

The numerical solution of Sturm-Liouville problems and Schrödinger problems using high order CP methods

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Outline

- 1 Introduction
 - Sturm-Liouville Problems (SLP)
 - Solving SLP and Schrödinger problems
- 2 Piecewise Perturbation Methods (PPM)
 - PPM for Schrödinger equations
 - CPM for Schrödinger equations
 - CPM extended to other problems
- 3 MATSLISE
 - Numerical solution of SLP and Schrödinger problems
 - Some experiments
 - Summary

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The Sturm-Liouville problem (SLP)

The classical SLP

$$-\frac{d}{dx} \left(p(x) \frac{dy}{dx} \right) + q(x)y = \lambda w(x)y, \quad a < x < b$$

- BC's: $a_0 y(a) + b_0 p(a) y'(a) = 0$,
 $a_1 y(b) + b_1 p(b) y'(b) = 0$.
- λ for which there is a nontrivial solution: **eigenvalue**
- corresponding solution y : **eigenfunction**

Aim

- calculate the set of eigenvalues
- compute the associated eigenfunctions

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The Schrödinger problem

The one-dimensional Schrödinger problem

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

- SLP with $p(x) = w(x) = 1$ and $q(x) = V(x)$
- $V(x)$: potential function
- E : energy level (**eigenvalue**)
- y : wave function (**eigenfunction**)

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Solving SLPs using the classical methods?

Classical methods for linear 2nd order diff. eqs.

- Runge Kutta (RK) or multistep methods
- piecewise polynomial approximation of the exact solution
- only applicable when h is so small that the piecewise polynomial approx. to the solution is a good approx. !!!

Special techniques for oscillatory problems

- Mathematical Physics: perturbation approximation



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



Approximation of
the **equation**
(piecew. perturb. methods)

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Perturbation approximation

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



Approximation of
the **equation**
(piecew. perturb. methods)

Basic principle

- The given diff. eq. is replaced (piecewisely) by another **reference** diff. eq. which can be solved exactly
- The deviation of the solution of the reference eq. from the solution of the original eq. is estimated by means of the **perturbation theory**

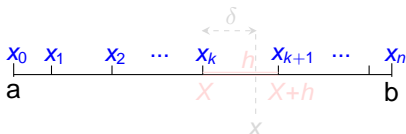
The Schrödinger equation

Initial Value Problem

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

- $V(x)$: potential (a well behaved function)
- E : energy (constant)
- Aim: construct a PPM for the calculation of y

Propagators



propagators

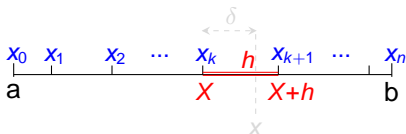
$u(\delta)$ and $v(\delta)$ with $\delta = x - X \in [0, h]$: **propagators**, i.e. solutions of

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

with the initial values

$$u(0) = 1, u'(0) = 0, v(0) = 0, v'(0) = 1.$$

Propagators



propagators

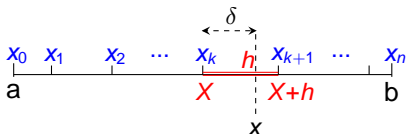
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Propagators

- 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

PPM for Schrödinger equations

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

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

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

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

- The 2 indep. solutions of (2) have known analytic forms: $u_0(\delta)$ and $v_0(\delta)$
- The desired $u(\delta)$ and $v(\delta)$ of (1) are generated by adding corrections from the perturbation

$$\Delta V(X + \delta) = V(X + \delta) - \bar{V}(X + \delta)$$

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PPM for Schrödinger equations

$$\begin{aligned}
 u(\delta) &= u_0(\delta) + \underbrace{u_1(\delta) + u_2(\delta) + \dots}_{\text{correction terms}} \\
 v(\delta) &= v_0(\delta) + \underbrace{v_1(\delta) + v_2(\delta) + \dots}_{\text{correction terms}}
 \end{aligned}$$

\uparrow $\bar{V}(X + \delta)$ \uparrow $\Delta V(X + \delta)$

- The accuracy increases with the number of correction terms included

Different PPM versions

- CPM: piecewise constant for $\bar{V}(x)$
- LPM: piecewise line for $\bar{V}(x)$
- ...

