Dedicated to Academician Aureliu Sandulescu's 80th Anniversary

CONTEXT-DEPENDENT QUADRATURE RULES. A WAY TO IMPROVE THE QUALITY OF SCIENTIFIC CODES

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We show how the exponential fitting technique can be used for building up quadrature rules of prerequisite forms and with constant coefficients. This includes forms where not only the values of the integrand are accepted in input, as in standard formulas, but also the values of some derivatives of the integrand. The new rules are of substantial help in practical computations because quite often such extra data are available from the previous steps of the computation chain but they are ignored when evaluating integrals. We also give a numerical illustration which clearly demonstrates the accuracy gain to be obtained from the new rules.

1. INTRODUCTION

The exponential fitting (*ef* for short) is a powerful technique for the construction of approximation formulas for operations on functions with special behavior, in particular when these are oscillatory functions. The following simple examples are of help for understanding the object of this technique.

First derivative. The simplest approximation for this operation is the popular central difference formula

$$f'(X) \approx \frac{1}{2h}[f(X+h) - f(X-h)], \tag{1}$$

which gives good results when f has a slow, smooth variation on $[X-h, X+h]$. Much less known is the fact that when f is an oscillatory function of form

$$f(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x) \tag{2}$$

with smooth f_1 and f_2, then the slightly modified formula

$$f'(X) \approx \frac{\theta}{2h\sin(\theta)}[f(X+h) - f(X-h)], \text{ where } \theta = \omega h, \tag{3}$$

becomes appropriate; it tends to the former when $\theta \to 0$.

Second derivative. Three-point approximation

$$f''(X) \approx \frac{1}{h^2}\{a_1[f(X+h) + f(X-h)] + a_2 f(X)\}, \tag{4}$$

has the constant coefficients $a_1 = 1$, $a_2 = -2$ for the classical case, and the θ dependent

$$a_1(\theta) = \frac{\theta}{\sin\theta} \qquad \text{and} \qquad a_2(\theta) = \frac{\theta(\sin\theta - 2\cos\theta)}{\sin\theta}$$

for oscillatory functions of form (2).

Quadrature. Trapezium rule

$$\int_{X-h}^{X+h} f(z)dz \approx h[a_1 f(X+h) + a_2 f(X-h)], \tag{5}$$

has the classical coefficients $a_1 = a_2 = 1$ but

$$a_1(\theta) = a_2(\theta) = \frac{\sin(\theta)}{\theta\cos(\theta)},$$

for functions of form (2).

Interpolation. Let $f(X \pm h)$ be given and we want to interpolate at some $x' \in (X-h, X+h)$ with the formula

$$f(x') \approx a_- f(X-h) + a_+ f(X+h). \tag{6}$$

In the classical case (usual linear interpolation) the coefficients $a_\pm$ depend only on x'. With $t = (x'-X)/h$ these are $a_\pm(x') = (1 \pm t)/2$ but for treating oscillatory functions they depend also on θ,

$$a_\pm(x', \theta) = \frac{\sin[(1 \pm t)\theta]}{\sin(2\theta)}.$$

These were only a few simple examples but the literature is very vast, of several hundred papers. A short selection is [1]- [34], and a book is also available, [35]. Interesting enough, the procedure was seen for long as one for building up suited algorithms for differential equations, in particular for the Schrödinger equation, and this explains why the vast majority of papers are concerned with this case. The fact that the procedure is applicable for other numerical operations (differentiation, quadrature, interpolation *etc.*) became clear only later on, [5], thus shaping up a direction of increasing concern in the last years.

The expression 'exponential fitting' indicates that the procedure has a larger area than dealing with oscillatory functions: in general it covers the cases where f is a linear combination of exponential functions with different frequencies. Expression (2) represents only some possible linear combination of exponential functions: only two imaginary frequencies $\pm i\omega$ are involved in this case. (Notice that in *ef* the term frequency has a different meaning than that usually adopted in physics; it represents the factor of x in the exponent). Still, in practice this was the case that has been the most extensively exploited up to now due to the tremendous large variety of problems where oscillatory functions are involved; think, for example, of phenomena involving oscillations, rotations, vibrations, wave propagation, behavior of quantum particles *etc.*

