Efficient computation of Sturm-Liouville eigenvalues using modified Neumann schemes

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The Sturm-Liouville problem

Jacques Sturm (1803-1855)

Joseph Liouville (1809-1882)

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

The Sturm-Liouville problem

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

- One-dimensional model of many important physical processes which often exhibit a pronounced oscillatory behaviour
  - behaviour of pendulum-like systems
  - vibrations
  - resonances
  - wave propagation
- Description of quantum mechanical systems (atoms, transistors): the Schrödinger equation

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

The Sturm-Liouville 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):

$$\begin{cases} a_0 y(a) + b_0 p(a) y'(a) = 0, \\ a_1 y(b) + b_1 p(b) y'(b) = 0 \end{cases}$$

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

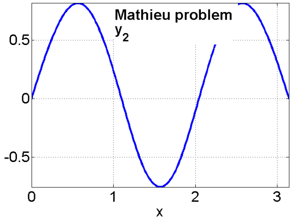
Oscillatory character of the eigenfunctions

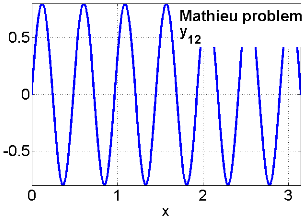
For a regular Sturm-Liouville problem

- The E_k can be ordered as an increasing sequence tending to infinity,

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

- The eigenfunction $y_k(x)$ corresponding to E_k has exactly k zeros on (a, b).
- A higher eigenfunction is oscillating 'more rapidly' than a lower eigenfunction.





Numerical solution of SLPs

Naive methods

- The oscillatory behaviour of the solutions forces a standard integrator to take increasingly smaller steps.

Coefficient approximation

- Special techniques are needed which adequately take into account the oscillatory character of the solution.
- Replace the diff. eq. (piecewisely) by a diff. eq. which can be solved exactly.

Approximation of the solution (classical methods)	→	Approximation of the equation (coefficient approximation)

Coefficient approximation methods

$$-(p(x)y'(x))' + q(x)y(x) = Ew(x)y(x)$$

p, q, w are replaced piecewisely by **low degree polynomials**

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Constants (Pruess method)

S. Pruess and C. T. Fulton, ACM Trans. Math. Software 19 (1993)

- The problem is solved analytically on the piecewise-constant intervals
- Eigenvalues E_k are computed in a shooting process
- The accuracy is maintained or even improves when k increases.
- But only second order

Coefficient approximation methods

$$-(p(x)y'(x))' + q(x)y(x) = Ew(x)y(x)$$

p, q, w are replaced piecewisely by **low degree polynomials**

Higher order polynomials?

- Analytic integration not so easy
- Schrödinger: piecewise perturbation methods

  L. Gr. Ixaru, H. De Meyer and G. Vanden Berghe, JCAM 88 (1997)
  V. L., M. Van Daele and G. Vanden Berghe, CPC 162 (2004)

  ...
- General SLP: Modified Neumann schemes

Neumann expansion

Consider a matrix linear ODE

$$y' = A(t)y, \quad y(0) = y_0 \in \mathbb{R}$$

The Neumann expansion is

$$\begin{aligned} y(t) = & y_0\Big(1 + \int_0^t A(\tau)\mathrm{d}\tau + \int_0^t A(\tau)\int_0^\tau A(\tau_1)\mathrm{d}\tau_1\mathrm{d}\tau \\ & + \int_0^t A(\tau)\int_0^\tau A(\tau_1)\int_0^{\tau_1} A(\tau_2)\mathrm{d}\tau_2\mathrm{d}\tau_1\mathrm{d}\tau + \dots\Big) \end{aligned}$$

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- A SLP can be written in the form $Y' = A(x)Y$:

$$\begin{bmatrix} y(x) \\ p(x)y'(x) \end{bmatrix}' = \begin{bmatrix} 0 & 1/p(x) \\ q(x) - Ew(x) & 0 \end{bmatrix} \begin{bmatrix} y(x) \\ p(x)y'(x) \end{bmatrix}.$$

- Apply Neumann series integrator directly?

The modified Neumann method

Iserles (2002), Degani and Schiff (2006): when the solution of $y' = A(x)y$ oscillates rapidly, a modified scheme should be used

Over each step:

- The variables are changed locally:

$$Y(x) = e^{(x-x_i)\bar{A}} U(x - x_i), \quad x \in [x_i, x_{i+1}]$$

  where

$$\bar{A}(E) = \begin{bmatrix} 0 & 1/\bar{p} \\ \bar{q} - E\bar{w} & 0 \end{bmatrix}$$

  i.e. we precondition Y locally by the known solution of a linear system with constant coefficients.

