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In Memoriam Adelina Georgescu

APPROXIMATION FORMULAE GENERATED BY EXPONENTIAL FITTING*

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Abstract

We present the main elements of the exponential fitting technique for building up linear approximation formulae. We cover the two main components of this technique, that is the error analysis and the way in which the coefficients of the new formulae can be determined. We present briefly the recently developed error analysis of Coleman and Ixaru, whose main result is that the error of the formulae based on the exponential fitting (ef, for short) is a sum of *two* Lagrange-like terms, in contrast to the case of the classical formulae where it consists of a *single* term. For application we consider the case of two quadrature formulae (extended Newton-Cotes and Gauss), which are indistinguishable in the frame of the traditional error analysis, to find out that the Gauss rule is more accurate. As for the determination of the coefficients, we show how the *ef* procedure can be applied for deriving formulae of *classical* type. We re-obtain wellknown formulae and also derive some new ones.

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1 Introduction

The exponential fitting (ef for short) is a powerful technique for the construction of approximation formulae for operations on functions with special behaviour, 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

$$f'(X) \approx \frac{1}{2h}[f(X+h) - f(X-h)]\,, \tag{1.1}$$

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

$$f(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x) \tag{1.2}$$

with smooth f_1 and f_2, then the slightly modified formula

$$f'(X) \approx \frac{\theta}{2h\sin(\theta)}[f(X+h) - f(X-h)], \text{ where } \theta = \omega h\,, \tag{1.3}$$

becomes appropriate; it tends to the former when $\theta \to 0$.
Second derivative. Three-point approximation

$$f''(X) \approx \frac{1}{h^2}\{a_1[f(X+h) + f(X-h)] + a_2 f(X)\}, \tag{1.4}$$

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

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

for oscillatory functions of form (1.2).
Quadrature. Trapezium rule

$$\int_{X-h}^{X+h} f(z)dz \approx h[a_1 f(X+h) + a_2 f(X-h)]\,, \tag{1.5}$$

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 (1.2).

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

$$f(x') \approx a_- f(X-h) + a_+ f(X+h). \tag{1.6}$$

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

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

For other examples see e.g. [1], [2], [3].

The purpose of the exponential fitting procedure is to produce such new forms for the approximation formulae and to evaluate their error. The expression 'exponential fitting' indicates that the procedure has a larger area: in general it covers the cases where f is a linear combination of exponential functions with different frequencies. The oscillatory function (1.2) represents only one of the possible combinations of such functions (two imaginary frequencies $\pm i\omega$ are actually involved in it) but in practice this case is by far the most popular of all. The reason is related to the existence of a tremendously large variety of phenomena governed by oscillatory functions; think, for example, of phenomena involving oscillations, rotations, vibrations, wave propagation, behavior of quantum particles etc.

The paper is organized in two parts. In the first part (Section 2) we consider the error analysis while in the second part (Sections 3-5) we show how the ef technique is used to build up new formulae. In the first part we present briefly the recently developed error analysis of Coleman and Ixaru [4], whose results might be of interest well beyond the area covered by the ef procedure. The main finding of this analysis is that the error of the ef-based approximation formulae is a sum of two Lagrange-like terms, in contrast to the case of the classical formulae (that is where the coefficients are constants) where it consists of a single term. For application we consider the case of two quadrature formulae (extended Newton-Cotes and Gauss), which are indistinguishable in the frame of the existing error analysis, to find out that the Gauss rule is more accurate.

The unusual feature in the second part is that we apply the ef procedure for deriving formulae of classical type. We re-obtain wellknown formulae and also derive some new ones.

2 A two-term Lagrange-like formula of the error

When the value of a function f at $X+h$ is approximated by a truncated Taylor expansion about X, that is by $f_K(X+h)=\sum_{k=0}^{K} h^k f^{(k)}(X)/k!$, the resulting error may be expressed in the Lagrange form

$$E[f]=f(X+h)-f_K(X+h)=\frac{h^{K+1}}{(K+1)!}f^{(K+1)}(\eta)\,, \tag{2.7}$$

for some $\eta\in(X,\,X+h)$, if $f^{(K+1)}(x)$ is continuous on $(X,\,X+h)$. That error may also be written, less usefully, as the formal expansion

$$E[f]=\sum_{k=K+1}^{\infty}\frac{h^k}{k!}f^{(k)}(X)\,. \tag{2.8}$$

Expressions of Lagrange type are also available for the truncation errors of many other classical approximations. For example, the error of the simplest approximation for the first derivative, eq.(1.1), has the Lagrange-like expression

$$E[f]=-\frac{1}{6}h^2 f^{(3)}(\eta) \tag{2.9}$$

where $\eta\in(X-h,\,X+h)$, but a formal expansion as in eq.(2.8) can also be written, whose leading term is

$$lte=-\frac{1}{6}h^2 f^{(3)}(X)\,. \tag{2.10}$$

Note that in both cases considered above the expression of the leading term is the same as that in the Lagrange form except for the interchange of X and η.

