

Error curves for Lanczos' "selected points" method*

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The solution of ordinary differential equations by polynomials is discussed from the point of view of constructive function theory. The paper shows how to obtain two new families of "selected points", one of which tends to minimize the absolute maximum error of the solution, and the other of which tends to minimize the absolute value of the error at the final time point.

1. Introduction

Various investigators (Clenshaw, 1957; Fox, 1962; Clenshaw and Norton, 1963; Kizner, 1964a; Wright, 1964) have made use of Lanczos' method of "selected points" (Lanczos, 1956) or in related methods in the solution of ordinary differential equations. The choice of these points has been either the zeroes of $T_n(x)$ or the maxima of $T_n(x)$. Recently, Filippi (1964) recommended another choice which is close to optimal. Here we find two other choices of "selected points" and indicate their advantages.

Wright (1964) attempts a justification of the choice of the zeroes of $T_n(x)$, but his form of the residual,

$$E = \prod_{i=1}^n (x - x_i)\psi(x),$$

where $\psi(x)$ is an unknown function which depends on the differential equation, is incorrect. In fact we will show that local extrema occur near the x_i .

Some of our conclusions about the form of error curves are similar to Lanczos (1956). Whereas his discussion (p. 477) is concerned with a particular equation, we consider the question more generally.

Other topics that we consider concern estimates of the error when the length of the interval in which the solution is sought is changed, and the degree of the approximating polynomial changed.

2. Results from the constructive theory of functions

We wish to solve

$$\dot{Y} = F(Y, x) \quad (1)$$

where $Y = (y^{(1)}, y^{(2)}, \dots, y^{(m)})$ is the vector of the m unknown functions, \dot{Y} is the derivative of Y with respect to x , the independent variable. We also assume that equation (1) holds for $-1 \leq x \leq 1$.

To simplify matters we will assume that $m = 1$, and call our solution $y(x)$. In solving a differential equation by Lanczos' method, using n evaluation of derivatives, we obtain a polynomial approximation of degree $n, p_n(x)$, for the solution. In order to specify how

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"good" an approximation is, we adopt the uniform norm. Thus

$$\|y(x) - p_n(x)\| = \max_x |y(x) - p_n(x)| \quad (2)$$

where we assume that $y(x)$ is a continuous function. Thus our problem is to choose the "selected points" so that equation (2) is as small as possible, if not for all $F(y, x)$ of equation (1), then for sufficiently "well behaved" functions $F(y, x)$.

In order to see how good these approximations can be, we make use of results from the constructive theory of functions. A good source for learning the theory at about the level of a real-variables course is Natanson (1955). Golomb (1962) provides a functional-analysis-oriented treatment with many new results. The following fundamental theorem is due to Chebyshev and Borel.

Theorem 1. Let $y(x)$ be a continuous function on $[a, b]$ or $y(x) \in C[a, b]$, and let the integer n be given. Define

$$E_n = \inf_{p_n} \|y(x) - p_n(x)\|$$

where $p_n(x)$ is any polynomial of degree n or less. Then

(a) There exists a polynomial \bar{p}_n contained in the set of p_n such that

$$E_n = \|y(x) - \bar{p}_n(x)\|.$$

(b) For $\bar{p}_n(x)$ to have this property, it is necessary and sufficient that $y(x) - \bar{p}_n(x)$ attain its maximum absolute value M at least $n + 2$ points of $[a, b]$, and that the maxima alternate with the minima at these points.

(c) The polynomial $\bar{p}_n(x)$ is unique.

The Weierstrass approximation theorem tells us that E_n tends to zero for any continuous function. However, there is a theorem due to Bernstein, which tells us that for any number sequence

$$A_0 \geq A_1 \geq A_2 \geq \dots \quad \lim_{n \rightarrow \infty} A_n = 0$$

there exists a function $y(x) \in C[a, b]$ with the best approximations $E_n(y) = A_n$. Thus if all we know about the function is that it is continuous, it may be impractical to try to find a polynomial approximation for it.

The rate at which E_n tends to zero depends largely on the "degree of smoothness" of the function approxi-

mated. In order of increasing smoothness we list continuous functions, differentiable functions, n -times differentiable functions, infinitely differentiable functions, analytic functions, entire functions, and polynomials of restricted degree. The following is an abstract of results due to Jackson. The form of the theorem as stated here can be found in Golomb (1962). By $y(x) \in C^n[a, b]$ we denote functions that have continuous n th order derivatives in $[a, b]$.

Theorem II.

(a) If $y(x) \in C^1[a, b]$ such that for $x \in [a, b]$, $|y'(x)| \leq M_1$, then

$$E_n \leq \frac{\pi(b-a)M_1}{(n+1)2}$$

(b) If $y(x) \in C^p[a, b]$, $|y^{(p)}(x)| \leq M_p$ for $x \in [a, b]$, and $n \geq p, p = 1, 2, \dots$

$$E_n \leq \frac{\pi^p M_p}{(n+1)n \dots (n-p+2)} \left(\frac{b-a}{2}\right)^p$$

(c) Under the assumptions for (b) and $n \geq 2p - 4$

$$E_n \leq \pi^p M_p \left(\frac{b-a}{n+1}\right)^p$$

Thus we have bounds on E_n which tell us how rapidly E_n goes to zero. From (c) we see that for any $y(x) \in C^p[a, b]$, E_n goes to zero at least as fast as $(n+1)^{-p}$. When $y(x)$ is infinitely differentiable on $[a, b]$, or $y(x) \in C^\infty[a, b]$, we have

$$\lim_{n \rightarrow \infty} (n^p E_n) = 0$$

for all p .

Bernstein has proved a converse theorem: If

$$E_n < \frac{A}{(n+1)n \dots (n-p+2)}$$

for a constant A , then $y(x) \in C^p[a, b]$.

We next see what the convergence is for functions analytic on the line. $y(x)$ defined on $[a, b]$ is said to be analytic on the interval if for any $x_0 \in [a, b]$ there is a power series

$$\sum_{i=0}^{\infty} C_i(x_0)(x-x_0)^i$$

convergent for $|x-x_0| < R$, which represents the function at all points belonging simultaneously to $[a, b]$ and (x_0-R, x_0+R) . We denote by $A[a, b]$ the class of functions analytic in the segment $[a, b]$. If $R = \infty$, the function is said to be an entire function. Then we have:

Theorem III. Let $y(x) \in C[a, b]$. Then $f(x) \in A[a, b]$ if and only if

$$E_n < Kq^n$$

where K and $q < 1$ are constants.

