frac{t^{2n}}{(2n+1)!} + O(t^{2N+2}) \right) e^{-\lambda t}\, dt + EST \\
&= \int_0^{\lambda T} \sum_{n=0}^N (-1)^n \frac{u^{2n}}{(2n+1)!\lambda^{2n+1}} e^{-u}\, du + O(\lambda^{-2N-3}) \\
&= \int_0^\infty \sum_{n=0}^N (-1)^n \frac{u^{2n}}{(2n+1)!\lambda^{2n+1}} e^{-u}\, du + O(\lambda^{-2N-3}) + EST \\
&= \sum_{n=0}^N (-1)^n \frac{\Gamma(2n+1)}{(2n+1)!\lambda^{2n+1}} + O(\lambda^{-2N-3}) \\
&= \sum_{n=0}^N (-1)^n \frac{(2n)!}{(2n+1)!\lambda^{2n+1}} + O(\lambda^{-2N-3}) \\
&= \sum_{n=0}^N \frac{(-1)^n}{(2n+1)\lambda^{2n+1}} + O(\lambda^{-2N-3})
\end{aligned}$$

Here, the function $\Gamma(x)$ is called the Gamma function and is defined by

$$\Gamma(x) := \int_0^\infty t^{x-1} e^{-t}\, dt.$$

This function is well defined for $x > 0$. By using integration by part, we get

$$\Gamma(x+1) = x\Gamma(x).$$

2. Asymptotic expansion for error function. The error function is defined as

$$\text{erfc}(\lambda) = \frac{2}{\sqrt{\pi}} \int_{\lambda}^{\infty} e^{-t^2}\, dt.$$

We make a change of variable $\tau = (t - \lambda)/2$. Then

$$\text{erfc}(\lambda) = \frac{1}{\sqrt{\pi}} e^{-\lambda^2} \int_{0}^{\infty} e^{-\tau^2/4} e^{-\lambda\tau}\, d\tau.$$

We find the important part is localated near $\tau = 0$. We can decompose the integral region into $[0, T]$ and $[T, \infty)$. The latter part is a EST. In the formal integral, we make Taylor expansion for $e^{-\tau^2/2}$ for $\tau \in [0, T]$, then integrate the integral, we get

$$\text{erfc}(\lambda) \sim \frac{2}{\sqrt{\pi}} e^{-\lambda^2} \sum_{n=0}^{\infty} (-1)^n \frac{(2n)!}{n!(2\lambda)^{2n+1}}$$

Method of steepest descent for integrals In the case that $g(t)$ has interior local minima, the important parts of the integral (2.1) are near these local minima. Let us suppose there is only one inimum, say t_0. If there are more than one (but still finite many), we just add the asymptotic formulation for each one together. We break the integral into $(t_0 - \delta, , t_0 + \delta)$ and its exterior part. In the exterior region: $|t - t_0| \geq\geq \delta$ and t is bounded,

$$g(t) - g(t_0) \geq M,$$

and the integral

$$\int_{(a,b)\cap|t-t_0|\geq\delta} f(t) e^{-\lambda t} \leq C e^{-\lambda M}.$$

For unbounded region (a, b), we can require that that the asymptotic behavior of g is some power growth, say $g(t) - g(t_0) \geq M|t - t_0|$. Then we still have the above estimate.

In the interior region: $|t - t_0| < \delta$, let us expand g by

$$g(t) = g(t_0) + \frac{1}{2} g''(t_0)(t - t_0)^2 + O(t - t_0)^3, \text{ for } |t - t_0| \leq \delta.$$

We can replace $g - g(t_0)$ by the quadratic term in the Laplace integral:

$$\int_{|t-t_0|<\delta} f(t) e^{-\lambda g(t)} = e^{-\lambda(g(t_0)+O(\delta^3))} \int_{|t-t_0|<\delta} f(t) e^{-\lambda(t-t_0)^2/2}\, dt.$$

The term

$$e^{-\lambda O(\delta^3)} = 1 + O(\lambda\delta^3).$$

The choice of δ should depend on λ. We shall determine it later.

For the integral

$$\int_{t_0-\delta}^{t_0+\delta} f(t) e^{-\lambda g''(t_0)(t-t_0)^2/2}\, dt,$$

we make a change of variable $\sqrt{\lambda g''(0)}t - t_0 = s$. Then the above becomes

$$\int_{-\delta\sqrt{\lambda g''(t_0)}}^{\delta\sqrt{\lambda g''(t_0)}} f\left(t_0 + \frac{s}{\sqrt{\lambda g''(t_0)}}\right) e^{-s^2/2}\, d\left(\frac{s}{\sqrt{\lambda g''(t_0)}}\right).$$

We need the domain of integral goes to the whole line. This require $\delta\sqrt{\lambda} \to \infty$ as $\lambda \to \infty$. On the other hand, we should also require $\lambda\delta^3 \to 0$ as $\lambda \to \infty$. So, we can choose $\delta = \lambda^{-\alpha}$ with $1/3 < \alpha < 1/2$. We may choose $\alpha = 1/2 - \epsilon/3$ for any small $\epsilon > 0$. Then

$$O(\lambda\delta^3) = O(\lambda^{-1/2+\epsilon}).$$

With this, we get

$$I(\lambda) \sim f(t_0)e^{-\lambda g(t_0)} \left(\frac{2\pi}{\lambda g''(t_0)}\right)^{1/2} (1 + O(\lambda^{-1/2+\epsilon})).$$

Here, we have used

$$\int_{-\infty}^{\infty} e^{-s^2/2}\, ds = \sqrt{2\pi}.$$

Remark. The error $O(\lambda^{-1/2+\epsilon})$ can be improved. Indeed, we can expand g as

$$g(t) = \sum_{i=0}^{3} \frac{g^{(i)}(t_0)}{i!}(t - t - t_0)^i + O(\delta^4).$$

We claim that the third order term can be removed by a qradratic translation. For simplicity, let us assume $t_0 = 0$. We have

$$\begin{aligned} g(t) &= g(0) + \frac{g''(0)}{2}t^2 + \frac{g'''(0)}{3!}t^3 + O(t^4) \\ &= g(0) + \frac{g''(0)}{2}\left(t + at^2\right)^2 + O(t^4) \end{aligned}$$

where

$$a = \frac{g'''(0)}{3!g''(0)}.$$

Using the change-of-variable $(t + at^2) \leftarrow t$, we can remove the third order term. Thus we get

$$I(\lambda) = \int_{-\delta\sqrt{\lambda g''(t_0)}}^{\delta\sqrt{\lambda g''(t_0)}} f(t_0 + \frac{s}{\sqrt{\lambda g''(t_0)}})e^{-s^2/2}\, d\frac{s}{\sqrt{\lambda g''(t_0)}} \left(1 + O(\lambda\delta^4)\right).$$

We can choose $\delta = M/\sqrt{\lambda}$ for large M. Then we can get the asymptotic formula

$$I(\lambda) \sim f(t_0)e^{-\lambda g(t_0)} \left(\frac{2\pi}{\lambda g''(t_0)}\right)^{1/2} (1 + O(\lambda^{-1})).$$

Stirning formula The Stirnling formula is

$$n! \sim \sqrt{2\pi} n^{n+1/2} e^{-n} (1 + O(\frac{1}{n})).$$

This formula is very useful to connect discrete phenomena to continuous phenomena. Since $\Gamma(n+1) = n!$, we shall study the asymptotic expansion of the Gamma function. The Gamma function is defined to be

$$\Gamma(s) = \int_0^\infty x^{s-1} e^{-x}\, dx = \int_0^\infty e^{-sF(x,s)}\, dx$$

where

$$F(x,s) = -\ln x + \frac{\ln x}{s} + \frac{x}{s}.$$

The minimum of F w.r.t. x is $x = s-1$. We rescale x by setting $t = x/(s-1)$. Then

$$\begin{aligned} F(t(s-1), s) &= -\ln(t(s-1)) + \frac{1}{s}\ln(t(s-1)) + \frac{t(s-1)}{s} \\ &= -\ln(s-1) + \frac{\ln(s-1)}{s} + (-\ln t + \frac{\ln t}{s} + \frac{t(s-1)}{s}) \end{aligned}$$

Therefore,

$$\Gamma(s) = (s-1)^s J(s),$$

where

$$J(s) = \int_0^\infty e^{-(s-1)g(t)}\, dt,\ g(t) = t - \ln t.$$

The minimum of $g(t)$ is $g'(t) = 1 - 1/t = 0$. This gives the extremal point $t_0 = 1$. At $t = 1$, $g''(1) = 1 > 0$. Thus, $t = 1$ is a mimimum. From the Laplace asymptotic formula, we get

$$J(s) \sim e^{-(s-1)} \left(\frac{2\pi}{s-1}\right)^{1/2}$$

Thus,

$$\ln \Gamma(s) = \left(s - \frac{1}{2}\right)\ln(s-1) - (s-1) + \frac{1}{2}\ln(2\pi) + O(\frac{1}{s-1}).$$

Homework.

- pp. 149: 3, 6, 7(a), 8, 11, 12.

