MATSLISE, a Matlab package for solving Sturm-Liouville and Schrodinger equations

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MATSLISE

This talk is based on the paper

V. Ledoux, M. Van Daele

Solving Sturm-Liouville problems
by piecewise perturbation methods, revisited

Computer Physics Communications **181** (2010) 1335-1345.

MATSLISE is a Matlab package that has been developed by Veerle Ledoux under the supervision of Guido Vanden Berghe and VD in a close collaboration with Liviu Ixaru (Bucharest).

Outline

Sturm-Liouville problems

Find an eigenvalue E and corresponding eigenfunction $y(x)$ $\not\equiv 0$ such that

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

with boundary conditions

$$a_1 y(a) + a_2 p(a) y'(a) = 0, \quad b_1 y(b) + b_2 p(b) y'(b) = 0,$$

where $|a_1| + |a_2| \neq 0 \neq |b_1| + |b_2|$.

J.D. Pryce, Numerical Solution of Sturm-Liouville Problems, Oxford University Press, 1993

Regular Sturm-Liouville problems

The eigenvalues of a regular SLP can be ordered as an increasing sequence tending to infinity

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

E_k has index k.

The corresponding $y_k(x)$ has exactly k zeros on the open interval (a, b).

Distinct eigenfunctions are orthogonal with respect to $w(x)$

$$\int_a^b y_i(x) y_j(x) w(x) dx = 0, \quad i \neq j.$$

Special case : for the Schrödinger equation $p = w = 1$ (this is the so-called normal form of an SLP).

Singular Sturm-Liouville problems

The integration interval (a, b) may be infinite,

or at least one of the coefficients p^{-1}, q or w may not be integrable up to one of the endpoints . . .

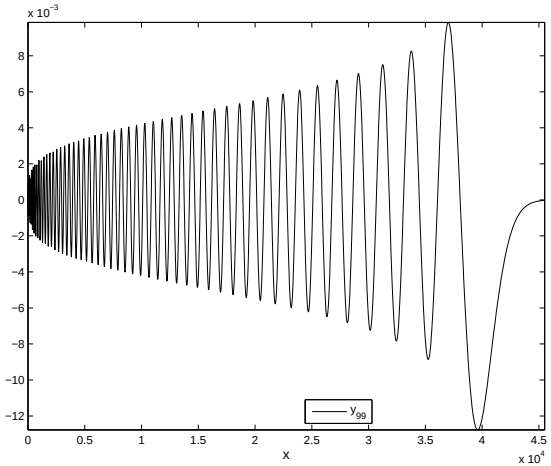
For SLP, there is an important classification : problems may be regular or singular, limit point or limit circle, oscillatory or non-oscillatory. Problems may have a discrete spectrum or a continuous set of eigenvalues, etc.

At the moment, not all singular problems can be solved by MATSLISE, but since we started with the MATSLISE project, we managed to tackle more and more problems . . .

In this talk, we mainly concentrate on regular problems.

How to solve Sturm-Liouville problems

Problem: as the index k increases, the corresponding y_k become increasingly oscillatory.



Standard numerical methods for ODEs encounter difficulties in efficiently estimating the higher eigenvalues.

Naive integrators will be forced to take increasingly smaller steps, thereby rendering them exceedingly expensive.

Matrix methods

Consider the SL problem in normal form :

$$-y'' + q(x)\,y = E\,y \qquad y(0) = y(\pi) = 0 \tag{1}$$

Solving this problem with the Numerov method leads to

$$A\,v + B\,Q\,v = \Sigma\,B\,v \tag{2}$$

of size N, whereby $(N+1)\,h = \pi$

The eigenvalues $E_1 < E_2 < E_3 < \cdots$ of (1) are approximated by the eigenvalues $\tilde{E}_1 < \tilde{E}_2 < \tilde{E}_3 < \cdots < \tilde{E}_N$ of (2).

$$|\tilde{E}_k - E_k| = \mathcal{O}(k^6\,h^4)$$

Several correction techniques were developed (asymptotic correction by Paine, de Hoog and Anderssen; EF by Vanden Berghe and De Meyer; ...)

