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SOME ASPECTS OF THE BOUNDARY LOCUS METHOD

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Abstract.

The boundary locus method for determining the stability region of a linear multistep method is considered from several viewpoints. In particular we show how it is related to the order of the method. These ideas are extended to Runge–Kutta and other methods.

1. Introduction.

Consider the linear k-step method for the numerical integration of ordinary differential equations

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \tag{1.1}$$

where α_j, β_j are real, $j=0,\ldots,k$, and $\alpha_k \neq 0$, $|\alpha_0|+|\beta_0|>0$. Assume that its characteristic polynomials $\varrho(r)$, $\sigma(r)$ have no common factor, and denote by $\pi(r,\bar{h}) = \varrho(r)-\bar{h}\sigma(r)$ the stability polynomial, The absolute stability set $\mathscr{R}$ of the method consists of all complex numbers $\bar{h}$ for which all roots r_s, $s=1,2,\ldots,k$, of $\pi(r,\bar{h})=0$ lie in U, the open unit disk (see [8], p. 82).

A widely used method for determining $\mathscr{R}$ is the "boundary locus method", (see e.g. [8], p. 82), which can be described as follows. If $\bar{h} \in \partial\mathscr{R}$ (the boundary of $\mathscr{R}$), then by continuity at least one of the roots r_s must lie on the unit circle ∂U, and so there exists a $\theta \in [-\pi,\pi]$ such that $\varrho(e^{i\theta})-\bar{h}\sigma(e^{i\theta})=0$. Introduce the function $q(r) =\varrho(r)/\sigma(r)$ and plot on the complex plane the parameter curve $\gamma(\theta)=q(e^{i\theta})$, $\theta \in [-\pi,\pi]$; then it follows that $\bar{h}$ lies in the image set $\Gamma=\gamma([-\pi,\pi])$ and so $\partial\mathscr{R}$ is contained in Γ. Thus $\mathscr{R}$ consists of one or more of the connected domains in which Γ divides the plane. The problem of deciding which of the various domains form $\mathscr{R}$ is solved by studying the roots r_s at appropriate spot values $\bar{h}$. In some cases an expansion of the functions $r_s=r_s(\bar{h})$ is helpful.

In this paper we shall look at several aspects of the boundary locus method, from a geometrical point of view. In section 2 we develop an alternative approach and show its relevance for some theoretical purposes. In section 3 the relationship between the locus $\gamma(\theta)$ and the order of the corresponding method is studied. These ideas are extended in section 4 to cover Runge–Kutta and other methods.

Reference [7] studies the local behaviour of $\partial\mathscr{R}$ near $\bar{h}=0$, and reference [13] shows a beautiful geometrical relationship between stability and order.

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2. Use of the argument principle.

Assume first that no zero of σ lies on ∂U. If $\bar{h} \notin \Gamma$, the rational function $q(r)-\bar{h}$ has no zero and no pole on ∂U and a straightforward application of the argument principle (see for instance [4], 9.17.12) yields

$$n(\gamma-\bar{h},0) = N(\bar{h})-Z \tag{2.1}$$

where $n(\gamma-\bar{h},0)$ is the index of the cycle $\gamma(\theta)-\bar{h}$, $\theta \in [-\pi,\pi]$, with respect to the origin; $N(\bar{h})$ and Z the number of zeros and poles of $q(r)-\bar{h}=0$ in U. Now by translation $n(\gamma-\bar{h},0)=n(\gamma,\bar{h})$, the index of γ with respect to $\bar{h}$. Clearly $N(\bar{h})$ is the number of roots r_s in U and Z is the number of zeros of σ in U. Hence we have

THEOREM 2.1. *Assume that no zero of σ lies on the unit circle and let $\bar{h} \notin \Gamma$. Then the number of roots of the stability polynomial $\pi(r,\bar{h})$ having modulus less than one, equals the index of γ with respect to $\bar{h}$ plus the number of zeros of σ in the unit disk.*

In particular $\mathscr{R}$ will consist of the points $\bar{h} \notin \Gamma$ such that

$$n(\gamma,\bar{h}) = k-Z\,. \tag{2.2}$$

When σ vanishes on ∂U, the curve γ passes through infinity and a result analogous to Theorem 2.1 can be proved by introducing a Möbius transformation T in such a way that $T(\gamma(\theta))$ remains finite for $\theta \in [-\pi,\pi]$.

The boundary locus method, either combined with (2.2) or not, can be of theoretical interest in several instances. As an example we provide a proof of a result of Liniger [9].

THEOREM 2.2 (Liniger). *Assume*

i) *All zeros of σ lie in the open unit disk,*
ii) $\beta_k \neq 0$,
iii) $\operatorname{Re} q(e^{i\theta}) \geqq 0$, $\theta \in [-\pi,\pi]$.

Then the method is A-stable.

