

计算物理

Lecture 11

傅子文

fuziwen@scu.edu.cn



Today's lecture

- Challenges in numerical integration
 - Using a change of variables
 - Dealing with singularities & improper integrals
- Multidimensional integration

Change of variables: motivation

- Romberg integration works especially well when $f'(a)=f'(b)$ since the first error term must cancel

$$\int_a^b f(x)dx = \frac{h}{2} [f(a) + f(b)] + h \sum_{i=1}^{n-1} f(a + ih)$$

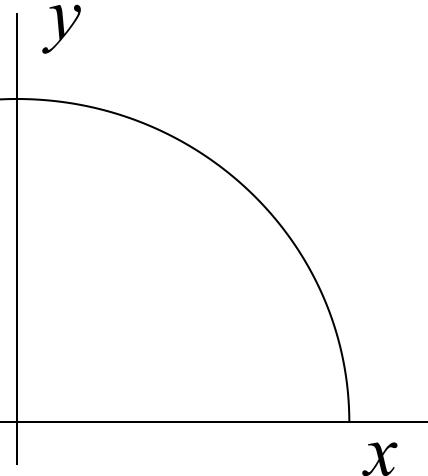
$$+ \boxed{\frac{h^2}{12} [f'(a) - f'(b)]}$$

$$+ \frac{h^4}{720} [f'''(a) - f'''(b)] + \dots$$

Euler-Maclaurin integration rule.

Change of variables: motivation

However, if derivatives become infinite at the end points there can be trouble converging



Consider $f(x) = \sqrt{1 - x^2}$,

Area of half circle :

$$A = \int_{-1}^1 \sqrt{1 - x^2} dx$$

$$\text{But } f'(x) = -\frac{x}{\sqrt{1 - x^2}} \rightarrow \infty$$

for $x = \pm 1$

In fact *all* derivatives are ∞ at ± 1

- so error is not determined by the power of h !

Apply a change of variables

Let $x = \cos\theta$, $\Rightarrow \sqrt{1-x^2} = \sin\theta$, and $dx = -\sin\theta d\theta$

At $x = 1$, we have $\theta = 0$

At $x = -1$, we have $\theta = \pi$

$$\therefore A = \int_{-1}^1 \sqrt{1-x^2} dx = - \int_{\pi}^0 \sin^2 \theta d\theta = \int_0^{\pi} \sin^2 \theta d\theta \quad (1)$$

Derivatives are now:

$$f'(\theta) = 2\sin\theta \cos\theta, \text{ and } f'(0) = f'(\pi) = 0$$

$$f''(\theta) = 2\cos 2\theta,$$

$$\text{so } f'''(\theta) = -4\sin 2\theta, \text{ and } f'''(0) = f'''(\pi) = 0$$

- All odd derivatives are zero – we can expect the trapezoid rule to be very accurate!
 - In fact it gives the exact answer with just 2 zones!

Check for convergence: Romberg Ratio

- The Romberg integrator needs to know whether things are converging or not
- Define the Romberg ratio:

$$Rt_j = \frac{R_{j-1,1} - R_{j,1}}{R_{j,1} - R_{j+1,1}} = \frac{\text{error at step } j}{\text{error at step } j+1}$$
$$\approx \frac{h_{j-1}^2 - (h_{j-1}^2 / 4)}{(h_{j-1}^2 / 4) - (h_{j-1}^2 / 16)} \sim 4$$

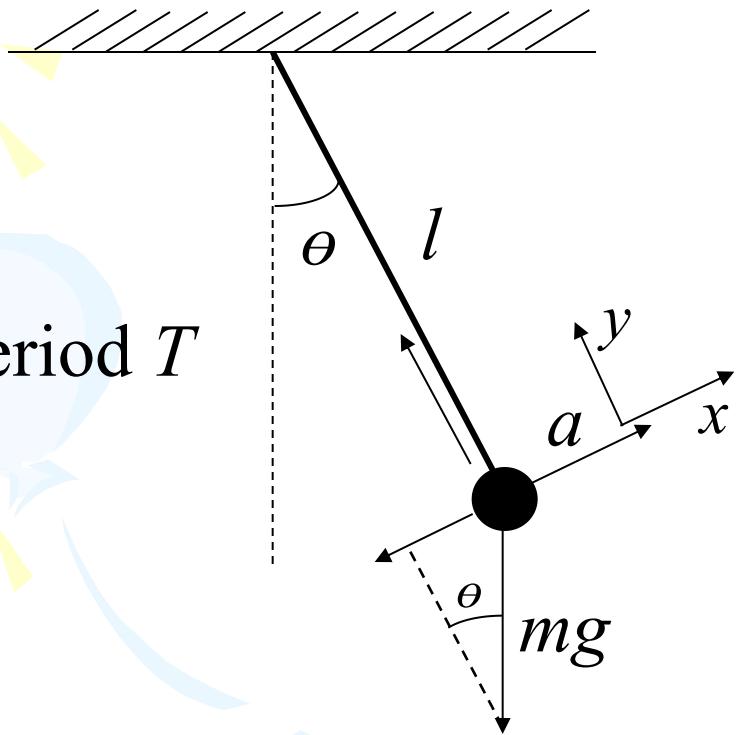
- So provided this ratio stays around 4 things are converging as they should
- If $Rt_j < 3.5$ (say) then that is a signal things are not converging and we need to check some things...

