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SCIENTIFIC NOTES

ON THE USE OF GAUSS QUADRATURE IN ADAPTIVE AUTOMATIC INTEGRATION SCHEMES

JARLE BERNTSEN* and TERJE O. ESPELID

Institutt for Informatikk, Universitetet i Bergen, Allégate 53-55, N-5000 Bergen, Norway

Abstract.

The use of Kronrod's scheme for automatic adaptive integration is well known. In this paper we introduce Gauss integration rules combined with a new way of estimating the errors as basic rules in automatic adaptive integration schemes. On the basis of very limited numerical experiments it seems that our scheme may be as efficient and reliable as the Kronrod scheme.

1. Introduction.

A well-known objection to the use of Gauss quadrature in automatic integration schemes is that in proceeding from one computation of a Gauss approximation using n points $G_n(f)$ to $G_m(f)$ with $m > n$, almost all the information obtained in computing the former value is discarded. (See Davis and Rabinowitz [1] p. 82). A partial answer to this objection is given by Kronrod [2]. Kronrod starts with an n-point Gauss rule, G_n, of polynomial degree $2n-1$, adds $n+1$ new points and arrives at a rule, K_{2n+1}, of polynomial degree $3n+1$. The Kronrod rule, K_{2n+1}, combined with G_n is well suited for adaptive integration. The value given by K_{2n+1} is taken as the approximation of the integral over each sub-interval, and the value given by G_n is used to estimate the error.

In the NAG library, [3], K_{2n+1} is used in adaptive schemes for $n = 10$ and $n = 30$. In adaptive schemes we need an integration rule together with a way to estimate the error in the computed value. In this paper we have tried to construct the integration rule and the error estimator from a new point of view. We demand full freedom in all abscissas and weights when constructing the integration rule. To get as high polynomial degree as possible using the same number of points as Kronrod, that is $2n+1$, we therefore choose the Gauss rule G_{2n+1} of polynomial degree $4n+1$ as integration rule.

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Now, if we change one of the weights in this Gauss rule, using the same abscissas, the other weights of a rule Q of polynomial degree $2n-1$ are uniquely given. The weights of this rule Q are functions of the perturbation in one of the weights in the Gauss rule. Therefore we have a one-parameter family of rules of degree $2n-1$. If one of the weights in Q is 0 the rule is an interpolatory rule, otherwise it is not. The difference $Qf-G_{2n+1}f$ may be used to estimate the error in $G_{2n+1}f$.

It is necessary to decide which member of the family Q should be used. We have found by numerical experiments that the choice which assigns zero weight to the midpoint is not unreasonable.

2. The rule of degree $2n-1$.

The abscissas in the $2n+1$ points Gauss rule, defined on $[-1,1]$, may be numbered

$$-1 < x_{-n} < x_{-n+1} < \ldots < x_{-1} < x_0 = 0 < x_1 < \ldots < x_{n-1} < x_n < 1.$$

Both Gauss abscissas and weights, w_i, $i = -n(1)n$, are symmetric, that is $x_{-i} = -x_i$ and $w_i = w_{-i}$, $i = 1(1)n$. They also satisfy

$$\text{(2.1)} \qquad \begin{cases} w_0'+2\sum_1^n w_i' = 2 \\ 2\sum_1^n w_i x_i^{2k} = 2/(2k+1), \qquad k = 1(1)n. \end{cases}$$

Define the new rule

$$Q_{2n+1}\{f\} = \sum_{-n}^{n} w_i' f(x_i), \qquad \text{with } w_i' = w_{-i}', \quad i = 1(1)n.$$

In order to be a rule of polynomial degree $2n-1$ the new weights have to satisfy

$$\text{(2.2)} \qquad \begin{cases} w_0'+2\sum_1^n w_i' = 2 \\ 2\sum_1^n w_i' x_i^{2k} = 2/(2k+1), \qquad k = 1(1)n-1. \end{cases}$$

Taking the difference between corresponding equations in (2.2) and (2.1) we get, with $\Delta w_i \equiv w_i' - w_i$,

$$\text{(2.3)} \qquad \sum_{i=1}^{n} x_i^{2k} \Delta w_i = \begin{cases} -\frac{1}{2}\Delta w_0, & k = 0 \\ 0, & k = 1(1)n-1. \end{cases}$$

Thus, given Δw_0, the changes in the other weights are uniquely defined by (2.3). Using Cramer's rule and a wellknown result of the Vandermonde determinant we may solve (2.3) to get

$$(2.4)\qquad \begin{cases} \Delta w_k \equiv c_k \Delta w_0, & k = 0(1)n. \\ c_k = (-1)^n \frac{1}{2} \prod\limits_{\substack{i=1 \\ i \neq k}}^{n} x_i^2/(x_k^2 - x_i^2), & k = 1(1)n. \end{cases}$$

Using the theory of Legendre polynomials, see Krylov [4], we get

$$(2.5)\qquad c_k = (-1)^k \frac{(2n+2)!}{2^{2n+1} n!(n+1)!} \{(1-x_k^2)w_k/2\}^{\frac{1}{2}}, \qquad k = 1(1)n.$$

(2.5) then gives us an easy way to compute the weights of Q_{2n+1} given Δw_0 and (x_k, w_k), $k = 1(1)n$.

3. Numerical experiment.

In the numerical experiment we have used an adaptive strategy due to Cranley and Patterson [5]. The subinterval with the greatest estimated error is divided into two halves until the sum of the estimated errors is less than a given error-bound.

The results produced by Kronrod's scheme are compared to the results obtained using Gauss quadrature with our way of estimating the error and $\Delta w_0 = -w_0$. As an illustration we have chosen $n = 10$ and $n = 30$ to approximate the integrals

$$\int_0^1 \frac{2}{2+\sin(\lambda \pi x)}\,dx$$

with $\lambda = 10$ and $\lambda = 70$. The requested relative error is 10^{-3}.

Integration rule	Number of function evaluations		Actual relative error	
	$\lambda = 10$	$\lambda = 70$	$\lambda = 10$	$\lambda = 70$
K_{21}	147	1197	$.26 \times 10^{-7}$	$.45 \times 10^{-4}$
G_{21}	147	1197	$.11 \times 10^{-6}$	$.34 \times 10^{-4}$
K_{61}	183	915	$.69 \times 10^{-9}$	$.24 \times 10^{-6}$
G_{61}	183	915	$.63 \times 10^{-9}$	$.15 \times 10^{-6}$

4. Conclusions.

In this paper we have presented a way of estimating the error in G_{2n+1} without adding new points that may be useful. Substantial numerical testing is, however, needed in order to reveal whether or not this new idea can be used in numerical software. The theoretical properties of the rule Q_{2n+1}, e.g. convergence, have not been examined.

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