Exponentially-fitting matrix methods

To obtain a better approximation for E_k we first compute ω_n^2 from the error-expression of the EF Numerov method

$$y_k^{(6)}(t_n)+\omega_n^2\, y_k^{(4)}(t_n) = 0, \qquad n = 1, \ldots, N\,.$$

Then, we solve the problem with the EF Numerov method. This leads to

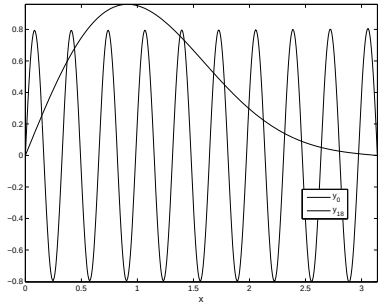
$$A_{EF}\, v + B_{EF}\, Q\, v_{EF} = \Sigma_{EF}\, B_{EF}\, v_{EF} \tag{3}$$

The eigenvalues $E_1 < E_2 < E_3 < \cdots$ of (1) are approximated by the eigenvalues $E_{EF,1} < E_{EF,2} < E_{EF,3} < \cdots < E_{EF,N}$ of (3).

$$|E_{EF,k} - E_k| = \mathcal{O}(k^3\, h^4)$$

Example : the Paine problem

$$-y'' + \exp(x)\, y = E\, y \qquad y(0) = y(\pi) = 0$$



The errors ($\times 10^3$) obtained with the Numerov algorithm, the Numerov method with correction technique and the EF-Numerov scheme.

k	E_k	$10^3\,(E_k - \tilde{E}_k)$	$10^3\,(E_k - \tilde{E}_{CT,k})$	$10^3\,(E_k - E_{EF,k})$
0	4.8966694	0.0028	0.0027	0.0014
2	16.019267	0.2272	0.1114	0.0424
4	32.263707	2.8802	0.3879	0.1959
6	56.181594	19.687	0.8159	0.4535
8	88.132119	87.276	1.4108	0.8115
10	128.10502	290.92	2.1961	1.2859
12	176.08900	797.57	3.2082	1.9073
14	232.07881	1898.8	4.5015	2.6947
16	296.07196	4063.9	6.1589	3.7168
18	368.06713	8000.6	8.3076	5.0273

How to solve Sturm-Liouville problems

Taking into account the characteristic features of the SL problem, one can construct specialized numerical algorithms having some crucial advantages over general-purpose codes.

Some early codes (from the nineties) on SLP :
SLEIGN (Bailey et al.), SLEDGE (Fulton-Pruess),
SL02F (Marletta-Pryce)
SLCP12 (Ixaru-Vanden Berghe-De Meyer)

MATSLISE originates from SLCP12.

In the next slides we focus on the special techniques used in SLCP12.

Shooting methods

Shooting methods transform the boundary value problem into an initial value problem.

One solves the differential equation for a succession of trial values of E which are adjusted till the boundary conditions at both ends can be satisfied at once, at which point we have an eigenvalue.

The simplest technique is to shoot from a to b, but multiple shooting is preferred.

Shooting methods

One chooses initial conditions for a function

- $y_L(x, E)$ which satisfy the boundary condition in a:

$$y_L(a, E) = -a_2, \quad p(a)y_L'(a, E) = a_1$$

- $y_R(x, E)$ which satisfy the boundary condition in b:

$$y_R(b, E) = -b_2, \quad p(b)y_R'(b, E) = b_1$$

and one searches for a value of E for which, at a matching point x_m, both functions and their first derivatives agree, i.e. we have find the roots of the mismatch function

$$\phi(E) = y_L(x_m, E)p(x_m)y_R'(x_m, E) - y_R(x_m, E)p(x_m)y_L'(x_m, E).$$

Prüfer transformation

Suppose we have found an eigenvalue : $\phi(E) = 0$.

What is its index?

To solve this problem, we use a polar coordinate substitution, known as the (scaled) Prüfer transformation.

$$y = S^{-1/2}\rho\sin\theta, \quad py' = S^{1/2}\rho\cos\theta,$$

leading to

$$\begin{aligned}\theta' &= \frac{S}{p}\cos^2\theta + \frac{(Ew-q)}{S}\sin^2\theta + \frac{S'}{S}\sin\theta\cos\theta,\\ \frac{2\rho'}{\rho} &= \left(\frac{S}{p} - \frac{(Ew-q)}{S}\right)\sin 2\theta - \frac{S'}{S}\cos 2\theta.\end{aligned}$$

$$\theta(a) = \alpha, \quad \theta(b) = \beta \qquad \tan\alpha = -\frac{S(a)a_2}{a_1}, \quad \tan\beta = -\frac{S(b)b_2}{b_1}.$$

Prüfer transformation

Theorem

Consider the scaled Prüfer equations of a regular SL problem. Let the boundary values α and β satisfy $\alpha \in [0, \pi)$, $\beta \in (0, \pi]$.

