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AERONOMICA ACTA

A - N° 38 - 1965

An iterative method for the solution of eigenvalue problems

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FOREWORD

The paper entitled "An iterative method for the solution of eigenvalue problems" has been submitted for publication in "Mathematics of Computation".

AVANT PROPOS

L'article "An iterative method for the solution of eigenvalue problems" a été soumis pour publication dans "Mathematics of Computation".

VOORWOORD

Het artikel "An iterative method for the solution of eigenvalue problems" is ter publicatie voorgelegd aan "Mathematics of Computation".

VORWORT

Die Arbeit "An iterative method for the solution of eigenvalue problems" wurde für Veröffentlichung in "Mathematics of Computation" eingegelen.

AN ITERATIVE METHOD FOR THE SOLUTION OF EIGENVALUE PROBLEMS

By

M. GODART

Abstract

A new simple iterative method is developed for the determination of proper elements associated with the solution of Sturm-Liouville problems. The convergence of the iteration process is rapid and each eigenvalue can be estimated independently of all the other eigenvalues. The involved accuracy is determined by the method used for the solution of an ordinary first order differential equation.

Zusammenfassung

Um die, mit der Lösung Sturm-Liouvilleschen Problemen, verbundenen Eigenelemente zu rechnen, stellen wir ein neues Iterationsverfahren vor. Die Konvergenz dieses Verfahren ist sehr gut und jede Eigenwert kann unabhängig von den anderen gerechnet werden. Die Genauigkeit hängt meistens von der Lösung einer gewöhnlichen Differentialgleichung erster Ordnung ab.

Résumé

Nous présentons une nouvelle méthode iterative simple pour déterminer les éléments propres associés à la résolution des problèmes de Sturm-Liouville. La convergence du processus est rapide et chaque valeur propre peut être calculée indépendamment de toutes les autres. La précision atteinte est déterminée principalement par la technique utilisée pour résoudre une équation différentielle ordinaire du premier ordre.

Samenvatting

Wij stellen een eenvoudige iteratiemethode voor om de eigenwaarden en -funkties te bepalen van vraagstukken welke leiden tot vergelijkingen van Sturm-Liouville. De convergentie van het iteratieproces is snel en iedere eigenwaarde kan onafhankelijk van de overige berekend worden. De bereikte nauwkeurigheid wordt hoofdzakelijk bepaald door de methode die gebruikt werd om een gewone differentiaalvergelijking van de eerste orde op te lossen.

1.- INTRODUCTION

Many boundary value problems of interest in mathematical physics can be finally reduced to the determination of the proper elements of a Sturm-Liouville equation. The most general form of these equations is :

$$\frac{d}{d\,x}\left[\,p(x)\,\frac{dy(x)}{d\,x}\,\right] + q(x)\;y(x) + \lambda r(x)\;y(x) = 0\;, \tag{1}$$

with $a \leq x \leq b$, and the problem is to determine the particular values of the λ parameter (eigenvalues) for which equation (1) possesses non identically zero solutions (eigenfunctions) obeying two boundary conditions of the type :

$$A_1\;y(a) + A_2\;p(a)\,\frac{dy(a)}{dx} = 0\;, \tag{2,a}$$

$$B_1\;y(b) + B_2\;p(b)\,\frac{dy(b)}{dx} = 0\;, \tag{2,b}$$

where the values of the constants A_1, A_2 and B_1, B_2 are not simultaneously zero.

Several methods have been proposed to determine the proper elements (i.e. eigenvalues and eigenfunctions) of Sturm-Liouville equations. Most of them have been reviewed by Kopal[1], but we shall examine one of them, the so called Rayleigh-Ritz method, in order to explain the main defect they have in common and to judge their general efficiency. This method was originally proposed by Ritz[2]. By transformations whose details will not be given here but which are described in many classical texts it leads to the solutions of equations of the form :

$$\det \| D_{ik} - \lambda H_{ik} \| = 0, \qquad (3)$$
$$1 \leq i, \quad k \leq n$$

