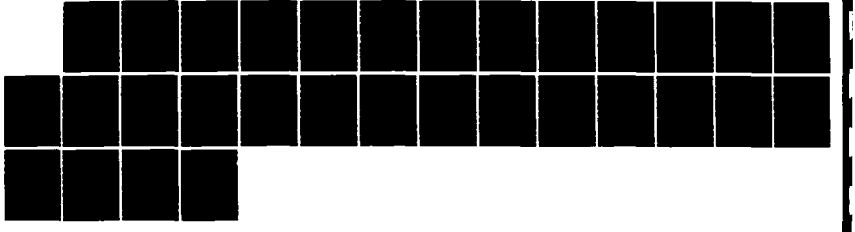
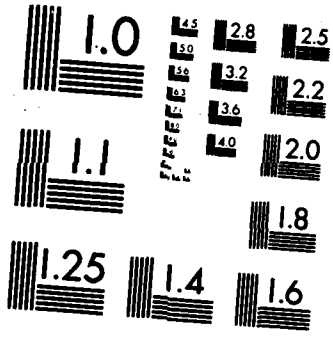
AD-A173 404 A CONTINUOUS ANALOGUE OF STURM SEQUENCES IN THE CONTEXT OF STURM-LIOUVILL..(U) MARYLAND UNIV COLLEGE PARK DEPT OF MATHEMATICS I GREENBERG ET AL. AUG 86 MD86-14-LG/IB 1/1

UNCLASSIFIED N00014-85-K-0169 F/G 12/1 NL





A CONTINUOUS ANALOGUE OF STURM SEQUENCES IN THE CONTEXT OF STURM-LIOUVILLE EQUATIONS

by

L. Greenberg
Mathematics Department
University of Maryland
College Park, Maryland 20742

and

I. Babuška
Institute for Physical Science and Technology
University of Maryland
College Park, Maryland 20742

August 1986

MD86-14-LG/IB

TR86-14

Encl (1)

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER MD86-14-LG/IB - TR86-14	2. GOVT ACCESSION NO. A173 404	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) A Continuous Analogue of Sturm Sequences in the Context of Sturm-Liouville Equations		5. TYPE OF REPORT & PERIOD COVERED Final life of the contract 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) L. Greenberg (University of Washington) I. Babuska (IPST)		8. CONTRACT OR GRANT NUMBER(s) UMCP N00014-85-K-0169
9. PERFORMING ORGANIZATION NAME AND ADDRESS Mathematics Department University of Maryland College Park, MD 20742		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Department of Naval Research Office of Naval Research Arlington, VA 22217		12. REPORT DATE August 1986 13. NUMBER OF PAGES 28
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release: distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Eigenvalue, eigenfunction, Sturm-Liouville equation, Sturm sequence, closure.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A closure of the Sturm sequence algorithm is found, leading to a shooting method for the n^{th} eigenvalue and eigenfunction of a Sturm-Liouville operator. The method works for general (separated) boundary conditions, and provides an a-posteriori error estimate for the approximate value of the n^{th} eigenvalue. A related method, which involves critical lengths in the invariant imbedding method, is shown to be incorrect for general boundary conditions.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-LF-014-6601

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

A Continuous Analogue of Sturm Sequences in the Context of Sturm-Liouville Equations

L. Greenberg[1] and I. Babuška[2]

Abstract. A closure of the Sturm sequence algorithm is found, leading to a shooting method for the n^{th} eigenvalue and eigenfunction of a Sturm-Liouville operator. The method works for general (separated) boundary conditions, and provides an a-posteriori error estimate for the approximate value of the n^{th} eigenvalue. A related method, which involves critical lengths in the invariant imbedding method, is shown to be incorrect for general boundary conditions.

Key words. Eigenvalue, eigenfunction, Sturm-Liouville equation, Sturm sequence, closure.

AMS (MOS) subject classification. 65L15.

[1] Mathematics Department, University of Maryland, College Park, Maryland 20742.

[2] Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742. The work of this author was supported in part by the Office of Naval Research, under contract N00014-85-K-0169.

1. Introduction.

Two point boundary value problems are often solved by finite difference or finite element methods. Sometimes one can find a "closure" or "limit" of the method as the mesh size $h \longrightarrow 0$. Such closures are often shooting methods which provide more flexibility and adaptability than the finite difference or finite element method. The double sweep method (see, for example, Babuška, Práger and Vitásek [3], Babuška amd Majer [2], Keller and Lentini [10]) is an example of this, which is also related to the invariant imbedding method (see Scott [11]).

In this paper, we shall give a closure of the Sturm sequence algorithm for computing the n^{th} eigenvalue and eigenfunction of the finite difference discretization of a Sturm-Liouville problem. The resulting shooting method is related to the critical (or characteristic) lengths in the invariant imbedding method. However, a simple counting of critical lengths does not produce a correct algorithm for calculating the n^{th} eigenvalue (for general boundary conditions). We shall discuss this in detail in section 3. In addition, our method gives an a-posteriori error estimate for the approximate value of the n^{th} eigenvalue.

Standard methods by finite differences or finite elements usually find the first n eigenvalues λ_k, $1 \leq k \leq n$. Shooting methods, such as those discussed in Keller [9], find one eigenvalue, but do not determine which one it is. We are aware of only one other shooting method which finds the n^{th} eigenvalue. That method, which uses the Prüfer transformation, was given by Bailey [5] and Godart [7], and was also discussed by Scott, Shampine and Wing [12]. Our method has the advantage that it generalizes to higher order problems and systems. Such generalizations will be discussed elsewhere.

In section 2 of this paper, we formulate the problem and describe the shooting method (which is a closure of the Sturm

sequence algorithm). In section 3, a plausible but incorrect algorithm is discussed. This is related to critical lengths. In section 4, we discuss closures of numerical processes. In this context, we outline the proof of our main theorem (Theorem 1), which is the basis for our shooting method. In sections 5 and 6, we recall details of the finite difference discretization and the Sturm sequence algorithm. Section 7 deals with the closure of the Sturm sequence algorithm, and the proof of Theorem 1. In section 8, we summarize our results, and state some conclusions.

