Diss. ETH No. 18347

# Adaptive Quadrature Re-Revisited

*A dissertation submitted to the*
SWISS FEDERAL INSTITUTE OF TECHNOLOGY
ZÜRICH

*for the degree of*
DOCTOR OF SCIENCES

*presented by*
**Pedro Gonnet**

Dipl. Inf. Ing., ETH Zürich
born on January 6th, 1978
citizen of Zürich, Switzerland

*Accepted on the recommendation of*
Prof. Dr. W. Gander, examiner
Prof. Dr. J. Waldvogel, co-examiner
Prof. Dr. D. Laurie, co-examiner

2009

ISBN 978-0-557-08761-7

# Acknowledgments

First and foremost I would like to thank my thesis advisor, Prof. Walter Gander who gave me the opportunity to switch to his group and offered me an interesting topic. I also thank him for introducing me to his many friends and acquaintances in what is, in my opinion, more of a *family* than a field.

From this family and the Department of Computer Science at large, I would also like to thank Oscar Chinellato, Prof. Jörg Waldvogel, Michael Bergdorf, Urs Zimmerli, Marco Wolf, Martin Müller, Marcus Wittberger, Cyril Flaig, Dirk Zimmer and Prof. François Cellier who all contributed in some part, through discussions or support, to the completion of this thesis.

I would also like to thank Prof. Milovanovic, Prof. Bojanov, Prof. Nikolov and Aleksandar Cvetkovic, as well as the many participants of the SCOPES meetings in Serbia, Bulgaria and here in Zurich for giving me a chance to present my work and learn from their questions and their criticisms.

Many thanks also go to E. H. A. Venter, F. J. Smith, E. de Doncker, P. Davis, T. O. Espelid and R. Jaffe for their help in retrieving and understanding some of the older or less accessible publications referenced in this thesis.

Many thanks go to my family: My mother, Marta, my younger brothers Julio and Ignacio for their support. Very special thanks go to my older sister Ariana, who took the time to proofread this dissertation. I thank my father, Gaston, for his support, advice and long conversations over coffee regarding computing, research, science, politics and life.

Most importantly, I would like thank Joanna, whom I love very much, for her patience and understanding, for standing by me and for pushing me forward.

Pedro Gonnet
Zurich, December 2008

# Abstract

The goal of this thesis is to explore methods to improve on the reliability of adaptive quadrature algorithms. Although adaptive quadrature has been studied for several years and many different algorithms and techniques have been published, most algorithms fail for a number of relatively simple integrands.

The most important publications and algorithms on adaptive quadrature are reviewed. Since they differ principally in their error estimates, these are tested and analyzed in detail and their similarities and differences are discussed.

In order to construct a more reliable error estimate, we start with a more complete and explicit representation of the integrand. To this extent, we **explicitly construct the interpolatory polynomial over the nodes of a quadrature rule**, which is constructed implicitly when the quadrature rule is evaluated.

The interpolatory polynomial is represented as a linear combination of orthogonal polynomials satisfying a three-term recurrence relation. Two new algorithms are presented for the efficient and numerically stable **construction, update and downdate** of such interpolations.

This representation can be easily **transformed** to any interval, thus allowing for its re-use inside the sub-intervals. The interpolation updates can be used to increase the degree of a quadrature rule by adding more nodes and the downdates can be used to remove nodes for which the integrand is not defined.

Based on this representation, **two new error estimates** based on the $L_2$-norm of the difference between the interpolant and the integrand (as opposed to using the integral of the difference between the interpolant and the integrand) are derived and shown to be more reliable than previously published error estimates. The space of possible integrands for which the new estimators will fail is shown to be smaller than that of previous error estimators.

A mechanism for the **detection of divergent integrals**, which may cause the algorithm to recurse infinitely and are usually caught by artificially limiting the number of function evaluations, is also included and tested.

These new improvements are implemented in **three new quadrature routines** and tested against several other commonly used routines. The results show that the new algorithms are **all more reliable** than previously published algorithms.

# Zusammenfassung

Das Ziel dieser Dissertation ist es, Verfahren zu untersuchen, um die Zuverlässigkeit von Algorithmen zur adaptiven Quadratur zu verbessern. Obwohl an der adaptiven Quadratur seit mehreren Jahren geforscht wird und eine Vielzahl von Algorithmen und Techniken schon publiziert wurden, versagen die gängigen Verfahren für zum Teil sehr einfache Integranden.

Die wichtigsten Publikationen und Algorithmen werden hier besprochen. Da sie sich hauptsächlich in der Art der Fehlerschätzung unterscheiden, werden die Verfahren zur Fehlerschätzung im Detail untersucht und getestet. Die Gemeinsamkeiten und Unterschiede zwischen den einzelnen Verfahren werden diskutiert.

Um einen genaueren Fehlerschätzer zu konstruieren, wird zuerst eine vollständige und explizite Darstellung des Integranden angefangen. Um diese zu erhalten, wird das Interpolationspolynom über die Knoten der Quadraturregel explizit konstruiert, welches sonst von dieser nur implizit berechnet wird.

Das Interpolationspolynom wird als Linearkombination einer orthogonalen Polynomialbasis dargestellt. Die Polynome dieser Basis erfüllen eine dreigliedrige Rekursionsformel. Zwei neue Algorithmen zur Berechnung, zur Erweiterung und zur Reduktion einer solchen Interpolation werden vorgestellt und getestet.

Diese Darstellung kann später auf ein beliebiges Intervall transformiert werden, was die Wiederverwertung in den Subintervallen ermöglicht. Die Interpolations-Erweiterung kann dazu benutzt werden, den Grad einer Quadraturformel zu erhöhen, indem zusätzliche Punkte zur Interpolation hinzugefügt werden und die Reduktion kann benutzt werden, um Punkte zu entfernen an denen der Integrand nicht definiert ist.