Chapter 3

Calculus of Variation

3.1 Examples of Functionals

Many physical problems can be formulated as variational problems.

Example 1. Minimum arc length problem Consider the set

$$\mathcal{A} = \{y : [a, b] \to \mathbb{R} \text{ in } C^1, y(a) = y_a, y(b) = y_b\}$$

For $y \in \mathcal{A}$, we define its arc length by

$$J(y) = \int_a^b \sqrt{1 + y'(x)^2}\, dx$$

The function J maps a "path" $y \in \mathcal{A}$ to a real number. That is, $J : \mathcal{A} \to \mathbb{R}$. We call J is a functional. The problem is to find a minimum of J in the set $\mathcal{A}$. Certainly, the answer of this is the straight line connecting (a, y_a) and (b, y_b).

Example 2. Minimum area problem Consider the minimum area problem defined on a domain $\Omega \subset \mathbb{R}^2$. Let

$$\mathcal{A} = \{u : \Omega \to \mathbb{R} \text{ in } C^1, \text{ with } u = u_0, \text{ on } \partial\Omega\}$$

where u_0 is a precribed function defined on $\partial\Omega$. For a function $u \in \mathcal{A}$, the area of its graph on Ω is

$$J(u) = \int_\Omega \sqrt{1 + |\nabla u(x)|^2}\, dx.$$

The minimum of J in $\mathcal{A}$ is called the minimum surface with prescribed boundary value u_0. This problem is much nontrivial.

Example 3. The Brachistochrone The Brachistochrone problem is to find a curve on which a ball sliding down under gravitation to a point with depth h takes least time. The word "brachistochrone" means the "the shortest time delay" in Greek. It was one of the oldest problem in Calculus of Variation. Its solution is a section of a cycloid. This was founded by Leibnitz, L'Hospital, Newton and two Bernoullis. Suppose the curve starts from $A = (0, 0)$ and ends at $B = (a, -h)$. Let s be the arc length of the curve. The equation of motion is

$$m\ddot{s} = -mgy'(s).$$

This gives the conservation of energy

$$\frac{1}{2}m\dot{s}^2 + mgy(s) = E.$$

At point A, we take $s = 0$, $\dot{s} = 0$ and $y(0) = 0$. With this normalization, $E = 0$. Thus, we have the speed

$$v = \dot{s} = \sqrt{-2gy}.$$

Notice that $y \leq 0$ under our consideration. The traveling time from A to B is given by

$$T(y) = \int_0^T dt = \int_0^S \frac{ds}{\dot{s}} = \int_0^s \frac{ds}{\sqrt{-2gy}}.$$

Here, S is the arc length of the curve $\{(x, y(x))|x \in (0, a)\}$. We can also express the functional using parameter x:

$$T(y) = \int_0^S \frac{ds}{v} = \int_0^a \frac{\sqrt{1 + y'(x)^2}}{\sqrt{-2gy(x)}}\, dx$$

The admissible class is

$$\mathcal{A} = \{y : (0, a) \to \mathbb{R} \in C^1 | y(0) = 0, y(a) = -h\}.$$

In the above examples, we encounter a functional defined as

$$J(y) = \int_a^b L(x, y(x), y'(x))\, dx$$

for functions y in an addmissible class $\mathcal{A}$. The class of functions should be continuously differentiable so that $L(x, y(x), y'(x))$ is well-defined. In addition, some boundary conditions of y at a and b are imposed. The integrand is called the Lagrangian. The functional J has the names "cost functional", "action", ... in different applications.

Homework. pp. 158: 1

3.2 Banach Spaces

Normed linear space The above functionals are defined in a function space. In abstract, the function space is a vector space V over a scalar field. The scalar field we consider is either the real field $\mathbb{R}$ or the complex field $\mathbb{C}$. In a vector space, we can associat each vector y a norm $\|y\|$, which measures the length of the vector y. It is required to satisfy the following properties:

1. $\|y\| \geq 0$, and $\|y\| = 0$ if and only if $y = 0$,
2. $\|\alpha y\| = |\alpha| \|y\|$,
3. Triangle inequality: $\|y_1 + y_2\| \leq \|y_1\| + \|y_2\|$.

A vector space V associated with a norm $\|\cdot\|$ is called a normed linear space.

Examples

1. $\mathbb{R}^n$ with $\|x\| = \sqrt{x_1^2 + \cdots + x_n^2}$ is a normed linear space.
2. $\mathbb{R}^n$ with $\|x\|_p := (|x_1|^p + \cdots + |x_n|^p)^{1/p}$ for $p \geq 1$ is a normed linear space.
3. $C[a, b] = \{y : [a, b] \to \mathbb{R} \text{ is continuous}\}$ with the norm
$$\|y\|_\infty := \max_{x \in [a,b]} |y(x)|$$
is a normed linear space.
4. $C^1[a, b] := \{y : [a, b] \to \mathbb{R} \text{ is continuously differentiable}\}$ with the norm
$$\|y\| := \max_{x \in [a,b]} \big(|y(x)| + |y'(x)|\big)$$
is a normed linear space.
5. The space ℓ^p is defined to be
$$\ell^p = \{(x_n)_{n=1}^\infty | \sum_n |x_n|^p < \infty\}$$
associated with the norm
$$\|x\|_p := \left(\sum_{n=1}^\infty |x_n|^p\right)^{1/p}$$
The space ℓ^p with $p \geq 1$ is a normed linear space.
6. The ℓ^∞ space is
$$\ell^\infty = \{(x_n)_{n=1}^\infty | \sup_n |x_n| < \infty\}$$
associated with the norm
$$\|x\|_\infty := \sup_n |x_n|.$$

7. The space $L^p(a,b)$ defined to be

$$L^p(a,b) = \{y : (a,b) \to \mathbb{R} | \int_a^b |y(x)|^p \, dx < \infty\}$$

associated with the norm

$$\|y\|_p := \left(\int_a^b |y(x)|^p \, dx \right)^{1/p}$$

is a normed linear space for $p \geq 1$.

8. The space $L^\infty(a,b)$ is defined as

$$L^p(a,b) = \{y : (a,b) \to \mathbb{R} | \sup_{x \in (a,b)} |y(x)| < \infty\}$$

associated with the norm

$$\|y\|_\infty := \sup_{x \in (a,b)} |y(x)| < \infty.$$

9. The Sobolev space $H^m(a,b)$ is defined as

$$H^m(a,b) := \left\{ y : (a,b) \to \mathbb{R} \, \middle| \int_a^b |y(x)|^2 + \cdots + |y^{(m)}|^2 \, dx < \infty \right\}$$

with the norm

$$\|y\|_{H^m} := \left(\int_a^b |y(x)|^2 + \cdots + |y^{(m)}|^2 \, dx \right)^{1/2}$$

Homework

1. Show that $\|x\|_p \to \|x\|_\infty$ as $p \to \infty$.

Banach spaces In a normed linear space V, we can define the concept of limits.

- Limit: A sequence $\{y_n\}$ in V is said to have a limit $y \in V$ if $\|y_n - y\| \to 0$. We denote it by $\lim_{n\to\infty} y_n = y$.
- Cauchy sequence: A sequence $\{y_n\}$ in is called Cauchy sequence if all but finite of them are closed to each other. In mathematical languish, for any $\epsilon > 0$, there exists an N such that for all $n, m > N$, we have $\|y_n - y_m\| < \epsilon$.
- Completeness: A normed linear space V is said to be complete if all its Cauchy sequences have limits in V. Such spaces are also called Banach spaces.
- Theorem [Completion of normed linear space] For any normed linear space V, there exists a minimal complete normed linear space $\tilde{V}$ containing V. One way to construct such a space is to define

$$\tilde{V} = \{(y_n) | (y_n) \text{ is a Cauchy sequence in } V\} / \sim .$$

Here $\sim$ is the notation of equivalence. Two Cauchy sequences (y_n) and (z_n) are called equivalent if for any $\epsilon > 0$ there exists N such that for all $n \geq N$, we have $\|y_n - z_n\| < \epsilon$.

Examples

1. The space $C[a,b]$ under the $\|\cdot\|_\infty$ is a Banach space.

2. The space $C[-1,1]$ under $\|\cdot\|_1$ is not a Banach space. Because the sequence $\tanh(x/\epsilon)$ with $\epsilon = 1/n$ is a Cauchy sequence, but its limit is a discontinuous function which is not in $C[-1,1]$.

3. The spaces $L^p(a,b)$ under $\|\cdot\|_p$, $1 \le p \le \infty$ are Banach spaces. In fact, the $L^p(a,b)$, $1 \le p < \infty$ is the completion of $C[a,b]$ under the norm $\|\cdot\|_p$.

4. The Sobolev space $H^m(a,b)$ the completion of $C^m[a,b]$ under the norm:

$$\|y\|_{H^m} := \left(\int_a^b |y(x)|^2 + \cdots + |y^{(m)}|^2 \, dx \right)^{1/2}$$

Homework: Find the function classes (as shown in the above examples) of the following functions they belong to.