Check derivatives

- First thing to check is the first derivatives at $x=a$ & $x=b$
 - If large or infinite then a change of variables is probably necessary
- It is possible that you may hit a point where $f'(a), f'(b), f''(a), f''(b)$ are still well behaved but convergence is slow
 - In this case you force your integrator to proceed but keep a check on the interim results
 - Eventually if there is convergence you will get back to a Romberg ratio of $Rt_j \sim 4$

Example: Pendulum without small angle approximation

Period T



- Along x direction:

$$-mg \sin \theta = ma$$

Since $dx = ld\theta$, we get

$$a = \frac{d^2 x}{dt^2} = l \frac{d^2 \theta}{dt^2}$$

$$\Rightarrow \frac{d^2 \theta}{dt^2} = -\frac{g}{l} \sin \theta \quad (1)$$

Note under small angle approx. $\sin \theta \rightarrow \theta$, to give a solution:

$$\theta(t) = \theta_0 \cos \sqrt{\frac{g}{l}} t \equiv \theta_0 \cos \omega t \quad \text{where } \omega = \sqrt{\frac{g}{l}}$$

Rewriting as an integral

- Eqn (1) is a second order ODE which we could solve using a numerical ODE solver
- However we can translate this particular problem into an integral as follows:

Multiply (1) by $\dot{\theta}$

$$\Rightarrow \dot{\theta}\ddot{\theta} = -\frac{g}{l}\dot{\theta}\sin\theta$$

$$\Rightarrow \int \dot{\theta} \frac{d\dot{\theta}}{dt} dt = -\frac{g}{l} \int \sin\theta \frac{d\theta}{dt} dt$$

cancel dt 's & integrate wrt $\dot{\theta}, \theta$

$$\Rightarrow \frac{1}{2}\dot{\theta}^2 = \frac{1}{2}\left(\frac{d\theta}{dt}\right)^2 = \frac{g}{l}\cos\theta + c$$

Further manipulation

We can establish the constant c by imposing that

at $t = 0$, $\theta = \theta_0$, $\dot{\theta} = 0$ hence $c = -\frac{g}{l} \cos \theta_0$

Substitute for c and take square roots to get

$$\frac{d\theta}{dt} = \sqrt{\frac{2g}{l} (\cos \theta - \cos \theta_0)}$$
$$\Rightarrow dt = \sqrt{\frac{l}{2g}} \frac{d\theta}{\sqrt{\cos \theta - \cos \theta_0}}$$

Since we set $\theta = \theta_0$ at $t = 0$, the period, T , must be 4 times the time taken to go from $\theta = 0$ to $\theta = \theta_0$.

$$\therefore T = 4 \int_{t=0}^{t=\theta_0} dt = 4 \sqrt{\frac{l}{2g}} \int_0^{\theta_0} \frac{d\theta}{\sqrt{\cos \theta - \cos \theta_0}} \quad (2)$$

Immediate problems

- This is an *elliptic integral of the first kind* and must be evaluated numerically – however the upper limit produces a singularity so change variables:

We first rearrange using the trig identity

$$\cos \theta = 1 - 2 \sin^2(\theta / 2)$$

$$\Rightarrow \cos \theta - \cos \theta_0 = 2[\sin^2(\theta_0 / 2) - \sin^2(\theta / 2)],$$

so we now have

$$T = 4 \sqrt{\frac{l}{g}} \int_0^{\theta_0} \frac{d\theta}{2\sqrt{\sin^2(\theta_0 / 2) - \sin^2(\theta / 2)}} \quad (2)$$

We next set $\sin \xi = \frac{\sin(\theta / 2)}{\sin(\theta_0 / 2)}$

Change of variables to x

- Here are all the steps:

Setting $\sin \xi = \frac{\sin(\theta/2)}{\sin(\theta_0/2)}$ gives

at $\theta = 0$, $\sin \xi = 0 \Rightarrow \xi = 0$

at $\theta = \theta_0$, $\sin \xi = 1 \Rightarrow \xi = \frac{\pi}{2}$

and for the differential substitution $\cos \xi d\xi = \frac{\cos(\theta/2)}{\sin(\theta_0/2)} \frac{d\theta}{2}$

$$\Rightarrow d\theta = \frac{2\sin(\theta_0/2)\sqrt{1-\sin^2 \xi}}{\sqrt{1-\sin^2(\theta/2)}} d\xi = \frac{2\sqrt{\sin^2(\theta_0/2)-\sin^2(\theta/2)}}{\sqrt{1-k^2 \sin^2 \xi}} d\xi$$

where $k = \sin(\theta_0/2) \Rightarrow k < 1$

$$\therefore T = 4 \sqrt{\frac{l}{g}} \int_0^{\pi/2} \frac{2\sqrt{\sin^2(\theta_0/2)-\sin^2(\theta/2)}}{2\sqrt{\sin^2(\theta_0/2)-\sin^2(\theta/2)}\sqrt{1-k^2 \sin^2 \xi}} d\xi \quad (2)$$

Arrive at numerically tractable integral

- After cancelling like terms in the numerator & denominator we get

$$T = 4 \sqrt{\frac{l}{g}} \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2 \xi}} d\xi \quad (3)$$

- (3) is a perfectly well behaved function: there are no issues at the end points or the interior ($k=1$ is impossible since $k=\sin(\theta_0/2)$ and $\theta_0 < \pi/2$)
 - Thus amenable to numerical (e.g. Romberg) integration
- Note that the integral of the form

$$K(k) = \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2 \xi}} d\xi$$

is called a *complete elliptic integral of the first kind* and can be found tabulated for various k