Moreover, $y(x)$ is an entire function if and only if

$$\lim_{n \rightarrow \infty} \sqrt[n]{E_n} = 0.$$

To apply these theorems to solutions of differential equations (1), where the solution is not available, we can make use of the following two theorems (Lefschetz, 1962).

Theorem IV. Let $F(y, x)$ of (1) be C^p in y and x in a certain region Ω of the product space of y and x . Then the solution $y(x, x^0, y^0)$, where x^0 and y^0 are the initial conditions, such that $y(x^0, x^0, y^0) = y^0$ belongs to C^p in x^0 and y^0 and belongs to C^{p+1} in x .

Theorem V. If $F(y, x)$ is analytic in both variables and Δ is the domain of analyticity then the solution $y(x, x^0, y^0)$ such that $[y(x), x] \in \Delta, y(x^0, x^0, y^0) = y^0$, is analytic in all three arguments.

Having found good estimates of how E_n varies with increasing n for a particular function defined in a given interval, we ask how E_n behaves when we vary the interval, or vary a and b . Here we have in mind the claims made that "global" methods are more efficient than "local" methods. Here Theorem II tells us what to expect if these bounds are close to the best possible bounds. But it is easy to show cases where these bounds are a poor indication of the actual error. Theorem II does suggest that for a given $y(x) \in C^p[a, b]$ and M_p more or less independent of the interval, that E_n is proportional to $(b-a)^{\min(n,p)}$ where by $\min(n,p)$ we mean choosing the minimum value from the collection of values n and p . This result is consistent with our experimental findings.

Another approach that we might take is to assume that we have a "well behaved" function which can be expanded in a Chebyshev series such that the norm of the error in using the truncated series is close to E_n . Elliott (1963) has derived the following bound for a_n , the coefficient of $T_n(x)$ in the expansion of $y(x)$ where $y(x) \in C^\infty[a, b]$:

$$a_n \leq \frac{M_n}{2^{n-1}n!} \tag{3}$$

and, as before, $\max |y^n(x)| = M_n$.

Sharper bounds are derived by Elliott (1964) which depend on the behaviour of the function in the complex plane.

3. The form of optimum error curves for solutions of differential equations

Let us now see how the practical limitations involved in solving an ordinary differential equation on a computer affect our results. Since the error curve for the optimum $\bar{p}_n(x)$ may resemble $T_{n+1}(x)$ and usually will have maxima or minima at the end points, we cannot obtain this curve without modifying the initial conditions. For practical reasons let us agree not to modify the initial conditions.

Another constraint which may be needed comes about if the time interval for which a solution is sought is so large that the desired accuracy cannot be achieved by a

polynomial of limited degree, thus necessitating the subdivision into smaller intervals, and the approximation on each of these. Here we would like the error at the end of each subinterval to be as small as possible so that errors do not propagate. Thus we postulate that we wish a modified extremal approximation where the initial error and final error is zero.

4. Properties of the optimal error curve

There is a fundamental theorem similar to Theorem I: *Theorem VI.* Let $y(x) \in C[a, b]$ and let the integer $n \geq 1$ be given. Define

$$\bar{E}_n = \inf_{q_n} ||y(x) - q_n(x)||$$

where $q_n(x)$ is any polynomial of degree n or less that satisfies $q_n(a) = y(a)$ and $q_n(b) = y(b)$. Then

- (a) There exists a polynomial \bar{q}_n contained in the family of q_n such that

$$\bar{E}_n = ||y(x) - \bar{q}_n(x)||.$$

- (b) For $\bar{q}_n(x)$ to have this property, it is necessary and sufficient that $y(x) - \bar{q}_n(x)$ attain its maximum absolute value M at at least n points of $[a, b]$, and that the maxima alternate with the minima at these points.
- (c) The polynomial $\bar{q}_n(x)$ is unique.

Proof: The proof of existence (a) follows from a theorem in functional analysis (Theorem 1.1 of Golomb, 1962) which states that when the manifold of approximants is finite dimensional, the set of best approximations is non-empty. Incidentally the search for \bar{q}_n can be made from the set $c_2 T_2^{**}(x) + c_3 T_3^{**}(x) + \dots + c_n T_n^{**}(x)$, where c_2, c_3, \dots, c_n are unknown coefficients and $T_i^{**}(x)$ are polynomials which are similar to the Chebyshev polynomials but are zero at the end points (see equation 6). To this must be added a straight-line solution satisfying the boundary conditions.

Next we prove the sufficiency of condition (b). Suppose $\bar{q}_n(x)$ is a polynomial such that it satisfies the boundary conditions, and $y(x) - \bar{q}_n(x)$ attains its maximum modulus M , with alternating signs, at n points of (a, b) . If $q_n(x)$ is any other polynomial of degree n satisfying the boundary conditions, we cannot have $|y(x) - q_n(x)| < M$ throughout $[a, b]$ because the polynomial

$$q_n(x) - \bar{q}_n(x) = [y(x) - \bar{q}_n(x)] - [y(x) - q_n(x)]$$

would be of alternating sign at the n points in question, and would therefore vanish at $n - 1$ in (a, b) in addition to vanishing at the end points, which is impossible.

Next we show that condition (b) is necessary. Suppose the maximum error M is attained at fewer than n points having alternating sign. Then the interval $[a, b]$ can be subdivided into $n - 1$ subintervals, in each of which we have one or the other of the inequalities:

$$-M \leq y(x) - \bar{q}_n(x) < M - \epsilon$$

$$\text{or} \quad -M + \epsilon < y(x) - \bar{q}_n(x) \leq M$$

satisfied alternately, where ϵ is a positive number. This can be done by taking each subinterval to include one extremum of $y(x) - \bar{q}_n(x)$. Let $q_n(x)$ be a polynomial which vanishes only at the end points and the $n - 2$ points common to two of these subintervals. Therefore for some choice of parameter η , we have

$$|y(x) - \bar{q}_n(x) - \eta q_n(x)| < M$$

contradicting the extremal property of $\bar{q}_n(x)$.