1. The Heviside function (i.e. the step function).

2. Find the condition on α such that the function $|x|^\alpha \in L^p(-1,1)$

Approximation and Subspaces In applications, we usually approximate a function by nice smooth functions. For instance, $u \in C[a,b]$ can be approximated by $C^\infty[a,b]$ by the norm $\|\cdot\|_\infty$. That is, for any $\epsilon > 0$, we can find a function $u_\epsilon \in C^\infty[a,b]$ such that $\|u - u_\epsilon\| < \epsilon$. We can choose, for instance, $u_\epsilon = \rho_\epsilon * u$, where $\rho_\epsilon(x) := \rho(x/\epsilon)/\epsilon$ and $\rho \in C^\infty(\mathbb{R})$, has compact supported in $(-1,1)$, $\rho(x) > 0$ for $|x| < 1/2$ and $\int \rho \, dx = 1$.

The space $C^\infty \subset C[a,b]$ as a subspace. Moreover, from the discussion above, we say that $C^\infty[a,b]$ is dense in $C[a,b]$. Some commonly used examples are:

1. $H^m(a,b)$ is dense in $L^2(a,b)$ for $0 \le m < \infty$,

2. $L^p(a,b)$ is dense in $L^q(a,b)$ for $1 \le q \le p \le \infty$. Here, we require the interval (a,b) being bounded.

Homework. Prove the assertion:

1. $u_\epsilon \in C^\infty$.

2. $\rho_\epsilon * u \to u$ in $\|\cdot\|_\infty$ for $u \in C[a,b]$.

Boundary conditions and Subspaces In variational problems, we usually impose some boundary condition such as Dirichlet, Neumann or Robin conditions. They come naturally from the process of integration-by-part. We will explain this latter. We would like to point out here is that the set which satisfies the boundary condition usually form a subspace, provided the problem is linear. Here are some examples:

1. $C_0[a,b] = \{u \in C[a,b], u(a) = u(b) = 0\}$ is a closed subspace in $C[a,b]$.
2. $H_0^1[a,b] = \{u \in H^1(a,b), u(a) = u(b) = 0\}$ is a closed subspace in $H^1(a,b)$.
3. $C_0^m[a,b] = \{u \in C^m[a,b], u(a) = u(b) = 0\}$ is a subspace in $C^m[a,b]$.

In general, the boundary condition gives a constraint. The set $\mathcal{A}$ of those vectors satisfying the constraint forms a manifold (or an admissible class) in the Banach space.

3.3 Linear operators

Linear functionals Let V be a normed linear space over $\mathbb{R}$. Let ℓ be a linear function from V to $\mathbb{R}$. Such a function is called a linear functional. A linear functional ℓ is said to be bounded if there exist a constant C such that $|\ell(x)| \leq C\|x\|$ for all $x \in V$.

Proposition 1. *ℓ is bounded if and only if it is continuous.*

Examples

1. Let $x_0 \in [a,b]$. Consider the mapping defined by $\ell(f) = f(x_0)$ for any $f \in C[a,b]$. Then ℓ is a bounded linear functional on $C[a,b]$.
2. Let $\epsilon > 0$ be small number. Define
$$\ell(f) = \frac{1}{2\epsilon}\int_{-\epsilon}^{\epsilon} f(x_0 + y)\, dy$$
Then ℓ is a bounded linear functional on $L^1(\mathbb{R})$.
3. Let $\rho \in C^\infty$ with the properties: $\rho > 0$ in $(-1/2, 1/2)$, supp $\rho \subset (-1,1)$, and $\int \rho = 1$. Let ϵ be a small positive number, and define $\rho_\epsilon(x) := \frac{1}{\epsilon}\rho(x/\epsilon)$. Define
$$\ell(f) = \rho_\epsilon * f(x_0) := \int f(x_0 - y)\rho_\epsilon(y)\, dy.$$
Then ℓ is a bounded linear functional on $L^1(\mathbb{R})$.
4. The mapping: $\ell(f) := Df(x_0)$ is a linear functional on $C^1[a,b]$ but not bounded. Here, $x_0 \in (a,b)$ and Df is the derivative of f.

Bounded Operators Let V and W be two normed linear spaces. A linear operator $A : V \to W$ is said to be bounded if there exist a constant C such that $\|Av\| \leq C\|v\|$ for all $v \in V$.

Proposition 2. *A linear operator $A : V \to W$ is bounded if and only if it is continuous.*

Examples

1. Integral operator: Let $k(x, y)$ be a continuous function defined on $[a, b] \times [a, b]$. the operator defined by
$$Af(x) = \int_a^b k(x, y)f(y)\, dy$$
maps $f \in C[a, b]$ into $Af \in C[a, b]$. This operator is bounded.

2. Consider the interval $[0, 1]$. Let $k(x, y)$ be defined as
$$k(x, y) = \begin{cases} (1 - y)x & \text{for } x < y \\ (1 - x)y & \text{for } x > y \end{cases}$$
You can show that $Af \in C^1[0, 1]$ if $f \in C[a, b]$.

For a bounded operator $A : V \to W$, we can define its operator norm by
$$\|A\| := \sup \frac{\|Af\|_W}{\|f\|_V}.$$
One can show that the set $B(V, W) := \{A : V \to W \text{ is a bounded operator}\}$ endow with this operator norm is a normed linear space. If W is complete, so is $B(V, W)$.

Unbounded Operators The unbounded operators are those differential operators. They usually define on a dense subspace of a Banach space. Here is the definition:

Examples

1. $u \mapsto Du$ is defined on $C^1(a, b)$ whose range is in $C^0(a, b)$. We may think $D : C^1(a, b) \subset C^0(a, b) \to C^0(a, b)$.

2. D can also be thought as a mapping defined on $H^1(a, b) \subset L^2(a, b)$ to $L^2(a, b)$.

3.4 Variation of Functionals

As we have seen in Section 1 of this chapter that variational problems involve a functional J defined on an admissible set $\mathcal{A}$ in a Banach space V. Our goal is to look for extremals of J in $\mathcal{A}$. A vector y_0 is said to be a local minimum of J in $\mathcal{A}$ if $J(y_0) \leq J(y)$ for all y in a small neighborhood of y_0 in $\mathcal{A}$.

Tangent space Suppose y_0 is a local extremal in $\mathcal{A} \subset V$. A function $h \in V$ such that $y_0 + \epsilon h \in \mathcal{A}$ for all sufficiently small ϵ, such a function h is called a variation of $\mathcal{A}$ at y_0. In other words, h lies on the tangent space of $\mathcal{A}$ at y_0. For example, let us consider the set

$$\mathcal{A} = \{y : [a, b] \mapsto \mathbb{R}^3 \mid y \in C^1[a, b] \text{ and } y(a) = A, y(b) = B\}$$

where A and B are two points in $\mathbb{R}^3$. The admissible variations are

$$\mathcal{T}(y_0) = \{h : [a, b] \mapsto \mathbb{R}^3 \mid h \in C^1[a, b] \text{ and } h(a) = 0, h(b) = 0\}$$

Sometimes, we denote a variation h by δy.

Directional Derivatives The directional derivative of J at y_0 in a direction $h \in \mathcal{T}(y_0)$ is defined to be $dJ(y_0 + \epsilon h)/d\epsilon$ at $\epsilon = 0$, if it exists. We denote it by $\delta J(y_0, h)$. If $\delta J(y_0, h)$ exists for all the admissible variations $h \in \mathcal{T}$, one can show that $\delta J(y_0, \alpha h) = \alpha \delta J(y_0, h)$. However, it may not be linear in h. Even if it is linear in h, it may not be continuous in h. In most applications, it is indeed a bounded linear in h. In this case, we can express $\delta J(y_0, h)$ by $\delta J(y_0) \cdot h$. The functional $\delta J(y_0)$ is called the first variation (or the Gâteaux derivative) of J at y_0. Notice that the linear functional $\delta J(y_0)$ may not be bounded.

Another relevant definition is the Fréchet's derivative. A functional J uis said to be Fréchet differentiable at y_0 if there exists a bounded linear functional ℓ such that for any sufficiently small h, we have

$$J(y_0 + h) = J(y_0) + \ell(h) + o(\|h\|).$$

The functional ℓ is also denoted by δJ, or DJ. It is clear that Fréchet differentiability implies Gâteaux differentiability. Conversely, if J is Gâteaux differentiable at y_0, Further, the corresponding Gáteaux derivative $\delta J(y_0, h)$ is continuous in both y_0 and h, then J is also Fréchet differentiable.

Necessary Conditions for Extremals

Theorem 3.4. *Let $J : \mathcal{A} \to \mathbb{R}$ be a functional. If y be its local minimum in $\mathcal{A}$, then $\delta J(y, h) = 0$ for all admissible variation h.*

Let now study one dimensional variational problem. Let $L : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ called the Lagragian. We look for minimum of the functional

$$J(y) = \int_a^b L(x, y(x), y'(x))\, dx$$

in the admissible class

$$\mathcal{A} = \{y : [a, b] \to \mathbb{R}^n | y \in C^1, y(a) = y_0, y(b) = y_1\}.$$

The argument of L is $(x, y, v) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$. Later, we shall take partial derivative of L with respect to v. However, since y' is used for the argument v, we commonly use $L_{y'}$ to represent L_v.

