On certain numerical technique to solve Sturm-Liouville systems (1)

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Abstract. This note deals with the generalization of a numerical technique to compute approximated eigenvalues and eigenfunctions of second order linear differential operators in one dimension recently proposed. This technique now uses a finite matrix representation of the operator d/dx built out of N numbers obtained by imposing a condition where the coefficients of the differential equation play the main part. It is shown numerically that this method can now be applied to eigenvalue problems with difficult–to–handle boundary conditions.

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Recently, M. Bruschi, R.G. Campos and E. Pace [1], have improved a numerical method to compute eigenvalues of linear ordinary differential equations proposed some years ago by F. Calogero [2]. This method consists in the substitution of the differential operator d/dx and the variable x by the $N \times N$ matrices

$$D_{ij} = \begin{cases} \sum_{k=1}^{N}{}' \dfrac{1}{(x_i - x_k)}, & i = j, \\ \dfrac{1}{(x_i - x_j)}, & i \neq j, \end{cases} \qquad X_{ij} = x_i \delta_{ij}, \tag{1}$$

built out of the N arbitrary different numbers $x_1, x_2, \ldots, x_N$, (the prime of the sum sign means that the term with $i = k$ is excluded) in the differential equation to convert it into a matricial problem. (A similar method was proposed independently by one of us [3]). The improvement frees this method of its main drawback: the presence of complex eigenvalues for an hermitian operator as the Schrödinger-like differential operator

$$-\varphi_n''(x) + q(x)\varphi_n(x) = \lambda_n \omega(x)\varphi_n(x), \qquad x \in (a, b), \tag{2}$$

where $\omega(x) > 0$, and $\varphi(a) = \varphi(b) = 0$. It takes advantage of the arbitrariness in the

selection of the points x_j and of the fact that the method embodies the homogeneous boundary conditions of such a problem through the *ansatz*

$$\varphi(x) = \gamma(x)f(x), \qquad a \leq x \leq b, \tag{3}$$

where $\gamma(a) = \gamma(b) = 0$ and $f(x)$ is a supposed regular function at the boundary points. The matrices given in Eq. (1) replace the operators d/dx and x in the differential equation for $f(x)$ obtained by the substitution of (3) in (2). In Ref. [1] it is shown that if $\gamma(x) = (x-a)^{\mu}(b-x)^{\nu}$, $\mu > 0, \nu > 0$ and the points x_j are chosen to satisfy the nonlinear equations

$$\sum_{k=1}^{N}{}' \frac{1}{(x_i - x_k)} = -\frac{\gamma'(x_i)}{\gamma(x_i)}, \qquad i = 1, 2, \ldots, N, \tag{4}$$

then a really fast convergence of the approximated eigenvalues to those of Eq. (2) is obtained for functions $q(x)$ and $\omega(x)$ satisfying certain boundary conditions.

Our purpose in this note is to report the numerical results yielded by a generalization of this method when it is applied to a unidimensional two-point boundary problem with nonhomogeneous conditions like this one

$$[(1-x^7)\varphi'(x)]' + \lambda x^7 \varphi(x) = 0, \quad \varphi(0) = 0, \quad \varphi(x) \text{ continuous at } x = 1. \tag{5}$$

This equation, concerning a heat conduction problem, [4] does not meet the conditions for which the results of Ref. [1] are valid. Besides the strong singularity, the lack of a *quantitative* condition on $\varphi(x)$ at $x = 1$, makes this problem difficult to handle even with other methods [4]. But this is not beyond remedy, because we can obtain good results, in agreement with those obtained by other authors, if we extend the numerical procedure as follows.

We begin by considering the general form of the Sturm-Liouville equation

$$[p(x)\varphi'(x)]' + q(x)\varphi(x) = \lambda\omega(x)\varphi(x) \qquad x \in (a, b), \tag{6}$$

where $p(x), \omega(x) > 0$ for $x \in (a, b)$. In the ansatz (3), the function $f(x)$ is supposed to be approximated by polynomials, *i.e.*, a polynomial of degree N that satisfies approximately the equation

$$A_2(x)f''(x) + A_1(x)f'(x) + A_0(x)f(x) = \lambda\omega(x)f(x)$$

where

$$A_2(x) = p(x), \qquad A_1(x) = 2p(x)\frac{\gamma'(x)}{\gamma(x)} + p'(x),$$

$$A_0(x) = p(x)\frac{\gamma''(x)}{\gamma(x)} + p'(x)\frac{\gamma'(x)}{\gamma(x)} + q(x),$$

is supposed to exist. This means that the N points x_j obtained through

$$\sum_{k=1}^{N}{}' \frac{1}{(x_i - x_k)} = -\frac{1}{2}\frac{A_1(x_i)}{A_2(x_i)}, \qquad i = 1, 2, \ldots, N, \tag{7}$$

are the N approximated zeros of $f(x)$ [5]. Therefore, these points should be a better choice than those yielded by Eq. (4). It is an easy matter to show that the matrices D and X built out of these numbers yield real eigenvalues for