Special values

$$K(0) = \frac{\pi}{2}$$

$$K\left(\frac{\sqrt{2}}{2}\right) = \frac{1}{4\sqrt{\pi}} \Gamma\left(\frac{1}{4}\right)^2$$

$$K\left(\frac{1}{4}(\sqrt{6} - \sqrt{2})\right) = \frac{3^{\frac{1}{4}}}{2^{\frac{7}{3}}\pi} \Gamma\left(\frac{1}{3}\right)^3$$

$$K\left(\frac{1}{4}(\sqrt{6} + \sqrt{2})\right) = \frac{3^{\frac{3}{4}}}{2^{\frac{7}{3}}\pi} \Gamma\left(\frac{1}{3}\right)^3$$

$$K\left(2\sqrt{-4 - 3\sqrt{2}}\right) = \frac{(2 - \sqrt{2})\pi^{\frac{3}{2}}}{4\Gamma\left(\frac{3}{4}\right)^2}$$

The **complete elliptic integral of the second kind** E
is defined as

$$E(k) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 \xi} d\xi$$

$$E(0) = \frac{\pi}{2}$$

$$E(1) = 1$$

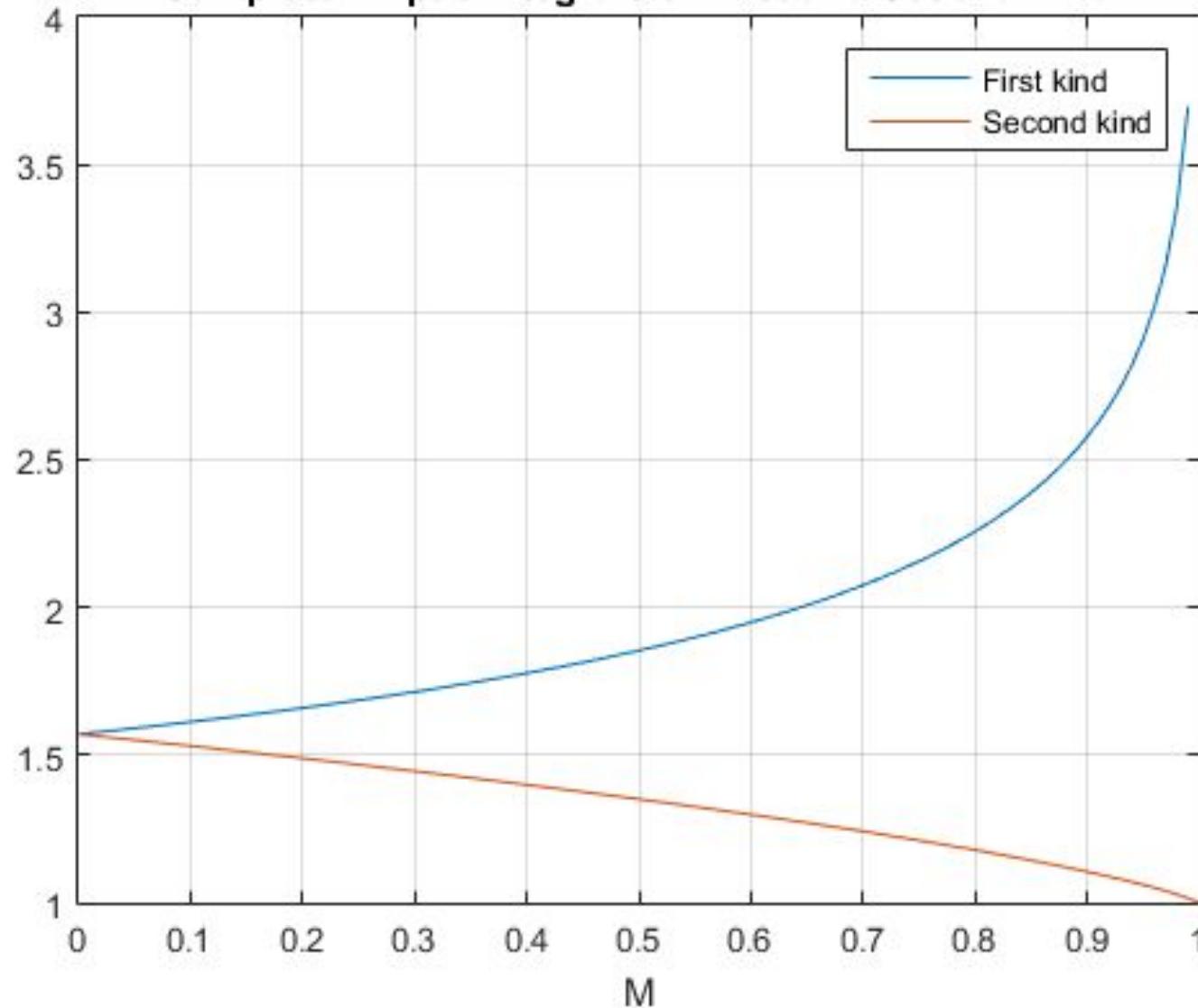
$$E\left(\frac{\sqrt{2}}{2}\right) = \pi^{\frac{3}{2}} \Gamma\left(\frac{1}{4}\right)^{-2} + \frac{1}{8\sqrt{\pi}} \Gamma\left(\frac{1}{4}\right)^2$$

$$E\left(\frac{1}{4}(\sqrt{6} - \sqrt{2})\right) = 2^{\frac{1}{3}} 3^{-\frac{3}{4}} \pi^2 \Gamma\left(\frac{1}{3}\right)^{-3} + 2^{-\frac{10}{3}} 3^{-\frac{1}{4}} \pi^{-1} (\sqrt{3} + 1) \Gamma\left(\frac{1}{3}\right)^3$$

