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Abstract

Depending on the nature of the coefficients and forcing term, many differential equations cannot be solved analytically, especially, when forcing term is nonsmooth. In such cases, numerical approximations and graphical visualization of the solution are highly desirable. Spectral method based on Gauss-Legendre points is presented and implementation strategies to explicitly impose different boundary conditions is given. Techniques using several domains and solving problems with constant as well as variable coefficients are described. Various types of boundary conditions are considered, for example, Dirichlet, Dirichlet–Neumann, Neumann, and Robin. Numerical solution of several nontrivial problems having smooth as well as nonsmooth forcing terms with random Gaussian noise is computed and graphs of their exact and numerical solutions are presented.

Key words: Gauss– Legendre, Spectral, Numerical Differentiation, Boundary Value Problems.

1 Introduction

A short introduction to spectral methods with particular emphasize on practical examples having nonsmooth data is described. Several books have been written about spectral methods. Therefore our aim is not to present an exhaustive mathematical presentation of the method. With an efficient boundary conditions implementation strategy, the presented material should instead be considered as a toolkit for implementing spectral methods in simple and efficient way.

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Many differential equations cannot be solved analytically, in which case we have to satisfy ourselves with an approximation to the solution. The basic idea of all the numerical methods is to approximate a function by polynomials. Finite difference method converts BVP into system of algebraic equations by replacing the derivatives with finite difference approximations. These formulas are based on local representation of functions–usually by low–order polynomials. Derivatives are approximated at a given grid point or node through combinations of values at the neighboring points. More neighboring points are required to achieve better accuracy. Use of second order central finite difference formulas results in a tridiagonal system which is easy to solve and saves on both work and storage compared to general system of equations. But much smaller step size and many more mesh points would be required to achieve acceptable accuracy.

The spectral methods make use of global representation, usually by higher order polynomials or Fourier series. A derivative calculated at a given grid point will make use of information from the entire spatial domain of the problem. Under suitable conditions the result of spatial approximation is a degree of accuracy that local methods cannot match. In particular, they allow to reach very good accuracy with only moderate computational resources.

A collocation method is to choose a finite-dimensional space of basis functions and a mesh of points in the domain and approximates solution to BVP by finite linear combination of basis functions. Basis functions with global support, such as polynomials or trigonometric functions, yield spectral method. Mesh of points, called collocation points, can be equally spaced or Chebyshev points or Gaussian quadrature points. Since smooth basis functions can be differentiated analytically, therefore approximate solution and its derivatives can be substituted into ODE and BC to obtain system of algebraic equations. We shall use Gauss–Legendre points x_i to discretize the domain and construct a Lagrange polynomial interpolating y_i at these mesh points. The numerical solution y_i is computed such that it satisfy the given differential equation along with boundary conditions.

It would be hard to overemphasized the difficulties caused by boundary conditions in scientific computing. Boundary conditions can easily make the difference between a successful and an unsuccessful computation or between a fast and a slow one. Yet in many important cases, there is little agreement about what the proper treatment of the boundary should be. Spectral methods are affected far more than finite difference methods in the presence of boundary conditions. This can cause stability problems that are ill-understood and sometimes highly restrictive as regards time step. The reason that spectral methods have not replaced their lower-accuracy competition in most applications is the difficulty with boundaries.

Since the mesh points (Gauss–Legendre or Chebyshev) are more congested near boundaries, the spectral methods are more sensitive to boundary conditions. Boundary conditions implementation makes the method more complicated. A BVP with inhomogeneous boundary conditions can be transformed into a similar problem with homogeneous boundary conditions using a linear transformation, see (1; 2). A BVP with the Dirichlet–Neumann and Robin boundary conditions, we cannot find such transformation which make it difficult to implement spectral methods.

We are presenting implementation strategies to resolve boundary conditions issues. Using these techniques, we can not only implement inhomogeneous Dirichlet boundary conditions without transforming the problem but also implement mixed Dirichlet–Neumann or Robin boundary conditions efficiently. A Legendre-collocation method is employed to obtain highly accurate numerical approximations to the exact solution.

Organization of this paper is as follows: In section 2 we mention the spectral method and an algorithm to construct differentiation matrix. Various implementation strategies to implement different boundary conditions are given in section 3. Several problems are solved in section 4 to show the performance of the method. Finally we provide concluding remarks in section 5.