Expressions of the leading term of the error can be easily built up for both classical and new forms of the coefficients. Also, since the new coefficients tend to the classical ones when $\theta\to 0$ the same holds true for the leading term of the error. For example, approximation (1.3) has

$$lte=h^2\frac{\sin(\theta)-\theta}{\theta^2\sin(\theta)}[f^{(3)}(X)+\omega^2 f'(X)]\,, \tag{2.11}$$

see [1]. When $\theta\to 0$ (for fixed h this implies $\omega\to 0$ and viceversa) this lte obviously tends to (2.10) which is the same as the whole $E[f]$ of (2.9) except for the interchange of X and η. This induces the impression that such a link may be more general, in the sense that for any ef-based approximation formula it is sufficient to build up the expression of the *lte* (which, as said, can be derived without difficulty) and to accept simply that this expression represents also the whole error $E[f]$ if X is replaced by some η.

The problem of whether the suggested link can be sustained has been investigated recently by Coleman and Ixaru [4] for linear ef-based approximation formulae on the basis of a theory developed in the book of Ghizzetti and Ossicini [5]. Coleman and Ixaru have shown that $E[f]$ can be written as a sum of two Lagrange-like terms from which only one survives in the limit $\theta \to 0$. The consequence is that the link is justified in the limit case but it does not hold true for big θ, that is, in the region where the ef-based approximation formulae are actually helpful.

The work [5] is concerned with quadrature formulae of the form

$$\int_a^b g(x)f(x)\,dx \approx \sum_{i=1}^{n}\sum_{k=0}^{m-1} A_{ki}f^{(k)}(x_i), \tag{2.12}$$

whose error

$$E[f] = \int_a^b g(x)f(x)\,dx - \sum_{i=1}^{n}\sum_{k=0}^{m-1} A_{ki}f^{(k)}(x_i) \tag{2.13}$$

is such that $E[f] = 0$ when f is a solution of a linear differential equation $Lf = 0$ of order m. It is assumed that

$$a \le x_1 < x_2 < \cdots < x_n \le b$$

and it is convenient to define $x_0 = a$ and $x_{n+1} = b$, to allow for cases where the end-points of the integration interval are not quadrature abscissas.

The operator L has the form

$$L = \sum_{k=0}^{m} w_k(x)D^{m-k}\,,\ x \in [a,\,b]\,,\ \text{ where }\ D^p = \frac{d^p}{dx^p}, \tag{2.14}$$

with $w_0(x) = 1$. Smoothness conditions on the coefficients w_k are specified in [5].

We place the discussion on the case when the coefficients A_{ki} corresponding to the given L are known, to find the expression of the error $E[f]$. The presence of $g(x)$ in the integrand allows for considerable flexibility. Not only the quadrature formulae are covered by (2.12) but many others, including any known linear approximation formula which is consistent with L of the given form, for operations such as the numerical differentiation, quadrature, solving differential or integral equations, interpolation etc.

For illustration let us examine the approximation formulae listed above from this perspective.

- *First derivative.* The classical and ef-based formulae, eqs.(1.1) and (1.3), respectively, are of form (2.12) for $g(x) \equiv 0$, $n = m = 3$, $x_1 = X - h$, $x_2 = X$, $x_3 = X + h$, $A_{02} = A_{11} = A_{13} = A_{21} = A_{22} = A_{23} = 0$, and $A_{12} = -1$. The other coefficients are $-A_{01} = A_{03} = 1/(2h)$ for the classical formula and $-A_{01} = A_{03} = \theta/[2h\sin(\theta)]$ for the other. Since the classical formula is exact for $f = 1,\, x, x^2$ i.e. when f satisfies $f^{(3)}(x) = 0$, it follows that $L = D^3$. Likewise, the ef-based formula is exact when $f = 1$, $\sin(\omega x)$, $\cos(\omega x)$ and since these are three linear independent solutions of differential equation $f^{(3)} + \omega^2 f' = 0$ it results that $L = D(D^2 + \omega^2)$ in this case.

- *Second derivative*, eq.(1.4). This corresponds to (2.12) if we take $g(x) \equiv 0$, $n = 3$, $m = 4$, $x_1 = X - h$, $x_2 = X$, $x_3 = X + h$, $A_{22} = -1$, $A_{21} = 0 = A_{23}$ and $A_{1k} = A_{3k} = 0$ for $k = 1, 2, 3$. The other coefficients are $A_{01} = A_{03} = 1/h^2$, $A_{02} = -2/h^2$ for the classical case, and $A_{01} = A_{03} = a_1(\theta)/h^2$, $A_{02} = a_2(\theta)/h^2$ for the ef-based case. The expressions of the operator are $L = D^4$ and $L = (D^2 + \omega^2)^2$, respectively.