In this paper we want to exploit this procedure in a special context, which does not actually fit the standard purpose of the exponential fitting procedure. We are actually interested in explaining how the procedure can be used as a tool for obtaining approximation formulas *of the classical type*, that is when the involved frequencies vanish. Of course, in this way we reobtain known formulas but the advantage is that the procedure is much simpler and direct than the standard one. The knowledge of this procedure has actually a very large area of potential applications and the most important of these is that it allows approaching the case when numerical formulas with *prerequisite forms* are demanded.
To understand the importance of the demand for prerequisite forms we focus on the quadrature case. When approaching problems in natural sciences (physics, chemistry, biology *etc.*) a succession of numerical operations has to be carried out, where the output from some step is used as input in the next step. For example, let us assume that at some moment we have to solve a second order differential equation, let this be $y'' = f(x,y)$ on $[a,b]$, and just after that we are interested in the evaluation of the integral of y over this interval. If the differential equation is solved by the Runge-Kutta method, then we get not only the values of the solution y at the mesh points but also of its first and second derivative; the latter results directly by computing the right-hand side of the differential equation. If, alternatively, the equation is solved by a finite difference scheme, then we obtain the values of y and y'' but not those of y'. As for the calculation of the integral, plenty of versions are presented in the standard literature, see [36] for example, but, surprisingly enough, these typically use only the values of the integrand. Formulas which use also the values of sets of successive derivatives appeared only recently, [16–18, 22], while formulas in which some of these are missing are nearly ignored although it is clear that all such extended formulas are potentially more accurate whereas they exploit richer input information than that contained in the integrand alone. Expressed in other words, the new formulas (we call them context-dependent) provide an advantageous alternative to the standard formulas which, for comparable accuracy, impose repeating the whole computation on finer partitions, thus increasing the computational effort.

2. BUILDING UP CONTEXT-DEPENDENT QUADRATURE RULES

As said, for chains of numerical operations it is advantageous to use approximation formulas which take into account as much information as is available from the previous steps of the chain. In the following we take the case of quadrature formulas which make use not only of the values of the integrand but also of its first and second derivative.

To fix the things we consider the interval $[-h, h]$, a partition of this by the mesh points $x_1 = -h$, $x_2 = 0$, $x_3 = h$, and a quadrature rule of the announced form. This is

$$Q[y] = \int_{-h}^{h} y(z)dz \approx \sum_{k=0}^{2} h^{k+1}[a_{k1}y^{(k)}(-h) + a_{k2}y^{(k)}(0) + a_{k3}y^{(k)}(h)], \quad (7)$$

where a_{k1}, a_{k2}, a_{k3} ($k = 0,1,2$) are coefficients to be determined in order to get the closest approximation. The choice $[-h,h]$ of the interval represents no restriction at all. The interval can be well taken in its general form $[X-h, X+h]$ but the chosen form makes the notations simpler. The final values of the coefficients are unchanged, of course. The error of this rule is the difference between the exact value of the integral and the approximation of this,

$$E[h,\mathbf{a};y] = \int_{-h}^{h} y(z)dz - \sum_{k=0}^{2} h^{k+1}[a_{k1}y^{(k)}(-h) + a_{k2}y^{(k)}(0) + a_{k3}y^{(k)}(h)]$$

where the parameters h and $\mathbf{a}$ (this collects all nine coefficients) are explicitly mentioned.

The problem consists in the determination of the coefficients such that the error is minimal in a certain sense. Various particular forms are of interest in terms of the available data. For example, if only the values of y at the three points are known we have to impose from the very beginning that all coefficients of the derivatives equal zero, *i.e.* only a_{01}, a_{02} and a_{03} have to be determined.

Our investigation, inspired from the exponential fitting procedure, follows three steps:

1. Find the expressions of $E[h,\mathbf{a};y]$ for $y(x) = x^n$, $n = 0,1,2,3,\cdots$.
2. Evaluate the values of the coefficients such that $E[h,\mathbf{a};y] = 0$ for as many successive $y(x) = x^n$, $n = 0,1,2,\ldots$, as possible; it is assumed that this is actually the way which leads to coefficients which ensure the minimal error for the considered rule.
3. Determine the Lagrange-like expression of the error.

Step 1 regards the general form (7) while steps 2-3 will treat each particular case separately.