Gestützt auf diese Darstellung werden zwei neue Fehlerschätzer konstruiert. Es wird gezeigt, dass die neuen Fehlerschätzer zuverlässiger als die bisher publizierten Verfahren funktionieren und dass der Raum aller Funktionen, für die sie nicht funktionieren, stärker eingeschränkt ist als bei anderen Verfahren.

Ein neuer Mechanismus zur Erkennung divergenter Integrale, die bei anderen Verfahren zu einer unendlichen Rekursion führen können und durch willkürliche Rekursionsbeschränkungen abgefangen werden, wird ebenfalls vorgestellt und getestet.

Diese Neuerungen werden in drei neue Quadraturverfahren implementiert und gegen mehrere etablierte Verfahren getestet. Die Resultate zeigen, dass die drei neue Algorithmen zuverlässiger sind als die anderen im Test.

# Table of Contents

# Chapter 1

# Introduction

## 1.1 Goals

Since the publication of the first adaptive quadrature routines in 1962 [55, 68], much work has been done and published on the subject, introducing new quadrature rules, new termination criteria, new error estimates, new data types and new extrapolation algorithms.

With these improvements, adaptive quadrature has advanced both in terms of reliability and efficiency, yet for most algorithms it is still relatively simple to find integrands for which they will *fail*. These integrands are not just pathological cases that would rarely occur in normal applications, but include relatively simple functions which *do* appear in every day use.

The goal of this thesis is to explore new methods in adaptive quadrature to make the process *more reliable* as a whole. This should be done, if possible, without aversely impacting its *efficiency*.

To this end, we will focus on computing better *error estimates* by using an *explicit representation of the integrand*. In doing so, we will also be able to *re-use* more information over several levels of recursion and be able to treat singularities, non-numerical function values, divergent integrals and other problems in a more efficient way.

The resulting algorithms should be able to integrate a larger set of integrands reliably with little or no performance penalty as compared to current “state-of-the-art” algorithms.

## 1.2 Notation, Definitions and Fundamental Concepts

In the following, we will use the notation

$$Q_n^{(m)}[a,b] \approx \int_a^b f(x)\,\mathrm{d}x$$

For a quadrature rule $Q$ of *degree* $n$ and *multiplicity* $m$ over the interval $[a,b]$.

In several publications the notations $Q_n^{(m)}[a,b]f$ or $Q_n^{(m)}[a,b](f(x))$ are used to specify which function the quadrature rule is to be applied to. Since in most cases it is usually clear what integrand is intended, we will use the latter notation only when it is not obvious, from the context, to which function the quadrature rule is to be applied.

We will use the term **degree** to denote the *algebraic degree of precision* of a quadrature rule. A quadrature rule is of degree $n$ when it integrates all polynomials of degree $\leq n$ exactly, but not all polynomials of degree $n+1$. This is synonymous with the *precise degree of exactness* as defined by Gautschi in [39] or the *degree of accuracy* as defined by Krommer and Überhuber in [53].

We will use the term **multiplicity** to denote the number of *sub-intervals* or *panels* of equal size in $[a,b]$ over which the quadrature rule is applied. Hence,

$$Q_n^{(m)}[a,b] = \sum_{k=1}^{m} Q_n[a+(k-1)h, a+kh], \quad h = \frac{b-a}{m}. \tag{1.1}$$

In [12], $Q_n^{(m)}[a,b]$ is referred to as a *compound* or *composite* quadrature rule.

The quadrature rule itself is evaluated as the linear combination of the integrand evaluated at the **nodes** $x_i \in [-1, 1]$, $i = 0 \dots n$

$$Q_n[a,b] = \frac{b-a}{2} \sum_{i=0}^{n} w_i f\left(\frac{a+b}{2} + \frac{b-a}{2} x_i\right)$$

where the $w_i$ are the weights of the quadrature rule $Q_n$. For notational simplicity, we have assumed that a quadrature rule of degree $n$ has $n+1$ nodes. This is of course not always true: The degree of interpolatory quadrature rules over a symmetric set of an odd number of nodes is equal to the number of nodes, and for Gauss quadratures, Gauss-Lobatto quadratures and their Kronrod extensions, the degree is much larger than the number of nodes. The opposite may of course also be true: a quadrature rule need not be interpolatory and the degree may therefore be smaller than the number of nodes used by the rule (*e.g.* see Section 2.19).

Given a quadrature rule $Q_n^{(m)}[a,b]$ of degree $n$ and multiplicity $m$ applied to an integrand $f(x)$ which has $n+1$ continuous derivatives in $[a,b]$ and for which the $n+1$st derivative does not change sign in $[a,b]$, we model the error of the quadrature rule as

$$Q_n^{(m)}[a,b] - \int_a^b f(x)\,\mathrm{d}x = \kappa_n \left(\frac{b-a}{m}\right)^{n+2} f^{(n+1)}(\xi), \quad \xi \in [a,b]. \quad (1.2)$$

where the factor $\kappa_n$ is the integral of the *Peano kernel* of the quadrature rule $Q_n^{(m)}$ over the interval $[a,b]$ (see [12], Section 4.3). If $f^{(n+1)}(x)$ is more or less constant and does not change sign for $x \in [a,b]$, the integrand is usually said to be "*sufficiently smooth*".