PPM for Schrödinger equations

$$\begin{aligned}
 u(\delta) &= \boxed{u_0(\delta)} + \boxed{u_1(\delta) + u_2(\delta) + \dots} \\
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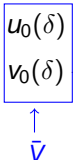
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CPM for Schrödinger equations

$$u(\delta) = u_0(\delta) + u_1(\delta) + u_2(\delta) + \dots$$

$$v(\delta) = v_0(\delta) + v_1(\delta) + v_2(\delta) + \dots$$



u_0 and v_0

- solutions of $y''(\delta) = (\bar{V} - E) y(\delta)$
- initial values $u_0(0) = 1$, $u_0'(0) = 0$, $v_0(0) = 0$, $v_0'(0) = 1$

$$u_0 = \xi(Z(\delta)), \quad v_0 = \delta \eta_0(Z(\delta)), \quad Z(\delta) = (\bar{V} - E) \delta^2$$

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\uparrow
 \bar{V}

u_0 and v_0

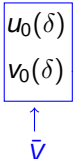
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 \bar{V}

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CPM for Schrödinger equations

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

- Set of **basic functions** in $Z(\delta) = (\bar{V} - E) \delta^2$:
 - $\xi(Z)$ and $\eta_0(Z)$
 - $\eta_1(Z) = [\xi(Z) - \eta_0(Z)]/Z$
 $\eta_m = [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z$
- These functions are all **oscillating** for negative Z

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Calculation of the corrections

$$\begin{aligned} u(\delta) &= u_0(\delta) + \boxed{u_1(\delta) + u_2(\delta) + \dots} \\ v(\delta) &= v_0(\delta) + \boxed{v_1(\delta) + v_2(\delta) + \dots} \end{aligned}$$

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 $\Delta V(X + \delta)$

Calculation of the propagators

$$u(h) = \xi(Z) + \sum_{m=1}^{\infty} C_m^{(u)} \eta_m(Z),$$

$$hu'(h) = Z\eta_0(Z) + \sum_{m=0}^{\infty} C_m^{(u')} \eta_m(Z),$$

$$v(h)/h = \eta_0(Z) + \sum_{m=2}^{\infty} C_m^{(v)} \eta_m(Z),$$

$$v'(h) = \xi(Z) + \sum_{m=1}^{\infty} C_m^{(v')} \eta_m(Z),$$

- Only contributions proportional to h^p , $p \leq P$, are retained.

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CPM for Schrödinger equations

different CPM versions: CPM{P,Q}

- order P when $Z(h) = (\bar{V} - E)h^2 \rightarrow 0$
- order Q when $-Z(h) \rightarrow +\infty$
- L.Gr. Ixaru et al. (1997): CPM{12,10}
- Higher order versions (2004): CPM{14,12}, CPM{16,14} and CPM{18,16}

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CPM extended to other problems

The CP-algorithm for the (regular) Schrödinger problem is extended to

- 1 Regular Sturm-Liouville problems
- 2 Radial Schrödinger equations with distorted coulomb potential
- 3 Systems of coupled Schrödinger equations
(not discussed here)

CPM extended to other problems

The Sturm-Liouville problem

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

Liouville's transformation:

$$x = \int_{r_{min}}^r \sqrt{w(s)/p(s)} ds$$

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

CPM extended to other problems

a problem with a distorted Coulomb potential

$$y'' = \left(\frac{l(l+1)}{r^2} + V(r) - E \right) y, \quad r > 0$$

With

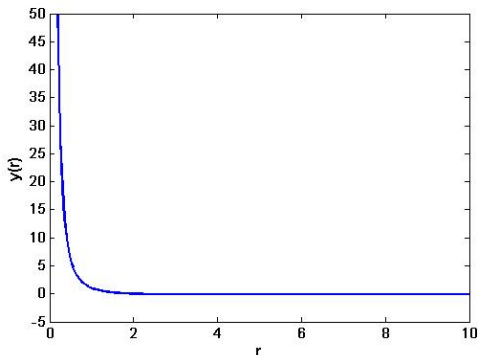
$$V(r) = \frac{S(r)}{r} + R(r)$$

Example (Hydrogen atom)

- $y''(r) = \left(\frac{2}{r^2} - \frac{1}{r} - E \right) y(r), \quad r > 0$
- $S(r) = -1, \quad R(r) = 0, \quad l = 1$