2 Spectral Method

The idea of spectral methods arise from the problem of approximating a function using interpolating polynomials. In this section we shall describe the Gauss–Legendre spectral method. The idea is similar to the Chebyshev spectral method *cf.*(1, Ch. 6), (2, Ch. 8), and (3). We shall use Gauss–Legendre points to construct the differentiation matrices to approximate the derivatives. For Gauss–Legendre spectral method the grid points used are the Gauss–Legendre points, also known as Gaussian quadrature points. These points are the eigenvalues of the triangular matrix, (1)

$$A = \begin{bmatrix} 0 & \frac{0.5}{\sqrt{(1-(2\times1)^{-2})}} & & & & \\ \frac{0.5}{\sqrt{(1-(2\times1)^{-2})}} & 0 & \frac{0.5}{\sqrt{(1-(2\times2)^{-2})}} & & & \\ & \frac{0.5}{\sqrt{(1-(2\times2)^{-2})}} & 0 & \frac{0.5}{\sqrt{(1-(2\times3)^{-2})}} & & \\ & & \ddots & \ddots & \ddots & \\ & & \frac{0.5}{\sqrt{(1-(2\times(N-2))^{-2})}} & 0 & \frac{0.5}{\sqrt{(1-(2\times(N-1))^{-2})}} \\ & & & \frac{0.5}{\sqrt{(1-(2\times(N-1))^{-2})}} & 0 \end{bmatrix},$$

which are not equally spaced. These points are used to construct the differentiation matrices. Given a function u defined on the Gauss–Legendre points, a discrete derivative denoted by w is obtained in two steps as follows:

- Let P be the unique polynomial of degree $\leq N$ with $P(x_j) = y_j$, $0 \leq j \leq N$.
- Define $w_j = P'(x_j)$.

Since this is a linear operation, it can be represented using matrix notation $\mathbf{w} = D_N\mathbf{y}$. We shall use $P(x)$ as the Lagrange interpolation polynomial interpolating y_j at $x_j,\ j = 0, 1, 2, ..., N$,

$$P(x) = y_0 l_0(x) + y_1 l_1(x) + y_2 l_2(x) + ... + y_N l_N(x), \tag{1}$$

where

$$l_j(x) = \prod_{\substack{k=0\\k\neq j}}^{N} \left(\frac{x - x_k}{x_j - x_k}\right) = \frac{1}{a_j}\prod_{\substack{k=0\\k\neq j}}^{N}(x - x_k), \quad a_j = \prod_{\substack{k=0\\k\neq j}}^{N}(x_j - x_k). \tag{2}$$

Differentiating (2) using logarithm, we get,

$$l_j'(x) = l_j(x)\sum_{\substack{k=0\\k\neq j}}^{N}\left(\frac{1}{x - x_k}\right) = \frac{1}{a_j}\sum_{\substack{k=0\\k\neq j}}^{N}\Big[\prod_{\substack{k=0\\k\neq i,j}}^{N}(x - x_k)\Big]. \tag{3}$$

For N = 2,

$$\begin{aligned}
P'(x) &= l_0'(x)y_0 + l_1'(x)y_1 + l_2'(x)y_2\\
&= \frac{1}{a_0}\Big[(x - x_1) + (x - x_2)\Big]y_0 + \frac{1}{a_1}\Big[(x - x_0) + (x - x_2)\Big]y_1\\
&+ \frac{1}{a_2}\Big[(x - x_0) + (x - x_1)\Big]y_2.
\end{aligned}$$

At x_0, x_1, and x_2,

$$\begin{aligned}
P'(x_0) &= \frac{1}{a_0}\Big[(x_0 - x_1) + (x_0 - x_2)\Big]y_0 + \frac{1}{a_1}\Big[(x_0 - x_2)\Big]y_1 + \frac{1}{a_2}\Big[(x_0 - x_1)\Big]y_2\\
&= \frac{(x_0 - x_1) + (x_0 - x_2)}{(x_0 - x_1)(x_0 - x_2)}y_0 + \frac{(x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)}y_1 + \frac{(x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)}y_2\\
&= \frac{(x_0 - x_1) + (x_0 - x_2)}{(x_0 - x_1)(x_0 - x_2)}y_0 + \frac{(x_0 - x_1)(x_0 - x_2)}{(x_0 - x_1)(x_1 - x_0)(x_1 - x_2)}y_1\\
&+ \frac{(x_0 - x_2)(x_0 - x_1)}{(x_0 - x_2)(x_2 - x_0)(x_2 - x_1)}y_2\\
&= \Big((x_0 - x_1)^{-1} + (x_0 - x_2)^{-1}\Big)y_0 + \frac{a_0}{a_1(x_0 - x_1)}y_1 + \frac{a_0}{a_2(x_0 - x_2)}y_2.
\end{aligned}$$