Finally concerning uniqueness, suppose $\bar{q}_n(x), q_n(x), \bar{q}_n(x) \neq q_n(x)$ are both extremals of our problem satisfying the boundary conditions. Then so is

$$R_n(x) = \frac{1}{2}[\bar{q}_n(x) + q_n(x)].$$

But $y(x) - R_n(x)$ attains its extrema at fewer than n points, which is impossible.

We now ask how much larger is \bar{E}_n than E_n ? We can see immediately that $\bar{E}_n \leq 2E_n$, since if we start out with \bar{p}_n and add a first-degree polynomial to satisfy the boundary conditions, then the maximum increase in the error modulus is E_n .

By making some assumptions about the form of the error curves we can obtain a more realistic estimate of the relationship of E_n and \bar{E}_n . We assume that the error curve for $\bar{q}_n(x)$ for $[a, b]$ is the same as for $\bar{p}_n(x)$, but with a larger interval $[A, B]$, where $A < a$, and $B > b$. In general we can find an A and B which will satisfy these conditions, assuming that the function $y(x)$ can be continued beyond the original interval. If in addition we assume that the ratio of the lengths of the intervals is $\cos\{\pi/2[1/(n+1)]\}$ [assuming that $\bar{p}_n(x)$ results in an error curve resembling $T_{n+1}(x)$], and that E_n is proportional to the $n + 1$ the power of the ratio of the lengths of the interval, then

$$\begin{aligned} \frac{\bar{E}_n}{E_n} &= \left[\frac{1}{\cos\left(\frac{\pi}{2} \frac{1}{n+1}\right)} \right]^{n+1} \\ &= 1 + \frac{\pi^2}{8} \frac{1}{n+1} + O\left(\frac{1}{n+1}\right)^2. \end{aligned} \tag{5}$$

Thus for large n it appears that \bar{E}_n tends to E_n .

5. Choices of "selected points"

At this point we have a clear picture of the optimum error curve, associated with $\bar{q}_n(x)$. This error curve has n extrema alternating in sign and is zero at the initial and final values of x . Now we seek to choose "selected points" to achieve this form of error curve.

Consider the differential equation (1) with $F \in C^\infty$ in y and x in a region containing the solution of the differential equation for the fixed initial conditions. Then Theorem IV implies that $y(x) \in C^\infty[a, b]$, which indicates that $y(x)$ and $\dot{y}(x)$ have rapidly converging polynomial approximations.

We construct the error curve by starting out with the exact solution, and using Picard's method of successive approximations to see how the errors enter. Hopefully this method will converge rapidly for a large enough n and a good choice of "selected points." This assumption will appear more reasonable when certain matrices are derived in Section 6.

Thus we calculate the n values of the derivatives at the "selected points" using the exact solution to obtain \hat{Q}_1 , the first $(n - 1)$ th degree polynomial approximation for the derivative, and Q_1 , the first n th degree polynomial approximation for $y(x)$.

Q_1 will differ from $y(x)$ because \hat{Q}_1 is inexact, except at some few points. Hence the error curve associated with Q_1 will have extrema at the "selected points," where \hat{Q}_1 is exact.

The next approximation is determined by equating \hat{Q}_2 and $f(Q_1, x)$ at the "selected points." If a good choice of points has been made then, for large enough n , we expect that, because of averaging, the integrated values, Q_1 , should not differ much from $y(x)$ even though \hat{Q}_1 may differ considerably from $y(x)$. This implies that Q_2 will not differ much from Q_1 . It is then our task to choose the points so that averaging does occur.

If we have only one dependent variable, then one choice of "selected points" might be the n extremal points referred to in Theorem VI(b). This would make the maximum absolute error of Q_1 at the "selected points" as small as possible while satisfying the boundary conditions. Thus when \bar{E} is small enough so that $f(Q_1, x)$ is close enough to $f[y(x), x]$, Q_2 will not differ appreciably from Q_1 , and the process will have converged in a practical sense. Unfortunately it may not be practical to calculate these "selected points," except in an approximate manner to be described.

Thus we assume that the error curve $y(x) - \hat{Q}_1(x)$ can be adequately represented by an n th degree polynomial. We can now easily calculate the "selected points" since we know the form of the integrated error curves, $y(x) - Q_1(x)$. We guess that the integrated error curve is of the form $T_{n+1}(x)$ with a change in scale. We define a new "stretched" Chebyshev polynomial by

$$T_{n+1}^{**} \left[\frac{x}{\cos \left(\frac{\pi}{2} \frac{1}{n+1} \right)} \right] \equiv T_{n+1}(x) \quad n \geq 1 \quad (6)$$

From Theorem VI we see that $T_{n+1}^{**}(x)$, $-1 \leq x \leq 1$, is the unique error curve, since it has the required number (n) of extrema with the alternation property. Thus the "selected points" are given by

$$x_i = \frac{\cos \left(\frac{\pi i}{n+1} \right)}{\cos \left(\frac{\pi}{2} \frac{1}{n+1} \right)} \quad i = 1, 2, \dots, n \quad (7)$$

We call this distribution the "extremal."

Filippi (1964), in considering a specialized case of solving an ordinary differential equation, that of finding

an indefinite integral, has arrived at a distribution of "Stützstellen," or "selected points" which is similar to equation (7):

$$x_i = \cos \left(\frac{\pi i}{n+1} \right) \quad i = 1, 2, \dots, n \quad (7a)$$

It is clear that this choice will result in an error curve which is similar to T_{n+1} except that it will be displaced either up or down due to choice of initial values. Filippi's Fig. 1 shows this clearly. Thus Filippi's choice results in a maximum error about twice the size of \bar{E}_n .

We shall call the usual distribution, based on the zeroes of T_n , the Chebyshev. This choice tends to make $\|y(x) - \hat{Q}_1(x)\|$ small, but not necessarily the integrated error curve. Another distribution that we might use is based on zeroes of the Legendre polynomials $P_n(x)$, as used in Gaussian quadrature. If we are particularly concerned with the accuracy of end-point values, and the partial derivatives $\frac{\partial f(x, y)}{\partial y}$ are small, then this choice has much to commend it. Because of the properties of Gaussian quadrature we expect to obtain excellent accuracy at the end points provided the partial derivatives are small. We now seek to show that

$$\begin{aligned} \|y(x) - Q_1(x)_{\text{Chebyshev}}\| &> \|y(x) - Q_1(x)_{\text{Legendre}}\| \\ &> \|y(x) - Q_1(x)_{\text{extremal}}\| \quad n > 2 \end{aligned}$$

where by $Q_1(x)_{\text{Chebyshev}}$ we mean Q_1 determined by using the zeroes of $T_n(x)$, and the corresponding quantities using the Gaussian abscissas and the extremal points (7). For $n = 2$ the zeroes of $P_2(x)$ and the extremal points coincide.