Then the k-th eigenvalue is the value of E giving a solution of

$$\theta' = \frac{S}{p}\cos^2\theta + \frac{(Ew - q)}{S}\sin^2\theta + \frac{S'}{S}\sin\theta\cos\theta$$

satisfying

$$\theta(a; E) = \alpha, \quad \theta(b; E) = \beta + k\pi.$$

Shooting with Prüfer mismatch function

One chooses initial conditions for a

- a function $y_L(x)$ which satisfy the boundary condition in a:

$$y_L(a) = -a_2, \quad p(a)y_L'(a) = a_1 \qquad \theta_L(a;E) = \alpha \in [0,\pi)$$

- a function $y_R(x)$ which satisfy the boundary condition in a:

$$y_R(b) = -b_2, \quad p(b)y_R'(b) = b_1 \qquad \theta_R(b;E) = \beta \in [0,\pi)$$

and E_k is the unique value for which,at a matching point x_m, $\phi(E) = k\,\pi$, whereby

$$\phi(E) = \theta_L(x_m;E) - \theta_R(x_m;E)$$

is the Prüfer mismatch function.

Solving the θ equation

The SLEIGN code (and its successor SLEIGN2) e.g. uses an (explicit) Runge-Kutta method to integrate

$$\theta' = \frac{S}{p}\cos^2\theta + \frac{(Ew - q)}{S}\sin^2\theta + \frac{S'}{S}\sin\theta\cos\theta$$

However, this equation may becomes stiff ...

This problem can be circumvented if the equation can be solved analytically.

Therefore we need an extra technique:

coefficient approximation.

Coefficient Approximation methods

Basic idea : replace the coefficient functions $p(x)$, $q(x)$, $w(x)$ of the SL equation piecewisely by low degree polynomials so that the resulting equation can be solved analytically.

Gordon (1969), Canosa and De Oliveira (1970), Ixaru (1972), Pruess (1973)

The Pruess method

Let $a = x_0 < x_1 < x_2 < \cdots < x_n = b$ be a partition of $[a, b]$.

Replace

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

in the interval (x_{i-1}, x_i), $i = 1, \ldots, n$ by

$$-(\bar{p}y'(x))' + \bar{q}y(x) = E\bar{w}y(x).$$

where $\bar{p}$, $\bar{q}$, $\bar{w}$ are constant.

The Pruess method

The solution y of this approximating problem over $[x_{i-1}, x_i]$ is then advanced by the relation

$$\begin{pmatrix} y(x_i) \\ p(x_i)y'(x_i) \end{pmatrix} = \begin{pmatrix} \xi(Z) & h\eta_0(Z)/\bar{p} \\ \bar{p}Z\,\eta_0(Z)/h & \xi(Z) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix}$$

$$Z = h^2(\bar{q} - E\bar{w})/\bar{p}$$

The functions ξ and η_0 are introduced by Ixaru (1984).

Ixaru's basis functions ξ and η_0

$$\xi(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \leq 0 \\ \cosh(Z^{1/2}) & \text{if } Z > 0 \end{cases}$$

$$\eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 \end{cases}$$

The Pruess method

The solution y is advanced by

$$\begin{pmatrix} y(x_i) \\ p(x_i)y'(x_i) \end{pmatrix} = \begin{pmatrix} \xi(Z) & h\eta_0(Z)/\bar{p} \\ \bar{p}Z\eta_0(Z)/h & \xi(Z) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix}$$

and inverse of the transfer matrix is easily obtained :

$$\begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix} = \begin{pmatrix} \xi(Z) & -h\eta_0(Z)/\bar{p} \\ -\bar{p}Z\eta_0(Z)/h & \xi(Z) \end{pmatrix} \begin{pmatrix} y(x_i) \\ p(x_i)y'(x_i) \end{pmatrix}$$

Both relations can then be used in a shooting process, as in Pruess's Fortran solver SLEDGE

Convergence and error analysis of CA methods

S. Pruess, Estimating the eigenvalues of Sturm-Liouville problems by approximating the differential equation. SIAM J. Numer. Anal., 10 (1973) 55-68.

For CA methods based on piecewise polynomials of degree m the following holds when applied to SL problems:

- $|E_k - \tilde{E}_k| \leq C_k\, h^{2m+2}$.
- for the Pruess method ($m = 0$) this means $|E_k - \tilde{E}_k| \leq C\, h^2\, |E_k|$, but in practice $|E_k - \tilde{E}_k| \leq C\, h\, |E_k|$
- the relative error in E_k is of order $\mathcal{O}(h^{m+1})$, and is thus independent of k.