2. A Shooting Method for Eigenvalues and Eigenfunctions.

Consider the eigenvalue problem

$$-(p(x)u')' + q(x)u = \lambda\, r(x)u \quad \text{for } 0 \le x \le 1, \tag{2.1a}$$

$$\begin{cases} \alpha_0\, u(0) + \beta_0\, u'(0) = 0, \\ \alpha_1\, u(1) + \beta_1\, u'(1) = 0, \end{cases} \tag{2.1b}$$

where we suppose that:

(a) $p(x)$, $q(x)$, $r(x)$ are continuous, and $p(x)$ is piecewise differentiable on $[0,1]$.

(b) $p(x) > 0$ and $r(x) > 0$ on $[0,1]$.

(c) The boundary conditions are normalized as follows: If $\beta_i \neq 0$, then $\beta_i = 1$; if $\beta_i = 0$, then $\alpha_i = 1$ (for $i = 0,1$).

It is well-known that the eigenvalues of (2.1) form an increasing sequence:

$$\lambda_1 < \lambda_2 < \lambda_3 < \ldots < \lambda_n < \ldots$$

and $\lim_{n\to\infty} \lambda_n = \infty$.

Remark 1. Without any difficulty, we could assume that p, q, r are piecewise continuous functions, instead of continuous functions. For simplicity, we have assumed they are continuous.

Remark 2. The boundary conditions in (2.1) could also be written in the form

$$\begin{cases} \alpha_0\, u(0) + \beta_0\, p(0)u'(0) = 0, \\ \alpha_1\, u(1) + \beta_1\, p(1)u'(1) = 0, \end{cases} \tag{2.1c}$$

which would be more natural, for physical reasons. Obvicusly, conditions (2.1b) and (2.1c) are equivalent. We have chosen (2.1b) for simplicity.

We shall now describe the shooting method for finding the n^{th} eigenvalue and eigenfunction of (2.1). Choose a number λ_0, and let $u_0(x)$ be a nontrivial solution of the initial value

problem:

$$(2.2)\qquad \begin{cases} -(p(x)u')' + q(x)u = \lambda_0\, r(x)u\ , \text{ for } 0 < x < 1, \\ \alpha_0\, u(0) + \beta_0\, u'(0) = 0. \end{cases}$$

(Choose any initial conditions which satisfy the boundary condition $\alpha_0\, u(0) + \beta_0\, u'(0) = 0$.) Let $N_0 = N_0(\lambda_0)$ be the number of zeros of $u_0(x)$ in the open interval $(0,1)$. (Note that the uniqueness theorem implies that all zeros have multiplicity 1.) Let $v = v(\lambda_0) = \alpha_1\, u_0(1) + \beta_1\, u_0'(1)$, and

$$\sigma = \sigma(\lambda_0) = \begin{cases} 0 & \text{if } v\, u_0(1) > 0 \text{ or } v = 0, \\ 1 & \text{if } v\, u_0(1) < 0 \text{ and } v \neq 0. \end{cases}$$

(Note that λ_0 is an eigenvalue if and only if $v = 0$.) Finally, let $N(\lambda_0) = N_0 + \sigma$. Thus, $N(\lambda_0)$ is the number of zeros of $u_0(x)$ in $(0,1)$, with a correction which depends on the boundary condition at $x = 1$. The shooting method depends on the following theorem, which will be proved in §7.

Theorem 1. $N(\lambda_0)$ equals the number of eigenvalues of (2.1) which are less than λ_0.

We can now describe the shooting method:

Step 0. Find values $L_0 < R_0$, such that $N(L_0) = n-1$ and $N(R_0) = n$. This implies that $L_0 < \lambda_n < R_0$.

Step k. For given values $L_{k-1} < R_{k-1}$, with $N(L_{k-1}) = n-1$, $N(R_{k-1}) = n$, find values L_k, R_k, such that $N(L_k) = n-1$, $N(R_k) = n$, $L_{k-1} < L_k < R_k < R_{k-1}$, and $R_k - L_k < R_{k-1} - L_{k-1}$.

STOP when $R_k - L_k < \tau$, where τ is a given tolerance.

To implement the above steps, we need an initial value solver to compute $u_0(x)$ and a nonlinear solver for L_k and R_k. The approximate eigenvalue λ_n will be either the midpoint of the last interval $[L_k, R_k]$, or the last approximation λ_n found by a

nonlinear solver. The approximate eigenfunction $\phi_n(x)$ will be the solution of (2.2), with $\lambda_0 = \lambda_n$.

STEP 0 can be carried out either by using estimates of λ_n which the user may have, or by using a related boundary value problem whose eigenvalues are known. For STEP k, we can use the bisection method for the integer-valued function $N(\lambda)$, or we can combine this with a nonlinear solver, such as the secant method, for the function $v(\lambda)$.

Assuming that the ODE's under consideration are solved exactly, the method gives a sharp a-posteriori error esimate for the eigenvalue λ_n. Of course, the ODE's will be solved numerically. An effective implementation of this method must relate the accuracy of the initial value solver (governed by an input tolerance parameter) to the value $R_k - L_k$, and to the accuracy of the nonlinear solver for finding L_k, R_k. A detailed analysis is required to determine the effects of the approximate solution of ODE's on this method, and on the a-posteriori error estimation. Such an analysis, together with a program implementing the method, will be published elsewhere.

Remark 3. If we are only interested in the eigenvalue λ_n, and not the eigenfunction ϕ_n, then we need only concern ourselves with the count of the zeros of $u(x)$ and the correction term σ. This can be obtained by solving various transformed formulations (such as that used in the invariant imbedding method).

Remark 4. The method resembles a count of the critical lengths in the invariant imbedding method (see [11], chap. V). However, a simple count of the critical lengths (with no correction term) does not produce a correct algorithm, for general boundary conditions. We shall return to this point in §3.

Remark 5. Theorem 1 leads immediately to the following corollary, which is a classical theorem about eigenfunctions.

Corollary. The n^{th} eigenfunction $\phi_n(x)$ of (2.1) has exactly n-1 zeros in the interval (0,1).

