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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

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

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

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