TOWARDS NON-LINEAR QUADRATURE FORMULAE

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Abstract. Prompted by an observation about the integral of exponential functions of the form \( f(x) = \lambda e^{\alpha x} \), we investigate the possibility to exactly integrate families of functions generated from a given function by scaling or by affine transformations of the argument using nonlinear generalizations of quadrature formulae. The main result of this paper is that such formulae can be explicitly constructed for a wide class of functions, and have the same accuracy as Newton-Cotes formulae based on the same nodes. We also show how Newton-Cotes formulae emerge as the linear case of our general formalism, and demonstrate the usefulness of the nonlinear formulae in the context of the Padé-Laplace method of exponential analysis.

1. Motivation

One of the most basic tasks in numerical analysis is the approximate evaluation of definite integrals by quadrature formulae. Since one of the most fundamental properties of integration is its linearity, typical quadrature formulae consist of taking linear combinations of the values of the integrand at specific values of the integration variable. Depending on whether only the linear coefficients (weights) or also the abscissae (nodes) are adjusted to minimize the error made in the numerical evaluation, one gets families of quadrature formulae such as the Newton-Cotes or Gaussian quadrature formulae. These are then exact on polynomials of a given degree.

However, the case sometimes arises that one needs to evaluate the integral of some numerically given function which is known to be very close to a family of functions (other than polynomials) whose integrals are known analytically. As an example, which arises for instance in the analysis of time series known to consist of a sum of exponentially decaying components using the Padé-Laplace method \([1]\) or in certain calculations in theoretical high-energy physics \([2]\), consider a function \( f \) which is known to be very close to an exponential, \( |f(x) - \lambda e^{\alpha x}| < \epsilon \). Then the integral of this function can be approximated by

\[
\int_a^b f(x) \, dx \approx f(b) - f(a) \log f(b) - \log f(a) \frac{b - a}{\log f(b) - \log f(a)}.
\]

This approximation is still useful even if \( \lambda \) and \( \alpha \) are not known beforehand, because they can be estimated from \( f \). Indeed, within the bound given by \( \epsilon \), we can replace \( \lambda e^{\alpha a} \) and \( \lambda e^{\alpha b} \) by \( f(a) \) and \( f(b) \), respectively, and estimate \( \alpha \) from the numerical derivative of the logarithm of \( f \) as \( \alpha = \frac{1}{h} (\log f(x + h) - \log f(x)) + O(h) \). Putting these ingredients together, we arrive at a non-linear quadrature formula

\[
\int_a^b f(x) \, dx \approx f(b) - f(a) \log f(b) - \log f(a) \frac{b - a}{\log f(b) - \log f(a)}.
\]

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We note that this formula is exact for functions of the form \( f(x) = \lambda e^{\alpha x} \), which form a non-linear family. In the following, we will try to develop a more general theoretical background for non-linear quadrature formulae of this kind.

Even though the results we will obtain do not require more than standard undergraduate analysis and therefore ought to be well-known, there appears to be hardly any literature on the topic of non-linear quadrature formulae, apart from two papers by Werner [3] and Wuytack [4], which relate to the use of rational interpolants or Padé approximants instead of interpolating polynomials to integrate functions known to have a singularity at one end of the integration interval. Our approach here will be much more general and will take eq. (2) as its exemplary case.

To this end, we will first define the class of non-linear quadrature formulae we will be considering, and will derive some general results on their accuracy and analytical properties as a consequence of their behaviour on certain families of functions. As an excursion, we will consider the traditional Newton-Cotes formulae as special (linear) cases of the general (non-linear) case and rederive some well-known results in this way. Finally, we give some explicit examples and perform some numerical experiments to investigate the potential usefulness of non-linear quadrature rules.

2. General results

We will typically consider integration over an interval of length \( h > 0 \) and write

\[
I[f] = \int_a^{a+h} f(x) \, dx
\]

for the definite integral. We will approximate this by a (generally non-linear) function \( q: \mathbb{R}^n \to \mathbb{R} \) of \( \hat{f} = (f(a + \xi_0 h), \ldots, f(a + \xi_{n-1} h)) \in \mathbb{R}^n \) via

\[
\hat{I}[f] = hq(\hat{f})
\]

in the sense that

\[
|\hat{I}[f] - I[f]| = o(h^r)
\]

for some \( r > 1 \). We will assume throughout that \( q \) and \( f \) are sufficiently smooth.