CPM extended to other problems

a problem with a distorted Coulomb potential



Hydrogen atom:
The potential function

$$\frac{2}{r^2} - \frac{1}{r}$$

CPM extended to other problems

a problem with a distorted Coulomb potential

The integration interval is split up into **two subintervals**:

- 1 A narrow subinterval around the origin: I_1
 - The algorithm to be used on I_1 is consistent with the singular nature of the problem around the origin
- 2 The remaining interval: I_2
 - cut at some large r_{\max}
 - On I_2 one of the CP algorithms is chosen

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MATSLISE

- A Matlab package for the numerical solution of
 - Regular Sturm-Liouville problems
 - Regular (one-dimensional) Schrödinger problems
 - Radial Schrödinger equations with a distorted Coulomb potential
- Computation / visualization of the **eigenvalues** and **eigenfunctions**
- Based on high order **CP-methods**
- <http://allserv.ugent.be/~vledoux/MATSLISE/>

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The Schrödinger problem in MATSLISE

Boundary Value Problem (BVP)

$$y'' = (V(x) - E)y$$

With BC's:

$$a_0 y(a) + b_0 y'(a) = 0, \quad |a_0| + |b_0| \neq 0,$$

$$a_1 y(b) + b_1 y'(b) = 0, \quad |a_1| + |b_1| \neq 0,$$

Solution of this BVP in MATSLISE (3 stages)

- 1 Construction of the partition
- 2 Eigenvalue calculation
- 3 Eigenfunction calculation

Stage 1: construction of the partition

Construction of the partition

- in terms of the tolerance required by the user (i.e. higher accuracy = more steps)
- It can be shown that (for a fixed partition) *the errors are bounded vs. energy E*
 - The partition is dictated only by the behaviour of the potential; the value of E is **NOT** involved
 - For a finite integration interval **the partition should be generated only once !** (and is never modified further on).

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Stages 2 - 3: Eigenvalues - Eigenfunctions

Calculation eigenvalues: **Shooting** procedure

- $a \rightarrow$ matching point $\leftarrow b$
- using the CP theory for IVP

Evaluation eigenfunctions

- Using the propagation matrix algorithm

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

- $y(x)$ can be evaluated for every x -value very easily

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Example 1: The Mathieu equation

Example (Mathieu equation)

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

- calculation eigenvalues
- calculation / visualization eigenfunctions
- CPM{16,14} - CPM{18,16}

The screenshot shows a software window titled "Mathieu" with a menu bar containing "File", "Options", and "Help". The main area is labeled "Input" and contains the following sections:

- 1. Potential**
 $V(x) = 2 \cdot \cos(2 \cdot x)$
- 2. Integration interval**
 $a = 0$ $b = \text{pi}$
- 3. Boundary Conditions**
 $y(a) +$ $y'(a) = 0$
 $y(b) +$ $y'(b) = 0$
- 4. Parameter**
parameter name(s) =
parameter value(s) =
- 5. Accuracy**
tol =

At the bottom of the input area are four buttons: "Construct", "Stop", "Plot potential", and "Exit". Below the input area is a status bar that says "Ready" and a scroll bar.

Example 1: The Mathieu equation

Mathieu: eigenvalues

File Edit Help

Input

Indices between

0 and 10

Eigenvalues between

Calculate eigenvalues >> Stop

Results

Index	Eigenvalue	Estimated Error
0	-0.110248816980986	1.1e-11
1	3.917024772994192	-4.7e-12
2	9.047739259778009	-3.1e-11
3	16.032970081355053	-4.9e-11
4	25.020840823258268	-3.0e-11
5	36.014289910651023	2.3e-11
6	49.010418249453139	2.8e-11
7	64.007937189280455	2.9e-11
8	81.006250326656797	2.3e-11
9	100.005050675168330	7.8e-12
10	121.004166761279820	1.1e-11

