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A Matrix Method for the Solution of Sturm-Liouville Problems [1]

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Abstract: We investigate the numerical solution of regular and singular Sturm-Liouville problems by means of finite difference schemes of high order. In particular, a set of difference schemes is used to approximate each derivative independently so to obtain an algebraic problem corresponding to the original continuous differential equation. The endpoints are treated depending on their classification and in case of limit points, no boundary condition is required. Several numerical tests are finally reported on equispaced grids show the convergence properties of the proposed approach.

Keywords: Sturm-Liouville problems, finite difference schemes, matrix method.

Mathematics Subject Classification: 65L15, 65L10, 65L12, 65Z05

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1 Introduction

We study the general Sturm-Liouville equation

$$-(p(x)y')' + q(x)y = \lambda r(x)y, \qquad x \in I \subseteq \mathbb{R}, \quad y, \lambda \in \mathbb{R}. \tag{1}$$

Here I can be a compact interval $[a, b]$ or a open, bounded or unbounded, interval (a, b) (i.e., $-\infty \leq a < b \leq \infty$). We assume that the set of Sturm-Liouville coefficients $p, q, r : I \to \mathbb{R}$ satisfy $p^{-1}, q, r \in L_{loc}(I)$, $p > 0$ and $r > 0$ in (a, b). The equation (1) is subjected to separated boundary conditions

$$\begin{array}{ll} a_1[y,u](a) + a_2[y,v](a) = 0, & (a_1, a_2) \neq (0, 0), \\ b_1[y,u](b) + b_2[y,v](b) = 0, & (b_1, b_2) \neq (0, 0), \end{array} \tag{2}$$

where the Wronskian $[f, g]$ is defined for two admissible functions as $[f, g](x) = f(x)(pg')(x) - (pf')(x)g(x)$, and u and v are two linearly independent solutions of the Sturm-Liouville equation for some arbitrary λ, $[u, v](a) \neq 0$ and $[u, v](b) \neq 0$.

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The unspecified parameter λ, called eigenvalue, exists for non-trivial solution of (1)-(2), whereas the solution is called eigenfunction associated with λ. We consider a Sturm-Liouville problem with an infinite but countable number of eigenvalues, which are real and bounded below, so that they can be ordered as

$$-\infty < \lambda_0 < \lambda_1 < \lambda_2 < \lambda_3 < \dots \quad \text{with} \quad \lim_{n\to\infty} \lambda_n = \infty. \tag{3}$$

In addition, the associated eigenfunctions $Y_n(x)$ are orthogonal to each other with respect to the *weight function* $r(x)$,

$$\int_a^b r(x)Y_m(x)Y_n(x)dx = 0 \qquad \text{if } m \neq n, \text{ and } m, n = 1, 2, \dots.$$

As for the usual algebraic eigenvalue problem, the eigenfunctions are uniquely computed according to a specified normalization function.

The Sturm-Liouville boundary value problems are important in applied mathematics and in mathematical physics where they are involved in the description of many phenomena. Typical examples of Sturm-Liouville problems are Bessel equation, Legendre equation, Laguerre equation and Hermite equation, whose eigenfunctions are the homonym functions or polynomials, respectively.

We distinguish between a regular problem and a singular one through the classification of the endpoints. Speaking about the left endpoint a (for the right endpoint b the treatment is similar), we say that it is regular if $p^{-1}, q, r \in L([a, c])$ for $c \in (a, b)$. If both the endpoints of the interval are regular, then the separated boundary conditions (2) become

$$\begin{array}{ll} a_1 y(a) + a_2 (py')(a) = 0, & (a_1, a_2) \neq (0, 0), \\ b_1 y(b) + b_2 (py')(b) = 0, & (b_1, b_2) \neq (0, 0). \end{array} \tag{4}$$

Vice versa an endpoint is singular if it is not regular, and this means that either it is infinite or it is finite, but at least one of p^{-1}, q or r is not integrable in any neighborhood of the endpoint. If the singular endpoint a is classified as limit circle (LC), it means that the solution of (1) is in $L^2_r(a, c)$ for $c \in (a, b)$, and then a left boundary condition (2) is required. It is possible that a LC endpoint is oscillatory (LCO), namely the nontrivial solution of (1) has an infinite number of zeros in any neighborhood of it. In this paper we do not treat LCO endpoints, but LC non oscillatory (LCNO) endpoints satisfying the property (3). Moreover, a singular endpoint is a limit point (LP) if it is not LC, and then no boundary condition is needed.

