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Paul Luger

August 8, 1971

AEC Contract No. W-7405-eng-48

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APPLICATION OF CUBIC SPLINES TO A STURM-LIOUVILLE SYSTEM

Paul Luger

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

and
Seattle University
Seattle, Washington 98105

ABSTRACT

In a general Sturm Liouville System approximations for the least characteristic value and a corresponding characteristic function are obtained. The method begins with the construction of a cubic spline with uniformly spaced knots in the interval of definition. Then the generalized Rayleigh quotient is minimized in an iterative process to obtain the final solution approximation.

INTRODUCTION

We consider a Sturm-Liouville system

$$py'' + fy' + (g + h\lambda)y = 0 \tag{1}$$

$$y(0) = 0 \quad \text{and} \quad y(1) = 0 \tag{2}$$

with p, f, g and h continuous, and where $p > 0$, f is the derivative of p, and $h > 0$, $g \leq 0$, insuring a positive λ on [0, 1]. It is noted that most second order differential equations can be put in this form. Note also that (2) implies

$$py''(0) + f(0)\cdot y'(0) = 0 \quad \text{and} \quad py''(1) + f(1)\, y'(1) = 0 \tag{3}$$

obviously the system (1), (2) is always satisfied by the trivial solution

$$y(0) \equiv 0 \tag{4}$$

We seek (characteristic) values for λ for which there are (characteristic) non-trivial functions which satisfy the system. The theory of Sturm-Liouville systems as presented in references 1 and 2, establishes the following

(a) There are a countably infinite number of characteristic values.

(b) They are all real and distinct.

(c) No more than a finite number are negative. Hence there is a least characteristic value.

(d) The space, $U = \left\{ u \,\middle|\, \begin{array}{l} u \in C_2[0,1] \\ u(0)=0 \\ u(1)=0 \end{array} \right\}$ is spanned by the set of characteristic functions and for the scalar product of u, $v \in U$ defined as:

$$\hat{uv} = \int_0^1 uv\,dx$$

a countable orthonormal basis for the space can be found in the set.

(e) For the least characteristic value we have

$$\underline{\lambda} = \min_{u \in U} R(u) \tag{6}$$

where R is the generalized Rayleigh quotient and

$$R(u) = -\int_0^1 [u''u + fu'u + gu^2]dx \Big/ \int_0^1 hu^2 dx \tag{7}$$

We propose to find an approximation for $\underline{\lambda}$ by use of cubic splines with uniformly spaced knots in the interval [0, 1].

THE SPACE OF SPLINES

For $n \geq 3$ and with the knots

$$x_i = \{{}^{i-1}/_{n-1}\} \text{ for } i=1,\ldots n \tag{8}$$

we consider the space, S, of cubic splines which satisfy the boundary conditions:

$$\begin{aligned} s(0) &= 0 \\ s(1) &= 0 \end{aligned} \tag{9}$$

for all $s \epsilon S$. In reference 3, it is established that for a general space of cubic splines on a specified interval and having n knots has dimension n+2. But for the particular subspace of S, because of the boundary conditions (9), the dimension must be n.

A convenient basis for the space s consists of the cubic splines, t_j, $j=1,\ldots n$ defined as follows:

$$\begin{array}{llllll} t_1(x_i) = 0 & \text{all } x_i, & t_1'(0) = 1, & t_i'(1) = 0 & & \\ t_j(x_i) = \delta_{ij}, & & t_j'(0) = 0, & t_j'(1) = 0 & & j=2,\ldots n-1 \\ t_n(x_i) = 0 & \text{all } x_i, & t_n'(0) = 0, & t_n'(1) = -1 & & \end{array} \tag{10}$$

It may be readily verified that $\{t_j\}$ is a linearly independent set which spans S. It is further obvious that any linear combination of the t_j is in S.

Now, it is well known that any $u \epsilon U$ can be approximated by some $s \epsilon S$, consequently the least characteristic value, $\underline{\lambda}$ can be approximated by

$$\underline{\lambda}^* = \min_{s \epsilon S} R(s) = R(s^*), \tag{11}$$

We note that s^* is not unique since for any $c \neq 0$

$$R(cs) = R(s)$$

However any s^* is an approximation of a characteristic function $\underline{y}$ corresponding to $\underline{\lambda}$.