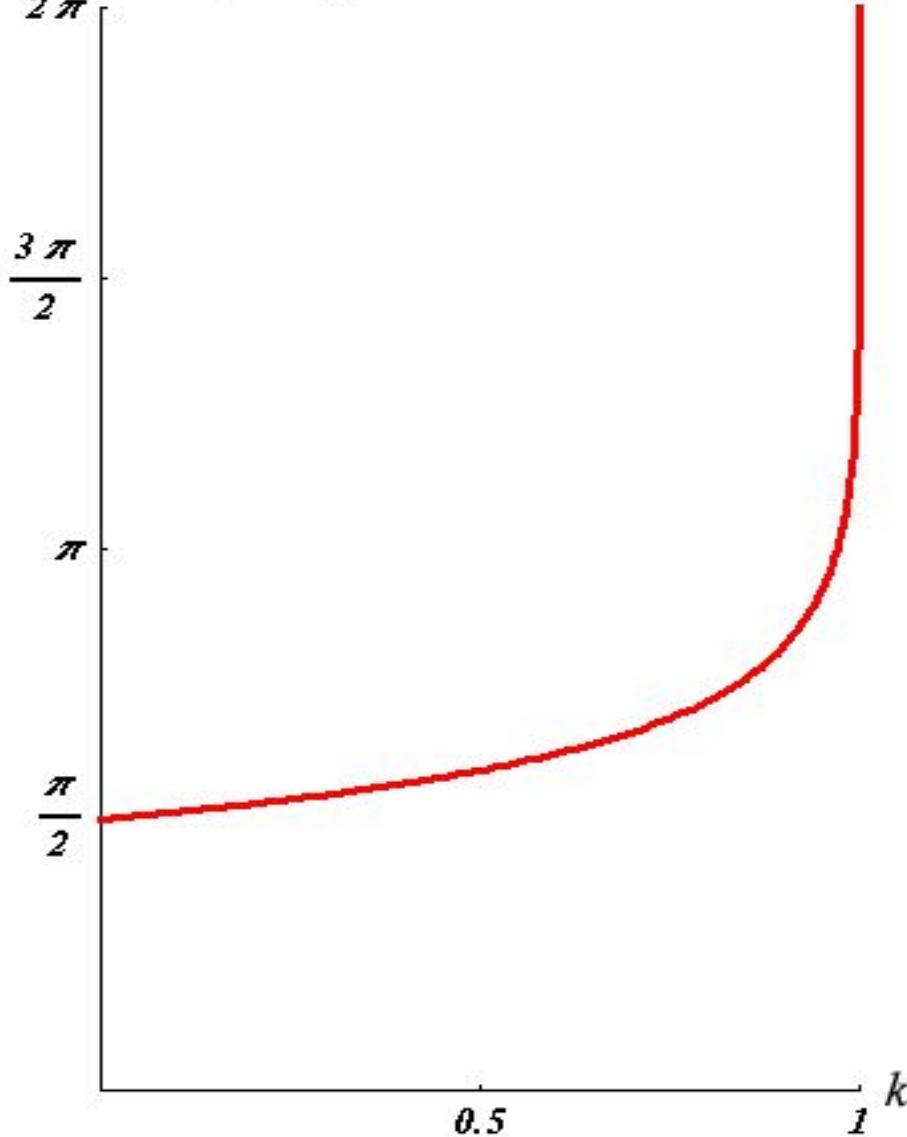
$$E\left(\frac{1}{4}(\sqrt{6} + \sqrt{2})\right) = 2^{\frac{1}{3}} 3^{-\frac{1}{4}} \pi^2 \Gamma\left(\frac{1}{3}\right)^{-3} + 2^{-\frac{10}{3}} 3^{\frac{1}{4}} \pi^{-1} (\sqrt{3} - 1) \Gamma\left(\frac{1}{3}\right)^3$$

$$E\left(2\sqrt{-4 - 3\sqrt{2}}\right) = \frac{(2 + \sqrt{2})(\pi^2 + 4\Gamma\left(\frac{3}{4}\right)^4)}{4\sqrt{\pi}\Gamma\left(\frac{3}{4}\right)^2}$$

Complete Elliptic Integrals of First and Second Kind




$$K(k) = F(\pi/2|k)$$



Improper integrals

- Thus far we have considered only definite integrals with finite limits, what about

$$I = \int_0^{\infty} f(x)dx$$

- Firstly, if I is divergent then a numerical integration is pointless
- If I is convergent we must still handle the upper limit somehow
- There are two ways of handling this type of integral
 - Break up the integral into two parts
 - Use a single change of variables to make the limits tractable

Split the integral

Write $I = \int_0^\infty f(x)dx = \underbrace{\int_0^a f(x)dx}_{\text{Proper integral } I_1} + \underbrace{\int_a^\infty f(x)dx}_{\text{Improper integral } I_2}$

- The value of a needs to be chosen with care
- I_1 we can evaluate numerically, with say a Romberg integrator (provided f is finite everywhere!)
- For I_2 we apply a change of variables to turn the integral into one with finite limits

Change of variables

Suppose we set $x = 1/y$, then
at $x = a$, $y = 1/a$

$$x = \infty, y = 0 \quad \text{and} \quad dx = -\frac{dy}{y^2}$$

Then we write I_2 as follows :

$$I_2 = \int_a^\infty f(x)dx = \int_0^{1/a} \frac{f(1/y)}{y^2} dy$$

- Provided $f(1/y) \sim y^n$ & $n > 1$ then there are no singularities in the integrand and we can apply Romberg integration
 - This is a reasonable expectation. We really asking for asymptotic behaviour of $f(x) \sim 1/x^2$ or lower. Without a fairly rapid approach to zero we wouldn't expect the integral to be bounded.