The aim is to analyze the numerical solution of various (regular and singular) Sturm-Liouville problems by means of finite difference schemes [2, 3]. In this context, the idea is to transform the continuous problem (1) in a discrete one approximating each derivative by means of an appropriate difference scheme. This kind of approach, typical of several methods for PDEs approximation, has been proposed in the last few years for the solution of general second order evolutionary problems

$$f(x, y, y', y'') = 0 \tag{5}$$

subject to initial or boundary conditions (see [8, 9, 4, 5, 6]). Since the methods considered emphasize a nice behavior when applied to both second order initial and boundary value problems, firstly we have applied them to eigenvalue IVPs (see [7]), showing that the obtained methods maintain the order of accuracy of the underlined schemes for regular problems, while often the order of accuracy decays for singular problems. The main advantage with respect to the classical Runge-Kutta and linear multistep methods is that this approach does not require the reformulation of equation (5) as an equivalent first order one with y and y' as unknowns. This is useful to lower the computational cost (the size of the continuous problem is halved) and to simplify step variation because y and

y' have in general a different behavior. Another positive feature of this approach is that not only each derivative is obviously discretized with a different scheme, but also each derivative may be discretized at each grid point with a different scheme depending on the position of the point itself. This aspect, typical of BVMs (see, for example, the main reference [10]) where a main method is used in the central points of the grid and is associated to initial and final methods used once in the other points, allows to reach high orders of accuracy easily.

The paper is organized as follows: in the next section high order finite difference schemes are briefly described. In the successive section we explain how to derive a matrix method to compute the eigenvalues and the eigenfunction of the Sturm-Liouville problem. Finally, the last section is devoted to several examples to emphasize the behavior of the method on classical examples.

2 High order finite difference schemes

In this section we describe high order finite difference schemes for the approximation of general second order differential equations. These schemes will be used in the next section to solve Sturm-Liouville problems. For simplicity, we first suppose problem (5) is solved for $x \in [a, b]$ with boundary conditions $y(a) = y_a$ and $y(b) = y_b$. Then, we discretize $[a, b]$ by means of $n + 1$ equispaced points $x_i = a + ih$, $i = 0, \ldots, n$, where $h = (b - a)/n$.

Finite differences are linear multistep schemes approximating the derivatives of (5) in the points x_i, $i = 1, \ldots, n - 1$. For a fixed number k of points, it is possible to define k alternative schemes approximating $y^{(\nu)}(x_i)$ and depending on the considered stencil $x_{i-s+1}, \ldots, x_{i-s+k}$ (here we suppose $0 < s \leq k$)

$$y^{(\nu)}(x_i) \approx y_i^{(\nu)} = \frac{1}{h^\nu} \sum_{j=1}^{k} \alpha_{j,s}^{(\nu)} y_{i-s+j}, \qquad \nu = 1, 2, \tag{6}$$

where the coefficients $\alpha_{j,s}^{(\nu)}$ in (6) are always chosen in order the above formula have maximum order. The order of each formula is $k - \nu$ with the exception of the formulae for $\nu = 2$, k odd and $s = (k + 1)/2$ which have order $k - 1$. The idea carried on in [8] and the subsequent papers is to select a combination of schemes of the same order with the best stability properties. In the following we will use schemes of even order p, that is $k = p + 1$ odd for the first derivative while, for the second derivative, $k = p + 1$ odd for the scheme with symmetric stencil and $k = p + 2$ even for the others.

For the second derivative just the schemes with symmetric stencil have the best stability properties. For the first derivative, in [9, 4, 5, 6] it is suggested to use schemes with $s = (k - 1)/2$ or $s = (k+3)/2$ depending on the sign of the coefficient multiplying the derivative. For Sturm-Liouville problems, symmetry reasons suggest to use schemes with symmetric stencil ($s = (k + 1)/2$). The formula selected to approximate each derivative is called *main scheme*.

For $p \geq 4$ the main scheme cannot be used on all the points of the grid: for example, for the order 4, main schemes approximating the derivatives in x_1 and x_{n-1} would require the values in x_{-1} and x_{n+1}. Consequently is necessary to use different formulae (called *initial* and *final schemes*) to approximate derivatives in the initial and final points of the mesh. So, in general, the approximation of a derivative in all the internal points of the grid requires a combination of formulae, some of them used once in the initial and final gridpoints. As an example, for the order

4 we use the schemes

$$y'(x_i) \approx y'_i = \frac{1}{h}\begin{cases} \left(-\frac{1}{4}y_0 - \frac{5}{6}y_1 + \frac{3}{2}y_2 - \frac{1}{2}y_3 + \frac{1}{12}y_4\right), & i = 1 \\ \left(\frac{1}{12}y_{i-2} - \frac{2}{3}y_{i-1} + \frac{2}{3}y_{i+1} - \frac{1}{12}y_{i+2}\right), & i = 2, \ldots, n-2, \\ \left(-\frac{1}{12}y_{n-4} + \frac{1}{2}y_{n-3} - \frac{3}{2}y_{n-2} + \frac{5}{6}y_{n-1} + \frac{1}{4}y_n\right), & i = n-1 \end{cases}$$

which in matrix form is represented as

$$Y' = \bar{A}_1 \bar{Y}, \tag{7}$$

where $Y' = \left(y'_1, \ldots, y'_{n-1}\right)^T$, $\bar{Y} = (y_0, \ldots, y_n)^T = \left(y_0, Y^T, y_n\right)^T$ and

$$\bar{A}_1 = \frac{1}{h}\begin{pmatrix} -\frac{1}{4} & -\frac{5}{6} & \frac{3}{2} & -\frac{1}{2} & \frac{1}{12} & & & \\ \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} \\ & & & -\frac{1}{12} & \frac{1}{2} & -\frac{3}{2} & \frac{5}{6} & \frac{1}{4} \end{pmatrix}_{(n-1)\times(n+1)}. \tag{8}$$