THE CUBIC SPLINE APPROXIMATION

Every s in S is a linear combination of the t_j,

$$s = \Sigma \alpha_j t_j \tag{12}$$

and an s^* is determined by that set of α_j, $j=1,\ldots n$ for which R is minimized.

We wish to avoid the trivial solution where $\alpha_j=0$, all j. By the non-unicity of s^* it is permissible to assign a non-zero value to some one of the α_j. We elect to set

$$\alpha_1 = 1$$

since $\alpha_1 = 0$ might easily lead to the trivial solution. This selection will leave us with n-1 coefficients α_j $(j \neq 1)$ to be determined.

A minimization process on R(s) involving n-1 variables, α_j, $j=2,\ldots n$ must be employed.

THE MINIMIZATION PROCESS

The general R(s) is the quotient of two quadratic expressions in the unknown α_j of the form

$$R(S) = A(\alpha_2,\ldots\alpha n)/B(\alpha_2,\ldots\alpha n) \tag{13}$$

and

$$\frac{\partial R}{\partial \alpha_j} = (B\,\frac{\partial A}{\partial \alpha_j} - A\,\frac{\partial B}{\partial \alpha_j})/B^2 \tag{14}$$

For that set of particular α_j which minimizes R we must have

$$\frac{\partial R}{\partial \alpha_j} = 0 \quad \text{for } j=2,\ldots n$$

or

$$B\,\frac{\partial A}{\partial \alpha_j} - A\,\frac{\partial B}{\partial \alpha_j} = 0 \quad \text{for } \alpha_j=2,\ldots n \tag{15}$$

We employ a minimizing procedure, reference 4, due to W.C. Davidon in order to compute the minimizing set $\{\alpha_j\}$.

This procedure permits us, initially, to set $\alpha_1 = 1$ in constraint, to assign guesses to the other α_j, j=2,...n values and, then, permitting the guesses to vary, to generate sets of α_j scalars, thus minimizing R.

In the Fortran code written for this problem, Eq. (12) takes on this contracted form:

$$R(\alpha_j) = \frac{\sum_{j=1}^{n}\sum_{k=1}^{n} A_{jk}\,\alpha_j\alpha_k}{\sum_{j=1}^{n}\sum_{k=1}^{n} B_{jk}\,\alpha_j\alpha_k} \tag{16}$$

where the coefficients are defined by the following integrals

$$A_{jk} = \int_0^1 [s_j s_k'' + f s_j s_k' + g s_j s_k]\,dx \tag{17}$$

$$B_{jk} = \int_0^1 h s_j s_k\,dx \tag{18}$$

The coefficients of equations (17) and (18) are calculated prior to minimization. Except for the input guesses where the α_j's are specified, the minimization routine computes and optimizes on each iteration a new set of α_j. Thereupon our Fortran code uses equation (16) to calculate a new $R(\alpha_j)$, and also the partial derivatives of equation (14). (There are as many of these partials as there are dimensions in the cubic spline space.) Once the partial derivatives are calculated they are returned to the minimization routine where a new set of α_j's are obtained. This process is repeated until there is no significant reduction in the value of R. Then the current set of α_j is accepted as minimized.

The cubic spline, which minimizes R is obtained by

$$s^* = \Sigma\alpha_j\, t_j \tag{19}$$

where the t_j are the basic splines. We then approximate $\underline{\lambda}$ by the corresponding R and finally the eigen function itself by (19), where $y \simeq s^*$.

Error Discussion

Once we have found $\underline{\lambda}^*$ an approximation for $\underline{\lambda}$ and s^* an approximation for the eigen function y, we may substitute in Eq. (1) for mid-point values between knots. In the examples we give we will calculate s", s' and s at mid-points. Then we calculate as a measure of the error

$$e_m = p_m s_m + f_m s_m + (g_m + h_m \underline{\lambda}^*)\, s_m \tag{20}$$

and as an overall measure of the error

$$e = \text{Max}\ |e_m|. \tag{21}$$

This approach to error analysis is direct and gives in one figure a measure of approximation errors from the eigenvalue and the α_j coefficients.

The details of the process described thus far will be made clearer in the numerical examples of the next section.

