

The numerical solution of Sturm-Liouville and Schrödinger eigenvalue problems

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Outline

- 1 Introduction
 - The Sturm-Liouville equation
 - The Sturm-Liouville boundary value problem
- 2 Matrix methods
 - Discretization methods
 - Pros and Cons
- 3 Shooting methods
 - The shooting principle
 - Coefficient approximation methods
- 4 Summary

Outline

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Introduction

- The Sturm-Liouville equation
- The Sturm-Liouville boundary value problem

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- Discretization methods
- Pros and Cons

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- The shooting principle
- Coefficient approximation methods

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Summary

Sturm-Liouville equations



Jacques Sturm (1803-1855)



Joseph Liouville (1809-1882)

$$-\frac{d}{dx} \left[p(x) \frac{dy(x)}{dx} \right] + q(x)y(x) = Ew(x)y(x)$$

Sturm-Liouville equations

$$-\frac{d}{dx} \left[p(x) \frac{dy(x)}{dx} \right] + q(x)y(x) = Ew(x)y(x)$$

- Description of a lot of important physical phenomena which exhibit a pronounced **oscillatory** character.
 - behaviour of pendulum-like systems
 - vibrations
 - resonances
 - wave propagation
- Description of quantum mechanical systems (atoms, transistors,...) → **The Schrödinger problem**

The Schrödinger problem



Erwin Schrödinger (1887 - 1961)

The Schrödinger problem

$$\frac{d^2 y}{dx^2} = [V(x) - E]y(x)$$

- fundamental equation in quantum mechanics
- $V(x)$: potential function
- E : energy level
- y : wavefunction

The boundary value problem

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

- Boundary conditions (BCs):

$$\begin{cases} a_0y(a) + b_0p(a)y'(a) = 0, & (y' = dy/dx) \\ a_1y(b) + b_1p(b)y'(b) = 0 \end{cases}$$

- **Eigenvalue**: E for which there exists a nonzero solution y satisfying the BCs.
- **Eigenfunction**: corresponding solution y .

The boundary value problem

Example

$$\frac{d^2 y}{dx^2} + Ey = 0, \quad y(0) = 0, \quad y(\pi) = 0,$$

- This equation represents the physics of a vibrating elastic string.
- **Eigenvalues:** $E_k = (k + 1)^2$, $k = 0, 1, 2, \dots$
- **Eigenfunctions:** $y_k(x) = \sin((k + 1)x)$, $k = 0, 1, 2, \dots$

Fundamental theorem

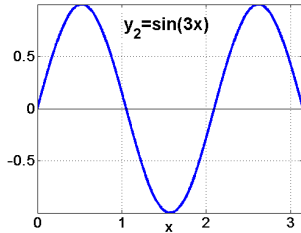
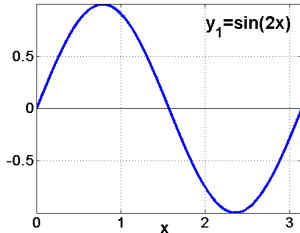
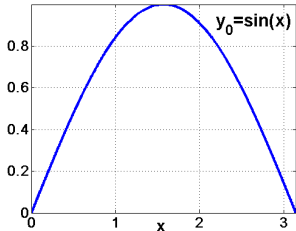
- The eigenvalues E_k are real and simple and can be ordered as an increasing sequence:

$$E_0 < E_1 < E_2 < \dots$$

Oscillatory character of the eigenfunctions

- The eigenfunction $y_k(x)$ corresponding to E_k has **exactly k zeros** on (a, b)
- The eigenfunctions are thus more oscillatory as the eigenvalue increases

$$d^2y/dx^2 + Ey = 0, \quad y(0) = 0, \quad y(\pi) = 0$$



Numerical solution of Sturm-Liouville problems

- Most Sturm-Liouville eigenvalue problems cannot be solved analytically \implies numerical methods are used to approximate the eigenvalues.
- Many numerical methods are constructed for a Sturm-Liouville problem in the Schrödinger form:

$$-\frac{d}{dr} \left(p(r) \frac{dz}{dr} \right) + q(r)z = Ew(r)z, \quad r_{min} < r < r_{max}$$

Liouville's transformation:

$$x = \int_{r_{min}}^r \sqrt{w(s)/p(s)} ds, \quad y = (pw)^{1/4} z$$

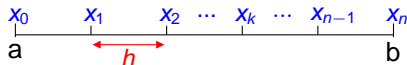
$$y'' = (V(x) - E) y, \quad x_{min} \leq x \leq x_{max}$$

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Simple matrix methods

- Equally spaced mesh:



- Methods based on finite differences (or finite elements).
- Typically they lead to ordinary matrix eigenvalue problems $\mathbf{A}\mathbf{y} = E\mathbf{y}$ or generalized matrix eigenvalue problems $\mathbf{A}\mathbf{y} = E\mathbf{B}\mathbf{y}$ with a matrix of band structure.
- The bandwidth of the matrix increases with the number of points used in the finite difference approximation.