We have the following

Lemma 1 *The expressions of* $E[h,\mathbf{a};y]$ *for* $y(x) = x^n$, $n = 0,1,2,3,\cdots$ *are of the form*

$$E[h,\mathbf{a};x^n] = h^{n+1}E_n(\mathbf{a}), \quad (8)$$

where $E_n(\mathbf{a})$, called reduced moments, are

$$
\begin{aligned}
&E_0(\mathbf{a}) = 2-(a_{01}+a_{02}+a_{03}),\\
&E_1(\mathbf{a}) = -(-a_{01}+a_{03}+a_{11}+a_{12}+a_{13}),\\
&E_2(\mathbf{a}) = \frac{2}{3}-[a_{01}+a_{03}+2(-a_{11}+a_{13}+a_{21}+a_{22}+a_{23})],\\
&E_n(\mathbf{a}) = -[-a_{01}+a_{03}+n(a_{11}+a_{13})+n(n-1)(-a_{21}+a_{23})], \textit{odd } n\geq 3,\\
&E_n(\mathbf{a}) = \frac{2}{n+1}-[a_{01}+a_{03}+n(-a_{11}+a_{13})+n(n-1)(a_{21}+a_{23})], \textit{even } n\geq 4.
\end{aligned}
\tag{9}
$$

Proof: Elementary evaluations on $y(x)=x^n$ give:

$$
\begin{aligned}
y(h) &= (-1)^n y(-h) = h^n, & y(0) &= \delta_{n0},\\
y'(h) &= (-1)^{n-1} y'(-h) = nh^{n-1}, & y'(0) &= \delta_{n1},\\
y''(h) &= (-1)^n y''(-h) = n(n-1)h^{n-2}, & y''(0) &= 2\delta_{n2},
\end{aligned}
$$

for all $n=0,1,2,\ldots$, and

$$
\int_{-h}^{h} y(z)dz = \begin{cases} \dfrac{2}{n+1}h^{n+1} & \text{for even } n,\\ 0 & \text{for odd } n. \end{cases}
$$

If these are introduced in (2) the expressions under eq.(9) result directly.

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Remark: The knowledge of the expressions of the moments plays a central role in the procedure. First, it allows determining the coefficients by equating to zero as many successive moments as needed and then solving the resulting algebraic system. Second, after the coefficients are determined, the next coming moments have to be calculated and, if $E_m(\mathbf{a})$ is the first nonvanishing coefficient, then the Lagrange-like error formula is

$$
E[h,\mathbf{a};y] = \frac{1}{m!}E_m(\mathbf{a})h^{m+1}y^{(m)}(\eta), \tag{10}
$$

where $\eta \in (-h,h)$. If the interval is $[X-h, X+h]$ then the error has the same form but $\eta \in (X-h, X+h)$. For the general expression of the error for *ef*-based approximation formulas see [21].

In the following we examine two families of quadrature rules of the form (7). These are the two-point rules, denoted Q^2_s, where only data at the mesh points $\pm h$ are accepted, and three-point rules, denoted Q^3_s, where data at all three mesh points are accepted. Index $s=1,2,3,4$ identifies versions in the corresponding family in terms of what are actually the data accepted for input:

- Versions Q^2_1 and Q^3_1. Accepted input data: y. These are the trapezium and Simpson rule, respectively.

- Versions Q_2^2 and Q_2^3. Accepted input data: y and y'.
- Versions Q_3^2 and Q_3^3. Accepted input data: y and y''.
- Versions Q_4^2 and Q_4^3. Accepted input data: y, y' and y''.

3. TWO-POINT RULES

For the trapezium rule Q_1^2 the following result is well-known, *e.g.* [36] :
Theorem 1 *The coefficients and the Lagrange-like expression of the error for version Q_1^2 are*

$$a_{01} = a_{03} = 1 \ \text{ and } \ E[h, \mathbf{a}; y] = -\frac{2}{3} h^3 y''(\eta)\,,$$

for some $\eta \in (-h, h)$.
Proof: This result can be proved in various ways but here we reconsider the proof again mainly as a first and simple illustration on how the *ef*-based procedure works. Since only the values $y(\pm h)$ are accepted, all coefficients in eq.(7) are set to zero except for a_{01} and a_{03} which have to be determined.
We now cover the above mentioned steps 2-3.
Step 2. Since the number of coefficients to be determined is 2 the same is the number of the involved successive reduced moments. For brevity reasons hereinafter the reduced moments will be called simply moments and the parameter $\mathbf{a}$ will be omitted when they are written.
The first two moments are $E_0 = 2-(a_{01}+a_{03})$, $E_1 = -(-a_{01}+a_{03})$, and the linear system $E_0 = E_1 = 0$ has the solution $a_{01} = a_{03} = 1$.
Step 3. With these coefficients the first nonvanishing moment is $E_2 = -4/3$, that is, $m = 2$. Error expression (10) results directly in the announced form.

