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Numerical Treatment od Singular ODE EVPs Using `bvpsuite`

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Numerical Treatment of Singular ODE EVPs Using `bvpsuite`

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Abstract. We put forward a new method for the solution of eigenvalue problems for (systems of) ordinary differential equations, where our main focus is on eigenvalue problems for singular Schrödinger equations arising, for example, in electronic structure computations. Here, the generation of the starting values for the computation of eigenvalues of higher index is a critical issue. Our approach comprises two stages: First we generate rough approximations by a matrix method. These approximations are used as starting values for an adaptive collocation method which yields approximations of high accuracy together with a reliable error estimate. We successfully apply our method to the solution of the coupled ODE Stark problem for the hydrogen atom.

Keywords: electronic structure computation – polynomial collocation – fullpotential core solver – singular eigenvalue problems
PACS: 31.15ae – 31.15es – 32.60.+i

EIGENVALUE PROBLEMS FOR SINGULAR ODES

We study eigenvalue problems for systems of linear ordinary differential equations

$$Ly = \lambda y, \quad B_a y(a) + B_b y(b) = 0, \tag{1}$$

where L is a linear differential operator of order one or order two which may be singular, particularly we allow $a = -\infty$ and/or $b = \infty$[1]. The application that we focus on is the radial Schrödinger equation

$$Ly(r) := \left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) \right) y(r) = \lambda y(r), \quad r \in (0,\infty), \quad y(0) = y(\infty) = 0, \tag{2}$$

where $l \in \mathbb{N}_0$. This represents a *singular eigenvalue problem* [1]. Since the differential operator L is *self-adjoint*, the spectrum is real [2]. Our aim is to compute the point spectrum of L numerically.

Our approach uses first a *matrix method*, which replaces the continuous problem by a finite discretization whose eigenvalues converge to those of the original problem. This provides crude approximations of a large number of eigenvalues and eigenfunctions simultaneously, which serve as starting values for a solution based on collocation on adaptive meshes with reliable error control.

Alternative to our approach, there is a number of successful codes for the solution of (singular) Sturm-Liouville problems: SLEIGN2, SLEDGE, SL02F, MATSLISE and MATSCS. For more information and references see [11]. All these codes have in common that intricate procedures are integrated to enable computation of particular eigenvalues and eigenfunctions of higher index.

COLLOCATION METHOD

In the approach put forward and analyzed in [3], we rewrite the problem (1) by introducing the following auxiliary quantities: We formally interpret λ as a function of r and add the auxiliary differential equation $\lambda'(r) = 0$ and define $x(r) := \int_a^r |y(\tau)|^2 \, d\tau$, whence we have a further differential equation involving a quadratic nonlinearity, and

[1] In the second-order case, the boundary conditions in (1) may additionally depend on $y'(a)$, $y'(b)$; for notational simplicity, we restrict ourselves to Dirichlet boundary conditions.

two additional boundary conditions $x'(r) = |y(r)|^2,\ x(a) = 0,\ x(b) = 1$ to realize the usual normalization condition $\int_a^b |y(\tau)|^2 d\tau = 1$. The resulting augmented system is a boundary value problem in standard form (not an eigenvalue problem) for the set of unknowns $y(r)$, $\lambda(r)$ and $x(r)$ without any further unknown parameters. This system is subsequently solved by polynomial collocation. In this way, at some extra cost we can make use of the elaborate theory and practical usefulness of these methods, particularly for singular problems, and use a code developed by the authors featuring asymptotically correct error estimation and adaptive mesh selection for an efficient and reliable solution of the problem [4].

To treat the unbounded interval, we use an approach successfully applied for example in [5]: We split the interval at the point $r = 1$ and transform the problem posed on $[1,\infty)$ by $r \mapsto 1/r$. This yields a system of doubled size on the finite interval $(0,1]$, where the differential operator now has an *essential singularity* at zero.

As the problem is nonlinear it is sensitive to the starting values for the solution of the associated discrete nonlinear algebraic system. Particularly, for many problems (2), the eigenvalues accumulate at some finite number, which means that for the computation of eigenvalues of higher index, very accurate starting guesses are required. We propose to provide these by the *matrix method* introduced in the next section.