$$L = A_2(X)D^2 + A_1(X)D + A_0(X).$$

Firstly, we note that the right-hand side of (7) can be written as $-\Gamma'(x_i)/\Gamma(x_i)$ where $\Gamma(x) = \gamma(x)\sqrt{p(x)}$, and this function is usually zero at the extreme. Therefore, a solution of (7) there exists [6], with $a < x_1 < x_2 < \cdots < x_N < b$ (if $\ln(\Gamma(x))$ is a concave function, the solution is unique), and this implies that the matrices $p(X)$ and $\omega(X)$ are positive definite. Because L can be written as a product of the positive definite matrix $p(X)[\omega(X)]^{-1}$ and the hermitian matrix $(D^2 + Dd - dD - d^2 + A_0(X)[A_2(X)]^{-1})$, where d is the diagonal matrix whose nonzero elements are given by Eq. (7), its eigenvalues are all real, having the same inertia as those yielded by the hermitian matrix.

Note that Eq. (4) is one case of Eq. (7). the function $\gamma(x)$ should be chosen to embody the boundary conditions in such a way that the ansatz (3) satisfies the differential equation at the extreme, as stated in Ref. [1].

Thus, for the problem given in Eq. (5), we choose $\gamma(x) = x$ and build the matrices D and X out of the points obtained through

$$\sum_{k=1}^{N}{}' \frac{1}{(x_i - x_k)} = \frac{1}{x_i} - \frac{7x_i^6}{2(1 - x_i^7)}, \qquad i = 1, 2, \ldots, N.$$

According to this method [2], we proceed to diagonalize the matrix

$$L = (1 - X^{-7})D^2 + (9X^{-1} - 2X^{-8})D + 7X^{-2}. \tag{8}$$

The first eigenvalues λ_n^* of this matrix (approximants of those of Eq. (5), λ_n) are shown in Tables I and II for some values of the number of points N. The components $(\mathbf{v}_n)_i$ of the eigenvectors $\mathbf{v}_n$ of (8) are related to the values $\varphi_n^*(x_i)$ of the

n	λ_n^* $(N = 10)$	λ_n^L	λ_n^U
1	8.72747035	8.721575	8.727471
2	152.423	128.2512	152.4231
3	435.	208.3475	435.0634

TABLE I. The first three stabilized eigenvalues λ_n^* of the matrix given in Eq. (8) obtained with a 10–point mesh are shown in the second column. they can be compared with the lower and upper bounds λ_n^L and λ_n^U, obtained [4] by the orthogonal invariants method and the Rayleigh-Ritz method respectively.

n	$\lambda_n^*(N = 20)$
1	8.727470352642
2	152.42307087862
3	435.063332175
4	855.68572

TABLE II. The first four stabilized eigenvalues of the matrix given in Eq. (8) obtained with a 20–point mesh. The stabilization was established by comparing them with the eigenvalues computed with a 25–point mesh.

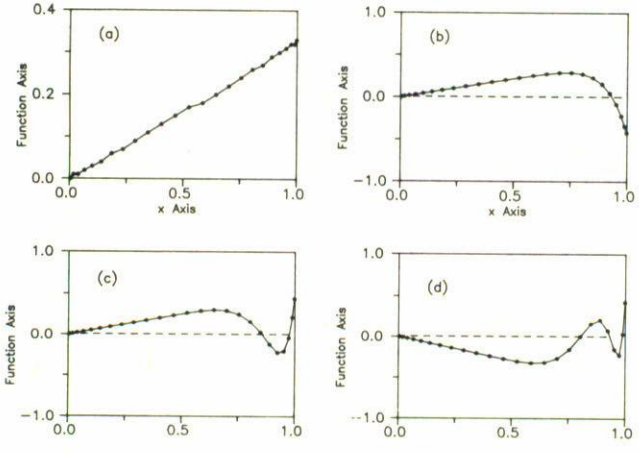

FIGURE 1. (a)–(d): Piecewise linear interpolations of the first four normalized vectors $\varphi_n^*(x_i)$, $n = 1, \ldots, 4$, yielded by Eq. (9). They are the approximants to the corresponding eigenfunctions $\varphi_n(x)$, $n = 1, \ldots, 4$ of Eq. (5).

approximated eigenfunctions of (5) through [2,1]

$$\varphi_n^*(x_i) = C_n \gamma(x_i) \left[\prod_{k \neq i} (x_i - x_k) \right] (\mathbf{v}_n)_i \tag{9}$$

where C_n is a normalization constant.

In Fig. 1 we show a graphic description of the first four normalized eigenvectors $\varphi_n^*(x_i)$ obtained for $N = 25$.

We conclude this note pointing out the simplicity of this procedure. The results presented in this work have been performed on a personal computer using standard FORTRAN 77 routines to solve Eq. (7) and to diagonalize Eq. (8).

References

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Resumen. Esta nota trata con la generalización de una técnica numérica recientemente propuesta para calcular eigenvalores y eigenfunciones aproximados de operadores diferenciales lineales en una dimensión. Esta técnica ahora usa una representación matricial finita del operador d/dx construida con N números obtenidos a partir de una condición donde los coeficientes de la ecuación diferencial juegan el papel principal. Este método puede ser aplicado a problemas de eigenvalores con condiciones a la frontera difíciles de manejar, como se muestra numéricamente.