For problems in Schrödinger form, there is an improved error bound :

- For the Pruess method ($m = 0$) : $|E_k - \tilde{E}_k| \leq C\, h^2\, |E_k|/k$.

The Pruess method - SLEDGE

Advantage of the Pruess method: the step size is not restricted by the oscillations in the solution.

Drawback: step sizes must be sufficiently small such that the error introduced by the approximation by piecewise constants is not too large.

For problems with strongly varying coefficient functions the number of intervals in a mesh can be quite large.

Conclusion: higher order CA methods are needed.

How to construct higher order CA methods?

Important contributions :

- Constant perturbation methods, especially designed for SL problems in normal form (i.e. Schrödinger problems)
- Constant perturbation methods, designed for general SL problems
- integral series methods such as modified Neumann methods, directly applicable to regular SL problems

PPM for Schrödinger problems

Constant perturbation methods and Line Perturbation methods are particular cases of Piecewise Perturbation Methods.

Piecewise Perturbation Methods (PPM) are based on an idea from mathematical physics: the perturbation approximation.

These PPM are CA methods : the original differential equation is replaced piecewisely by another differential equation, the reference equation, which can be solved exactly.

Some perturbation corrections are then added to the solution of the reference equation, which gives a more accurate approximation to the solution of the original equation.

PPM for Schrödinger problems

The PPM are identified by the type of piecewise approximation:

- if the coefficients are approximated by piecewise constants the method is referred to as a constant perturbation method (CPM)
- if piecewise lines are used the method is called a line perturbation method (LPM)

The CPM are generally considered to be more convenient for applications than the LPM.

PPM for Schrödinger problems

$$y'' = (q(x) - E)y\,, \quad x \in [a,b]\,, \quad y(a) = \alpha, \quad y'(a) = \beta\,,$$

where $q(x)$ is supposed to be a well behaved function.

On the mesh interval $[x_{i-1}, x_i]$ we rewrite this problem as

$$y''(\delta) = (q(x_{i-1} + \delta) - E)y(\delta)\,, \quad \delta \in [0,h]\,.$$

Suppose $u(\delta)$ and $v(\delta)$ are two linear independent solutions of the local problem with the initial values $y(0) = 1, y'(0) = 0$ for u and $y(0) = 0, y'(0) = 1$ for v.

Then the solution is advanced by the algorithm

$$\begin{pmatrix} y(x_i) \\ y'(x_i) \end{pmatrix} = \begin{pmatrix} u(h) & v(h) \\ u'(h) & v'(h) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix}, \quad h = x_i - x_{i-1}.$$

PPM for Schrödinger problems

$$y''(\delta) = (q(x_{i-1} + \delta) - E)y(\delta), \quad \delta \in [0, h]$$

$$\begin{pmatrix} y(x_i) \\ y'(x_i) \end{pmatrix} = \begin{pmatrix} u(h) & v(h) \\ u'(h) & v'(h) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix}, \quad h = x_i - x_{i-1}.$$

The inverse propagation algorithm is given by

$$\begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix} = \begin{pmatrix} v'(h) & -v(h) \\ -u'(h) & u(h) \end{pmatrix} \begin{pmatrix} y(x_i) \\ y'(x_i) \end{pmatrix}.$$

The knowledge of the propagators u and v and their first derivatives is thus sufficient to advance the solution in both directions.

PPM for Schrödinger problems

However, analytic forms of these u and v are known only for a restricted number of expressions for the function $q(x)$, let such functions be denoted by $\bar{q}(x)$.

The idea is to replace $q(x)$ piecewisely by a $\bar{q}(x)$. The propagators corresponding to this approximating problem are called the reference propagators and denoted by $\bar{u}$ and $\bar{v}$.

To further improve the accuracy, some extra correction terms, which are derived from the perturbation $\Delta_q = q(x) - \bar{q}(x)$, are added to $\bar{u}$ and $\bar{v}$.

From this point on, we assume that we apply constant approximations.