Similarly,

$$\begin{aligned}
P'(x_1) &= \frac{a_1}{a_0(x_1 - x_0)}y_0 + \Big((x_1 - x_0)^{-1} + (x_1 - x_2)^{-1}\Big)y_1 + \frac{a_1}{a_2(x_1 - x_2)}y_2\\
P'(x_2) &= \frac{a_2}{a_0(x_2 - x_0)}y_0 + \frac{a_2}{a_1(x_2 - x_1)}y_1 + \Big((x_2 - x_0)^{-1} + (x_2 - x_1)^{-1}\Big)y_2.
\end{aligned}$$

Which can be written as $\mathbf{w} = D_2\mathbf{y}$, where

$$D_2 = \begin{bmatrix} (x_0-x_1)^{-1}+(x_0-x_2)^{-1} & \frac{a_0}{a_1(x_0-x_1)} & \frac{a_0}{a_2(x_0-x_2)} \\ \frac{a_1}{a_0(x_2-x_1)} & (x_1-x_0)^{-1}+(x_1-x_2)^{-1} & \frac{a_1}{a_2(x_1-x_2)} \\ \frac{a_2}{a_0(x_2-x_0)} & \frac{a_2}{a_1(x_2-x_1)}y_1 & (x_2-x_0)^{-1}+(x_2-x_1)^{-1} \end{bmatrix},$$

For $x_0 = -1, x_1 = 0, x_2 = 1$, this matrix simplifies to

$$D_2 = \begin{bmatrix} -1.5 & 2 & -0.5 \\ -0.5 & 0 & 0.5 \\ 0.5 & -2 & 1.5 \end{bmatrix}.$$

Similarly, for $x_0 = -1, x_1 = -\frac{1}{\sqrt{3}} = -0.5774, x_2 = \frac{1}{\sqrt{3}} = 0.5774, x_3 = 1$, the differentiation matrix becomes,

$$D_3 = \begin{bmatrix} -3.5000 & 4.0981 & -1.0981 & 0.5000 \\ -1.3660 & 0.8660 & 0.8660 & -0.3660 \\ 0.3660 & -0.8660 & -0.8660 & 1.3660 \\ -0.5000 & 1.0981 & -4.0981 & 3.5000 \end{bmatrix}.$$

From these three examples we find that the differentiation matrices are in general not symmetric or skew-symmetric. A more general statement is that they are not normal, which is a reason that stability analysis is difficult for spectral methods.

For an arbitrary N, the differentiation matrix is given by the following theorem.

Theorem 1 *(1) For $N \geq 2$ any integer, the first order spectral differentiation matrix D_N has the following entries*

$$(D_N)_{ij} = \frac{1}{a_j}\prod_{\substack{k=0\\k\neq i,j}}^{N}(x_i - x_k) = \frac{a_i}{a_j(x_i - x_j)} \quad i \neq j,$$
$$(D_N)_{jj} = \sum_{\substack{k=0\\k\neq j}}^{N}\left(\frac{1}{x_j - x_k}\right).$$

The second order spatial derivative can be approximated via D_N^2, the square of the matrix D_N.

3 Implementation Strategies

I this section various implementation strategies are given to solve second order boundary value problems

$$p(x)y'' + q(x)y' + r(x)y = f(x), \quad a \le x \le b \tag{4}$$

3.1 Constant Coefficients Case

For the case when $p(x), q(x)$, and $r(x)$ are constant, we can write the problem (4) as $\mathbf{Ay} = \mathbf{f}$, where $\mathbf{A} = pD^2 + qD + rI$, $\mathbf{y} = [y_0\ y_1\ \ldots\ y_n]^T$, and $\mathbf{f} = [f(x_0)\ f(x_1)\ \ldots\ f(x_n)]^T$.