To make such approximations useful, one typically has to require that they become exact in some limiting case. We therefore define several properties that will become useful in the following:

**Definition 1.** A non-linear quadrature formula \( \hat{I} \) is

1. exact on a function \( f^* \) if \( \hat{I}[f^*] = I[f^*] \) for all \( h > 0 \),
2. scalably exact on a function \( f^* \) if there exist \( \lambda_- < 1 < \lambda_+ \) such that \( \hat{I}[\lambda f^*] = I[\lambda f^*] \) for all \( \lambda \in (\lambda_-; \lambda_+) \) and all \( h > 0 \),
3. affinely exact on a function \( f^* \) if with \( f_{\alpha,\beta}^*(x) = f^*(\alpha x + \beta) \) we have \( \hat{I}[f_{\alpha,\beta}^*] = I[f_{\alpha,\beta}^*] \) for all \( \alpha, \beta \in \mathbb{R} \) and \( h > 0 \),
4. symmetric if \( \xi_{n-k-1} = -\xi_k \) for all \( k \in \{0, \ldots, n-1\} \) and \( q(f_{n-1}, \ldots, f_0) = q(f_0, \ldots, f_{n-1}) \) for all \( f \in \mathbb{R}^n \), and
5. quasilinear if \( q(\lambda \hat{f}) = \lambda q(\hat{f}) \) for all \( \lambda \in \mathbb{R} \) and all \( \hat{f} \in \mathbb{R}^n \).

The idea behind these definitions is that we will take exactness on a family of target functions as our guide as to the goodness of a quadrature rule (while noting that this has recently been pointed out by Trefethen [5] to not be an entirely reliable heuristic in the case of traditional linear quadrature rules), and we will attempt to preserve at least some of the linear properties of integration when acting on these target functions.

First, we show that scalably exact quadratures are at least no worse than the trapezoidal rule on general functions:
Lemma 1. Let \( n = 2, \xi_0 = 0, \xi_1 = 1 \). If there exists a function \( f^* \) with \( f^*(a) \neq 0 \) and \( f^*(a) \neq 0 \) such that \( \hat{I} \) is scalably exact on \( f^* \), then \( |\hat{I}[f] - I[f]| = o(h^2) \) for all \( f \in C^2(a,a + h) \).

Proof. The Taylor expansion in \( h \) of the exact integration is given by

\[
I[f] = f(a)h + \frac{1}{2} f'(a)h^2 + \frac{1}{6} f''(a)h^3 + o(h^3)
\]

whereas that of the two-point quadrature formula is given by

\[
\hat{I}[f] = q(\bar{f})h + q^{(0,1)}(\bar{f})f'(a)h^2 + \frac{1}{2} \left( q^{(0,2)}(\bar{f})f''(a) + q^{(0,1)}(\bar{f})f'''(a) \right) h^3 + o(h^3)
\]

where \( \bar{f} = (f(a), f(a)) \) and we understand \( q(\bar{f}) \) to denote \( \lim_{b \to f(a)} q(f(a), f_b) \) in the case where \( q(\bar{f}) \) itself is ill-defined. In order for these to be identical for all \( f = \lambda f^* \), we need to have \( q(\bar{f}) = f(a) \) and \( q^{(0,1)}(\bar{f}) = \frac{1}{2} \) for all \( f \). Hence, we have for arbitrary \( f \in C^2(a,a + h) \) that

\[
|\hat{I}[f] - I[f]| = \left| \frac{1}{2} q^{(0,2)}(\bar{f})[f'(a)]^2 + \frac{1}{12} f''(a) \right| h^3 + o(h^3) = o(h^2).
\]

\[\Box\]

Noting that the exactness of \( \hat{I} \) on functions of the form \( \lambda f^* \) requires linearity of \( q \) in the vicinity of \( f^* \) since \( \hat{I}[\lambda f^*] = I[\lambda f^*] = \lambda I[f^*] = \lambda \hat{I}[f^*] \), we find relationships between the partial derivatives of \( q \):

Lemma 2. Let \( \hat{I} \), \( f^* \) be as in Lemma 1. Then

\[
q^{(1,0)}(\bar{f}^*) + q^{(0,1)}(\bar{f}^*) = 1,
\]

\[
q^{(0,2)}(\bar{f}^*) + q^{(1,1)}(\bar{f}^*) = 0,
\]

\[
q^{(0,2)}(\bar{f}^*) + 2q^{(1,1)}(\bar{f}^*) + q^{(2,0)}(\bar{f}^*) = 0
\]

\[
q^{(0,3)}(\bar{f}^*) + 3q^{(1,2)}(\bar{f}^*) + 3q^{(2,1)}(\bar{f}^*) + q^{(3,0)}(\bar{f}^*) = 0
\]

\[
q^{(0,3)}(\bar{f}^*) + 2q^{(1,2)}(\bar{f}^*) + q^{(2,1)}(\bar{f}^*) = 0
\]

