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SOME STABILITY RESULTS FOR EXPLICIT RUNGE-KUTTA METHODS

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Abstract.

The theory of positive real functions is used to provide bounds for the largest possible disk to be inscribed in the stability region of an explicit Runge-Kutta method. In particular, we show that the closed disk $|\zeta + r| \leq r$ can be contained in the stability region of an explicit m-stage Runge-Kutta method of order two if and only if $r \leq m - 1$.

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1. Introduction.

It is well known that an explicit m-stage Runga-Kutta method applied to the linear test equation, $y' = \lambda y$, $\lambda \in \mathbf{C}$, results in a recursion formula of the form $y_{n+1} = P(\lambda h) y_n$ where $P(\zeta)$ is a polynomial of degree m and h is the step size. The region of absolute stability S_P for such a method is given by

$$S_P = \{\zeta \in \mathbf{C} : |P(\zeta)| \leq 1\}.$$

When designing a Runge-Kutta method one will usually have some freedom in choosing the coefficients of the method. One might wish to utilize this freedom to optimize S_P in some sense. It is impossible to find an optimization criterion that would be appropriate in general, since the desired shape of the stability region will depend on the problem at hand. In this paper we consider the largest disk centered at $(-r, 0)$ with radius r that can be contained in the stability region of the method. In doing this, we compromise between stretching the stability region in the real and in the imaginary direction, and in addition the problem is relatively simple to analyze.

This idea was introduced by Jeltsch and Nevanlinna [4]. They proved that the closed disk $|\zeta + r| \leq r$ can be contained in the stability region of a consistent m-stage explicit Runge-Kutta method if and only if $r \leq m$. This largest disk is obtained only if the stability polynomial is given by

$$P(\zeta) = (1 + \zeta/m)^m. \tag{1}$$

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As pointed out in [5], this can be viewed as a simple consequence of Bernstein's inequality [1, p. 91] in conjunction with the following result of [5]: $S_P \not\subset S_Q$ whenever $P \neq Q$ and the two corresponding methods have the same number of stages.

The above result is clearly of great theoretical value. But it does not provide much information for the most commonly used Runge-Kutta methods, since (1) can only be the stability polynomial of an m-stage first order method. Thus it would be of interest to know the corresponding result under the additional requirement that the method be of order $p > 1$.

The aim of this paper is to seek this optimal disk for general p. We shall see how the proof of [4] can be modified to cover the case $p = 2$. We also intend to illustrate to what extent the technique of [4] is applicable in the general case. This approach leads to a study of polynomials closely related to the generalized Bessel polynomials yielding upper bounds for the optimal radii. For some special cases we provide numerical values for the optimal radii and for the corresponding stability polynomial.

In order to put the problem into a precise setting, let $\mathscr{P}_{m,p}$ be the class of polynomials

$$P(\zeta) = \sum_{n=0}^{m} \alpha_n \frac{\zeta^n}{n!} \qquad (2)$$

where $\alpha_0 = \alpha_1 = \ldots = \alpha_p = 1$, and $1 \leq p < m$ (obviously, the stability polynomials of m-stage explicit Runge-Kutta methods of order p constitute a subclass of $\mathscr{P}_{m,p}$, possibly empty due to the order barriers. Introducing the disk $D_r = \{\zeta \in \mathbf{C} : |\zeta + r| \leq r\}$, we may define

$$\rho = \rho(\mathrm{m}, \mathrm{p}) = \sup_{P \in \mathscr{P}_{m,p}} \{r : D_r \subset S_P\}$$

which is our main object of interest.

We close this introduction by making the reader aware of an interesting connection between this paper and a work of Kraaijevanger [6]. One could make a comparison with the various bounds for the *optimal threshold-factor* $R_{m,p}$ in [6] since some of these are quite similar to our results and since obviously $R_{m,p} \leq \rho(m,p)$.

2. Preliminary results.

As in [4] we shall make use of the theory of positive real functions. For details on this subject in general, we recommend the survey by Dahlquist [2]. We define $\mathbf{C}^-$ and $\mathbf{C}^+$ as the open left and right half-planes, respectively. Next we remind the reader that $f(z)$ is a positive function if it is analytic in $\mathbf{C}^+$ and maps $\mathbf{C}^+$ into $\mathbf{C}^+$. If such a function is real-valued for real z, we say that it is a positive real function. The following well-known facts [2] about positive real functions will be needed.