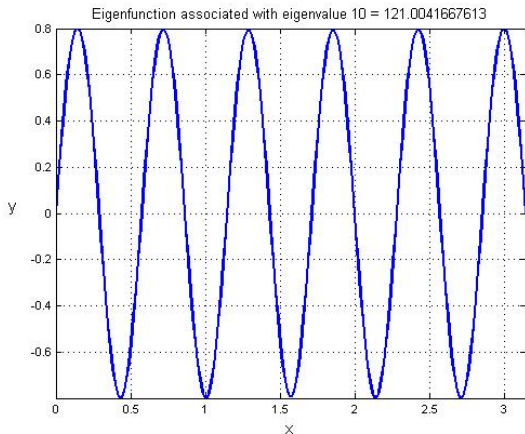
Select All Plot Eigenfunction Workspace

Succeeded -- calculated 11 eigenvalues in 0.84 (s) time

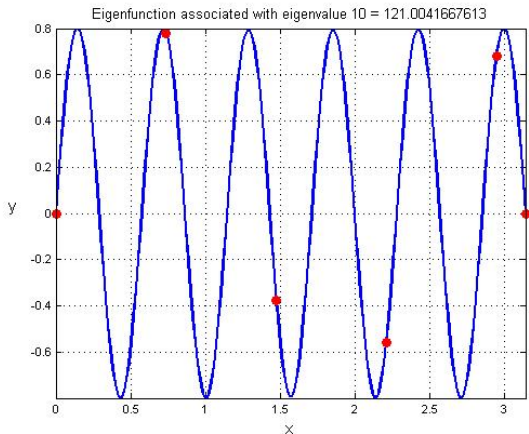
Help Close

$$tol = 10^{-8}$$

Example 1: The Mathieu equation



Example 1: The Mathieu equation



Example 2: Harmonic Oscillator

Example (Harmonic Oscillator)

$$y'' = (x^2 - E)y, \quad a = -\infty, \quad b = +\infty$$

- Exact eigenvalues: $E_k = 2k + 1, \quad k = 0, 1, \dots$

$a = -\infty, b = +\infty$ (singular endpoints)

- regularization: truncating the interval
- truncate where?

Example 2: Harmonic Oscillator

Example (Harmonic Oscillator)

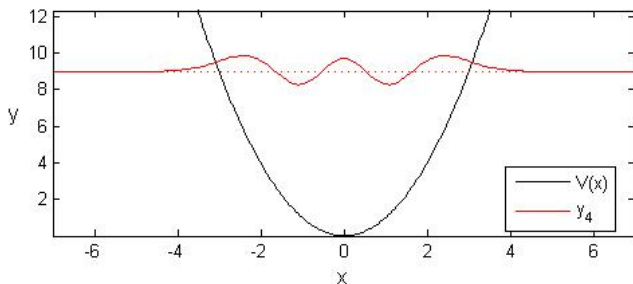
$$y'' = (x^2 - E) y, \quad a = -\infty, \quad b = +\infty$$

- Exact eigenvalues: $E_k = 2k + 1, \quad k = 0, 1, \dots$

$a = -\infty, \quad b = +\infty$ (singular endpoints)

- **regularization**: truncating the interval
- truncate where?

Example 2: Harmonic Oscillator



truncate where? **two-pass process**

- form a *cheap* estimation of the eigenvalue: E^*
- truncation point must be chosen beyond the point x where $V(x) - E^*$ becomes positive

