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NEWTON'S METHOD AND GAUSS-KRONROD QUADRATURE*

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1. Introduction

One of us, jointly with CALIÒ and MARCHETTI (1986), considered the application of Newton's method (for large nonlinear systems of equations) in the context of computing Gauss-Kronrod quadrature rules. With the equations set up in an appropriate manner, it was found that, by careful choice of initial approximations and continued monitoring of the iteration process, the method could be made to work for rules with up to 81 nodes (40 Gauss and 41 Kronrod nodes). This was documented for the Legendre weight on $[-1,1]$ (where in fact formulae with up to 161 nodes were computed) and for weight functions on $[0,1]$ involving logarithmic and algebraic singularities. Further evidence of the feasibility of Newton's method, also for Kronrod extension of Gauss-Radau and Gauss-Lobatto formulae, is contained in NOTARIS's thesis (1988). If one attempts, however, to repeat Kronrod extension in the manner of PATTERSON (1968), one discovers that Newton's method quickly deteriorates and

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eventually fails to converge. The purpose of this note is to shed some light on the reasons for this failure of Newton's method. One of these is the excessive magnitude of the inverse Jacobian of the nonlinear system (evaluated at the solution) which comes about because of a peculiar behavior of a certain polynomial responsible for the magnitude of this inverse. Graphical evidence is provided to underscore the phenomenon.

For simplicity we consider only integrals over a finite interval (standardized by $[-1,1]$) with constant weight function.

2. Extension of quadrature rules

Given an N-point quadrature rule $Q_N(f)$ of the form

$$Q_N(f) = \sum_{\nu=1}^{N} \omega_\nu f(\tau_\nu), \quad -1 < \tau_N < \tau_{N-1} < \cdots < \tau_1 < 1, \tag{2.1}$$

approximating the integral $I(f)$,

$$Q_N(f) \approx I(f) = \int_{-1}^{1} f(t)dt, \tag{2.2}$$

we call *Kronrod extension* of Q_N, in notation

$$Q_N(f) \subset Q_{N'}(f), \tag{2.3}$$

the quadrature rule $Q_{N'}(f)$ with $N' = N + (N+1) = 2N + 1$ nodes, N of which being the given

nodes τ_ν in (2.1) and the additional $N+1$ (the "Kronrod nodes") and all $2N+1$ weights being determined to achieve maximum algebraic degree of exactness for $Q_{N'}(f)$. Hopefully, the $N+1$ Kronrod nodes are all real and fit nicely into the $N+1$ spaces between the nodes τ_ν and between the extreme nodes τ_1, τ_N and the corresponding endpoints 1, -1 of the interval of integration. Unfortunately, however, this is not guaranteed in general. Letting

$$\pi_N(t) = \prod_{\nu=1}^{N} (t - \tau_\nu) \tag{2.4}$$

denote the (given) node polynomial, it is known that the Kronrod nodes must be the zeros of the (monic) polynomial π^*_{N+1} of degree $N+1$ (if it exists) satisfying the orthogonality property

$$\int_{-1}^{1} \pi^*_{N+1}(t) p(t) \pi_N(t) dt = 0 , \quad \text{all} \quad p \in \mathbf{P}_N . \tag{2.5}$$

Since this is orthogonality with respect to a sign-changing "weight function", π_N, the usual properties of classical orthogonal polynomials can no longer be expected to hold. Even the existence of π^*_{N+1} is in doubt, unless the Hankel matrix $H_{N+1}(\pi_N dt) = \left[\int_{-1}^{1} t^{i+k} \pi_N(t) dt \right]_{i,k=0}^{N}$ is known to be nonsingular.

By *repeated Kronrod extension* we mean a sequence of Kronrod extensions (all assumed to exist),

$$Q_{N_0}(f) \subset Q_{N_1}(f) \subset Q_{N_2}(f) \subset \cdots , \tag{2.6}$$

where

$$N_0 = n , \quad N_k = 2N_{k-1} + 1 , \quad k = 1, 2, 3, \ldots . \tag{2.7}$$

Example 2.1: Gauss-Kronrod formula [KRONROD (1964)].

