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The role of orthogonal polynomials in numerical ordinary differential equations

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Abstract

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Orthogonal polynomials have many applications to numerical ordinary differential equations. Some of these, especially those connected with the quadrature formulae on which many differential equation methods are based, are to be expected. On the other hand, there are many surprising applications, quite unlike traditional uses of orthogonal polynomials. This paper surveys many of these applications, especially those related to accuracy and implementability of Runge–Kutta methods.

Keywords: Orthogonal polynomials; ordinary differential equations; Legendre polynomials; Jacobi polynomials; Laguerre polynomials; Chebyshev polynomials; Runge–Kutta methods; Gaussian quadrature; Radau quadrature; Lobatto quadrature; stiff problems; implementation costs.

1. Introduction

It is not surprising that orthogonal polynomials have a place in numerical ordinary differential equations. This is not only because orthogonal polynomials have an all-pervasive role in applied mathematics generally, but also because differential equation solutions are closely related to quadratures where the particular significance of orthogonal polynomials is well known. What is surprising, however, is that various classical orthogonal polynomial systems have a particular place because of special properties not directly related to orthogonality.

In this review we will concentrate our attention on the choice of abscissae in the construction of implicit Runge–Kutta methods. The choice of the zeros of shifted Legendre polynomials leads to methods with optimal order of accuracy. However, various other choices, all related to the zeros of particular orthogonal polynomial sequences, have some interesting properties and some specific computational advantages.

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In Section 2 we will establish a notation for the polynomial sequences that we will consider in this survey. Much of the notation is standard but, because some polynomials are written in different ways by different authors, we are specifying some terminology of our own, but only for the purposes of this paper.

In Section 3 we will discuss implicit Runge–Kutta methods based on shifted Legendre polynomials and on some closely related Jacobi polynomials. These Runge–Kutta methods have excellent stability but do have some shortcomings in practical computation because of their implementation costs when used for the solution of stiff problems.

In Section 4 differential equation methods based on the zeros of Laguerre and generalized Laguerre polynomials are discussed. These methods seem to be credible competitors to standard linear multistep methods because they have acceptable stability, relatively low implementation costs and some other desirable properties.

The use of Chebyshev polynomials in the selection of abscissae for implicit Runge–Kutta methods is discussed in Section 5 and, finally, in Section 6, a number of miscellaneous applications of orthogonal polynomials in this subject are briefly introduced.

2. Some orthogonal polynomial sequences

Let I be an interval on the real line and let w denote a "weight function" on I. Under certain conditions, it is possible to define a sequence of polynomials $p_0, p_1, p_2, \ldots$ of degrees $0, 1, 2, \ldots$ such that they are orthogonal in the sense that $\int_I p_i(x)p_j(x)w(x)\,dx = 0$ if $i \neq j$. In all the examples discussed in this section, $I = [0, 1]$ or $I = [0, \infty)$. Note that the formula given for $T_n^*(x)$ applies only when $n > 0$ and that $T_0^*(x) = 1$.

Table 1

I	$w(x)$	Name	Symbol	Formula
[0,1]	1	Shifted Legendre	$P_n^*(x)$	$\sum_{i=0}^{n}(-1)^{n-i}\binom{n+i}{i}\binom{n}{i}x^i$
[0,1]	x	Jacobi I	$G_n^{(1)}(x)$	$\sum_{i=0}^{n}(-1)^{n-i}\binom{n+i+1}{i+1}\binom{n}{i}x^i$
[0,1]	$1-x$	Jacobi II	$G_n^{(2)}(x)$	$\sum_{i=0}^{n}(-1)^{n-i}\binom{n+i+1}{i}\binom{n}{i}x^i$
[0,1]	$x(1-x)$	Jacobi III	$G_n^{(3)}(x)$	$\sum_{i=0}^{n}(-1)^{n-i}\binom{n+i+2}{i}\binom{n+1}{i+1}x^i$
[0,1]	$(x-x^2)^{-1/2}$	Shifted Chebyshev (1st kind)	$T_n^*(x)$	$\sum_{i=0}^{n}(-1)^{n-i}\frac{n}{n+i}\binom{n+i}{2i}(4x)^i$
[0,1]	$(x-x^2)^{1/2}$	Shifted Chebyshev (2nd kind)	$U_n^*(x)$	$\sum_{i=0}^{n}(-1)^{n-i}\binom{n+i+1}{2i+1}(4x)^i$
$[0,\infty)$	$\exp(-x)$	Laguerre	$L_n(x)$	$\sum_{i=0}^{n}\frac{1}{i!}\binom{n}{i}(-x)^i$
$[0,\infty)$	$\exp(-x)$	Generalized Laguerre	$L_n^{(1)}(x)$	$\sum_{i=0}^{n}\frac{1}{i!}\binom{n+1}{i+1}(-x)^i$