3. An Incorrect Algorithm.

We consider an alternative algorithm for calculating the n^{th} eigenvalue of (2.1). Let $u_0(x)$ denote a solution of the initial value problem (2.2), as before, and let $v_0(x) = \alpha_1 u_0(x) + \beta_1 u_0'(x)$. It might seem natural to count the zeros of $v_0(x)$, rather than counting the zeros of $u_0(x)$, with a correction using $v_0(1)$, as in the previous section. In other words, if $N'(\lambda_0)$ denotes the number of zeros of $v_0(x)$ in $(0,1)$, we might conjecture the following:

Hypothetical Theorem. $N'(\lambda_0)$ equals the number of eigenvalues of (2.1) which are less than λ_0.

This would lead to an alternative algorithm for finding λ_n, by replacing $N(\lambda_0)$ by $N'(\lambda_0)$ in STEP 0 and STEP k (previous section). However, the above Hypothetical Theorem turns out to be false. It depends on monotonicity properties of eigenvalues, which are valid for Dirichlet boundary conditions, but not for general boundary conditions. At the end of this section, we shall give an example where the alternative algorithm (using $N'(\lambda_0)$) fails.

Note that if $v_0(x_0) = 0$, then λ_0 is an eigenvalue on the interval $[0,x_0]$, and x_0 is a critical length (as used in the invariant imbedding method). Thus $N'(\lambda_0)$ is the number of critical lengths (corresponding to λ_0) which are less than 1. We see that a simple count of the critical lengths does not produce a correct algorithm for calculating the n^{th} eigenvalue of (2.1).

We shall now indicate the role played by monotonicity properties of eigenvalues. For $0 < y \leq 1$, let $\lambda_n(y)$ denote the n^{th} eigenvalue of the same operator as before, with the same boundary conditions, but on the interval $[0,y]$. In other words, $\lambda_n(y)$ is the n^{th} eigenvalue for the problem:

$$(3.1)\qquad \begin{cases} -(p(x)u')' + q(x)u = \lambda\, r(x)u\ , \text{ for } 0 \le x \le y, \\ \alpha_0\, u(0) + \beta_0\, u'(0) = 0, \\ \alpha_1\, u(y) + \beta_1\, u'(y) = 0. \end{cases}$$

For a given n, we ask the following question:

(Q) Is $\lambda_n(y)$ a decreasing function on $(0,1]$?

If the answer to (Q) is yes, for all n, then the Hypothetical Theorem is true and the alternative algorithm is correct. For suppose that x_0 $(0 < x_0 < 1)$ is a zero of $v_0(x) = \alpha_1\, u_0(x) + \beta_1\, u_0'(x)$, where $u_0(x)$ is a solution of (2.2). Then λ_0 is an eigenvalue on $[0,x_0]$, i.e., $\lambda_0 = \lambda_k(x_0)$, for some k. Since $\lambda_k(y)$ is a decreasing function, $\lambda_k = \lambda_k(1) < \lambda_k(x_0) = \lambda_0$. In this way, each zero of $v_0(x)$ corresponds to an eigenvalue less than λ_0. This shows that the Hypothetical Theorem and alternative algorithm are correct, if $\lambda_n(y)$ is a decreasing function, for all n. Unfortunately, this is not true for general boundary conditions.

If the boundary condition at the right endpoint is a Dirichlet condition: $u(y) = 0$, then the classical monotonicity theorem tells us that $\lambda_n(y)$ is a decreasing function, for all n. But Greenberg [8] has shown that if the boundary condition at the right endpoint is not a Dirichlet condition (i.e., $\beta_1 \neq 0$), then for given $n_0 \ge 1$, there exist coefficient functions $p(x)$, $q(x)$, $r(x)$ and a subinterval $[a,b] \subset (0,1]$, so that the eigenvalues $\lambda_1(y), \lambda_2(y), \ldots, \lambda_{n_0}(y)$ are increasing functions in $[a,b]$. (On the other hand, for given $p(x)$, $q(x)$, $r(x)$, α_0, β_0, α_1, β_1, there exists $n_1 \ge 1$, so that for $n \ge n_1$, $\lambda_n(y)$ is a decreasing function on $(0,1]$.) Thus, we cannot expect the Hypothetical Theorem and alternative algorithm to be correct for general boundary conditions. We now give a concrete example where they fail.

Example. For $0 < y \leq 1$, consider the eigenvalue problem:

$$(3.2) \qquad \begin{cases} -(p(x)u')' = \lambda u, & \text{for } 0 \leq x < y, \\ u(0) + u'(0) = 0, \\ u'(y) = 0. \end{cases}$$

The energy norm is given by

$$(3.3) \qquad B(v,v) = -p(0)v(0)^2 + \int_0^y p(x)v'(x)^2 dx,$$

and

$$(3.4) \qquad \lambda_1(y) = \inf_{v \in C^1[0,y]} \frac{B(v,v)}{\|v\|^2},$$

where $\|v\|^2 = \int_0^y v(x)^2 dx$.

Putting $v(x) \equiv 1$, we find that $\lambda_1(y) \leq \frac{B(v,v)}{\|v\|^2} = \frac{-p(0)}{y}$. Thus

$$(3.5) \qquad \lambda_1(y) < 0.$$

We now consider the two algorithms (given by Theorem 1 and the Hypothetical Theorem) for finding the number of eigenvalues $\lambda < 0$ (for the interval $[0,y]$). We must solve the initial value problem:

$$(3.6) \qquad \begin{cases} -(p(x)u')' = 0 \\ u(0) = 1, \ u'(0) = -1. \end{cases}$$

Denote the solution by $u_0(x)$, and let $v_0(x) = u_0'(x)$. We obtain: $-p\,u_0' = \text{constant} = p(0)$, so that

$$(3.7) \qquad \begin{cases} v_0(x) = u_0'(x) = \frac{-p(0)}{p(x)}, \\ u_0(x) = 1 - \int_0^x \frac{p(0)}{p(t)}\, dt. \end{cases}$$

Since $u_0'(x) < 0$, $u_0(x)$ is a decreasing function (with $u_0(0) = 1$). For a given y $(0 < y \leq 1)$, either

(A) $u_0(y) \geq 0$ and $u_0'(y) < 0$, or

(B) $u_0(y) < 0$ and $u_0'(y) < 0$.