This is the Kronrod extension

$$Q_n(f) \subset Q_{2n+1}(f) \tag{2.8}$$

of the n-point Gauss formula $Q_n(f)$. It has all the desirable properties – interlacing of nodes [SZEGÖ (1935)] and positivity of weights [MONEGATO (1978)] – for each $n = 1, 2, 3, \ldots$.

Example 2.2: Gauss-Kronrod-Patterson formulae.

These are the repeated Kronrod extensions (2.6), (2.7) for $n = 3$ and $Q_3(f)$ the 3-point Gauss formula,

$$Q_3(f) \subset Q_7(f) \subset Q_{15}(f) \subset Q_{31}(f) \subset \cdots \quad . \tag{2.9}$$

The chain of quadrature rules has been computed numerically by PATTERSON (1968), (1973) through $Q_{255}(f)$. Remarkably, both the interlacing and positivity properties appear to hold for each extension, although no proof of this has ever been given.

3. Extension by Newton's method

Traditionally, the Kronrod extension (2.3) is computed by first obtaining π^*_{N+1} in (2.5), for example by expansion in Legendre or Chebyshev polynomials, then applying a rootfinding procedure to compute the zeros of π^*_{N+1} and finally (if the zeros are all real) computing the weights of the Kronrod extension as those of an interpolatory quadrature rule. The first two

steps can be combined into one by using eigenvalue techniques [see, e.g., ELHAY and KAUTSKY (1984), FREY, and WALDVOGEL and FREY].

Here we try to obtain all quantities of interest at once, by applying Newton's method to an appropriate system of nonlinear equations. If we write (2.3) as

$$Q_N(f) \subset Q_{2N+1}(f) = \sum_{\nu=1}^{N} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{N+1} \sigma_\mu^* f(\tau_\mu^*) , \tag{3.1}$$

where the τ_ν are prescribed and σ_ν, σ_μ^*, τ_μ^* are unknowns, the system of equations is taken to be

$$Q_{2N+1}(p_k) = m_k, \quad k = 0, 1, 2, \ldots, 3N+1 , \tag{3.2}$$

where p_k is the normalized Legendre polynomial of degree k and $m_k = \int_{-1}^{1} p_k(t)dt = \sqrt{2}\ \delta_{k,0}$ with $\delta_{0,0} = 1$, $\delta_{k,0} = 0$ for $k > 0$. Letting $x^T = [\sigma_1, \ldots, \sigma_N;\ \sigma_1^*, \ldots, \sigma_{N+1}^*;\ \tau_1^*, \ldots, \tau_{N+1}^*] \in \mathbf{R}^{3N+2}$ denote the vector of unknowns, we write (3.2) in the form

$$g(x) = 0 , \quad g: \mathbb{R}^{3N+2} \to \mathbf{R}^{3N+2} , \tag{3.3}$$

where g has as kth component $Q_{2N+1}(p_k) - m_k$, $k = 0, 1, \ldots, 3N+1$. We assume here that the extension (3.1) exists and has real nodes τ_μ^*.

Newton's method for (3.3) can then be written in the form

$$x_{i+1} = x_i - \Delta_i , \ \Delta_i = [g'(x_i)]^{-1} g(x_i) , \ i = 0, 1, 2, \ldots , \tag{3.4}$$

where $x_0 \in \mathbf{R}^{3N+2}$ is a suitable initial approximation and g' denotes the Jacobian matrix of g.

If symmetry is present, as in Examples 2.1 and 2.2, the system (3.3) can be reduced to essentially half its size, and in practice Newton's method need only be applied to this reduced system. For our qualitative study we shall ignore this simplification since Newton's method applied to the full system produces the same approximations as Newton's method applied to the reduced system, if the initial approximation of the former is the symmetric extension of that of the latter. Neither shall we concern ourselves here with other practical matters, such as the choice of initial approximations, for which we refer to CALIÒ et al. (1986).

