High order finite difference schemes for the numerical solution of eigenvalue problems for IVPs in ODEs

Pierluigi Amodio and Giuseppina Settanni

Dipartimento di Matematica, Università di Bari, I-70125 Bari, Italy

Abstract. In this short note we describe how to apply high order finite difference methods to the solution of eigenvalue problems with initial conditions. Finite differences have been successfully applied to both second order initial and boundary value problems in ODEs. Here, based on the results previously obtained, we outline an algorithm that at first computes a good approximation of the eigenvalues of a linear second order differential equation with initial conditions. Then, for any given eigenvalue, it determines the associated eigenfunction.

Keywords: Initial value problems, eigenvalue problems, finite difference schemes.
PACS: 02.60.Lj, 02.70.Bf

INTRODUCTION

Eigenvalue problems with boundary conditions are quite important and widely studied since they describe many physical phenomena, both in classical and quantum mechanics, and also engineering problems such as wave functions in signal processing. They are defined by means of an ODE which depends on a parameter λ called eigenvalue. A classical example is the Sturm-Liouville problem [9] which is described by a second order ODE and is in general subject to separated boundary conditions. The main properties of Sturm-Liouville problems are that the eigenvalues are real and ordered as $\lambda_1 < \lambda_2 < \dots$. The eigenfunction associated with λ_i has $i-1$ zeros.

Different numerical approaches for solving BVODE eigenvalue problems have been developed over the years. For example, the shooting-type algorithms which reduce the solution of a boundary value problem to an initial value one (see, for example, [7]), and the so called matrix methods, where finite difference or finite element methods are considered to transform the original problem into the computation of the eigenvalues of a matrix [1, 2]. Most of the available code for boundary value problems have been adapted to the solution of eigenvalue problems. As an example, if the eigenvalue problem is singular, the code BVPSUITE1.1 [10] for singular boundary value problems has been successfully applied.

In this note our interest is to determine the numerical solution of eigenvalue problems where initial conditions are known. Although IVODE eigenvalue problems are less considered in the literature, they are of practical interest. We study the linear problem

$$p(t)y'' + q(t)y' + r(t)y = \lambda y, \qquad t \in [0,\ 1], \quad y, \lambda \in \mathbb{R} \tag{1}$$

subject to homogenous initial conditions

$$y(0) = y'(0) = 0, \tag{2}$$

where p, q and r are sufficiently smooth functions. In the following sections we describe a numerical method based on high order finite difference schemes proposed in [4, 5, 6] for boundary value problems, which have been generalized to initial value problems in [3]. The idea of this approach is to approximate each derivative of the original problem by a high order finite difference involving a finite set of discrete values of the solution. Therefore, it is not necessary to transform the original problem into a system of first order ODEs.

Depending on the position in the interval of integration, we use symmetric finite differences for the feasible inner points and one-sided finite differences at the boundaries, see [8]. Furthermore, for the IVPs in ODEs of second order, an appropriate use of $y'(0)$ has to be provided.

HIGH ORDER FINITE DIFFERENCES

Given an ODE

$$f(t,y,y',y'')=0, \qquad t\in[0,\ 1], \quad y\in\mathbb{R} \tag{3}$$

with initial conditions

$$y(0)=y_0, \qquad y'(0)=y'_0, \tag{4}$$

we fix a constant stepsize partition of $[0,\ 1]$

$$0=t_0<t_1<\cdots<t_n=1, \qquad t_i=t_0+ih=ih, \quad h=\frac{t_n-t_0}{n}=\frac{1}{n}, \tag{5}$$

and the following vector of approximations

$$Y=[y'_0,y_0,y_1,\ldots,y_n],$$

where $y_i\approx y(t_i)$ and y'_0 and y_0 are the known values in (4).

Then, based on the mesh specified in (5) and for a fixed number k we use central finite differences (called ECDFs in [5]) to approximate the first and the second derivative,

$$y'(t_i)\approx y'_i=\frac{1}{h}\sum_{j=-k}^{k}\beta_{j+k}y_j, \qquad i=k,\ldots,n-k,$$

$$y''(t_i)\approx y''_i=\frac{1}{h^2}\sum_{j=-k}^{k}\alpha_{j+k}y_j, \qquad i=k,\ldots,n-k,$$

where α_j and β_j are chosen in such a way that the formulae are consistent with the maximum order $2k$.