Equation 1.2 can be derived using the Taylor expansion of $f(x)$ around $x = a$:

$$\begin{aligned} &f(a+x) = \\ &\quad f(a) + f'(a)x + \dots + \frac{f^{(n)}(a)}{n!}x^n + \frac{f^{(n+1)}(\xi)}{(n+1)!}x^{n+1}, \quad \xi \in [a,b]. \quad (1.3) \end{aligned}$$

Integrating both sides of Equation 1.3 from 0 to $b-a$, we obtain

$$\begin{aligned}
&\int_0^{b-a} f(a+x)\,\mathrm{d}x \\
&= f(a)\int_0^{b-a}\mathrm{d}x + f'(a)\int_0^{b-a} x\,\mathrm{d}x + \dots \\
&\quad + \frac{f^{(n)}(a)}{n!}\int_0^{b-a} x^n\,\mathrm{d}x + \frac{f^{(n+1)}(\xi)}{(n+1)!}\int_0^{b-a} x^{n+1}\,\mathrm{d}x, \quad \xi\in[a,b] \\
&= f(a)(b-a) + f'(a)\frac{(b-a)^2}{2} + \dots \\
&\quad + \frac{f^{(n)}}{n!}\frac{(b-a)^{n+1}}{n+1} + \frac{f^{(n+1)}(\xi)}{(n+1)!}\frac{(b-a)^{n+2}}{n+2}\,\mathrm{d}x, \quad \xi\in[a,b]. \qquad (1.4)
\end{aligned}$$

Note that se can only extract $f^{(n+1)}(\xi)$ from the last term using the mean value theorem if $f^{(n+1)}(x)$ does not change sign in $x\in[a,b]$. Applying the *basic* (*i.e.* non-compound) quadrature rule $Q_n[0,b-a]$ on both sides of Equation 1.3 we obtain:

$$\begin{aligned}
&Q_n[0,b-a](f(a+x)) \\
&= f(a)Q_n[0,b-a](1) + f'(a)Q_n[0,b-a](x) + \dots \\
&\quad + \frac{f^{(n)}(a)}{n!}Q_n[0,b-a](x^n) + \frac{f^{(n)}(\xi)}{(n+1)!}Q_n[0,b-a](x^{n+1}).
\end{aligned} \qquad (1.5)$$

Subtracting Equation 1.4 from Equation 1.5 we then obtain

$$\begin{aligned}
&Q_n[0,b-a](f(a+x)) - \int_0^{b-a} f(a+x)\,\mathrm{d}x \\
&= \sum_{i=0}^{n+1}\frac{f^{(i)}(a)}{i!}Q_n[0,b-a](x^i) - \sum_{i=0}^{n+1}\frac{f^{(i)}(a)}{i!}\frac{(b-a)^{i+1}}{i+1} \\
&= \frac{f^{(n+1)}(\xi)}{(n+1)!}\left(Q_n[0,b-a](x^{n+1}) - \frac{(b-a)^{n+2}}{n+2}\right) \\
&= \kappa_n(b-a)^{n+2}f^{(n+1)}(\xi). \qquad (1.6)
\end{aligned}$$

Since $Q_n$ is exact for all polynomials of degree up to $n$, the first $n+1$ terms in the right-hand sides of Equation 1.4 and Equation 1.5 cancel each other out. The remaining, final term of Equation 1.5, when inserted in Equation 1.1, results in a multiple of $(b-a)^{n+2}$:

$$\begin{aligned} Q_n[0,b-a](x^{n+1}) &= \frac{b-a}{2}\sum_{i=0}^{n} w_i \left(\frac{b-a}{2}x_i\right)^{n+1} \\ &= \left(\frac{b-a}{2}\right)^{n+2} \sum_{i=0}^{n} w_i x_i^{n+1} \\ &= (b-a)^{n+2} C \end{aligned}$$

where $C$ is a constant which is independent of the interval of integration. This easily extends to the compound rule $Q_n^{(m)}$, the error of which can be computed as

$$\begin{aligned} & Q_n^{(m)}[a,b] - \int_a^b f(x)\,\mathrm{d}x \\ = {} & \sum_{i=1}^{m} \left[ Q_n[a+(i-1)h, a+ih] - \int_{a+(i-1)h}^{a+h} f(x)\,\mathrm{d}x \right], \quad h = \frac{b-a}{m} \\ = {} & \sum_{i=1}^{m} \kappa_i h^{n+2} f^{(n+1)}(\xi_i), \quad \xi_i \in [a+(i-1)h, a+ih] \\ = {} & \kappa h^{n+2} f^{(n+1)}(\xi), \quad \xi \in [a,b] \\ = {} & \kappa \left(\frac{b-a}{m}\right)^{n+2} f^{(n+1)}(\xi) \end{aligned}$$

which is the error in Equation 1.2.

If a quadrature rule is of degree $n$, then its *order of accuracy* as defined by Skeel and Keiper in [93], to which we will simply refer to as its *order*, is the exponent of the interval widht $b-a$ in the error expression. For a quadrature rule of degree $n$, the order is $n+2$.

To avoid confusion regarding the nature of the degree vs. the number of nodes, we will use the following symbols to describe some special quadrature rules:

- $\mathsf{S}^{(m)}[a,b]$: compound Simpson rule of degree 3 over $m$ sub-intervals,

- $\mathsf{NC}_n^{(m)}[a,b]$: compound Newton-Cotes rule of degree $n$ over $m$ sub-intervals (usually $n$ will be odd and the number of nodes will also be $n$),
- $\mathsf{CC}_n[a,b]$: Clenshaw-Curtis quadrature over $n$ *nodes* (note that here the subscript denotes the number of *nodes*, not the *degree*),
- $\mathsf{G}_n[a,b]$: Gauss quadrature over $n$ *nodes* (note that here the subscript denotes the number of *nodes*, not the *degree*),
- $\mathsf{GL}_n[a,b]$: Gauss-Lobatto quadrature over $n$ *nodes* (note that here the subscript denotes the number of *nodes*, not the *degree*),
- $\mathsf{K}_n[a,b]$: Kronrod extension over $n$ *nodes* (note that here the subscript denotes the number of *nodes*, not the *degree*).

