LAB 6

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Sturm-Liouville Problems

"Sturm-Liouville problems" are homogeneous boundary-value problems that naturally arise when solving certain partial differential equation problems using a "separation of variables" method. It is the theory behind Sturm-Liouville problems that, ultimately, justifies the "separation of variables" method for these partial differential equation problems.

Sturm-Liouville Boundary Value Problem (SL-BVP) is written as

$$L[y] = \frac{d}{dx}\left[p(x)\frac{dy}{dx}\right] + q(x)\,y = -\lambda\, w(x)\, y \qquad x \in [a,b]$$

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0$$

$$\beta_1 y(b) + \beta_2 y'(b) = 0$$

where p(x), q(x) and w(x) are continuous functions on [a,b] and both p and w are positive on [a,b]

$y(x) = 0$ is a solⁿ of this eqⁿ

A non-trivial solution exists for certain values of λ but not for others

Those values of λ for which nontrivial solutions do exist are called eigenvalues and the corresponding nontrivial solutions are callled eigenfunctions.

Solving the eigenvalue problem means finding all eigenvalues and associated eigenfunctions of Equation

Properties ;

1. THe eigenvalues of a Sturm-Liouville problem are all real and non-negative

2. THe eigenvalues of Sturm-Liouville problem can be arranged to form a strictly increasing sequence

$$0 \le \lambda_1 < \lambda_2 < \dots \qquad \lambda_n \to \infty \quad \text{as} \quad n \to \infty$$

3. For each eigenvalue of a Sturm-Liouvilee problem, there exists one and only one linearly independent eigenfunctions.

For Example

$$y'' + \lambda y = 0 \quad ; \quad y(0) = y(\pi) = 0$$

This has the trivial solution y(x) = 0, but for some values of λ , there are non-trivial solutions.

If y(x) is a solution of this BVP, then a constant times y(x) is also

Hence we need a normalizing condition to specify a solution of interest for example

$y'(0) = 1$

For $\lambda > 0$, the solution of IVP with

$y(0) = 0$, $y'(0) = 1$ is $y(x) = \frac{1}{\sqrt{\lambda}} \sin(x\sqrt{\lambda})$.

Now BC $y(\pi) = 0$ amounts to

$$\sin(\pi\sqrt{\lambda}) = 0 \Rightarrow \pi\sqrt{\lambda} = n\pi \Rightarrow \lambda = n^2; \; n = 1, 2, \ldots$$

Thus, when solving a Sturm-Liouville problem, we have to specify not only a normalizing condition, but also which eigenvalue interests us.

One way to solve these problems is shooting method

However, the basic difficulty with shooting is that a perfectly nice BVP can require the integration of IVPs that are unstable. That is, the solution of a BVP can be insensitive to the changes in boundary values, yet the solutions of the IVPs of shooting are sensitive to changes in initial values.

Example

$$y'' - 100y = 0 \qquad y(0) = 1, \; y(1) = \beta$$

Shooting involves the solution

$$y(x,s) = \cosh(10x) + 0.1s\sinh(10x)$$

of IVP with IV

$$y(0) = 1, \quad y'(0) = s$$

$\frac{\partial y}{\partial s} = 0.1 \sinh(10x)$ which may be as large as

$$0.1 \sinh(10) \simeq 1101$$

It may be shown that the slope that results in satisfaction of the boundary condition at x = 1 is

$$s = 10\left(\beta - \cosh(10)\right) / \sinh(10)$$

And for the solution of the BVP

$$\left|\frac{\partial y}{\partial \beta}\right| = \left|\frac{\sinh(10x)}{\sinh(10)}\right| \leq 1$$

Thus the solutions of the IVPs are considerably more sensitive to changes in the initial slope s than the solution of the BVP is to changes in the boundary value β .