NUMERICAL EXAMPLES

Example 1

In this example we treat the very simple case where in (1)

$$\begin{aligned} p &= 1 \\ f &= 0 \\ g &= 0 \\ h &= 1 \end{aligned} \quad \text{on } [0, 1]$$

yielding $\qquad y'' + \lambda y = 0 \qquad (22)$

with $\qquad y(0) = 0 \ , \ y(1) = 0$

from (20), $\qquad y''(0) = 0$ and $y''(1) = 0$.

Our equation has an analytic solution:

$$\underline{\lambda} = \pi^2 = 9.869604 \quad \text{with}$$

$$y = C \text{ Sin } \pi X. \qquad C \neq 0$$

Suppose n=3, where knots are 0, 1/2 and 1; let us compute the basic splines, where, we assume

$$t_1(0) = 0 \ , \ t_2(0) = 0 \ , \ t_3(0) = 0$$

$$t_1(1) = 0 \ , \ t_2(1) = 0 \ , \ t_3(0) = 0$$

We arrange values for the splines in three arrays. The spline function array together with the underlined values in the first derivative array define the splines. The other values are calculated:

	t_1	t_2	t_3
0	$\underline{0}$	$\underline{0}$	$\underline{0}$
.5	$\underline{0}$	$\underline{1}$	$\underline{0}$
1	$\underline{0}$	$\underline{0}$	$\underline{0}$

	t_1'	t_2'	t_3'
0	$\underline{1}$	$\underline{0}$	$\underline{0}$
.5	$\underline{-.2}$	$\underline{0}$	$\underline{.25}$
1	$\underline{0}$	$\underline{0}$	$\underline{-1}$

	t_1''	t_2''	t_3''
0	-7	24	-1
.5	2	-24	2
1	-1	24	-7

Any linear combination of the basic splines with any α_1, α_2 and α_3 automatically satisfies the boundary conditions. Arbitrarily choosing $\alpha_1 = 1$,

$$s = t_1 + \alpha_2 t_2 + \alpha_3 t_3$$

$$s'' = t_1'' + \alpha_2 t_2'' + \alpha_3 t_3''$$

Substituting s for y and s" for y" in equation (22), we have

$$t_1'' + \alpha_2 t_2'' + \alpha_3 t_3'' + \lambda(t_1 + \alpha_2 t_2 + \alpha_3 t_3) = 0$$

Evaluating at x=0, and 1 we obtain

$$t_2''(0)\alpha_2 + t_3''(0)\alpha_3 = -t_1''(0)$$

$$t_2''(1)\alpha_2 + t_3''(1)\alpha_3 = -t_1''(1)$$

Employing computed values of the second derivative,

$$\alpha_2 = 1/3 \quad \text{and} \quad \alpha_3 = 1.$$

Hence $$s = t_1 + 1/3 t_2 + t_3$$

Then $R(s) = -\int_0^1 ss''dx \Big/ \int_0^1 s^2 dx = 9.882353$. Since no minimization is possible $s^* = s$ and $\underline{\lambda}^* = 9.882353$.

With 5 knots (n=5), x=0, 1/4, 1/2, 3/4 and 1. The basic spline functions are chosen as shown, with the two boundary conditions imposed: $t_j(0) = 0$ and $t_j(1) = 0$, j=1,...5

	t_1	t_2	t_3	t_4	t_5
0	0	0	0	0	0
.25	0	1	0	0	0
.5	0	0	1	0	0
.75	0	0	0	1	0
1	0	0	0	0	0

	t_1'	t_2'	t_3'	t_4'	t_5'
0	1	0	0	0	0
.25	-.27	-.86	3	-.86	-.018
.5	-.07	-3.4	0	3.4	-.07
.75	-.018	-.86	-3	-.86	-.27
1	0	0	0	0	-1

In the array of first derivatives $t_1'(0) = 1$ and $t_5'(1) = -1$ so that at none of the basic splines will be zero to avoid the trivial solution. All other values of $t_j'(0) = 0$ and $t_j'(1) = 0$. Choose these for convenience.

Here again, as with 3 knots, the entire spline function array together with the underlined values of the first derivative array define the splines. The other values of the first derivative are calculated, as are all the second derivative values:

	t_1''	t_2''	t_3''	t_4''	t_5''
0	13.8	89	-24	6.8	-.14
.25	3.7	-82	48	-14	-.28
.5	-1	48	-72	48	-1
.75	.28	-14	48	-82	3.7
1	-.14	6.8	-24	89	-14

These values completely determine a set of five basic splines shown in the plots of Figure 1. The second derivatives are necessary for computing the integrals of equations (17) and (18).