Removable singularities

- It is still possible that after our substitution we wind up with removable singularities

- Consider

$$\frac{y \sin y}{y^2} \sim \frac{\sin y}{y} \rightarrow 1 \text{ as } y \rightarrow 0$$

- However, when you calculate $\sin 0/0$ the computer will give a divide by zero error
- There is clearly no “magic algorithm” that works in all cases
 - Different substitutions may be required, series expansions may be necessary or even other methods be employed before invoking numerical integration

Other useful substitutions

1) Set $x = \frac{1+y}{1-y}$, then $dx = \frac{2dy}{(1-y)^2}$ & $y = \frac{x-1}{x+1}$

at $x = 0, y = -1$

$x = \infty, y = +1$

2) Set $x = \frac{y}{1-y}$, then $dx = \frac{dy}{(1-y)^2}$ & $y = \frac{x}{x+1}$

at $x = 0, y = 0$

$x = \infty, y = +1$

- Notice that both these substitutions can be used on the entire range $[0, \infty)$ – there is no need to break up the integral
 - It may be the case though that it is better to do this for numerical convergence reasons

Singularities in the integrand

Consider,

$$I = \int_0^\infty \frac{1}{(1+x)\sqrt{x}} dx, \text{ break this up as suggested before}$$

$$= \int_0^a \frac{1}{(1+x)\sqrt{x}} dx + \int_a^\infty \frac{1}{(1+x)\sqrt{x}} dx$$



I_1



I_2

- Our primary concern is I_1 due to the singularity at 0
- Firstly though, let's look at I_2 and how we would approach that

Try substitutions in I_2

$x = 1/y$, gives

$$I_2 = \int_0^{\frac{1}{a}} \frac{\sqrt{y}}{y^2(1+1/y)} dy = \int_0^{\frac{1}{a}} \frac{1}{\sqrt{y}(1+y)} dy$$

Exactly the same form as I_1 , which has singularity at $x = 0$!

$$x = 1/y^2, \Rightarrow dx = -2dy/y^3$$

$$I_2 = 2 \int_0^{\frac{1}{\sqrt{a}}} \frac{y}{y^3(1+1/y^2)} dy = 2 \int_0^{\frac{1}{\sqrt{a}}} \frac{1}{(1+y^2)} dy$$

- The latter example is perfectly well behaved (no singularities in $[0, 1/\sqrt{a}]$)
 - So we can deal with I_2 without a problem

Approaches to help us integrate I_1

- Use another substitution
- Can do a power series expansion
 - Not covered here, but see some references?
- We may be able to isolate the singularity (say by using a partial fraction expansion)
- We'll look at both substitution (again) and isolation

Substitution

Let's try $x = y^2$

$$\Rightarrow y = \sqrt{x}, \quad \text{and} \quad dx = 2ydy$$

Limits $x = [0, a]$ become

$$y = [0, \sqrt{a}]$$

$$I_1 = \int_0^a \frac{1}{(1+x)\sqrt{x}} dx = 2 \int_0^{\sqrt{a}} \frac{1}{(1+y^2)} dy$$

- We have removed the singularity and the result can easily be calculated via Romberg integration

Isolation

We know that as $x \rightarrow 0$, so $f(x) = \frac{1}{(1+x)\sqrt{x}} \rightarrow \frac{1}{\sqrt{x}}$

Try adding and subtracting the singularity:

$$f(x) = \frac{1}{(1+x)\sqrt{x}} = \frac{1}{(1+x)\sqrt{x}} - \frac{1}{\sqrt{x}} + \frac{1}{\sqrt{x}} = \frac{-\sqrt{x}}{(1+x)} + \frac{1}{\sqrt{x}}$$

$$\Rightarrow I_1 = \int_0^a f(x) dx = - \int_0^a \frac{\sqrt{x}}{(1+x)} dx + \int_0^a \frac{1}{\sqrt{x}} dx$$

This has isolated the singularity. If I_1 is tractable, the singularity must be integrable. Clearly here

$$\int_0^a \frac{1}{\sqrt{x}} dx = 2\sqrt{x} \Big|_0^a = 2\sqrt{a} \Rightarrow I_1 = 2\sqrt{a} - \int_0^a \frac{\sqrt{x}}{(1+x)} dx$$

What to take away from this...

- Every integral will be different
- You must be prepared to handle each one individually!