If the IVPs are not too unstable, shooting can be quite effective. Unstable IVPs can cause a shooting code to fail because the integration “blows up” before reaching the end of the interval. More often, though, the IVP solver reaches the end, but is unable to compute an accurate result there and because of this, the nonlinear equation solver is unable to find accurate initial values

Specific case of BVP: Eigenvalue-eigenfunction problem

Aim: Find a number λ and a non-zero function y solutions to the boundary value problem

$$y'' = \lambda y \qquad \frac{d^2}{dx^2} \text{ is operator}$$

$$L y = \lambda y \qquad L = \frac{d^2}{dx^2}$$

-- Siimilar to the eigenvalue-eigenvector problem in Linear Algebra:
Given an n × n matrix A, find λ and a non-zero n-vector v solutions of

$$Av = \lambda v$$

Example
Find every $\lambda \in R$ and corresponding non-zero functions y solutions of the BVP

$$y''(x) + \lambda y(x) = 0, \qquad y(0) = 0, \; y(L) = 0, \qquad L > 0.$$

$\underline{\lambda = 0}$ $\quad y(x) = c_1 + c_2 x$

$y(0) = 0 \Rightarrow c_1 = 0 \quad \& \quad y(L) = 0 \Rightarrow c_2 = 0$

$\therefore y(x) = 0 \quad \forall x$

There are NO non-zero solutions for λ = 0.

$\underline{\lambda < 0}$ $\qquad \lambda = -\alpha^2$ & $\alpha^2 > 0$

$$y'' - \alpha^2 x = 0$$

general sol^n is $\quad y(x) = c_1 e^{\alpha x} + c_2 e^{-\alpha x}$

$$y(0) = c_1 + c_2 = 0$$

& $y(L) = c_1 e^{\alpha L} + c_2 e^{-\alpha L} = 0$

TO find C_1 and C_2, we need to solve the homogeneous linear system

$$\underbrace{\begin{pmatrix} 1 & 1 \\ e^{\alpha L} & e^{-\alpha L} \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}}_{C} = \underbrace{\begin{pmatrix} 0 \\ 0 \end{pmatrix}}_{Z} \quad \Rightarrow A.C = Z$$

$\mathrm{Det}(A) = e^{-\alpha L} - e^{\alpha L} \neq 0$ for any $\alpha \neq 0$

Thus matrix A is invertible, and the linear system has a unique solution

$$C_1 = C_2 = 0$$

Since y = 0, there are NO non-zero solutions for $\lambda < 0$.

Case $\lambda > 0$

$$y'' + \lambda y = 0$$

$$\lambda = k^2 > 0$$

The general solution is

$$y = C_1 \cos(kx) + C_2 \sin(kx)$$

$$y(0) = 0 \Rightarrow C_1 = 0$$

& $y(L) = 0 \Rightarrow C_2 \sin(kL) = 0$

$C_2 = 0$ gives $y(x) = 0$ solution

Non-zero solution exists for

$$k = \frac{n\pi}{L} \quad \text{or} \quad \lambda = \frac{n^2\pi^2}{L^2}$$

So sol^n is $\quad y(x) = C_2 \sin\left(\frac{n\pi}{L}x\right)$

C_2 may be detyermined from a normalisation condition.

Conclusion:

(i) If $\lambda \leq 0$, then the BVP has no solution.

(ii) If $\lambda > 0$, then there exist infinitely many eigenvalues λ_n and eigenfunctions y_n ,
with n any positive integer, given by

$$\lambda_n = \frac{n^2\pi^2}{L^2}, \qquad y_n(x) = \sin\left(\frac{n\pi}{L}x\right)$$

HW

Find every $\lambda \in R$ and corresponding non-zero functions y solutions of the BVP

(i) $y''(x) + \lambda y(x) = 0, \qquad y(0) = 0, \; y'(L) = 0, \qquad L > 0.$

(ii) $y''(x) + \lambda y(x) = 0, \qquad y(0) = y(L), \; y'(0) = y'(L)$ -- Periodic BC

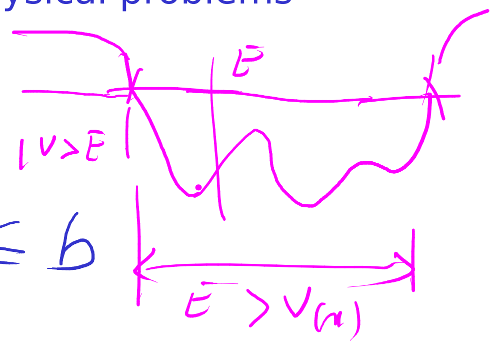
Numerov Method

$$RK4 \quad - \quad \mathcal{O}(h^4)$$

$$FD \quad - \quad \mathcal{O}(h^2)$$

Special Problem -- Without the first order derivative term y' -- appear in various physical problems