First we derive the form of the error curves for the first iteration. For the Chebyshev case we obtain

$$\begin{aligned} e(x) &= \int_{-1}^x T_n(x^1) dx^1 \quad n \geq 2 \\ &= \frac{1}{2} \left[\frac{T_{n+1}(x)}{n+1} - \frac{T_{n-1}(x)}{n-1} \right] \\ &\quad + \frac{(-1)^n}{2} \left[\frac{1}{n+1} - \frac{1}{n-1} \right]. \quad (8) \end{aligned}$$

Using the zeroes of the Legendre polynomials we obtain

$$\begin{aligned} e(x) &= \int_{-1}^x P_n(x^1) dx^1 \quad n \geq 1 \\ &= \frac{1}{2n+1} [P_{n+1}(x) - P_{n-1}(x)]. \quad (9) \end{aligned}$$

From equation (8) we see that if n is odd there is no truncation error at the end point $x = 1$. For large n the term involving $1/(n+1) - 1/(n-1)$ can be neglected. It is easily shown from equation (8) that the signs of the extremal points alternate and the magnitudes

are given by

$$C \sin \left\{ \frac{\pi}{2} \left(\frac{2i + 1}{n} \right) \right\} \quad (10)$$

$$i = 0, 1, \dots, n - 1$$

where C depends only on n and i is the number of the "selected point." Thus the magnitudes of the extrema are small at the ends and are largest at the middle of the interval. From equation (10) it follows that for large n about 29% of the extrema will have a magnitude between M , the maximum of the extrema and $0.9M$.

In Table 1 we show the results for other magnitudes and compare with the case using the zeroes of the Legendre polynomials.

Table 1

Distribution of the magnitudes of the extrema for large n

	FRACTION HAVING MAGNITUDES			
	$\geq 0.90M$	$\geq 0.75M$	$\geq 0.50M$	$\geq 0.25M$
Chebyshev	0.29	0.46	0.67	0.84
Legendre	0.40	0.62	0.84	0.96

To find a formula analogous to equation (10) for the Legendre case we make use of the well-known asymptotic formula

$$P_n(\cos \theta) \cong \left(\frac{2}{n\pi \sin \theta} \right)^{1/2} \cos \left[n \left(\frac{1}{2} \theta \right) - \frac{1}{4} \pi \right]. \quad (11)$$

Using equation (11) to find the zeroes of P_n and the amplitudes of P_{n+1} we find that the maximum and minimum points of $P_{n+1}(x) - P_{n-1}(x)$ are given by

$$\cong \frac{2n + 1}{n} \left\{ \frac{2}{(n+1)\pi \sin \left[\frac{\pi}{2} \frac{(3 + 4i)}{(2n + 1)} \right]} \right\}^{1/2}$$

$$\cos \left[\frac{\pi}{2} \frac{(2n + 3)(3 + 4i)}{4n + 2} - \frac{\pi}{4} \right] \quad (12)$$

$$i = 0, 1, \dots, n - 1.$$

After some manipulation the formula analogous to equation (10) is found to be

$$\left\{ \sin \left[\frac{\pi}{2} \left(\frac{3 + 4i}{2n + 1} \right) \right] \right\}^{1/2} \quad (13)$$

$$i = 0, 1, \dots, n - 1$$

which for large n is like the square root of equation (10).

Equation (13) was evaluated for various n and compared with the exact results. The maximum error of (13) for $n = 6, 24,$ and 96 is about $0.03, 0.01,$ and $0.003,$ respectively. The results of Table 1 hold surprisingly well for very small n for the Legendre choice.

On the basis of the distribution of the magnitudes of the extrema we might guess that $\|y(x) - Q_1(x)_{\text{Chebyshev}}\| > \|y(x) - Q_1(x)_{\text{Legendre}}\|$. For $n = 1$ the points coincide.

It is possible to prove these results by expanding the error curve in $T_n^{**}(x)$ polynomials, and note that if the term of highest n , $cT_n^{**}(x)$ is neglected, then we can compare the magnitude of c with the magnitude of the largest extrema of the error curve. This is similar to approximating an n th degree polynomial by an $n - 1$ th degree polynomial by finding K the coefficient of T_n , and subtracting KT_n . The results of these calculations are shown in Fig. 1, where we give the ratio of $\|y(x) - Q_1(x)_{\text{Chebyshev}}\|$ to $\|y(x) - Q_1(x)_{\text{extremal}}\|$ and $\|y(x) - Q_1(x)_{\text{Legendre}}\|$ to $\|y(x) - Q_1(x)_{\text{extremal}}\|$. The limits of these ratios as n approaches infinity are 2 and $\sqrt{2}$, respectively.

6. Numerical results

We now consider some examples to show how well the model error curves, equations (8) and (9) and T_n^{**} , agree with actual error curves. First, we expect that the extrema of the actual error curves occur close to the "selected points." In addition, if $y'(x)$ has a very rapidly converging polynomial expansion, then the error curve should resemble the model error curve for our choices of "selected points."