where the D_{ik} and H_{ik} are the values of quadratic functionals for the i-th and k-th elements of a sequence of trial functions chosen once for all. Under rather general conditions, it can be shown that for indefinitely increasing values of n, the solutions of equation (3) decrease monotonically and converge to the eigenvalues of the originally stated problem. More precisely, if $\lambda_m^{(n)}$ is the m-th solution of equation (3) when the solutions are ranged in increasing order, then the sequence of all the numbers $\lambda_m^{(n)}$ with $n = m, m + 1, \ldots\ldots$ is decreasing and converges to the m-th eigenvalue of the corresponding Sturm-Liouville equation when its eigenvalues are also ranged in increasing order. The big defect of this approximation method is its inability to furnish any estimate of the difference between one of the numbers $\lambda_m^{(n)}$ and the corresponding eigenvalue λ_m.
A theoretical convergence is not sufficient because the solution of equation (3) gets extremely complicated when n increases. A rapid convergence is thus required but this can only be reasonably expected if we possess beforehand a rather precise knowledge of the general behaviour of the eigenfunctions. This is not usually the case.
An even more serious defect of this method is that high values of n are necessary to obtain the higher order eigenvalues and to reduce a truncation-like error for the low order eigenvalues appreciably. When however such large values of n are used, the determinantal equation (3) for λ turns out to be of a correspondingly high degree and its solution may then entail such an accumulation of round-off errors as to prevent any further diminution of the total error affecting the computed eigenvalues. The necessity to compromise between these two sources of error severely restricts the accuracy obtainable. Similar restrictions are encountered when other previously developed methods are applied.

The methos currently in the mathematical literature devoted to the approximation of the proper elements of a Sturm-Liouville problem are thus not very reliable. The present work will describe a very simple method which does not suffer from the main defects of the calculation methods used previously. In what follows, the underlying principle of the method will be explained and it will be shown how it can be applied. A particularly simple case will then be treated in order to illustrate the efficiency of the new method. It will finally be shown that it can be extended to singular Sturm-Liouville equations.

2.- THE NEW APPROXIMATION METHOD.

The method is based on the remarkable properties of a function introduced in a change of dependent variables that considerably simplifies the theoretical study of those equations. Continual reference will be made to references [4] and [5] where all details and proofs omitted here for sake of brevity can be found. It will be assumed that in the interval $a \leq x \leq b$, the function $p(x)$ is positive and possesses a first continuous derivative, that the function $r(x)$ is positive and continuous and that the function $q(x)$ is continuous. The new dependent variables $\rho(x)$ and $\theta(x)$ may be introduced by means of the defining equations :

$$y(x) = \rho(x) \sin \theta(x), \tag{5,a}$$

$$p(x) \frac{dy(x)}{dx} = \rho(x) \cos \theta(x). \tag{5,b}$$

According to equation (1) and boundary conditions (2,a) and (2,b), the function $\theta(x)$ obeys the differential equation :

$$\frac{d\theta(x)}{dx} = \frac{1}{p(x)} \cos^2 \theta(x) + \left[q(x) + \lambda\, r(x) \right] \sin^2 \theta(x) \tag{6}$$

and satisfies the boundary conditions :

$$A_1 \sin\theta(a) + A_2 \cos\theta(a) = 0, \tag{7,a}$$

$$B_1 \sin\theta(b) + B_2 \cos\theta(b) = 0, \tag{7,b}$$

while the function $\rho(x)$ obeys the differential equation :

$$\frac{d\rho(x)}{dx} = \rho(x)\,\sin\theta(x)\,\cos\theta(x)\left[\frac{1}{p(x)} - q(x) - \lambda\, r(x)\right] \tag{8}$$

and satisfies the condition of never being zero in the interval $a \leq x \leq b$.

Let us now determine a priori permissible initial and final values for the function $\theta(x)$ by means of the auxiliary conditions :

$$0 \leq \alpha < \pi\,, \tag{9,a}$$

$$0 < \beta \leq \pi\,, \tag{9,b}$$

Boundary conditions (7,a) and (7,b) can then be replaced by the equivalent conditions :

$$\theta(a) = \alpha, \tag{10,a}$$

$$\theta(b) = \beta + n\pi\,, \tag{10,b}$$

where n is any integer (positive, negative or null).