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The following theorem covers the three extensions of the trapezium rule:
Theorem 2 *The extended trapezium rules and the Lagrange-like expression of their errors are as follows:*

- Version Q_2^2 :

$$\begin{aligned} &Q[y] \approx h[y(-h)+y(h)] + \frac{1}{3}h^2[y'(-h) - y'(h)], \\ &E[h, \mathbf{a}; y] = \frac{2}{45}h^5 y^{(4)}(\eta); \end{aligned} \tag{11}$$

- *Version Q_3^2 :*

$$\begin{aligned} &Q[y] \approx h[y(-h)+y(h)] - \frac{1}{3}h^3[y''(-h)+y''(h)], \\ &E[h,\mathbf{a};y] = \frac{4}{15}h^5 y^{(4)}(\eta); \end{aligned} \tag{12}$$

- *Version Q_4^2 :*

$$\begin{aligned} &Q[y] \approx h[y(-h)+y(h)] + \frac{2}{5}h^2[y'(-h)-y'(h)] + \frac{1}{15}h^3[y''(-h)+y''(h)], \\ &E[h,\mathbf{a};y] = -\frac{2}{1575}h^7 y^{(6)}(\eta), \end{aligned} \tag{13}$$

for some $\eta \in (-h,h)$. The value of η may vary from one version to another.
Remark: The coefficients of the rules Q_2^2 and Q_4^2 are known, [18], but the Lagrange-like expression of their error and rule Q_3^2 are new.

Proof: This follows the same pattern as for the previous theorem.

Version Q_2^2. Here four parameters have to be determined: a_{01}, a_{03}, a_{11} and a_{13}. The first four moments are $E_0 = 2-(a_{01}+a_{03})$, $E_1 = -(-a_{01}+a_{03}+a_{11}+a_{13})$, $E_2 = 2/3-[a_{01}+a_{03}+2(-a_{11}+a_{13})]$, $E_3 = -[-a_{01}+a_{03}+3(a_{11}+a_{13})]$, and the algebraic system $E_0 = E_1 = E_2 = E_3 = 0$ has the solution

$$a_{01} = a_{03} = 1,\ a_{11} = -a_{13} = \frac{1}{3},$$

as in (11). An extra check gives $E_4 = 16/15 \neq 0$ and therefore $m = 4$.

Version Q_3^2. Four parameters have to be determined also in this case: a_{01}, a_{03}, a_{21} and a_{23}. The first four moments are $E_0 = 2-(a_{01}+a_{03})$, as before, but $E_1 = -(-a_{01}+a_{03})$, $E_2 = 2/3-[a_{01}+a_{03}+2(a_{21}+a_{23})]$, $E_3 = -[-a_{01}+a_{03}+6(-a_{21}+a_{23})]$. The algebraic system $E_0 = E_1 = E_2 = E_3 = 0$ has the solution

$$a_{01} = a_{03} = 1,\ a_{21} = a_{23} = -\frac{1}{3}.$$

With these we get $E_4 = 32/5 \neq 0$ and therefore $m = 4$.

Version Q_4^2. Six parameters have to be determined: a_{01}, a_{03}, a_{11}, a_{13}, a_{21} and a_{23} and then the same number of successive moments have to be considered: $E_0 = 2-(a_{01}+a_{03})$, $E_1 = -(-a_{01}+a_{03}+a_{11}+a_{13})$, $E_2 = 2/3-[a_{01}+a_{03}+2(-a_{11}+a_{13}+a_{21}+a_{23})]$, $E_3 = -[-a_{01}+a_{03}+3(a_{11}+a_{13})+6(-a_{21}+a_{23})]$, $E_4 = 2/5-[a_{01}+a_{03}+4(-a_{11}+a_{13})+12(a_{21}+a_{23})]$ and $E_5 = -[-a_{01}+a_{03}+5(a_{11}+a_{13})+20(-a_{21}+a_{23})]$. The algebraic system $E_0 = E_1 = E_2 = E_3 = E_4 =$

$E_5 = 0$ has the solution

$$a_{01} = a_{03} = 1,\ a_{11} = -a_{13} = \frac{2}{5},\ a_{21} = a_{23} = \frac{1}{15}\,.$$

With these the next moment is $E_6 = -32/35 \neq 0$ and therefore $m = 6$.