MATRIX METHOD

In this approach [6], the continuous problem (1) is replaced by an algebraic eigenvalue problem, whose eigenvalues and eigenvectors are approximations to the eigenvalues and eigenfunctions of the original problem. This can be done by any suitable discretization scheme. For simplicity, we describe the (singular) problem that results after transformation to a finite interval. We first consider a linear first order eigenvalue problem

$$Lz(t) = z'(t) - \frac{M(t)}{t^\alpha} z(t) = \lambda G(t) z(t), \quad t \in (0,1],\ \alpha \geq 1, \quad B_0 z(0) + B_1 z(1) = 0, \tag{3}$$

where z is a vector–valued function of dimension n. This general formulation also includes the case when eigenvalue problems for higher order equations are transformed to a first order system, and also the case of problems on unbounded intervals after transformation to the finite interval $(0,1]$, see [7].

The differential problem (3) is discretized by any suitable discretization scheme [6]. Since our main interest is in singular problems, we choose the *box scheme*, which is known to have beneficial convergence properties for this problem class [8, 9]. The eigenvalues of the resulting generalized algebraic eigenvalue problem

$$Av = \lambda Bv, \tag{4}$$

can be shown to converge to the eigenvalues of the continuous problem [6, 8] as the discretization parameter tends to zero. For the MATLAB computations reported in this paper, we used the MATLAB built-in function `eig(A,B)`, which computes the full spectrum of most general, non–Hermitian algebraic eigenvalue problems. For many problems in our scope, the matrix B in (4) is singular, whence standard convergence theory for this approach cannot be applied. According to the results in [8], B may be any square matrix. However, standard solution routines for the algebraic eigenvalue problem are commonly designed for the case where A is symmetric and B is symmetric and positive definite.

In detail, the approximation scheme for the singular first order problem is given by

$$\frac{z_{j+1} - z_j}{h_j} - \frac{1}{2} \frac{M(t_{j+1/2})}{t_{j+1/2}^\alpha} (z_{j+1} + z_j) = \lambda \frac{1}{2} G(t_{j+1/2})(z_{j+1} + z_j), \quad B_0 z_0 + B_1 z_N = 0. \tag{5}$$

Since this numerical scheme uses no evaluation at $t_0 = 0$, it can be applied straight forwardly to singular problems. The resulting matrix eigenvalue problem is given by

$$\begin{pmatrix} D_0 & R_0 & & & & \\ & D_1 & R_1 & & & \\ & & \ddots & \ddots & & \\ & & & & D_{N-1} & R_{N-1} \\ B_0 & & & & & B_1 \end{pmatrix} \begin{pmatrix} z_0 \\ z_1 \\ \vdots \\ z_N \end{pmatrix} = \lambda \begin{pmatrix} G_0 & G_0 & & & & \\ & G_1 & G_1 & & & \\ & & \ddots & \ddots & & \\ & & & & G_{N-1} & G_{N-1} \\ 0 & & & & & 0 \end{pmatrix} \begin{pmatrix} z_0 \\ z_1 \\ \vdots \\ z_N \end{pmatrix}, \tag{6}$$

where D_j, G_j and R_j are properly defined $n \times n$ matrices. Here h_j denotes the (not necessarily equidistant) step width and I is the identity matrix. Subsequently we will actually use equidistant step-sizes for the matrix method. A truly adaptive mesh refinement based on the solution behavior for this method is computationally demanding, and is not necessary for our purpose, as we use the matrix method only as a routine to provide starting values for an adaptive solution method with reliable error control. An a priori choice of a graded mesh is not appropriate here, as the underlying discretization is robust with respect to the singularity [8].

APPLICATIONS

In this section, we illustrate the performance of our approximation method by considering examples of interest in the physics literature. We first discuss the Schrödinger equation for the radially symmetric *Yukawa potential*,

$$-\frac{1}{2}y''(r)+\left(\frac{l(l+1)}{2r^2}+V(r)\right)y(r)=\lambda y(r), \quad r\in(0,\infty), \quad y(0)=0,\, y(\infty)=0, \quad V(r)=-\frac{\mathrm{e}^{-\alpha r}}{r}, \tag{7}$$

where the parameter $\alpha > 0$ is called *screening parameter*. Bound states exist only for values of α below a threshold α_c. The number of elements in the point spectrum varies with α.