LEMMA 1. *If $f(z) = r(z)/s(z)$ is a positive real rational function, all coefficients of r and s have the same sign.*

LEMMA 2. *If $g(z) = f(z) - az$ is regular at ∞, then $f(z)$ is positive or an imaginary constant if and only if $a \geq 0$ and $g(z)$ is positive or an imaginary constant.*

LEMMA 3. *A rational function $f(z) = r(z)/s(z)$ where r and s are relatively prime and at least one of them is not a constant is positive if and only if $r + s$ has all its roots in $\mathbf{C}^-$ and $Re(f(iy)) \geq 0$ for all y such that $s(iy) \neq 0$.*

Following [4] we introduce the transformation $\zeta = -2r/(1 + z)$ mapping $\overline{\mathbf{C}^+}$ one-to-one onto D_r. If $D_r \subset S_P$ then

$$f(z) = \left[1 + P\left(\frac{-2r}{1+z}\right)\right] \Big/ \left[1 - P\left(\frac{-2r}{1+z}\right)\right]$$

is a positive real function. Defining

$$q(z) = \sum_{n=0}^{m-1} \beta_n z^n = -\sum_{i=1}^{m} \frac{\alpha_i}{i!}(-2r)^i(1+z)^{m-i} \tag{3}$$

we may write

$$f(z) = \frac{2(1+z)^m - q(z)}{q(z)} \tag{4}$$

3. Some stability theorems.

We start by deducing a general upper bound for ρ. To this end we define the polynomial

$$H_{m,p}(r) = \binom{m}{m-p} - (-1)^p \sum_{n=0}^{p} \frac{(-2r)^n}{n!} \binom{m-n}{m-p}.$$

Then Lemma 1 immediately yields

PROPOSITION 4. *$\rho \leq r_0(m,p)$ where $r_0(m,p)$ is the unique positive root of $H_{m,p}$.*

PROOF. These polynomials are discussed in some detail in the appendix of [7], to which we refer for a proof of the existence and uniqueness of positive roots. The inequality follows from Lemma 1 applied to (4) by observing that for odd p, $H_{m,p}(r)$ equals $2\binom{m}{m-p} - \beta_{m-p}$ and that for even p it equals β_{m-p}. ■

The polynomials of Proposition 4 are closely related to the generalized Bessel polynomials, see [3]. By making use of this connection one may prove the following general localization result. Again we refer to [7] for details.

THEOREM 5. *We have* $m - p + 1 \leq r_0(m,p) \leq m - (1 + (-1)^p)/2$.
As $m \to \infty$ *we have* $m - p + 1 - r_0(m,p) = O(m^{-1})$.

As already mentioned it is known from [4] that the bound of Proposition 4 is sharp for $p = 1$. We shall now prove that this is also so for $p = 2$ and that the corresponding optimal polynomial is unique. One may notice that in this case the question of uniqueness cannot be settled by using the previously quoted result from [5].

THEOREM 6. *Let* $P \in \mathscr{P}_{m,2}$. *Then* $D_{m-1} \subset S_P$ *if and only if*

$$P(\zeta) = \frac{m-1}{m}\left(1 + \frac{\zeta}{m-1}\right)^m + \frac{1}{m}.$$

REMARK. It has been pointed out to us that part of this result was proved by Miss Rueckstadt-Pakmor in [8].[1])

In the proof of this theorem we shall need the following lemma.

LEMMA 7. *Let*

$$f(z) = \frac{2(1+z)^m - q(z)}{q(z)} \quad \textit{where} \quad q(z) = \sum_{n=0}^{m-1} \beta_n z^n$$

and $0 < \beta_{m-1} \leq 2m, \quad \beta_{m-2} = 0$.
Then $f(z)$ *is a positive real function if and only if*

$$q(z) = \frac{\beta_{m-1}}{2m}((1+z)^m - (-1)^m(1-z)^m).$$

PROOF. Assume that $f(z)$ is a positive real function. Then, as in the proof of the lemma in [4], we deduce that $q(z)$ is an even (odd) polynomial with nonnegative coefficients if $m - 1$ is even (odd). We next make use of Lemma 3. Since $q(z)$ is either even or odd with nonnegative coefficients, -1 is not a root of $q(z)$, thus $(1+z)^m - q(z)$ and $q(z)$ are relatively prime. The roots of $(1+z)^m$ are definitely in $\mathbf{C}^-$, hence it remains to be checked when $\mathrm{Re}(f(iy)) \geq 0$. *If* $m - 1$ is even, then

$$\mathrm{Re}(f(iy)) = \frac{(1+iy)^m + (1-iy)^m - q(iy)}{q(iy)}.$$

We observe that the roots of $(1+iy)^m + (1-iy)^m$ are real and distinct since $\dfrac{1+iy}{1-iy}$ is a one-to-one transformation of $\mathbf{R} \cup \{\infty\}$ onto the unit circle. Thus $q(iy)$

[1]) Added in proof: Recently the authors have proved the existence of a unique optimal polynomial for all $P_{m,p}$, a result that will appear elsewhere.

must vanish at each of these roots and we conclude that

$$q(z) = \frac{\beta_{m-1}}{2m}((1 + z)^m + (1 - z)^m).$$

The argument is completely analogous when $m - 1$ is odd.