Moreover, we approximate the first and second derivatives at points t_i, $i=1,\ldots,k-1$, by

$$y'(t_i)\approx y'_i=\beta_*^{(i)}y'_0+\frac{1}{h}\sum_{j=0}^{2k-1}\beta_j^{(i)}y_j,$$

$$y''(t_i)\approx y''_i=\frac{1}{h}\alpha_*^{(i)}y'_0+\frac{1}{h^2}\sum_{j=0}^{2k}\alpha_j^{(i)}y_j,$$

and at points t_i, $i=n-k+1,\ldots,n$, by

$$y'(t_i)\approx y'_i=\frac{1}{h}\sum_{j=0}^{2k}\beta_j^{(i-n+2k)}y_{n-j},$$

$$y''(t_i)\approx y''_i=\frac{1}{h^2}\sum_{j=0}^{2k+1}\alpha_j^{(i-n+2k)}y_{n-j}.$$

We again choose the coefficients such that the formulae have maximum order.

Substituting y'_i and y''_i in (3) we obtain the following nonlinear system

$$f(t_i,y_i,y'_i,y''_i)=0, \qquad i=1,\ldots,n$$

that, together with the initial conditions (4), provide (in the linear case) a unique solution of the problem in the meshpoints (5).

EIGENVALUE COMPUTATION

If we apply the numerical method of the previous section to the left hand side of (1), we obtain a $n \times n$ matrix. The eigenvalues of such matrix are in general good approximations of the first eigenvalues of (1)-(2). Then, in order to improve the approximation of these values and to compute the corresponding eigenfunctions, we solve, for each λ_k of interest, the following nonlinear problem with unknowns $y_1, \ldots, y_n, \lambda_k$:

$$\begin{aligned} &p(t_i)y_i'' + q(t_i)y_i' + r(t_i)y_i = \lambda_k y_i, \qquad i = 1, \ldots, n, \\ &\sum_{i=0}^{n} y_i^2 = 1, \end{aligned} \tag{6}$$

where the last row is a normalization condition on the eigenfunction.

Since for the solution of (6) a very good approximation for λ_k is available, only few iterations are sufficient to compute the corresponding eigenfunction too.

TEST EXAMPLE

In this section we consider the following test problem (in the class of Sturm-Liouville problems)

$$(t^2-1)y'' + 2ty' - y = \lambda y \qquad t \in [0,1], \tag{7}$$

with initial conditions $y(0) = y'(0) = 0$. All the eigenvalues are real and positive.

We have computed the first 10 eigenvalues (and the corresponding eigenvectors) by using the previous formulae for the discretization of the derivatives. If we are interested in obtaining the eigenvalues with an error less than 10^{-2}, then very small sizes (at most 30 for the 10th eigenvalue) of the coefficient matrices are required. Viceversa, around 200 meshpoints were necessary to decrease the error to less than 10^{-3}. In Table 1 we show the computed value of each eigenvalue (approximated to 4 digits), the value of n required to obtain the prescribed tolerance for the orders 4, 6 and 8, and the relative errors.

TABLE 1. Relative error obtained approximating the eigenvalues with fixed order and n.

Eigenvalue	λ_1 1.001e0	λ_2 1.100e1	λ_3 2.901e1	λ_4 5.501e1	λ_5 8.902e1	λ_6 1.310e2	λ_7 1.811e2	λ_8 2.391e2	λ_9 3.051e2	λ_{10} 3.791e2
order 4 $n = 205$	7.72e-4	9.36e-4	9.63e-4	9.72e-4	9.76e-4	9.79e-4	9.80e-4	9.81e-4	9.81e-4	9.75e-4
order 6 $n = 170$	7.83e-4	9.48e-4	9.76e-4	9.86e-4	9.90e-4	9.92e-4	9.94e-4	9.95e-4	9.96e-4	9.96e-4
order 8 $n = 180$	7.76e-4	9.41e-4	9.67e-4	9.77e-4	9.81e-4	9.83e-4	9.84e-4	9.85e-4	9.85e-4	9.86e-4

We emphasize that, by using the orders and the number of meshpoints n shown in Table 1 for the above problem (7), a much greater number of eigenvalues is approximated with an error smaller than 10^{-4}. In particular, 16 eigenvalues are well approximated with order 4 and $n = 170$, 23 eigenvalues with order 6 and $n = 170$, and 24 eigenvalues with order 8 and $n = 180$. As an example, Figures 1 and 2 depict the eigenfunctions associated with λ_4 and λ_9, respectively.