- *Trapezium rule for the quadrature*, eq.(1.5): $g(x) \equiv 1$, $n = m = 2$, $a = x_0 = x_1 = X - h$, $b = x_2 = x_3 = X + h$, $A_{11} = 0 = A_{12}$. The other coefficients depend on the version. They are $A_{01} = A_{02} = h$ for the classical version and $A_{01} = A_{02} = h\sin(\theta)/[\theta\cos(\theta)]$ for the ef-based version. As for the expression of the operator, this is $L = D^2$ and $L = D^2 + \omega^2$, respectively.

- *Two point interpolation*, eq.(1.6): $g(x) \equiv \delta(x - x')$, $n = m = 2$, $a = x_0 = x_1 = X - h$, $b = x_2 = x_3 = X + h$, $A_{11} = A_{12} = 0$. For the classical version we have $A_{01} = a_-(x')$, $A_{02} = a_+(x')$ and $L = D^2$ while $A_{01} = a_-(x', \theta)$, $A_{02} = a_+(x', \theta)$ and $L = D^2 + \omega^2$ for the ef-based version.

The theory of Ghizzetti and Ossicini allows writing $E[f]$ in integral form,

$$E[f] = \int_a^b \Phi(x) L f(x)\, dx, \tag{2.15}$$

where function $\Phi(x)$ is determined piecewise in terms of some other functions, namely

$$\Phi(x) = \phi_i(x) \qquad \text{for} \quad x_i < x < x_{i+1}, \quad i = 0, \ldots, n.$$

The functions $\phi_i(x)$ are constructed as follows. Let K be the resolvent kernel corresponding to the operator L, i.e., $K(x, z)$ is the solution of $Lu(x) = 0$ such that

$$\left[\frac{\partial^k}{\partial x^k} K(x, z)\right]_{x=z} = \delta_{k,m-1}, \tag{2.16}$$

for $k = 0, 1, \ldots, m-1$. This is used to build up function $\phi_0(x)$ by

$$\phi_0(x) = -\int_a^x K(t, x) g(t)\, dt\,. \tag{2.17}$$

Once $K(t, x)$ and $\phi_0(x)$ are known the other ϕ-functions are generated by recurence,

$$\phi_{i+1}(x) = \phi_i(x) + \sum_{k=0}^{m-1} A_{k,i+1} \left[\frac{\partial^k}{\partial t^k} K(t, x)\right]_{t=x_{i+1}}. \tag{2.18}$$

Let us denote

$$T_0 = \int_a^b \Phi(x) dx.$$

The significance of this T_0 is that it represents the front factor in the expression of the leading term of the error. This is easily seen if we take some reference point X on $(a,\, b)$, and use the Taylor series for $Lf(x)$ around X,

$$Lf(x) = Lf(X) + \frac{(x-X)}{1!}\frac{d}{dx} Lf(x)|_{x=X} + \frac{(x-X)^2}{2!}\frac{d^2}{dx^2} Lf(x)|_{x=X} + \ldots$$

The leading term of the error is integral (2.15) in which only the first term of this expansion is retained:

$$lte = \int_a^b \Phi(x)\, dx \times Lf(X) = T_0\, Lf(X) \tag{2.19}$$

Indeed, the integrals with the next terms will result in higher order contributions, proportional to h, h^2, ...; to see this use the second mean-value theorem. On the other hand, if $\Phi(x)$ does not change the sign on $(a,\, b)$, then, assuming that $f \in C^m(a, b)$, the same second mean-value theorem applied on integral (2.15) gives that

$$E[f] = T_0\, Lf(\eta) \tag{2.20}$$

for some $\eta \in (a,\, b)$, such that only in this case one can say that the expressions of *lte* and of $E[f]$ coincide except for the interchange of X and η. However, $\Phi(x)$ may not be of constant sign. For illustration, function $\Phi(x)$ corresponding to the ef-based approximation of the second derivative (1.4) is

$$\Phi(x) = h\frac{\theta(1-|x^*|)\cos[\theta(1-|x^*|)] - \sin[\theta(1-|x^*|)]}{2\theta^2 \sin\theta}\,,$$

where $x^* = (x - X)/h \in [-1,\, 1]$ is associated to $x \in [X - h,\, X + h]$, see [4]. Experimental evidence, also presented in [4], shows that this $\Phi(x)$ is of constant sign if $\theta \in (0,\, \theta_1 \approx 4.4934)$ but it changes the sign for bigger values of θ.