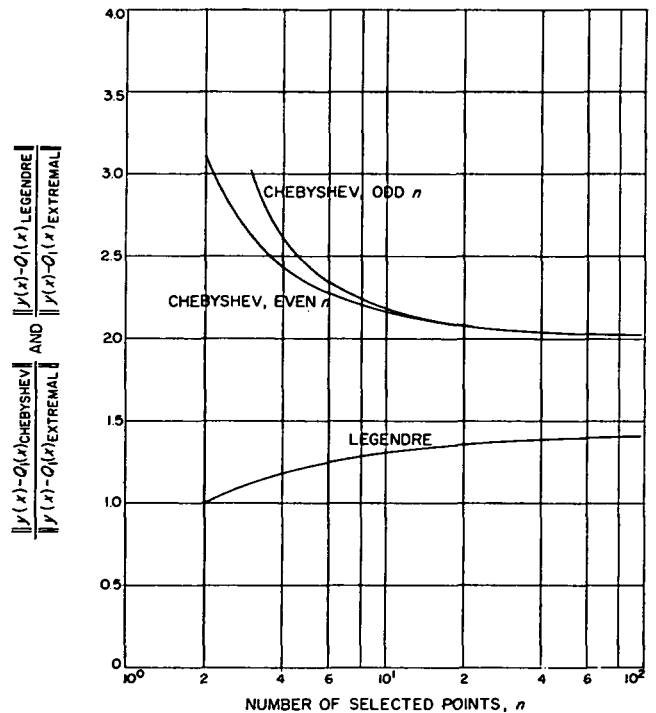


Fig. 1.—Ratio of Chebyshev and Legendre maximum absolute errors to extremal maximum absolute error for various numbers of selected points

Table 2

Error curves for e^t , $n = 5$, $0 \leq t \leq 1$

NUMBER OF POINTS	CHEBYSHEV CASE		LEGENDRE CASE		EXTREMAL CASE	
	VALUE OF t AT SELECTED POINT	ERROR $\times 10^6$	VALUE OF t AT SELECTED POINT	ERROR $\times 10^6$	VALUE OF t AT SELECTED POINT	ERROR $\times 10^6$
1	0.0245	-0.31	0.0469	-1.17	0.0517	-1.45
2	0.2061	3.13	0.2308	1.61	0.2412	1.36
3	0.5	-1.78	0.5	-1.71	0.5	-1.44
4	0.7939	3.55	0.7692	1.55	0.7588	1.31
5	0.9755	0.81	0.9531	-1.10	0.9483	-1.47

An example where both assumptions are fulfilled is the solution for e^t :

$$\frac{dy}{dt} = y, \quad y(0) = 1, \quad 0 \leq t \leq 1.$$

In Table 2 we show the results taking the number of points, n , equal to five. The errors given in Table 2 are calculated at the "selected points," but would not vary much if calculated at the extremal points.

Thus we see that for the extremal case the magnitude of the peaks of the error curve are nearly constant. For the Legendre case we choose a constant for the model curve of equation (9) to match the middle residual to obtain -1.12, 1.57, -1.71, 1.57, and -1.12. If we do the same for the Chebyshev case we obtain -0.24, 2.25, -1.78, 2.25, and -0.24. Thus the Chebyshev case exhibits the poorest agreement with the model curve, and the Legendre case the best. In other examples that we calculated the Legendre and extremal cases had also error curves much closer to the model curves than the Chebyshev case. Another quantity that is of interest is the ratio of $\|y(x) - Q(x)_{\text{Chebyshev}}\|$ to $\|y(x) - Q(x)_{\text{extremal}}\|$ and the corresponding ratio for the Legendre case. Here $Q(x)$ is

$$\lim_{i \rightarrow \infty} Q_i(x)$$

If we assume that $Q(x)$ does not differ much from $Q_i(x)$, we can compare the observed ratios from Table 2, $\frac{3.55}{1.47} = 2.41$ and $\frac{1.71}{1.47} = 1.16$, with the curves of Fig. 1, which yield 2.43 and 1.22, respectively. Thus we have good agreement for this example.

Let us now consider the error at the end point for the same equation. In Table 3 we show the results for different n . Here we underline the first digit that must be changed. The exact value for e is 2.71828182845904 . . ., so that the last result using the zeroes of the Legendre polynomials is good to 12 decimal places.

Various other differential equations were integrated. If the interval was chosen small enough to assume rapid convergence similar results were found. Where the interval was large and convergence was slow the

Table 3

Solutions of $\dot{y} = y$, $y(0) = 1$, evaluated at $t = 1$

NUMBER OF POINTS	CHEBYSHEV CASE	LEGENDRE CASE	EXTREMAL CASE
1	<u>3</u>	<u>3</u>	not defined
2	<u>2.777</u>	<u>2.7143</u>	2.7143
3	<u>2.7168</u>	<u>2.71831</u>	2.71845
4	<u>2.71836</u>	<u>2.71828172</u>	2.718279
5	<u>2.7182807</u>	<u>2.71828182874</u>	2.71828195
6	<u>2.718281890</u>	<u>2.7182818284586</u>	2.7182818270

results were erratic. But in all cases the peaks in the error curves occurred close to the "selected points." And in all cases where the interval was fixed and n varied, the end-point error decreased more rapidly for the Legendre case than for the other two.

7. The practical calculation of solutions by the Picard method

One method of solution which is applicable to a wide range of problems is based on the Picard method of successive approximations (Clenshaw and Norton, 1963). Other methods in which the equations are linearized will be discussed in the next section.

We seek a solution of

$$\frac{dY}{dt} = \bar{F}(Y, t), \quad Y(a) = Y_0 \quad (1)$$

$a \leq t \leq b$, where Y_0 are the initial conditions. With the change of variable

$$t = \frac{a+b}{2} + \frac{b-a}{2}x$$

we obtain

$$\frac{dY}{dx} = \dot{Y} = hF(Y, x), \quad Y(a) = Y_0 \quad (1a)$$

where

$$-1 \leq x \leq 1, h = \frac{b-a}{2}, F(Y, x) = \bar{F}[Y, t(x)].$$

Next we evaluate $F(Y, x)$ at the "selected points," fit the derivatives with polynomials, and integrate to obtain the next approximation. Instead of carrying out these operations explicitly we can simplify the calculations, and thereby gain in accuracy and speed, by precalculating the results of these operations in the form of matrices. The amount of simplification depends on the choice of "selected points." We illustrate this first for the Legendre case (using the zeroes of the Legendre polynomials for the "selected points"). If we assume that Y has only one component, then the i th approximation

$$\dot{Q}_i = \sum_{j=0}^{n-1} a_j P_j(x) \tag{14}$$

$$a_j = \frac{h(2j+1)}{2} \sum_{k=1}^n P_j(x_k) F(Q_{i-1}, x_k) \mu_{n,k} \tag{15}$$

where $\mu_{n,k}$ are the weight factors for Gaussian integration, n being the total number of points, and k the index of the point. Abscissas and weights for Gaussian quadratures are tabulated in Gawlik (1958) and Davis and Rabinowitz (1956 and 1958). Equation (15) can be derived using the property of Gaussian quadrature that

$$\int_{-1}^1 y(x) dx = \sum_{k=1}^n \mu_{n,k} y(x_{n,k})$$

whenever $y(x)$ is a polynomial of degree $\leq 2n-1$, and the orthogonal relations of Legendre polynomials

$$\int_{-1}^1 P_m(x) P_n(x) dx = \frac{2}{2n+1} \delta_{mn}$$

where δ_{mn} is the Kronecker delta function. Integrating equation (14)

$$Q_i(x) = \sum_{j=0}^n b_j P_j(x) \tag{16}$$

$$b_0 = y_0 - a_0 - \frac{a_1}{3}$$

$$b_j = \frac{a_{j-1}}{2j-1} - \frac{a_{j+1}}{2j+3} \quad j = 1, 2, \dots, n \tag{17}$$

where $a_j = 0$ for $j \geq n$.