For the minimization routine a set of guesses must be made for the coefficients α_j, j=2,...5 with α_1 always kept at 1, thus preventing the trivial solution. We submit as guesses:

$$\{\alpha_{jo}\} = \{1,1,1,1,1\}$$

The following values of $\{\alpha_{jk}\}$ and the corresponding values of $\underline{\lambda} \simeq R_k = \Sigma\, \alpha_j t_j$ are shown for several of 26 total computer iterations:

$\{\alpha_{jk}\} = \{\alpha_1,$	$\alpha_2,$	$\alpha_3,$	$\alpha_4,$	$\alpha_5\}$;	$\underline{\lambda}$
k=1 {1,	.865,	1.25,	.865	1.01}	10.7365
k=5 {1	.601	.869	.612	.146}	10.3502
k=15 {1	.340	.501	.363	1.85}	9.99320
k=20 {1	.219	.311	.225	1.06}	9.87747
k=25 {1	.225	.318	.225	1}	9.869700
k=26 {1	.225	.318	.225	1}	9.869700

We note that five basic splines yield a better approximation to the analytic solution for $\underline{\lambda}$ than did three.

Figure 2 shows the solution of $y'' + \lambda y = 0$. To better show continuity in a plot on a given interval, two methods might be employed: a) interpolate by a Taylor's expansion for values between the knots, or, b) employ a sufficiently large number of knots, i.e. basic splines.

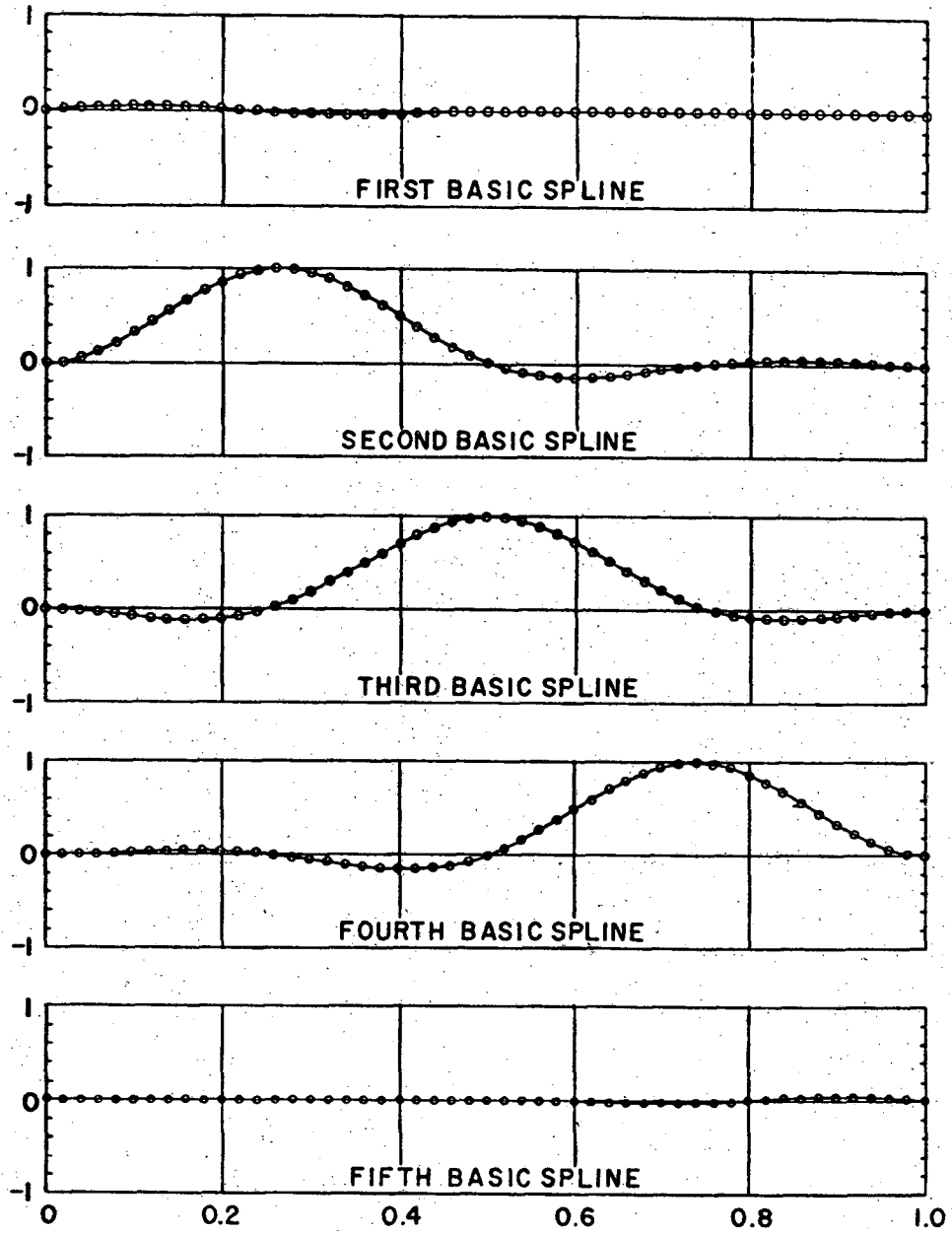
FIRST BASIC SPLINE
SECOND BASIC SPLINE
THIRD BASIC SPLINE
FOURTH BASIC SPLINE
FIFTH BASIC SPLINE
1
0
-1
0
0.2
0.4
0.6
0.8
1.0