The polynomials that we need to consider are displayed in Table 1.

Note that the names Jacobi I, II and III, together with the symbols used here for these polynomials, are not standard and $L_n^{(1)}(x)$ is only one of a family of generalized Laguerre polynomials. The names and symbols for the remaining polynomials given in the table are standard (see, for example, [1]).

Although we refer the reader to standard results on orthogonal polynomials, it is convenient to introduce in Theorem 2.1 below the famous Christoffel–Darboux formula. The proof of this makes use of the well-known three-term recurrence relation

$$p_n(x) = \frac{\gamma_n}{\epsilon_n}\left(x - \frac{\delta_{n-1}}{\gamma_{n-1}}\right)p_{n-1}(x) - \frac{\gamma_n \epsilon_{n-1}}{\epsilon_n \gamma_{n-2}}p_{n-2}(x), \tag{2.1}$$

where

$$\gamma_n = \int_I p_n(x)^2 w(x)\,\mathrm{d}x, \qquad \delta_n = \int_I x p_n(x)^2 w(x)\,\mathrm{d}x,$$

$$\epsilon_n = \int_I x p_n(x) p_{n-1}(x) w(x)\,\mathrm{d}x.$$

The identity (2.1) holds for $n = 1, 2, \ldots$ where the convention is used that $p_{-1} = 0$.

Theorem 2.1. *Let $p_0, p_1, p_2, \ldots$ be an orthogonal polynomial sequence. Then for $n = 1, 2, 3, \ldots$ and real x and y,*

$$\frac{\epsilon_n}{\gamma_n \gamma_{n-1}}\left(p_n(x)p_{n-1}(y) - p_n(y)p_{n-1}(x)\right) = (x-y)\sum_{k=0}^{n-1}\frac{p_k(x)p_k(y)}{\gamma_k}. \tag{2.2}$$

Proof. Let $p_0(x) = c_0$, $p_1(x) = c_1 x + d$ so that

$$\epsilon_1 = \int_I x p_1(x) p_0(x) w(x)\,\mathrm{d}x$$

$$= \frac{c_0}{c_1}\int_I p_1(x)^2 w(x)\,\mathrm{d}x - \frac{d}{c_1}\int_I p_1(x)p_0(x)w(x)\,\mathrm{d}x = \frac{c_0}{c_1}\gamma_1.$$

To prove (2.2) for $n = 1$, we evaluate the left-hand side as

$$\frac{\epsilon_1}{\gamma_1\gamma_0}\left((c_1x + d)c_0 - (c_1y + d)c_0\right) = \frac{c_0^2}{\gamma_0}(x-y) = (x-y)\frac{p_0(x)p_0(y)}{\gamma_0}.$$

For $n > 1$, (2.2) is proved by induction. It must be shown that

$$\frac{\epsilon_n}{\gamma_n\gamma_{n-1}}\left(p_n(x)p_{n-1}(y) - p_n(y)p_{n-1}(x)\right)$$

$$- \frac{\epsilon_{n-1}}{\gamma_{n-1}\gamma_{n-2}}\left(p_{n-1}(x)p_{n-2}(y) - p_{n-1}(y)p_{n-2}(x)\right) = (x-y)\frac{p_{n-1}(x)p_{n-1}(y)}{\gamma_{n-1}},$$

and this is easily proved by substituting for $p_n(x)$ and $p_n(y)$ from (2.1). □

Because the zeros of p_n are real and distinct, it is possible to form a real matrix using the values of $p_0, p_1, \ldots, p_{n-1}$ evaluated at these zeros. We now show how to form a useful orthogonal matrix using a modified form of this generalized Vandermonde matrix.