In evaluating a Legendre series or any series of polynomials $p_0(x), p_1(x), \dots$, satisfying a recursion of the form

$$p_0(x) \equiv 1 \tag{18}$$

$$p_1(x) \equiv (a_0 + b_0 x) p_0(x) \tag{19}$$

$$p_j(x) \equiv (a_{j-1} + b_{j-1} x) p_{j-1} - c_{j-2} p_{j-2}(x), \tag{20}$$

$$j = 2, 3, \dots,$$

where the $a_j, b_j,$ and c_j are constants independent of x , Theorem VII may be applied. The motivation for the theorem is due to Clenshaw (1955). The proofs given

here are due to Drs. J. R. Rice, Purdue University, and C. L. Lawson, Jet Propulsion Laboratory. *Theorem VII.* An expression of the form

$$q(x) = \sum_{i=0}^n d_i p_i(x)$$

can be evaluated by the following recursion formulas:

$$w_n = d_n$$

$$w_{n-1} = (a_{n-1} + b_{n-1} x) w_n + d_{n-1} \tag{21}$$

$$j = n-2, n-3, \dots, 0$$

$$w_j = (a_j + b_j x) w_{j+1} - c_j w_{j+2} + d_j$$

$$q(x) = w_0.$$

To verify that w_0 is equal to

$$\sum_{i=0}^n d_i p_i(x)$$

multiply the equation containing d_i by $p_i(x)$ and sum these $n+1$ equations obtaining

$$\sum_{j=0}^n w_j p_j(x) = \sum_{j=0}^{n-1} (a_j + b_j x) w_{j+1} p_j(x) - \sum_{j=0}^{n-2} c_j w_{j+2} p_j(x) + \sum_{j=0}^n d_j p_j(x).$$

Then collect terms on the w_j 's obtaining

$$\sum_{j=2}^n w_j [p_j(x) - (a_{j-1} + b_{j-1} x) p_{j-1}(x) + c_{j-2} p_{j-2}(x)] + w_1 p_1(x) - (a_0 + b_0 x) p_0(x) + w_0 p_0(x) = \sum_{j=0}^n d_j p_j(x).$$

The coefficient of $w_j, j = 2, \dots, n$, is zero because of equation (20), the coefficient of w_1 is zero because of equation (19), and the coefficient of w_0 is one because of equation (18). Thus this equation reduces to

$$w_0 = \sum_{j=0}^n d_j p_j(x)$$

which is the desired result. For Chebyshev polynomials $T_0(x) = 1, T_1(x) = x, T_2(x) = 2x^2 - 1$, etc., this recursion becomes particularly simple because with the exception of b_0 all of the a_i 's, b_i 's, and c_i 's are independent of i .

$$a_i = 0 \quad i = 0, 1, \dots$$

$$b_0 = 1$$

$$b_i = 2 \quad i = 1, 2, \dots$$

$$c_i = 1 \quad i = 0, 1, \dots$$

For Legendre polynomials $P_0(x) = 1, P_1(x) = x, P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$, etc., the constants are

$$a_i = 0 \quad i = 0, 1, \dots$$

$$b_i = \frac{2i+1}{i+1} \quad i = 0, 1, \dots$$

Table 4

Legendre case

$$G = \begin{pmatrix} 0.17392742 & -0.053208360 & 0.025254925 & -0.0071102994 \\ 0.37623623 & 0.32607258 & -0.055760857 & 0.013471001 \\ 0.33438384 & 0.70790601 & 0.32607258 & -0.028381390 \\ 0.35496514 & 0.62689023 & 0.70535352 & 0.17392742 \end{pmatrix}$$

$$H = \begin{pmatrix} 0.29205613 & 0.39453250 & 0.25761265 & 0.055798711 \\ 0.10736392 & 0.39263608 & 0.39263608 & 0.10736392 \\ -0.08142227 & -0.14187965 & 0.14187965 & 0.089142227 \\ 0.066563505 & -0.066563505 & -0.066563505 & 0.066563505 \\ -0.028986485 & 0.073419724 & -0.073419724 & 0.028986485 \end{pmatrix}$$

$$c_i = \frac{i+1}{i+2} \quad i = 0, 1, \dots$$

We note that the calculation of the coefficients and the evaluation of the series are linear processes which relate calculated values of derivatives to the values of the functions at the "selected points." Thus there exists an $n \times n$ matrix G such that

$$\begin{aligned} Q_{i+1}(x_1) &= h[G_{11}F(Q_i, x_1) \\ &\quad + G_{12}F(Q_i, x_2) + \dots] + y_0 \\ Q_{i+1}(x_2) &= h[G_{21}F(Q_i, x_1) \\ &\quad + G_{22}F(Q_i, x_2) + \dots] + y_0 \\ Q_{i+1}(x_n) &= h[G_{n1}F(Q_i, x_1) \\ &\quad + G_{n2}F(Q_i, x_2) + \dots] + y_0. \end{aligned} \tag{21}$$

G is obtained by calculating each column in turn. For the j th column set $h = 1$, $F(Q_i, x_k) = \delta_{kj}$, $y_0 = 0$. The a 's and b 's are calculated by equations (15) and (17) and the resulting series for Q_{i+1} is evaluated at the "selected points." These are the elements of the j th column of G .