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4. THREE-POINT RULES

The following theorem exists:
Theorem 3 *The set of three-point rules and the Lagrange-like expression of their errors are as follows:*

- Version Q_1^3 (standard Simpson rule):

$$\begin{aligned} &Q[y] \approx h[y(-h) + 4y(0) + y(h)]/3, \\ &E[h, \mathbf{a}; y] = -\frac{1}{90} h^5 y^{(4)}(\eta); \end{aligned} \tag{14}$$

- Version Q_2^3

$$\begin{aligned} &Q[y] \approx \frac{1}{15} h[7y(-h) + 16y(0) + 7y(h)] + \frac{1}{15} h^2[y'(-h) - y'(h)], \\ &E[h, \mathbf{a}; y] = \frac{1}{4725} h^7 y^{(6)}(\eta); \end{aligned} \tag{15}$$

- Version Q_3^3

$$\begin{aligned} &Q[y] \approx \frac{1}{21} h[5y(-h) + 32y(0) + 5y(h)] - \frac{1}{315} h^3[y''(-h) - 32y''(0) + y''(h)], \\ &E[h, \mathbf{a}; y] = \frac{1}{396900} h^9 y^{(8)}(\eta); \end{aligned} \tag{16}$$

- Version Q_4^3

$$\begin{aligned} Q[y] \approx\ & \frac{1}{105} h[41y(-h) + 128y(0) + 41y(h)] + \frac{2}{35} h^2[y'(-h) - y'(h)] \\ & + \frac{1}{315} h^3[y''(-h) + 16y(0) + y''(h)], \\ E[h, \mathbf{a}; y] =\ & -\frac{1}{130977000} h^{11} y^{(10)}(\eta), \end{aligned} \tag{17}$$

for some $\eta \in (-h, h)$. The value of η may vary from one version to another.

Remark: the coefficients of the Simpson rule Q_1^3 and the expression of its error can be found in any standard textbook, *e.g.*, [36]. The coefficients of versions Q_2^3 and Q_4^3 are also known, [18], but the Lagrange-like expression of their error and rule Q_3^3 are new.

Proof: Technically, this follows the same steps as for the previous theorem but the volume of calculations is a bit larger. This is due to the fact that the number of involved moments is bigger. In the following we examine each version and give the main results for each step.

Version Q_1^3:

- Parameters to be determined and their total number N: a_{01}, a_{02}, a_{03}, *i.e.*, $N = 3$ parameters.
- Expressions of the first N moments: $E_0 = 2-(a_{01}+a_{02}+a_{03})$, $E_1 = -(-a_{01}+a_{03})$, $E_2 = 2/3-(a_{01}+a_{03})$.
- Solution of the algebraic system $E_n = 0$, $n = 0,1,\cdots,N-1$: $a_{01} = a_{03} = 1/3$, $a_{02} = 4/3$.
- Extra checks and the value of m: $E_3 = 0$ but $E_4 = -4/15 \neq 0$, therefore $m = 4$.

Note the importance of the extra checks. Without them we might have been tempted to assign the wrong value $m = 3$.

Version Q_2^3:

- Parameters to be determined and their total number N: a_{k1}, a_{k2}, a_{k3}, $k = 0,1$, *i.e.*, $N = 6$ parameters.
- Expressions of the first N moments: $E_0 = 2-(a_{01}+a_{02}+a_{03})$, $E_1 = -(-a_{01}+a_{03}+a_{11}+a_{12}+a_{13}))$, $E_2 = 2/3-[a_{01}+a_{03}+2(-a_{11}+a_{13})]$, $E_3 = -[-a_{01}+a_{03}+3(a_{11}+a_{13})]$, $E_4 = 2/5-[a_{01}+a_{03}+4(-a_{11}+a_{13})]$, $E_5 = -[-a_{01}+a_{03}+5(a_{11}+a_{13})]$.
- Solution of the algebraic system $E_n = 0$, $n = 0,1,\cdots,N-1$: $a_{01} = a_{03} = 7/15$, $a_{02} = 16/15$, $a_{11} = -a_{13} = 1/15$, $a_{12} = 0$.
- Extra checks and the value of m: $E_6 = 16/105 \neq 0$, therefore $m = 6$.