Now, let us compute the first variation of J.

$$\begin{aligned}\frac{d}{d\epsilon}|_{\epsilon=0}J(y+\epsilon h) &= \frac{d}{d\epsilon}|_{\epsilon=0}\int_a^b L(x,y(x)+\epsilon h(x),y'(x)+\epsilon h'(x))\,dx \\ &= \int_a^b \frac{\partial}{\partial\epsilon}|_{\epsilon=0}L(x,y(x)+\epsilon h(x),y'(x)+\epsilon h'(x))\,dx \\ &= \int_a^b \left[L_y(x,y(x),y'(x))\cdot h(x)+L_{y'}(x,y(x),y'(x))\cdot h'(x)\right]\,dx\end{aligned}$$

Since the boundary $y+\epsilon h$ is required to be admissible, we will have $(y+\epsilon h)(a)=y_0$ and $(y+\epsilon h)(b)=y_1$ for all small ϵ. Thus, admissible variation h should satisfies $h(a)=h(b)=0$.

Thus, a local minimum y should satisfy

$$\delta J(y)\cdot h=\int_a^b \left[L_y(x,y,y')\cdot h+L_{y'}(x,y,y')\cdot h'\right]\,dx=0$$

for all $h\in C^1[a,b]$ with $h(a)=h(b)=0$.

If $y\in C^2$, then we can take integration-by-part on the second term and use $h(a)=h(b)=0$ to get

$$\begin{aligned}\delta J(y)\cdot h &= \int_a^b \left[L_y(x,y(x),y'(x))\cdot h(x)+L_{y'}(x,y(x),y'(x))\cdot h'(x)\right]\,dx \\ &= \int_a^b L_y(x,y,y')\cdot h-\frac{d}{dx}L_{y'}(x,y,y')\cdot h\,dx+L_y(x,y,y')\cdot h(x)|_{x=a}^{x=b} \\ &= \int_a^b \left[L_y(x,y,y')-\frac{d}{dx}L_{y'}(x,y,y')\right]\cdot h\,dx=0.\end{aligned}$$

A fundamental lemma states that

Lemma 3.1. *If f is continuous on $[a,b]$ and if $\int_a^b f(x)h(x)\,dx=0$ for all smooth function h with $h(a)=h(b)=0$, then $f\equiv 0$.*

Proof. If $f(x_0)\neq 0$ for some $x_0\in(a,b)$ (say $f(x_0)=C>0$), then there is small neighborhood $(x_0-\epsilon,x_0+\epsilon)$ such that $f(x)>C/2$. We can choose h to be a hump such that $h(x)=1$ for $|x-x_0|\leq\epsilon/2$ and $h(x)\geq 0$ and $h(x)=0$ for $|x-x_0|\geq\epsilon$. The test function still satisfies the boundary constraint if ϵ is small enough. Using this h, we get

$$\int_a^b f(x)h(x)\,dx\geq\frac{C\epsilon}{2}>0.$$

This contradicts to our assumption. □

Thus, we get a necessary condition for y being a local minimum. That is y should satisfies

$$-\frac{d}{dx}L_{y'}(x,y,y')+L_y(x,y,y')=0$$

with the boundary condition

$$y(a) = y_0,\ y(b) = y_1.$$

The above equation is called the *Euler-Lagrange equation* for the functional J. The variational problem is transformed to solving a differential equation with certain boundary conditions.

Example 1. For the problem of minimizing arc length, the functional is

$$J(y) = \int_a^b \sqrt{1 + y'^2}\, dx,$$

where $y(a) = y_0, y(b) = y_1$. The corresponding Euler-Lagrange equation is

$$-\frac{d}{dx} L_{y'} = \frac{d}{dx}\left(\frac{y'}{\sqrt{1 + y'^2}}\right) = 0.$$

This yields

$$\frac{y'}{\sqrt{1 + y'^2}} = Const.$$

Solving y', we further get

$$y' = C \text{ (a constant)}.$$

Hence $y = Cx + D$. Applying boundary condition, we get

$$C = \frac{y_1 - y_0}{b - a}, D = \frac{by_0 - ay_1}{b - a}.$$

Thus, the minimal arc length curve is a straight line.

Example 2 In classical mechanics, we define the Lagrangian L to be

$$L(t, y, \dot{y}) := \frac{1}{2} m\dot{y}^2 - V(y),$$

where V is the potential. The corresponding Euler-Lagrange equation is

$$-\frac{d}{dt} m\dot{y} - V_y = 0.$$

This is exactly the Newton's law of motion, where $\partial L/\partial \dot{y} = m\dot{y} = p$ is the momentum and $\partial L/\partial y = -V_y$ is the force. This equation admits an time invariant quantity, namely the total energy is unchanged along physical trajectory. To see this, we multiply the above Newton's equation by $\dot{y}$. We get

$$m\ddot{y}\dot{y} = -V_y\dot{y}$$

This can be rewritten as

$$\frac{d}{dt}\left(\frac{1}{2} m\dot{y}^2 + V(y)\right) = 0.$$

Thus, we have

$$\frac{1}{2}m\dot{y}^2 + V(y) = E(aConst).$$

The quantity $\frac{1}{2}m\dot{y}^2 + V(y)$ is the total energy. The advantage of the existence of first integral is that the Euler-Lagrange equation is integrated once and the first integral is a first order equation, which is much easier to solve. To be precise, we can solve y' in terms of y from the above energy equality:

$$y' = \pm\sqrt{2(E - V(y))/m}$$

Uing separation of variable, we get

$$\frac{dy}{\sqrt{2(E - V(y))/m}} = \pm dt$$

This can be integrated to get $y(t)$.

Such a property is in general true for a Lagrangian which is independent of time. The invariant is called the first integral. We have the following theorem.

Theorem 3.5 (The first integral)**.** *If L is independent of x, then the quantity*

$$I(y, y') := -y'L_{y'}(y, y') + L(y, y')$$

is independent of x along the solution of the Euler-Largange equation.

Example: Barchistochrone The Barchistochrone problem is to minimize the travel time from $(0, 0)$ to $(a, -h)$. The functional of the travel time for a path $y(\cdot)$ connecting the above two points is given by

$$T(y) = \int_0^S \frac{ds}{v} = \int_0^a \frac{\sqrt{1 + y'^2}}{\sqrt{-2gy}}\, dx.$$

The Lagrangian

$$L(y, y') = \frac{\sqrt{1 + y'^2}}{\sqrt{-2gy}}$$

is independent of x. Thus, the solution admits the first integral which is independent of x:

$$\frac{\sqrt{1 + y'^2}}{\sqrt{-2gy}} - y'\left(\frac{y'}{\sqrt{1 + y'^2}\sqrt{-2gy}}\right) = Const.$$

which can be simplified to

$$y'^2 = \frac{1 + ky}{-ky}$$

where k is a constant. Using separation of variable

$$\frac{\sqrt{-ky}}{\sqrt{1 + ky}}dy = \pm dx.$$

We make a substitution:

$$y = -\frac{1}{k}\sin^2\frac{\phi}{2},$$

then the above differential equation becomes

$$\frac{\sin\frac{\phi}{2}}{\cos\frac{\phi}{2}}\frac{1}{k}\sin\frac{\phi}{2}\cos\frac{\phi}{2}d\phi = \pm dx$$

This yields

$$\pm dx = \frac{1}{k}\sin^2\frac{\phi}{2}d\phi = \frac{1}{2k}(1-\cos\phi)\,d\phi.$$

This leads to

$$x = \pm\frac{1}{2k}(\phi - \sin\phi) + C,$$

whereas we have parametrized

$$y = -\frac{1}{k}\sin^2\frac{\phi}{2} = \frac{1}{2k}(\cos\phi - 1)$$

This is the parametric form of a cycloid. The portion we want is to take

$$x = \frac{1}{2k}(\phi - \sin\phi).$$

Example In electrostatics, given a charge density function f in Ω, the boundary $\partial\Omega$ is a conductor. We are interested in the induced electric potential ϕ. The energy induced by f is $-\int f\phi\,dx$ and the energy induced by ϕ is $\int |\nabla\phi|^2/2\,dx$. The total energy is

$$\mathcal{E}[\phi] = \int (\frac{1}{2}|\nabla\phi|^2 - f\phi)\,dx.$$

The variation of $\mathcal{E}$ with respect to ϕ is

$$\begin{aligned}
\delta\mathcal{E}\cdot h &= \int_\Omega (\nabla\phi\cdot\nabla h - f\cdot h)\,dx \\
&= \int_\Omega (-\nabla^2\phi\cdot h - f\cdot h)\,dx + \int_\Omega \nabla\cdot(\nabla\phi\cdot h)\,dx \\
&= \int_\Omega (-\nabla^2\phi\cdot h - f\cdot h)\,dx + \int_{\partial\Omega} h\,\nabla\phi\cdot n\,dx
\end{aligned}$$

There are two kinds of natural boundary conditions:

