A THESIS ON

FINITE DIFFERENCE METHODS AND THEIR CONVERGENCE ANALYSIS FOR CERTAIN TWO-POINT BOUNDARY VALUE PROBLEMS

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CERTIFICATE

This is to certify that the thesis entitled "Finite Difference Methods and Their Convergence Analysis For Certain Two-Point Boundary Value Problems" which is being submitted by Mr. Chittaranjan P. Katti for the award of Doctor of Philosophy (Mathematics) to the Indian Institute of Technology, Hauz Khas, New Delhi, is a record of bonafide research work. He has worked for the last three and a half years under my guidance and supervision.

The thesis has reached the standard, fulfilling the requirements of the regulations relating to the degree. The results obtained in the thesis have not been submitted to any other University or Institute for the award of any degree or diploma.

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S Y N O P S I S

The thesis is concerned with the development of finite difference methods and their convergence analysis for certain two-point boundary value problems. In Chapter I we study the development of finite difference methods and their convergence analysis for two-point boundary value problems involving fourth-order differential equation with boundary conditions prescribing either y, y' or y, y''. For the purpose we consider a more general problem and give a systematic development for the construction of "(2n+1)-diagonal" finite difference methods for two-point boundary value problems involving the 2n-th order differential equation: $y^{(2n)}+f(x,y) = 0, n \geqslant 2$. For use with these discretizations of the differential equation, we also consider obtaining general discretizations for the boundary conditions prescribing either $y, y'', \ldots, y^{(2n-2)}$ or $y, y', \ldots, y^{(2n-3)}$. We then consider in detail obtaining finite difference methods of orders two, four and six for two-point boundary value proble involving fourth order differential equations and study the convergence of these methods. The five-diagonal sixth order methods thus obtained involve certain off-step abscissas. We then consider obtaining sixth order methods which are not based on any off-step abscissas. By suitably lowering the order of the local truncation errors in the boundary discretizations, and by suitably modifying the usual convergence arguments, we give five-diagonal sixth order methods which do not involve any off-step abscissas. In Chapter II we consider the convergence of some existing finite difference methods and the development of some new finite difference methods for computing eigenvalues of certain two-point boundary value problems. We first consider the eigenvalue problem: $y''+(\lambda q(x)-r(x))y = 0$, $y(a) = y(b) = 0$. Noumerov's method is often used to compute approximations for the eigenvalues λ of this problem. No proof showing that Noumerov's method applied to this problem provides $O(h^4)$-convergent approximations for λ seems to have been given so far. We give a proof establishing that Noumerov's method provides real, positive and $O(h^4)$-convergent approximations for λ for all $q(x) > 0$. Again, we note that for computing eigenvalues of this two-point boundary value problem Noumerov's method is used expressed in the form: $(B^{-1}D+h^2R)\,\tilde{Y} - h^2\Lambda Q\tilde{Y} = \underline{0}$. Now, even though both B and D are (symmetric) tridiagonal matrices, $B^{-1}D+h^2R$ is a "completely filled" matrix. Therefore, for computing eigenvalues of this two-point boundary value proble it is natural to ask for an alternative method of the form $(C+h^2R)\,\tilde{Y} - h^2\Lambda Q\tilde{Y} = \underline{0}$, in which the matrix C is a suitable "band matrix". We present such a new method in which the matrix C is symmetric and five-diagonal. We then consider the eigenvalue problem involving a fourth-order differential equation: $y^{(4)}-(\lambda q(x)-r(x))y = 0$, $y(a) = y(b) = y'(a) = y'(b) = 0$. For this problem, the coefficient matrices for all the existing finite difference methods (even for a method of order two) are unsymmetric. We present a new finite difference method for which the coefficient matrix is symmetric and five-diagonal; it is shown that the resulting method provides $O(h^2)$-convergent approximations for the eigenvalues of this problem. Finally, in Chapter II we study the convergence of a finite difference method for computing eigenvalues of Sturm-Liouville problems: $(p(x)y')'+(\lambda q(x)-r(x))y = 0$, subject to mixed boundary conditions. In Chapter III we discuss the construction of three-point finite difference approximations for the class of two-point boundary value problems: $(p(x)y')' = f(x,y)$, $\alpha_0 y(a)-\alpha_1 y'(a) = A$, $\beta_0 y(b)+\beta_1 y'(b) = B$. We first establish a certain identity from which, by making use of suitable cubature formulas, a family of fourth-order discretizations for the differential equation are obtained; appropriate discretizations for the boundary conditions are also obtained. From this family of methods, a "simplest" fourth-order method is given and its convergence is established. In Chapter IV we discuss the construction of three-point finite difference approximations and their convergence for the class of (weakly) singular two-point boundary value problems: $(x^{\alpha}y')' = f(x,y)$, $y(0) = A$, $y(1) = B$, $0 < \alpha < 1$. Again, employing a general (nonuniform) mesh, we first establish a certain identity from which various methods can be obtained. Our main objective here is to obtain methods having order two for <u>all</u> $\alpha \in (0,1)$. It turns out that a method of order two for <u>all</u> $\alpha \in (0,1)$, and based on just one evaluation of f, is possible only if an appropriate non-uniform mesh is employed. Such a method is obtained and its convergence is established. On the other hand, it turns out that any method having order two for <u>all</u> $\alpha \in (0,1)$ and employing uniform mesh must be based on, at least, three evaluation of f; two such second order methods are obtained and their convergence is established.