The $f(z)$ thus constructed is clearly a positive real function, and the proof is finished. ■

PROOF TH. 6. We observe that $D_{m-1} \subset S_P$ if $P(\zeta) = \frac{m-1}{m}\left(1 + \frac{\zeta}{m-1}\right)^m + \frac{1}{m}$. We next assume that $D_{m-1} \subset S_P$ and proceed as above, that is we find that

$$f(z) = \frac{2(1 + z)^m - q(z)}{q(z)}$$

must be a positive real function with $q(z)$ given by (3). From this we see that $\beta_{m-1} = 2(m - 1)$ and $\beta_{m-2} = 0$. By Lemma 7 we thus have $q(z) = \frac{m-1}{m}((1 + z)^m - (z - 1)^m)$. By using (3) and the transformation $\zeta = -2(m - 1)/(1 + z)$ we arrive at the desired result. ■

For $p > 2$ the bounds of Proposition 4 will not be sharp. This is illustrated by considering th simplest case $p = 3$ and $m = 4$. Then if $\beta_1 = 8$ (corresponding to the bound of Proposition 4), $f(z) = 2z/\beta_3 + g(z)$ where

$$g(z) = \frac{(8 - \beta_3 - 2\beta_2/\beta_3)z^3 + (12 - \beta_2 - 2\beta_1/\beta_3)z^2 - 2\beta_0 z/\beta_3 + 2 - \beta_0}{\beta_3 z^3 + \beta_2 z^2 + \beta_1 z + \beta_0}.$$

By Lemma 1 we must have $\beta_0 = 0$ for f to be positive real. But then it turns out that the numerator of g has zeros in $\mathbf{C}^+$, which is impossible if f is to be positive.

We are thus left with the problem of how to estimate ρ for $p > 2$. A naturally related question is that of the sharpness of the bound of Proposition 4. Do we have $\rho - (m - p + 1) \to 0$ as $m \to \infty$? The numerical experiments of the next section may be in agreement with an affirmative answer to this question, but they are of course too few to indicate much. The complexity of such computations increases rapidly with $m - p$, making it difficult to use them as a guideline for further investigations. From these experiments it may however be suggested that the bound of Proposition 4 is "reasonably" good.

So far we have not been able to provide answers to the above questions, which should be interesting issues for future research.

4. Numerical results.

For some special (m, p)-pairs we have computed the bounds $r_0(m, p)$. In addition we have used some routines from the NAG-library to seek for the optimal radii and

Table 1: *Numerical results for some selected values of m and p.*

p	m	$r_0(m,p)$	$\rho(m,p)$	α_{p+1}	α_{p+2}
3	4	2.19	2.07	0.5698	
3	5	3.15	2.94	0.7374	0.2771
4	5	2.34	2.22	0.5806	
4	6	3.30	3.06	0.7707	0.3053
5	6	2.53	2.37	0.6083	
5	7	3.47	3.17	0.7956	0.3305
6	7	2.71	2.55	0.6185	

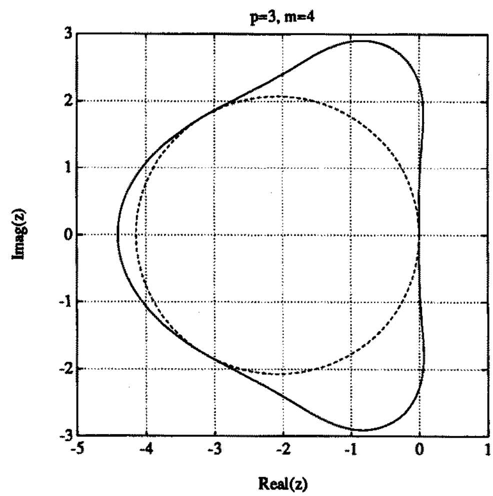

Fig. 1: The stability region and the largest inscribed disk for $p = 3, m = 4$.

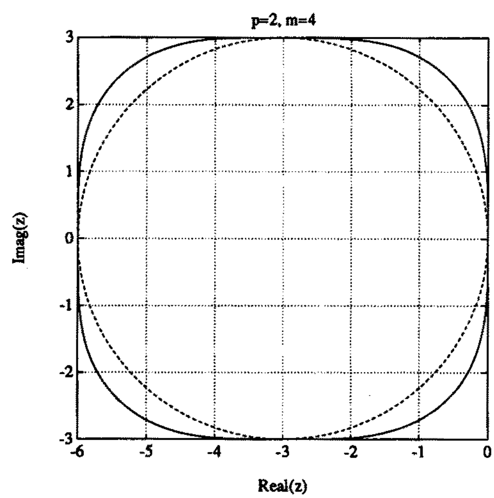

Fig. 2: The stability region and the largest inscribed disk for $p = 2, m = 4$.

the corresponding polynomials. These tests were run on a CRAY XMP-28. Some of the results are presented in the table below, and we have plotted the stability region with the corresponding largest disk for two examples.

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