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Stratified nested and related quadrature rules

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Abstract

The stratified nested quadrature procedure due to Laurie is discussed together with an alternative computational procedure which leads to the concept of hybrid GKP rules. In the context of the approximation of stratified nested sequences the work of Krogh and Van Snyder on the representation of the GKP rules is considered and a generalisation of this employing hybrid rules of special form is discussed. © 1999 Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

Sequences of *nested* quadrature rules are of interest in automatic integration and other areas of numerical analysis. They approximate the weighted integral

$$If = \int_a^b \Omega(x)f(x) dx,$$

by a sequence of rules S_1, S_2, \dots with the property that nodes used by S_i are a subset of those used by S_{i+1} . Generally, they have at least interpolatory degree. An example is the sequence for $\Omega(x)$ constant and the interval $[-1, 1]$ produced by the optimal extension of the Gauss 1-point rule given by Patterson [6] (referred to later as the GKP rules) with rule k having $n_k = 2^k - 1$ nodes and integrating degree $(3n_k + 1)/2$. An attraction of nested rules is that no integrand evaluations are wasted in proceeding down the sequence and the convergence (or otherwise) of the results obtained by each may be used to give an indication of their accuracy.

An interesting variation of the concept of *nested rules* has been proposed by Laurie [5] for which the term *stratified nested rules* has been coined. These stratified nested rules have the property that

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the weights associated with the nodes of a particular rule are a prescribed fraction of the weights for those same nodes in its successor. The effect of this is to greatly reduce the amount of information which must be stored to calculate the integration sequence. Of course, the nodes of stratified nested rules clearly have implicit constraints imposed upon them to achieve the relationships between the weights. In turn this implies a constraint on the maximum integrating degree achievable.

In this paper we discuss the calculation of the Laurie rules and outline an alternative computational procedure which leads to the concept of hybrid rules, viz., rules which combine the properties of Laurie and the GKP methods. In the context of approximate stratified nested sequences we consider the work of Krogh and Van Snyder [4] on the representation of the GKP rules together with a related procedure arising from judiciously formed hybrid rules. We also comment briefly on the sequence proposed by Pérez-Jordá et al. [8,9] based on a transformation of the integrand. The results of applying some of the rules to two simple basis functions are discussed.

2. Laurie's calculations

Using a moments formulation, Laurie [5] discussed an algorithm for the construction of the stratified nested rules related in the simplest case by

$$If = \int_{-1}^1 \Omega(x)f(x) dx \approx Q_k f = \theta Q_{k-1} f + \sum_{i=0}^{n_k-1} w_{i,k} f(x_{i,k}). \quad (1)$$

Briefly, the rules are computed by requiring that Q_k integrates exactly a set of basis polynomials $p_j(x)$ for $j = 0, \dots, n_k$. Using (1), this gives the equation for the moments μ_j ,

$$\sum_{i=0}^{n_k-1} w_{i,k} p_j(x_{i,k}) = I p_j - \theta Q_{k-1} p_j = \mu_j \quad \text{for } j = 0, 1, \dots, n_k$$

from which the nodes and weights can be determined.

Laurie generated a number of these rules for the interval $[-1, 1]$ with $\Omega(x)$ constant and $n_k = 2^k - 1$ and listed those using $1, 3, 7, \dots, 255$ nodes corresponding to Q_1, \dots, Q_8 for $\theta = \frac{1}{2}$. These parallel the nonstratified GKP sequence [6]. The constraints placed on the weights results in the rules having algebraic degree n_k compared to $(3n_k + 1)/2$ for the nonstratified sequence.

The choice of $\theta = \frac{1}{2}$ is appropriate in that, as for the GKP rules, the nodes are then found empirically to interlace, lie inside $[-1, 1]$ and the weights are positive. Unfortunately, this case turns out to be computationally ill-conditioned and the sequence was not taken beyond Q_8 using the 200 digit precision then available for the calculations.