Analogously,

$$y''(x_i) \approx y''_i = \frac{1}{h^2}\begin{cases} \left(\frac{5}{6}y_0 - \frac{5}{4}y_1 - \frac{1}{3}y_2 + \frac{7}{6}y_3 - \frac{1}{2}y_4 + \frac{1}{12}y_5\right), & i = 1 \\ \left(-\frac{1}{12}y_{i-2} + \frac{4}{3}y_{i-1} - \frac{5}{2}y_i + \frac{4}{3}y_{i+1} - \frac{1}{12}y_{i+2}\right), & i = 2, \ldots, n-2, \\ \left(\frac{1}{12}y_{n-5} - \frac{1}{2}y_{n-4} + \frac{7}{6}y_{n-3} - \frac{1}{3}y_{n-2} - \frac{5}{4}y_{n-1} + \frac{5}{6}y_n\right), & i = n-1 \end{cases}$$

or

$$Y'' = \bar{A}_2 \bar{Y}, \tag{9}$$

where $Y'' = \left(y''_1, \ldots, y''_{n-1}\right)^T$ and

$$\bar{A}_2 = \frac{1}{h^2}\begin{pmatrix} \frac{5}{6} & -\frac{5}{4} & -\frac{1}{3} & \frac{7}{6} & -\frac{1}{2} & \frac{1}{12} & & \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ & & \frac{1}{12} & -\frac{1}{2} & \frac{7}{6} & -\frac{1}{3} & -\frac{5}{4} & \frac{5}{6} \end{pmatrix}_{(n-1)\times(n+1)}. \tag{10}$$

Hence, the differential equation (5) is substituted by a nonlinear system of equations

$$f(X, Y, Y', Y'') = 0 \tag{11}$$

in the unknown vector Y.

Sometimes boundary conditions also involve first derivatives in the extreme points. So, for example, we have

$$\gamma_0 y(a) + \delta_0 y'(a) = y_a, \qquad \gamma_1 y(b) + \delta_1 y'(b) = y_b. \tag{12}$$

The values $y'(a)$ and $y'(b)$ were not considered in the previous formulae. So the simplest thing to do is to approximate them by means of (6) with $s = 1$ and $s = k$, respectively; in such a case boundary conditions (12) are approximatively satisfied. In this case it is however preferable to treat $y'(a)$ and $y'(b)$ as additional unknowns. We use the following initial and final schemes in place of the previous ones:

$$y'(x_i) \approx y'_i = \frac{1}{h}\begin{cases} hy'_0, & i = 0 \\ \left(-\frac{h}{3}y'_0 - \frac{17}{18}y_0 + \frac{1}{2}y_1 + \frac{1}{2}y_2 - \frac{1}{18}y_3\right), & i = 1 \\ \left(\frac{1}{18}y_{n-3} - \frac{1}{2}y_{n-2} - \frac{1}{2}y_{n-1} + \frac{17}{18}y_n - \frac{h}{3}y'_n\right), & i = n-1 \\ hy'_n, & i = n \end{cases}$$

and

$$y''(x_i) \approx y''_i = \frac{1}{h^2}\begin{cases} \left(-\frac{25h}{6}y'_0 - \frac{415}{72}y_0 + 8y_1 - 3y_2 + \frac{8}{9}y_3 - \frac{1}{8}y_4\right), & i = 0 \\ \left(\frac{5h}{12}y'_0 + \frac{257}{144}y_0 - \frac{10}{3}y_1 + \frac{7}{4}y_2 - \frac{2}{9}y_3 + \frac{1}{48}y_4\right), & i = 1 \\ \left(\frac{1}{48}y_{n-4} - \frac{2}{9}y_{n-3} + \frac{7}{4}y_{n-2} - \frac{10}{3}y_{n-1} + \frac{257}{144}y_n - \frac{5h}{12}y'_n\right), & i = n-1 \\ \left(-\frac{1}{8}y_{n-4} + \frac{8}{9}y_{n-3} - 3y_{n-2} + 8y_{n-1} - \frac{415}{72}y_n + \frac{25h}{6}y'_n\right), & i = n \end{cases}$$