REFERENCES

1. L. Aceto, P. Ghelardoni and C. Magherini, *BVMs for Sturm-Liouville eigenvalue estimates with general boundary conditions*, JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 1644–1656 (2009).
2. L. Aceto, P. Ghelardoni and C. Magherini, *Boundary value methods as an extension of Numerov's method for Sturm-Liouville eigenvalue estimates*, Appl. Numer. Math. **59**, 113–127 (2009).
3. P. Amodio and G. Settanni, *High order finite difference schemes for the solution of second order initial value problems*, JNAIAM J. Numer. Anal. Ind. Appl. Math. (2010), in press.
4. P. Amodio and G. Settanni, *Variable step/order generalized upwind methods for the numerical solution of second order singular perturbation problems*, JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 65–76 (2009).
5. P. Amodio and I. Sgura, *High-order finite difference schemes for the solution of second-order BVPs*, J. Comput. Appl. Math. **176**, 59–76 (2005).
6. P. Amodio and I. Sgura, *High order generalized upwind schemes and numerical solution of singular perturbation problems*, BIT **47**, 241–257 (2007).

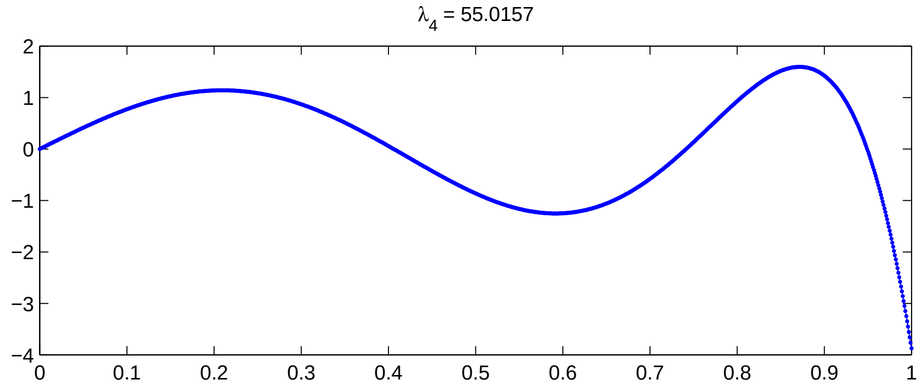

FIGURE 1. Eigenfunction associated with λ_4 in (7)

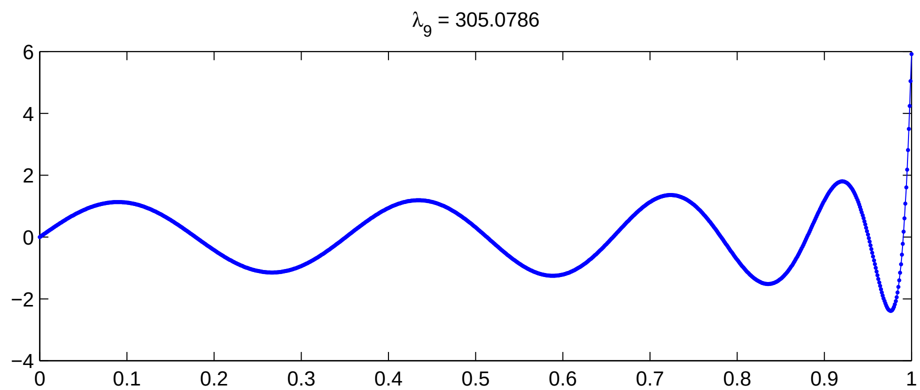

FIGURE 2. Eigenfunction associated with λ_9 in (7)

7. P. B. Bailey, M. K. Gordon and L. F. Shampine, *Automatic solution of the Sturm-Liouville problem*, ACM Trans. Math. Software **4**, 193–208 (1978).
8. L. Brugnano and D. Trigiante, *Solving Differential Problems by Multistep Initial and Boundary Value Methods*, Gordon and Breach Science Publishers, Amsterdam, 1998.
9. W. N. Everitt, *A catalogue of Sturm-Liouville differential equations*, in: Sturm-Liouville theory, W.O. Amrein, A.M. Hinz and D.B. Pearson Editors. Birkhäuser, Basel, 271–331, 2005.
10. G. Kitzhofer, O. Koch, G. Pulverer, C. Simon and E. B. Weinmüller , *BVPSUITE1.1 A new matlab solver for singular implicit boundary value problems*, `http://www.math.tuwien.ac.at/~ewa`.