The solution $\theta(x, \lambda)$ of equation (6) satisfying an initial condition deduced from (10,a) and (9,a) possess the following interesting properties.

As is shown in [4] and [5], $\theta(x, \lambda)$ is a monotonically increasing function of the argument λ and satisfies the equalities :

$$\lim_{\lambda \to -\infty} \theta(b, \lambda) = 0, \tag{11,a}$$

$$\lim_{\lambda \to +\infty} \theta(b, \lambda) = +\infty. \tag{11,b}$$

Moreover, the function :

$$\chi(x, \lambda) = \frac{\partial\theta(x, \lambda)}{\partial\lambda} \tag{12}$$

is a solution of the differential equation :

$$\frac{d\chi(x, \lambda)}{dx} = \chi(x, \lambda)\left[q(x) + \lambda r(x) - \frac{1}{p(x)} \right] \sin 2\theta(x, \lambda) + r(x) \sin^2 \theta(x, \lambda) \tag{13}$$

and it obviously satisfies the initial condition :

$$\chi(a, \lambda) = 0 \tag{14}$$

From this, we can deduce that $\chi(x, \lambda)$ is positive everywhere in the interval $a < x \leq b$. Equation (13) and initial condition (14) lead to the expression :

$$\chi(x, \lambda) \exp \int_a^x \left[q(\xi) + \lambda r(\xi) - \frac{1}{p(\xi)} \right] \sin 2\theta(\xi, \lambda)\, d\xi$$

$$\int_a^x r(\eta) \sin^2 \theta(\eta, \lambda) \exp\left\{ -\int_a^\eta \left[q(\xi) + \lambda r(\xi) - \frac{1}{p(\xi)} \right] \sin 2\theta(\xi,\lambda)d\xi \right\} d\eta \tag{15}$$

Because of our hypothesis concerning the functions $p(x)$, $q(x)$ and $r(x)$, this function is certainly non negative in the interval $a < x \leq b$. Moreover, it can be zero at a point $x = c$ of this interval only if the function $\sin \theta(x, \lambda)$ is identically zero and thus constant in the interval $a < x \leq c$. This cannot happen however because at all points where the function $\sin \theta(x, \lambda)$ vanishes, we have according to (6) :

$$\frac{d\theta(x, \lambda)}{dx} = \frac{1}{p(x)} > 0, \tag{16}$$

and also :

$$\frac{d \sin \theta(x, \lambda)}{dx} = \pm \frac{1}{p(x)} \neq 0 \tag{17}$$

and this would contradict the previous deduction that $\sin\theta(x, \lambda)$ must be constant in the interval $a < x \leq c$.

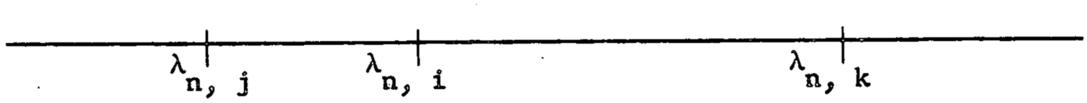
Now, the derivative $\chi(b, \lambda)$ of the function $\theta(b, \lambda)$ with respect to λ is positive. When this is considered with the relations (11,a) and (11,b) it may be clearly seen that the second boundary condition (10,b) considered as an equation for λ is solvable only for non negative values of the integer n and that it then possesses one and only one solution. The calculation of the (n + 1) - th eigenvalue λ_n is thus equivalent to the solution of the equation :

$$\beta + n\pi - \theta(b, \lambda) = 0 \tag{18}$$

In the present case, the Newton-Raphson approximation method leads to the algorithm :

$$\lambda_{n,\, k+1} = \lambda_{n,\, k} + \left[\beta + n\pi - \theta(b, \lambda_{n,\, k}) \right] \chi^{-1}(b, \lambda_{n,\, k}), \tag{19}$$