During adaptive integration, the interval $[a,b]$ is divided into a number of *sub-intervals* $[a_k,b_k]$ such that

$$\bigcup_k [a_k,b_k] = [a,b],$$

over which the quadratures are computed. The sum of the *local* quadratures is an approximation to the *global* integral:

$$\sum_k Q_n^{(m)}[a_k,b_k] \approx \int_a^b f(x)\,\mathrm{d}x.$$

The sub-division occurs either recursively or explicitly. Most algorithms follow either the *recursive* scheme in Algorithm 1 or the *non-recursive* scheme in Algorithm 2.

In both cases, the decision whether to sub-divide an interval or not is made by first approximating the integral over the sub-interval (Line 1 in Algorithm 1 or Lines 7 and 8 in Algorithm 2) and then approximating the *integration error* over the sub-interval (Line 2 in Algorithm 1 or Lines 9 and 10 in Algorithm 2). If this *error estimate* is larger than the accepted tolerance (Line 3 in Algorithm 1) or the largest error of all sub-intervals (Line 5 in Algorithm 2), then that interval is sub-divided.

**Algorithm 1** integrate $(f, a, b, \tau)$

```
1: $Q_n^{(m)}[a,b] \approx \int_a^b f(x)\,\mathrm{d}x$    ($\textit{approximate the integral}$)
2: $\varepsilon \approx \left|Q_n - \int_a^b f(x)\,\mathrm{d}x\right|$    ($\textit{approximate the integration error}$)
3: if $\varepsilon < \tau$ then
4:     return $Q_n$    ($\textit{accept the estimate}$)
5: else
6:     $m \leftarrow (a+b)/2$
7:     return integrate$(f, a, m, \tau')$ + integrate$(f, m, b, \tau')$    ($\textit{recurse}$)
8: end if
```

**Algorithm 2** integrate $(f, a, b, \tau)$

```
1: $I \leftarrow Q_n^{(m)}[a,b] \approx \int_a^b f(x)\,\mathrm{d}x$    ($\textit{initial approximation of } I$)
2: $\varepsilon \leftarrow \varepsilon_0 \approx \left|Q_n - \int_a^b f(x)\,\mathrm{d}x\right|$    ($\textit{initial approximation the error}$)
3: initialize $H$ with interval $[a,b]$, integral $Q_n[a,b]$ and error $\varepsilon_0$
4: while $\varepsilon > \tau$ do
5:     $k \leftarrow$ index of interval with largest $\varepsilon_k$ in $H$
6:     $m \leftarrow (a_k + b_k)/2$
7:     $I_{\mathsf{left}} \leftarrow Q_n^{(m)}[a,m] \approx \int_{a_k}^m f(x)\,\mathrm{d}x$    ($\textit{evaluate } Q_n^{(m)} \textit{ on the left}$)
8:     $I_{\mathsf{right}} \leftarrow Q_n^{(m)}[m,b] \approx \int_m^{b_k} f(x)\,\mathrm{d}x$    ($\textit{evaluate } Q_n^{(m)} \textit{ on the right}$)
9:     $\varepsilon_{\mathsf{left}} \approx \left|Q_n[a_k,m] - \int_{a_k}^m f(x)\,\mathrm{d}x\right|$    ($\textit{approximate } \varepsilon \textit{ on the left}$)
10:    $\varepsilon_{\mathsf{right}} \approx \left|Q_n[m,b_k] - \int_m^{b_k} f(x)\,\mathrm{d}x\right|$    ($\textit{approximate } \varepsilon \textit{ on the right}$)
11:    $I \leftarrow I - I_k + I_{\mathsf{left}} + I_{\mathsf{right}}$    ($\textit{update the global integral}$)
12:    $\varepsilon \leftarrow \varepsilon - \varepsilon_k + \varepsilon_{\mathsf{left}} + \varepsilon_{\mathsf{right}}$    ($\textit{update the global error}$)
13:    push interval $[a_k, m]$ with integral $I_{\mathsf{left}}$ and error $\varepsilon_{\mathsf{left}}$ onto $H$
14:    push interval $[m, b_k]$ with integral $I_{\mathsf{right}}$ and error $\varepsilon_{\mathsf{right}}$ onto $H$
15: end while
16: return $I$
```

In the following, we will distinguish between the *local* and *global* error in an adaptive quadrature routine. The *local error* $\varepsilon_k$ of the $k^{\text{th}}$ interval $[a_k, b_k]$ is defined as

$$\varepsilon_k = \left| Q_n[a_k, b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x \right| \tag{1.7}$$

and the *global error* $\varepsilon$ is

$$\varepsilon = \left| \sum_k Q_n[a_k, b_k] - \int_a^b f(x)\,\mathrm{d}x \right|. \tag{1.8}$$

Since the local errors may be of different sign, the sum of the local errors forms an upper bound for the global error.

$$\varepsilon \leq \sum_k \varepsilon_k.$$

We further distinguish between the absolute errors (1.7) and (1.8), the *locally relative local error*

$$\varepsilon_k^{\mathsf{lrel}} = \left| \frac{Q_n[a_k, b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x}{\int_{a_k}^{b_k} f(x)\,\mathrm{d}x} \right|, \tag{1.9}$$

and the *globally relative local error*

$$\varepsilon_k^{\mathsf{grel}} = \left| \frac{Q_n[a_k, b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x}{\int_a^b f(x)\,\mathrm{d}x} \right|. \tag{1.10}$$

We also define the *global relative error* which is bounded by the sum of the globally relative local errors:

$$\varepsilon^{\mathsf{grel}} = \frac{\left|\sum_k Q_n[a_k, b_k] - \int_a^b f(x)\,\mathrm{d}x\right|}{\int_a^b f(x)\,\mathrm{d}x} \leq \sum_k \left| \frac{Q_n[a_k, b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x}{\int_a^b f(x)\,\mathrm{d}x} \right|.$$

The sum of the *locally relative local errors*, however, form no such bound: If the integral in a sub-interval is larger than the global integral, then the local error therein will be smaller relative to the local integral than relative to the global integral and may cause the sum of locally relative local errors to be smaller than the global relative error.