1. **Dirichlet boundary condition:** We impose $\phi(x) = g(x)$ for $x \in \partial\Omega$. In this case, the admissible ϕ should satisfy this boundary. Its variation h should satisfies $h(x) = 0$ for $x \in \partial\Omega$. In this case, the variational of the energy is

$$\delta\mathcal{E}\cdot h = \int_\Omega (-\nabla^2\phi\cdot h - f\cdot h)\,dx$$

The Euler-Lagrange is

$$-\nabla^2\phi = f.$$

This together with the Dirichlet boundary condition

$$\phi(x) = g(x), x \in \partial\Omega$$

constitute the well-known Dirichlet problem. Indeed, solving this Dirichlet is equivalent to solving

$$\min_{\phi\in\mathcal{A}} \mathcal{E}[\phi],\ \mathcal{A} = \{\phi \in C^1(\Omega), \phi(x) = g(x), x \in \partial\Omega\}$$

We have seen one side of the equivalent. Indeed, if ϕ solves the Dirichlet problem, then for any $\psi \in \mathcal{A}$, we express $\psi = \phi + h$ with h vanishing on $\partial\Omega$. Then

$$\begin{aligned}
\mathcal{E}[\phi + h] - \mathcal{E}[\phi] &= \int_\Omega \frac{1}{2}\left(\nabla(\phi + h)\cdot\nabla(\phi + h) - |\nabla\phi|^2\right) - fh\,dx \\
&= \int_\Omega \left(\nabla\phi\cdot\nabla h + \frac{1}{2}|\nabla h|^2\right) - fh\,dx \\
&= \int_\Omega \left(-\nabla^2\phi\cdot h + \frac{1}{2}|\nabla h|^2\right) - fh\,dx + \int_{\partial\Omega} h\phi_n\,dx \\
&= \int_\Omega \left((-\nabla^2\phi - f)\cdot h + \frac{1}{2}|\nabla h|^2\right)\,dx \\
&= \int_\Omega \frac{1}{2}|\nabla h|^2\,dx \geq 0.
\end{aligned}$$

This shows that if ϕ solves the Dirichlet problem, ϕ is the minimum of $\mathcal{E}$ in $\mathcal{A}$.

2. **The Neumann boundary condition.** The second natural boundary condition is to prescribe $\nabla\phi(x)\cdot n = \sigma(x)$ on the boundary. In this case, σ is the surface charge. So, we should modify our energy functional to be

$$\mathcal{E}_1[\phi] = \int_\Omega (\frac{1}{2}|\nabla\phi|^2 - f\phi)\,dx - \int_{\partial\Omega}\sigma\phi\,dx.$$

Now, we choose the admissible class to be

$$\mathcal{A} = \{\phi \in C^1(\Omega)\}.$$

Its variation class is still the same $\mathcal{A}$, no restriction on the boundary. The variation of $\mathcal{E}$ with respect to a variation h now read

$$\delta\mathcal{E}.h = \int_\Omega (-\nabla^2\phi - f)\cdot h\,dx + \int_{\partial\Omega}(\phi_n - \sigma)\cdot h\,dx$$

We can first choose those h which are vanish on $\partial\Omega$. This leads to the Euler-Lagrange equation

$$-\nabla^2\phi(x) = f(x),\ \text{in } \Omega.$$

Next, we have

$$\int_{\partial\Omega} (\phi_n - \sigma) h \, dx = 0$$

for arbitrary function h. This leads to

$$\phi_n = \sigma \text{ on } \partial\Omega.$$

This PDE with the boundary condition above is called the Neumann problem.

Remark. The condition $y \in C^2$ in Lemma **??** is only for the classical solutions of the Euler-Lagrange equations. Indeed, the condition for having the functional J well-defined is weaker, say we only need $y \in C^1$. In this case, the Euler-Lagrange equation is still meaningful, but in *weak sense*. This means that the equation is valid when it is tested by smooth functions. More precisely, the Euler-Lagrange

$$-\frac{d}{dx} L_{y'}(x, y, y') + L_y(x, y, y') = 0$$

is valid if

$$\int_a^b \left[L_{y'}(x, y, y') \cdot h' + L_y(x, y, y') \cdot h \right] \, dx = 0,$$

for any smooth compact supported function h defined on (a, b). In the latter definition, we only need $y \in C^1$. The logic of the approach to this problem is that we find solution in weak class. Then if it is indeed a smooth function, we prove so-called the regularity result.

Homework You can show that if ϕ solves the Neumann problem, then ϕ is the minimum of the energy functional $\mathcal{E}_1$.

Homework

1. pp. 167: 7, 9, 13.
2. pp. 176: 8, 12, 14.

3.5 Lagrange Mechanics and Hamilton Mechanics

3.5.1 Noether's Theorem

To solve the Euler-Lagrange equation for problems arisen from mechanics, an important technique is to find invariants of the system. This will reduce the degree of freedom, or to reduce a high-order differential equation to a lower order one. There are two examples which are fundamental.

- The *first integral* is one of such examples. When the Lagrangian $L(x, \dot{x})$ is *independent of* t, then the quantity

$$I(x, \dot{x}) := \dot{x} \cdot \frac{\partial L}{\partial \dot{x}} - L.$$

is independent of t along physical trajectories. To see this, we differentiate I along a physical trajectory:

$$\begin{aligned}\frac{d}{dt}\left[\dot{x}L_{\dot{x}} - L\right] &= \ddot{x}L_{\dot{x}} + \dot{x}\frac{d}{dt}L_{\dot{x}} - L_x\dot{x} - L_{\dot{x}}\ddot{x} \\ &= \dot{x}\left(\frac{d}{dt}L_{\dot{x}} - L_x\right) = 0.\end{aligned}$$

- Suppose the Lagrangian $L(t, x, \dot{x})$ is *independent of x_i for some i*, then we have

$$\frac{d}{dt}L_{\dot{x}_i} = L_{x_i} = 0.$$

This means that the quantity

$$p_i := L_{\dot{x}_i}(t, x, \dot{x})$$

is invariant in time along physical trajectories.

In the latter example, the condition that L is independent x_i can be reformulated as that L is invariant under the group action: $g^s(x_1, .., x_i, ..) = (x_1, ..., x_i + s, ...)$. That is

$$L(x_1, ..., x_i + s, ..., \dot{x}_1, ..., \dot{x}_i, ...) = L(x_1, ..., x_i + s, ..., x_1, ..., \dot{x}_i, ...).$$

The mapping g^s maps $\mathbb{R}^n$ to $\mathbb{R}^n$ satisfying

$$g^s \circ g^t = g^{s+t},\ g^0 = id.$$

is a one-parameter of group on $\mathbb{R}^n$. The rotation R^s with axis n and rotating angle s is also a one-parameter family of group. If L is invariant under such group action, it also admits an invariant. This is the Noether theorem.

Theorem 3.6 (Noether)**.** *Let $g^s : M \to M$ be a group such that $L(g^s(x), g^s\dot{x})) = L(x, \dot{x})$ for all s. Let $\ell(x) = \frac{d}{ds}|_{s=0}g^s(x)$ be its generator. Then the quantity*

$$\frac{\partial L}{\partial \dot{x}}(x, \dot{x}) \cdot \ell(x)$$

is invariant along physical trajectory.

Proof. Let $\Phi(s, t) = g^s(x(t))$. By assumption, we have

$$\frac{d}{ds}L(\Phi(s, t), \dot{\Phi}(s, t)) = 0.$$

This gives

$$\frac{\partial L}{\partial \dot{x}}\frac{d}{dt}\Phi'(s, t) + \frac{\partial L}{\partial x}\Phi'(s, t) = 0.$$

Here, we denote d/ds by '.

On the other hand, $\Phi(s,\cdot)$ satisfies the Euler-Lagrange equation:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0.$$

Taking inner product with $\Phi'(s,t)$, from these two, we obtain

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}} \cdot \Phi'(s,t)\right) = 0.$$

In particular, $s = 0$ is the case we look for. □

Remarks

1. Suppose the trajectory $g^s(x)$ is tranversal to the hyperplane $(0, x^2, \cdots, x^n)$ locally. Let us denote $(x^2, \cdots, x^n)$ by x'. Then we can make a local coordinate transformation:

   $$x(s, x') = g^s(0, x').$$

   Let us call the new coordinate $q = (s, x')$. Then this transformation is locally invertible. With this, then we see in the new coordinate system, the Lagrangian

   $$L(q, \dot{q}) = L(g^s(0,x), \dot{g}^s(0,x))$$

   is independent of s, which is q^1. Therefore, the quantity

   $$\partial L/\partial \dot{q}^1$$

   is invariant. That is,

   $$\frac{\partial L}{\partial \dot{q}^1} = \frac{\partial L}{\partial \dot{x}}\frac{g^s(0,x')}{ds} \text{ (TOBE PROVEN)}$$

   is invariant in time.