Theorem 2.2. *Let Q denote the $n \times n$ matrix with elements given by*

$$q_{ij} = \sqrt{\frac{\gamma_n \gamma_{n-1}}{\gamma_{i-1} \epsilon_n p_n'(x_j) p_{n-1}(x_j)}}\, p_{i-1}(x_j),$$

where $x_1, x_2, \ldots, x_n$ are the zeros of p_n. Then Q is an orthogonal matrix; that is, $Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I$.

Proof. Let ξ and η be two distinct zeros of p_n. The result is equivalent to

$$\sum_{k=0}^{n-1} \frac{p_k(\xi) p_k(\eta)}{\gamma_k} = 0 \tag{2.3}$$

and

$$\sum_{k=0}^{n-1} \frac{p_k(\xi)^2}{\gamma_k} = \frac{\epsilon_n p_n'(\xi) p_{n-1}(\xi)}{\gamma_n \gamma_{n-1}}. \tag{2.4}$$

To prove (2.3), substitute $x = \xi$, $y = \eta$ in (2.2) and note that the left-hand side is zero. To prove (2.4), substitute $y = \xi$ and divide both sides of (2.2) by $x - \xi$. Evaluate the limit as $x \to \xi$ using l'Hôpital's rule. □

3. Runge–Kutta methods based on Jacobi polynomials

Consider the s-stage Runge–Kutta method with tableau

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathrm{T}} \end{array}$$

where

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1s} \\ a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & & \vdots \\ a_{s1} & a_{s2} & \cdots & a_{ss} \end{bmatrix}, \quad c = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_s \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_s \end{bmatrix}.$$

It is known that if $c_1, c_2, \ldots, c_s$ are chosen as the distinct zeros of P_n^*, then it is possible to choose the elements of A and of b^{T} in such a way that the resulting method has order $2s$. Since such a method would include, as a special case, the Gaussian quadrature formula

$$\int_0^1 \phi(t)\, \mathrm{d}t \approx \sum_{i=1}^{s} b_i \phi(c_i),$$

it is clear how the elements of b^{T} must be chosen. It is also known that the elements in each row of A must also be chosen as weights for order s quadrature formulas with the same

abscissae but with different intervals of integration:

$$\int_0^{c_i} \phi(t)\,\mathrm{d}t \approx \sum_{j=1}^{s} a_{ij}\phi(c_j).$$

That the order for these methods is as stated is shown, for example, in [5].

In a similar way, it is possible to construct methods whose abscissae are given by $c_1 = 0$ and $c_{i+1} = \xi_i$, where ξ_i, for $i = 1, 2, \ldots, s-1$, are the zeros of $G_{s-1}^{(1)}$. These are known as Radau IA [8] methods if the a_{ij} matrix is chosen in a suitable way. Further to these, Radau IIA [8] and Lobatto IIIC [6] methods exist related to Jacobi II and Jacobi III polynomials.

Because of the high orders of accuracy of these methods, and in particular when applied to the standard linear test problem

$$y' = qy,$$

with $z = hq$, it is possible to show that the rational function associated with the stability of the method,

$$R(z) = 1 + zb^{\mathrm{T}}(I - zA)^{-1}e,$$

where $e = [1, 1, \ldots, 1]^{\mathrm{T}}$, satisfies the approximation property

$$R(z) = \exp(z) + \mathrm{O}(z^{2s+1-d}),$$

where $d = 0$ in the Gauss case, $d = 1$ in the Radau IA and IIA cases and $d = 2$ in the Lobatto IIIC case. Furthermore, the degrees in $R(z)$ are $s - d$ for the numerators and s for the denominators.