1. For homogeneous boundary conditions $y(x_0) = y_0 = 0$ and $y(x_n) = y_n = 0$, first and last columns of the matrix A have no effect and therefore these columns are deleted. Also first and last rows deleted since these rows corresponds to y_0 and y_n. See (1) for more details.
2. For inhomogeneous boundary conditions $y(x_0) = y_0$ and $y(x_n) = y_n$ when not both y_0 and y_n are zero, we replace the first and last rows of A by the first and last rows of an Identity matrix I of the same size and replace $f(x_0)$ by y_0 and $f(x_n)$ by y_n.
3. For Neumann boundary conditions $y'(x_0) = d_1$ and $y'(x_n) = d_2$, we replace the first and last rows of A by the first and last rows of D and replace $f(x_0)$ by d_1 and $f(x_n)$ by d_2.
4. For Dirichlet boundary condition on one side and Neumann boundary condition on the other side, say $y(x_0) = y_0$ and $y'(x_n) = d_2$, we replace the first row of A by the first row of I and last row of A by the last row of D. Also replace $f(x_0)$ by y_0 and $f(x_n)$ by d_2.

3.2 Nonconstant Coefficients Case

For the case when $p(x)$, $q(x)$, and $r(x)$ are not all constant, we compute the matrix A as:

$$\mathbf{A} = \begin{bmatrix} p(x_0)D^2(1,:) + q(x_0)D(1,:) + r(x_0)I(1,:) \\ p(x_1)D^2(2,:) + q(x_1)D(2,:) + r(x_1)I(2,:) \\ \vdots \qquad \vdots \qquad \vdots \\ p(x_{N-1})D^2(N,:) + q(x_{N-1})D(N,:) + r(x_{N-1})I(N,:) \\ p(x_N)D^2(N+1,:) + q(x_N)D(N+1,:) + r(x_N)I(N+1,:) \end{bmatrix},$$

and solve the system $\mathbf{Ay} = \mathbf{f}$ for all cases mentioned in the previous subsection. Note that $D(i,:)$ denotes the $i - th$ row of D.

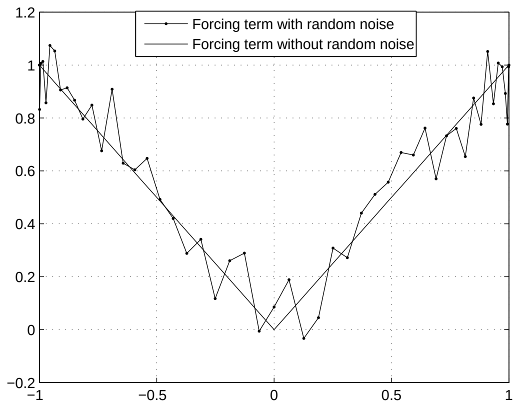

Fig. 1. Example 1. Nonsmooth forcing term with and without random noise.

4 Numerical Experiments

Numerical experiments are performed on various nontrivial examples, particularly examples with nonsmooth forcing term. We have checked the stability of the method by perturbing the forcing term. Stability has also been checked by adding White Gaussian Random noise to the forcing term.

Example 1. This is a Sturm–Liouville differential equation with inhomogeneous boundary conditions and nonsmooth forcing term. We consider the differential equation,

$$x^2y'' + 2xy' - 6y = |x| \tag{5}$$

with

$$y(-1) = 1, \quad y(1) = 1. \tag{6}$$

having the exact solution

$$y(x) = \frac{5}{4}x^2 + \frac{1}{5x^3}\begin{cases} \frac{5x^4}{4} & \text{if } x < 0 \\ \text{undefined} & \text{if } x = 0 \\ -\frac{5x^4}{4} & \text{if } x > 0 \end{cases}$$

Figure 1 shows graph of the forcing term with and without random noise. Solution of (5) is shown in figure 2.