To treat the case when $\Phi(x)$ changes the sign on $(a,\, b)$ we follow [4] to write $\Phi(x) = \Phi_+(x) + \Phi_-(x)$, where

$$\Phi_+(x) := \begin{cases} \Phi(x) & \text{for all } x \text{ such that } \;\Phi(x) \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\Phi_-(x) := \begin{cases} \Phi(x) & \text{for all } x \text{ such that } \;\Phi(x) \leq 0 \\ 0 & \text{otherwise} \end{cases}$$

The integral in (2.15) can be expressed as the sum of two integrals,

$$E[f] = \int_a^b \Phi_+(x) Lf(x)\, dx + \int_a^b \Phi_-(x) Lf(x)\, dx\,. \tag{2.21}$$

and, since functions $\Phi_\pm(x)$ are of constant sign, the mean-value theorem can be applied to both integrals to give

$$E[f] = Lf(\eta_+) \int_a^b \Phi_+(x)\, dx + Lf(\eta_-) \int_a^b \Phi_-(x)\, dx, \tag{2.22}$$

for some $\eta_+\,, \eta_- \in (a\,, b)$. With

$$T_\pm = \int_a^b \Phi_\pm(x)\, dx$$

this reads simply

$$E[f] = T_+ Lf(\eta_+) + T_- Lf(\eta_-)\,, \tag{2.23}$$

which is the announced two-term Lagrange-like expression of the error.

To summarize, the error of approximation formula (2.12) admits a Lagrange-like expression whose number of terms depends on the behavior of $\Phi(x)$ on (a, b): it consists of a single term if $\Phi(x)$ does not change the sign but of two terms otherwise. As a matter of fact, no case in which $\Phi(x)$ changes its sign is known to us if L is of the simple form $L = D^m$ (this covers the familiar formulae with constant coefficients such as Simpson, Newton-Cotes or Gauss). In all these cases the error expressions consist in a single Lagrange-like term.

As for new applications, note that the expression of $\Phi(x)$ can be build up in analytic form but the determination of functions $\Phi_\pm(x)$ needs a numerical approach. A final check for the accuracy of the later determination consists in verifying that $T_0 = T_+ + T_-$.

Note also that formula (2.23), whose derivation uses for start the work of Ghizzetti and Ossicini [5], is more general than needed for linear ef-based approximations since it assumes that the coefficients w_k in the operator L may depend on x, while in the exponential fitting these are simply constants.

Application

We consider two ef-based quadrature rules, see also [4].

• Extended Newton-Cotes rule, [7], [2]:

$$\int_a^b f(x)dx = \int_{X-h}^{X+h} f(x)dx \approx h\sum_{n=1}^{N}[a_n^{(0)} f(X + x_n^* h) + h a_n^{(1)} f'(X + x_n^* h)]\,, \tag{2.24}$$

on evenly-spaced abscissas $x_n^* = 2(n-1)/(N-1) - 1 \quad (n = 1, 2, \ldots, N)$. The rule is called extended because it uses the values of f and its derivative, to underline that its structure contrasts that of the versions in current use, where only the values of f are used. As a matter of fact, the Simpson rule is a particular case of the later ($N = 3$); for an adaptation of the Simpson rule to oscillatory integrals see [9] and [10].

• Gauss rule, [11], [2]:

$$\int_a^b f(x)dx = \int_{X-h}^{X+h} f(x)dx \approx h \sum_{n=1}^{N} a_n^{(0)} f(X + x_n^* h)\,. \qquad (2.25)$$

The $2N$ coefficients, that is $a_n^{(0)}$, $a_n^{(1)}$ for the first rule, and $a_n^{(0)}$, x_n^* for the second ($n = 1, \ldots, N$) are determined from the condition that the rule is exact if f satisfies $Lf = 0$ for

$$L = (D^2 + \omega^2)^N = h^{-2N}(D^{*2} + \theta^2)^N.$$

In the last member we have used the dimensionless $x^* = (x - X)/h$ and $D^{*p} = d^p/dx^{*p} = h^p D^p$. Both rules are exact if the integrand f is of form (1.2) where f_1, f_2 are polynomials of degree $N - 1$ or less. The coefficients of each rule depend on θ only.

The *lte* can be expressed either as in (2.19) or in terms of x^*,

$$lte = T_0(D^2 + \omega^2)^N f(X) \; = hT_0^*(D^{*2} + \theta^2)^N f(X)\,,$$

where $T_0^* = h^{-(2N+1)}T_0$. The advantage of the second representation is that it makes the θ dependence more obvious. Indeed, T_0^* depends on θ only, and its expression is formally the same in both rules,

$$T_0^*(\theta) = \frac{2 - \sum_{n=1}^{N} a_n^{(0)}(\theta)}{\theta^{2N}}.$$

As said, the niche for such quadrature rules is that of highly oscillatory integrands, i.e., when big values of θ are involved. Let then keep h fixed and examine the behaviour of *lte* when ω (or θ) tends to infinity. Factor $T_0^*(\theta)$ decreases as θ^{-2N} in both formulae because in each of these the coefficients $a_n^{(0)}(\theta)$ tend to 0 when $\theta \to \infty$. The last factor, $(D^{*2} + \theta^2)^N f(X)$, which is identical in the two, increases as θ^N, see [2], such that the prediction based on the expression of the leading term is that the error should decrease as θ^{-N} in both formulae.
However, the two-term form of the error, eq.(2.23), leads to a different picture. It is convenient to write this equation under the equivalent form