Simple centred difference approximation

$$y'' = [V(x) - E]y, \quad y(a) = y(b) = 0$$

The centred difference approximation:

$$y''_i \approx \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}, \quad y_i = y(x_i)$$

$$\mathbf{A}y = Ey$$

\mathbf{A} : symmetric tridiagonal

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{pmatrix}, \quad \mathbf{A} = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} + \begin{pmatrix} V(x_1) & & & & \\ & V(x_2) & & & \\ & & \ddots & & \\ & & & & V(x_{n-1}) \end{pmatrix}$$

The Numerov method

$$y'' = [V(x) - E]y, \quad y(a) = y(b) = 0$$

Numerov for $y'' = f(x, y)$:

$$y_{i-1} - 2y_i + y_{i+1} = \frac{h^2}{12}(f_{i-1} + 10f_i + f_{i+1}), \quad f_i = f(x_i, y_i)$$

$$\mathbf{A}y = \mathbf{E}By$$

\mathbf{A} and \mathbf{B} are tridiagonal: $\mathbf{A} = \frac{1}{h^2}\mathbf{M} + \mathbf{B}V$, $\mathbf{B} = \mathbf{I} - \frac{1}{12}\mathbf{M}$,

$$\mathbf{M} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} V(x_1) & & & & \\ & V(x_2) & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & V(x_{n-1}) \end{pmatrix}$$

Experiments

Table: Eigenvalues obtained with simple centred differences for $y'' + Ey = 0, y(0) = y(\pi) = 0$.

k	E_k	$n = 10$	$n = 20$	$n = 40$
0	1	0.99180234	0.99794552	0.99948606
1	4	3.87012484	3.96720936	3.99178209
2	9	8.35321723	8.83467838	8.95843958
3	16	14.0022432	15.4804993	15.8688374
4	25	20.2642367	23.7410301	24.6803708

$O(k^4 h^2)$

Table: Eigenvalues obtained with Numerov for $y'' + Ey = 0, y(0) = y(\pi) = 0$.

k	E_k	$n = 10$	$n = 20$	$n = 40$
0	1	0.99995926	0.99999746	0.99999984
1	4	3.99736290	3.99983702	3.99998984
2	9	8.96943979	8.99813471	8.99988417
3	16	15.8246732	15.9894516	15.9993481
4	25	24.3170841	24.9594385	24.9975077

$O(k^6 h^4)$

Higher eigenvalues?

The AAdHP correction

- Anderssen, Andrew, de Hoog and Paine (1980-1985).
- They showed that the error, when $V(x) = 0$, has the same asymptotic form (for $k \rightarrow \infty$) as the error for general $V(x)$.
- The known error for $V(x) = 0$ is used to correct the eigenvalue estimates for general $V(x)$:
 - Simple centred differences: $O(k^4 h^2) \rightarrow O(kh^2)$
 - Numerov: $O(k^6 h^4) \rightarrow O(k^3 h^4)$

Modified / Exponentially-fitted Numerov method

- Vanden Berghe, De Meyer, Van Daele
- delivers more accurate eigenvalues than the classical Numerov method: $O(k^6 h^4) \rightarrow O(k^3 h^4)$.

Experiments

Table: Errors ($\times 10^3$) obtained with $n = 40$ for $V(x) = e^x$, $y(0) = y(\pi) = 0$.

k	E_k	Numerov	AAAdHP corr.	Exp. fitted
0	4.8966694	0.0028	0.0027	0.0014
1	10.045190	0.0427	0.0325	0.0127
2	16.019267	0.2272	0.1114	0.0424
3	23.266271	0.8837	0.2317	0.1040
4	32.263707	2.8802	0.3879	0.1959
5	43.220020	8.0432	0.5820	0.3132
6	56.181594	19.6872	0.8159	0.4535
7	71.152998	43.2849	1.0913	0.6197
8	88.132119	87.2765	1.4108	0.8115
9	107.11668	164.0239	1.7778	1.0373
		$O(k^6 h^4)$	$O(k^3 h^4)$	$O(k^3 h^4)$

Matrix methods: conclusion

Pros

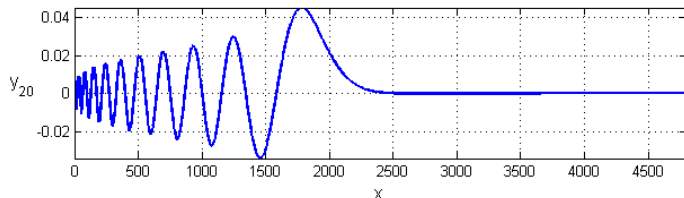
- Simple to set up.
- Reliable and efficient software for eigenvalues and eigenvectors of a tridiagonal matrix can be used. (Typically, NAG or other standard library codes are used).