Now the approximation (7) and (9) are defined for $Y' = (y'_0, \ldots, y'_n)^T$, $\bar{Y} = (y'_0, y_0, \ldots, y_n, y'_n)^T = \left(y'_0, Y^T, y'_n\right)^T$ and

$$\bar{A}_1 = \frac{1}{h}\begin{pmatrix} h & & & & & & & & & \\ -\frac{h}{3} & -\frac{17}{18} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{18} & & & & & \\ & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & \\ & & & & & \frac{1}{18} & -\frac{1}{2} & -\frac{1}{2} & \frac{17}{18} & -\frac{h}{3} \\ & & & & & & & & & h \end{pmatrix}_{(n+1)\times(n+3)}, \tag{13}$$

$$\bar{A}_2 = \frac{1}{h^2}\begin{pmatrix} -\frac{25h}{6} & -\frac{415}{72} & 8 & -3 & \frac{8}{9} & \frac{1}{8} & & & & \\ \frac{5h}{12} & \frac{257}{144} & -\frac{10}{3} & \frac{7}{4} & -\frac{2}{9} & \frac{1}{48} & & & & \\ & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & \\ & & & & \frac{1}{48} & -\frac{2}{9} & \frac{7}{4} & -\frac{10}{3} & \frac{257}{144} & -\frac{5h}{12} \\ & & & & -\frac{1}{8} & \frac{8}{9} & -3 & 8 & -\frac{415}{72} & \frac{25h}{6} \end{pmatrix}_{(n+1)\times(n+3)}. \tag{14}$$

Obviously the absence of one of the first derivative term in the boundary conditions allows us to simplify initial and final schemes as said previously.

3 Algebraic solution of Sturm-Liouville problems

In this section we apply high order finite difference schemes to Sturm-Liouville equations (1). The main difference with respect to the equation (5) is the presence of the unknown parameter λ in the equation as well as possible singularities in the extreme points.

Supposing, for simplicity, that the problem is regular on a finite interval and (4) contains $a_2 = b_2 = 0$. Then (1) is equivalent to

$$-p(x)y'' - p'(x)y' + q(x)y = \lambda r(x)y, \qquad x \in [a,b], \quad y, \lambda \in \mathbb{R} \tag{15}$$

and it is approximated by

$$R^{-1}\left(-PA_2 - P_1A_1 + Q\right)Y = \lambda Y \tag{16}$$

where R, P, P_1 and Q are diagonal matrices of size $n-1$ containing $r(x_i)$, $p(x_i)$, $p'(x_i)$ and $q(x_i)$, $i = 1, \ldots, n-1$, respectively, A_1 and A_2 are square matrices extracted by (8) and (10) neglecting the first and the last column (which are multiplied by $y_0 = y_n = 0$), and $Y = (y_1, \ldots, y_{n-1})^T$.

Eigenvalues and eigenfunctions of (15) are eigenvalues and eigenvectors of the sparse matrix $M = R^{-1}\left(-PA_2 - P_1A_1 + Q\right)$ in (16). Hence they will be computed in the next section by means of a linear algebra tool. Anyway, we stress that the same result could be reached by solving the nonlinear system (16) in the unknowns λ and Y by using a normalization condition on the vector Y as additional equation and a suitable initial guess for the eigenvalue required.

For general boundary conditions (4), where a_1, a_2, b_1 and b_2 are all different from 0, the idea is always to reduce the size of the problem and use an algebraic tool. In this case the approximation of (15) is given by

$$\bar{R}^{-1}\left(-\bar{P}\bar{A}_2 - \bar{P}_1\bar{A}_1 + \bar{Q}\hat{I}\right)\bar{Y} = \lambda Y, \tag{17}$$

where $\bar{A}_1$ and $\bar{A}_2$ are the rectangular matrices (13) and (14), $\bar{Y} = (y_0', Y, y_n')^T$, $Y = (y_0, y_1, \ldots, y_n)^T$, $\hat{I} = [o\ I_{n+1}\ o]$ and $\bar{R}$, $\bar{P}$, $\bar{P}_1$ and $\bar{Q}$ are diagonal matrices of size $n+1$ containing $r(x_i)$, $p(x_i)$, $p'(x_i)$ and $q(x_i)$, $i = 0, \ldots, n$. As a consequence of (4), we consider a matrix of transformation

$$D = \begin{pmatrix} a_2p(a) & a_1 & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & b_1 & b_2p(b) \end{pmatrix}_{(n+3)\times(n+3)} .$$

such that $D\bar{Y} = (a_1y_0 + a_2p(a)y_0',\ y_0,\ \ldots,\ y_n,\ b_1y_n + b_2p(b)y_n')^T$ contains the first and the last element which are zero. Then (17) is equivalent to

$$\bar{R}^{-1}\left(-\bar{P}\bar{A}_2 - \bar{P}_1\bar{A}_1 + \bar{Q}\hat{I}\right)D^{-1}D\bar{Y} = \bar{R}^{-1}\left(-\bar{P}A_2 - \bar{P}_1A_1 + \bar{Q}\right)Y = \lambda Y,$$

where again a square matrix is extracted by the original rectangular one erasing the first and the last column; as in the previous case we obtain an algebraic eigenvalue problem whose eigenvalues and eigenvectors are the eigenvalues and eigenfunctions of the original problem (15).