Theorem 1: CPM algorithm for Schrödinger problems

The solution of

$$y''(\delta) = (q(x_{i-1} + \delta) - E)y(\delta), \quad \delta \in [0, h]$$

with the initial conditions $y(x_{i-1}) = \alpha$ and $y'(x_{i-1}) = \beta$ can be written as

$$\begin{pmatrix} y(x_{i-1} + \delta) \\ y'(x_{i-1} + \delta) \end{pmatrix} = \begin{pmatrix} u(\delta) & v(\delta) \\ u'(\delta) & v'(\delta) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix}$$

where u and v are written as perturbation series:

$$u(\delta) = \sum_{k=0}^{\infty} u_k(\delta), \; v(\delta) = \sum_{k=0}^{\infty} v_k(\delta).$$

...

Theorem 1: CPM algorithm for the Schrödinger problem

...

The zeroth order propagators are exactly the reference propagators:

$$u_0(\delta) = \bar{u}(\delta) = \xi(Z(\delta)) \qquad v_0(\delta) = \bar{v}(\delta) = \delta\eta_0(Z(\delta)),$$
$$u_0'(\delta) = \bar{u}'(\delta) = Z(\delta)\eta_0(Z(\delta))/\delta \qquad v_0'(\delta) = \bar{v}'(\delta) = \xi(Z(\delta))$$

with $Z(\delta) = (\bar{q} - E)\delta^2$.

The correction terms ($z = u, v$, $k = 1, 2, \ldots$) are computed as follows:

$$z_k'' = (\bar{q} - E)z_k + \Delta_q(\delta)z_{k-1}\,, \quad z_k(0) = z_k'(0) = 0\,.$$

Ixaru's basis functions

For the construction of the perturbation corrections, some additional functions have to be defined first:

$$\begin{aligned} \eta_1(Z) &= [\xi(Z) - \eta_0(Z)]/Z, \\ \eta_m(Z) &= [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z, \quad m = 2, 3, \ldots. \end{aligned}$$

For negative Z, the function $\eta_m(Z)$ is an oscillating function whose amplitude damps out when $Z \to -\infty$.

For positive Z, all these functions increase exponentially with Z.

It will become clear that $\{\eta_m | m = 0, 1, \ldots\}$ is a suitable basis to develop higher order CP methods.

Theorem 2: CPM algorithm for the Schrödinger problem

If the potential function $q(\delta)$ is a polynomial in δ, then

$$\begin{aligned} z_k(\delta) &= \sum_{m=0} C_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)), \\ z_k'(\delta) &= C_0(\delta)\xi(Z(\delta)) + \sum_{m=0}[C_m'(\delta) + \delta C_{m+1}(\delta)]\delta^{2m+1}\eta_m(Z(\delta)) \end{aligned}$$

with a finite number of terms.
This means that the product $\Delta_q z_{k-1}$ is of the form

$$\Delta_q(\delta)z_{k-1}(\delta) = G(\delta)\xi(Z(\delta)) + \sum_{m=0} S_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)),$$

...

Theorem 2: CPM algorithm for the Schrödinger problem

...

and the coefficients $C_0(\delta), C_1(\delta), \ldots$ are then polynomials in δ which are given by quadrature

$$
\begin{aligned}
C_0(\delta) &= \frac{1}{2}\int_0^\delta G(\delta_1)d\delta_1, \\
C_m(\delta) &= \frac{1}{2}\delta^{-m}\int_0^\delta \delta_1^{m-1}[S_{m-1}(\delta_1) - C''_{m-1}(\delta_1)]d\delta_1, \quad m = 1, 2, \ldots
\end{aligned}
$$

in $\Delta_q u_0(\delta)$: $G(\delta) = \Delta_q(\delta), S_0(\delta) = S_1(\delta) = \cdots = 0$
in $\Delta_q u_0(\delta)$: $G(\delta) = 0, S_0(\delta) = \Delta_q(\delta), S_1(\delta) = S_2(\delta) = \cdots = 0$.

How to compute the integrals?

How to ensure that the correction terms $z_k(\delta)$ have an analytic solution?

There is an intermediate stage in the procedure in which $q(x_{i-1}+\delta)$ is approximated by a polynomial (expressed in terms of shifted Legrendre functions) in δ:

$$q(x_{i-1}+\delta) \approx \sum_{n=0}^{\nu-1} Q_n h_i^n P_n^*(\delta/h_i), \quad \delta = x - x_{i-1}.$$

$$\text{whereby } Q_n = \frac{(2n+1)}{h_i^{n+1}} \int_0^h q(x_{i-1}+\delta) P_n^*(\delta/h_i) d\delta.$$

We then take $\bar{q} = Q_0$ and $\Delta_q(\delta) \approx \sum_{n=1}^{\nu-1} Q_n h_i^n P_n^*(\delta/h_i)$.