Although the solution is available in the form of a Legendre series, it is preferable to have it in the form of a Chebyshev series because a Chebyshev series requires fewer multiplications for its evaluation. Another reason is that the user can specify the accuracy he desires more easily with a Chebyshev series. Again, it is a straightforward matter to evaluate the solution Q_{i+1} at the zeroes of $T_{n+1}(x)$ and fit them with Chebyshev polynomials, thus obtaining the H matrix defined by

$$Q_{i+1}(x) = \sum_{i=0}^n c_i T_i(x) \tag{22}$$

$$c = hHF(Q_i, x) + \begin{pmatrix} Y_0 \\ 0 \\ 0 \\ \dots \end{pmatrix}$$

where c is the column vector of c_0, c_1, \dots, c_n , and F is the column vector of $F(Q_i, x_1), F(Q_i, x_2), \dots$

We exhibit in Table 4 the G and H matrices for $n = 4$ for the Legendre case, the numbers being correctly rounded off to eight decimal digits. The points are numbered starting with the point closest to -1 .

Similar matrices can be derived for the extremal case. But here there is a difficulty in fitting Q with a polynomial. The problem can be handled as follows:

By a change of scale

$$t = x \cos\left(\frac{\pi}{2} \frac{1}{n+1}\right)$$

the points are given by

$$t_i = \cos\left(\frac{\pi i}{n+1}\right) \quad i = 1, 2, \dots, n. \tag{23}$$

If we include the points $t_0 = 1$ and $t_{n+1} = -1$ we can determine an $(n+1)$ th degree polynomial $y(t) = 1/2c_0 + c_1 T_1(t) + \dots + c_n T_n(t) + 1/2c_{n+1}(t)$ which takes on prescribed values at the $n+2$ points by

$$c_j = \frac{2}{n+1} \sum_{i=0}^{n+1} y(t_i) \cos\left(ji \frac{\pi}{n+1}\right) \quad j = 0, 1, \dots, n+1 \tag{24}$$

with the understanding that the end points are taken with half weight. We now define $y(t_0)$ and $y(t_{n+1})$ so that c_n and c_{n+1} are both zero. Thus to obtain the k th column of G we let $y(t_k) = 1, y(t_i) = 0$ for $i = 1, 2, \dots, n, i \neq k$, and

$$\begin{aligned} \frac{y(t_0)}{2} &= -\frac{1}{2} \left[\cos\left(\frac{\pi nk}{n+1}\right) + \cos \pi k \right] \\ \frac{y(t_{n+1})}{2} &= \frac{1}{2} \left[\cos \pi k - \cos\left(\frac{\pi nk}{n+1}\right) \right]. \end{aligned} \tag{25}$$

The Chebyshev series is integrated with respect to dx and the constant of integration chosen arbitrarily. The series may then be converted to power form and the transformation made from t to x and then transformed into a Chebyshev series in x . Or the function can be

Table 5

Extremal case

$$G = \begin{pmatrix} 0.19031666 & -0.063801399 & 0.031304253 & -0.0084703186 \\ 0.39297441 & 0.32498835 & -0.055434256 & 0.012551802 \\ 0.35597247 & 0.68690999 & 0.30648738 & -0.024450139 \\ 0.376994519 & 0.60017148 & 0.69527713 & 0.17820761 \end{pmatrix}$$

$$H = \begin{pmatrix} 0.30776329 & 0.37711809 & 0.25435764 & 0.060760981 \\ 0.11684405 & 0.38315595 & 0.38315595 & 0.11684405 \\ -0.093780638 & -0.13918955 & 0.13918955 & 0.093780638 \\ 0.067418083 & -0.067418083 & -0.067418083 & 0.067418083 \\ -0.029720516 & 0.077809321 & -0.077809321 & 0.029720516 \end{pmatrix}$$

evaluated at the points

$$t_i = \cos\left(\frac{\pi}{2} \frac{2i+1}{n+1}\right) \cos\left(\frac{\pi}{2} \frac{1}{n+1}\right)$$

and then fitted with a polynomial in x . Lastly the constant term is evaluated. We exhibit in Table 5 the G and H matrices for $n = 4$ for the extremal case. Again the points are renumbered starting with the point closest to -1 .

An elegant alternative method is given by Filippi (1964) for doing this sort of problem.

These matrices have been calculated up to $n = 48$ using the curve-fitting procedure. The calculations were in double precision (16 decimal places) and were checked using extended precision. The final results were always good to about 14 decimal places.

For large n it may be desirable to store the matrices on tape, since the elements are used in a fixed order. Also it is clear that for large n we may estimate the size of the elements in the H matrix by neglecting the difference between x and t . Thus for large n the elements of k th column of H are approximately given by

$$H_{jk} \approx \frac{1}{2} \frac{c_{j-1} - c_{j+1}}{j} \quad j, k = 1, 2, \dots, n \quad (26)$$

with $H_{0k} = H_{1k} - H_{2k} + H_{3k} - \dots$

From equations (24) to (26)

$$H_{jk} \leq \frac{3}{j(n+1)},$$

$j \geq 1$ when n is sufficiently large. This assures us that the roundoff error will be small.

8. Linearization of the equations

An approach to the solution of nonlinear ordinary differential equations, especially those that are (two-point) boundary-value problems is based on linearizing the equations. One method of linearization depends on a generalization of Newton's iteration formula to

operator equations in Banach spaces obtained by Kantorovich (1948). Hestenes (1949), Kalaba (1959), McGill and Kenneth (1964), and others applied this method to boundary-value problems. Norton (1964) showed how to implement this method using Chebyshev series.

The method consists of solving equation (1) by iterations, the iteration being indicated by a subscript:

$$\dot{y}_i = F(y_{i-1}, x) + (y_i - y_{i-1})F_y(y_{i-1}, x). \quad (27)$$

By adding to any solution of equation (27) a suitable solution of the homogeneous equation

$$\dot{z} = zF_y(y_{i-1}, x) \quad (28)$$

one can hope to satisfy the boundary conditions for each iteration.

Kizner (1964a) has shown another method for linearizing the equations for the initial-value problem. Let us rewrite equation (1) as

$$\dot{y}_i = \dot{y}_{i-1} + \lambda[F(y_i, x) - \dot{y}_{i-1}] \quad (29)$$

where λ is a parameter that takes on values $0 \leq \lambda \leq 1$. For $\lambda = 1$ equation (29) is identical to equation (1). For $\lambda = 0$, $y_i = y_{i-1}$. Now consider y_i as a function of both x and λ .