Examples (Rotational symmetry and conservation of angular momentum) Consider the Lagrangian $L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}|\dot{\mathbf{x}}|^2 - \Phi(|\mathbf{x}|)$. The system does not change under the rotation: $\mathbf{x} \mapsto R^s\mathbf{x}$, where R^s is a rotation with axis $\mathbf{n}$ and angle s. To find the infinitesimal generator of $R^s\mathbf{x}$, suppose R^s is a rotation with axis n by an angle s, let $\mathbf{y}(s) = R^s\mathbf{x}$. then $\mathbf{y}(s)$ satisfies

$$\frac{d\mathbf{y}}{ds} = \mathbf{n} \times \mathbf{y},\ \mathbf{y}(0) = \mathbf{x}.$$

Thus, the infinitesimal generator of R^s, which is $d\mathbf{y}/ds(0)$ is

$$\frac{dR^s\mathbf{x}}{ds} = \mathbf{n} \times \mathbf{x}.$$

According to Noether theorem, the quantity

$$\frac{\partial \mathbf{L}}{\partial \dot{\mathbf{x}}} \cdot (\mathbf{n} \times \mathbf{x})$$

is invariant in time. That is

$$\mathbf{p} \cdot \mathbf{n} \times \mathbf{x} = \mathbf{n} \cdot (\mathbf{x} \times \mathbf{p}) = \mathbf{n} \cdot \mathbf{L}.$$

Here, $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ is the angular momentum. Since we can choose three independent $\mathbf{n}$'s, thus, $\mathbf{L} = (L_x, L_y, L_z)$ are the three invariants.

Centrally directed force and conservation of angular momentum The motion of planets or stars can be viewed as a particle moving under a centrally directed field of force:

$$\mathbf{F} = F(r)\hat{\mathbf{e}}_r,$$

where r is the distance from the star to the center, $\mathbf{r}$ is the position vector from the center to the star and

$$\hat{\mathbf{e}}_r = \frac{\mathbf{r}}{r},$$

is the unit director. The equation of motion of the star is

$$\ddot{\mathbf{r}} = F(r)\hat{\mathbf{e}}_r.$$

Define the angular momentum $\mathbf{L} = \mathbf{r} \times \dot{\mathbf{r}}$. We find

$$\frac{d\mathbf{L}}{dt} = \dot{\mathbf{r}} \times \dot{\mathbf{r}} + \mathbf{r} \times \ddot{\mathbf{r}} = F(r)\mathbf{r} \times \hat{\mathbf{e}}_r = 0.$$

Hence , $\mathbf{L}$ is a constant. A function in the state space $(\mathbf{r}, \dot{\mathbf{r}})$ is called an integral if it is unchanged along any orbits. *The integrals can be used to reduce number of unknowns of the system.* The conservation of angular momentum provides us three integrals. Let us write $\mathbf{L} = L\mathbf{n}$ where $L = |\mathbf{L}|$ and $\mathbf{n}$ is a unit vector. The position vector $\mathbf{r}$ and the velocity $\dot{\mathbf{r}}$ always lie on the plane which is perpendicular to $\mathbf{n}$. This plane is called the orbital plane. We use polar coordinates (r, θ) on this plane. Thus, by using the integrals $\mathbf{n}$, which has two parameters, we can reduce the number of unknowns from 6 to 4, that is, from $(\mathbf{r}, \dot{\mathbf{r}})$ to $(r, \theta, \dot{r}, \dot{\theta})$. To find the equation of motion on this plane, we express

$$\mathbf{r} = r\hat{\mathbf{e}}_r = r(\cos\theta, \sin\theta).$$

Define

$$\hat{\mathbf{e}}_\theta := (-\sin\theta, \cos\theta)$$

be the unit vector perpendicular to $\hat{\mathbf{e}}_r$. Then a particle motion on a plane with trajectory $\mathbf{r}(t)$ has the following velocity

$$\dot{\mathbf{r}} = \dot{r}\hat{\mathbf{e}}_r + r\dot{\hat{\mathbf{e}}}_r = \dot{r}\hat{\mathbf{e}}_r + r\dot{\theta}\hat{\mathbf{e}}_\theta.$$

where $\dot{r}$ is the radial speed and $r\dot{\theta}$ is the circular speed. Here, we have used

$$\dot{\hat{\mathbf{e}}}_r = \frac{d}{dt}(\cos\theta, \sin\theta) = \dot{\theta}\hat{\mathbf{e}}_\theta.$$

The acceleration is

$$\begin{aligned}\ddot{\mathbf{r}} &= \ddot{r}\hat{\mathbf{e}}_r + \dot{r}\dot{\hat{\mathbf{e}}}_r + \dot{r}\dot{\theta}\hat{\mathbf{e}}_\theta + r\ddot{\theta}\hat{\mathbf{e}}_\theta + r\dot{\theta}\dot{\hat{\mathbf{e}}}_\theta \\ &= (\ddot{r} - r\dot{\theta}^2)\hat{\mathbf{e}}_r + (2\dot{r}\dot{\theta} + r\ddot{\theta})\hat{\mathbf{e}}_\theta.\end{aligned}$$

Here, we have used $\dot{\hat{\mathbf{e}}}_\theta = -\hat{\mathbf{e}}_r\dot{\theta}$. In this formula, $\ddot{r}$ is the radial acceleration, and $-r\dot{\theta}^2$ is the centripetal acceleration. The term

$$r(2\dot{r}\dot{\theta} + r\ddot{\theta}) = \frac{d}{dt}(r^2\dot{\theta})$$

is the change of angular momentum. Indeed, the angular momentum is

$$\mathbf{L} = \mathbf{r} \times \dot{\mathbf{r}} = r\hat{\mathbf{e}}_r \times (\dot{r}\hat{\mathbf{e}}_r + r\dot{\theta}\hat{\mathbf{e}}_\theta) = r^2\dot{\theta}\mathbf{n}.$$

The equation of motion $\ddot{\mathbf{r}} = F(r)\hat{\mathbf{e}}_r$ gives

$$\ddot{r} - r\dot{\theta}^2 = F(r), \tag{3.1}$$

$$\frac{d}{dt}(r^2\dot{\theta}) = 0. \tag{3.2}$$

These are the two second-order equations for the unknowns $(r, \theta, \dot{r}, \dot{\theta})$. The θ equation (3.2) can be integrated and gives the conservation of angular momentum

$$r^2\dot{\theta} = \text{ constant } = L. \tag{3.3}$$

If we prescribe an L, the trajectory lies on the set

$$\{(r, \theta, \dot{r}, \dot{\theta}) \,|\, \dot{\theta} = L/r^2\}.$$

We may project this set to the $(r, \theta, \dot{r})$-space and our unknowns now are reduced to $(r, \theta, \dot{r})$. The equations of motion in this space are (3.1) and (3.3).

The integral L can be used to eliminate $\dot{\theta}$ from the first equation. We get

$$\ddot{r} = F(r) + \frac{L^2}{r^3}, \tag{3.4}$$

where the second term on the right-hand side is the centrifugal force. Notice that this equation is independent of θ. Thus, given initial data $(r_0, \theta_0, \dot{r}_0)$ at time $t = 0$, we can find $r(t)$ and $\dot{r}(t)$ from (3.4) by using $(r_0, \dot{r}_0)$ only. We can then use $r^2\dot{\theta} = L$ to find $\theta(t)$:

$$\theta(t) = \theta_0 + \int_0^t \frac{L}{r(t)^2}\, dt.$$

The equation (3.4) can be solved by the energy method. We multiply (3.4) by $\dot{r}$ on both sides to obtain

$$\frac{d}{dt}\left(\frac{1}{2}\dot{r}^2 + \Phi(r) + \frac{1}{2}\frac{L^2}{r^2}\right) = 0,$$

where Φ with $\Phi'(r) = -F(r)$ is the potential. We obtain the law of conservation of energy:

$$\frac{1}{2}\dot{r}^2 + \Phi(r) + \frac{1}{2}\frac{L^2}{r^2} = \text{ constant } = E. \tag{3.5}$$

This energy is another integral. A prescribed energy E defines a surface in the $(r, \theta, \dot{r})$-space. Since the energy $\frac{1}{2}\dot{r}^2 + \Phi(r) + \frac{1}{2}\frac{L^2}{r^2}$ is *independent of* θ (a consequence of centrally forcing), this energy surface is a *cylinder* $C_E \times \mathbb{R}_\theta$, where C_E is the curve defined by (3.5) on the phase plane r-$\dot{r}$.