The integrals are then computed using ν-point Gauss-Legendre quadrature.

CPM[N,Q] : Convergence results

Let N be the degree of the polynomial approximating $q(x)$ and let Q be the number of correction terms. The corresponding CPM method is denoted is CPM[N,Q].

L.Gr. Ixaru, H. De Meyer and G. Vanden Berghe, CP methods for the Schrödinger equation, revisited, *J. Comput. Appl. Math.* **88** (1997) 289–314.

The error in the eigenvalue E_k, obtained with CPM[N,Q],

- is of order $\mathcal{O}(h^{2N+2})$ for small E if $Q \geq \lfloor \frac{2}{3}N \rfloor + 1$
- is of order $\mathcal{O}(h^{2N})/\sqrt{E}$ for large E if $Q \geq \delta_{N0}$

Liouville's transformation

The CP methods developed so far can only be applied to SLP in normal form, i.e. Schrödinger problems.

They can be applied to an SLP only if the SL equation

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

can be converted to the Schrödinger form

$$-z''(u) + V(u)z(u) = Ez(u)\,.$$

The conversion is possible and is achieved via the so-called Liouville's transformation:

$$u = \int_a^x \sqrt{w(x)/p(x)}\,dx\ .$$

Then $y(x) = m(x)z(u(x))$.

The Schrödinger problem has the same eigenvalues as the original SL problem.

CPM for SL problems

The CPM were extended to solve the more general SLP using the Liouville transformation and were implemented in the Fortran code SLCPM12.

The SLCPM-code is a method of order 12 for low energies and order 10 for high energies.

L. Gr. Ixaru, H. De Meyer, and G. Vanden Berghe. SLCPM12 - a program for solving regular Sturm-Liouville problems. Comput. Phys. Commun., 118 (1999) 259–277.

Later, the SLCPM12-code was extended to higher order methods and a Matlab package MATSLISE was produced.

V. Ledoux, M. Van Daele, and G. Vanden Berghe. Matslise, A matlab package for the numerical solution of Sturm-Liouville and Schrödinger equation. ACM Trans. Math. Software, 31 (2005), 532-554.

CPM for SL problems

The Liouville's transformation is rather expensive due to the quadrature which is needed for the conversion between old and new variables.

Moreover the transformation can only be realized for sufficiently well-behaved (and non-singular) p, q and w functions : q must be continuous and p and w should have a continuous second order derivative.

As a consequence the software packages based on CPM still have a smaller range of applicability in comparison with e.g. SLEDGE, which applies the Pruess method directly to an SL problem.

CPM for SL problems

In order to really outperform the software packages based on the second-order Pruess method, higher order CA methods must be constructed for general SL problems.

This has been done in

V. Ledoux, M. Van Daele
Solving Sturm-Liouville problems
by piecewise perturbation methods, revisited
Computer Physics Communications **181** (2010) 1335-1345.

and this algorithm (a method of order 6) will be implemented in a new version of MATSLISE (to be released in 2014).

CPM for SLP: Convergence results

V. Ledoux, M. Van Daele. Solving Sturm-Liouville problems by piecewise perturbation methods, revisited. Computer Physics Communications **181** (2010) 1335-1345.

For large eigenvalues, the error behaves like $\mathcal{O}(E)$ for general SLP.

In the special case of Schodinger problems, the error is $\mathcal{O}(|E|^{-1/2})$.

For well behaved SLP it is still a good idea to transform the problem into Schrödinger form, especially when large eigenvalues are computed.

CPM and Neumann series methods

Degani and Schiff (2006) have shown, in theory, that PPM applied to Schrödinger equations is equivalent to the application of a modified Neumann Series.

In (2010) Ledoux and V.D. have shown that, in theory, PPM applied directly to SLP is equivalent to the application of a modified Neumann Series.

However, the application of PPM is, from a computational point of view more interesting . . .