Example 2. This example has constant coefficients and homogeneous Dirichlet boundary conditions. We consider the problem

$$y'' + y' - 6y = |x| \tag{7}$$

with

$$y(-1) = 0, \quad y(1) = 0, \tag{8}$$

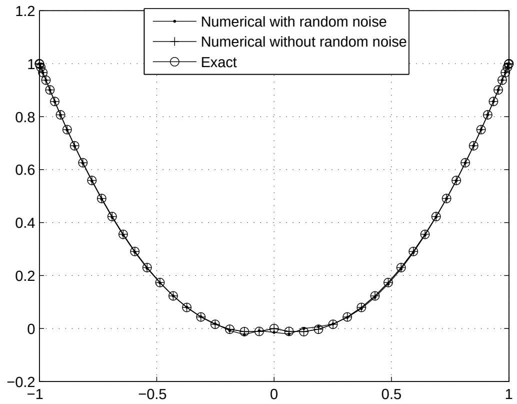

Fig. 2. Example 1. Exact and Numerical solution with and without random noise.

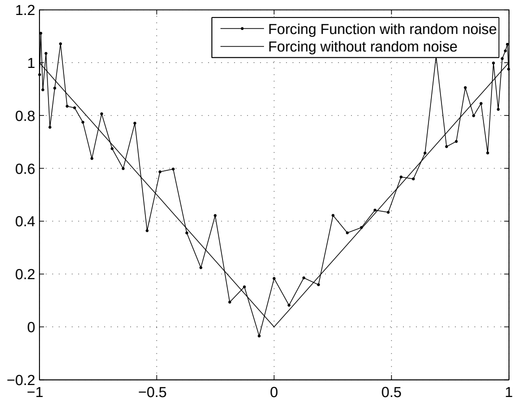

Fig. 3. Example 2. Graph of forcing term.

having the exact solution

$$
\begin{aligned}
y(x) = & -\frac{1}{180}\,\frac{e^{2x-3}\left(-18\,e^{8}-25+35\,(e^{6})+8\,e^{3}\right)}{e^{-5}-e^{5}} \\
& +\frac{1}{180}\,\frac{e^{-3\,x}\left(-18\,+35\,e^{-2}+8\,e^{-5}-25\,e^{2}\right)}{e^{-5}-e^{5}} \\
& +\begin{cases} \frac{1+6x}{36} & \text{if } x \le 0 \\ -\frac{1}{180}\,(5+30x+8-18e^{2\,x}) & \text{if } x > 0 \end{cases}
\end{aligned}
$$

We also compute the numerical solution of the perturbed problem

$$y'' + y' - 6y = (1+\epsilon)|x|$$

with same boundary conditions. We find that the perturbed solutions converge to the unperturbed solution as $\epsilon \to 0$ as is shown in the figure 5.

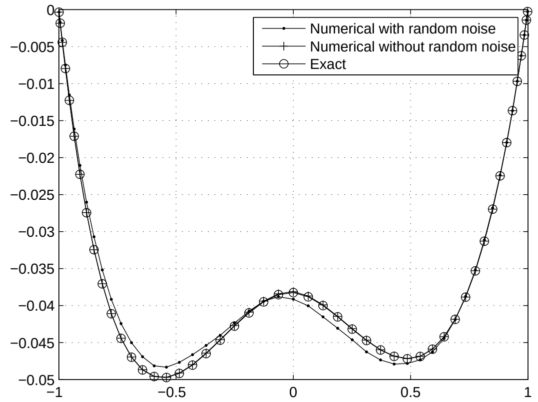

Fig. 4. Example 2. Exact and Numerical solution with and without random noise.

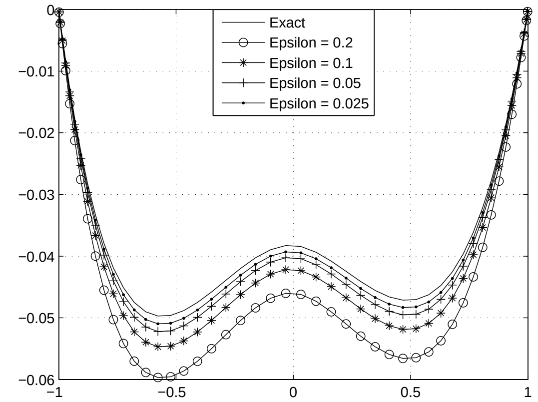

Fig. 5. Example 2. Perturbed numerical solutions converge to the exact solution as $\epsilon \to 0$.