Harmonic_oscillator

File Options Help

Input

1. Potential
 $V(x) = x^2$

2. Integration interval
a = -inf b = inf

3. Boundary Conditions
 $y(a) +$ $y'(a) = 0$
 $y(b) +$ $y'(b) = 0$

4. Parameter
parameter name(s) =
parameter value(s) =

5. Accuracy
tol = 1e-12

Construct Stop Plot potential Exit

Ready

Example 2: Harmonic Oscillator

Harmonic_oscillator: eigenvalues

File Edit Help

Input

Indices between

0 and 20

Eigenvalues between

Calculate eigenvalues >> Stop

Results

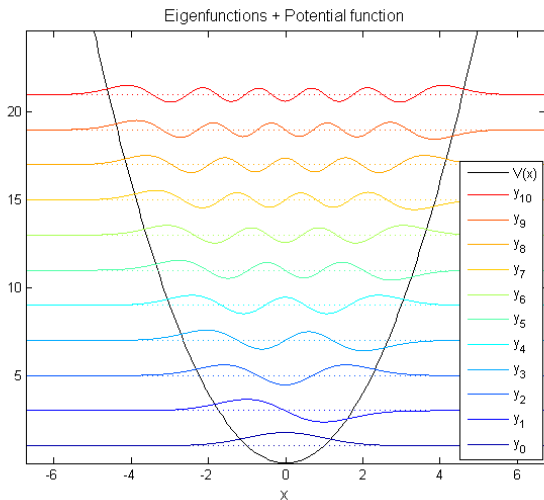
Index	Eigenvalue	Estimated Error
0	0.999999999999993	-7.0e-15
1	3.000000000000000	6.7e-16
2	5.000000000000010	8.9e-15
3	7.000000000000015	1.4e-14
4	9.000000000000016	1.1e-14
5	11.000000000000018	1.8e-14
6	13.000000000000037	3.6e-14
7	15.000000000000039	3.9e-14
8	17.000000000000032	2.9e-14
9	19.000000000000032	2.9e-14
10	21.000000000000032	2.9e-14
11	23.000000000000043	3.9e-14
12	25.000000000000071	6.4e-14
13	27.000000000000057	6.1e-14
14	29.000000000000082	7.9e-14

Select All Plot Eigenfunction Workspace

Succeeded -- calculated 21 eigenvalues in 12.42 (s) time Help Close

$$tol = 10^{-12}$$

Example 2: Harmonic Oscillator



Example 3: Hydrogen atom equation

Example (Hydrogen atom)

- $y''(r) = \left(\frac{2}{r^2} - \frac{1}{r} - E \right) y(r), \quad r > 0$
- Exact eigenvalues: $E_k = -1/(2k + 4)^2, \quad k = 0, 1, \dots$

Example 3: Hydrogen atom equation

The screenshot shows a software window titled "hydrogen: eigenvalues" with a menu bar (File, Edit, Help). The interface is divided into two main sections: "Input" and "Results".

Input Section:

- Radio button selected: "Indices between"
 - Input field 1: 10000
 - Text: and
 - Input field 2: 10000
- Radio button unselected: "Eigenvalues between"
 - Input field 1: (empty)
 - Text: and
 - Input field 2: (empty)
- Buttons: "Calculate eigenvalues >>" and "Stop" (disabled)

Results Section:

Index	Eigenvalue	Estimated Error
10000	-0.000000002499000	2.2e-16

Buttons below the table: "Select All", "Plot", "Eigenfunction", "Workspace".

Status Bar:

Succeeded -- calculated 1 eigenvalues in 235.47 (s) time

Buttons: "Help", "Close"

Example 4: A parameter example

Use of **parameters** in MATSLISE

- facilitate the input process
- study the behaviour of the eigenvalue(s) or eigenfunction(s) when the parameter changes

Example (Mathieu equation)

- $y'' = (2r \cos(2x) - E)y, \quad y(0) = 0 = y(\pi)$
- $r = 1 : 20$
- compare eigenvalues / eigenfunctions

Example 4: A parameter example

Use of **parameters** in MATSLISE

- facilitate the input process
- study the behaviour of the eigenvalue(s) or eigenfunction(s) when the parameter changes

Example (Mathieu equation)

- $y'' = (2r \cos(2x) - E)y, \quad y(0) = 0 = y(\pi)$
- $r = 1 : 20$
- compare eigenvalues / eigenfunctions

parameter_example1 {2}

File Options Help

Input

1. Potential
 $V(x) = 2^*r^*\cos(2^*x)$

2. Integration interval
a = 0 b = pi

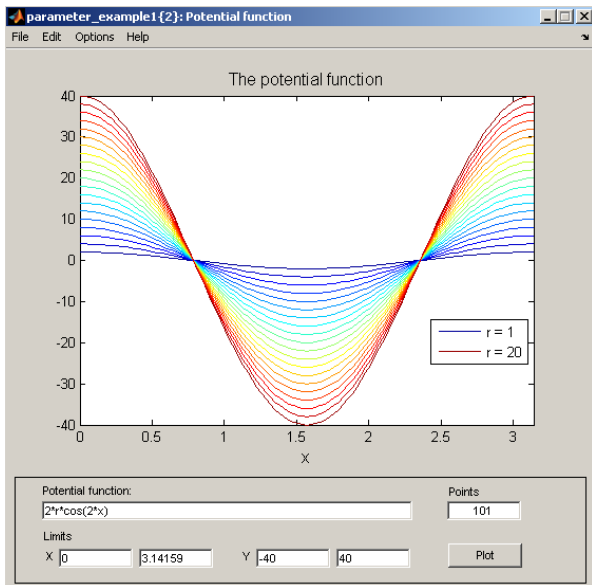
3. Boundary Conditions
 1 $y(a) +$ 0 $y'(a) = 0$
 1 $y(b) +$ 0 $y'(b) = 0$