## 1.3 Outline

In Chapter 2, a detailed history of the most significant advances in adaptive quadrature algorithms from the past 45 years is given.

In Chapter 3 different ways in which the integrand is represented in different algorithms are discussed, as well as how it may be explicitly represented using orthogonal polynomials. A new algorithm for the efficient and stable construction, update and downdate (*i.e.* the addition or removal of a node, respectively) of such interpolations is described, as well as a new algorithm for their construction. Both algorithms are tested against previous efforts in the field.

In Chapter 4 the different types of error estimates described and used to date are discussed and categorized. A new type of error estimate is proposed and described in two distinct variants. These two new estimates are compared to all of the error estimators discussed previously. The results are then analyzed and a further classification of the error estimators is suggested.

In Chapter 5 some common problems of adaptive quadrature algorithms are discussed and strategies for dealing with singularities and non-numerical function values, as well as divergent integrals, are presented.

In Chapter 6 some general design considerations are discussed and three new algorithms are presented. These algorithms are compared to other widely-used algorithms on several sets of test-functions and shown to be more reliable.

In Chapter 7 we summarize the results from the previous chapters and draw some general conclusions.

Appendices A and B contain the Matlab source of the different error estimators and quadrature algorithms as they were implemented and tested for this thesis.

# Chapter 2

# A Short History of Adaptive Quadrature

## 2.1 A Word on the "First" Adaptive Quadrature Algorithm

There seems to be some confusion as to who actually published the first adaptive quadrature algorithm. Davis and Rabinowitz [12] cite the works of Villars [100], Henriksson [45] and Kuncir (see Section 2.2), whereas other authors [24, 20, 22, 21, 5, 66] credit McKeeman (see Section 2.3).

Although no explicit attribution is given, Henriksson's algorithm seems to be an unmodified ALGOL-implementation of the algorithm described by Villars. The algorithm described by Villars is, in turn, as the author himself states, only a slight modification of a routine developed by Helen Morrin [72][1] in 1955. These three algorithms already contain a number of features, *e.g.* the use of an analytical scaling factor for the error and subtraction the error from the integral estimate (in effect using Romberg extrapolation), which were apparently forgotten and later re-discovered

[1]This reference is only given for the sake of completeness since the author was not able to obtain a copy of the original manuscript. The routine presented therein is, however, described in detail by Villars in [100].

by other authors.

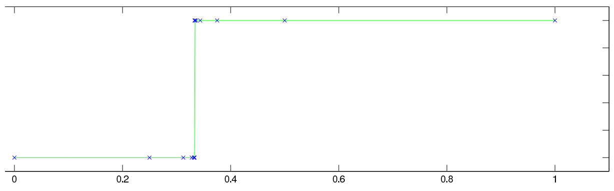
The algorithms of Morrin, Villars and Henriksson, however, are more reminiscent of ODE-solvers. Following the general scheme in Algorithm 3, they integrate the function stepwise from left to right using Simpson's rule and adapting (doubling or halving) the step-size whenever an estimate converges or fails to do so. These algorithms effectively discard function evaluations and so lose information on the structure of the integrand (see Figure 2.1). We will therefore not consider them to be "genuine" adaptive integrators.

**Algorithm 3** ODE-like integration algorithm

```
$h \leftarrow b - a$                                                          (*initial step size*)
$I \leftarrow 0$                                                              (*initial integral*)
**while** $a < b$ **do**
    $Q_n^{(m)}[a, a+h] \approx \int_a^{a+h} f(x)\,\mathrm{d}x$                (*approximate the integral*)
    $\varepsilon \approx \left| Q_n^{(m)}[a, a+h] - \int_a^{a+h} f(x)\,\mathrm{d}x \right|$   (*approximate the error*)
    **if** $\varepsilon < \tau$ **then**
        $I \leftarrow I + Q_n^{(m)}[a, b]$                                    (*increment the global integral*)
        $a \leftarrow a + h$                                                  (*move the left boundary*)
        $h \leftarrow \min\{2h, b - a\}$                                      (*increase the step size*)
    **else**
        $h \leftarrow h/2$                                                    (*use a smaller step size*)
    **end if**
**end while**
**return** $I$                                                                (*return the accumulated integral*)
```

This is not the case with Kuncir's algorithm (see Section 2.2), which follows the recursive scheme presented in Algorithm 1, and seems to be the first published algorithm to do so.

Kuncir predates McKeeman by approximately six months. Interestingly enough, the very similar works of both Kuncir and McKeeman were both published in the same journal (Communications of the ACM) in the same year (1962) in different issues of the same volume (Volume 5), both edited by the same editor (J.H. Wegstein). This duplication of efforts does not seem to have been noticed at the time.

a)


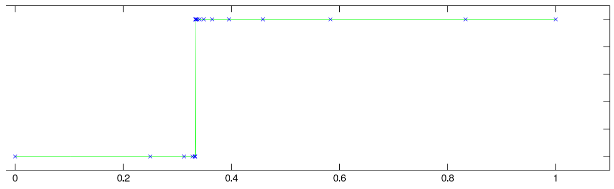
b)


**Figure 2.1:** Boundaries of the intervals generated in (a) a recursive scheme using bisection and in (b) an ODE-like scheme halving or doubling the interval size depending on the success of integration in that interval as per Algorithm 3. If we subdivide up to an interval width of $10^{-5}$ around a difficulty at $x = 1/3$, the ODE-like scheme generates 25 intervals whereas the recursive scheme generates only 18.