Example 3. (Nonconstant Coefficients and Homogeneous Dirichlet Boundary) Consider the differential equation,

$$y'' + y' - 6y = Heaviside(x) \tag{9}$$

with homogeneous boundary conditions

$$y(-1) = 0, \quad y(1) = 0, \tag{10}$$

and the exact solution

$$\begin{aligned} y(x) = 1/30\, \frac{e^{2\,x} e^{3} \left(-5 + 3\,e^{2} + 2\,e^{-3}\right)}{-e^{2}e^{3} + e^{-3}e^{-2}} - 1/30\, \frac{e^{-3\,x} e^{-2} \left(-5 + 3\,e^{2} + 2\,e^{-3}\right)}{-e^{2}e^{3} + e^{-3}e^{-2}} \\ + 1/30\, Heaviside\,(x) \left(-5 + 3\,e^{2\,x} + 2\,e^{-3\,x}\right) \end{aligned}$$

Example 4.(Constant Coefficient and Inhomogeneous Neumann Boundary) Consider

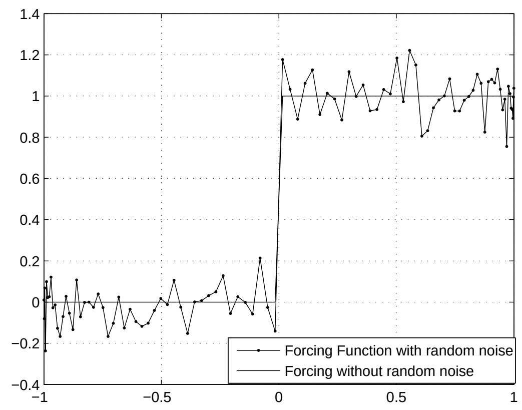

Fig. 6. Example 3. Discontinuous forcing term with and without random noise.

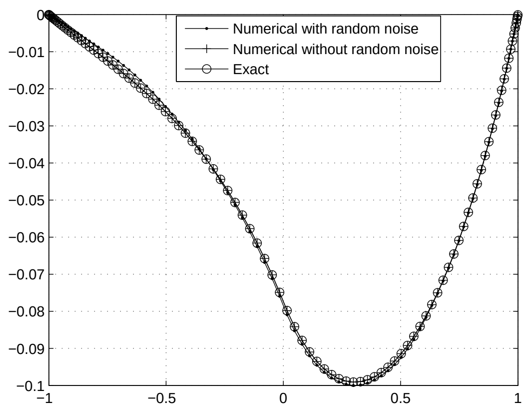

Fig. 7. Example 3. Exact and Numerical solution with and without random noise.

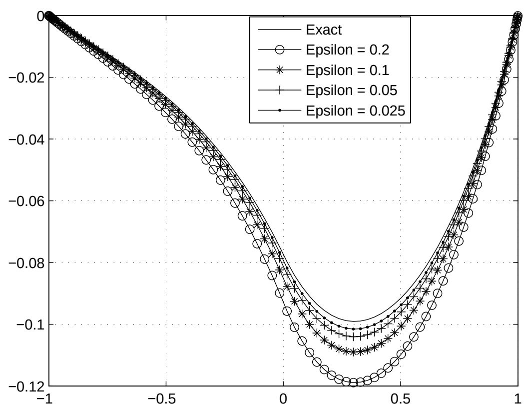

Fig. 8. Example 3. Perturbed numerical solutions converge to the exact solution as $\epsilon \to 0$.

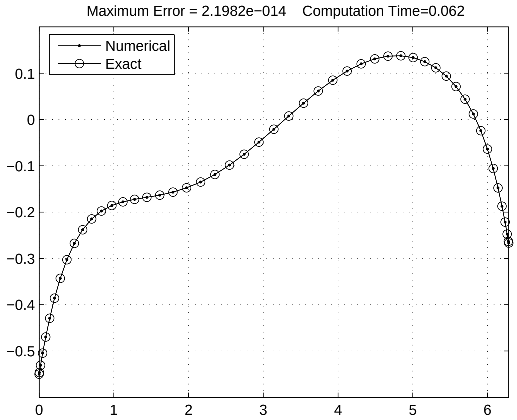

Fig. 9. Example 4. Exact and Numerical Solutions.