Fig. 1

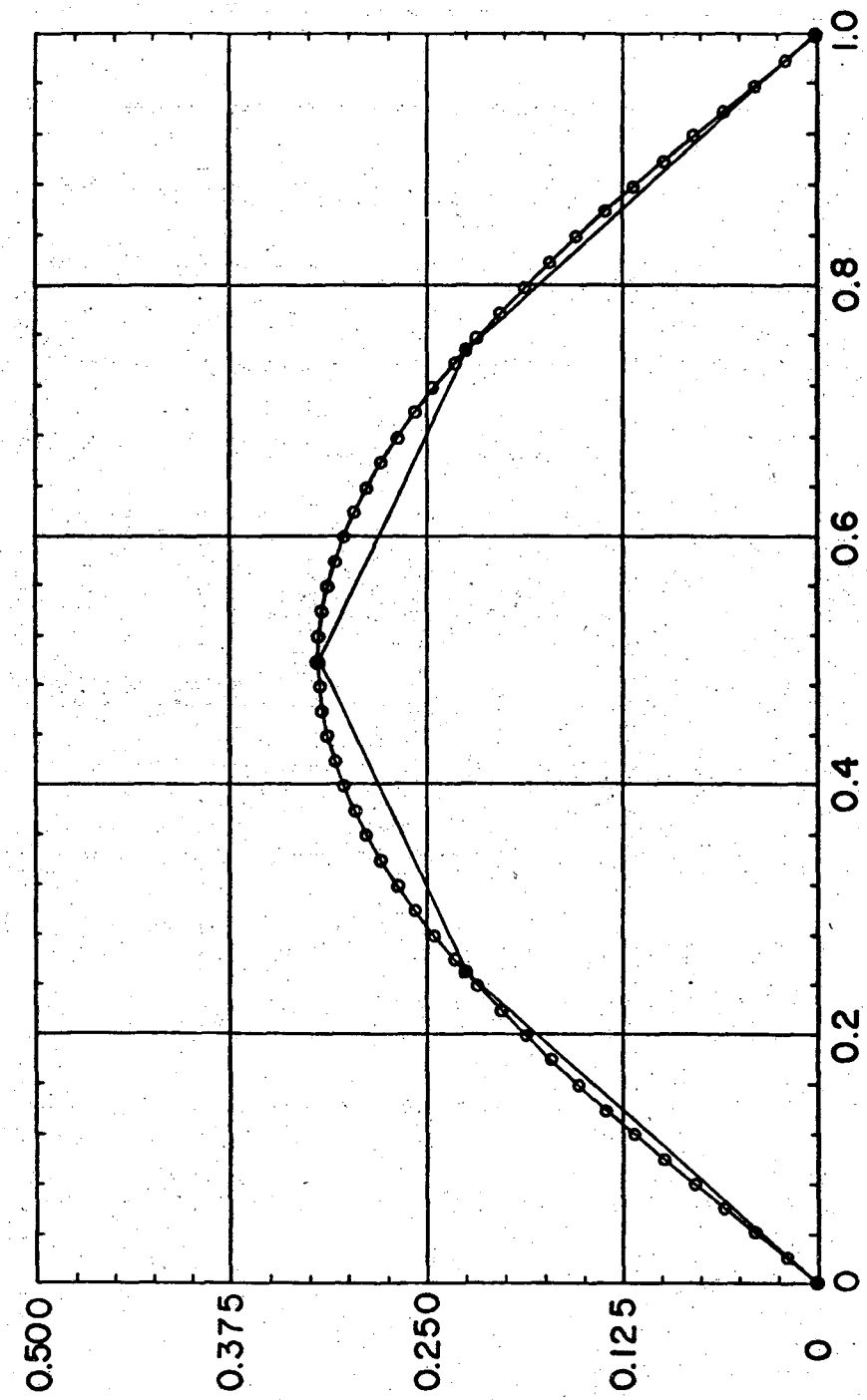
0.500
0.375
0.250
0.125
0
0
0.2
0.4
0.6
0.8
1.0