In case (A), N_0 = [number of zeros of $u_0(x)$ in $(0,y)$] = 0, $\sigma = 1$, and $N = N_0 + \sigma = 1$.
In case (B), $N_0 = 1$, $\sigma = 0$, and $N = N_0 + \sigma = 1$.
Thus we see that the algorithm of Theorem 1 counts 1 negative eigenvalue on $[0,y]$, for all y in the interval $(0,1]$.

On the other hand, the alternative algorithm, based on the Hypothetical Theorem counts the zeros of $v_0(x) = u_0'(x)$ in $(0,y)$. Since $v_0(x) < 0$, $N' = 0$, predicting no negative eigenvalues! Here we have an example where the Hypothetical Theorem and alternative algorithm are incorrect.

Remark. Greenberg [8] has shown that in the above example, $\lambda_1(y)$ is an increasing function on $(0,1]$. Thus we have "reverse monotonicity" in this example!

4. Closure of a Numerical Process.

Standard methods for solving boundary value problems involve two stages:

(A) A discretization method (such as finite differences or finite elements) which approximates the continuous problem by a finite-dimensional algebraic problem.

(B) An algorithm for solving the algebraic problem.

It may happen that the algebraic algorithm is equivalent to finding a numerical solution u_h of an initial value problem, and manipulating this solution in some way to find some desired approximate value z_h. Perhaps $z_h = F_h(u_h)$, where F_h is some function. As the mesh size $h \longrightarrow 0$, suppose that $F_h \longrightarrow F$ (some function), $u_h \longrightarrow u$ (the solution of the initial value problem), and $z_h \longrightarrow z$ (the value we wish to compute). Of course we then have $z = F(u)$. Thus we obtain an alternate method for calculating z, which we call a closure of the numerical process. This method consists in solving the initial value problem to find u, and then calculating $F(u)$ to find z.

We have in mind situations where the initial value problem is hidden in the numerical process. Finding a closure amounts to discovering a hidden initial value problem. If we find a closure, then we gain a better understanding of various properties of the algorithm, and we can improve it. The algebraic algorithm may have involved a low order method, such as Euler's method. We can choose a higher order initial value solver, or one which is especially adapted to the particular problem.

We shall show that Theorem 1 is a closure of a numerical process. In the next section, we review the discretization by finite differences. In the following section, we discuss the algebraic algorithm, using Sturm sequences. In this context, z_h is the number of eigenvalues (of the finite difference equation) which are less than λ_0. The Sturm sequence turns out to be

related to the initial value problem (2.2). F_h counts the number of sign changes in the Sturm sequence. This turns out to be the same as the number of sign changes in the numerical solution u_h of (2.2), except for the last term. This last term gives rise to the correction term σ (mentioned in §2, where $N(\lambda_0)$ is defined).

The general notion of closure is probably due to S.L. Sobolev [13], [14]. In [14], Sobolev defines closure and applies it to the elimination method for solving a discretized integral equation. Babuška, Práger and Vitásek [3], [4] find closures of several algorithms. The closure method seems to have many other possibilities for application. We plan to return to some of them in the future.

5. Discretization.

We shall discretize the boundary value problem (2.1) by finite differences. We use uniform mesh of size $h = 1/n$, and the finite difference operator:

$$\Delta\ (u_i) = \frac{1}{h}\ (u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}).$$

Approximate the differential equation by the difference equation:

$$-\Delta\ (p_i\ \Delta\ (u_i) + q_i u_i = \lambda\ r_i u_i,$$

or equivalently:

$$(5.1)\quad -p_{i-\frac{1}{2}} u_{i-1} + (p_{i-\frac{1}{2}} + p_{i+\frac{1}{2}} + h^2 q_i) u_i - p_{i+\frac{1}{2}} u_{i+1} = \lambda\ h^2 r_i u_i.$$

The boundary condition $\alpha_0\ u(0) + \beta_0\ u'(0) = 0$ is approximated by the difference equation

$$\alpha_0\ u_0 + \beta_0 \left[\frac{u_1 - u_0}{h}\right] = 0\ ,\ \text{or}\ \ u_0 = \frac{\beta_0 u_1}{\beta_0 - h\alpha_0}\ .$$

Substituting this into (5.1), with $i = 1$, we obtain

$$(5.2)\qquad \left[\frac{-h\alpha_0}{\beta_0 - h\alpha_0}\ p_{\frac{1}{2}} + p_{\frac{3}{2}} + h^2 q_1\right] u_1 - p_{\frac{3}{2}} u_2 = \lambda\ h^2 r_1 u_1.$$

The boundary condition $\alpha_1\ u(1) + \beta_1\ u'(1) = 0$ is approximated by the difference equation

$$\alpha_1\ u_n + \beta_1 \left[\frac{u_n - u_{n-1}}{h}\right] = 0\ ,\ \text{or}\ \ u_n = \frac{\beta_1 u_{n-1}}{\beta_1 + h\alpha_1}\ .$$

Substituting this into (5.1), with $i = n-1$, we obtain

$$(5.3)\qquad -p_{n-\frac{3}{2}} u_{n-2} + (p_{n-\frac{3}{2}} + \frac{h\alpha_1}{\beta_1 + h\alpha_1}\ p_{n-\frac{1}{2}} + h^2 q_{n-1}) u_{n-1}$$
$$= \lambda\ h^2 r_{n-1} u_{n-1}.$$

Thus, we have a finite-dimensional eigenvalue problem:

$$(5.4)\qquad Au = \lambda\ Ru,$$

where A is the finite difference matrix

$$A = \begin{bmatrix} a_1 & b_1 & & & & \\ b_1 & a_2 & b_2 & & & \\ & b_2 & a_3 & b_3 & & \\ & & \ddots & & & \\ & & & b_{n-3} & a_{n-2} & b_{n-2} \\ & & & & b_{n-2} & a_{n-1} \end{bmatrix}$$

with $a_1 = \frac{-h\alpha_0}{\beta_0 - h\alpha_0} p_{\frac{1}{2}} + p_{\frac{3}{2}} + h^2 q_1$,