Such problems can be solved by a better algorithm -- the Numerov Meethod



$$y'' + \overbrace{[k(x)]^2}^{k^2(x)} y = F(x) \qquad a \leq x \leq b$$

$$y(a) = \alpha, \quad y(b) = \beta$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

$$F(x) = 0$$

$$\& \quad k^2(x) = \frac{2m}{\hbar^2}[E - V(x)]$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)\psi = E\psi$$

We can interpret F(x) as an inhomogenous driving force

k(x) is a real function.
If it is positive the solutions y(x) will be oscillatory functions, and
if negative they are exponentionally growing or decaying functions.

First consider the case

$$F(x) = 0$$

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

Numerov’s method is designed to solve such an equation numerically, achieving a

local truncation error $O(h^6)$

$$y^{(n)}(x) \equiv \frac{d^n y}{dx^n}$$

Taylor expansion

$$y(x+h) = y(x) + h\, y^{(1)}(x) + \frac{h^2}{2}\, y^{(2)}(x)$$

$$+ \frac{h^3}{3!}\, y^{(3)}(x) + \frac{h^4}{4!}\, y^{(4)}(x) + \frac{h^5}{5!}\, y^{(5)}(x)$$

$$+ \cdots$$

$$y(x-h) = y(x) - h\,y^{(1)}(x) + \frac{h^2}{2}\,y^{(2)}(x) - \frac{h^3}{3!}\,y^{(3)}(x) + \frac{h^4}{4!}\,y^{(4)}(x) - \frac{h^5}{5!}\,y^{(5)}(x) + \cdots$$

$$y(x+h) - y(x-h) = 2y(x) + h^2\,y^{(2)}(x) + \frac{h^4}{12}\,y^{(4)}(x) + O(h^6)$$

$$y^{(2)}(x) = \frac{y(x+h) + y(x-h) - 2y(x)}{h^2} - \frac{h^2}{12} y^{(4)}(x) + O(h^4)$$

$$y^{(2)} + \frac{h^2}{12} y^{(4)}(x) = \left(1 + \frac{h^2}{12}\frac{d^2}{dx^2}\right) y^{(2)}(x)$$

To eliminate the fourth-derivative term we apply the operator

$$\left(1 + \frac{h^2}{12}\frac{d^2}{dx^2}\right)$$

on the differential equation $y'' + k^2(x)\, y = 0$

$$\underline{y^{(2)}(x) + \frac{h^2}{12} y^{(4)}(x)} + k^2(x)\, y(x) + \frac{h^2}{12}\frac{d^2}{dx^2}\left[k^2 y\right] = 0$$

$$\Rightarrow y(x+h) + y(x-h) - 2y(x) + h^2 k^2 y(x) + \frac{h^4}{12}\frac{d^2}{dx^2}(k^2 y) \approx 0$$

approximate the second derivative of $k^2_{(x)}\, y(x)$

$$\frac{d^2}{dx^2}(k^2 y) = \frac{1}{h^2}\left[(k^2 y)\big|_{x+h} + (k^2 y)\big|_{x-h} - 2(k^2 y)\big|_{x} + O(h^2)\right]$$

$$\frac{d^2}{dx^2}(k^2 y) \simeq \frac{1}{h^2}\Big[\left\{k^2(x+h)\, y(x+h) - k^2(x)\, y(x)\right\}$$

$$+ \left\{k^2(x-h)\, y(x-h) - k^2_{(x)}\, y(x)\right\}\Big]$$

Writing $x = x_i$, $x+h = x_{i+1}$, $x-h = x_{i-1}$

$y(x) = y_i$, $y(x+h) = y_{i+1}$, $y(x-h) = y_{i-1}$

$$y_{i+1} = \frac{1}{\left[1 + \frac{h^2}{12} k^2_{i+1}\right]}\left[2\left(1 - \frac{5}{12} h^2 k_i^2\right) y_i - \left(1 + \frac{1}{12} h^2 k^2_{i-1}\right) y_{i-1}\right] + O(h^6)$$