the differential equation,

$$y'' - y' - 6y = sin(x) \tag{11}$$

with homogeneous boundary conditions

$$y'(0) = 1, \quad y'(2\pi) = -1, \tag{12}$$

and the exact solution

$$y(x) = -\frac{1}{150}\,\frac{e^{3\,x}(43 + 57\,e^{-4\,\pi})}{e^{6\,\pi} - e^{-4\,\pi}} - \frac{1}{100}\,\frac{e^{-2\,x}(57\,e^{6\,\pi} + 43)}{e^{6\,\pi} - e^{-4\,\pi}} + \frac{1}{50}\,\cos(x) - \frac{7}{50}\,\sin(x) \tag{13}$$

Example 5. (Hermite Differential Equation) Consider the differential equation,

$$y'' - 2xy' + \lambda y = 0 \tag{14}$$

with homogeneous boundary conditions

$$y(0) = 0, \quad y(1) = 1. \tag{15}$$

Exact solution of this problem for $\lambda = 3$ computed by Maple 10 consists of several Bessel–I functions.

$$y(x) = -\frac{e^{\frac{x^2}{2}}\sqrt{x}\left[2\,x^2 BesselI(-\frac{3}{4}, -\frac{x^2}{2}) + 2\,BesselI(\frac{1}{4}, -\frac{x^2}{2})x^2 - BesselI(\frac{1}{4}, -\frac{x^2}{2})\right]}{e^{\frac{1}{2}}(BesselI(\frac{1}{4}, -\frac{1}{2}) - 2\,BesselI(\frac{5}{4}, -\frac{x^2}{2}))} \tag{16}$$

Exact solution corresponding to $\lambda = 8$ consists of $erfi(x)$ function,

$$y(x) = -\frac{(10\,x - 4\,x^3)e^{x^2} + 4\,\mathit{erfi}(x)(\frac{3}{4} - 3\,x^2 + x^4)\sqrt{\pi}}{-6\,e + 5\,\mathit{erfi}(1)\sqrt{\pi}} \tag{17}$$

Note: $erfi(x)$ is not a Matlab function.

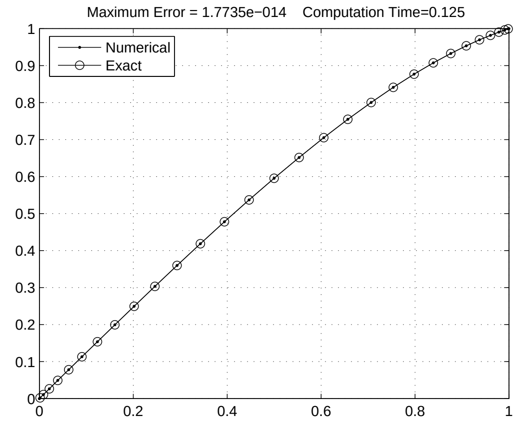

Fig. 10. Example 5. Numerical and Exact Solutions for $\lambda = 3$.

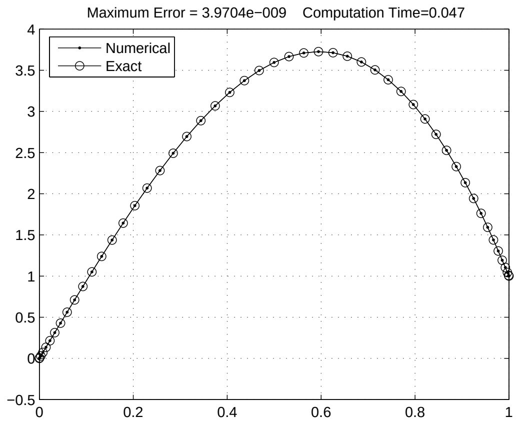

Fig. 11. Example 5. Exact and Numerical Solutions corresponding to $\lambda = 8$.

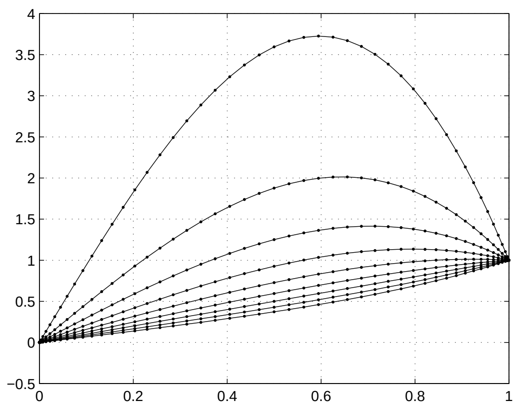

Fig. 12. Example 5. Numerical Solutions corresponding to $\lambda = 0, 1, 2, 3, 4, 5, 6, 7, 8$.