In case of singular Sturm-Liouville problems with (for simplicity both) LP endpoints, no boundary condition is required and hence it is necessary to add two finite difference schemes to (7) and (9). To this aim we consider initial and final methods approximating equation (15) in both the endpoints (here we again use order 4):

$$\begin{aligned} y'(x_0) \approx y_0' &= \frac{1}{h}\left(-\frac{25}{12}y_0 + 4y_1 - 3y_2 + \frac{4}{3}y_3 - \frac{1}{4}y_4\right), \\ y'(x_n) \approx y_n' &= \frac{1}{h}\left(\frac{1}{4}y_{n-4} - \frac{4}{3}y_{n-3} + 3y_{n-2} - 4y_{n-1} + \frac{25}{12}y_n\right), \end{aligned}$$

$$
\begin{aligned}
y''(x_0) \approx y_0'' &= \frac{1}{h^2}\left(\frac{15}{4}y_0 - \frac{77}{6}y_1 + \frac{107}{6}y_2 - 13y_3 + \frac{61}{12}y_4 - \frac{5}{6}y_5\right), \\
y''(x_n) \approx y_n'' &= \frac{1}{h^2}\left(-\frac{5}{6}y_{n-5} + \frac{61}{12}y_{n-4} - 13y_{n-3} + \frac{107}{6}y_{n-2} - \frac{77}{6}y_{n-1} + \frac{15}{4}y_n\right),
\end{aligned}
$$

Matrices (8) and (10) becomes

$$
A_1 = \frac{1}{h}\begin{pmatrix}
-\frac{25}{12} & 4 & -3 & \frac{4}{3} & -\frac{1}{4} & & & & \\
-\frac{1}{4} & -\frac{5}{6} & \frac{3}{2} & -\frac{1}{2} & \frac{1}{12} & & & & \\
\frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & & & \\
 & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\
 & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & \\
 & & & -\frac{1}{12} & \frac{1}{2} & -\frac{3}{2} & \frac{5}{6} & \frac{1}{4} & \\
 & & & \frac{1}{4} & -\frac{4}{3} & 3 & -4 & \frac{25}{12} &
\end{pmatrix}_{(n+1)\times(n+1)}, \tag{18}
$$

and

$$
A_2 = \frac{1}{h^2}\begin{pmatrix}
\frac{15}{4} & -\frac{77}{6} & \frac{107}{6} & -13 & \frac{61}{12} & -\frac{5}{6} & & & \\
\frac{5}{6} & -\frac{5}{4} & -\frac{1}{3} & \frac{7}{6} & -\frac{1}{2} & \frac{1}{12} & & & \\
-\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & & \\
 & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\
 & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & \\
 & & \frac{1}{12} & -\frac{1}{2} & \frac{7}{6} & -\frac{1}{3} & -\frac{5}{4} & \frac{5}{6} & \\
 & & -\frac{5}{6} & \frac{61}{12} & -13 & \frac{107}{6} & -\frac{77}{6} & \frac{15}{4} &
\end{pmatrix}_{(n+1)\times(n+1)}. \tag{19}
$$

Consequently, equation (15) is approximated by

$$
\bar{R}^{-1}\left(-\bar{P}A_2 - \bar{P}_1A_1 + \bar{Q}\right)Y = \lambda Y,
$$

where $Y = (y_0, \ldots, y_n)^T$ and $\bar{P}$, $\bar{P}_1$ $\bar{Q}$ are the same matrices used in (17).

We observe that it could happen that the coefficients of Sturm-Liouville problems are not defined in the endpoints, so we have to consider a truncated interval $[\alpha, \beta]$ with $a < \alpha < \beta < b$.

4 Numerical examples

In this section we examine some examples of Sturm-Liouville problems with one or both the endpoints regular, LCNO or LP. Except for unbounded problems, we have always considered constant step size in order to estimate the numerical order of convergence. Unbounded intervals are transformed into limited ones before a constant stepsize is applied. Methods of order 4, 6 and 8 are considered and, as explained in Section 3, the matlab tool for sparse matrices *eigs* is used to evaluate both the eigenvalues and the eigenvectors.

At the beginning, we test the methods on a regular problem (Problem 1) and on a regular one that looks singular (Problem 2). Afterwards, we solve the same Sturm-Liouville problem (the hydrogen equation) on a truncated interval (Problem 3) and on an upper unbounded one (Problem

Table 1: Numerical results for Test problem 1.

		$p=4$		$p=6$		$p=8$	
	Mesh	Error	Order	Error	Order	Error	Order
λ_0	200	1.01e-05	3.45	4.26e-07	6.16	1.61e-07	8.65
	400	9.19e-07	3.89	5.97e-09	6.91	4.01e-10	9.08
	600	1.90e-07	3.96	3.63e-10	7.35	1.01e-11	1.45
	800	6.08e-08	-	4.38e-11	-	1.55e-13	-
λ_4	300	2.88e-04	7.13	9.14e-05	12.22	2.64e-05	8.05
	600	2.05e-06	1.92	1.92e-08	2.34	9.95e-08	9.96
	900	9.42e-07	2.38	7.42e-09	7.57	1.75e-09	10.81
	1.200	4.75e-07	3.24	8.39e-10	11.22	7.82e-11	12.97
	1.500	2.31e-07	-	6.86e-11	-	4.33e-12	-
λ_{24}	2000	5.69e-05	3.19	5.53e-06	6.85	3.33e-07	7.27
	2500	2.79e-05	3.53	1.20e-06	6.92	6.58e-08	8.84
	3000	1.47e-05	3.70	3.40e-07	6.85	1.31e-08	9.51
	3500	8.30e-06	3.79	1.18e-07	6.74	3.03e-09	9.93
	4000	5.00e-06	-	4.81e-08	-	8.05e-10	-

4). Here the left endpoint is LP while the right one is regular in the first case and LP in the second. We point out again that no boundary condition is required in a LP endpoint, and this is substituted by an initial or a final method. Finally, in the last example the endpoints are both LCNO and boundary conditions are needed.