## 2.2 Kuncir's Simpson Rule Integrator

In 1962, Kuncir [55] publishes the first adaptive quadrature routine following the scheme in Algorithm 1 and using Simpson's compound rule over two sub-intervals to approximate the integral

$$\int_a^b f(x)\,\mathrm{d}x \approx \mathsf{S}^{(2)}[a,b]$$

and the *locally relative* local error estimate

$$\varepsilon_k = \left|\mathsf{S}^{(1)}[a_k,b_k] - \mathsf{S}^{(2)}[a_k,b_k]\right| \frac{2^d}{|\mathsf{S}^{(2)}[a_k,b_k]|} \tag{2.1}$$

where $d$ is the recursion depth of the $k$th interval $[a_k, b_k]$. The function values of the compound rule can be re-used to compute the basic rule $\mathsf{S}^{(1)}$ in the sub-intervals after bisection.

Replacing every evaluation of the integrand in the un-scaled error estimate (Equation 2.1) with an appropriate $f(a+h)$ and expanding it in a

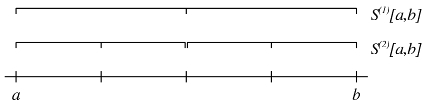


**Figure 2.2:** Kuncir's error estimate uses the difference between Simpson's rule applied once ($\mathsf{S}^{(1)}[a,b]$) and Simpson's rule applied twice ($\mathsf{S}^{(2)}[a,b]$) in the same interval.

Taylor expansion around $a$, as is done in [32], we obtain

$$\mathsf{S}^{(1)}[a_k,b_k] - \mathsf{S}^{(2)}[a_k,b_k] = \frac{(b_k-a_k)^5}{3072} f^{(4)}(\xi), \quad \xi \in [a_k,b_k], \tag{2.2}$$

from which we see that the error is a function of the fourth derivative of the integrand. Inserting the Taylor expansion into the *actual* error gives a similar result:

$$\mathsf{S}^{(2)}[a_k,b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x = \frac{(b_k-a_k)^5}{46\,080} f^{(4)}(\xi), \quad \xi \in [a_k,b_k]. \tag{2.3}$$

If we assume that $f^{(4)}(x)$ is more or less constant for $x \in [a_k,b_k]$ and both Equation 2.2 and Equation 2.3 therefore have similar values for $f^{(4)}(\xi)$, then the error estimate is 15 times larger than the actual integration error. This factor of 15 might seem large, but in practice it is a good guard against bad estimates when $f^{(4)}(x)$ is *not* constant for $x \in [a_k,b_k]$.

The scaling factor $2^d$, which is implemented implicitly by scaling the local tolerance ($\tau'$ in Line 7 of Algorithm 1) by a factor of 1/2 upon recursion (*i.e.* $\tau' \leftarrow \tau/2$), was probably chosen to ensure that, after subdividing an interval, the sum of the interval error estimates can not exceed the requested tolerance. However, since a *locally relative* error estimate is used, this is only true if the integral over the sub-intervals is of approximately the same magnitude. If the integral over any sub-interval is larger in magnitude than the global integral, then its local error, while still below the locally relative tolerance, may exceed the global relative tolerance.

This can lead the algorithm to fail to converge for integrals which tend to zero locally. Consider, for example, the integration of $f(x) = x^{1.1}$ over the interval $[0,1]$. The expansion of the error of the leftmost interval

$[0,h]$ results in:

$$\begin{aligned}\varepsilon &= \left|\mathsf{S}^{(1)}[0,h](x^{1.1}) - \mathsf{S}^{(2)}[0,h](x^{1.1})\right| \frac{2^d}{|\mathsf{S}^{(2)}[0,h](x^{1.1})|} \\ &= \left|\mathsf{S}^{(1)}[0,2^{-d}](x^{1.1}) - \mathsf{S}^{(2)}[0,2^{-d}](x^{1.1})\right| \frac{2^d}{|\mathsf{S}^{(2)}[0,2^{-d}](x^{1.1})|} \\ &\approx 0.0024 \times 2^d. \end{aligned} \tag{2.4}$$

where the error estimate *grows exponentially* with each subdivision. If the error criterion is not met in the first step of the algorithm, it never will be met. Kuncir guards against this problem by using a user-supplied maximum recursion depth $N$. This prevents the algorithm from recursing indefinitely, yet does not guarantee that the requested tolerance will indeed have been achieved.

## 2.3 McKeeman's Adaptive Integration by Simpson's Rule

In the same year, McKeeman [68] publishes a similar recursive algorithm (following Algorithm 1, yet using trisection instead of bisection) using the compound Simpson's rule over three panels to approximate the integral

$$\int_a^b f(x)\,\mathrm{d}x \approx \mathsf{S}^{(3)}[a,b]$$

and the *globally relative* local error estimate

$$\varepsilon_k = \left|\mathsf{S}^{(1)}[a_k,b_k] - \mathsf{S}^{(3)}[a_k,b_k]\right| \frac{3^d}{\hat{I}_d} \tag{2.5}$$

(see Figure 2.3) where $\hat{I}_d$ is an approximation to the integral of the absolute value of $f(x)$:

$$\hat{I}_d \approx \int_a^b |f(x)|\,\mathrm{d}x.$$

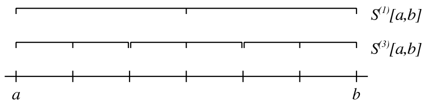


**Figure 2.3:** McKeeman's error estimate uses the difference between Simpson's rule applied once ($\mathsf{S}^{(1)}[a,b]$) and Simpson's rule applied three times ($\mathsf{S}^{(3)}[a,b]$) in the same interval.

This estimate is updated in every recursion step using

$$\hat{I}_d = \hat{I}_{d-1} - \left|\mathsf{S}^{(1)}[a_k,b_k]\right| + \sum_{i=1}^{3}\left|\mathsf{S}^{(1)}[a_k+(i-1)h, a_k+ih]\right|, \quad h = \frac{b_k-a_k}{3}. \tag{2.6}$$

The main differences with respect to Kuncir's error estimator can be summed-up as follows:

1. The use of *trisection* as opposed to bisection,
2. The use of a *globally* relative local error estimate as opposed to a locally relative error estimate,
3. The error is computed relative to the global integral of the *absolute value* of $f(x)$ as opposed to the local integral of $f(x)$.