As to convergence of Newton's method (3.4), suppose that

$$\| g''(x_0) \|_F \leq M_0 \quad \text{on} \quad U_0 = \{ x \in \mathbf{R}^{3N+2} : \| x - x_0 \| \leq 2 \| \Delta_0 \| \} , \tag{3.5}$$

where $\| g'' \|_F^2$ is the sum of the squares of all second partial derivatives of all components of g, and vector norms are Euclidean norms. A sufficient condition for convergence then is [OSTROWSKI (1966, p. 187)]

$$\theta_0 < 1 , \quad \theta_0 := 2M_0 \| \Delta_0 \| \cdot \| [g'(x_0)]^{-1} \|_F , \tag{3.6}$$

where now $\| \cdot \|_F$ denotes the Frobenius matrix norm.

If we denote by $\hat{x} \in \mathbf{R}^{3N+2}$ the exact solution of (3.3) and assume that $\hat{\sigma}_\mu^* \neq 0$, $\mu = 1, 2, \ldots, N+1$, then a straightforward adaptation of an argument in GAUTSCHI (1982, Thm. 3.1) yields

$$\| [g'(\hat{x})]^{-1} \|_F = \left\{ \int_{-1}^{1} \phi_N(t) dt \right\}^{1/2} , \tag{3.7}$$

where

$$\phi_N = \sum_{\nu=1}^{N} \alpha_\nu^2 + \sum_{\mu=1}^{N+1} \left[\beta_\mu^2 + \frac{1}{\hat{\sigma}_\mu^{*2}} \gamma_\mu^2 \right] \tag{3.8}$$

is a polynomial of degree $6N + 2$ expressed in terms of elementary Hermite interpolation polynomials α_ν, β_μ, γ_μ defined by

$$\begin{aligned} &\alpha_\nu(\hat{\tau}_\lambda) = \delta_{\nu\lambda}\,, \quad \alpha_\nu(\hat{\tau}_\mu^*) = 0\,, \quad \alpha_\nu'(\hat{\tau}_\mu^*) = 0\,; \\ &\beta_\mu(\hat{\tau}_\lambda) = 0\,, \quad \beta_\mu(\hat{\tau}_\kappa^*) = \delta_{\mu\kappa}\,, \quad \beta_\mu'(\hat{\tau}_\kappa^*) = 0\,; \\ &\gamma_\mu(\hat{\tau}_\lambda) = 0\,, \quad \gamma_\mu(\hat{\tau}_\kappa^*) = 0\,, \quad \gamma_\mu'(\hat{\tau}_\kappa^*) = \delta_{\mu\kappa}\,. \end{aligned} \tag{3.9}$$

From the definition (3.8) of ϕ_N, and (3.9), it readily follows that

$$\begin{aligned} &\phi_N(t) > 0\,, \quad \text{all } t \in \mathbf{R}\,, \\ &\phi_N(\hat{\tau}_\nu) = 1\,, \quad \nu = 1, 2, \ldots, N\,, \\ &\phi_N(\hat{\tau}_\mu^*) = 1\,, \quad \phi_N'(\hat{\tau}_\mu^*) = 0\,, \quad \mu = 1, 2, \ldots, N+1\,. \end{aligned} \tag{3.10}$$

We emphasize that (3.7) is an *equality,* not an inequality, and that it holds for *any* Kronrod extension with real distinct nodes and $\hat{\sigma}_\mu^* \neq 0$, including those that may arise as links in a chain of repeated Kronrod extensions.