Integrals over infinite ranges

$$I = \int_0^\infty f(x)dx$$

solution is to change variables: $y = \frac{x}{1+x} \Rightarrow x = \frac{y}{1-y}$ & $dx = \frac{dy}{(1-y)^2}$

$$\int_0^\infty f(x)dx = \int_0^1 \frac{1}{(1-y)^2} f\left(\frac{y}{1-y}\right) dy$$

We can make two changes of variables: $y = x - a$ & $z = y/(1+y)$ to calculate

$$\int_a^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f\left(\frac{z}{1-z} + a\right) dy$$

Multidimensional Numerical Integration

- At first it seems a straightforward extension of $1d$ ideas
 - However, if in $1d$ we needed say a 100 function evaluations $2d$ will require 100×100 !
 - $3d$ $100 \times 100 \times 100 \dots$ etc
 - Quickly gets very numerically expensive – sometimes we have to resort to guestimating using Monte Carlo methods
 - Secondly, multidimensional integrals often have unusual boundaries
 - Defining the limits may be tricky
- As a first step lets consider integration over a rectangle

Multidimensional Numerical Integration

“Divide and Conquer”

$$\int_{x_a}^{x_b} \int_{y_a}^{y_b} f(x, y) dy dx$$

$$f(x) = \int_{y_a}^{y_b} f(x, y) dy$$

$$\int_{x_a}^{x_b} f(x) dx$$

Solve by Series Integration

Newton-Cotes

Trapezoidal

3-Point Simpson

For N points in each integral calculation there are N^2 calculations

Simple 2d integration

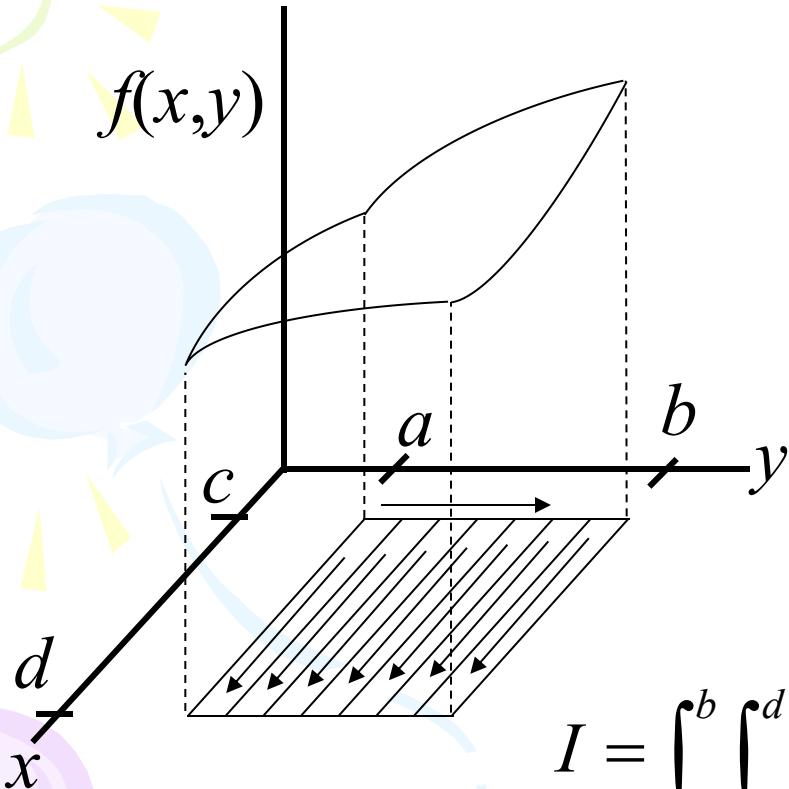
Consider,

$$I = \int_a^b \int_c^d f(x, y) dx dy$$

$$= \int_a^b F(y) dy \quad \text{where } F(y) = \int_c^d f(x, y) dx$$

- Thus there are two “sweeps”
 - 1d integrator evaluates $F(y)$ from $f(x, y)$ (clearly we must do this for all values of y)
 - 1d integrator evaluates I from $F(y)$

2d integration illustrated

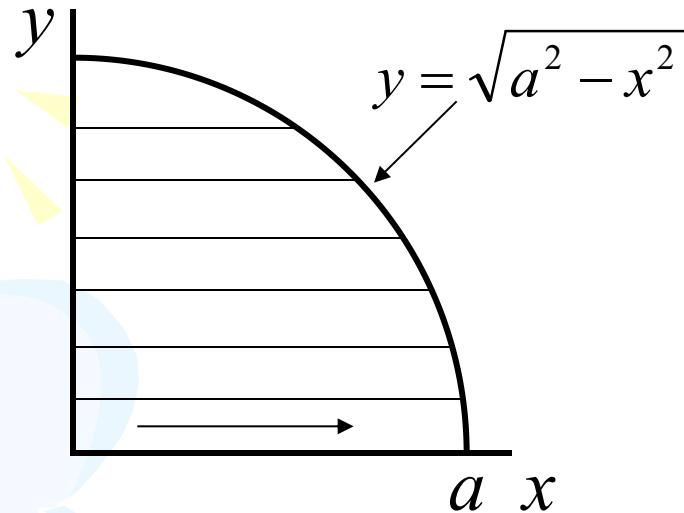


- This diagram shows precisely how the “sweeps” come about
- There are N x -sweeps followed by a single y sweep
- We of course could do things the other way round
 - i.e. y -sweeps before the x -sweeps:

$$I = \int_a^b \int_c^d f(x, y) dx dy$$

$$= \int_c^d G(x) dx \quad \text{where } G(x) = \int_a^b f(x, y) dy$$

Other integration limits (in 2d)