PROOF. By iii) $\eta(\gamma,\bar{h})=0$ for $\operatorname{Re}\bar{h}<0$. By i) and ii) $Z=k$ and then (2.2) shows that $\mathscr{R}$ contains the left half plane. ∎

In the same way we have (cf. Nørsett [10]).

THEOREM 2.3. *Assume that conditions* i) *and* ii) *in theorem* 2.2 *hold and* iii) *becomes* $|\operatorname{Im} q(e^{i\theta})|+\tan(\alpha)\ \operatorname{Re} q(e^{i\theta}) \geqq 0$, $\theta \in [-\pi,\pi]$. *Then the method is $A(\alpha)$-stable.*

3. Boundary locus and order.

The derivatives of the mapping γ are related to the order of the method. Namely

THEOREM 3.1. *Assume* $\sigma(1) \neq 0$. *Then*

i) *All derivatives* $\gamma^{(2n)}(0)$ *are purely real, and all derivatives* $\gamma^{(2n-1)}(0)$ *are purely imaginary*; $n=1,2,\ldots$.

ii) *The method is consistent if and only if* $\gamma(0)=0$, $\gamma'(0)=i$.

iii) *If the method is consistent, it has exact order p if and only if* $\gamma''(0)=0,\ldots,\gamma^{(p)}(0)=0$, $\gamma^{(p+1)}(0)\neq 0$.

PROOF. By definition $\gamma(\theta)=\varrho(e^{i\theta})/\sigma(e^{i\theta})$. Clearly for $-\pi \leqq \theta \leqq \pi$ $\operatorname{Re}\gamma(\theta)=\operatorname{Re}\gamma(-\theta)$, $\operatorname{Im}\gamma(\theta)=-\operatorname{Im}\gamma(-\theta)$ and i) follows. It is easily checked that $\gamma(0)=0$, $\gamma'(0)=i$ are a reformulation of the consistency conditions $\varrho(1)=0$, $\sigma(1)=\varrho'(1)$. To prove iii) consider any function $\varphi(r)$, analytic in the neighbourhood of 1, with Taylor series

$$\varphi(r) = \sum_{n=0}^{\infty} a_n (r-1)^n . \tag{3.1}$$

Then $\hat{\varphi}(\theta)=\varphi(e^{i\theta})$ is an analytic function of θ in the neighbourhood of the origin and will have an expansion

$$\varphi(e^{i\theta}) = \sum_{n=0}^{\infty} c_n \theta^n . \tag{3.2}$$

Substitution of the exponential series in (3.1) and comparison with (3.2) gives

$$c_1 = ia_1$$

$$c_k = i^k a_k + \Gamma_{k-1}(a_1,\ldots,a_{k-1}), \qquad k=2,3,\ldots$$

where Γ_{k-1} are functions of the stated arguments. These relations show recursively that the values $a_k=\varphi^{(k)}(1)/k!$ determine the coefficients $c_k=\hat{\varphi}^{(k)}(0)/k!$, $j=1,2,\ldots$ in a one-to-one way. Therefore the functions $i\theta=\log e^{i\theta}$ and $\gamma(\theta)=q(e^{i\theta})$ will have the same first, second, ... pth derivatives at $\theta=0$ if and only if the first p derivatives at $r=1$ of the functions $\log r$, $q(r)$ are the same, i.e. if the order is at least p ([6] p. 225). (Here $\log r$ denotes the principal branch of the logarithm.) ∎

In particular any consistent linear multistep method whose function $\gamma(\theta)$ exhibits nonzero curvature in $\theta=0$ is first order.

The conditions iii) of the theorem imply a pth order contact at the origin between $\gamma(\theta)$ and the imaginary axis, but are not to be confused with the necessary and sufficient conditions for such a contact to exist, these being independent of the particular parameterization of the curve. For instance the trapezoidal rule, for which the graph Γ of $\gamma(\theta)$ is precisely the imaginary axis, is only second order.

More generally consider a consistent method for which Γ is contained in the imaginary axis, (for example a symmetric method [8] p. 84). All derivatives

$\gamma^{(2n)}(0)$, $n=1,2,\ldots$ are real by i) in the theorem, and consequently must vanish. Then iii) shows that such a method has *even order*. On the other hand, according to the boundary locus method the absolute stability region must be either void or the left half plane. It is well known ([3]) that the order for an A-stable method cannot exceed 2, and therefore must be 2. We have

THEOREM 3.2. *A consistent linear multistep method having the left half plane as absolute stability region has order two.*

PROOF. According to the previous analysis it suffices to prove that $\gamma(\theta)$ is purely imaginary, $-\pi \leqq \theta \leqq \pi$. Now $\partial\mathcal{R}$ is the imaginary axis and since $\partial\mathcal{R}$ is contained in Γ, $\operatorname{Re}\gamma(\theta)=0$ for a continuum set of θ values. Let T be a Möbius transformation mapping the real axis onto the unit circle. Then $q(T(z))$ is a rational function taking purely imaginary values for a continuum set of real values of z and hence for every real value of z, other than a pole (see [1], theorem 8, page 190). Therefore $\operatorname{Re}\gamma(\theta)=0$ for all θ. ∎