Integral series solutions

One can rewrite

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

as

$$\mathbf{y}'(x) = A(x)\mathbf{y}(\mathbf{x}), \quad \mathbf{y}(\mathbf{a}) = \mathbf{y_0},$$

with

$$A(x) = \begin{pmatrix} \mathbf{0} & \mathbf{1}/p(x) \\ q(x) - Ew(x) & \mathbf{0} \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y(x) \\ p(x)y'(x) \end{pmatrix}.$$

Integral series solutions

A Neumann series method gives the solution of

$$\mathbf{y}'(x) = A(x)\mathbf{y}(\mathbf{x}), \quad \mathbf{y}(\mathbf{a}) = \mathbf{y_0},$$

in the form of an integral series :

$$\begin{aligned}
\mathbf{y}(\delta) &= \mathbf{y}(\mathbf{0}) + \int_{\mathbf{0}}^{\delta} A(x)\,\mathbf{y}(x)dx \\
&= \mathbf{y}(\mathbf{0}) + \int_{\mathbf{0}}^{\delta} A(x)\left(\mathbf{y}(\mathbf{0}) + \int_{\mathbf{0}}^{x} A(x_{\mathbf{2}})\,\mathbf{y}(x_{\mathbf{2}})dx_{\mathbf{2}}\right)dx \\
&= \ldots
\end{aligned}$$

When the solution of a linear system $\mathbf{y}' = A(x)\mathbf{y}$ oscillates rapidly, a Neumann method should not be applied directly to the problem but modified schemes should be used.

Modified Neumann series method

Suppose that we have already computed $\mathbf{y}_{i-1} \approx \mathbf{y}(x_{i-1})$ and that we wish to advance the numerical solution to $x_i = x_{i-1} + h$.

The first step in the modified Neumann scheme is to change the variables locally

$$\mathbf{y}(x) = e^{(x-x_{i-1})\bar{A}}\mathbf{u}(x - x_{i-1}), \quad x_{i-1} \leq x \leq x_i$$

where $\bar{A}(E)$ is a (piecewise) constant approximation of A :

$$\bar{A}(E) = \begin{pmatrix} \mathbf{0} & \bar{P} \\ \bar{r} & \mathbf{0} \end{pmatrix}, \quad P(x) = \mathbf{1}/p(x).$$

Then

$$\mathbf{y}(x_i) = e^{h\bar{A}}\mathbf{u}(h) \qquad e^{h\bar{A}} = \begin{pmatrix} \xi(Z(h)) & h\bar{P}\eta_{\mathbf{0}}(Z(h)) \\ \dfrac{Z(h)\eta_{\mathbf{0}}(Z(h))}{h\bar{P}} & \xi(Z(h)) \end{pmatrix}.$$

Modified Neumann series method

We treat $\mathbf{u}$ as our new unknown which itself obeys the equation

$$\mathbf{u}'(\delta) = B(\delta, E)\mathbf{u}(\delta), \quad \delta \in [\mathbf{0}, h], \quad \mathbf{u}(\mathbf{0}) = \mathbf{y}_{i-\mathbf{1}}$$

where

$$B(\delta, E) = e^{-\delta\bar{A}} \left(A(x_{i-\mathbf{1}} + \delta) - \bar{A}\right) e^{\delta\bar{A}} = e^{-\delta\bar{A}} \Delta_A(\delta) e^{\delta\bar{A}}.$$

Over each interval $[x_{i-\mathbf{1}}, x_i]$, we apply a Neumann method to the modified equation $\mathbf{u}'(\delta) = B(\delta)\mathbf{u}(\delta), \mathbf{u}(\mathbf{0}) = \mathbf{y}_{i-\mathbf{1}}$:

$$\mathbf{u}_i = \mathbf{y}_{i-\mathbf{1}} + \int_{\mathbf{0}}^{h} B(x)dx\mathbf{y}_{i-\mathbf{1}} + \int_{\mathbf{0}}^{h}\int_{\mathbf{0}}^{x_{\mathbf{1}}} B(x_{\mathbf{1}})B(x_{\mathbf{2}})dx_{\mathbf{2}}dx_{\mathbf{1}}\mathbf{y}_{i-\mathbf{1}} + \ldots$$

Modified Neumann series method

$$\mathbf{u}_i = \mathbf{y}_{i-1} + \int_0^h B(x)dx\,\mathbf{y}_{i-1} + \int_0^h \int_0^{x_1} B(x_1)B(x_2)dx_2dx_1\,\mathbf{y}_{i-1} + \dots$$

The coefficients of the $B(x)$ matrix become highly oscillatory.
The integrals are computed in an efficient way making use of Filon quadrature

Modified Neumann Series method

$$\mathbf{u}_i = \mathbf{y}_{i-1} + \int_0^h B(x)dx\,\mathbf{y}_{i-1} + \int_0^h \int_0^{x_1} B(x_1)B(x_2)dx_2dx_1\,\mathbf{y}_{i-1} + \dots$$

Retaining only one term, one agains obtains the second order Pruess method.