$a_i = p_{i-\frac{1}{2}} + p_{i+\frac{1}{2}} + h^2 q_i \quad (2 \le i \le n-2)$,

$a_{n-1} = p_{n-\frac{3}{2}} + \frac{h\alpha_1}{\beta_1 + h\alpha_1} p_{n-\frac{1}{2}} + h^2 q_{n-1}$,

$b_i = -p_{i+\frac{1}{2}} \quad (1 \le i \le n-2)$,

and R is the diagonal matrix

$$R = h^2 \begin{bmatrix} r_1 & & & & \\ & r_2 & & & \\ & & r_3 & & \\ & & & \ddots & \\ & & & & r_{n-1} \end{bmatrix} .$$

6. Sturm Sequences.

The finite difference discretization has approximated the continuous eigenvalue problem by the finite-dimensional eigenvalue problem

$$Au = \lambda Ru. \tag{6.1}$$

The algebraic algorithm we shall use for this is the method of Sturm sequences. We shall briefly recall the definition and main theorem on Sturm sequences, in the context of (6.1). Details about Sturm sequences can be found in Bathe, Wilson [6], Stoer, Bulirsch [15] and Wilkinson [16].

For a given number λ_0, the Sturm sequence $S_0(\lambda_0), S_1(\lambda_0), \ldots, S_{n-1}(\lambda_0)$ is defined by: $S_0(\lambda_0) = 1$, and for $1 \le i \le n-1$, $S_i(\lambda_0)$ is the leading i i principal minor of $A-\lambda_0 R$. In other words, $S_i(\lambda_0)$ is the determinant:

$$S_i(\lambda_0) = \begin{vmatrix} (a_1-\lambda_0 h^2 r_1) & b_1 & & & \\ b_1 & (a_2-\lambda_0 h^2 r_2) & b_2 & & \\ & \ddots & & & \\ & & b_{i-2} & (a_{i-1}-\lambda_0 h^2 r_{i-1}) & b_{i-1} \\ & & & b_{i-1} & (a_i-\lambda_0 h^2 r_i) \end{vmatrix} .$$

The following theorem is the main fact that we shall need.

Sturm Sequence Theorem. Let $c(\lambda_0)$ be the number of sign changes in the sequence $S_0(\lambda_0), S_1(\lambda_0), \ldots, S_{n-1}(\lambda_0)$. Then $c(\lambda_0)$ equals the number of eigenvalues (of the problem (6.1)) which are less than λ_0.

Note: If $S_i(\lambda_0) = 0$, then it counts as a sign change, in the above theorem.

7. Closure of the Sturm-Sequence Algorithm. Proof of Theorem 1.

For a given number λ_0, consider the initial value problem

$$(7.1)\qquad \begin{cases} -(p(x)u')' + q(x)u = \lambda_0\, r(x)u \ , \text{ for } 0 \le x \le 1, \\ u(0) = \beta_0 \ , \ u'(0) = -\alpha_0. \end{cases}$$

Note that the initial conditions were chosen to satisfy the boundary condition $\alpha_0\, u(0) + \beta_0\, u'(0) = 0$. Thus, equation (7.1) is essentially the same as (2.2).

Consider a finite difference approximation to (7.1). We obtain the same difference equations (5.1), including the first equation (5.2), but with λ_0 replacing λ. We do not obtain the last equation (5.3), because u is not required to satisfy the boundary condition at $x = 1$. Thus, the finite difference approximation u_i satisfies:

$$(7.2)\qquad (a_1 - \lambda_0\, h^2 r_1)u_1 + b_1 u_2 = 0,$$

and

$$(7.3)\qquad b_{i-1}u_{i-1} + (a_i - \lambda_0\, h^2 r_i)u_i + b_i u_{i+1} = 0 \ , \text{ for } 2 \le i \le n-2.$$

It also satisfies a last equation

$$-p_{n-\frac{3}{2}}u_{n-2} + (p_{n-\frac{3}{2}} + p_{n-\frac{1}{2}} + h^2 q_{n-1})u_{n-1} - p_{n-\frac{1}{2}}u_n = \lambda_0\, h^2 r_{n-1}u_{n-1},$$

which can be written

$$(7.4)\qquad b_{n-2}u_{n-2} + \left[a_{n-1} + \frac{\beta_1}{\beta_1 + h\alpha_1}\, p_{n-\frac{1}{2}} - \lambda_0\, h^2 r_{n-1}\right]u_{n-1} + b_{n-1}u_n = 0.$$

We shall relate the Sturm sequence $S_0(\lambda_0), S_1(\lambda_0), \ldots, S_{n-1}(\lambda_0)$ to the solution $u_1, u_2, \ldots, u_n$ of the above finite difference equations. We first consider the case where all $S_i(\lambda_0)$ are nonzero. We shall use the notation

$$(7.5)\qquad A_i = a_i - \lambda_0\, h^2 r_i.$$

For $1 \le i \le n-2$, consider the first i equations:

$$\begin{cases} A_1u_1 + b_1u_2 = 0 \\ b_1u_1 + A_2u_2 + b_2u_3 = 0 \\ \quad \ddots \qquad\qquad \vdots \\ b_{i-2}u_{i-2} + A_{i-1}u_{i-1} + b_{i-1}u_i = 0 \\ b_{i-1}u_{i-1} + A_iu_i = -b_iu_{i+1} \ . \end{cases}$$

By Cramer's rule:

$$u_i = \frac{-b_iu_{i+1}S_{i-1}(\lambda_0)}{S_i(\lambda_0)} \ , \text{ or}$$

$$\frac{u_i}{S_{i-1}(\lambda_0)} = -b_i \frac{u_{i+1}}{S_i(\lambda_0)} \ , \text{ for } 1 \le i \le n-2. \tag{7.6}$$

Let $t_i = \dfrac{u_i}{S_{i-1}(\lambda_0)}$. Then $t_{i+1} = -\dfrac{t_i}{b_i} = \dfrac{t_i}{p_{i+\frac{1}{2}}}$.

$$t_{i+1} = \frac{t_i}{p_{i+\frac{1}{2}}} \ , \ 1 \le i \le n-2. \tag{7.7}$$

This implies that

$$t_i = \frac{t_1}{p_{i-\frac{1}{2}}p_{i-\frac{3}{2}} \cdots p_{\frac{3}{2}}p_{\frac{3}{2}}} \ , \ 1 \le i \le n-1 \tag{7.8}$$

Thus, all the ratios $t_i = \dfrac{u_i}{S_{i-1}(\lambda_0)}$ $(1 \le i \le n-1)$ have the same sign. This implies that the sequences $S_0(\lambda_0)$, $S_1(\lambda_0)$, ..., $S_{n-2}(\lambda_0)$ and u_1, u_2, ..., u_{n-1} have the same number of sign changes.