Version Q_3^3:

- Parameters to be determined and their total number N: a_{k1}, a_{k2}, a_{k3}, $k = 0,2$, *i.e.*, $N = 6$ parameters.
- Expressions of the first N moments: $E_0 = 2-(a_{01}+a_{02}+a_{03})$, $E_1 = -(-a_{01}+a_{03})$, $E_2 = 2/3-[a_{01}+a_{03}+2(a_{21}+a_{22}+a_{23})]$, $E_3 = -[-a_{01}+a_{03}+6(-a_{21}+a_{23})]$, $E_4 = 2/5-[a_{01}+a_{03}+12(a_{21}+a_{23})]$, $E_5 = -[-a_{01}+a_{03}+20(-a_{21}+a_{23})]$.
- Solution of the algebraic system $E_n = 0$, $n = 0,1,\cdots,N-1$: $a_{01} = a_{03} = 5/21$, $a_{02} = 32/21$, $a_{21} = a_{23} = -1/315$, $a_{22} = 32/315$.
- Extra checks and the value of m: $E_6 = E_7 = 0$ but $E_8 = 32/315 \neq 0$, therefore $m = 8$.

Version Q_4^3:

- Parameters to be determined and their total number N: a_{k1}, a_{k2}, a_{k3}, $k = 0,1,2$,

i.e., $N = 9$ parameters.
- Expressions of the first N moments: see eq.(9).
- Solution of the algebraic system $E_n = 0$, $n = 0, 1, \cdots, N-1$: $a_{01} = a_{03} = 41/105$, $a_{02} = 128/105$, $a_{11} = a_{13} = -2/35$, $a_{12} = 0$, $a_{21} = -a_{23} = 1/315$, $a_{22} = 16/315$.
- Extra checks and the value of m: $E_8 = E_9 = 0$ but $E_{10} = -32/1155 \neq 0$, therefore $m = 10$.

The results obtained above for the quadrature rules Q^2 and Q^3 allow drawing some conclusions. First, we see that, as expected, the accuracy increases with the *number* of input data in the corresponding versions. Thus the three-point versions are more accurate than their two-point counterparts (compare the orders, *i.e.*, the powers of h in the error expressions) and within each of these two families the order increases with the number of data at each point; the latter are one for Q_1^p versions, two for versions Q_2^p and Q_3^p and three for Q_4^p, $p = 2, 3$. Second, and this is a new issue, the results allow answering a question of a different nature: how does the *type* of data used in versions with the same number of input data/point influence the accuracy? This is the case of versions Q_2^p and Q_3^p where the two data are y and y', and y and y'', respectively. For the two-point versions the order is not modified but the error constant is smaller for Q_2^2 and therefore the use of y' is more advantageous. This is in contrast with the three-point versions where the use of y'' is more advantageous because the corresponding version, that is Q_3^3, has a bigger order than Q_2^3.

5. NUMERICAL ILLUSTRATION

We compute the integral

$$Q = \int_0^1 e^{5x} \sin 5x \, dx = \frac{1}{10} e^{5x} [\sin(5x) - \cos(5x)]|_0^1 \tag{18}$$

by all versions of two and three-point rules. We use $h = 1/2, 1/4, 1/8, 1/16$, $1/32$ and $1/64$, that is with $N = 1, 2, 4, 8, 16$ and 32 two-step intervals. Once the version and h are fixed the integral is computed numerically by that version on each of the N two-step intervals and the individual results are summed. Let denote the value computed this way as $Q^{comput}(h)$. This and its error, $\Delta Q(h) = Q - Q^{comput}(h)$, depend also on the version, of course.