From this it follows that each of these $R(z)$ functions is identical with the corresponding entry in the Padé table of rational approximations to $\exp(z)$ and are thus known to correspond to A-stable, and in the cases that $d > 0$, L-stable Runge–Kutta methods.

Some examples of Gauss, Radau IA, Radau IIA and Lobatto IIIC methods are given in the following table. In each case, s is the number of stages, p is the order and $R(z)$ is the stability function.

Gauss method, $s = 1$, $p = 2$, $R(z) = (1 + \frac{1}{2}z)/(1 - \frac{1}{2}z)$

$\frac{1}{2}$	$\frac{1}{2}$
	1

Gauss method, $s = 2$, $p = 4$, $R(z) = (1 + \frac{1}{2}z + \frac{1}{12}z^2)/(1 - \frac{1}{2}z + \frac{1}{12}z^2)$

$\frac{1}{2} - \frac{1}{6}\sqrt{3}$	$\frac{1}{4}$	$\frac{1}{4} - \frac{1}{6}\sqrt{3}$
$\frac{1}{2} + \frac{1}{6}\sqrt{3}$	$\frac{1}{4} + \frac{1}{6}\sqrt{3}$	$\frac{1}{4}$
	$\frac{1}{2}$	$\frac{1}{2}$

Gauss method, $s = 3$, $p = 6$, $R(z) = (1 + \frac{1}{2}z + \frac{1}{10}z^2 + \frac{1}{120}z^3)/(1 - \frac{1}{2}z + \frac{1}{10}z^2 - \frac{1}{120}z^3)$

$\frac{1}{2} - \frac{1}{10}\sqrt{15}$	$\frac{5}{36}$	$\frac{2}{9} - \frac{1}{15}\sqrt{15}$	$\frac{5}{36} - \frac{1}{30}\sqrt{15}$
$\frac{1}{2}$	$\frac{5}{36} + \frac{1}{24}\sqrt{15}$	$\frac{2}{9}$	$\frac{5}{36} - \frac{1}{24}\sqrt{15}$
$\frac{1}{2} + \frac{1}{10}\sqrt{15}$	$\frac{5}{36} + \frac{1}{30}\sqrt{15}$	$\frac{2}{9} + \frac{1}{15}\sqrt{15}$	$\frac{5}{36}$
	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

Radau IA method, $s = 2$, $p = 3$, $R(z) = (1 + \frac{1}{3}z)/(1 - \frac{2}{3}z + \frac{1}{6}z^2)$

$$\begin{array}{c|cc} 0 & \frac{1}{4} & -\frac{1}{4} \\ \frac{2}{3} & \frac{1}{4} & \frac{5}{12} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

Radau IA method, $s = 3$, $p = 5$, $R(z) = (1 + \frac{2}{5}z + \frac{1}{20}z^2)/(1 - \frac{3}{5}z + \frac{3}{20}z^2 - \frac{1}{60}z^3)$

$$\begin{array}{c|ccc} 0 & \frac{1}{9} & -\frac{1}{18} - \frac{1}{18}\sqrt{6} & -\frac{1}{18} + \frac{1}{18}\sqrt{6} \\ \frac{3}{5} - \frac{1}{10}\sqrt{6} & \frac{1}{9} & \frac{11}{45} + \frac{7}{360}\sqrt{6} & \frac{11}{45} - \frac{43}{360}\sqrt{6} \\ \frac{3}{5} + \frac{1}{10}\sqrt{6} & \frac{1}{9} & \frac{11}{45} + \frac{43}{360}\sqrt{6} & \frac{11}{45} - \frac{7}{360}\sqrt{6} \\ \hline & \frac{1}{9} & \frac{4}{9} + \frac{1}{36}\sqrt{6} & \frac{4}{9} - \frac{1}{36}\sqrt{6} \end{array}$$