The equation of motion with a prescribed energy E is

$$\frac{dr}{dt} = \pm\sqrt{2(E - \Phi(r)) - \frac{L^2}{r^2}}. \tag{3.6}$$

It is symmetric about the r-axis. Let us suppose that r_1 and r_2 ($r_1 < r_2$) are two roots of the right-hand side of the above equation:

$$2(E - \Phi(r)) - \frac{L^2}{r^2} = 0$$

and no other root in between. Then the curve defined by (3.6) is a closed curve connecting $(r_1, 0)$ and $(r_2, 0)$. The radial period is defined to be the time the particle travels from $(r_1, 0)$ to $(r_2, 0)$ and back. That is,

$$T_r = 2\int_{r_1}^{r_2} \frac{dr}{\sqrt{2(E - \Phi(r)) - L^2/r^2}}.$$

Next, we shall represent this orbit on the orbital plane (r, θ). From the conservation of angular momentum

$$\frac{d\theta}{dt} = \frac{L}{r^2} \neq 0,$$

we can invert the function $\theta(t)$ and use θ as our independent variable instead of the time variable t. The chain rule gives

$$\frac{d}{dt} = \frac{L}{r^2}\frac{d}{d\theta}.$$

The equation of motion now reads

$$\frac{L}{r^2}\frac{d}{d\theta}\left(\frac{L}{r^2}\frac{dr}{d\theta}\right) - \frac{L^2}{r^3} = F(r). \tag{3.7}$$

The energy equation (3.6) becomes

$$\frac{dr}{d\theta} = \pm\frac{r^2}{L}\sqrt{2(E - \Phi(r)) - \frac{L^2}{r^2}}. \tag{3.8}$$

We can integrate this equation by separation of variable to obtain the trajectory $r = r(\theta)$ in the orbital plane. Sometimes, it is convinient to introduce $u = 1/r$ to simplify the equation (3.7):

$$\frac{d^2u}{d\theta^2} + u = -\frac{F\left(\frac{1}{u}\right)}{L^2u^2}. \tag{3.9}$$

Multiplying $du/d\theta$ on both sides, we get the conservation of energy in u variable:

$$\frac{1}{2}\left(\frac{du}{d\theta}\right)^2 + \frac{u^2}{2} + \frac{\Phi}{L^2} = \frac{E}{L^2}. \tag{3.10}$$

Homework When the potential is a polynomial of $u = 1/r$, in some cases, (3.10) can be integrated to get an exact form.

1. Solve equation (3.10) with $\Phi(r) = -G/r$.

Next, we check the variation of θ as r changes for a radial period. The roots of the right-hand side of (3.8) are equilibria. From (3.6) and (3.8), we see that $dr/d\theta = 0$ if and only if $dr/dt = 0$. Hence these roots are exactly r_1 and r_2 in (3.6). The orbit $r = r(\theta)$ defined by (3.6) must lie between its two extremals where $dr/d\theta = 0$. That is, the orbit $r = r(\theta)$ must lie between the inner circle $r \equiv r_1$ and the outer circle $r \equiv r_2$. The inner radius r_1 is called the pericenter distance, whereas r_2 the apocenter distance.

As the particle travels from pericenter to apocenter and back (i.e. one radial period T_r), the azimuthal angle θ increases by an amount

$$\begin{aligned} \Delta\theta &= 2\int_{r_1}^{r_2} \frac{d\theta}{dr} dr = 2\int_{r_1}^{r_2} \frac{L}{r^2}\frac{dt}{dr}\, dr \\ &= 2L\int_{r_1}^{r_2} \frac{dr}{r^2\sqrt{2(E-\Phi(r)) - L^2/r^2}}. \end{aligned}$$

The azimuthal period is defined as the time that θ varies 2π:

$$T_\theta := \frac{2\pi}{\Delta\theta} T_r.$$

In general, $2\pi/\Delta\theta$ is not a rational number. Hence, the orbit may not be closed.

3.6 Variational Problems with Constraints

In variational problems, there are usually accompanied with sopme constraints.

Examples

1. **Isoperimeteric problem** A typical problem is the *isoperimetric problem*, which states that find the maximum area enclosed by a closed curve with prescribed perimeter. Suppose the curved is described by $(x(t), y(t))$, $0 \le t \le 1$ with $x(1) = x(0)$ and $y(1) = y(0)$. The arc length is

   $$\mathcal{W}(x, y) = \int_0^1 \sqrt{\dot{x}(t)^2 + \dot{y}(t)^2}$$

   The area it encloses is

   $$\mathcal{J}(x, y) = \frac{1}{2}\int_0^t y(t)\dot{x}(t) - x(t)\dot{y}(t)\, dt$$

   The problem is

   $$\max \mathcal{J}(x, y) \text{ subject to } \mathcal{W}(x, y) = \ell.$$

2. **Hanging Rope problem** A rope given by $y(x)$, $a \le x \le b$ hangs two end points (a, y_0) and (b, y_1). Suppose the rope has length ℓ and with density $\rho(x)$. Suppose the rope is in equilibrium, then it minimizes its potential energy, which is

$$\mathcal{J}(y) = \int_0^\ell \rho g y \, ds = \int_a^b \rho g y \sqrt{1 + y'^2} \, dx.$$

The rope is subject to the length constraint

$$\mathcal{W}(y) = \int_a^b \sqrt{1 + y'^2} \, dx = \ell.$$

In dealing with such problems, it is very much like the optimization in finite dimension with constraints. Let us start with two dimensional examples. Suppose we want to minimize $f(x, y)$ with constraint $g(x, y) = 0$. The method of Lagrange multiplier states that a necessary condition for (x_0, y_0) being such a solution is that there exists a constant λ_0 such that (x_0, y_0, λ_0) is the extremal of the un-cosntraint function $F(x, y, \lambda) := f(x, y) + \lambda g(x, y)$. That is, (x_0, y_0, λ_0) solves

$$\frac{\partial F}{\partial x} = 0, \ \frac{\partial F}{\partial y} = 0, \ \frac{\partial F}{\partial \lambda} = 0.$$

For variational problem, we have much the same. We can reduce the problem to the above two dimensional problem. Let us consider a variational problem in an abstract form:

$$\min \mathcal{J}(y) \text{ subject } \mathcal{W}(y) = 0$$

in some admissible class $\mathcal{A} = \{y | y(a) = y_0, y(b) = y_1\}$ in some function space. We consider two-parameter variations

$$z(x) = y(x) + \epsilon_1 h_1(x) + \epsilon_2 h_2(x).$$

the variation h_i should satisfy the boundary conditions: $h_i(a) = h_i(b) = 0$.. For arbitrarily chosen such variations h_i, we should also require ϵ_i satisfying

$$W(\epsilon_1, \epsilon_2) = \mathcal{W}(y + \epsilon_1 h_1 + \epsilon_2 h_2) = 0.$$

Such ℓ_i can be found in general by the implicit function theorem. On the variational subspaces spanned by h_i, $i = 1, 2$, the functional $\mathcal{J}$ becomes

$$J(\epsilon_1, \epsilon_2) := \mathcal{J}(y + \epsilon_1 h_1 + \epsilon_2 h_2).$$

Thus the original problem is reduced to

$$\min J(\epsilon_1, \epsilon_2) \text{ subject to } W(\epsilon_1, \epsilon_2).$$

on this variational subspace. By the method of Lagrange multiplier method, there exists a λ such that an extremal of the original problem solves the unconstraint optimization problem $\min J + \lambda W$.

This leads to three equations

$$\begin{aligned} 0 &= \frac{\partial}{\partial \epsilon_1}(J + \lambda W) = \left(\frac{\delta \mathcal{J}}{\delta y} + \lambda \frac{\delta \mathcal{W}}{\delta y}\right) \cdot h_1 \\ 0 &= \frac{\partial}{\partial \epsilon_2}(J + \lambda W) = \left(\frac{\delta \mathcal{J}}{\delta y} + \lambda \frac{\delta \mathcal{W}}{\delta y}\right) \cdot h_2 \\ 0 &= \frac{\partial}{\partial \lambda}(J + \lambda W) = \mathcal{W}(y) \end{aligned}$$

The first two conditions give the same Euler-Lgrange equation:

$$\frac{\delta \mathcal{J}}{\delta y} + \lambda \frac{\delta \mathcal{W}}{\delta y} = 0.$$

Thus, we obtain that if y_0 is an extremal of $\mathcal{J}$ subject to the constraint $\mathcal{W}(y) = 0$, then there exists a constant λ_0 such that (y_0, λ_0) is the extremal of the functional $\mathcal{J}(y) + \lambda \mathcal{W}(y)$ with respect to (y, λ).

Examples

1. **Hanging rope problem** By the method of Lagrangian multiplier, we consider the extremal problem of new Lagragian

   $$L(y, y', \lambda) = \rho g y \sqrt{1 + y'^2} + \lambda \sqrt{1 + y'^2}$$

   The Lagragian is independent of x, thus it admits the first integral $L - y' L_{y'} = C$, or

   $$(\rho g y + \lambda) \left(\sqrt{1 + y'^2} - \frac{y'^2}{\sqrt{1 + y'^2}} \right) = C.$$

   Solving for y' gives

   $$y' = \pm \frac{1}{C} \sqrt{(\rho g y + \lambda)^2 - C^2}$$

   Using method of separation of variable, we get

   $$\frac{dy}{\sqrt{(\rho g y + \lambda)^2 - C^2}} = \pm \frac{dx}{C}$$

   Change variable $u = \rho g y + \lambda$, we get

   $$\frac{1}{\rho g} \cosh^{-1}\left(\frac{u}{C}\right) = \pm \frac{x}{C} + C_1.$$

   Hence

   $$y = -\frac{\lambda}{\rho g} + \frac{C}{\rho g} \cosh\left(\frac{\rho g x}{C} + C_2\right).$$

   The cosntrants C, C_2 and the Lagrange multiplier λ are then determined by the two bopundary conditions and the cosntraint. The shape of this hanging rope is called a *catenary*.