The error $\Delta Q(h)$ behaves as h^m because it is the sum of the N individual errors and $N \cdot h^{m+1} \sim h^m$. As a consequence the ratio of the errors from the same version at $2h$ and h, $\Delta Q(2h)/\Delta Q(h)$, should be around 2^m. Possible deviations from this value are due to the influence of the variation of factor $y^{(m)}$ over four successive intervals of width h. This variation tends to be less and less important when $h \to 0$ and therefore that ratio will tend to the theoretical value in this limit.

Table 1.

Step width dependence of the absolute errors of the results given by the four versions of rule Q^2 for integral (18). Notation $a(b)$ means $a \cdot 10^b$.

h	Q_1^2	Q_2^2	Q_3^2	Q_4^2
1/ 2	0.53(+02)	0.11(+02)	0.14(+03)	-0.16(+02)
1/ 4	0.14(+02)	0.30(+01)	0.20(+02)	-0.29(+00)
1/ 8	0.29(+01)	0.24(+00)	0.14(+01)	-0.35(-02)
1/16	0.67(+00)	0.15(-01)	0.93(-01)	-0.50(-04)
1/32	0.17(+00)	0.97(-03)	0.58(-02)	-0.76(-06)
1/64	0.41(-01)	0.61(-04)	0.36(-03)	-0.12(-07)

Table 2.

The same as in Table 1 for the versions of rule Q^3. The error from Q_4^3 for $h = 1/64$ is zero within machine accuracy for double precision computations (of approximately 16 decimal figures).

h	Q_1^3	Q_2^3	Q_3^3	Q_4^3
1/ 2	0.52(+00)	0.25(+01)	0.98(-01)	0.14(-01)
1/ 4	-0.70(+00)	0.50(-01)	-0.14(-02)	0.18(-04)
1/ 8	-0.59(-01)	0.60(-03)	-0.80(-05)	0.13(-07)
1/16	-0.38(-02)	0.83(-05)	-0.33(-07)	0.12(-10)
1/32	-0.24(-03)	0.13(-06)	-0.13(-09)	0.11(-13)
1/64	-0.15(-04)	0.20(-08)	-0.52(-12)	0.00(+00)

We have written a FORTRAN program in double precision and in Table 1 we give the error $\Delta Q(h)$ for the two-point versions. It is seen that, as expected, the decrease of the error with h becomes faster and faster when the number of accepted data is increased. It is also confirmed the fact that the error decrease is similar for versions Q_2^2 and Q_3^2 and that for each step width h the error for the latter is by a factor 6 larger. Table 2 gives the same data for the three-point versions. The errors decrease faster than for the two-point formulas and also, as predicted but in contrast to the two-point case, the errors from Q_3^3 are massively better than from Q_3^3, especially for small h.

Table 3 collects the ratios $\Delta Q(2h)/\Delta Q(h)$. The theoretical predictions that these should tend to $4, 16, 16, 64$ for Q^2 versions, and to $16, 64, 256, 1024$ for Q^3

Table 3.

The ratio $\Delta Q(2h)/\Delta Q(h)$ for various values of the step width h.

h	Q_1^2	Q_2^2	Q_3^2	Q_4^2	Q_1^3	Q_2^3	Q_3^3	Q_4^3
1/ 4	3.9	3.5	7.2	54.7	-0.7	51.1	-67.6	742.3
1/ 8	4.7	12.9	13.7	81.8	12.0	83.4	180.3	1361.9
1/16	4.3	15.4	15.6	70.8	15.3	71.6	242.4	1159.7
1/32	4.1	15.9	15.9	65.8	15.8	66.1	253.0	1081.7
1/64	4.0	16.0	16.0	64.5	16.0	64.5	254.0	–

versions when $h \to 0$ are nicely confirmed.

6. CONCLUSIONS

We have presented a list of unusual quadrature rules whose main peculiarity is that they accept not only the values of the integrand at the mesh points, as the standard rules, but also those of some of its derivatives. Since in many scientific codes the latter data are often available as output from earlier stages of the current run, the replacement in such codes of the standard rules with the new, context-dependent ones leads to an increase of the accuracy at no extra cost. The procedure used for building up these rules can be extended without difficulty on cases when more restrictions are demanded, for example when the partition has non-equidistant steps.