Fig. 2

Figure 2 shows a double plot. One is based on five knots or five points without interpolation. The other results from a Taylor's expansion about these five points and is plotted for 5- points within the interval.

Example 2

For a second example, start with

$$y = e^x \sin \gamma x \tag{23}$$

from the first and second derivatives of (23), setting $\lambda = 1 + \gamma^2$, we obtain

$$y'' - 2y' + \lambda y = 0 \tag{24}$$

or

$$e^{-2x}y'' - 2e^{-2x}y' + e^{-2x}\lambda y = 0 \tag{25}$$

on [0,1] with $y(0) = y(1) = 0$. Then

$$\begin{aligned} p &= e^{-2x} \\ f &= -2p \\ g &= 0 \\ h &= p \end{aligned} \tag{26}$$

Equations (26), specific for each problem, are entered into the Fortran code by a separate routine.

We note that identical boundary conditions on the interval [0,1] permit use of the same basic spline space as discussed in example 1. The Fortran code is generalized to accomodate any reasonable number of basic splines. As in example 1, initial guesses

for the α_j's are inputted, one for each α.

The analytic answers for example 2 are:

$$\underline{\lambda} = 1 + \pi^2 = 10.869604$$

$$y = \frac{1}{\pi} e^x \sin \pi x$$

The following values of $\underline{\lambda}$ are shown for several of the 37 iterations k:

k	$\underline{\lambda}$
1	20.074721
5	11.297976
15	11.092549
20	10.993930
25	10.871439
30	10.871063
35	10.869790
36	10.869606
37	10.869604

Figure 3 shows the solution of Equation (24). Note that the plot of Figure 3 employing 11 knots has practically the same resolution as the 50 point plot derived from these 11 knots by a Taylor's expansion.

In all the examples tried with our Frotran code the error by equation (20) is reduced by taking a greater number of basic splines. In examples 1 and 2 the maximum error, e (21) is shown in the following table:

Basic Splines	Example 1 e	Example 2 e
3	0.154	0.124
5	0.078	0.029
11	0.013	0.0099
21	0.003	0.003