$$E[f](\theta) = h[T_+^*(\theta)(D^{*2} + \theta^2)^N f(\eta_+) + T_-^*(\theta)(D^{*2} + \theta^2)^N f(\eta_-)]\,, \quad (2.26)$$

where functions $T_\pm^*(\theta)$ satisfy $T_+^*(\theta) \geq 0$, $T_-^*(\theta) \leq 0$, and $T_0^*(\theta) = T_+^*(\theta) + T_-^*(\theta)$. The picture is different because the asymptotic behaviours of $T_0^*(\theta)$,

on one hand, and those of its components $T^*_\pm(\theta)$, on the other, are not necessarily similar.
Indeed, Coleman and Ixaru have shown that for large θ and $N \geq 2$ the sign conserving functions $T^*_\pm(\theta)$ are well described by the approximation

$$T^*_\pm(\theta) \approx \pm c(\theta)\theta^{-(2N-\bar{N})} + c_\pm(\theta)\theta^{-2N}, \tag{2.27}$$

where $\bar{N} \geq 0$, and the functions $c(\theta)$ and $c_\pm(\theta)$, with $c_+(\theta) \neq -c_-(\theta)$, are oscillating between constant limits; think, for example, of functions of the form $c(\theta) = c_+(\theta) = 1 + \cos\theta$ and $c_-(\theta) = -1 + \cos\theta$. Consequently, the errors will damp out as $\theta^{\bar{N}-N}$, and this is slower than the rule θ^{-N} suggested by the behaviour of the *lte*.
Coleman and Ixaru have also shown that the values of $\bar{N}$ are different in the two rules. They are $\bar{N} = N - 2$ for the extended Newton-Cotes rule but $\bar{N} = \lfloor (N-1)/2 \rfloor$ for the Gauss rule, that is $\bar{N} = 0$ for $N = 2$, $\bar{N} = 1$ for $N = 3$, 4, and $\bar{N} = 2$ for $N = 5$, 6 etc. Thus the error damps out like θ^{-2} for the extended Newton-Cotes rule with any $N \geq 2$ but faster and faster when N is increased for the Gauss rule: θ^{-2} for $N = 2$, 3, θ^{-3} for $N = 4$, 5 etc. All these theoretical predictions are nicely confirmed in practice.
We can then conclude that the two-term Lagrange-like expression of the error [4] allows a solid theoretical understanding of the experimental evidence that the ef-based approximation formulae are so well suited for operations on oscillatory functions. It also warns us that the characterization of the error in terms of the *lte*, as largely used in the literature, is often misleading.
The presented application is however rather special: only functions with *one* frequency were involved and also the two selected quadrature rules (extended Newton-Cotes and Gauss) share the property of being defined for any θ. However, such a property is quite exceptional in the family of the ef-based formulae. The typical situation is when some values of θ exist at which the formulae cannot be defined; these are called critical values, see [1], [2]. For example, $\theta_n = (n + 1/2)\pi,\ n = 0, 1, 2, \ldots$ are the critical values for the trapezium rule (1.5) because the coefficients exhibit a factor $\cos(\theta)$ in the denominator. It would be then interesting to see applications on such cases, and also on cases when linear combinations of functions of form (1.2) with *different* frequencies are involved. Situations of the later type also appear in some applications, as in the computation of the normalization constant (two frequencies) or of the Slater integrals (eight frequencies) in quantum mechanics, see, e.g. [2], [12], [13].

It is also important to notice that the approach which has lead to the two-term error formula is restrictive because in the present form it does not give a direct answer for nonlinear approximations. For example, the two-step hybrid algorithm for differential equations in which the phase-fitting technique is used [14], the conditionally P-stable ef-based method for differential equations of form $y'' = f(x, y)$ [15], the ef-based extensions of Runge-Kutta methods as in [16], [6],[17], [18], and references therein, cannot be approached at this moment, and an adaptation is needed.

3 Exponential fitting technique for the construction of the coefficients of approximation formulae

In the previous section we were concerned with the determination of the expression of the error when the coefficients of the approximation formulae are assumed known. The complementary problem, that is the determination of the coefficients, is of equal importance and this is what we consider in this and the next sections in the frame of the ef approach. To fix the ideas we continue to focus our attention on quadrature formulae and, to make the things even simpler, we restrict our concern on the two and three-point formulae with constant coefficients, that is on the classically allowed extensions (in the sense that the frequencies are simply set to zero) of the familiar trapezium and Simpson rules, respectively.

There is a direct practical motivation for such extensions. 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 second derivative results directly from the expression of function $f(x, y)$. If, alternatively, the equation is solved by a finite difference scheme, then we get 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 [19] for example, but, surprisingly enough, these typically use only the values of the integrand. Formulae which use also the values of sets of successive derivatives appeared only recently while formulae in which some of these are missing do not exist although it is clear that all such extended formulae are potentially more accurate whereas they exploit richier input information than that contained in the integrand alone. Expressed in other words, the new formulae provide an advantageous alternative to the standard formulae which, for comparable accuracy, will need repeating the whole computation on finer partitions, thus increasing the computational effort.