Proof. We expand the exact integral (which is of course linear) in powers of \( h \)

\[
I[\lambda f^*] = h\lambda f^*(a) + \frac{1}{2} h^2 \lambda f''(a) + \frac{1}{6} h^3 \lambda f'''(a) + o(h^3)
\]

and perform a double expansion of \( \hat{I}[\lambda f^*] \) into powers of \( h \) and \( \lambda - 1 \),

\[
\hat{I}[\lambda f^*] = h \left[ q(f^*) + (\lambda - 1) f(a) \left( q^{(1,0)}(\bar{f}^*) + q^{(0,1)}(\bar{f}^*) \right) \right. \\
\left. + \frac{(\lambda - 1)^2}{2} f(a)^2 \left( q^{(0,2)}(\bar{f}^*) + 2q^{(1,1)}(\bar{f}^*) + q^{(2,0)}(\bar{f}^*) \right) \right. \\
\left. + \frac{(\lambda - 1)^2}{6} f(a)^3 \left( q^{(0,3)}(\bar{f}^*) + 3q^{(1,2)}(\bar{f}^*) + 3q^{(2,1)}(\bar{f}^*) + q^{(3,0)}(\bar{f}^*) \right) \right] \\
\frac{1}{2} h^2 f'''(a) \left[ \lambda + 2(\lambda - 1) f(a) \left( q^{(0,2)}(\bar{f}^*) + q^{(1,1)}(\bar{f}^*) \right) \right. \\
\left. + (\lambda - 1)^2 \lambda f(a)^2 \left( q^{(0,3)}(\bar{f}^*) + 2q^{(1,2)}(\bar{f}^*) + q^{(2,1)}(\bar{f}^*) \right) \right] \\
\left. + o(h^2) + o(h(\lambda - 1)^3) + o(h^2(\lambda - 1)^2) \right.
\]

and equality for all \( \lambda \) and \( h \) is only possible if the given relations hold.

\[\Box\]

We therefore find that scalably exact non-linear quadratures locally resemble the trapezoidal rule:
Corollary 1. Let $n = 2$, $\xi_0 = 0$, $\xi_1 = 1$, and let $\hat{I}$ be scalably exact on $f^*$ with $f^{*'}(a) \neq 0$. Then

$$q(f(a), f(b)) = \frac{f(a) + f(b)}{2} - \frac{1}{12} \frac{f^{*''}(a)}{[f^{*'}(a)]^2} (f(b) - f(a))^2 + o((f(b) - f(a))^2).$$

Proof. Since $\hat{I}[f^*] = I[f^*]$, we must have

$$\frac{1}{2} \left( q^{(0,2)}(\hat{f}^*)[f^{*'}(a)]^2 + q^{(0,1)}(\hat{f}^*) f^{*''}(a) \right) = \frac{1}{6} f^{*''}(a)$$

and using $q^{(0,1)}(\hat{f}) = \frac{1}{2}$ then yields

$$q^{(0,2)}(\hat{f}^*) = -\frac{1}{6} \frac{f^{*''}(a)}{[f^{*'}(a)]^2}.$$

Substituting this into the Taylor expansion of $q(f(a), f(b))$ around $f(b) = f(a)$ and using the relations between the partial derivatives of $q$ found above yields the result. \hfill \square

We note that this corollary can be used to construct an improved trapezoidal rule for functions known a priori to be close to multiples of a given function $f^*$ for which no explicit form of $q$ satisfying $I[\lambda f^*] = I[\lambda f^*]$ is known by simply setting

$$q(f(a), f(b)) = \frac{f(a) + f(b)}{2} - \frac{1}{12} \frac{f^{*''}(a)}{[f^{*'}(a)]^2} (f(b) - f(a))^2$$

(15)

to reduce the integration error of the trapezoidal rule by using the known curvature behaviour of $f^*$.

Essentially identical results can be shown for affinely exact non-linear quadrature formulæ.

Lemma 3. Let $n = 2$, $\xi_0 = 0$, $\xi_1 = 1$. If there exists a function $f^*$ with $f^*(a) \neq 0$ and $f^{*'}(a) \neq 0$ such that $\hat{I}$ is affinely exact on $f^*$, then $|\hat{I}[f] - I[f]| = o(h^2)$ for all $f \in C^2(a, a + h)$. Moreover,

$$q^{(1,0)}(\hat{f}^*) + q^{(0,1)}(\hat{f}^*) = 1,$$

(16)

$$q^{(0,2)}(\hat{f}^*) + q^{(1,1)}(\hat{f}^*) = 0,$$

$$q^{(0,3)}(\hat{f}^*) + 3q^{(1,2)}(\hat{f}^*) + 3q^{(2,1)}(\hat{f}^*) + q^{(3,0)}(\hat{f}^*) = 0,$$

$$q^{(0,3)}(\hat{f}^*) + q^{(1,2)}(\hat{f}^*) + q^{(2,1)}(\hat{f}^*) = 0.$$

Proof. We start by noting that the Taylor expansion of $I[f_{a,\beta}^*]$ in $h$ is

$$I[f_{a,\beta}^*] = hf^*(\alpha a + \beta) + \frac{\alpha h^2}{2} f^{*'}(\alpha a + \beta) + o(h^2)$$