We have confirmed Laurie's calculations using 500 decimal digit arithmetic and the numerical procedures given in the ORTHPOL package of Gautschi [3]. The calculations were accomplished using the excellent multiprecision arithmetic package developed by Bailey [1,2] which allows standard working FORTRAN code to be translated directly into its multiprecision counterpart with relatively little effort. Additionally, the computations have been continued successfully to obtain the 511 and 1023 node rules although these are likely to be only of theoretical interest, simply confirming their existence with the desirable properties of positive weights and interlacing nodes. We shall comment later on new high precision calculations for the GKP rules based on the Bailey package.

3. The hybrid rules

Laurie [5] has posed a number of questions concerning the stratified nested rules and in particular, speculated on the existence of an alternative and possibly better computational algorithm. In this context, we have examined another technique following the general procedures discussed in [7] which combines the ideas of stratified nested quadrature and the optimal GKP rules. We shall use the notation R_1, R_2, \dots to refer to the GKP rule sequence.

Suppose a given quadrature rule has n nodes x_1, \dots, x_n and we wish to form a new $n + m$ node rule (with $m > n$) composed from these n nodes together with an additional m nodes chosen subject to some prescribed conditions. Let $H_n(x)$ and $E_m(x)$ be polynomials whose roots are, respectively, the n original nodes and the m new nodes expressed in terms of the polynomials $\phi_j(x)$ orthogonal over $[a, b]$ with respect to $\Omega(x)$ as,

$$H_n(x) = \sum_{j=0}^n (\tau_j/h_j) \phi_j(x), \quad E_m(x) = \sum_{j=0}^m \varepsilon_j \phi_j(x). \quad (2)$$

The moments which conveniently scale the coefficients of $H_n(x)$ are defined by

$$h_j = \int_a^b \Omega(x) \phi_j^2(x) dx.$$

Let w_i and W_i , respectively, be the interpolatory weights associated with x_i in the original and extended rule. The objective is to *pre-assign* $l \leq n$ of the weights of the extended rule in such a way that

$$W_i = \theta_i w_i \quad \text{for } i = 1, \dots, l. \quad (3)$$

This is done as follows. Since $x - x_i$ is a factor of $H_n(x)$ we can construct the polynomial $S_{n-1}^{(i)}(x)$ of degree $n - 1$ defined by

$$S_{n-1}^{(i)}(x) = \frac{H_n(x)}{x - x_i} = \sum_{j=0}^{n-1} (\gamma_{i,j}/h_j) \phi_j(x). \quad (4)$$

From the Lagrangian expression for the interpolatory weights for the old and new rules, (3) becomes

$$\int_a^b \Omega(x) S_{n-1}^{(i)}(x) E_m(x) dx = \theta_i E_m(x_i) \int_a^b \Omega(x) S_{n-1}^{(i)}(x) dx \quad \text{for } i = 1, \dots, l,$$

which, using (2) and (4) together with the orthogonality properties, can be expressed as

$$\sum_{j=0}^{n-1} \gamma_{i,j} \varepsilon_j = \theta_i \gamma_{i,0} \sum_{j=0}^m \varepsilon_j \phi_j(x_i) \quad \text{for } i = 1, \dots, l. \quad (5)$$

Arbitrarily taking $\varepsilon_m = 1$, this gives l linear equations to determine $\varepsilon_0, \dots, \varepsilon_{m-1}$. An additional $m - l$ equations are of course needed to provide a unique solution. These additional equations can be obtained, while achieving the maximum possible integrating degree, by imposing the *optimal extension* conditions

$$\int_a^b \Omega(x) H_n(x) E_m(x) \phi_s(x) dx = 0 \quad \text{for } s = 0, \dots, m - l - 1.$$