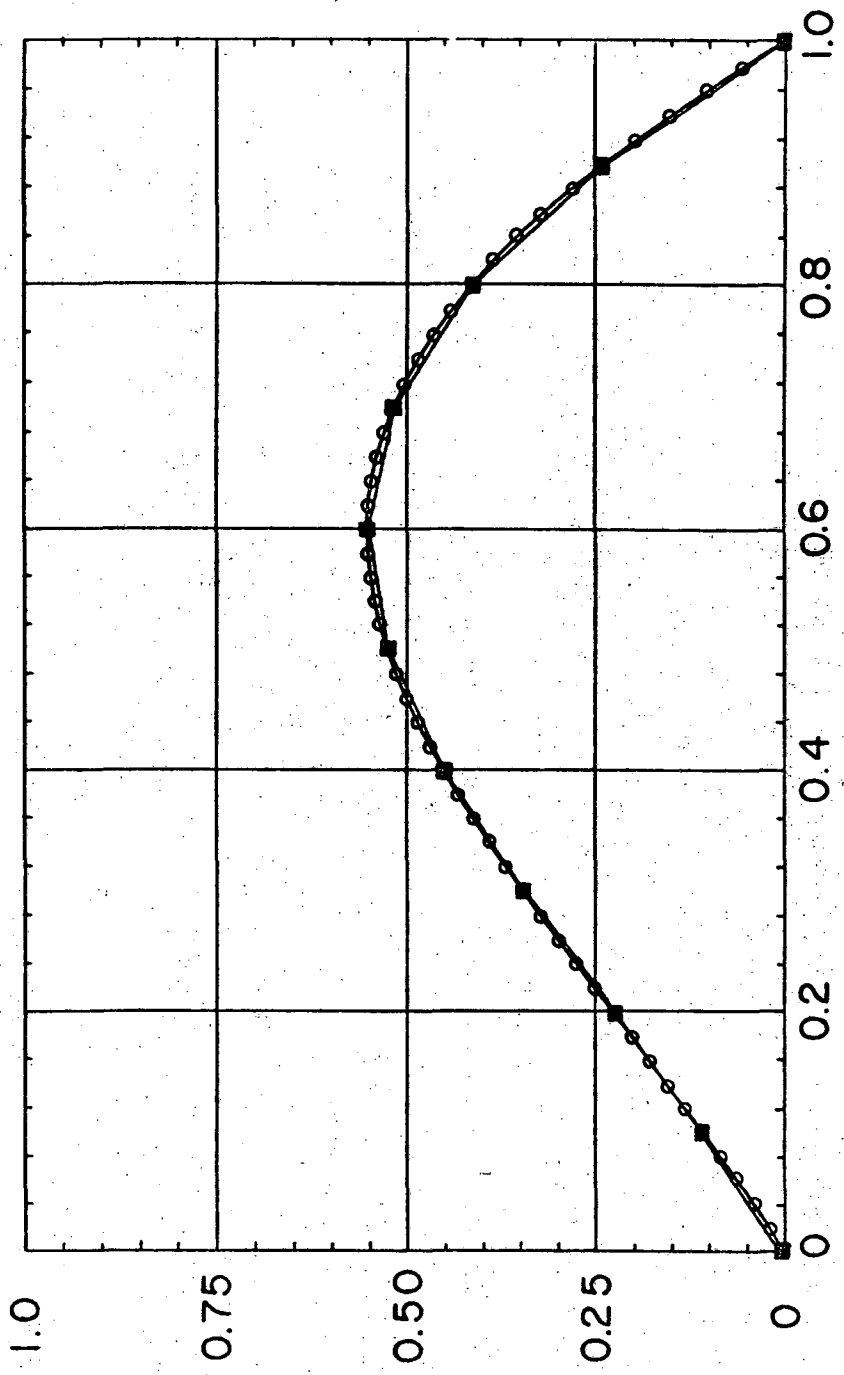

Fig. 3

Computer Code

Computer code EIGSLY (Eigenvalue by Splines) is written in Fortran for the CDC 6600. A listing of this program and the (Lawrence Berkeley) library subroutine VARMIT, an application of Davidon's minimization routine, reference 4, together with other called subroutines are available from the author.

Conclusion

The method presented here is a possible approach to the solution of eigenvalue problems of one dimension. It has the merit of simplicity in formulation and computation. The cubic spline approximation is amenable to interpolation, that is, it is easy to interpolate, since the spline is a cubic on each smaller segment in the interval in the independent variable. Thus we use terms to the third order in a Taylor's expansion and get an exact interpolation.

The smallness of the error at mid point shows that we have a reasonable approximation to the least eigenvalue and the corresponding eigen function.

Acknowledgements

This work was done in part under the auspices of the Atomic Energy Commission, U.S.A. The author is greatly indebted to the Lawrence Berkeley Laboratory for a six week visit for research, during the past summer in the Mathematics and Computing Group. I wish also to express my indebtedness to Dr. Jonathan Young for the invitation to join him at the Laboratory and for continuous aid and advice in attaining the purpose and goal of this research.

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Figure Captions

Figure 1. A set of five basic splines on the interval [0,1] used in solving $y'' + \lambda y = 0$ and $y'' - 2y' + \lambda y = 0$.

Figure 2. Solution of $y'' + \lambda y = 0$ on the interval [0,1], $y(0) = y(1) = 0$.

Figure 3. Solution of $y'' - 2y' + \lambda y = 0$ on the interval [0,1], $y(0) = y(1) = 0$.

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