Radau IIA method, $s = 2$, $p = 3$, $R(z) = (1 + \frac{1}{3}z)/(1 - \frac{2}{3}z + \frac{1}{6}z^2)$

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

Radau IIA method, $s = 3$, $p = 5$, $R(z) = (1 + \frac{2}{5}z + \frac{1}{20}z^2)/(1 - \frac{3}{5}z + \frac{3}{20}z^2 - \frac{1}{60}z^3)$

$$\begin{array}{c|ccc} \frac{2}{5} - \frac{1}{10}\sqrt{6} & \frac{11}{45} - \frac{7}{360}\sqrt{6} & \frac{37}{225} - \frac{169}{1800}\sqrt{6} & -\frac{2}{225} + \frac{1}{75}\sqrt{6} \\ \frac{2}{5} + \frac{1}{10}\sqrt{6} & \frac{37}{225} + \frac{169}{1800}\sqrt{6} & \frac{11}{45} + \frac{7}{360}\sqrt{6} & -\frac{2}{225} - \frac{1}{75}\sqrt{6} \\ 1 & \frac{4}{9} - \frac{1}{36}\sqrt{6} & \frac{4}{9} + \frac{1}{36}\sqrt{6} & \frac{1}{9} \\ \hline & \frac{4}{9} - \frac{1}{36}\sqrt{6} & \frac{4}{9} + \frac{1}{36}\sqrt{6} & \frac{1}{9} \end{array}$$

Lobatto IIIC method, $s = 2$, $p = 2$, $R(z) = 1/(1 - z + \frac{1}{2}z^2)$

$$\begin{array}{c|cc} 0 & \frac{1}{2} & -\frac{1}{2} \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Lobatto IIIC method, $s = 3$, $p = 4$, $R(z) = (1 + \frac{1}{4}z)/(1 - \frac{3}{4}z + \frac{1}{4}z^2 - \frac{1}{24}z^3)$

$$\begin{array}{c|ccc} 0 & \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{6} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

Because it is possible to attain such highly stable and high-order methods using methods based on shifted Legendre and the three types of Jacobi polynomials we have discussed here, it would seem that they would be ideal in practical applications to stiff problems. That this is not the case is a consequence of the excessive cost of implementing them.

To solve the algebraic equation arising in a single step of an implicit s-stage method applied to an N-dimensional problem, an iterative method is normally used based on some variant of the Newton–Raphson procedure. Because for many problems arising in practice, the Jacobian associated with the differential system is slowly varying, it is appropriate to avoid, as much as possible, the evaluation of this Jacobian matrix and the refactorization of matrices depending on it which are used in the modified Newton iterations. Even if it is possible to reduce the number of times these factorizations are carried out, the task when it arises may be considerable, since it involves a number of arithmetic operations equal to something like $\frac{2}{3}s^3N^3$. Furthermore, the cost of the back-substitutions required in each iteration of the Newton method is that of approximately $2s^2N^2$ arithmetical operations.

It was shown in [3] that these costs may be lowered considerably if the spectral structure of the A matrix is taken into account. Furthermore, if A has a one-point spectrum, the costs are cut down to approximately $\frac{2}{3}N^3$ for the factorizations and $2sN^2$ for the back-substitutions.

We will discuss methods of this type in the next section.