Using (2), this is equivalent to the set of $m - l$ equations

$$\sum_{j=0}^m \varepsilon_j \sum_{i=|s-j|}^{s+j} \tau_i a_i^{(s,j)} = 0 \quad \text{for } s = 0, \dots, m - l - 1,$$

where

$$h_i a_i^{(s,j)} = \int_a^b \Omega(x) \phi_i(x) \phi_j(x) \phi_s(x) dx.$$

The quantity $a_i^{(s,j)} = a_i^{(j,s)}$ is simply the coefficient of $\phi_i(x)$ in the expansion of the product $\phi_s(x)\phi_j(x)$ in terms of the orthogonal basis polynomials. Once $E_m(x)$ has been calculated it is easy to form the expansion of $H_n(x)E_m(x)$ and use this as the stepping point for generating the next member of a rule sequence using the same procedure. All the quantities needed in the calculation can be obtained from algorithms given in [7].

The integrating degree of the new rule is easily shown to be at least $d = n + 2m - l - 1$ ($d + 1$ if the integral is symmetric and d is even). For example, taking the common case of $m = n + 1$ we obtain $d = 3n + 1 - l$. If $l = n$ (Laurie rules) then $d = 2n + 1$. If $l = 0$ (GKP rules) then $d = 3n + 1$. For other values of l we get a hybridization of Laurie and GKP rules with intermediate integrating degree.

As an illustration for the case with $\Omega(x)$ constant and $[a, b] = [-1, 1]$, Table 1 gives a number of hybrid extensions of the basic 7-point GKP rule R_3 to 15-points with $\theta_i = \theta = \frac{1}{2}$ for all i in (5). We have given the full GKP extension R_4 with $l = 0$ and having degree 23 followed by the hybrid rules for $l = 2, 4, 6$ and 7 of respective degree 21, 19, 17 and 15. Of course the rule with $l = 7$ corresponds to a conventional Laurie rule and assumes the form of (1).

Extensive numerical experiments on these hybrid rules have shown the same computational ill-conditioning difficulties as experienced by Laurie so presumably the condition of the matrices involved is still critical. In common with the Laurie procedure, later rules are contaminated by errors in earlier rules and this must lead ultimately to breakdown.

The concept of hybrid rules can be used to exploit an observation of Krogh and Van Snyder [4] concerning the behaviour of the weights of high-order GKP rules. This will be discussed in Section 4.1.

4. Approximate stratified nested rules

4.1. The Krogh and Van Snyder procedure

Krogh and Van Snyder [4] have observed that the GKP sequence of rules approximates a stratified nested sequence when the number of nodes becomes large. Specifically, letting $w_{i,k}$ denotes the weight associated with x_i in rule R_k then the quantity

$$\omega_{i,k} = w_{i,k} - \frac{1}{2} w_{i,k-1}$$

is found to be very small when $k \geq 7$ except for a few of nodes near the end-points of the range $[-1, 1]$. The rule can then be expressed in the standard stratified nested form (1) for $\theta = \frac{1}{2}$ with a correcting contribution from those nodes for which the value of $\omega_{i,k}$ is regarded as significant.

Table 1

Various hybrid extensions to 15-points of the basic 7-point GKP rule R_3 (degree 11) with $\theta = \frac{1}{2}$. The 7-point rule is a GKP extension of the Gauss 3-point rule. The table gives the full GKP extension ($l = 0$, degree 23) followed by the hybrid rules for $l = 2, 4, 6$ and 7 of respective degree 21, 19, 17 and 15. Note that $l = 7$ corresponds to a conventional Laurie rule. The relationships of the weights to those of the original 7-point rules are highlighted by italisation. Only the positive nodes for these symmetric rules are shown