- You may frequently encounter integrals defined by a curve in the x - y plane

Limits on y : $0 \rightarrow a$

Limits on x : $0 \rightarrow \sqrt{a^2 - y^2}$

$$\text{Thus } I = \int_0^a \int_0^{\sqrt{a^2 - y^2}} f(x, y) dx dy$$

However, we could do y -sweeps
then x -sweeps

$$\text{Then } I = \int_0^a \int_0^{\sqrt{a^2 - x^2}} f(x, y) dy dx$$

In polar coordinates

- This particular problem strongly favours a change of variables:

$$r = \sqrt{x^2 + y^2}, \quad x = r\cos\theta$$

$$\theta = \tan^{-1}(y/x), \quad y = r\sin\theta$$

Which under this change of variables gives

$$dxdy = \frac{\partial(x,y)}{\partial(r,\theta)} drd\theta$$

where the Jacobian $\frac{\partial(x,y)}{\partial(r,\theta)}$ is given by

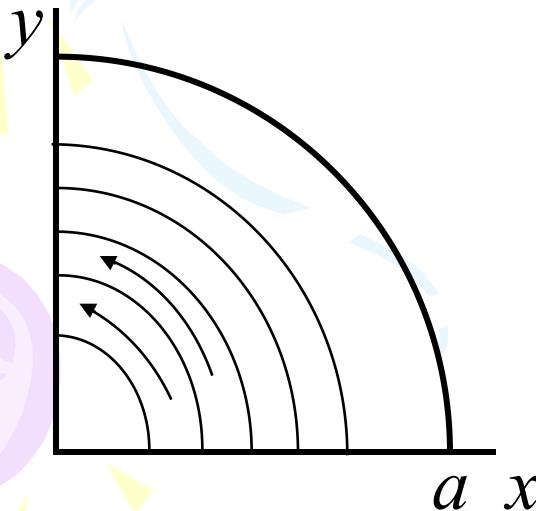
$$\begin{aligned}\frac{\partial(x,y)}{\partial(r,\theta)} &= \begin{vmatrix} \partial x / \partial r & \partial x / \partial \theta \\ \partial y / \partial r & \partial y / \partial \theta \end{vmatrix} \\ &= \begin{vmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{vmatrix} = r\cos^2\theta + r\sin^2\theta = r\end{aligned}$$

Change of limits

- The limits are obvious here: $r \in [0, a]$, $\theta \in [0, \pi/2]$
- Note that while the limits in x & y are from 0 to a respectively so that

min value for $y/x = 0$; $\tan^{-1} 0 = 0$

max value for $y/x = \infty$; $\tan^{-1} \infty = \pi/2$



$$\begin{aligned} \text{Thus } I &= \int_0^a \int_0^{\sqrt{a^2 - y^2}} f(x, y) dx dy \\ &= \int_0^a \int_0^{\pi/2} f(r \cos \theta, r \sin \theta) r d\theta dr \end{aligned}$$

Corresponds to $n \theta$ -sweeps
followed by 1 r -sweep.

Quickly gets very numerically expensive

Example: Atomic Physics

$$I = \int_0^1 dx_1 \int_0^1 dx_2 \dots \int_0^1 dx_{12} f(x_1, x_2, \dots, x_{12})$$