Then under very general conditions the following equation holds:

$$\frac{d}{dx} \frac{\partial y_i}{\partial \lambda} = F(y_i, x) - \dot{y}_{i-1} + \lambda \frac{\partial F(y_i, x)}{\partial y} \Big|_{y=y_i} \frac{\partial y_i}{\partial \lambda}. \quad (30)$$

Equation (30) may be interpreted as a matrix equation when the number of dependent variables is greater than one. Also

$$y_i(x) = y_i(x, 1) = y_{i-1}(x) + \int_0^1 \frac{\partial y_i(x, \lambda)}{\partial \lambda} d\lambda. \quad (31)$$

Thus far we have made no approximations and no linearization. Now let us formally solve equation (31) by a "Runge-Kutta integration" in λ . The classical Runge-Kutta fourth-order formula "applied" to equa-

tion (31), with step size $h = 1$ results in the following set of linear differential equations:

$$y_i(x, 1) = y_{i-1}(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad (32)$$

where k_i are solutions of equation (30) evaluated according to the following scheme:

$$\begin{aligned} \frac{d}{dx}k_1 &= F(y_{i-1}, x) - \dot{y}_{i-1} \\ \frac{d}{dx}k_2 &= F\left(y_{i-1} + \frac{k_1}{2}, x\right) - \dot{y}_{i-1} \\ &\quad + \frac{1}{2} \left. \frac{\partial F(y, x)}{\partial y} \right|_{y=y_{i-1} + (k_1/2)} k_2 \\ \frac{d}{dx}k_3 &= F\left(y_{i-1} + \frac{k_2}{2}, x\right) - \dot{y}_{i-1} \\ &\quad + \frac{1}{2} \left. \frac{\partial F(y, x)}{\partial y} \right|_{y=y_{i-1} + (k_2/2)} k_3 \\ \frac{d}{dx}k_4 &= F(y_{i-1} + k_3, x) - \dot{y}_{i-1} \\ &\quad + \left. \frac{\partial F(y, x)}{\partial y} \right|_{y=y_{i-1} + k_3} k_4 \end{aligned} \quad (33)$$

with the initial conditions $k_i = 0$ at $x = -1$, $i = 1, 2, \dots, 4$.

In other words (30) is linearized by substituting for y_i and λ the approximate expressions as given by a Runge-Kutta formula. This procedure can be justified in the same way that Runge-Kutta formulas are justified for the numerical solution of ordinary differential equations. Examples are given by Kizner (1964a).

The advantage of this method is that the convergence of the method is very rapid compared with the Picard method. A similar idea was applied by Kizner (1964b) to the solution of nonlinear equations. The reason for the success of "Runge-Kutta" type methods seems to be due to the use of Runge-Kutta formulas that take account in part of some of the higher-order terms. A collection of optimum Runge-Kutta formulas is given by Ralston (1962). Our experience with these formulas, which is mainly in solving nonlinear equations, bears out the theoretical results of Ralston about the size of the

truncation errors for different formulas. Also, the formulas are more widely applicable than the standard Newton-Raphson method.

9. Conclusions

Let us consider five choices for the n "selected points."

1. Zeroes of T_n , called the Chebyshev choice.
2. Zeroes of P_n , called the Legendre choice.
3. Extrema of the "stretched" Chebyshev polynomial T_{n+1}^{**} , called the extremal choice. This is equivalent to using the zeroes of the derivative of T_{n+1}^{**} .
4. The extrema of T_{n-1} , as used by Clenshaw and his associates, called the Clenshaw choice.
5. The zeroes of T'_{n+1} , advocated by Filippi (1964), which we call the Filippi choice.

For "well-behaved" functions and a proper choice of n the extremal choice yields the smallest maximum error, followed by the Legendre, Filippi, Chebyshev, and Clenshaw choices. The errors of the Filippi and Chebyshev are about the same size. Filippi (1964) discusses the Clenshaw choice and shows examples where it compares unfavourably.

If we are interested in keeping the end-point error as small as possible we should use the Legendre choice. Here the differences in accuracy are not something like a factor of 2, as for the previous criterion, but can amount to many orders of magnitude.

A possible drawback to the Legendre or the extremal choice for the Picard method using large n is that it requires the storage of large matrices. However, since the elements are used sequentially, the storage may be made on tape or other device without loss of machine time.

It was pointed out by Mr. C. W. Clenshaw that for second-order equations $\ddot{y} = f(y, x)$ the "extremal" choice would be the zeroes of the second derivative of the stretched Chebyshev polynomial, and similarly for higher degrees.

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Book Review

The Algebraic Eigenvalue Problem, by J. H. Wilkinson, 1965; 662 pages. (London: Clarendon Press; Oxford University Press, 110s.).

The first chapter of this book contains an account of the mathematical background to the algebraic eigenvalue problem, with emphasis on the manner in which the eigensystem is related to the various canonical forms of a matrix. The remainder of the book deals with the practical problems involved in computing eigenvalues and eigenvectors on a digital computer and in determining their accuracy.

Chapter 2 discusses the way in which the eigensystem is affected by small changes in the elements of the matrix. This leads to a chapter on error analysis of the type that the author has especially pioneered. In Chapter 4 the earlier material is applied to the problem of solving linear algebraic equations and some consideration is given to the various numerical methods that are available.

In Chapter 5 the author describes techniques for solving the eigenvalue problem for Hermitian matrices. This is one of the most important chapters in the book. In Chapter 6 the author passes to the more difficult problem of computing the eigensystem of a general matrix and deals in particular with its reduction to condensed (Hessenberg) form. He then

goes on to describe how eigenvalues and eigenvectors of the condensed matrix can be obtained. The two final chapters deal with the LR and QR algorithms and with iterative methods.

No review would give an adequate impression of this book if it did not emphasize its massive character. Most of the chapters are around 70 pages in length and the whole book runs to about 650 pages. The chapters start with the briefest of statements as to their scope and are packed with detailed information. The book is designed for the professional numerical analyst with research interests in the field, and in no way caters for the less specialized worker who would like to obtain an understanding of the problems at a less detailed level. However, an exception must be made in the case of the first chapter, which will undoubtedly be of real use to many people who will not make much of the rest of the book. In spite of all the detail, the author nowhere goes off into realms of purely mathematical interest; as anyone who knows him would expect, he keeps in sight throughout the ultimate objective of practical computation on a digital computer. The book is without doubt an important addition to the specialized literature on numerical analysis.

M. V. WILKES