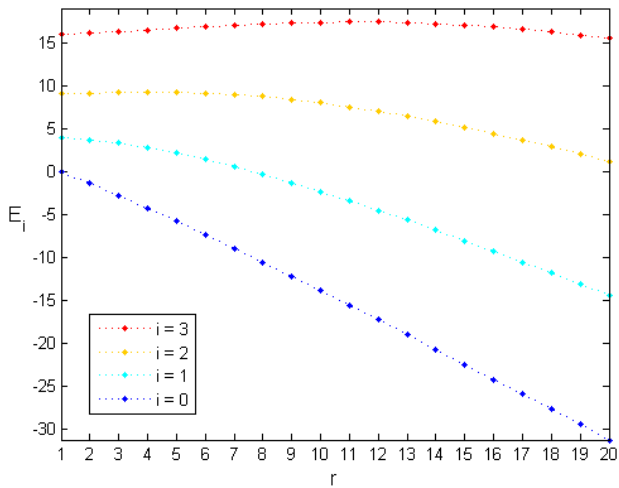
4. Parameter
parameter name(s) = r
parameter value(s) = 1:20

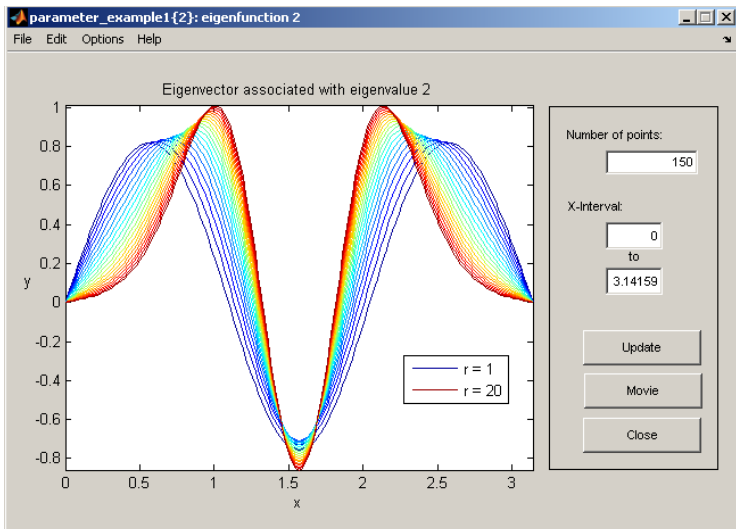
5. Accuracy
tol = 1e-8

Construct Stop Plot potential Exit

Ready







Outline

- 1 Introduction
 - Sturm-Liouville Problems (SLP)
 - Solving SLP and Schrödinger problems
- 2 Piecewise Perturbation Methods (PPM)
 - PPM for Schrödinger equations
 - CPM for Schrödinger equations
 - CPM extended to other problems
- 3 **MATSLISE**
 - Numerical solution of SLP and Schrödinger problems
 - Some experiments
 - **Summary**

Summary of the features of MATSLISE

- 1 GUI
 - simplifies input process
 - hides technical issues from the user
 - graphical features are built in
- 2 accurate eigenvalue calculation (even at high values of the eigenvalue-index)
- 3 visualization eigenfunctions
- 4 use of parameters
- 5 problems can be saved and reopened later

Outlook

- Outlook
 - other singular equations
 - systems of coupled Schrödinger equations
 - LPM
 - ...
- Some references
 - L.Gr. Ixaru, Numerical Methods for Differential Equations and Applications, Reidel, Dordrecht-Boston-Lancaster, 1984.
 - V. Ledoux, M. Van Daele and G. Vanden Berghe, CP methods of higher order for Sturm-Liouville and Schrödinger equations, *Comput. Phys. Commun.* 162 (2004).
 - V. Ledoux, M. Van Daele and G. Vanden Berghe, MATSLISE: A MATLAB package for the Numerical Solution of Sturm-Liouville and Schrödinger equations, *ACM Trans. Math. Softw.* (accepted).

Thank you for your attention...