Cons

- The infinite-dimensional problem is replaced by a matrix problem of dimension $n - 1$.
- The quality of E_k deteriorates as k increases.
- The use of a uniform mesh is not always a good idea.

Matrix methods: conclusion

An eigenfunction of a singular problem



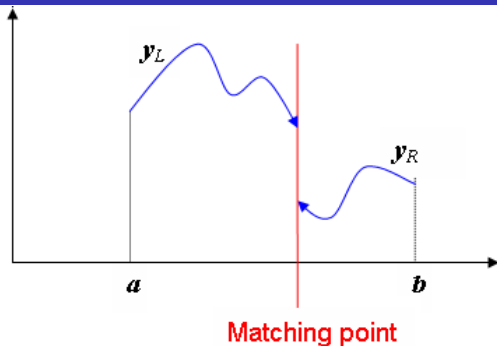
Conclusion

- For the computation of low-order eigenvalues of regular problems the matrix methods are competitive.
- For automatic software, and for most singular problems, more sophisticated methods are used.
- The challenge: uniform accuracy over the whole energy-range and large step sizes, even for high eigenvalues

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Shooting methods



- Reducing the solution of the boundary value problem (BVP) to the solution of two initial value problems (IVPs).
- The IVPs are solved for a succession of trial E values which are adjusted till y_L/y'_L and y_R/y'_R match in the matching point \Rightarrow we've found an eigenvalue.

Calculation of y_L, y'_L and y_R, y'_R

Classical methods

- Runge Kutta (RK) or multistep methods.
- Piecewise polynomial approximation of the exact solution.
- Very small step sizes have to be taken for high eigenvalues.

Special techniques are needed which adequately take into account the oscillatory character of the solution

- **coefficient approximation**: the given diff. eq. is replaced (piecewisely) by a diff. eq. which can be solved exactly.

Approximation of
the **solution**
(classical methods)



Approximation of
the **equation**
(coefficient approximation)

Calculation of y_L, y'_L and y_R, y'_R

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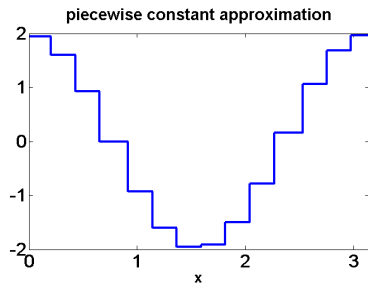
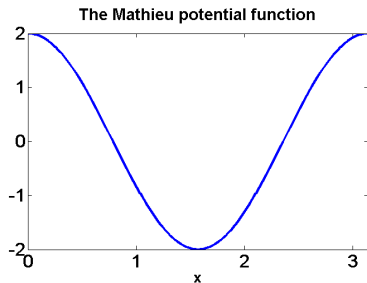
Approximation of
the **equation**
(coefficient approximation)



Coefficient approximation for the Schrödinger equation

$$y'' = (V(x) - E)y \xrightarrow{\text{(piecewisely)}} y'' = (\tilde{V}(x) - E)y$$

e.g. piecewise constant approximation of $V(x)$:

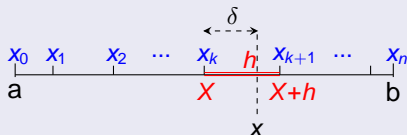


Coefficient approximation methods

$$y'' = (V(x) - E)y, \quad y(a) = \alpha, \quad y'(a) = \beta$$

- Aim: construct a method for the calculation of y .

Propagators



$u(\delta)$ and $v(\delta)$ (with $\delta = x - X \in [0, h]$) are the solutions of

$$y''(\delta) = (V(X + \delta) - E)y(\delta)$$

with initial values $u(0) = 1$, $u'(0) = 0$ and $v(0) = 0$, $v'(0) = 1$.

Propagators

- Forward propagation

$$\begin{bmatrix} y(X+h) \\ y'(X+h) \end{bmatrix} = \begin{bmatrix} u(h) & v(h) \\ u'(h) & v'(h) \end{bmatrix} \begin{bmatrix} y(X) \\ y'(X) \end{bmatrix}$$

- Backward propagation

$$\begin{bmatrix} y(X) \\ y'(X) \end{bmatrix} = \begin{bmatrix} v'(h) & -v(h) \\ -u'(h) & u(h) \end{bmatrix} \begin{bmatrix} y(X+h) \\ y'(X+h) \end{bmatrix}$$

- Knowledge of u , v , u' and v' is sufficient to advance the solution in both directions
- These matrix formulas are used to propagate y_L, y'_L and y_R, y'_R in the shooting procedure.