4. Extension to other methods.

For Runge–Kutta and other classes of one-step methods, the absolute stability region $\mathcal{R}$ is defined to consist of those $\bar{h}$ yielding $|r_1|<1$, where $r_1=Q(\bar{h})$ is a rational function associated with the method and approximating the exponential $\exp(\bar{h})$. We say that $Q(\bar{h})$ is an approximation of order p, if there exists a constant $C \neq 0$ such that

$$\exp(\bar{h})-Q(\bar{h}) = C\bar{h}^{p+1}+O(\bar{h}^{p+2}), \quad \text{for } \bar{h} \to 0 . \tag{4.1}$$

Furthermore we call an approximation consistent if its order is at least one. Note that p in (4.1) is not in general the order of the method; see for instance [2], where it is shown that certain implicit Runge–Kutta methods of order less than four give rise to the (2,2) Padé approximation to $\exp(\bar{h})$. We have

THEOREM 4.1. *Consider a consistent approximation $Q(\bar{h})$ as above. Then in the neighbourhood of $\bar{h}=0$, the boundary $\partial\mathcal{R}$ can be expressed as a parametric curve $\gamma(\theta)$, where θ is the argument $-\pi<\theta<\pi$ of $Q(\bar{h})$. Furthermore $Q(\bar{h})$ is an approximation of order p if and only if $\gamma(0)=0$, $\gamma'(0)=i$, $\gamma''(0)=0,\ldots,\gamma^{(p)}(0)=0$, $\gamma^{(p+1)}(0)\neq 0$.*

PROOF. Since $Q(0)=1$, $Q'(0)\neq 0$ there exist neighbourhoods V of $\bar{h}=0$, W of $r_1=1$ such that $Q(\bar{h})$ is a one-to-one analytic mapping of V onto W and has an analytic inverse $\bar{h}=Q^{-1}(r_1)$. It follows that $\partial\mathcal{R}\cap V$ will be mapped in a one-to-one way onto $\partial U \cap W$ and hence $\gamma(\theta)=Q^{-1}(e^{i\theta})$ will provide the necessary parameterization for θ small enough. On the other hand $Q(\bar{h})$ and $\exp(\bar{h})$ share precisely p derivatives at the origin iff the same happens to the inverse functions

$Q^{-1}(r_1)$, $\log r_1$ at $r_1 = 1$. The proof is concluded by considering the compositions $\gamma(\theta)$, $\log e^{i\theta} = i\theta$ as in Theorem 3.1. ∎

The ideas leading to Theorem 3.2 can also be applied to the present situation, provided that $Q(\bar{h})$ has real coefficients, to yield

THEOREM 4.2. *A consistent approximation to the exponential having the left half plane as absolute stability region has even order.*

Theorems 3.1 and 4.1 explain why for a high order method we should expect the boundary $\partial\mathscr{R}$ not to differ appreciably from the imaginary axis near the origin. This phenomenon has been observed in the past and led to the introduction of numerical A-acceptability (Nørsett [1]). We refer to Siemieniuch [12] for an analytical study of it in some particular cases. Note, however, that theorem 3.1 refers to Γ rather than $\partial\mathscr{R}$.

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REFERENCES

1. L. V. Ahlfors, *Complex Analysis*, McGraw–Hill (1953).
2. J. C. Butcher, *A class of implicit methods for ordinary differential equations*, Proceedings of the Dundee Conference on Numerical Analysis (Lecture Notes in Mathematics 506) Springer-Verlag (1975), 28–37.
3. G. Dahlquist, *A special stability problem for linear multistep methods*, BIT 3 (1963), 27–43.
4. J. Dieudonné, *Foundations of Modern Analysis*, Academic Press (1960).
5. A. Goetz, *Introduction to Differential Geometry*, Addison–Wesley (1970).
6. P. K. Henrici, *Discrete Variable Methods in Ordinary Differential Equations*, Wiley (1962).
7. R. Jeltsch, *A necessary condition for A-stability of multistep multiderivative methods*, Math. Comp. 30 (1976), 739–746.
8. J. D. Lambert, *Computational Methods in Ordinary Differential Equations*, Wiley (1973).
9. W. Liniger, *A criterion for A-stability of linear multistep integration formulae*, Computing 3 (1968), 280–285.
10. S. P. Nørsett, *A criterion for $A(\alpha)$-stability of linear multistep methods*, BIT 9 (1969), 259–263.
11. S. P. Nørsett, *One-step methods of Hermite type for numerical integration of stiff systems*, BIT 14 (1974), 63–77.
12. J. L. Siemieniuch, *Properties of certain rational approximations to e^{-z}*, BIT 16 (1976), 172–191.
13. G. Wanner, E. Hairer and S. P. Nørsett, *Order stars and stability theorems*, BIT 18 (1978), 475–489.

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