The thesis consists of four chapters; a brief description of the contents of each chapter follows:

<u>Chapter I</u>: Our main concern in Chapter I is to study the development of finite difference methods and their convergence for two-point boundary value problems involving fourth-order differential equations with boundary conditions prescribing either y, y' or y, y''. For the purpose we consider a more general problem from which the finite difference methods for fourth-order differential equations and the associated boundary conditi follow easily. We give a systematic development for the construction of "(2n+1)-diagonal" finite difference methods for two-point boundary value problems involving the 2n-th order differential equation:

(1) $$y^{(2n)} + f(x,y) = 0, \quad n \geq 2.$$

For use with these discretizations of the differential equation, we also consider obtaining general discretizations for the boundary conditions with either "even-derivatives prescribed":

(2) $$y^{(2j)}(a) = A_{2j}, \; y^{(2j)}(b) = B_{2j}, \; j = 0(1)n-1;$$

or, boundary conditions with "odd-derivatives prescribed";

(3) $y(a) = A_0,\ y(b) = B_0,\ y^{(2j-1)}(a) = A_{2j-1},\ y^{(2j-1)}(b)$

$= B_{2j-1},\quad j = 1(1)n-1.$

We then consider in detail obtaining finite difference methods of order two, four and six and study their convergence for two-point boundary value problems involving the fourth order differential equation: $y^{(4)}+f(x,y) = 0$, with boundary conditions prescribing y, y'' or y, y'. It turns out that the five-diagonal sixth order methods thus obtained involve certain off-step abscissas. We then consider obtaining sixth order methods which are not based on any off-step abscissas. By suitably lowering the order of the local truncation errors in the boundary discretizations (we show that it is enough to have the boundary conditions discretized with local truca - tion errors $O(h^{7+\alpha})$), we give five-diagonal sixth order methods, which do not involve any off-step abscissas, for each of the two-point boundary value problems:

(4a) $\quad y^{(4)} + f(x,y) = 0,$

(4b) $\quad y(a) = A_0,\ y^{(1+\alpha)}(a) = A_{1+\alpha},\ y(b) = B_0,\ y^{(1+\alpha)}(b) = B_{1+\alpha}$

$\alpha \in \{0,1\}.$

<u>Chapter II</u>: In Chapter II we consider the convergence of some existing finite difference methods and the development of some new finite difference methods for computing eigenvalues of certain two-point boundary value problems.

We first consider the eigenvalue problem:

$$(5)\qquad y'' + (\lambda q(x)-r(x))y = 0, \quad y(a) = y(b) = 0.$$

Noumerov's method is often used to compute approximations for the eigenvalues λ of (5). No proof showing that Noumerov's method applied to this problem provides $O(h^4)$-convergent, approximations for λ seems to have been given so far. We give a proof establishing that Noumerov's method provides real, positive and $O(h^4)$-convergent approximations for λ for all $q(x) > 0$ and $r(x) \geqslant 0$.

Again, we note that for computing eigenvalues of (5), Noumerov's method is used expressed in the form

$$(6)\qquad (B^{-1}D+h^2R)\,\tilde{Y} - h^2\Lambda Q\tilde{Y} = \underline{0},$$

where $D = (d_{ij})$ and $B = (b_{ij})$ are symmetric tridiagonal matrices with $d_{ii} = 2$, $d_{i,i\pm1} = -1$, $b_{ii} = \frac{10}{12}$; $b_{i,i\pm1} = \frac{1}{12}$, $R = \mathrm{diag}\{r_1,\dots,r_{N-1}\}$, $Q = \mathrm{diag}\{q_1,\dots,q_{N-1}\}$. Now, even though B and D are (symmetric) tridiagonal matrices, $B^{-1}D+h^2R$ is a "completely filled" matrix. Therefore for computing eigenvalues of (5) it is natural to ask for an alternative method of the form:

$$(7)\qquad (C+h^2R)\,\tilde{Y} - h^2\Lambda Q\tilde{Y} = \underline{0},$$

in which the matrix C is a suitable "band matrix". We present such a new method in which the matrix C is symmetric and five-diagonal; in fact, for present method,

$$C = D(I + \frac{1}{12} D).$$

A proof is given showing that this new method provides real, positive and $O(h^4)$-convergent approximations Λ for λ of (5).