Replacing the evaluations of the integrand $f(a+h)$ by their Taylor expansions around $a$ in Equation 2.5, as we did with Kuncir's error estimator (see Equation 2.2), we can see that

$$\left|\frac{\mathsf{S}^{(1)}[a,b] - \mathsf{S}^{(3)}[a,b]}{\mathsf{S}^{(3)}[a,b] - \int_a^b f(x)\,\mathrm{d}x}\right| \approx 80, \tag{2.7}$$

*i.e.* the error is overestimated by a factor of 80 for a sufficiently smooth integrand. This is significantly stricter than the factor of 15 in Kuncir's algorithm. Furthermore, although the scaling factor $3^d$ guarantees that the sum of the error estimates will not exceed the total tolerance, it is very strict in practice and will cause the algorithm to fail to converge around certain types of singularities.

Due to the *globally* relative error estimate, this algorithm has no difficulty integrating $f(x) = x^{1.1}$ (see Section 2.2, Equation 2.4), yet consider the case of integrating $f(x) = x^{-1/2}$ in $[\varepsilon_{\mathsf{mach}}, 1]$: The function has a singularity at $f(0) = \infty$ (which is why we integrate from $\varepsilon_{\mathsf{mach}}$) but its integral is bounded. Applying a similar analysis as for Kuncir's error estimate (Equation 2.4), we get, for the leftmost interval:

$$\begin{aligned} \varepsilon &= \left| \mathsf{S}^{(1)}[\varepsilon_{\mathsf{mach}}, 3^{-d}](x^{-1/2}) - \mathsf{S}^{(3)}[\varepsilon_{\mathsf{mach}}, 3^{-d}](x^{-1/2}) \right| 3^d \times 2 \\ &\approx 1.5 \times 10^7. \end{aligned} \tag{2.8}$$

The error estimate does not grow as it would using Kuncir's estimate ($\varepsilon \sim 2^d$) since the error is relative to the global integral, yet it still does not decrease with increasing recursion depth.

The same type of problem occurs with the integrand $f(x) = x^{1/2}$, which is smooth and has a bounded integral, yet also has a singularity in the first derivative at $x = 0$. Using the same analysis as above when integrating in $[0, 1]$ we obtain for the leftmost interval

$$\begin{aligned} \varepsilon &= \left| \mathsf{S}^{(1)}[0, 3^{-d}](x^{1/2}) - \mathsf{S}^{(3)}[0, 3^{-d}](x^{1/2}) \right| 3^d \times 2/3 \\ &\approx -0.725 \times 3^{d/2} \end{aligned} \tag{2.9}$$

in which the error grows *exponentially* with the increasing recursion depth. Similarly to Kuncir's algorithm, this type of problem is caught using a fixed maximum recursion depth of 7.

The use of a *globally relative* local error estimate is an important improvement. Besides forming a correct upper bound for the global error, it does not run into problems in sub-intervals where the integrand approaches 0, causing any *locally relative* error estimate to approach infinity.

Another uncommon yet beneficial feature is the use of the global integral of the *absolute* value of the function. This is a good guard against cancellation or *smearing* [44] when summing-up the integrals over the sub-intervals. Consider, for example, the computation of $\int_0^{2\pi} 10\,000\, sin(5x)\, \mathrm{d}x$: the integral itself is 0, yet when summing the non-zero integrals in the sub-intervals, we can expect cancellation errors of up to $10\,000\varepsilon_{\mathsf{mach}}$ or $10^{-12}$ for IEEE 754 double-precision machine arithmetic[2]. It would therefore make little sense to pursue a higher precision in the sub-intervals, which is what this estimate guards against. However, this error relative to $\hat{I}$ is generally *not* what the user wants or is willing to think about: he or she is usually only interested in the effective (and not the feasible) number of correct digits in the result.

## 2.4 McKeeman and Tesler's Adaptive Integrator

A year later, McKeeman and Tesler publish a non-recursive[3] [71] version of McKeeman's Simpson Integrator (see Section 2.3). This integrator is, in essence, almost identical to its predecessor, yet with one fundamental difference, which had been suggested by McKeeman himself as an improvement in [70], namely:

$$\varepsilon_k = \left| \mathsf{S}^{(1)}[a_k, b_k] - \mathsf{S}^{(3)}[a_k, b_k] \right| \frac{1.7^d}{\hat{I}} \tag{2.10}$$

where $\hat{I}$ is computed as in Equation 2.6 yet stored and updated *globally*. After each trisection, the error is no longer scaled with a factor of three, but with $1.7 \approx \sqrt{3}$. This small, uncommented[4] change is actually a significant improvement to the algorithm.

This relaxation can be derived statistically. Let us assume that the error of a quadrature rule $Q[a, b]$ can be described in terms of a normal distribution around 0:

$$Q[a, b] - \int_a^b f(x)\,\mathrm{d}x = \mathcal{N}(0, (\kappa\tau)^2) \tag{2.11}$$

[2]indeed, QUADPACK's `QAG`, for instance, achieves $-1.4 \times 10^{-11}$, MATLAB's `quad` achieves $-1.3 \times 10^{-12}$, both for a requested absolute tolerance of $10^{-15}$

[3]The algorithm of McKeeman and Tesler [71] is non-recursive in the sense that an explicit stack is maintained, analogous to the one generated in memory during recursion, and not as in the scheme presented in Algorithm 2

[4]A similar factor is later used by McKeeman (see Section 2.5) with a comment that dividing the tolerance by the number of sub-intervals, *i.e.* scaling by $m$ instead of $\sqrt{m}$, "*proves too strict in practice*".