Problem 1. The Klotter problem (see [14]) is defined as

$$-y''(x) + \frac{3}{4x^2}y(x) = \lambda\frac{64\pi^2}{9x^6}y(x), \quad x \in [8/7, 8],$$

$a = 8/7$ regular,

$b = 8$ regular,

with boundary conditions $y(8/7) = y(8) = 0$. The eigenvalues are

$$\lambda_k = (k+1)^2, \qquad k = 0, 1, \ldots$$

As shown in Table 1, the numerical order is preserved for each eigenvalue. Greater eigenvalues require more points than the smaller ones in order to obtain a good approximation. Anyway, it is clearly visible that a better accuracy is gained with the higher order methods.

Problem 2. The regular problem (see [14])

$$-\left(\frac{1}{\sqrt{1-x^2}}y'\right)'(x) = \lambda\frac{1}{\sqrt{1-x^2}}y(x), \quad x \in [-1, 1],$$

$a = -1$ regular,
$b = 1$ regular

has boundary conditions $y(-1) = y(1) = 0$. It is important to specify that, though being defined regular, it has the coefficients $p(x)$ and $r(x)$ not defined in the endpoints and hence it looks singular. This 'singular' behavior wreaks a loss of order. The results in Table 2 bear out the slow convergence and the numerical order reaches the same constant value for every eigenvalue and order of the method. Here it is known from [14] that $\lambda_0 = 3.559279966$, $\lambda_9 = 258.8005854$ and $\lambda_{24} = 1572.635284$.

Table 2: Numerical results for Test problem 2.

		$p=4$		$p=6$		$p=8$	
	Mesh	Error	Order	Error	Order	Error	Order
λ_0	1000	1.57e-05	1.50	1.41e-05	1.50	1.26e-05	1.50
	2000	5.56e-06	1.50	5.00e-06	1.50	4.44e-06	1.50
	3000	3.03e-06	1.50	2.72e-06	1.50	2.42e-06	1.50
	4000	1.97e-06	-	1.77e-06	-	1.57e-06	-
λ_9	6000	2.93e-06	1.50	2.63e-06	1.50	2.34e-06	1.50
	9000	1.59e-06	1.50	1.43e-06	1.50	1.27e-06	1.50
	12000	1.04e-06	1.50	9.31e-07	1.50	8.27e-07	1.50
	15000	7.41e-07	-	6.66e-07	-	5.92e-07	-
λ_{24}	10000	2.13e-06	1.50	1.91e-06	1.50	1.70e-06	1.50
	15000	1.16e-06	1.50	1.04e-06	1.50	9.25e-07	1.50
	20000	7.53e-07	1.50	6.76e-07	1.50	6.00e-07	1.50
	25000	5.38e-07	-	4.84e-07	-	4.30e-07	-

Problem 3. The truncated hydrogen equation (see [14]) is defined as,

$$-y''(x) + \left(\frac{2}{x^2} - \frac{1}{x}\right) y(x) = \lambda y(x), \quad x \in [0, 1000],$$
$$a = 0 \quad \text{LP},$$
$$b = 1000 \quad \text{regular}.$$

The only condition is $y(1000) = 0$. The eigenvalues are

$$\lambda_k = -\frac{1}{(2k+4)^2},\ k = 0, 1, \ldots$$

Since $a = 0$ is LP, no boundary condition is required and initial methods approximate the problem in the initial point. Since $q(x)$ is not defined in a, we also truncate the interval (see [13]) and choose $a > 0$ close to zero. Moreover, the results in Table 3 show that the numerical order is gained, the convergence for order 8 is rather faster and the accuracy improves with the higher order. We emphasize that, on a truncated interval, a good eigenvalue estimation is reached until $k = 9$, since when k increases the eigenfunction is not zero in the right endpoint and oscillations range on a greater interval. In order to compare the results with the next problem we have also drawn the eigenfunction associated to λ_4 in Figure 1 (left).

Problem 4. The Hydrogen atom equation in problem 3 is integrated for $x \in [0, \infty]$, where

$$b = \infty \quad \text{LP}$$

With respect to the previous example, both endpoints are LP and no boundary condition is given, so we consider one initial and final methods to approximate the problem in both endpoints. Moreover the upper unbounded interval is transformed by means of the simple change of variable

$$\tilde{x}_i = 1 - \frac{1}{\sqrt{1 + x_i}} \in [0, 1].$$

Obviously a constant step size in $[0, 1]$ gives a solution with variable step size in the original interval, as it is possible to see in Figure 1 (right). We note that the solution, obtained in the interval $(0, \infty)$, is truncated in $b = 1000$ in order to see the choice of the mesh selection in comparison to Figure 1 (left). Conversely to Problem 3 few points ensure a good approximation and numerical order is preserved. As noted in the other examples greatest accuracy is guaranteed by higher order methods.