(17)

whereas that of $\hat{I}[f_{a,\beta}^*]$ is

$$\hat{I}[f_{a,\beta}^*] = hq(f_{a,\beta}^*) + \alpha h^2 q^{(0,1)}(f_{a,\beta}^*) f^{*'}(\alpha a + \beta) + o(h^2)$$

(18)

and equality for all $h, \alpha, \beta$ is only possible if for all values of $\hat{f}$ with $f(a)$ in the range of $f^*$ the equalities $q(\hat{f}) = f(a)$ and $q^{(0,1)}(\hat{f}) = \frac{1}{2}$ hold, implying $|\hat{I}[f] - I[f]| = o(h^2)$ as in Lemma 1. Furthermore, the Taylor expansions around $\alpha = 0$ of the
coefficients of \( h \) and \( h^2 \) are
\[
q(f^*_a, \beta) = q(f^*_0, \beta) + \alpha a f''(\beta) \left( q^{(0,1)}(f^*_0, \beta) + q^{(1,0)}(f^*_0, \beta) \right) \\
+ \frac{(\alpha a)^2}{2} \left[ f'''(\beta) \left( q^{(0,1)}(f^*_0, \beta) + q^{(1,0)}(f^*_0, \beta) \right) \\
+ \left[ f''(\beta) \right]^2 \left( q^{(0,2)}(f^*_0, \beta) + 2q^{(1,1)}(f^*_0, \beta) + q^{(2,0)}(f^*_0, \beta) \right) \right] \\
+ \frac{(\alpha a)^3}{6} \left[ f^{(3)}(\beta) \left( q^{(0,1)}(f^*_0, \beta) + q^{(1,0)}(f^*_0, \beta) \right) \\
+ 3f''(\beta)f'''(\beta) \left( q^{(0,2)}(f^*_0, \beta) + 2q^{(1,1)}(f^*_0, \beta) + q^{(2,0)}(f^*_0, \beta) \right) \\
+ \left[ f''(\beta) \right]^3 \left( q^{(0,3)}(f^*_0, \beta) + 3q^{(1,2)}(f^*_0, \beta) + 3q^{(2,1)}(f^*_0, \beta) + q^{(3,0)}(f^*_0, \beta) \right) \right] \\
+ o(\alpha^3)
\]
and
\[
q^{(0,1)}(f^*_a, \beta) f''(\alpha + \beta) = f''(\beta) q^{(0,1)}(f^*_0, \beta) \\
+ \alpha a \left[ f'''(\beta) q^{(0,1)}(f^*_0, \beta) \\
+ \left[ f''(\beta) \right]^2 \left( q^{(0,2)}(f^*_0, \beta) + q^{(1,1)}(f^*_0, \beta) \right) \right] \\
+ \frac{(\alpha a)^2}{2} \left[ f^{(3)}(\beta) q^{(0,1)}(f^*_0, \beta) \\
+ 3f''(\beta)f'''(\beta) \left( q^{(0,2)}(f^*_0, \beta) + q^{(1,1)}(f^*_0, \beta) \right) \\
+ \left[ f''(\beta) \right]^3 \left( q^{(0,3)}(f^*_0, \beta) + 2q^{(1,2)}(f^*_0, \beta) + q^{(2,1)}(f^*_0, \beta) \right) \right] \\
+ o(\alpha^2),
\]
which must be equal to
\[
f^*(\alpha + \beta) = f^*(\beta) + \alpha a f''(\beta) + \frac{(\alpha a)^2}{2} f'''(\beta) + \frac{(\alpha a)^3}{6} f^{(3)}(\beta) + o(\alpha^3)
\]
and
\[
\frac{1}{2} f''(\alpha + \beta) = \frac{1}{2} f''(\beta) + \frac{\alpha a}{2} f'''(\beta) + \frac{(\alpha a)^2}{4} f^{(3)}(\beta) + o(\alpha^2)
\]
respectively, whence the relations immediately follow. \( \square \)

The equations for the partial derivatives of scalably or affinely exact \( q \) are readily solved, leading to the following

**Corollary 2.** Let \( n = 2, \xi_0 = 0, \xi_1 = 1, \) and let \( \tilde{I} \) be scalably or affinely exact on some function \( f^* \) with \( f^*(a) \neq 0 \) and \( f''^*(a) \neq 0 \). Then
\[
q(\tilde{f}) = f(a),
\]
\[
q^{(1,0)}(\tilde{f}) = q^{(0,1)}(\tilde{f}) = \frac{1}{2}, \\
q^{(2,0)}(\tilde{f}) = -q^{(1,1)}(\tilde{f}) = q^{(0,2)}(\tilde{f}).
\]
If \( \tilde{I} \) is moreover symmetric, then also
\[
q^{(3,0)}(\tilde{f}) = -3q^{(1,2)}(\tilde{f}) = -3q^{(2,1)}(\tilde{f}) = q^{(0,3)}(\tilde{f}).
\]
\( \square \)
At least for a certain class of functions, symmetric affinely exact non-linear quadrature formulae are readily constructed:

**Theorem 1.** Let \( f^* : \mathbb{R} \to \mathbb{R} \subseteq \mathbb{R} \) be bijective with inverse function \( f^{*-1} \), and let \( F^* \) be an antiderivative of \( f^* \). Define

\[
q_1(f_0, f_1) = \frac{F^*(f^{*-1}(f_1)) - F^*(f^{*-1}(f_0))}{f^{*-1}(f_1) - f^{*-1}(f_0)}.
\]

Then

\[
\hat{I}_1[f] = h q_1(f(a), f(a + h))
\]
is symmetric and affinely exact on \( f^* \), and with

\[
q_2(f_0, f_1, f_2) = \frac{2}{3} (q_1(f_0, f_1)) + q_1(f_1, f_2)) - \frac{1}{3} q_1(f_0, f_2)
\]
the three-point non-linear quadrature formula with \( \xi_0 = 0, \xi_1 = \frac{1}{2}, \xi_2 = 1 \) given by

\[
\hat{I}_2[f] = h q_2(f(a), f(a + h))
\]
is symmetric and affinely exact on \( f^* \) and has \( o(h^4) \) errors for \( f \in C^4(\mathbb{R}) \).

**Proof.** We have

\[
q_1(f^*(\alpha \alpha + \beta), f^*(\alpha \alpha + h \alpha + \beta)) = \frac{F^*(\alpha \alpha + h \alpha + \beta) - F^*(\alpha \alpha + \beta)}{\alpha \alpha + h \alpha - \alpha \alpha}
\]
and hence

\[
\hat{I}[f^*_{\alpha, \beta}] = \frac{F^*(\alpha \alpha + h \alpha + \beta) - F^*(\alpha \alpha + \beta)}{\alpha} = I[f^*_{\alpha, \beta}]
\]
as required. The symmetry of \( q_1 \) under an interchange of its two arguments is readily apparent.

Since \( q_1 \) is a symmetric affinely exact non-linear quadrature formula, its partial derivatives at each order are given by Corollary 2. We form the linear combination

\[
\hat{I}_2[\hat{f}] = \alpha_1 q_1(f(a), f(a + h)) \]

\[
+ \alpha_2 \left( q_1(f(a), f(a + \frac{1}{2} h)) + q_1(f(a + \frac{1}{2} h), f(a + h)) \right)
\]
and determine the weights \( \alpha_1 \) from expanding

\[
\hat{I}_2[\hat{f}] = \alpha_1 q_1(f(a), f(a + h))
\]

\[
+ \frac{1}{2} \alpha_1 + 2 \alpha_2 \right) h f(a) + \frac{1}{2} \left( \alpha_1 + 2 \alpha_2 \right) h^2 f'(a)
\]

\[
+ \frac{1}{8} h^3 \left( 2 (2 \alpha_1 + \alpha_2) f'(a)^2 q_1^{(0,2)}(f(a), f(a))
\]

\[
+ (2 \alpha_1 + 3 \alpha_2) f''(a) \right) + \frac{1}{48} h^4 \left( 4 (2 \alpha_1 + \alpha_2) f'(a)^3 q_1^{(0,3)}(f(a), f(a))
\]

\[
+ 12 (2 \alpha_1 + \alpha_2) f''(a) q_1^{(0,2)}(f(a), f(a))
\]

\[
+ (4 \alpha_1 + 5 \alpha_2) f^{(3)}(a) \right) + o(h^4)
\]

and equating this with

\[
I[f] = h f(a) + \frac{1}{2} h^2 f'(a) + \frac{1}{6} h^3 f''(a) + \frac{1}{24} h^4 f^{(3)}(a) + o(h^4)
\]

which yields the solution \( \alpha_1 = -\frac{1}{8}, \alpha_2 = \frac{2}{4} \).

Since each of the approximations across subintervals is affinely exact, so is their linear combination. The symmetry of \( q_2 \) follows from that of \( q_1 \) by inspection. \( \square \)
We note that the proof of eq. (27) only relied on \( q_1 \) being affinely exact and symmetric, and hence this construction could also be used to obtain an \( o(h^4) \) quadrature rule \( q_2 \) from an affinely exact symmetric quadrature rule \( q_1 \) that is not of the specific form (25). Similar constructions can be carried out to obtain analogues of higher-order Newton-Cotes rules using additional nodes.