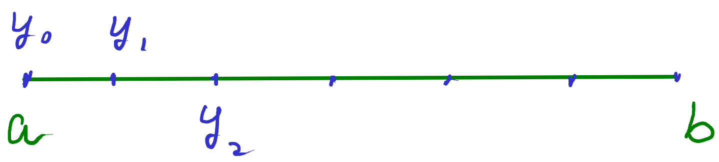
HW

$$\underline{F(x) \neq 0}$$

$$y_{i+1} = \frac{1}{\left[1 + \frac{h^2}{12} k_{i+1}^2\right]} \left[2\left(1 - \frac{5}{12} h^2 k_i^2\right) y_i - \left(1 + \frac{1}{12} h^2 k_{i-1}^2\right) y_{i-1} \right.$$

$$\left. + \frac{h^2}{12}\left(F_{i+1} + F_{i-1} - 2F_i\right) \right] + O(h^6)$$

The Numerov method can be used to determine y_p for $p = 2, 3, 4, \cdots$, given two initial values, y_0 & y_1.
We need two initial values because we are solving a second order differential equation.



The error in one x-step is $\mathcal{O}(h^6)$

However, the number of steps needed to integrate over a fixed range of x, from a to b is

$$\frac{b-a}{h} \propto \frac{1}{h}$$

One might expect that the errors at each step would be roughly comparable so so the total error in the Numerov method would be $\mathcal{O}(h^5)$.

Thus it is a 5-th order method, one higher than RK4.

local Truncation error $\sim \mathcal{O}(h^6)$

global error $\sim \mathcal{O}(h^5)$

Actually it turns out to be $\sim \mathcal{O}(h^4)$

↳ same as RK

there can be problems with roundoff errors in using algorithm so make sure you use double precision arithmetic

Solution of 1-d Time independent Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$\Rightarrow \quad \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0$$

of the form $y'' + k^2(x)\,y = 0$ with $k^2(x) = \frac{2m}{\hbar^2}\left[E - V(x)\right]$

Thus we can solve by Numerov method

Two additional Complexities

(i) Solution does not exist for all E. For Bound states, only certain discrete values of E give valid solution

Valid means -- satisying the conditions of continuity of ψ and ψ' and wave function should approach zero at $|x| \to \infty$

SO the numerical algorithm or code should be able to identify the valid values of E

(ii) In the classically forbidden regions the wavefunction should be exponentially decaying

Sch eq^n (1-d)

of the form

$$\psi''(x) = f(x)\,\psi(x)$$

$$H\psi = E\psi \qquad \text{TISE}$$

Dimensionless form

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad -\infty < x < \infty$$

$L \rightarrow$ typical length in the problem

Define $\quad \xi = \dfrac{x}{L}$

$$\frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi} = \frac{1}{L}\frac{d}{d\xi}$$

$$\frac{d^2}{dx^2} = \frac{1}{L^2}\frac{d^2}{d\xi^2}$$

$$H = -\frac{\hbar^2}{2m}\frac{1}{L^2}\underbrace{\frac{d^2}{d\xi^2}} + \underbrace{V(x)}$$

Dimensionless

$$\tilde{H} = \frac{mL^2}{\hbar^2} H = -\frac{1}{2}\frac{d^2}{d\xi^2} + \underbrace{\frac{mL^2}{\hbar^2} V(L\xi)}_{\tilde{V}}$$

$$\left(-\frac{1}{2}\frac{d^2}{d\xi^2}+\tilde{V}\right)\tilde{\psi} = \varepsilon\tilde{\psi}$$

$$\varepsilon = \frac{mL^2}{\hbar^2}E$$

$$\tilde{\psi} \equiv \psi(L\xi)$$

Sch eqn becomes

$$\frac{d^2\tilde{\psi}}{d\xi^2} + 2(\varepsilon - \tilde{V}(\xi))\tilde{\psi}(\xi) = 0$$

Compare with $\frac{d^2y}{dx^2} + k^2 y = 0$, we have

$$k^2 = 2(\varepsilon - \tilde{V}(x))$$

Use the iteration

$$y_{i+1} = \frac{1}{\left[1 + \frac{h^2}{12} k_{i+1}^2\right]} \left[2\left(1 - \frac{5}{12} h^2 k_i^2\right) y_i - \left(1 + \frac{1}{12} h^2 k_{i-1}^2\right) y_{i-1} \right] + O(h^6)$$

with N discrete points

$$\tilde{\psi}_0 = \tilde{\psi}_{N+1} = 1.$$