where $\lambda_{n,\, k}$ denotes the k - th approximation to the eigenvalue λ_n. The application of the algorithm (19) does not present any difficulties, especially when an electronic computer is available for the numerical integration of equations (6) and (13), or (6) and (15). Nothing can ensure the convergence of the successive estimates $\lambda_{n,\, k}$ to the corresponding eigenvalue λ_n, but obtaining a converging sequence of approximations is no longer a problem. In fact, it can be seen that the correction proposed by formula (19) for a known approximation is always in the right direction. In other words, this correction is positive (resp. negative, zero) if the chosen approximation is less than (resp. greater than, equal to) the sought eigenvalue. Then the only accident that must be avoided is to disturb or even to make the convergence impossible by obtaining successive approximation $\lambda_{n,\, i}$, $\lambda_{n,\, k}$ and $\lambda_{n,\, j}$ $(i < k < j)$ as shown in the following diagram :



Whenever such a situation occurs in the iteration process however, it is sufficient, in order to realise a sequence of successive approximations which certainly converges to the sought eigenvalue λ_n, to replace the value $\lambda_{n,j}$ computed with formula (19) by the arithmetical mean of the minimum and maximum values of all preceding approximations.

3.- APPLICATIONS

A. The efficiency of the proposed method for the approximation of the proper elements of Sturm-Liouville equations, will now be investigated on a particularly simple example.
Consider the differential equation :

$$\frac{d^2y(x)}{dx^2} + \lambda y(x) = 0 \tag{20}$$

and the boundary conditions :

$$y(0) = 0 \quad , \tag{21,a}$$

$$\frac{dy(1)}{dx} = 0. \tag{21,b}$$

Elementary calculations show that the proper elements of this problem are given by :

$$\lambda_n = (2n + 1)^2 \pi^2 /4 \quad , \tag{22,a}$$

$$y_n(x) = \sin (2n + 1) \pi x /2 \; . \tag{22,b}$$

In table I, we compare the eigenvalues as they have been determined by our method ($\lambda_{comp.}$) to their exact values ($\lambda_{theor.}$) for the first five values of the integer n. As an illustration, the estimated relative errors and the required numbers of iterations are also given.

TABLE I

n	$\lambda_{comp.}$	$\lambda_{theor.}$	$\varepsilon \times 10^6$	Iterations
0	2.46739	2.467401	4	9
1	22.2068	22.20661	8	1
2	61.6863	61.68503	21	3
3	120.907	120.9026	36	3
4	199.869	199.8595	48	3

It can thus be seen that the method provides good results in this case.

B. The theory as devoloped to this point is not applicable to cases for which the function p(x) can be zero at one or both of the extremities x = a or x = b. The method proposed is however applicable to these cases, after being slighty modified. For sake of brevity, the theoretical aspects will be omitted and only intuitive arguments will be used. These can, however, be estabiished rigorously. Two examples will be treated in order to indicate the suggested extension.

1° Consider the differential equation :

$$\frac{d}{dx}\left[x\,\frac{dy(x)}{dx}\right] + \lambda x y(x) = 0 \qquad (23)$$

and the boundary conditions :

$$|\,y(0)\,| < +\infty\,, \qquad (24,a)$$

$$y(1) = 0. \qquad (24,b)$$

It can easily be seen that the proper elements of this Sturm-Liouville problem are given by :

$$\lambda_n = j_n^2 , \tag{25,a}$$

$$y_n(x) = \sqrt{x}\, J_o\, (j_n\, x) , \tag{25,b}$$

where J_o is the Bessel function of order 0 and where j_n is its (n + 1) - th positive zero.

Equation (6) shows that the singularity at x = 0 can be avoided if we take :

$$\alpha = \pi /2. \tag{26,a}$$

By choosing β as explained in the second paragraph, the approximation method may be applied. The calculations have been performed and the obtained results are given in table II in the same form as used for table I.

TABLE II

n	$\lambda_{comp.}$	$\lambda_{theor.}$	$\varepsilon \times 10^6$	Iterations
0	5.78307	5.7831862	20	10
1	30.47111	30.471262	5	10
2	74.88676	74.887006	3	11
3	139.0414	139.04027	8	11
4	222.9352	222.93231	13	9

Once more, the method has given reliable results.