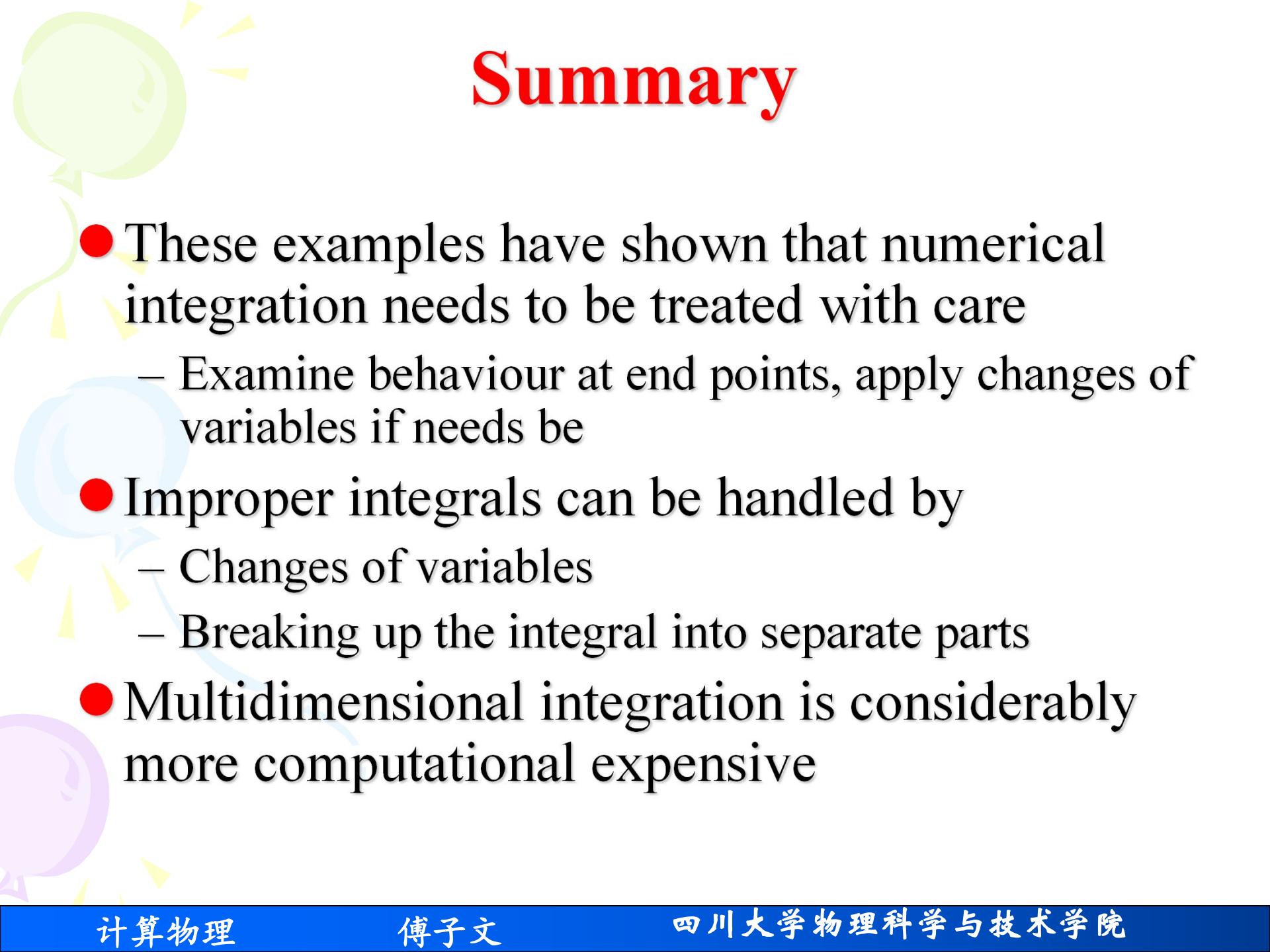


3 Dimension/electron * 4 electrons = 12 Dimensions

For 100 steps in each integration there are $100^{12} = 10^{24}$ calculations

Assuming 1 Giga evaluations/sec

It would take over 10^7 years!!!!



Summary

- These examples have shown that numerical integration needs to be treated with care
 - Examine behaviour at end points, apply changes of variables if needs be
- Improper integrals can be handled by
 - Changes of variables
 - Breaking up the integral into separate parts
- Multidimensional integration is considerably more computational expensive

Next Lecture

- ODE



Homework 11: 05/22/2019

Problem 1: Use the method discussed in this lecture to write the codes to integrate

a) $I = \int_{-1}^1 \sqrt{1-x^2} dx$

$$I = \int_0^\pi \sin^2 \theta d\theta$$

b) $T(\theta_0) = \int_0^{\theta_0} \frac{d\theta}{\sqrt{2\cos\theta - 2\cos\theta_0}}$

$$K(k) = \int_0^{\pi/2} \frac{1}{\sqrt{1-k^2 \sin^2 \xi}} d\xi$$

$$k = \sin(\theta_0/2) \quad \text{or} \quad \theta_0 = 2\arcsin(k)$$

Plot the results with different k (prefer to use xmGrace)

c) $I = \int_0^\infty \frac{1}{(1+x)\sqrt{x}} dx$

Problem 2. Gaussian integral via numerical integration

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

Write a program which uses your integration module to performs the Gaussian integral

$$f(x) = e^{-x^2}$$

from $-\infty$ to ∞ via numerical integration. The value for integral should be $\sqrt{\pi}$.

Have your program compare your results of the numerical integration to the true numerical value.

Problem 3. Volume of a n-dimensional hypersphere:

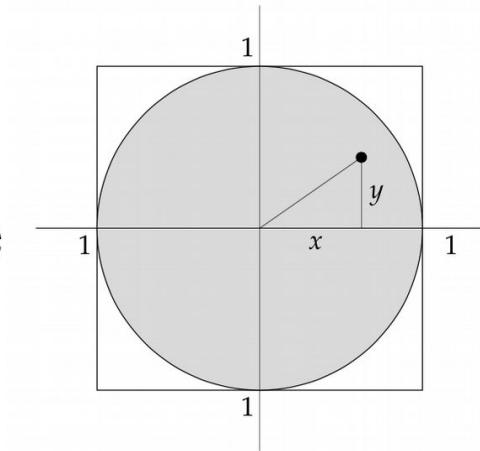
This exercise asks you to estimate the volume of a sphere of unit radius with any dimensions. Consider the equivalent problem in two dimensions, the area of a circle of unit radius:

$$I = \int \int_{-1}^1 f(x, y) dx dy$$

The area of the circle, the shaded area shown, is given by the integral I where $f(x, y) = 1$ everywhere inside the circle and zero everywhere outside, i.e,

$$f(x, y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{Otherwise} \end{cases}$$

- a) calculate hyper volume as a function of the dimensions from $n = 0$ to $n = 12$. (12,11,10...???)
- b) Print results to the screen and generate a graph of the hyper volume vs dimension.



(**Hints:** You will get high credit with higher n **project 3?**)

Volume of a n-dimensional hypersphere:

$$V_n = \frac{\pi^{\frac{n}{2}} R^n}{\Gamma(\frac{n}{2} + 1)} = C_n R^n$$

Where Γ is gamma function.

$$\Gamma\left(\frac{n}{2} + 1\right) = \left(\frac{n}{2}\right)! \quad (\text{For Even } n=2k),$$

$$\Gamma\left(\frac{n}{2} + 1\right) = \sqrt{\pi} \frac{n!!}{2^{(n+1)/2}} \quad (\text{For odd } n=2k+1)$$

$$C_n = \frac{\pi^k}{k!} \quad (\text{For Even } n=2k),$$

$$C_n = C_{2k+1} = \frac{2^{2k+1} k! \pi^k}{(2k+1)!} \quad (\text{For odd } n=2k+1)$$

Error Estimation

- Trapezoidal error for f on $[a, b]$
 - Where $M = \max$ value of $|f''(x)|$ on $[a, b]$

$$|E_n| \leq \frac{(b-a)^3}{12n^2} \cdot M$$

- Simpson's error for f on $[a, b]$
 - Where $K = \max$ value of $|f^{(4)}(x)|$ on $[a, b]$

$$|E_n| \leq \frac{(b-a)^5}{180n^4} \cdot K$$