4. Numerical behavior of Newton's method

Since notable differences were observed in the performance of Newton's method for one-time and repeated application of the Kronrod extension process, we carried out controlled experiments for the Gauss-Kronrod extension (2.8) and the Gauss-Kronrod-Patterson extensions (2.9) in order to (i) observe to what extent the sufficient condition of convergence (3.6) was satisfied (approximately) for various initial approximations at preassigned accuracy levels;

(ii) see how satisfaction or violation of (3.6) correlates with actual convergence or divergence of Newton's method; (iii) understand the principal factors responsible for convergence or divergence. All computations were carried out in double precision on the DEC VAX 11/780 computer (machine precision $\approx 2.78\times10^{-17}$).

Since accurate answers for the solutions $\hat{x}$ are available in the literature, it was easy to select initial approximations x_0 having preassigned accuracy, say $\|x_0 - \hat{x}\| \approx \varepsilon$. In reporting our results, we approximate M_0 in (3.5) by $\hat{M} = \|g''(\hat{x})\|_F$ and $\Gamma_0 = \|[g'(x_0)]^{-1}\|_F$ by $\hat{\Gamma} = \|[g'(\hat{x})]^{-1}\|_F$ as given in (3.7). The resulting approximation for θ_0 in (3.6) is denoted by $\hat{\theta}$; thus, $\hat{\theta} = 2\hat{M}\hat{\Gamma}\|\Delta_0\|$.

In our first experiment we applied Newton's method to compute the Gauss-Kronrod extension (2.8) for $n = 3, 7, 15, 31$, starting with initial approximations x_0 at accuracy levels $\varepsilon = 10^{-14}$, $\varepsilon = 10^{-10}$, and $\varepsilon = 10^{-6}$. In each case we computed the quantities $\|\Delta_0\|$, $\hat{M}$, $\hat{\Gamma}$, $\hat{\theta}$.

Table I. *Convergence study of Newton's method applied to* (2.8) *with* $n = 3, 7, 15, 31$

n	ε	$\|\Delta_0\|$	$\hat{M}$	$\hat{\Gamma}$	$\hat{\theta}$
3	10^{-14}	9.7(–15)	2.8(2)	1.6(0)	8.7(–12)
	10^{-10}	1.3(–10)			1.2(–7)
	10^{-6}	1.1(–6)			9.9(–4)
7	10^{-14}	2.1(–14)	2.4(3)	1.4(0)	1.4(–10)
	10^{-10}	1.7(–10)			1.1(–6)
	10^{-6}	1.8(–6)			1.2(–2)
15	10^{-14}	2.2(–14)	2.0(4)	1.4(0)	1.2(–9)
	10^{-10}	1.8(–10)			1.0(–5)
	10^{-6}	1.6(–6)			9.0(–2)
31	10^{-14}	2.1(–14)	1.6(5)	1.3(0)	8.7(–9)
	10^{-10}	1.9(–10)			7.9(–5)
	10^{-6}	2.4(–6)			1.0(0)

The results are displayed in Table I. (Integers in parentheses denote decimal exponents.) It can be seen that the sufficient condition (3.6) is amply satisfied at all accuracy levels shown, except for 6-digit initial approximation when $n = 31$, in which case it is just barely satisfied. Actually, Newton's method did in fact converge in all cases.

Our second experiment is an analogous study of the first four Gauss-Kronrod-Patterson extensions in (2.9), i.e., (3.1) with $N = 3$, 7, 15 and 31, and the nodes τ_ν on the right of (3.1) being those of the N-point Gauss-Kronrod-Patterson formula (the Gauss formula, when $N = 3$). The results obtained are shown in Table II. (The case $N = 3$ in Table II is identical with the case $n = 3$ in Table I.)