Table 1 shows the results of our hybrid method and compares them to values reported in [10]. The most remarkable advantage of our approach is the high accuracy which is confirmed by a reliable a posteriori error estimate. In the adaptive collocation method, 8 collocation points are used. For further comparisons see [11].

TABLE 1. Example (7): Comparison of the eigenvalues of the Yukawa potential for several values of α reported in [10]. For the computations we prescribed $tol_a = 10^{-15}$ and $tol_r = 10^{-10}$. $\lambda^{(0)}$ (MM) denotes the initial approximation for the eigenvalue computed by the matrix method.

α	n	l	$\lambda^{(0)}$ (MM)	N	bvpsuite	errest_λ	[10]
0.1	1	0	−0.4073	70	−0.40705803061326	$2.2\cdot10^{-19}$	−0.40705803061340
0.01	2	1	−0.1154	167	−0.11524522409056	$1.1\cdot10^{-19}$	−0.11524522409056
0.01	3	1	−0.0468	188	−0.04615310482916	$8.2\cdot10^{-20}$	−0.04615310482916
0.01	3	2	−0.0463	176	−0.04606145416066	$5.4\cdot10^{-20}$	−0.04606145416065
0.01	9	0	−0.00111	350	−0.00058524761250	$7.2\cdot10^{-21}$	−0.00058524761250
0.01	9	1	−0.00106	1034	−0.00056650762617	$2.5\cdot10^{-21}$	−0.0005665076261

The next example is the Schrödinger equation (7) with the *Hulthén potential*, $V(r)=-\frac{\alpha \mathrm{e}^{-\alpha r}}{1-\mathrm{e}^{-\alpha r}}$ [10]. Table 2 gives a comparison of our results with those from [10].

TABLE 2. Example (7): Comparison of the eigenvalues of the Hulthén potential for several values of α reported in [10]. For the computations we prescribed $tol_a = 10^{-15}$ and $tol_r = 10^{-10}$.

α	n	l	$\lambda^{(0)}$ (MM)	N	bvpsuite	errest_λ	[10]
0.002	1	0	−0.4993	67	−0.49900049999985	$8.7\cdot10^{-18}$	−0.49900050000000
0.15	3	2	−0.0015	235	−0.00139659246573	$1.9\cdot10^{-20}$	−0.00139659246573
0.02	8	1	−0.0016	1441	−0.0009868327076	$2.6\cdot10^{-21}$	−0.0009868327076

According to [12], for $l = 0$ exact eigenvalues can be determined analytically for the Hulthén potential. These are given by

$$\lambda_n^{exact}=-\frac{1}{2}\left(\frac{1}{n}-\frac{n\alpha}{2}\right)^2. \tag{8}$$

The resulting value corresponding to the first row in Table 2 is $\lambda = -0.49900050000000$. The error estimate computed by our numerical method is approximately equal to 10^{-18}, see Table 2, while the true error for $l = 0$ is 10^{-13}. This is no contradiction, since both errors are of the order of magnitude of round-off in double precision arithmetic.

Finally, we give numerical results for a Schrödinger equation with matrix-valued potential to demonstrate that systems of equations can be treated in a natural way by our code without any special handling. We discuss the hydrogen atom in a dc-electric field in x_3-direction, the *Stark effect* [13], which is given by the following PDE-operator

$$H(\mathscr{E})=-\frac{1}{2}\triangle-\frac{1}{r}-\mathscr{E}f_b(r)x_3=-\frac{1}{2}\triangle-\frac{1}{r}-\sqrt{\frac{4\pi}{3}}\mathscr{E}f_b(r)rY_{10}(x), \tag{9}$$

where $x = (x_1, x_2, x_3)$. The function $f_b(r)$ makes the perturbation decay to zero for large r and could be chosen as $f_b(r) := e^{-br^2}$, $b \geq 0$. The potential is no longer spherically symmetric and therefore no decoupled radial ODEs are obtained. Standard expansion into spherical harmonics $Y_{\ell m}$ and truncation at $l_{max} = 1$ lead to four, $(l_{max}+1)^2$, ODEs consisting of two decoupled ODEs and the following ODE system

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \begin{pmatrix} -\frac{1}{r} & -\frac{\mathscr{E}}{\sqrt{3}} r f_b(r) \\ \frac{\mathscr{E}}{\sqrt{3}} r f_b(r) & -\frac{1}{r} + \frac{1}{r^2} \end{pmatrix} \right] y(r) = \lambda y(r), \quad r \in (0,\infty), \quad y(0) = 0,\ y(\infty) = 0. \tag{10}$$

It turns out that our approach works equally well for $b = 0$ which we will henceforth use. Table 3 shows our numerical results for $\mathscr{E} = 10^{-4}$ as compared to the values determined by perturbation theory [13].