We must still determine what happens with regard to a possible sign change from $S_{n-2}(\lambda_0)$ to $S_{n-1}(\lambda_0)$. To find this, we shall consider all $(n-1)$ equations for the u_i. The last of these equations is (7.4), which can be written

$$b_{n-2}u_{n-2} + A_{n-1}u_{n-1} = -\left[b_{n-1}u_n + \frac{\beta_1}{\beta_1+h\alpha_1} p_{n-\frac{1}{2}}u_{n-1}\right] \ . \tag{7.9}$$

Let

$$v_n = -\left[b_{n-1}u_n + \frac{\beta_1}{\beta_1+h\alpha_1} p_{n-\frac{1}{2}}u_{n-1}\right] \ . \tag{7.10}$$

Then (7.9) can be written

$$b_{n-2}u_{n-2} + A_{n-1}u_{n-1} = v_n. \tag{7.11}$$

Now consider the $(n-1)$ equations for u_i:

$$\begin{cases} A_1u_1 + b_1u_2 = 0 \\ b_1u_1 + A_2u_2 + b_2u_3 = 0 \\ \quad\cdot\quad\cdot\quad\cdot \\ b_{n-3}u_{n-3} + A_{n-2}u_{n-2} + b_{n-2}u_{n-1} = 0 \\ b_{n-2}u_{n-2} + A_{n-1}u_{n-1} = v_n \,. \end{cases}$$

By Cramer's rule:

$$u_{n-1} = \frac{v_n S_{n-2}(\lambda_0)}{S_{n-1}(\lambda_0)} \,, \quad \text{or}$$

$$\frac{u_{n-1}}{S_{n-2}(\lambda_0)} = \frac{v_n}{S_{n-1}(\lambda_0)} \,. \tag{7.12}$$

Thus, the two sequences $S_0(\lambda_0), S_1(\lambda_0), \ldots, S_{n-1}(\lambda_0)$ and $u_1, u_2, \ldots, u_{n-1}, v_n$ have the same number of sign changes.

We now consider the case where some of the $S_i(\lambda_0)$ are zero. We first note that there is a recursion relation

$$S_i(\lambda_0) = (a_i - \lambda_0 h^2 r_i)S_{i-1}(\lambda_0) - b_{i-1}^2 S_{i-2}(\lambda_0), \tag{7.13}$$

which is obtained by calculating the determinant $S_i(\lambda_0)$ by cofactors of the last column. This implies that two consecutive terms $S_{i-1}(\lambda_0)$, $S_i(\lambda_0)$ cannot both be zero. For if $S_{i-1}(\lambda_0) = S_i(\lambda_0) = 0$, then the recursion relation implies that $S_{i-2}(\lambda_0) = 0$. (Note that $b_{i-1} = -p_{i-\frac{1}{2}} \neq 0$.) Similarly, it would follow that $S_{i-2}(\lambda_0) = S_{i-3}(\lambda_0) = \ldots = S_1(\lambda_0) = S_0(\lambda_0) = 0$. But $S_0(\lambda_0) = 1$. Therefore, two consecutive terms in the Sturm sequence cannot both be zero.

Similarly, two consecutive terms in the sequence $u_0, u_1, \ldots, u_n$ cannot both be zero. For if $u_i = u_{i+i} = 0$,

then (7.3) shows that $u_{i-1} = 0$. Similarly, this would imply that $u_i = u_2 = \ldots = u_{i+1} = 0$. The initial conditions $u(0) = \beta_0$, $u'(0) = -\alpha_0$ in (7.1) are implemented in the approximate solution by: $u_0 = \beta_0$, $\frac{u_1 - u_0}{h} = -\alpha_0$. Since $u_1 = 0$, this implies that $u_0 = h\alpha_0$ and $u_0 = \beta_0$, so that $\beta_0 = h\alpha_0$. This relation can be satisfied by at most one value of h, since α_0 and β_0 are not both zero. We assume that h is small enough so that $\beta_0 \neq h\alpha_0$. The assumption $u_i = u_{i+1} = 0$ now leads to a contradiction.

We have shown that two consecutive terms $S_i(\lambda_0)$, $S_{i+1}(\lambda_0)$ cannot both be zero, nor can two consecutive terms u_i, u_{i+1}. This fact, together with equation (7.6), written as

$$u_i S_i(\lambda_0) = -b_i u_{i+1} S_{i-1}(\lambda_0), \tag{7.14}$$

shows that $S_i(\lambda_0) = 0$ if and only if $u_{i+1} = 0$. Now suppose that $S_{i_0}(\lambda_0) = S_{i_1}(\lambda_0) = \ldots = S_{i_m}(\lambda_0) = 0$, and no other $S_i(\lambda_0)$ is zero. The argument given above, for the case where all $S_i(\lambda_0)$ are nonzero, shows that the sequences

S_{i_k+1}, $S_{i_k+2}(\lambda_0)$, ..., $S_{i_{k+1}-1}(\lambda_0)$, and

u_{i_k+1}, u_{i_k+2}, ..., $u_{i_{k+1}-1}$ have the same number of sign changes.