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- We solve

$$U'(\delta) = B(\delta)U(\delta), \quad U(0) = Y_i, \quad \delta = x - x_i \in [0, h_i]$$

  by the Neumann method

The modified Neumann method

The new linear system $U'(\delta) = B(\delta)U(\delta)$ has some crucial advantages over the original system:

- The entries of $B = e^{-\delta\bar{A}}\left(A(x_i + \delta) - \bar{A}\right)e^{\delta\bar{A}}$ are rapidly oscillating functions.
- Integration is a "smoothing" operator:
  The faster B oscillates, the smaller are the Neumann integrals, thus the faster the convergence and the smaller the error

The modified Neumann scheme

Over interval step size h:

1. $U(h) = Y_i + \int_0^h B(x)dx Y_i + \int_0^h \int_0^{x_1} B(x_1)B(x_2)dx_2 dx_1 Y_i + \ldots$
2. $Y_{i+1} = e^{h\bar{A}} U(h)$

Note: $e^{h\bar{A}}$ is known solution of system with constant coeff. functions

Practical Implementation

- Truncation of the integral series
- Replacement of integrals by quadrature:
    - Classical methods useless in the presence of high oscillation
    - Filon quadrature delivers accuracy which improves with higher oscillation. (A. Iserles, S. Nørsett,...)

Results: Collatz problem

$$y'' + \frac{3}{4x^2} y = -\frac{1}{x^6} E y \quad \text{in } [1,2],\ y(1) = y(2) = 0.$$

Collatz			
k	E_k	Pruess	MNM6
0	70.1836836876	2.1(-6)	1.9(-9)
25	47444.18579306	2.1(-6)	5.0(-6)
50	182548.2030025	2.1(-6)	3.3(-6)
75	405381.9379249	2.1(-6)	3.1(-6)
100	715945.489746	2.2(-6)	4.1(-6)
125	1114238.858465	2.2(-6)	3.0(-6)
150	1600262.044083	2.3(-6)	7.5(-7)
nsteps		1024	32
nfevs		3072	288

Table: The relative errors in some eigenvalue approximations computed by the second order Pruess method and the sixth order Modified Neumann Method (MNM6). The notation a(-b) stands for $a\,10^{-b}$.

Results: Paine problem

$$p(x) = (\gamma + x)^3, \quad q(x) = 4(\gamma + x), \quad w(x) = (\gamma + x)^5, \quad \gamma = \sqrt{0.2}$$

$$y(0) = y(-\gamma + \sqrt{\gamma^2 + 2\pi}) = 0$$

	Paine		
k	E_k	Pruess	MNM6
0	1.5198658211	3.4(-6)	1.2(-9)
5	37.9644258619	5.6(-6)	6.0(-8)
10	123.4977068009	6.0(-6)	2.1(-7)
20	443.8529598352	6.2(-6)	7.1(-7)
30	963.9644462621	6.2(-6)	1.7(-6)
40	1684.0120143379	6.2(-6)	2.4(-6)
50	2604.0363320246	6.2(-6)	5.2(-6)
nsteps		1024	48
nfevs		3072	432

Table: The relative errors in some eigenvalue approximations computed by the second order Pruess method and the sixth order Modified Neumann Method (MNM6).

Results: Collatz problem

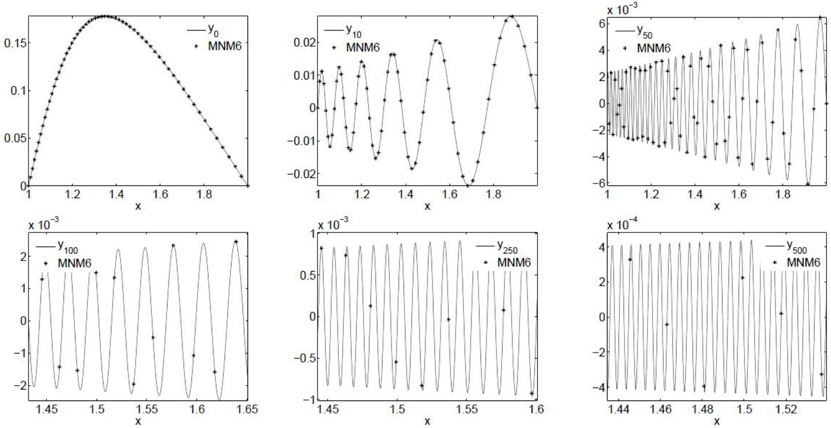

FIG. 6.1. *Sample eigenfunction computations of Collatz problem for* $k = 0, 10, 50, 100, 250, 500$. *For* $k = 100, 250, 500$ *only part of the eigenfunction is shown. The mesh contains only 31 mesh points.*

Summary

- For high eigenvalues the solution is severly oscillatory and standard numerical integrators have to advance in small steps.
- Better results are obtained using coefficient approximation methods in a shooting procedure.
- Neumann series integrators allow the construction of higher order coefficient approximation methods.
    - modified schemes should be used.
    - “Oscillation-proof” quadrature
    - Can be applied directly to a Sturm-Liouville problem (no expensive Liouville’s transformation needed)