TABLE 3. Example (10): The computed eigenvalues λ for $\mathscr{E} = 10^{-4}$ and $b = 0$ as compared to the results from perturbation theory. The tolerances were set to $tol_a = 10^{-15}$ and $tol_r = 10^{-10}$.

n	$\lambda^{(0)}$ (MM)	N	bvpsuite	errest$_\lambda$	λ_{per}
1	-0.5001	100	-0.500000022499859	$4.4 \cdot 10^{-19}$	-0.500000022500000
2	-0.1253	163	-0.125300320116262	$2.2 \cdot 10^{-19}$	-0.125300840000000
3	-0.1247	163	-0.124700319903047	$1.1 \cdot 10^{-19}$	-0.124700840000000

CONCLUSIONS

We have presented an alternative method for the solution of eigenvalue problems for singular ODEs which is very well suited for the radial Schrödinger equation. Our approach is based on a routine to determine rough approximations to several of the eigenvalues and eigenfunctions simultaneously, and subsequent refinement by an adaptive collocation method which additionally yields a reliable error estimate. This method can be efficiently applied to a more general class of singular boundary value problems, but can also compete with methods especially adapted to the linear second order radial Schrödinger equation.

REFERENCES

1. J. Pryce, Numerical Solution of Sturm-Liouville Problems, Oxford University Press, New York, 1993.
2. G. Teschl, Mathematical Methods in Quantum Physics, Graduate Studies in Mathematics, Amer. Math. Soc., Providence, 2009.
3. W. Auzinger, E. Karner, O. Koch, E. Weinmüller, Collocation methods for the solution of eigenvalue problems for singular ordinary differential equations, Opuscula Math. 26 (2) (2006) 229–241.
4. G. Kitzhofer, O. Koch, G. Pulverer, C. Simon, E. Weinmüller, The new MATLAB code BVPSUITE for the solution of singular implicit BVPs, accepted for JNAIAM J. Numer. Anal. Indust. Appl. Math.
5. C. J. Budd, O. Koch, E. Weinmüller, Computation of self-similar solution profiles for the nonlinear Schrödinger equation, Computing 77 (2006) 335–346.
6. H.-O. Kreiss, Difference approximations for boundary and eigenvalue problems for ordinary differential equations, Math. Comp. 26 (119) (1972) 605–624.
7. W. Auzinger, O. Koch, E. Weinmüller, Collocation methods for boundary value problems with an essential singularity, in: I. Lirkov, S. Margenov, J. Wasniewski, P. Yalamov (eds.), Large-Scale Scientific Computing, vol. 2907 of Lecture Notes in Computer Science, Springer Verlag, 2004.
8. F. d. Hoog, R. Weiss, Difference methods for boundary value problems with a singularity of the first kind, SIAM J. Numer. Anal. 13 (1976) 775–813.
9. F. d. Hoog, R. Weiss, The numerical solution of boundary value problems with an essential singularity, SIAM J. Numer. Anal. 16 (1979) 637–669.
10. A. Roy, The generalized pseudospectral approach to the bound states of the Hulthén and the Yukawa potentials, PRAMANA – J. Phys. 65 (2005) 1–15.
11. R. Hammerling, O. Koch, C. Simon, E. Weinmüller, Numerical Solution of Singular EVPs for ODEs with a Focus on Problems Posed on Semi-Infinite Intervals, ASC Report No. 8/2010, Vienna University of Technology, Vienna, Austria (2010).
12. O. Bayrak, I. Boztosun, Analytical solutions of the Hulthén and the Morse potentials by using the Asymptotic Iteration Method, J. Mol. Structure: THEOCHEM 802 (2007) 17–21.
13. L. D. Landau, L. M. Lifshitz, Quantum Mechanics: Non-Relativistic Theory, vol. 3, Butterworth-Heinemann, Oxford, U.K., 1981.