4. Runge–Kutta methods based on Laguerre polynomials

Let

$$p(z) = z^s - \alpha_1 z^{s-1} + \alpha_2 z^{s-2} - \cdots + (-1)^s \alpha_s \tag{4.1}$$

denote the polynomial with zeros equal to $c_1, c_2, \ldots, c_s$ and let

$$q(z) = z^s - \beta_1 z^{s-1} + \beta_2 z^{s-2} - \cdots + (-1)^s \beta_s \tag{4.2}$$

denote the characteristic polynomial of the A matrix of an implicit Runge–Kutta method. We will assume that the method in question has stage order equal to s. This means that

$$\sum_{j=1}^{s} a_{ij}\phi(c_j) = \int_0^{c_i} \phi(x)\,\mathrm{d}x,$$

for any polynomial ϕ of degree less than s. Substitute in turn $\phi(x) = 1, x, x^2, \ldots, x^{s-1}$, and we find that

$$Ac^{i-1} = \frac{1}{i}c^i, \tag{4.3}$$

for $i = 1, 2, \ldots, s$, where c^i denotes a component-by-component power. From (4.3) it follows that

$$A^i e = \frac{1}{i!}c^i, \quad i = 1, 2, \ldots, s. \tag{4.4}$$

Because $q(A) = 0$, it follows that

$$A^s e - \beta_1 A^{s-1} e + \beta_2 A^{s-2} e - \cdots + (-1)^s \beta_s e = 0,$$

and from (4.4) that

$$\frac{1}{s!}c^s - \frac{\beta_1}{(s-1)!}c^{s-1} + \frac{\beta_2}{(s-2)!}c^{s-2} - \cdots + (-1)^s \beta_s e = 0.$$

Thus, under the assumptions that have been made, the components of c satisfy the equation

$$\frac{1}{s!}z^s - \frac{\beta_1}{(s-1)!}z^{s-1} + \frac{\beta_2}{(s-2)!}z^{s-2} - \cdots + (-1)^s\beta_s = 0. \tag{4.5}$$

Comparing (4.5) with (4.1), we see that the coefficients α_i and β_i are related by

$$\alpha_i = \frac{s!}{(s-i)!}\beta_i. \tag{4.6}$$

Since there is an implementation cost advantage in all the zeros of the characteristic polynomial of A being equal (to λ say), we consider the case that

$$\beta_i = \binom{s}{i}\lambda^i, \quad i = 1, 2, \ldots, s.$$

From (4.6), it follows that

$$\alpha_i = \frac{s!}{(s-i)!}\binom{s}{i}\lambda^i, \quad i = 1, 2, \ldots, s, \tag{4.7}$$

so that, for $i = 1, 2, \ldots, s$, c_i is a zero of

$$L_s\left(\frac{z}{\lambda}\right) = 0.$$

It has been discussed in a number of papers [2,4] how this choice leads to a method which can be implemented cheaply. In this survey, we discuss the main ideas of this approach and explain how the matrix Q of Theorem 2.2 plays a role in the analysis of these methods.

For convenience, write $H = \lambda h$ and write the formulas for the Runge–Kutta method computation in terms of H rather than h. This means that the stage values $Y_1, Y_2, \ldots, Y_s$ in the first step of a method for which the initial values are given by $y(x_0) = y_0$ are approximations to $y(x_0 + hc_i) = y(x_0 + H\xi_i)$ for $i = 1, 2, \ldots, s$. If the A matrix is similarly scaled so that its spectrum is the one-point set 1, then it is known that

$$T^{-1}AT = \bar{A} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix},$$

where

$$T = \begin{bmatrix} L_0(\xi_1) & L_1(\xi_1) & L_2(\xi_1) & \cdots & L_{s-1}(\xi_1) \\ L_0(\xi_2) & L_1(\xi_2) & L_2(\xi_2) & \cdots & L_{s-1}(\xi_2) \\ L_0(\xi_3) & L_1(\xi_3) & L_2(\xi_3) & \cdots & L_{s-1}(\xi_3) \\ \vdots & \vdots & \vdots & & \vdots \\ L_0(\xi_s) & L_1(\xi_s) & L_2(\xi_s) & \cdots & L_{s-1}(\xi_s) \end{bmatrix},$$

and that the various quantities occurring in the computation may be transformed to corresponding quantities in which $\bar{A}$ takes the place of A in the transformed version of the implicit

algebraic equations for the Runge–Kutta method. In particular, if W denotes the vector made up of the s subvectors of Newton updates for the various stages and $\overline{W}$ is the vector of transformed updates, then

$$\overline{W} = (T^{-1} \otimes I)W.$$

Since the cost of the transformations is given approximately by $2s^2N$ (additions and multiplications), negligible for large N, the cost of the whole problem of carrying out modified Newton updates is effectively reduced from $2s^2N^2$ to $2sN^2$. Furthermore, the cost of carrying out the LU factorizations, in preparation for later iterations, is reduced from $\frac{2}{3}s^3N^3$ to $\frac{2}{3}N^3$.