Tabel II. *Convergence study of Newton's method applied to* (2.9)

N	ε	$\|\|\Delta_0\|\|$	$\hat{M}$	$\hat{\Gamma}$	$\hat{\theta}$
3	10^{-14}	9.7(–15)	2.8(2)	1.6(0)	8.7(–12)
	10^{-10}	1.3(–10)			1.2(–7)
	10^{-6}	1.1(–6)			9.9(–4)
7	10^{-14}	1.9(–14)	2.3(3)	1.5(0)	1.3(–10)
	10^{-10}	1.6(–10)			1.1(–6)
	10^{-6}	2.1(–6)			1.4(–2)
15	10^{-14}	2.2(–14)	1.7(4)	7.9(0)	5.9(–9)
	10^{-10}	2.0(–10)			5.4(–5)
	10^{-6}	2.3(–6)			6.2(–1)
31	10^{-14}	1.4(–10)	1.3(5)	9.6(5)	3.5(+1)
	10^{-10}	2.6(–10)			6.5(+1)
	10^{-6}	9.5(–5)			2.4(+7)

What is most notable in Table II is the large jump of $\hat{\Gamma}$ going from $N = 15$ to $N = 31$. The value of $\hat{\Gamma}$ for $N = 31$ is about 10^6 times as large as the corresponding value in Table I. This leads to values of the convergence index $\hat{\theta}$ considerably larger than 1. (For $\varepsilon = 10^{-14}$, the relatively large value of $\|\|\Delta_0\|\|$, and hence the large value of $\hat{\theta}$, is in part due to double-

precision rounding effects.) It was observed that Newton's method with initial approximations at the accuracy levels ε shown converges only when $N = 3, 7$ and 15, but not for $N = 31$.

In order to appreciate and to understand the well-behaved and ill-behaved nature of $\hat{\Gamma}$ in the contexts of (2.8) and (2.9), respectively, we display in Figures 1 and 2 the polynomial ϕ_N of (3.8) [which determines $\hat{\Gamma}$ according to (3.7)] in the case (2.8) for $n = 3, 7, 15, 31$ and in the respective cases of (2.9). [For $n = 3$, the graphs are identical.] Only half of the graphs are shown, since they are symmetric with respect to the origin.