2° Consider finally the differential equation :

$$\frac{d}{dx}\left[(1 - x^2) \frac{dy(x)}{dx} \right] + \lambda y(x) = 0 \tag{27}$$

and the boundary conditions :

$$| y(-1) | < + \infty , \tag{28,a}$$

$$| y(+1) | < + \infty , \tag{28,b}$$

It is well known that the proper elements of this problem are given by :

$$\lambda_n = n(n + 1) , \tag{29,a}$$

$$y_n(x) = P_n(x) , \tag{29,b}$$

where $P_n(x)$ is the Legendre polynomial of order n. Equation (6) shows that the singularity at x = - 1 can be avoided if as before :

$$\alpha = \pi /2. \tag{26,a}$$

The method however is no longer applicable in its original form because of the second singularity at x = + 1, yet its basic idea may be employed. For this, introduce some intermediate point, say x = 0. For an arbitrary value of λ, the equations (6) and (13) or (6) and (15) can be solved in the interval $- 1 \leq x \leq 0$ taking the initial conditions (14), (10,a) and (26,a) into account.
The values at x = 0 of the functions $\theta(x, \lambda)$ and $\chi(x, \lambda)$ just obtained are then denoted by $\theta_L(\lambda)$ and $\chi_L(\lambda)$.

In exactly the same manner, the singularity at x = 1 can be avoided by choosing :

$$\beta = \pi /2. \tag{26,b}$$

Taking into account the initial conditions (14), (10,b) and (26,b), the equations (6) and (13) or (6) and (15) can be solved in the interval $0 \leq x \leq 1$. The values at x = 0 of the new functions $\theta(x,\lambda)$ and $\chi(x,\lambda)$ that have been obtained are then denoted by $\theta_R(\lambda)$ and $\chi_R(\lambda)$.

It can be shown that the derivative $\chi_L(\lambda)$ of the function $\theta_L(\lambda)$ with respect to λ is always positive and that the derivative $\chi_R(\lambda)$ of the function $\theta_R(\lambda)$ with respect to λ is always negative. Moreover, the eigenvalues are the solutions of the equation :

$$\theta_L(\lambda) - \theta_R(\lambda) = 0. \tag{30}$$

Equation (19) can then be replaced by the new algorithm :

$$\lambda_{n,\ k+1} = \lambda_{n,\ k} - \left[\theta_R(\lambda) - \theta_L(\lambda) \right] \Big/ \left[\chi_R(\lambda) - \chi_L(\lambda) \right]. \tag{31}$$

This new form of the approximation method has been applied to the determination of the eigenvalues of the Sturm-Liouville problem defined by the relations (27) and (28, a and b). The results obtained in this case are summarized in table III.

TABLE III

n	$\lambda_{comp.}$	$\lambda_{theor.}$	$\varepsilon \times 10^6$	Iterations
0	0.	0.	-	1
1	1.99997	2.	15	8
2	5.99984	6.	27	10
3	11.9996	12	33	9
4	19.9991	20	45	13

Once more, the comparison shows that the method has provided excellent results.

4.- CONCLUSION

A new method of successive approximations has been proposed in order to solve eigenvalue and eigenfunction problem associated with

Sturm-Liouville equations. The examples treated show that the convergence is reasonably rapid and that the proper elements can be determined with an actual accuracy which is only limited by the errors inherent to the numerical resolution of equations (6), (13) and (15). It is thus highly recommended to replace numerical determinations by analytic expressions whenever this is possible. The rate of convergence of the approximation method is highly dependent on the first estimates chosen for the λ_n. These values must then be determined as accurately as possible either by comparison methods, by an asymptotic expression, or by any other means. In all cases, some theoretical study is always helpful for the numerical solution of a Sturm-Liouville problem.

5.- ACKNOWLEDGMENT

The author would like to express his thanks to the I.R.M. (Belgian Royal Meteorological Institute) for its assistance in making available its I.B.M. 7040 computer. It was used for the solution of the examples given above and for a practical case arising in the study of a diffusion problem.

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