Because of Theorem 2.2, it is a simple matter to write down the elements of T^{-1} in terms of the values of the elements of T itself. It is also possible, through the use of appropriate norms, to evaluate a measure of the size of $\overline{W}$ which transforms to a corresponding measure of the size of W. This further consequence of the orthogonal nature of Q in Theorem 2.2 enables convenient convergence testing to be performed during the iterations in the evaluation of the stage values of these methods.

It has been pointed out that many implicit Runge–Kutta methods, specifically those with order equal to at least s and stage order equal exactly to s, can be interpreted as collocation methods [14]. This applies, for example, to the Gauss and Radau IIA methods discussed in the previous section, and to the methods we are discussing in this section, as long as it is agreed to compute the final result for the step using the interpolational quadrature formula based on the given abscissae. One consequence of the collocation nature of singly-implicit methods based on Laguerre zeros is that the collocation polynomial is given explicitly and can be used for interpolation and extrapolation purposes. In particular, the final output from a step is given by the value of this polynomial at some appropriate point.

Because such a choice leads to methods with strong stability at infinity, it is desirable to choose the output point to correspond to one of the stage values. If such a choice is made, there may be a hope of achieving an L-stable method. The stability functions which arise in this way are exactly those for which Wolfbrandt investigated possible stable behaviour [13] and it is known that A-stability (and hence L-stability) arises for orders up to 8 (but with order 7 missing). Amongst other important contributions to the study of these approximations and to stability questions related to them is [11].

Because it is always possible to base collocation methods on nonconfluent choices of abscissae, the use of the zeros of various orthogonal polynomials naturally arises. The consequences of selecting Chebyshev polynomials is considered in the next setion.

5. Methods based on Chebyshev polynomials

In addition to their orthogonality properties, Chebyshev polynomials have some special optimality properties. In particular, we have the following four theorems. The first two are well known and no proof is given here. Theorems 5.3 and 5.4 are less known and outline proofs are given for these.

Theorem 5.1. *Let p be a polynomial of degree s such that $|p(x)| \leqslant 1$ for all $x \in [0, 1]$; then the coefficient of x^s is no more than 2^{2s-1} and equals this value only if $p = T_s^*$.*

Theorem 5.2. *Let p be a polynomial of degree s such that $\int_0^1 |\, p(x)|\,\mathrm{d}x \leqslant 1$; then the coefficient of x^s is no more than 2^{2s} and equals this value only if $p = U_s^*$.*

Theorem 5.3. *Let $c_1, c_2, \ldots, c_s$ denote a set of s real numbers in the interval $[0, 1]$ and let t be some real number not in this interval. Let $l_i(t)$, $i = 1, 2, \ldots, s$, denote the Lagrange interpolation basis polynomials for computing $\phi(t)$ as a linear combination of $\phi(c_1), \phi(c_2), \ldots, \phi(c_s)$. Then the value of $\sum_{i=1}^s |l_i(t)|$ is minimized when $c_1 = 0$, $c_s = 1$ and $c_2, c_3, \ldots, c_{s-1}$ are the zeros of U_{s-2}^*.*

Proof. Without loss of generality, assume that $t > 1$. The sum in equations is bounded by the magnitude of the interpolational polynomial through data points of the form (c_i, y_i), where $|y_i| \leqslant 1$. Thus optimality is achieved when the values of c_i are at the extrema of the interpolational polynomial. By Theorem 5.1, this polynomial is T_{s-1}^* and it is easy to verify that its extrema in the interval $[0, 1]$ occur at 0, 1 and at the zeros of U_{s-2}^*. □