GKP 7-point, R_3		$l = 0$ (GKP R_4)	
x_i	w_i	x_i	w_i
—	—	0.99383196	0.017001720
0.96049127	<i>0.10465623</i>	0.96049127	0.051603283
—	—	0.88845923	0.092927195
0.77459667	<i>0.26848809</i>	0.77459667	0.13441526
—	—	0.62110295	0.17151191
0.43424375	<i>0.40139741</i>	0.43424375	0.20062853
—	—	0.22338669	0.21915686
0.0	<i>0.45091654</i>	0.0	0.22551050
$l = 2$		$l = 4$	
x_i	w_i	x_i	w_i
0.99414505	0.016628953	0.99418427	0.016602634
0.96049127	<i>0.052328113</i>	0.96049127	<i>0.052328113</i>
0.88807672	0.092823086	0.88817419	0.092728602
0.77459667	0.13396873	0.77459667	<i>0.13424404</i>
0.62131682	0.17156690	0.62109763	0.17159758
0.43424375	0.20089844	0.43424375	0.20051997
0.22323635	0.21914347	0.22348686	0.21913795
0.0	0.22528462	0.0	0.22568222
$l = 6$		$l = 7$ (Laurie, Q_4)	
x_i	w_i	x_i	w_i
0.99420176	0.016592400	0.99421517	0.016585106
0.96049127	<i>0.052328113</i>	0.96049127	<i>0.052328113</i>
0.88819528	0.092726590	0.88820741	0.092728762
0.77459667	<i>0.13424404</i>	0.77459667	<i>0.13424404</i>
0.62115146	0.17153635	0.62116164	0.17153578
0.43424375	<i>0.20069871</i>	0.43424375	<i>0.20069871</i>
0.22332882	0.21916939	0.22334983	0.21915035
0.0	0.22540880	0.0	<i>0.22545827</i>

Letting $N(k, \delta)$ be the number of nodes in rule R_k for which $\omega_{i,k} \geq \delta$, Table 2 gives $N(k, \delta)$ for $\delta = 10^{-15}$ and 10^{-21} . It can be seen that only a small number of nodes need be involved in the correcting contribution. Exploiting this property allows the amount of information that must be stored to apply the sequence in an automatic integrator to be greatly reduced.

Krogh and Van Snyder [4] gave principal consideration to the cases $k = 7$ and 8 with $\delta \geq 10^{-21}$ corresponding to the highest members of the GKP sequence then available. We have included in Table 2 recently computed results for $k = 9$ and 10 which confirm empirically both the existence of these high-order rules and the continuing trend towards stratified nested form.

Table 2
Number of nodes, $N(k, \delta)$, common to R_k and R_{k-1} in the GKP sequence approximately satisfying the stratification criterion $\omega_{i,k} \geq \delta$

k	n_k	$N(k, 10^{-15})$	$N(k, 10^{-21})$
7	127	7	12
8	255	5	9
9	511	5	8
10	1023	4	7

Table 3
Order of magnitude of κ , the ratio of the absolute values of the largest to smallest coefficients in the expansion of $P_n(x)$ in powers of x

n	255	511	1023	2047
κ	10^{95}	10^{192}	10^{388}	10^{780}

These extensive calculations were completed again using the Bailey multiprecision package [1] and the algorithms given in [7]. High precision must be used to limit loss of accuracy and ensure meaningful results. Some idea of the potential for cancellation can be gauged by examining the expansion of the Legendre polynomial $P_n(x)$ in powers of x . Table 3 gives the order of magnitude, κ , of the ratios of the absolute values of the largest to smallest coefficients in the expansion for several values of n .

This gives a hint that when computing the GKP sequence through to R_{10} (1023 nodes) there is the possibility of a loss of around 388 decimal digits. As a precaution the calculations were carried out using 500 digit precision. This approach would appear to be somewhat pessimistic in that the highest monomial that should be integrated exactly by R_{10} was in fact integrated correctly to about 180 decimal digits. Wichura [10] has also confirmed the existence of R_9 (511 nodes) although the precision used is not stated. His results agree with the present calculations to the accuracy given (36 decimal digits).

4.2. Hybrid strategy

The attractiveness of the Krogh and Van Snyder approach is that the full precision of the GKP rules is preserved to the level detectable by the precision used in the calculations.