3. Traditional quadrature rules as linear approximations

We first note that when applying the construction of eq. (25) to the identity function \( f^*(x) = x \) with inverse \( f^{-1}(x) = x \) and antiderivative \( F^*(x) = \frac{1}{2}x^2 + C \), we obtain the trapezoidal rule,

\[
\hat{I}[f] = \frac{h}{2} (f(a) + f(a + h))
\]

which is affinely exact by construction, and hence is exact on all first-order polynomials \( f(x) = \alpha x + \beta \). We have thus given an alternative derivation of a well-known result:

**Corollary 3.** The trapezoidal rule

\[
\hat{I}[f] = \frac{h}{2} (f(a) + f(a + h))
\]

is exact for all first-order polynomials \( f(x) \) and has \( o(h^2) \) errors for \( f \in C^2(\mathbb{R}) \) otherwise.

We note that when the trapezoidal rule is used for \( q_1 \) in eq. (27), the rule \( q_2 \) obtained in this way is precisely Simpson’s rule, yielding another alternative proof of a well-known result:

**Corollary 4.** The quadrature rule

\[
\hat{I}[f] = \frac{h}{6} \left( f(a) + 4f(a + \frac{h}{2}) + f(a + h) \right)
\]

has \( o(h^4) \) errors for \( f \in C^4(\mathbb{R}) \).

Similarly, the higher-order Newton-Cotes rules can be obtained without any explicit reference to polynomial interpolation by linearly combining the different evaluations of the integral from \( a \) to \( a + h \) that can be formed using the trapezoidal rule on the nodes of the higher-order Newton-Cotes rule and optimizing the coefficients of the linear combination to minimize the total error:

**Corollary 5.** Let \( n \) be odd. Then the \( n \)-point quadrature rule

\[
\hat{I}[f] = h \sum_{k=0}^{n-2} \alpha_k \left( \xi_k f(a) + f(a + \xi_k h) + (1 - \xi_k) f(a + \xi_k h) + f(a + h) \right)
\]

with \( \xi_k = \frac{k}{n-1} \) and \( \alpha_k \) given by the solution of the linear equation system

\[
\sum_{k=0}^{n-2} \alpha_k \left( \xi_k^j - \xi_k + 1 \right) = \frac{2}{j+1}, \quad j = 2, \ldots, n
\]

is identical to the \( n \)-point Newton-Cotes rule with nodes \( \xi_k \) (taking \( \xi_{n-1} = 1 \)).

**Proof.** First, we note that by linearity, we can write

\[
\hat{I}[f] = h \sum_{k=0}^{n-1} w_k f(a + \xi_k h)
\]
determining a unique linear $n$-point quadrature formula. Next, we note that
\[
\xi_k^i h f(a) + f(a + \xi_k h) + (1 - \xi_k) h f(a + \xi_k h) + f(a + h) = \frac{1}{2} f(a) h + \frac{1}{2} f'(a) h^2 + \sum_{j=2}^{\infty} \frac{1}{2j!} f^{(j)}(a) \left[ \xi_k^j - \xi_k + 1 \right] h^{j+1}
\]
and hence demanding that the Taylor expansion of $\hat{I}[f]$ matches that of $I[f]$ up to order $h^n$ amounts to the $(n - 1) \times (n - 1)$ linear equation system
\[
\sum_{k=0}^{n-2} \alpha_k \left( \xi_k^j - \xi_k + 1 \right) = \frac{2}{j+1} \quad j = 2, \ldots, n
\]
which has a unique solution since the rows are polynomials of different orders in $\xi_k$ and hence must be linearly independent. This unique solution yields an $n$-point quadrature formula that is exact on polynomials of order $n - 1$ (whose derivatives from the $n^{th}$ on all vanish), and hence must be identical to the $n$-point Newton-Cotes rule on nodes $\xi_k$, which is defined by this exactness.

One easily verifies that Simpson’s ($n = 3$), Boole’s ($n = 5$) and Weddle’s ($n = 7$) rules are recovered in this way.

4. Explicit Non-linear Examples

The construction of Theorem 1 for $f^*(x) = e^x$ yields
\[
q_1(\hat{f}) = \frac{f(a + h) - f(a)}{\log f(a+h) / f(a)}
\]
which by construction is symmetric and affinely exact for $f^*(x) = e^x$. Since $\lambda e^{\alpha x} = e^{\alpha x + \beta}$ with $\beta = \log \lambda$, the corresponding non-linear quadrature formula is also scalably exact on all functions of the form $f(x) = e^{\alpha x}$. Finally, this quadrature formula is quasilinear since the numerator is linear and any scalar factor $\lambda$ cancels within the denominator.

In applications like the Padé-Laplace method we also require the momenta of multiexponential functions, and thus need to integrate products of multiexponential functions given as data points and monomials $x^n$. In this case, the integrand decays exponentially at large $x$, but grows polynomially at small $x$, so that nonlinear quadrature rules for exponentials will only work well at large $x$, while Newton-Cotes rules will be more appropriate at small $x$. One way to determine where the change in regime to exponential decay happens would be to consider numerical derivatives of the data $f_k = f(kh)$ and to use the nonlinear quadrature rule only in the convex decaying region where $f_k < f_{k-1}$ and $2f_k < f_{k-1} + f_{k+1}$, and to use Simpson’s rule otherwise.