Table 3: Numerical results for Test problem 3.

		$p=4$		$p=6$		$p=8$	
	Mesh	Error	Order	Error	Order	Error	Order
λ_0	500	2.18e-03	4.23	9.77e-04	6.89	2.00e-04	9.42
	1000	1.16e-04	2.96	8.22e-06	6.64	2.92e-07	11.15
	1500	3.49e-05	3.62	5.56e-07	6.37	3.17e-09	18.34
	2000	1.23e-05	-	8.91e-08	-	1.61e-11	-
λ_4	500	7.36e-04	4.64	1.17e-04	7.61	9.75e-06	10.18
	1000	2.95e-05	3.05	5.98e-07	6.90	8.38e-09	11.23
	1500	8.57e-06	3.68	3.64e-08	6.45	8.82e-11	14.28
	2000	2.97e-06	3.84	5.68e-09	6.24	1.45e-12	6.81
	2500	1.26e-06	-	1.41e-09	-	3.17e-13	-
λ_9	1000	1.44e-05	3.02	2.35e-07	6.98	2.54e-09	11.22
	1500	4.23e-06	3.67	1.39e-08	6.48	2.69e-11	10.95
	2000	1.47e-06	3.84	2.15e-09	6.27	1.15e-12	8.72
	2500	6.24e-07	-	5.31e-10	-	1.65e-13	-

Table 4: Numerical results for Test problem 4.

		$p=4$		$p=6$		$p=8$	
	Mesh	Error	Order	Error	Order	Error	Order
λ_0	100	2.79e-06	3.99	4.62e-08	5.96	1.60e-09	7.89
	150	5.53e-07	3.99	4.13e-09	5.98	6.51e-11	7.99
	200	1.75e-07	4.00	7.40e-10	5.99	6.53e-12	7.55
	250	7.19e-08	-	1.94e-10	-	1.21e-12	-
λ_4	200	3.16e-04	3.96	2.14e-05	5.90	2.21e-06	7.80
	400	2.03e-05	3.99	3.59e-07	5.97	9.88e-09	7.11
	600	4.03e-06	3.99	3.19e-08	5.98	5.53e-10	12.48
	800	1.28e-06	-	5.72e-09	-	1.52e-11	-
λ_9	500	8.14e-04	3.95	6.87e-05	5.89	7.70e-06	7.80
	1000	5.25e-05	3.98	1.16e-06	5.96	3.46e-08	7.80
	1500	1.04e-05	3.99	1.03e-07	5.98	1.46e-09	9.74
	2000	3.31e-06	-	1.85e-08	-	8.89e-11	-
λ_{24}	2000	2.76e-03	3.93	3.73e-04	5.84	6.09e-05	7.74
	4000	1.81e-04	3.97	6.53e-06	5.95	2.85e-07	7.93
	6000	3.61e-05	3.99	5.85e-07	5.97	1.15e-08	8.14
	8000	1.15e-05	-	1.05e-07	-	1.10e-09	-

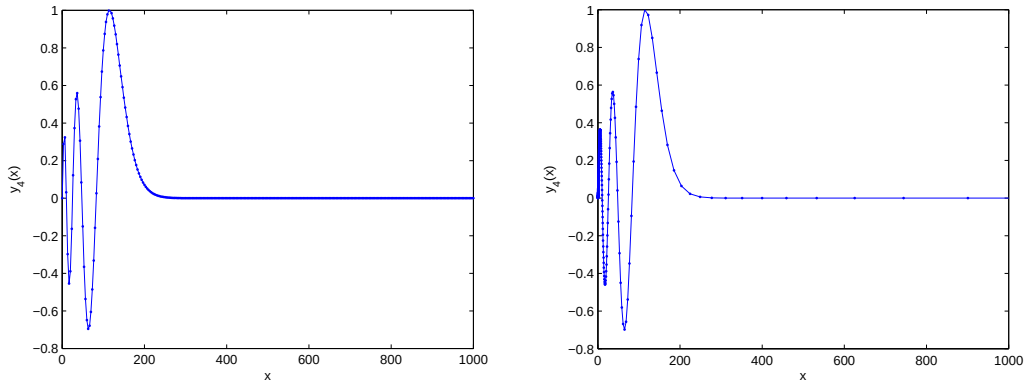

Figure 1: Eigenfunctions $y_4(x)$ computed by the order 6 method with 300 points in the interval $[0, 1000]$ (left) and in the interval $(0, \infty)$ truncated at $b = 1000$ (right).