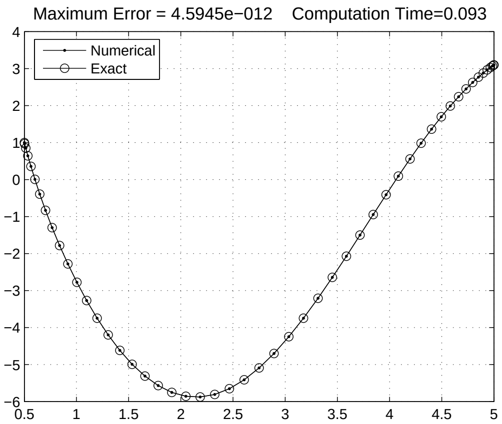

Fig. 13. Example 6. Exact and Numerical Solutions corresponding to v = 1.

Example 6.(Anger's Differential Equation) Consider the differential equation,

$$x^2y'' + xy' + (x^2 - v^2)y = \frac{x - v}{\pi}\sin(\pi v) \tag{18}$$

with Dirichlet–Neumann boundary conditions

$$y(0.5) = 1, \quad y'(5) = 2. \tag{19}$$

Exact solution of this problem computed by Maple 10 consists of several Bessel functions. The exact solution of (18) for $v = 1$ computed by Maple 10 is:

$$\begin{aligned} y(x) = -&\Big[\Big(-10BesselY(1,\frac{1}{2}) + 5BesselY(0,5) - BesselY(1,5)\Big)BesselJ(1,x)\Big] \\ &\Big/\Big[BesselY(1,\frac{1}{2})\Big(5BesselJ(0,5) - BesselJ(1,5)\Big) \\ &-\Big(5BesselY(0,5) - BesselY(1,5)\Big)BesselJ(1,\frac{1}{2})\Big] \\ &+\Big[\Big(-10BesselJ(1,\frac{1}{2}) + 5BesselJ(0,5) - BesselJ(1,5)\Big)BesselY(1,x)\Big] \\ &\Big/\Big[BesselY(1,\frac{1}{2})\Big(5BesselJ(0,5) - BesselJ(1,5)\Big) \\ &-\Big(5BesselY(0,5) - BesselY(1,5)\Big)BesselJ(1,\frac{1}{2})\Big] \end{aligned}$$

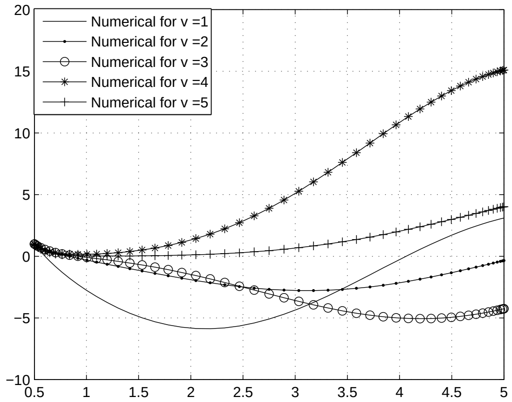

Fig. 14. Example 6. Numerical Solution corresponding to v = 1, 2, 3, 4, 5.

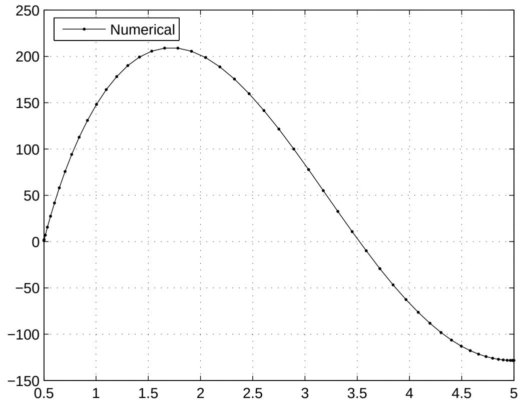

Fig. 15. Example 6. Numerical Solution corresponding to v = 0.1.

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