We can, however, do better than this by considering the integration-by-parts identity
\[
\int x^n e^{\alpha x} dx = \frac{x^n}{\alpha} e^{\alpha x} - \frac{n}{\alpha} \int x^{n-1} e^{\alpha x} dx
\]
with solution
\[
\int x^n e^{\alpha x} dx = \sum_{k=0}^{n} \frac{(-1)^k k!}{n-k} \frac{x^{n-k} e^{\alpha x}}{(n-k)! \alpha^{k+1}}
\]
and use the same heuristic that originally led us to consider eq. (12) in the first place to arrive at a quadrature formula for moments of functions that are close to
an exponential,

\[ \hat{I}^n[f] = \sum_{k=0}^{n} \frac{(-1)^k n! (a + h)^{n-k} f(a) - a^{n-k} f(a)}{n! (n-k)!} h^{k+1}. \]

This formula is scalably exact on functions of the form \( f(x) = e^{\alpha x} \), \( \hat{I}^n[\lambda e^{\alpha x}] = I[x^n \lambda e^{\alpha x}] \), and has \( O(h^3) \) errors,

\[ \left| \hat{I}^n[f] - \int_a^{a+h} x^n f(x) \right| = \frac{f(a)f''(a) - f'(a)^2}{12f(a)} a^n h^3 + O(h^4), \]

making it ideally suited for usage with the Padé-Laplace method.

Finally, we note that for the case (common in applications) where we need to estimate an improper integral out to infinity from a finite number of samples \( f(x_k) \), we can readily generalize eq. (42) in order to get a quadrature rule for improper integrals of the form

\[ \int_a^{\infty} f(x) \, dx \approx h \frac{f(a)}{\log \frac{f(a)}{f(a+h)}} \]

assuming that \( f \) is monotonically decaying with exponential speed such that the integral converges and \( f(a) > f(a+h) \). This rule is scalably exact on all functions of the form \( f(x) = e^{\alpha x}, \alpha < 0 \), but the error analysis for the case of the proper integral does not carry through (as there is notably no \( h \) dependence of the left-hand side).

5. Numerical Experiments

We have tested the accuracy of eq. (42), and of the corresponding three-point quadrature formula by comparison with the trapezoidal rule and Simpson’s rule, respectively. To this end we consider the integrals of

\[ f_1(x) = e^{-x} + \frac{1}{2} e^{-2x}, \]
\[ f_2(x) = \sum_{n=1}^{\infty} e^{-nx} = \frac{1}{e^x - 1}, \]
\[ f_3(x) = \cosh x, \]
\[ f_4(x) = \sin x, \]

over the intervals \([a; b] = [0, 1], [1; 2], [0; 1], \) and \([\frac{\pi}{8}; \frac{\pi}{4}]\), respectively.

First, we consider the accuracy of a single step \([a; a + h]\). Figures 1 and 2 show the comparison between the relative errors

\[ E(h) = \frac{|\hat{I}[f] - I[f]|}{|I[f]|} \]

for the \( o(h^2) \) and \( o(h^4) \) cases in their respective left columns. The right columns show the error ratios

\[ R(h) = \frac{|\hat{I}[f] - I[f]|}{|\hat{I}_0[f] - I[f]|} \]

where \( \hat{I} \) and \( \hat{I}_0 \) are the non-linear and linear quadrature formulae, respectively.

It can be seen that on \( f_1 \) and \( f_2 \), which are well described as being dominated by a leading exponential, the non-linear quadrature formulae outperform their linear counterparts by approximately an order of magnitude in error in the case of \( f_1 \) and a factor of 2 to 4 in the case of \( f_2 \). In the case of \( f_3 \), which is a sum of two
exponentials, but with opposite signs of the exponent, the advantage of the non-linear rules is very small in the \( o(h^2) \) case and non-existent in the \( o(h^4) \) case, where Simpson’s rule is more efficient by a factor of 4. In the case of \( f_4 \), which not a sum of real exponentials at all (although it is the sum of complex exponentials), the non-linear rules tailored to real exponentials fare very poorly, with one to two orders of magnitude larger errors than their linear counterparts (a large part of this likely being due to the fact that \( f_4 \) is positive and concave on the integration interval, while the non-linear rules implicitly assume a positive convex, or negative concave, function).

Given that the construction of Theorem 1 takes the quotient of two differences, the question of its numerical stability naturally arises. This is even more pronounced in the case of the higher-order rule, which involves an additional difference due to the negative coefficient \(-\frac{1}{3}\). This expectation is borne out by the numerical data, which show the advantage of the nonlinear rules over the linear ones vanishing as the step size \( h \) is reduced to below a point where the differences become numerically unstable.