Problem 5. The Legendre equation (see [11]) is defined as

$$\begin{aligned} &-((1-x^2)y')'(x) + \frac{1}{4}y(x) = \lambda y(x), \quad x \in [-1, 1], \\ &a = -1 \quad \text{LCNO} \\ &b = 1 \quad \text{LCNO} \end{aligned}$$

The boundary conditions $[y, u](-1) = -(py')(-1) = 0$ and $[y, u](1) = -(py')(1) = 0$ are obtained from (2) setting $a_1 = b_1 = 1$, $a_2 = b_2 = 0$, $u(x) = 1$ and $v(x) = \ln((1+x)/(1-x))$. The eigenvalues are

$$\lambda_k = \left(k + \frac{1}{2}\right)^2, \quad k = 0, 1, \ldots,$$

while the Legendre polynomials represent the eigenfunctions associated to λ_k. Since p is null in the endpoints, an initial and final method to approximate both endpoints substitute for the boundary conditions. The results obtained for small k show that 20 points are enough for a very good approximation, consequently the numerical order is estimated for $k = 9, 24, 49$. We underline that the numerical order is preserved and sometimes exceeds the order expected. Moreover, the number of points required to reach a prescribed accuracy is proportional to k and the higher order methods guarantee a better accuracy. Furthermore in Figure 2 the eigenfunctions associated to the eigenvalue λ_4 and λ_{24} are drawn, respectively.

5 Conclusion

The results shown in the section 4 highlight as the methods work well on regular and singular problems excepted when the Sturm-Liouville coefficients are not defined in the endpoints of the interval and it is not possible to consider a truncated interval (as, for example, in Problem 3 and Problem 5). This behavior is worth treating in a deeper way in a next paper. On the other hand it is important to point out that the number of mesh points is high unless the Problem 4. Consequently, we will consider a variable step size in order to reduce the number of points and to compare the used approach with other codes solving Sturm-Liouville problems as SLEIGN ([12]).

Table 5: Numerical results for Test problem 5.

		$p=4$		$p=6$		$p=8$	
	Mesh	Error	Order	Error	Order	Error	Order
λ_9	20	3.67e-02	3.61	5.69e-03	6.10	2.14e-04	8.93
	40	3.00e-03	5.55	8.28e-05	6.80	4.38e-07	9.25
	60	3.16e-04	6.76	5.27e-06	6.78	1.03e-08	9.43
	80	4.52e-05	9.22	7.49e-07	6.74	6.83e-10	9.54
	100	5.77e-06	-	1.66e-07	-	8.13e-11	-
λ_{24}	100	1.13e-02	1.19	2.81e-03	2.56	1.14e-03	4.97
	200	4.94e-03	4.50	4.75e-04	5.90	3.65e-05	7.93
	300	7.96e-04	5.53	4.33e-05	6.37	1.47e-06	8.59
	400	1.62e-04	6.40	6.94e-06	6.52	1.24e-07	8.91
	500	3.88e-05	-	1.62e-06	-	1.70e-08	-
λ_{49}	500	7.03e-03	2.70	1.72e-03	4.38	4.02e-04	6.37
	1000	1.08e-03	5.06	8.24e-05	6.13	4.85e-06	8.22
	1500	1.39e-04	6.05	6.87e-06	6.42	1.73e-07	8.73
	2000	2.44e-05	7.23	1.08e-06	6.51	1.41e-08	8.97
	2500	4.85e-06	-	2.54e-07	-	1.90e-09	-

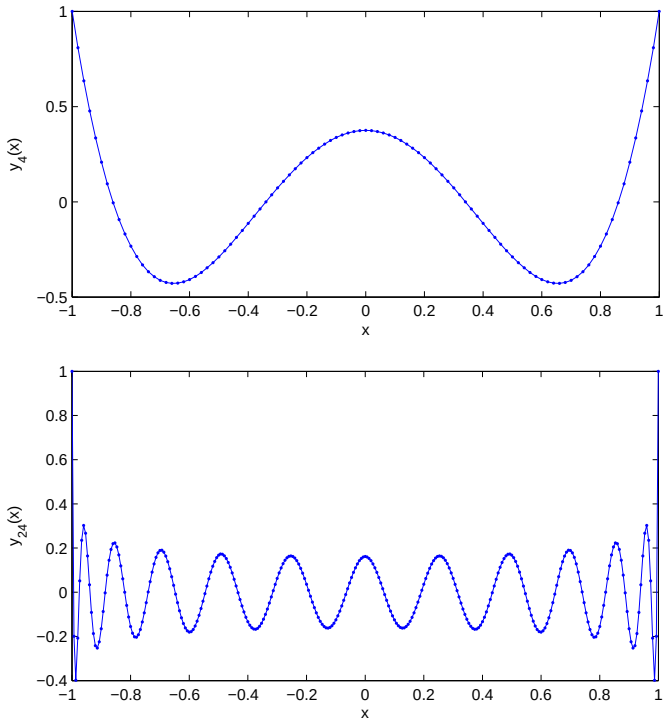

Figure 2: Eigenfunctions $y_4(x)$ and $y_{24}(x)$ computed by the order 6 method with 300 points.

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