We consider the interval $[-h, h]$, a partition of this by the meshpoints $x_0 = x_1 = -h$, $x_2 = 0$, $x_3 = x_4 = h$, and a quadrature rule of the form

$$Q[y] = \int_{-h}^{h} y(z)dz \approx \sum_{k=0}^{2} h^k [a_{k1} y^{(k)}(-h) + a_{k2} y^{(k)}(0) + a_{k3} y^{(k)}(h)] \,, \quad (3.28)$$

that is a rule which potentially allows the computation of the integral in terms of the values at the meshpoints of the integrand and of its first and second derivatives. The error of this rule is

$$\begin{aligned} &E[h, \mathbf{a};\, y] & (3.29) \\ &= \int_{-h}^{h} y(z)dz - \sum_{k=0}^{2} h^k [a_{k1} y^{(k)}(-h) + a_{k2} y^{(k)}(0) + a_{k3} y^{(k)}(h)] \end{aligned}$$

where the arguments 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, then we have to impose that all coefficients of the derivatives equal zero, i.e. only a_{01}, a_{02} and a_{02} have to be determined.

Our investigation 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 $y(x) = x^n$ as possible (it is assumed that this is actually the way which leads to coefficients which ensure the minimal error for the considered rule) and determine, on this basis, the expression of the operator L, eq.(2.14).
3. Determine the Lagrange-like expression of the error.

Step 1 regards the general form (3.28) 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*

$$E[h, \mathbf{a};\, x^n] = h^{n+1}\, E_n(\mathbf{a})\,, \tag{3.30}$$

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

$$\begin{aligned}
E_0(\mathbf{a}) &= 2 - (a_{01} + a_{02} + a_{03})\,, \\
E_1(\mathbf{a}) &= -(-a_{01} + a_{03} + a_{11} + a_{12} + a_{13})\,, \\
E_2(\mathbf{a}) &= \frac{2}{3} - [a_{01} + a_{03} + 2(-a_{11} + a_{13} + a_{21} + a_{22} + a_{23})]\,, \\
E_n(\mathbf{a}) &= -[-a_{01} + a_{03} + n(a_{11} + a_{13}) + n(n-1)(-a_{21} + a_{23})]\,, \\
&\qquad\qquad\qquad\qquad \text{for odd } n \geq 3\,, \\
E_n(\mathbf{a}) &= \frac{2}{n+1} - [a_{01} + a_{03} + n(-a_{11} + a_{13}) + n(n-1)(a_{21} + a_{23})]\,, \\
&\qquad\qquad\qquad\qquad \text{for even } n \geq 4\,.
\end{aligned} \tag{3.31}$$

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

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

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 (3.30) the expressions under eq.(3.31) result directly.
Q. E. D.
Another element of general interest in the subsequent considerations is the resolvent kernel of operator $L = D^m$. We have

Lemma 2. *The resolvent kernel of* $L = D^m$, $m \geq 1$ *is*

$$K(t, z) = \frac{1}{(m-1)!}(t - z)^{m-1}. \tag{3.32}$$

Proof The general solution of the differential equation $D^m u(x) = 0$ is the $(m-1)$-th degree polynomial

$$u(x) = \sum_{i=0}^{m-1} a_i x^i \,.$$

Its successive derivatives are

$$\frac{\partial^k}{\partial x^k} u(x) = \sum_{i=0}^{m-(k-1)} (i+1)(i+2)\cdots(i+k) a_{i+k} x^i, \;\; k = 1, 2, \cdots, m-1\,.$$

The particular solution which satisfies the initial conditions

$$\frac{\partial^k}{\partial x^k} u(x)|_{x=0} = \delta_{k,m-1}$$

is

$$u_p(x) = \frac{1}{(m-1)!} x^{m-1} \,,$$

and the resolvent kernel is this particular solution with argument $x = t - z$. Q. E. D.

For the construction of functions $\phi_i(x)$, eqs.(2.17)-(2.18), the expressions of the integral and successive partial derivatives of the kernel will often be involved:

$$\begin{aligned} I(X, x) \;&:=\; \int_X^x K(t, x) dt = -\frac{1}{m!}(X - x)^m \,, \\ K_k(X, x) \;&:=\; \frac{\partial^k}{\partial t^k} K(t, x)|_{t=X} = \frac{1}{(m-k-1)!}(X - x)^{m-k-1}, \\ &\qquad\qquad k = 0, 1, \cdots, m-1. \end{aligned} \tag{3.33}$$