A simple alternative strategy is to employ the full power of the GKP rules up to R_6 using 63 nodes which places minimal demands on storage. The majority of “well-behaved” integrals can be calculated very efficiently by this sub-set of rules. Then, referring to the $k = 7, \delta = 10^{-21}$ entry in Table 2, we calculate the hybrid rule, R'_7 , of degree 167 with $\theta = \frac{1}{2}$ using 127 nodes based on the extension of R_6 with $l = 24$ (corresponding to the largest 12 positive and negative symmetric nodes). This guarantees that the $\omega_{i,7}$ which were $\geq 10^{-21}$ in R_7 become exactly zero in R'_7 . Of course the other weights in R_7 which were $< 10^{-21}$ will change (increase) in the new rule. In fact, the calculations show that all $\omega_{i,7}$ in R'_7 are positive and $< 10^{-12}$ and thus, to that accuracy, we have a viable stratified nested rule with minimal loss of integrating degree compared to the GKP equivalent.

In practice, we would use the rule formed from R'_7 with all interlacing weights corresponding to $l > 24$ set to obey the $\theta = \frac{1}{2}$ relationship with R_6 . This will be referred to as R''_7 . The next member of the sequence could be obtained by extending the original R'_7 to give a standard Laurie rule of degree 255. This set of rules may form an adequate core integrator for a doubly adaptive procedure with moderate demands on storage.

A more conservative approach would be to base the start of the Laurie sequence on the GKP 63-node rule R_6 . The first rule in this sequence, referred to as Q'_7 , would have degree 255.

All the rules proposed in this section have been calculated to high precision and thus can be said to exist, at least empirically. Their nodes interlace and their weights are positive.

4.3. Pérez-Jordá and San-Fabián rules

A completely different approach to approximate stratified nested rules with $\Omega(x)$ constant and $[a, b] = [-1, 1]$ has been proposed by Pérez-Jordá et al. [8,9]. The essence of their procedure is to apply the simple transformation

$$dt = \frac{16}{3\pi}(1-x^2)^{3/2} dx,$$

giving

$$\int_{-1}^1 f(t) dt = \int_{-1}^1 f(t(x))(1-x^2)\sqrt{1-x^2} dx$$

with

$$t(x) = 1 + \frac{2}{\pi} \left\{ \left(1 + \frac{2}{3}(1-x^2) \right) x\sqrt{1-x^2} - \arccos x \right\}.$$

The integration is then carried out by applying Gauss–Chebyshev quadrature of the second kind with rule Z_k using $n_k = 2^k - 1$ nodes. The interlacing property of the Gauss–Chebyshev nodes and weights allows the rules sequence to be expressed the stratified nested form

$$Z_k f = \frac{1}{2} Z_{k-1} f + \sum_{i=0}^{n_k-1} w_{2i+1,k} f(t(x_{2i+1,k})),$$

where

$$x_{i,k} = \cos\left(\frac{i\pi}{n_k+1}\right), \quad w_{i,k} = \frac{\pi}{n_k+1} \sin^4\left(\frac{i\pi}{n_k+1}\right).$$

In contrast with the Laurie and GKP rules, these rules do not have polynomial precision. However, they do integrate a constant function exactly when the number of nodes exceeds unity and so could be used in doubly adaptive applications. Simple tests suggest that these rules are inherently less powerful than either the GKP or full Laurie rules in automatic integration.

5. Calculations

Testing numerical integrators can be very subjective and generally no single rule sequence can be regarded as ideal in all respects. Rather than expose rules to a barrage of particular test integrals