As the examples of the trapezoidal rule and Simpson’s rule in the previous section show, numerical instability is not a given since there may be a manifestly stable form of the quadrature rule that is mathematically equivalent to the construction of Theorem 1 in exact arithmetic. Whenever possible, it is therefore desirable to bring the quadrature rule derived from Theorem 1 into a form that involves as few differences as possible.

Next, we consider the convergence of the full integrals over \([a; b]\) evaluated using \( N \) steps from \( a + kh \) to \( a + (k+1)h \) with \( h = \frac{b-a}{N} \). Figure 3 shows the exact values of the integrals as dotted horizontal lines and the numerical evaluations using the \( o(h^2) \) and \( o(h^4) \) rules in the left and right columns, respectively (note that the vertical scales in the left and right columns differ markedly). The approach to the continuum limit is as expected from the previous two figures. We note that a form of Romberg quadrature based on the non-linear formulae should work as well (or better in the nearly-exponential cases where the extrapolation is much flatter) as traditional Romberg quadrature based on the linear formulae.

### 6. Conclusions and Outlook

We have defined general classes of non-linear quadrature rules that are exact on certain families of functions related by scaling of their value or affine transformations of their argument, and have shown that such non-linear quadrature rules must obey various relations between their partial derivatives. Our core result is Theorem 1 which gives an explicit construction of affinely exact non-linear quadrature rules for given target functions and demonstrates that these can be combined to yield higher-order non-linear quadrature rules. Numerical experiments demonstrate the superiority of the non-linear formulae on functions close to the families on which they are exact, while also indicating that their usefulness outside this intended domain of application is rather limited.

Future research should address the question of how to generalize Gaussian quadrature to the non-linear case. The most naive approach of simply varying the nodes \( \zeta_k \) and trying to reach higher-order accuracy by an optimal choice does not work in general. However, there is a tantalizing glimpse of what non-linear Gaussian integration could look like in the form of the \( o(h^2) \) two-point formula

\[
q(f_0, f_1) = \frac{f_0 - f_1}{\log \frac{f_0}{f_1}} - \frac{1}{12} (f_0 - f_1) \log \frac{f_0}{f_1}
\]

(54)
with $f_0 = f(a + \xi h)$, $f_1 = (a + (1 - \xi)h)$, $\xi = \frac{3 - \sqrt{3}}{6}$, which, however, is no longer scalably exact or affinely exact on exponential functions. It is probably no accident that the nodes $\xi, 1 - \xi$ are precisely those of $n = 2$ Gauss-Legendre quadrature, but a general theory of such quadrature rules is still elusive. Likewise, non-linear analogues of Clenshaw-Curtis quadrature would be an interesting direction of research.

**Conflicts of interest**

The author is not aware of any personal, professional, financial, political or other circumstances that could give rise to a relevant conflict of interest.

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**References**

[1] E. Yeramian and P. Claverie, Analysis of multiexponential functions without a hypothesis as to the number of components, Nature 326 (1987) 169–174.

[2] D. Bernecker and H. B. Meyer, Vector Correlators in Lattice QCD: Methods and applications, Eur. Phys. J. A 47 (2011) 148, doi:10.1140/epja/i2011-11148-6 [arXiv:1107.4388].

[3] H. Werner and L. Wuytack, Nonlinear Quadrature Rules in the Presence of a Singularity, Comp. & Maths. with Appl. 4 (1978) 237–245.

[4] L. Wuytack, Numerical integrator by using nonlinear techniques, J. Comp. Appl. Math. 1 (1975) 267–272.

[5] L. N. Trefethen, Exactness of Quadrature Formulas, SIAM Review 64 (2022) 132–150, doi:10.1137/20M1389522 [arXiv:2101.09501].

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Figure 1. Comparison between the non-linear exponential rule (blue) and the trapezoidal rule (red) of the relative error $|\hat{I}[f] - I[f]|/|I[f]|$ (left) and the ratio of the errors between the two rules (right) on a range of integrands (top to bottom: $e^{-x} + \frac{1}{2} e^{-2x}$, $(e^x - 1)^{-1}$, $\cosh x$, $\sin x$). See the text for details.
Figure 2. Comparison between the higher-order non-linear exponential rule (blue) and Simpson’s rule (red) of the relative error $|\hat{I}[f] - I[f]|/|I[f]|$ (left) and the ratio of the errors between the two rules (right) on a range of integrands (top to bottom: $e^{-x} + \frac{1}{2}e^{-2x}$, $[e^x - 1]^{-1}$, $\cosh x$, $\sin x$). See the text for details.
Figure 3. Comparison between the results from multistep evaluation of integrals using the non-linear exponential rule (blue) and the trapezoidal rule (red) on the left, and the higher-order non-linear exponential rule (blue) and Simpson’s rule (red) on the right. The integrands are (top to bottom) $e^{-x} + \frac{1}{2}e^{-2x}$, $[e^x - 1]^{-1}$, $\cosh x$, $\sin x$. Note the differences in scale. See the text for details.