We then consider the eigenvalue problem involving a fourth order differential equation:

$$(8) \qquad \begin{aligned} & y^{(4)} - (\lambda q(x) - r(x))y = 0 \\ & y(a) = y(b) = y'(a) = y'(b) = 0. \end{aligned}$$

For this problem, the coefficient matrices for all the existing finite difference methods (even for a method of order two) are unsymmetric. For computing approximations Λ for eigenvalues λ of (8), we present a new method in the form:

$$(9) \qquad (D + h^4 R)\,\tilde{Y} - h^4 \Lambda Q \tilde{Y} = \underline{0},$$

in which $D = (d_{ij})$ is a symmetric five-diagonal matrix with

$$d_{11} = d_{N-1,N-1} = 7,\ d_{12} = d_{N-1,N-2} = -4,\ d_{13} = d_{N-1,N-3} = 1$$

$$d_{k,k} = 6,\ \ d_{k,k\pm 1} = -4,\ \ d_{k,k\pm 2} = 1.$$

It is shown that this new method provides $O(h^2)$-convergent approximations Λ for eigenvalues λ of (8).

Finally, in this chapter we study the convergence of a finite difference method for computing eigenvalues of Sturm-Liouville problems:

$$(10a) \qquad (p(x)y')' + (\lambda q(x) - r(x))y = 0,$$

subject to the mixed boundary conditions:

$$\text{(10b)} \quad a_0 y(a) - a_1 p(a) y'(a) = 0, \quad b_0 y(b) + b_1 p(b) y'(b) = 0$$

A finite difference method with a symmetric tridiagonal coefficient matrix is described for computing eigenvalues λ of (10). A proof for the convergence of the method for the case of "natural boundary conditions", $(a_1 = b_1 = 0)$ has been given by Keller [H.B. Keller, "Two-Point Boundary Value Problems, Theorem 5.3.3]. A proof for the convergence of the present method for mixed boundary conditions can be given using stability analysis of Kreiss [H.O. Kreiss, "Difference Approximations for Boundary and Eigenvalue Problems for Ordinary Differential Equations", Math. Comp., V. 26, 1972, pp. 605-626]. However, the stability analysis of both Keller and Kreiss require a "proper normalization" of the discretization equations so that the local truncation errors are all $O(h^2)$. But this normalization destroyes symmetry of the coefficient matrix of our method. Thus our interest here is to offer an alternative proof showing that the convergence of the present method as such (without normalization) can be easily given by a slight modification of Keller's stability analysis.

Chapter III: In Chapter III we discuss the construction of three-point finite difference approximations for the class of two-point boundary value problems:

(11a) $\qquad (p(x)y')' = f(x,y),$

subject to the mixed boundary conditions:

(11b) $\qquad \alpha_0 y(a) - \alpha_1 y'(a) = A_1, \ \beta_0 y(b) + \beta_1 y'(b) = B.$

We first establish an identity from which general three-point finite difference approximations of various orders can be obtained by employing suitable cubature formulas to evaluate the double integrals occuring in this identity. We then consider in detail obtaining fourth order methods based on three evaluations of f. We obtain a family of fourth order discretizations for the differential equation; appropriate discretizations for the boundary conditions are also obtained. We select the free parameters available in these discretizations to obtain a "simplest" fourth order method. This method is described and its convergence is established; numerical examples are given to illustrate this new fourth order method.

Chapter IV: In Chapter IV we discuss the construction of three-point finite difference approximations and study their convergence, under appropriate conditions, for the class of (weakly) singular two-point boundary value problems:

(12) $\ (x^{\alpha}y')' = f(x,y), \ y(0) = A, \ y(1) = B, \ 0 < \alpha < 1.$

Again, employing a general (nonuniform) mesh, we first establish a certain identity from which various methods can be obtained.

Our main objective here is to obtain methods having order two for all $\alpha \varepsilon (0,1)$. Now, in order to obtain a method having order two for all $\alpha \varepsilon (0,1)$, there seem to be three possibilities. By employing an appropriate (nonuniform) mesh over $[0,1]$, we obtain a method M_1 based on just one evaluation of f. Alternatively, employing uniform mesh, we obtain the two methods M_2 and M_3 each based on three evaluations of f. The methods M_1 and M_2 have the property that for $\alpha = 0$ they reduce to the classical second order method based on one evaluation of f. These three methods are investigated in detail, their $O(h^2)$-convergence is established and illustrated by numerical examples.

Some of the results of the thesis have been published/ are to appear in:

BIT (1979), Math. Comp. (1980), BIT (1980), J. Comput. Appl. Math. (1980)

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