How to compute the propagators?

$u(\delta)$ and $v(\delta)$ are constructed via coefficient approximation:

$$y''(\delta) = (V(X + \delta) - E) y(\delta) \quad (1)$$

is approximated over $[X, X + h]$ by

$$y''(\delta) = (\bar{V} - E) y(\delta) \quad (2)$$

- When $\bar{V} = \text{constant}$, the 2 indep. solutions of (2) have known analytic forms: $u_0(\delta)$ and $v_0(\delta)$.
- Constant Perturbation Methods (CPM):
 - Perturbation theory is used to estimate the deviation of the solution of (2) from the solution of (1).
 - Correction terms are added to $u_0(\delta)$ and $v_0(\delta)$ to obtain a more accurate approximation to the desired $u(\delta)$ and $v(\delta)$.

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Coefficient approximation methods: advantages

- 1 The approximating problem has, like the original, an infinite spectrum.
- 2 The accuracy is maintained or even improves when k increases.
- 3 The mesh is fixed before the start of the shooting process and is used for all eigenvalue calculations (= big speed advantage).

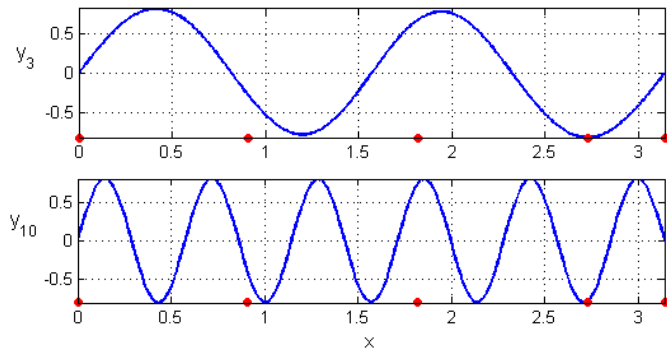


Illustration: the Mathieu problem

$$y'' = [2 \cos(2x) - E]y, \quad y(0) = y(\pi) = 0.$$

- The French mathematician E.L. Mathieu investigated this equation in 1868 while seeking a description of the vibrations of an elliptical membrane (drumheads).
- MATSLISE:
 - Matlab package for the numerical solution of Sturm-Liouville and Schrödinger problems.
 - Based on high order constant perturbation methods.
 - V. Ledoux, M. Van Daele and G. Vanden Berghe, ACM Trans. on Math. Software, 31 (2005).

The Mathieu problem in MATSLISE

Mathieu: eigenvalues

File Edit Help

Input

Indices between

and

Eigenvalues between

and

Calculate eigenvalues >> Stop

Results

Index	Eigenvalue	Estimated Error
0	-0.110248816990686	1.5e-12
1	3.917024772996808	-1.7e-12
2	9.047739259806463	-2.9e-12
3	16.032970081401817	-3.9e-12
4	25.020840823283084	-6.5e-12
5	36.014289910623226	-4.9e-12
6	49.010418249428675	4.9e-12
7	64.007937189252345	2.4e-12
8	81.006250326637215	4.5e-12
9	100.005050675169190	9.5e-12
10	121.004166761273440	4.2e-12

Select All Plot Eigenfunction Workspace

Succeeded -- calculated 11 eigenvalues in 0.20 (s) time

Help Close

input tolerance = 10^{-12}

The Mathieu problem in MATSLISE

Mathieu: eigenvalues

File Edit Help

Input

Indices between

100 and 110

Eigenvalues between

Calculate eigenvalues >> Stop

Results

Index	Eigenvalue	Estimated Error
100	10201.000049019611000	2.3e-12
101	10404.000048063062000	2.3e-12
102	10609.000047134241000	2.4e-12
103	10816.000046232088000	2.4e-12
104	11025.000045355589000	2.4e-12
105	11236.000044503788000	2.5e-12
106	11449.000043675755000	-2.5e-12
107	11664.000042870619000	2.6e-12
108	11881.000042087546000	2.6e-12
109	12100.000041325731000	-2.7e-12
110	12321.000040584418000	-2.7e-12

Select All Plot Eigenfunction Workspace

Succeeded -- calculated 11 eigenvalues in 0.21 (s) time

Help Close

input tolerance = 10^{-12}

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Summary

- Discretization methods reduce the Sturm-Liouville problem to a matrix eigenproblem.
 - They are very simple to set up and have been widely used in practice.
 - There have been many advances in such methods: AAdHP correction,...
 - However, for the calculation of high eigenvalues many stepsizes are needed.
- Constant perturbation methods are well suited to be used in a shooting procedure
 - uniform accuracy over the whole eigenvalue-range.
 - large stepsizes (due to the E -independent mesh).