Since $x_0 = x_1 = -h$ and $x_3 = x_4 = h$, the function $\Phi(x)$ will have only two piecewise determinations:

$$\Phi(x) = \begin{cases} \phi_1(x) = -I(-h, x) + \displaystyle\sum_{k=0}^{2} h^k a_{k1} K_k(-h, x) & \text{for } -h < x < 0 \\ \\ \phi_2(x) = \phi_1(x) + \displaystyle\sum_{k=0}^{2} h^k a_{k2} K_k(0, x) & \text{for } 0 < x < h \end{cases} \tag{3.34}$$

In the following we examine two families of quadrature rules of the form (3.28). These are the two-point rules, denoted Q^2_s, where only data at the meshpoints $\pm h$ are accepted, and three-point rules, denoted Q^3_s, where data at all three meshpoints 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^3_2. Accepted input data: y and y'.
- Versions Q^2_3 and Q^3_3. Accepted input data: y and y''.
- Versions Q^2_4 and Q^3_4. Accepted input data: y, y' and y''.

4 Two-point rules

Remark: Since for these rules we always have $a_{k2} = 0$, $k = 0, 1, 2$, function $\phi_2(x)$ has the same expression as $\phi_1(x)$ and therefore only one determination is active in eq.(3.34): $\Phi(x) = \phi_1(x)$ for $-h < x < h$.
For the trapezium rule Q^2_1 the following result is wellknown, e.g. [19] :

Theorem 1. *The coefficients and the Lagrange-like expression of the error for version Q^2_1 are*

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

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.(3.28) are set to zero except for a_{01} and a_{03} which have to be determined. We 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 $a_{01} = a_{03} = 1$. For these coefficients we have $E_2 = -4/3 \neq 0$ such that the error vanishes when $y(x)$ is a first degree polynomial or, equivalently, when $y(x)$ is any solution of the simple second order differential equation $y'' = 0$, that is $L = D^m$ with $m = 2$. As a matter of fact, after the coefficients have been determined a compulsory practice is to check how many next moments are also vanishing. This is because in some situations it may happen that this holds true for a number of such extra moments and therefore the degree of the polynomial may be higher than the number of coefficients. We will meet such a situation for version Q_3^3.
Step 3. For $m = 2$ we have:

$$I(-h,x) = -\frac{1}{2}(h+x)^2,\ K_0(-h,x) = -(h+x),$$

and then

$$\phi_0(x) = \frac{1}{2}(h+x)^2,\ \phi_1(x) = \phi_0(x) + ha_{01}K_0(-h,x) = \frac{1}{2}(x^2-h^2)\,.$$

$\phi_1(x)$ does not change the sign on $(-h,h)$ (it is negative) and therefore the error is of one-term Lagrange form (2.20) with

$$T_0 = \int_{-h}^{h} \phi_1(x)\,dx = -\frac{2}{3}h^3\,,$$

and this completes the proof.
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 *:*

$$\begin{aligned} Q[y] &\approx h[y(-h)+y(h)] + \frac{1}{3}h^2[y'(-h)-y'(h)], \\ E[h,\mathbf{a};y] &= \frac{2}{45}h^5 y^{(4)}(\eta)\,; \end{aligned} \tag{4.35}$$

- Version Q_3^2 *:*

$$\begin{aligned} Q[y] &\approx h[y(-h)+y(h)] - \frac{1}{3}h^3[y''(-h)+y''(h)], \\ E[h,\mathbf{a};y] &= \frac{4}{15}h^5 y^{(4)}(\eta)\,; \end{aligned} \tag{4.36}$$

- *Version Q_4^2 :*

$$Q[y] \approx h[y(-h)+y(h)] + \frac{2}{5}h^2[y'(-h)-y'(h)]$$
$$+\frac{1}{15}h^3[y''(-h)+y''(h)],$$
$$E[h,\mathbf{a};\,y] = -\frac{2}{1575}h^7 y^{(6)}(\eta)\,, \tag{4.37}$$

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

Remarks:

1. The coefficients of the rules Q_2^2 and Q_4^2 are known, [8], but the expressions of their error are new. The rule Q_3^2 is entirely new.

2. One should not remain with the impression that these rules apply only when the integration limits are $-h$ and h. If these are $X-h$ and $X+h$ the coefficients are the same. For example, Q_2^2 reads:

$$\int_{X-h}^{X+h} y(z)dz \approx h[y(X-h)+y(X+h)] + \frac{1}{3}h^2[y'(X-h)-y'(X+h)]$$

Its error is as in eq.(4.35) but $\eta \in (X-h, X+h)$.

Proof This follows the same pattern as for the previous theorem. However, hereinafter we treat explicitly only the rule Q_3^2 which is really new.

Four parameters have to be determined for this version, namely, a_{01}, a_{03}, a_{21} and a_{23}, and the first four moments are $E_0 = 2-(a_{01}+a_{03})$, $E_1 = -(-a_{01}+a_{03})$, $E_2 = 2/3-[a_{01}+a_{03}+2(a_{21}+a_{23})]$, $E_3 = -[-a_{01}+a_{03}+6(-a_{21}+a_{23})]$, see (3.31).