Table 4

Precision $D = -\log_{10}(\text{relative error})$ obtained in the integration of x^k over $[-1, 1]$ using the 63 node rules Q_6 (Laurie), R_6 (GKP) and Z_6 (Pérez-Jordá et al.) and the 127 node rules Q_7 , R_7 , R'_7 (hybrid), R''_7 (approximate hybrid), Q'_7 (Laurie from R_6) and Z_7

k	Q_6	R_6	Z_6	k	Q_7	R_7	R'_7	R''_7	Q'_7	Z_7
100	21.5	33.8	11.4	200	41.4	70.3	44.2	23.0	34.3	13.9
200	14.4	17.8	10.8	400	27.5	36.0	24.0	24.0	21.7	13.2
400	10.1	10.6	10.2	600	22.2	27.9	18.2	18.2	17.1	12.9
600	8.3	8.7	10.0	800	19.3	21.7	15.2	15.2	14.5	12.7
800	7.8	7.1	9.3	1000	17.3	19.9	13.3	13.3	12.9	12.4
1000	6.5	5.3	8.5	1800	13.0	12.7	9.6	9.6	9.4	11.9

Table 5

Precision $D = -\log_{10}(\text{relative error})$ obtained in the integration of $U_k(x)$ over $[-1, 1]$ using the 63 node rules Q_6 (Laurie), R_6 (GKP) and Z_6 (Pérez-Jordá et al.) as well as the 127 node rules Q_7 , R_7 , R'_7 (hybrid), R''_7 (approximate hybrid), Q'_7 (Laurie from R_6) and Z_7

k	Q_6	R_6	Z_6	k	Q_7	R_7	R'_7	R''_7	Q'_7	Z_7
62	490	486	2.3	200	-1.9	8.5	4.7	4.7	4.5	-1.5
64	12.2	486	1.4	202	-2.0	6.9	4.6	4.6	4.4	-0.5
66	11.1	486	0.6	204	-2.0	5.4	4.4	4.6	4.3	-1.5
94	-0.4	486	-1.4	206	-1.7	4.1	4.4	4.6	4.6	-1.5
96	-1.0	7.1	-1.1	208	-1.6	2.9	2.9	2.9	2.9	-0.2
98	-1.4	4.8	-1.3	210	-1.9	1.8	1.8	1.8	1.8	-1.5
100	-1.7	3.0	-1.4							
102	-1.8	1.6	-1.3							
104	-1.6	0.4	-1.2							

which have appeared over the years in the literature we have opted to focus on their performance on two simple polynomial basis functions.

Specifically, we give some results of integrating the elementary functions x^k and $U_k(x)$ over $[-1, 1]$ where $k \geq 0$ is an even integer and $U_k(x)$ is the Chebyshev polynomial of the second kind of algebraic degree k . The exact value of both integrals is $2/(k + 1)$. The calculations have been carried out using the same precision as used to generate the nodes and weights of the rules and the results have been expressed in terms of the precision defined by $D = -\log_{10}(\text{relative error})$ which is equivalent roughly to the number of correct decimal digits.

Table 4 gives the results of applying a variety of the 63 node and 127 node rules discussed earlier to integrate x^k . A general observation is that given that same number of nodes in two rules high precision seems to be a useful attribute. There is ultimately a cross-over in precision at high values of k between the 63 node rules R_6 (GKP, degree 95) and Q_6 (Laurie, degree 63) as pointed out by Laurie [5]. This also happens for Q_7 (degree 127) and R_7 (degree 191) at much higher values of k . The hybrid rules perform respectably given the compromises made in obtaining them as do the rules of Pérez-Jordá et al. [8]. There is little difference between R'_7 and R''_7 for high values of k . This is due to the nodes near the end-points of the range of integration making a dominant contribution and the weights for these, corresponding to $l = 24$, precisely satisfy the $\theta = \frac{1}{2}$ condition.

The performance when integrating $U_k(x)$, given in Table 5, is radically different. This basis function appears to have the property that the error increases very rapidly as k passes the value for which exactness is expected. The columns for R_6 , R_7 and Q'_7 (degree 127) illustrate this feature. High precision has a definite advantage for this function. Note that the negative numbers in the table essentially indicate that no accurate digits have been obtained. The large numbers, such as 490 for Q_6 and $k = 62$, correspond to exact evaluation apart from some small rounding in the multiprecision calculations.

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