Homeworks

- pp. 203: 4, 6, 7.

3.7 Variation Formulation of Elasticity

3.7.1 Flow maps

Lagrangian and Eulerian Coordinates We will derive a unified theory for both fluid and elasticity. We shall use the following notations.

- Let $x(\cdot, X)$ be the particle path of a piece of material (or fluid) with position X initially. X is called the Lagrangian coordinate, whereas x the Eulerian coordinate. It is assumed that the mapping satisfies $x(0, X) = X$.

- Ω_t: the region occupied by the material at time t. Thus, the mapping $x(t, \cdot) : \Omega_0 \to \Omega_t$. Or the mapping
$$x(\cdot, \cdot) : [0, T] \times \Omega_0 \to \cup_{t\in[0,T]}\Omega_t.$$
In most of case, we assume the whole region occupied by the material is unchanged. We denote this wholeregion by D. Thus, $x : [0, T] \times D \to D$. We always assume $x(t, \cdot)$ is 1-1 and onto from D to D.

- The deformation matrix $F := \frac{\partial x}{\partial X}$, or $F^i_\alpha(t, X) = \partial x^i(t, X)/\partial X^\alpha$.

- The Jacobian $J := \det F$. We have $dx = JdX$.

- The particle velocity is defined to be $\dot{x}(t, X)$. We shall use dot for the time derivative with the Lagrangian coordinate fixed.

- Internal energy W. The deformation F stores an internal energy W in the material. It is due to the strenching between atoms. This internal energy W is assumed to be a function of F.

  Examples

  - Hook's law:
  $$W(F) = \frac{k}{2}\sum |F^i_\alpha|^2 = \frac{k}{2}tr(F^TF).$$
  - St. Venant-Kirchhoff: we assume small variation, i.e. $x(t, X) - X$ is small. Let $E = \frac{1}{2}(F^TF - I)$.
  $$W(F) = \frac{\lambda}{2}(trE)^2 + \mu tr(E^2).$$

- The stress tensor. The derivative $P = W'(F)$ is called the Piola stress tensor. It is a surface force in Lagrange coordinate system.

3.7.2 Variation of Functionals w.r.t. the flow maps

Functionals Given a flow map $x(\cdot,\cdot)$, we define its kinetic energy, internal energy, action, total energy in the Lagrange coordinate as the follows.

- Kinetic energy: $\int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t,X)|^2\,dX$
- Internal energy: $\int_{\Omega_0} W(F)\,dX$
- Action:
$$A[x] = \int_0^T \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t,X)|^2 - W(F)\,dX\,dt$$
- Total energy:
$$E[x(t)] = \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t,X)|^2 + W(F)\,dX.$$

Variation w.r.t. flow maps We shall study the variation of these functionals with respect to the flow map $x(\cdot,\cdot)$. Let us perturb the flow map by $x_\epsilon(t,X)$ with $x_0(t,X) = x(t,X)$, the original unperturbed one. We call
$$\delta x(t,X) := \frac{\partial}{\partial\epsilon}|_{\epsilon=0} x_\epsilon(t,X),$$
the variation of the flow map $x(\cdot,\cdot)$. We write the variation of x by δx. The variation of a functional $I[x]$ in the direction of δx means that
$$\delta I[x]\cdot\delta x := \frac{d}{d\epsilon}|_{\epsilon=0} I[x_\epsilon].$$
Since, for small ϵ, $x_\epsilon(t,\cdot)$ are flow maps, its variation
$$\delta x(t,X) = \lim_{\epsilon\to 0}\frac{x_\epsilon - x_0}{\epsilon}$$
is an infinitesimal variation of position, thus, can be called a pseudo-velocity. Let us thus define the corresponding pseudo-velocity in the Eulerian coordinate as
$$v(t,x(t,X)) = \delta x(t,X).$$

- $\delta F = (\nabla v)F$, where ∇ is the abbreviation of ∇_x. From $\delta x(t,X) = v(t,x(t,X))$, we differentiate in X to get
$$\frac{\partial \delta x_i}{\partial X_j} = \frac{\partial v_i}{\partial x_k}\frac{\partial x_k}{\partial X_j}$$
Interchange ∂ and δ operators, we get $\delta F = (\nabla v)F$.
- Let $J = \det F$, then
$$\delta J = tr\left((\delta F)F^{-1}\right)J.$$
This follows from the following lemma.

Lemma 3.2. *Let $A(\epsilon)$ be a smooth $n \times n$ matrix-valued function. Then*

$$\frac{d}{d\epsilon}\det(A) = tr(\dot{A}A^{-1})\det(A)$$

Proof. We write $A = (a_{ij})$. First, we recall the expansion formula of $\det A$:

$$\sum_k a_{ik}A_{jk} = (\det A)\delta_{ij}$$

where A_{ij} is the signed cofactor of A at (i, j). That is, $A(cofA)^T = (\det A)I$.
We claim that $\partial \det(A)/\partial a_{ij} = A_{ij}$, To see that, we write $\det A$ as

$$\det(A) = \sum_k a_{ik}A_{ik},$$

and notice that A_{ik} does not involve a_{ij} for all k. Thus,

$$\frac{\partial \det A}{\partial a_{ij}} = A_{ij}.$$

Next,

$$\begin{aligned}\frac{d}{d\epsilon}\det A &= \sum_{ij}\frac{da_{ij}}{d\epsilon}\frac{\partial \det(A)}{\partial a_{ij}} = \sum_{ij}\dot{a}_{ij}A_{ij} = \sum_{ij}(\dot{A})_{ij}((cofA)^T)_{ij} \\ &= \sum_{ij}(\dot{A})_{ij}(A^{-1})_{ij}\det A = tr(\dot{A}A^{-1})\det A\end{aligned}$$

□

3.7.3 Equation of Motion

We shall take variation of action w.r.t. flow map (position). This will give us the equation of motion

Lagrange formulation. We take the variation δx satisfying $\delta x(t, X) = 0$ for $t = 0$ and $t = T$. We can take integration by part for t.

$$\begin{aligned}\delta A[x]\cdot\delta x &= \int_0^T\int_{\Omega_0}\left(\rho_0(X)\dot{x}(t,X)\cdot\delta\dot{x} - W'(F)\delta F\right)\,dX\,dt \\ &= \int_0^T\int_{\Omega_0}\left(-\frac{d}{dt}\rho_0(X)\dot{x}(t,X)\cdot\delta x - W'(F)\frac{\delta\partial x}{\partial X}\right)\,dX\,dt \\ &= \int_0^T\int_{\Omega_0}\left(-\frac{d}{dt}\rho_0(X)\dot{x}(t,X)\cdot\delta x + \left(\frac{\partial}{\partial X}W'(F)\right)\cdot\delta x\right)\,dX\,dt\end{aligned}$$

Here, we also choose $W'(F)\delta x \cdot n = 0$ on the boundary of Ω_0 so that no boundary terms show up in the integration-by-part for the integration in X over Ω_0. This leads to the Euler-Lagrange equation

$$\rho_0(X)\ddot{x}(t,X) = \nabla_X \cdot P\left(\frac{\partial x}{\partial X}\right).$$

Here, $P = W'(F)$ is the Piola stress tensor. In component form,

$$P^i_\alpha = \frac{\partial W}{\partial X^i_\alpha},\ (\nabla_X \cdot P)^i = \frac{\partial}{\partial X^\alpha} P^i_\alpha.$$

This is the equation of motion for an elastic material in Lagrange coordinate system.

We can also use the variable $u(t,X) := \dot{x}(t,X)$ and $F(t,X) = \frac{\partial x}{\partial X}(t,X)$ as the new unknowns to write the above equations as a first-order system. Notice that the velocity $u(t,X)$ is in Lagrange coordinate in this formulation. The equation of motion is

$$\rho_0(X)\dot{u}(t,X) = \nabla_X \cdot P(F).$$

By differentiate $\dot{x}(t,X) = u(t,X)$, we obtain the equation for F is

$$\dot{F}_{ij} = \frac{\partial u_i}{\partial X_j}(t,X).$$

Two special cases:

1. One dimension: In one dimension, let us call $v = F^1_1 - 1$ and $P(f^1_1) = \sigma(v)$. Then the equation of motion are

$$\begin{aligned} \rho_0(X)u_t &= \sigma(v)_X \\ v_t &= u_X \end{aligned}$$

   Such an equation is a 2×2 hyperbolic system. The stress $\sigma(v)$ satisfies $\sigma'(v) > 0$, but is a nonvex function of v in general. A shock wave attached to a rarefaction wave can be found.

2. Linear elasticity: In the Hook's case where $W(F) = \frac{k}{2}|F|^2$, the stress is $P(F) = kF$. The equation of motion becomes

$$\begin{aligned} \rho_0(X)u_t &= k\nabla_X \cdot F \\ F_t &= \nabla_X u \end{aligned}$$

   Eliminating F, we get

$$\rho_0(X)u_{tt} = k\nabla^2_X u$$

   This is the wave equation.