Methods with higher order terms were constructed in

V. Ledoux and M. Van Daele, Solution of Sturm-Liouville problems using Modified Magnus schemes.
SIAM J. Sci. Comput. **32** (2010) 563.

A fourth order modified Neumann series method

Retaining one term extra term, i.e.

$$\mathbf{u}_i = \mathbf{y}_{i-\mathbf{1}} + \int_{\mathbf{0}}^{h} B(x)dx\mathbf{y}_{i-\mathbf{1}}$$

one obtains a fourth order method :

$$\begin{pmatrix} y(x_i) \\ p(x_i)y'(x_i) \end{pmatrix} = T(h) \begin{pmatrix} y(x_{i-\mathbf{1}}) \\ p(x_{i-\mathbf{1}})y'(x_{i-\mathbf{1}}) \end{pmatrix}$$

where $T(h) = e^{h\bar{A}}(I + N_{\mathbf{1}})$, with I the identity matrix and $N_{\mathbf{1}}$ the approximation of the first Neumann integral

The fourth order modified Neumann series method

The transfer T matrix is given by

$$
\begin{aligned}
u(h) &= T_{11}(h) = \xi(Z)(1 + I_1) - h\eta_0(Z)\frac{I_2}{2} \\
v(h) &= T_{12}(h) = \xi(Z)\frac{I_2}{2\bar{r}} + h\bar{P}\eta_0(Z)(1 - I_1) \\
\mu(h) &= T_{21}(h) = \bar{r}h\eta_0(Z)(1 + I_1) - \xi(Z)\frac{I_2}{2\bar{P}} \\
\nu(h) &= T_{22}(h) = h\eta_0(Z)\frac{I_2}{2} + \xi(Z)(1 - I_1)
\end{aligned}
$$

$$
I_1 = \frac{2\eta_0(Z)\xi(Z) - 1 - (2\xi(Z)^2 - 1)}{4Z}U_1
$$

$$
I_2 = -\frac{2Z\eta_0(Z)\xi(Z) + 1 - (2\xi(Z)^2 - 1)}{2hZ}U_1
$$

$$
U_1 = h^3\left((Q_1 - EW_1)\bar{P} - P_1\bar{r}\right)
$$

The fourth order CPM[1,1] method

$$
\begin{aligned}
u(h) &= \xi(Z) - \frac{U_1}{2}\eta_1(Z) \\
v(h) &= \bar{P}h\eta_0(Z) \\
h\bar{P}\mu(h) &= Z\eta_0(Z) \\
\nu(h) &= \xi(Z) + \frac{U_1}{2}\eta_1(Z)
\end{aligned}
$$

$$
U_1 = h^3\left((Q_1 - EW_1)\bar{P} - P_1\bar{r}\right)
$$

Equivalence

As stated earlier, one can prove that the fourth order modified Neumann method and the fourth order CPM[1,1] method are equivalent.

However, the modified Neumann series methods lead to expressions which are highly nonlinear in ξ and $\eta_{\mathbf{0}}$, while the CPM methods give correction that are expressed in terms of ξ, $\eta_{\mathbf{0}}$ and $\eta_{\mathbf{1}}$.

This makes the CPM formula shorter, but a the method is also less sensitive to the numerical effect of near cancellation of large terms.

Singular problems

A reliable SLP solver should be able to solve also (most classes) of singular problems :

- infinite integration intervals
- singular endpoints

These singular problems require a special numerical treatment: an interval truncation procedure must be adopted.

Higher order CPM allow a very simple truncation algorithm for singular problems : the functions are not evaluated at the endpoints of the interval, but (for each meshinterval) in Legendre points and this effectively regularises the problem.

Conclusion

The CPM could originally only be applied on general SLP after a Liouville transformation.

Now there are CPM formulae which can be applied directly on the SL problem and which efficiently solve problems where a Liouville transformation is problematic or expensive.

Concluding remarks

For problems of the Schrödinger type, the orginal CPM for Schrödinger problems are the most efficient.

A Liouville's transformation can be a good idea for regular well-behaved SL problems, since for Schrödinger problem the error decreases with E.

The general CPM algorithms introduced in this paper are the best option for SL problems with discontinuities, singularities, or just strongly varying coefficient functions or with no second order derivatives of p and w available.

The Future of MATSLISE

The MATSLISE project started about ten years ago, based on the original CPM.

Also some singular problems with infinite intervals and specific singularities (e.g. distorted Coulomb potentials) could be handled.

The new CPM allow to solve new classes of problems, which could not be dealth with before.

A new release is planned in 2014.