The same holds for the beginning and end segments of the Sturm sequence, corresponding to $0 \leq i \leq i_0-1$ and $i_m + 1 \leq i \leq n-1$. Thus, if we count a zero as a sign change, then the two sequences $S_0(\lambda_0)$, $S_1(\lambda_0)$, ..., $S_{n-1}(\lambda_0)$ and u_1, u_2, ..., u_{n-1}, v_n have the same number of sign changes. The Sturm Sequence Theorem now implies that the number of sign changes in the sequence u_1, u_2, ..., u_{n-1}, v_n equals the number of eigenvalues of the approximate problem $Au = \lambda Ru$, which are less than λ_0.

We now consider what happens as the mesh size $h \longrightarrow 0$. Let $u_0(x)$ be the solution of (7.1), and $v = \alpha_1 u_0(1) + \gamma_1 u_0'(1)$. We shall consider four cases, according to the possibilities that

$u_0(1)$ and v are zero or not.

Case 1. $u_0(1) \neq 0$, $v \neq 0$.

The continuous problem has only finitely many (say m) eigenvalues less than λ_0. It is known that the first m eigenvalues of the approximate problem converge to the first m eigenvalues of the continuous problem as the mesh size $h \longrightarrow 0$. The number of sign changes in the sequence $u_1, u_2, \ldots, u_{n-1}$ converges to the number of zeros in $(0,1)$ of the solution $u_0(x)$ of the initial value problem (2.2) and (7.1).

We must find what happens to v_n as $h \longrightarrow 0$. Recall that $v_n = -\left[b_{n-1}u_n + \frac{\beta_1}{\beta_1+h\alpha_1} p_{n-\frac{1}{2}} u_{n-1}\right]$ and $b_{n-1} = p_{n-\frac{1}{2}}$. A simple calculation shows that

$$v_n = \frac{hp_{n-\frac{1}{2}}}{\beta_1+h\alpha_1} \left[\alpha_1 u_n + \beta_1 \left[\frac{u_n-u_{n-1}}{h}\right]\right] . \tag{7.15}$$

Recall that the boundary conditions are normalized: either $\beta_1 = 0$ and $\alpha_1 = 1$, or $\beta_1 = 1$. Thus

$$v_n = \begin{cases} p_{n-\frac{1}{2}} u_n \text{ , if } \beta_1 = 0 \\ \frac{hp_{n-\frac{1}{2}}}{1+h\alpha_1} \left[\alpha_1 u_n + \left[\frac{u_n-u_{n-1}}{h}\right]\right], \text{ if } \beta_1 = 1. \end{cases}$$

This shows that for small h , v_n has the same sign as $v = \alpha_1 u_0(1) + \beta_1 u_0'(1)$, where $u_0(x)$ is the solution of (7.1). Thus, for small h, the comparison of signs between u_{n-1} and v_n is the same as that between $u_0(1)$ and v. This shows that the correction term σ should be 1 if there is a sign change between $u(1)$ and v, and otherwise σ should be 0. This concludes the proof of the theorem, in Case 1.

Case 2. $u_0(1) = 0$, $v \neq 0$.

In this case, $\sigma = 1$ by definition, $\beta_1 = 1$ and

$v = \alpha_1 u_0(1) + u_0'(1)$. If $u_0(x)$ has positive values in some small interval $(1-\varepsilon,1)$, then $u_0'(1) < 0$, and $v = \alpha_1 u_0(1) + u_0'(1) = u_0'(1) < 0$. If $u_0(x)$ has negative values in $(1-\varepsilon,1)$, then $u_0'(1) > 0$ and $v > 0$. Thus there is always a change of sign between $u_0(x)$, for x close to 1, and v.

Now consider the sequence $u_1, u_2, \ldots, u_{n-1}, v_n$. For small h, the number of sign changes in this sequence equals the number of eigenvalues (of both the approximate and continuous problems) which are less than λ_0.

(7.16) #(eigenvalues $< \lambda_0$) = #(sign changes in $u_1, u_2, \ldots, u_{n-1}, v_n$).

Since $u_0'(1) \neq 0$, $u_0'(x) \neq 0$ for x near 1. Choose x_0 near 1, so that $u_0(x_0) \neq 0$ and $u_0'(x) \neq 0$ for $x_0 \leq x \leq 1$. Then $u_0(x)$ is monotone on $[x_0,1]$, and it has only one zero in this interval, namely at $x = 1$. We may suppose that $x_0 = i_0 h$. Then, for small h,

(7.17)
$$\begin{aligned} &\#(\text{sign changes in } u_1, u_2, \ldots, u_{i_0}) = \\ &\#(\text{zeros of } u_0(x) \text{ in } (0,x_0]) = \\ &\#(\text{zeros of } u_0(x) \text{ in } (0,1)). \end{aligned}$$

Also, from (7.16), we have

(7.18)
$$\begin{aligned} &\#(\text{eigenvalues} < \lambda_0) = \\ &\#(\text{sign changes in } u_1, u_2, \ldots, u_{i_0}) + \\ &\#(\text{sign changes in } u_{i_0}, \ldots, u_{n-1}, v_n). \end{aligned}$$

We claim that

$$\#(\text{sign changes in } u_{i_0}, \ldots, u_{n-1}, v_n) = 1.$$

If we can show this, then (7.17) and (7.18) imply that Theorem 1 is correct in this case.

Since $u_0'(x) \neq 0$ on $[x_0,1]$, the sequence $u_{i_0}, u_{i_0+1}, \ldots, u_{n-1}$ is monotone. Thus it can have at most one sign change. If there is a sign change, then either $u_{n-1} = 0$

(which counts as a sign change) or u_{n-1} has the opposite sign to that of $u_0(x)$, for $x_0 \le x < 1$. In this case, there is no sign change between u_{n-1} and v_n (since we have seen above that there is always a sign change between $u(x)$, for x near 1, and v). Thus #(sign changes in $u_{i_0}, \ldots, u_{n-1}, v_n$) = 1, in this case.

If there is no sign change in the sequence $u_{i_0}, u_{i_0+1}, \ldots, u_{n-1}$, then u_{n-1} and v_n have opposite signs. Again we have #(sign changes in $u_{i_0}, \ldots, u_{n-1}, v_n$) = 1. We have shown that

$$\#(\text{eigenvalues} < \lambda_0) = \#(\text{zeros of } u_0(x) \text{ in } (0,1)) + 1.$$

This proves the theorem in Case 2.