Theorem 5.4. *Let $c_1, c_2, \ldots, c_s$ denote a set of s real numbers in the interval $[0, 1]$ and let t be some real number such that $t > 1$. Let w_i, $i = 1, 2, \ldots, s$, denote the weights in the interpolational quadrature formula*

$$\int_1^t \phi(x)\,\mathrm{d}x = \sum_{i=1}^s w_i \phi(c_i).$$

Then the value of $\sum_{i=1}^s |w_i|$ is minimized when $c_1 = 0$, $c_s = 1$ and $c_2, c_3, \ldots, c_{s-1}$ are the zeros of U_{s-2}^*.

Proof. Because the result in Theorem 5.3 is independent of the choice of t and because $l_i(u)$ does not change sign for $u > 1$, the same optimum will occur for the sum of the magnitudes of the integrals $\int_1^t l_i(u)\,\mathrm{d}u$. □

The applications of these results to the construction of Runge–Kutta methods lie in the desirability of a number of criteria for numerical behaviour. The first of these criteria is the obtaining of uniformly low truncation errors for interpolated results found within the step. If a suitable adjustment is made from a local error estimate for the completed step, it is possible, by using the zeros of T_s^* as abscissae, to achieve this.

The second application we consider is the design of Runge–Kutta methods which permit accurate extrapolation of the results computed in one step to obtain starting values for the iteration of the stage values in the following step. This extrapolation may be carried out in one of two ways. The first is the taking of a linear combination of the stage values, and in this case the Lagrange interpolation formula would be used. The second is the taking of a linear combination of the derivative values at the stages. This involves a quadrature formula for each of the stages in the succeeding step. If our aim is to minimize the sum of the magnitudes of the Lagrange coefficients in the first option and the sum of the magnitudes of the quadrature weights in the second option, the result in each is the same. In fact from Theorems 5.3 and 5.4, the lowest values of the sums in question are obtained when the abscissae are placed at 0, 1 and at the zeros of U_{s-2}^*.

6. Miscellaneous applications

In addition to the construction of implicit Runge–Kutta methods, orthogonal polynomials have found their ways into the literature of numerical ordinary differential equations in several surprising ways.

In the proof of the "First Dahlquist Barrier" [7], which limits the possible order of stable linear multistep methods to $k+1$ if k is odd and to $k+2$ if k is even, orthogonal polynomials with respect to the weight function

$$w(x) = \frac{1}{\pi^2 + \left(\ln\left(\frac{1+x}{1-x}\right)\right)^2}$$

on the interval $[-1, 1]$ arise. This approach to the proof of this fundamental result leads directly also to a proof that order $2k$ would always be possible if stability were not a constraint.

A second application arises in the study of algebraically stable Runge–Kutta methods, where the W-transformation is used. This makes use of orthogonality with respect to a finite sum, rather than with respect to a continuous weight function and is used in investigations of the relationship between order, stability and implementability [9,10].

Finally, in the construction of explicit Runge–Kutta methods intended for the solution of mildly stiff problems, it is possible to extend the stability region so as to include a large interval of the negative real axis by limiting the order to $p < s$. If, for example, $p = 1$, then a stability function equal to $T_s^*(1 + z/(2s^2))$ is possible. In this case the stability interval is $[-2s^2, 0]$. Although the result is more complicated for $p = 2$, an interval $[-0.814\,s^2, 0]$ is found numerically in this case. It is remarkable that a good approximation to this optimal result, given [12] by a stability function

$$1 + \frac{z}{z-2}\left(T_s^*\left(\frac{1}{2}\left(\cos\frac{\pi}{s} + 1\right) - \tfrac{1}{4}z\left(\cos\frac{\pi}{s} - 1\right)\right) - 1\right),$$

yields an interval approximately equal to $[-0.810\,s^2, 0]$.

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