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 $L = D^m$ with $m = 4$. Function $\phi_1(x)$ is

$$\begin{aligned}\phi_1(x) &= -I(-h,x) + ha_{01}K_0(-h,x) + h^3 a_{21}K_2(-h,x)\\ &= \frac{1}{4!}(h+x)^4 - \frac{1}{3!}h(h+x)^3 - \frac{1}{3}h^3(h+x)\,.\end{aligned}$$

Separate investigation shows that this $\phi_1(x)$ is positive on $(-h,h)$ and then the error is of form (2.20) with

$$T_0 = \int_{-h}^{h} \phi_1(x)\,dx = \frac{4}{15}h^5\,.$$

Q. E. D.

5 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):

$$Q[y] \approx h[y(-h) + 4y(0) + y(h)]/3,$$
$$E[h, \mathbf{a};\, y] = -\frac{1}{90} h^5 y^{(4)}(\eta)\,; \tag{5.38}$$

- Version Q_2^3:

$$Q[y] \approx \frac{1}{15} h[7y(-h) + 16y(0) + 7y(h)] + \frac{1}{15} h^2 [y'(-h) - y'(h)],$$
$$E[h, \mathbf{a};\, y] = \frac{1}{4725} h^7 y^{(6)}(\eta)\,; \tag{5.39}$$

- Version Q_3^3:

$$Q[y] \approx \frac{1}{21} h[5y(-h) + 32y(0) + 5y(h)]$$
$$- \frac{1}{315} h^3 [y''(-h) - 32y''(0) + y''(h)]\,,$$
$$E[h, \mathbf{a};\, y] = \frac{1}{396900} h^9 y^{(8)}(\eta)\,; \tag{5.40}$$

- Version Q_4^3:

$$Q[y] \approx \frac{1}{105} h[41y(-h) + 128y(0) + 41y(h)] + \frac{2}{35} h^2 [y'(-h) - y'(h)]$$
$$+ \frac{1}{315} h^3 [y''(-h) + 16y(0) + y''(h)],$$
$$E[h, \mathbf{a};\, y] = -\frac{1}{130977000} h^{11} y^{(10)}(\eta)\,, \tag{5.41}$$

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., [19]. The coefficients of versions Q_2^3 and Q_4^3 are also known, [8], but the expressions of their error are new. The rule Q_3^3 is entirely 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, on one hand, and that function $\Phi(x)$ now has two piecewise expressions: $\phi_1(x)$ and $\phi_2(x)$. In the following we give details only on the new 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 $L = D^m$ with $m = 8$. (Notice that the extra check was crucial for this case. Otherwise we might have been tempted to wrongly assign the value $m = 6$.)
- Components of function $\Phi(x)$:

$$\begin{aligned}
\phi_1(x) &= -I(-h,x) + ha_{01}K_0(-h,x) + h^3 a_{21}K_2(-h,x) \\
&= \frac{1}{8!}(h+x)^8 - \frac{5}{21\cdot 7!}h(h+x)^7 + \frac{1}{315\cdot 5!}h^3(h+x)^5\,, \\
\phi_2(x) &= \phi_1(x) + ha_{02}K_0(0,x) + h^3 a_{22}K_2(0,x) \\
&= \phi_1(x) - \frac{32}{21\cdot 7!}hx^7 - \frac{32}{315\cdot 5!}h^3x^5\,.
\end{aligned}$$

By separate investigation we find that this $\Phi(x)$ is positive on $(-h, h)$ and then the error is of the form (2.20).
- Value of T_0:

$$T_0 = \int_{-h}^{0} \phi_1(x)\,dx + \int_0^h \phi_2(x)\,dx = \frac{1}{396900}h^9\,.$$

Q. E. D.

The results listed above for the quadrature rules Q^2 and Q^3 allow drawing some conclusions. First, in all cases the error has the one-term Lagrange form $Ch^{m+1}y^m(\eta)$ where C is some constant (called the error constant) and m is the order of the differential equation $Ly = 0$. Second, 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) and within each of these two families the order increases with the number of data at each point (one for Q_1^p versions, two for versions Q_2^p and Q_3^p and three for Q_4^p, $p = 2, 3$). Third, 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 values of y' are more helpful in increasing the accuracy than those of y''. 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_2^2.

Numerical illustration
We compute the integral

$$Q = \int_0^1 e^{5x} \sin 5x \, dx = \frac{1}{10} e^{5x} [\sin(5x) - \cos(5x)]|_0^1 \tag{5.42}$$

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.
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 acccepted data is increased. It is also confirmed the fact that the error

Table 1: Stepwidth dependence of the absolute errors of the results given by the four versions of rule Q^2 for integral (5.42). 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)

decrease is similar for versions Q_2^2 and Q_3^2 and that for each stepwidth 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 formulae 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 versions when $h \to 0$ are clearly confirmed.

Table 3: The ratio $\Delta Q(2h)/\Delta Q(h)$ for various values of the stepwith 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	–

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