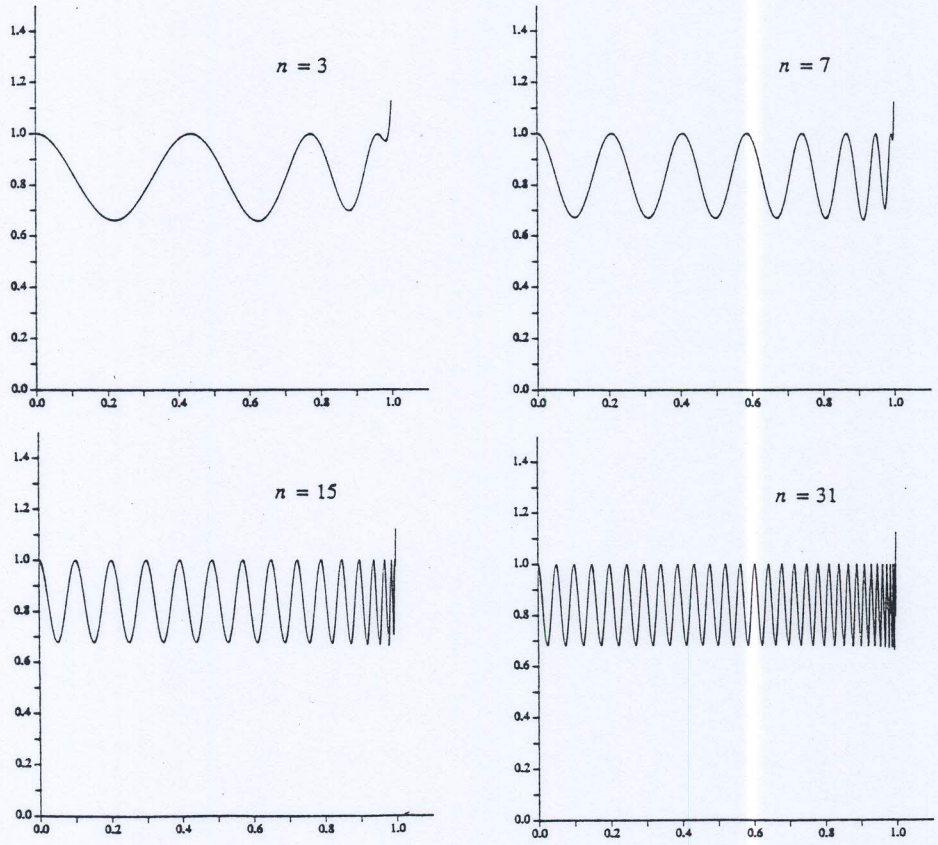

Fig. 1. *The behavior of* ϕ_N *in the case of* (2.8), $n = 3, 7, 15, 31$

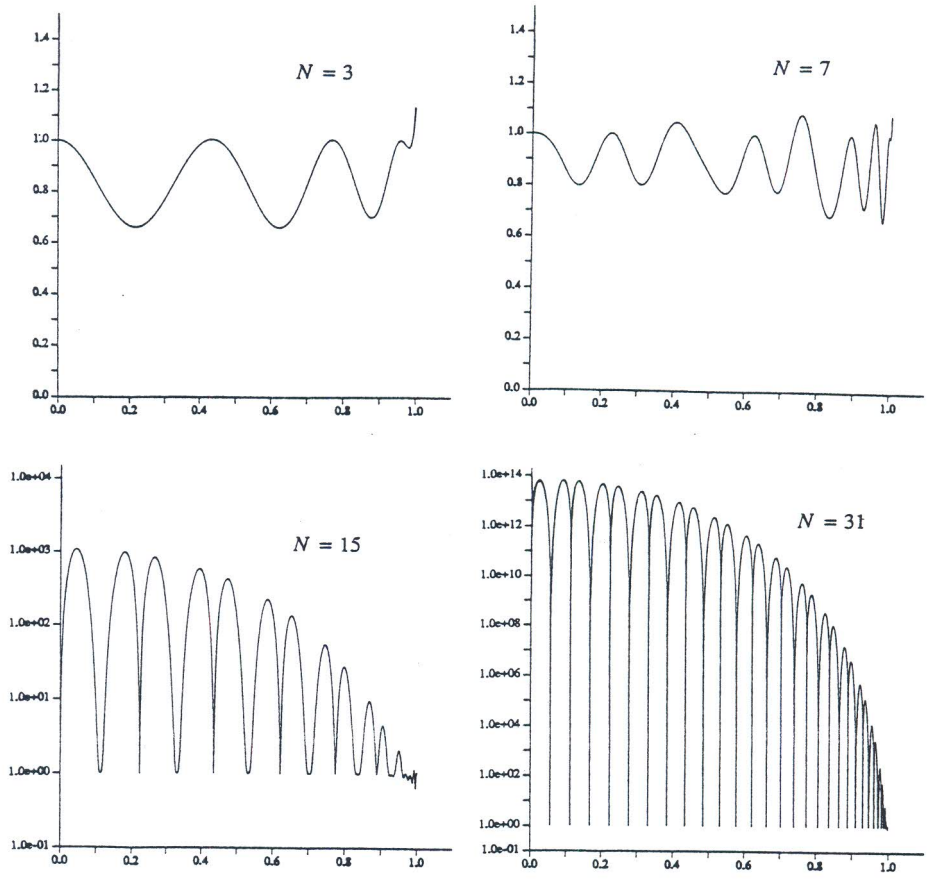

Fig. 2. *The behavior of* ϕ_N *in the first four extensions of* (2.9)

It can be seen that for one-time Kronrod extension, ϕ_N is less than 1 over most of the interval $[-1,1]$, the exceptions occurring very close to the endpoints ± 1. For repeated Kronrod extension, the story is quite different!

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