Case 3. $u_0(1) \neq 0$, $v = 0$.

In this case, $\sigma = 0$ by definition. Also λ_0 is an eigenvalue of the continuous problem, say $\lambda_0 = \lambda_k$. Thus, there are $k-1$ eigenvalues (of the continuous problem) less than λ_0. We must show that the eigenfunction $\phi_k(x) = u_0(x)$ has exactly $k-1$ zeros in $(0,1)$. Of course, this is a classical theorem. But we want to show that it follows from Sturm sequences.

Let $u_0(x,\lambda)$ denote the solution of (7.1), with λ replacing λ_0, and let $u_1(\lambda), u_2(\lambda), \ldots, u_{n-1}(\lambda), v_n(\lambda)$ be the corresponding sequence obtained from the finite difference solution. Let $c(\lambda)$ denote the number of sign changes in this sequence. Choose λ, λ' close to $\lambda_0 = \lambda_k$, such that $\lambda < \lambda_0 < \lambda'$. By Case 1, $c(\lambda) = k-1$ and $c(\lambda') = k$. Since $u_0(1,\lambda_0) \neq 0$, the number of zeros in $(0,1)$ is the same for $u_0(x,\lambda)$, $u_0(x,\lambda_0)$, $u_0(x,\lambda')$. Also, this number of zeros equals the number of sign changes in the sequences $u_1(\lambda), u_2(\lambda), \ldots, u_{n-1}(\lambda)$ and $u_1(\lambda'), u_2(\lambda'), \ldots, u_{n-1}(\lambda')$. Since $c(\lambda') = c(\lambda) + 1$, the extra sign change must come from a change in sign of v_n. This shows that $u_0(x,\lambda_0)$ has $k-1$ zeros

in (0,1), which proves the theorem in Case 3.

Case 4. $u_0(1) = 0$, $v = 0$.

Again λ_0 is an eigenvalue, say $\lambda_0 = \lambda_k$. In this case, we have a Dirichlet boundary condition: $\alpha_1 u(1) + \beta_1 u'(1) = u(1)$; $v = u_0(1)$, and $\sigma = 0$ by definition. We must show that $u_0(x,\lambda_0)$ has k-1 zeros in (0,1).

As in the previous case, choose λ, λ' close to λ_0, with $\lambda < \lambda_0 < \lambda'$. Then $v(\lambda) = u_0(1,\lambda) \neq 0$ and $v(\lambda') = u_0(1,\lambda') \neq 0$. By Case 1, $u_0(x,\lambda)$ has k-1 zeros in (0,1) and $u_0(x,\lambda')$ has k zeros in (0,1). The extra zero must arise from $u_0(x,\lambda_0)$, at x = 1. Therefore $u_0(x,\lambda_0)$ has k-1 zeros in (0,1). This concludes the proof of the theorem.

8. Conclusions.

A closure exists for any numerical process dealing with a matrix problem which comes from discretizing an ordinary differential equation. We have shown that the closure of the Sturm sequence algorithm for finding eigenvalues leads to a certain shooting method. Other numerical processes, such as vector iteration methods, transformation methods and polynomial iteration techniques also have closures. We have mentioned some closures (such as the double sweep method) of algorithms for solving systems of linear equations. A closure of an algorithm is important, because it leads to a new method for solving the continuous problem. The new method is often superior to the finite difference or finite element method, because it has greater flexibility.

References

[1] I. Babuška, The connection between finite difference like methods and methods based on initial value problems for ODE's, Numerical Solutions of Boundary Value Problems for Ordinary Differential Equations, ed. A.K. Aziz, Academic Press (1974), 149-176.

[2] I. Babuška and V. Majer, The factorization method for two point boundary value problems for ODE's and its relation to the finite difference method, Proceedings of the Centre for Mathematical Analysis, Australian National University, ed. A. Miller, vol. 7 (1984), 71-92.

[3] I. Babuška, M. Práger and E. Vitásek, The closure of numerical processes and the double sweep method, Zurn. Vyc. Mat. i Mat. Fiz. 4 (1964), 351-353, (in Russian).

[4] I. Babuška, M. Práger and E. Vitásek, Numerical Processes in Differential Equations, John Wiley (1966).

[5] P. Bailey, Sturm-Liouville eigenvalues via a phase function, SIAM J. Appl. Math. 14 (1966), 242-249.

[6] K.J. Bathe and E.L. Wilson, Numerical Methods in Finite Element Analysis, Prentice-Hall (1976).

[7] M. Godart, An iterative method for the solution of eigenvalue problems, Math. Comp. 20 (1966), 399-406.

[8] L. Greenberg, Monotonicity properties of eigenvalues of Sturm-Liouville equations, to appear.

[9] H.B. Keller, Numerical Solution of Two Point Boundary Value Problems, Reg. Conf. Ser. in Appl. Math. 24, SIAM (1976).

[10] H.B. Keller and M. Lentini, Invariant imbedding, the box scheme and an equivalence between them, SIAM J. Num. Anal. 19 (1982), 942-962.

[11] M.R. Scott, Invariant Imbedding and Its Applications to Ordinary Differential Equations, An Introduction, Addison-Wesley (1973).

[12] M.R. Scott, L.F. Shampine and G.M. Wing, Invariant imbedding and the calculation of eigenvalues for Sturm-Liouville systems, Computing 4 (1969), 10-23.

[13] S.L. Sobolev, The Closure of Numerical Processes and Some of Its Applications, USSR Academy of Sciences, Moscow (1955), (in Russian).

[14] S.L. Sobolev, Remarks on the numerical solution of integral equations, Izv. Akad. Nauk. SSSR Ser. Mat. 20 (1956), 413-436, (in Russian).

[15] J. Stoer and R. Bulirsch, Introduction to Numerical Analysis, Springer Verlag (1980).

[16] J.H. Wilkinson, The Algebraic Eigenvalue Problem, Oxford University Press (1965).

END

12-86

DTIC