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REFERENCES

1. A. Raptis and A. Allison, Comput. Phys. Commun. **14**, 1–5 (1978).
2. L. Gr. Ixaru and M. Rizea, Comput. Phys. Commun **19**, 23–27 (1980).
3. H. De Meyer *et al.*, J. Comput. Appl. Math. **32**, 407–415 (1990).
4. T. E. Simos, Int. J. Comput. Math. **46**, 77–85 (1992).
5. L. Gr. Ixaru, Comput. Phys. Commun. **105**, 1–19 (1997).
6. L. Gr. Ixaru *et al.*, Comput. Phys. Commun. **100**, 56–70 (1997).
7. B. Paternoster, Appl. Num. Math. **28**, 401–412 (1998).
8. L. Gr. Ixaru, H. De Meyer and G. Vanden Berghe, J. Comput. Appl. Math. **88**, 289–314 (1998).
9. L. Gr. Ixaru and B. Paternoster, J. Comput. Appl. Math. **106**, 87–98 (1999).
10. G. Vanden Berghe *et al.*, J. Comput. Appl. Math. **125**, 107–115 (2000).
11. L. Gr. Ixaru and B. Paternoster, Comput. Phys. Commun. **133**, 177–188 (2001).
12. L. Gr. Ixaru *et al.*, Comput. Phys. Commun. **100**, 71-80 (1997).
13. L. Gr. Ixaru, H. De Meyer and G. Vanden Berghe, J. Comput. Appl. Math. **132**, 95–105 (2001).
14. G. Vanden Berghe, L. Gr. Ixaru and M. Van Daele, Comput. Phys. Commun. **140**, 346–357 (2001).
15. L. Gr. Ixaru *et al.*, J. Comput. Appl. Math. **132**, 83–93 (2001).
16. J. K. Kim, R. Cools and L. Gr. Ixaru, J. Comput. Appl. Math. **140**, 479–497 (2002).
17. J. K. Kim, Comput. Phys. Commun. **153**, 135–144 (2003).
18. K. J. Kim, R. Cools and L. Gr. Ixaru, Appl. Num. Math. **46**, 59–73 (2003).
19. L. Gr. Ixaru, G. Vanden Berghe and H. De Meyer, Comput. Phys. Commun. **150**, 116–128 (2003).
20. H. Van de Vyver, J. Comput. Appl. Math. **184**, 442–463 (2005).
21. J. P. Coleman and L. Gr. Ixaru, SIAM J. of Numerical Analysis **44**, 1441–1465 (2006).
22. L. Gr. Ixaru, N. S. Scott and M. P. Scott, SIAM J. Sci. Comput. **28**, 1252–1274 (2006).
23. J. M. Franco, Comput. Phys. Commun. **177**, 479–492 (2007).

24. Kim Kyung Joong and Choi Seung Hoe, J. Comput. Appl. Math. **205**, 149–160 (2007).
25. Yonglei Fang, Yongzhong Song and Xinyuan Wub, Comput. Phys. Commun. **179**, 801–811 (2008).
26. J. Martin-Vaquero and J. Vigo-Aguiar, Numerical Algorithms **48**, 327–346 (2008).
27. M. K. El-Daou and N. R. Al-Matar, Appl. Math. and Comput. **216**, 1923–1937 (2010).
28. A. Cardone, L. Gr. Ixaru and B. Paternoster, Numerical Algorithms **55**, 467–480 (2010).
29. L. Gr. Ixaru, Romanian J. Phys. **55**, 619–630 (2010).
30. H. Ramos and J. Vigo-Aguiar, Appl. Math. Lett. **23**, 1378–1381 (2010).
31. D. Hollevoet, M. Van Daele and G. Vanden Berghe, J. Comput. Appl. Math. **235**, 5380–5393 (2011).
32. G. A. Panopoulos, Z. A. Anastassi and T. E. Simos, Comput. Phys. Commun. **182**, 1626–1637 (2011).
33. R. D'Ambrosio, E. Esposito and B. Paternoster, J. Comput. Appl. Math. **235**, 4888–4897 (2011).
34. Kim Kyung Joong, Appl. Math. and Comput. **217**, 7703–7717 (2011).
35. L. Gr. Ixaru and G. Vanden Berghe, *Exponential Fitting* (Kluwer, Dordrecht, 2004).
36. P. Davis and P. Rabinowitz, *Methods for numerical integration* (2nd edn., Academic Press, 1984).