where the variance $(\kappa\tau)^2$ is a function of the required tolerance $\tau$ with (hopefully) $\kappa < 1$. If we subdivide the interval into $m$ equally sized subintervals and compute the quadrature with some adjusted tolerance $\tau'$, the error should therefore behave as

$$\begin{aligned}\sum_{k=1}^{m} Q[a_k,b_k] - \int_a^b f(x)\,\mathrm{d}x &= \sum_{i=1}^{m}\left[Q[a_k,b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x\right] \\ &= \sum_{i=1}^{m}\mathcal{N}(0,(\kappa\tau')^2) \\ &= \mathcal{N}(0,m(\kappa\tau')^2) \qquad (2.12)\end{aligned}$$

*i.e.* the variance of the sum of the errors is the sum of the variances of the errors. If we now want the two estimates (Equation 2.11 and Equation 2.12) to have the same variance, we must equate

$$m(\kappa\tau')^2 = (\kappa\tau)^2 \quad \rightarrow \quad \tau' = \tau m^{-\frac{1}{2}} \qquad (2.13)$$

resulting in the scaling by $1.7 \approx \sqrt{3}$ used by McKeeman and Tesler. When applied to the problems in Equation 2.8 and Equation 2.9, this modification causes the error estimate in the former to converge and that of the latter to remain constant (as opposed to exponential growth). This simple idea has been, as we shall see, subsequently re-used by many authors.

Such a model was already introduced by Henrici in [43, Chapter 16] for the accumulation of rounding errors in numerical calculations. Whereas in such a case, the independence of the individual errors is a valid assumption, in the case of integration errors it is not[5].

## 2.5 McKeeman's Variable-Order Adaptive Integrator

Shortly after publishing the "non-recursive" recursive adaptive integrator, McKeeman publishes another recursive adaptive integrator [69] based

[5]Assume, for example, that the error behaves as in Equation 1.2 where $f^{(n+1)}(x)$ is of constant sign for $x \in [a,b]$, which is the usual assumption for a "sufficiently smooth" integrand.

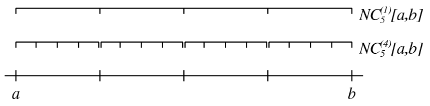


**Figure 2.4:** McKeeman's variable order error estimate uses the difference between a Newton-Cotes rule over $n$ points applied once ($NC_n^{(1)}[a,b]$) and the same Newton-Cotes rule applied $n-1$ times ($NC_n^{(n-1)}[a,b]$) in the same interval (shown here for $n=5$).

on Newton-Cotes rules over $n$ points, where $n$ is supplied by the user. In the same vein as the previous integrator, the integrand is computed using the compound Newton-Cotes rule over $n-1$ panels

$$\int_a^b f(x)\,\mathrm{d}x \approx \mathsf{NC}_n^{(n-1)}[a,b]$$

and the error estimate is computed as

$$\varepsilon_k = \left|\mathsf{NC}_n^{(1)}[a_k,b_k] - \mathsf{NC}_n^{(n-1)}[a_k,b_k]\right| \frac{\sqrt{n}^d}{\hat{I}_d} \tag{2.14}$$

where $\mathsf{NC}_n^{(m)}[a,b]$ is the Newton-Cotes rule over $n$ points applied on $m$ panels in the interval $[a,b]$ (see Figure 2.4). At every recursion level, the interval is subdivided into $n-1$ panels, effectively re-using the nodes of the composite rule as the basic rule in each sub-interval.

This algorithm is a good example of the pitfalls of using empirical error estimates of increasing degree without considering how the error estimate behaves analytically. Replacing the evaluations of the integrand $f(a+h)$ by their Taylor expansions around $a$ and inserting them into the expression

$$\left|\frac{\mathsf{NC}_n^{(1)}[a,b] - \mathsf{NC}_n^{(n-1)}[a,b]}{\mathsf{NC}_n^{(n-1)}[a,b] - \int_a^b f(x)\,\mathrm{d}x}\right|$$

we can see that for $n=3$ (*i.e.* applying Simpson's rule), we overestimate the actual error by a factor of 15 for sufficiently smooth $f(x)$, as we had already observed in Kuncir's algorithm (see Section 2.2).

For $n=4$, this factor grows to 80, as observed for McKeeman's first integrator (see Section 2.3). For $n=5$ it is 4 095 and for $n=8$, the

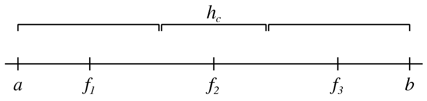


**Figure 2.5:** Gallaher's error estimate approximates the second derivative of $f(x)$ using divided differences over the three function evaluations $f_1$, $f_2$ and $f_3$.

maximum allowed in the algorithm, it is 5 764 800 (7 decimal digits!), making this a somewhat strict estimate, both in theory and in practice. Furthermore, the scaling by $\sqrt{n}$ is not justified if the interval is divided into $n-1$ panels (see Equation 2.13).

## 2.6 Gallaher's Adaptive Quadrature Procedure

In a 1967 paper [30], Gallaher presents a recursive adaptive quadrature routine based on the midpoint rule. In this algorithm, the interval is divided symmetrically into three sub-intervals with the width $h_c$ of the central sub-interval chosen randomly in

$$h_c \in \left[\frac{1}{6}h_k, \frac{1}{2}h_k\right], \quad h_k = (b_k - a_k).$$

The integrand $f(x)$ is evaluated at the center of each sub-interval and used to compute the midpoint rule therein (see Figure 2.5):

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{h_k - h_c}{2}\left(f(x_1) + f(x_3)\right) + h_c f(x_2)$$

where the $x_i$, $i = 1 \ldots 3$ are the centers of each of the three panels. If the error estimate is larger than the required tolerance, the interval is trisected into the three panels used to compute the midpoint rule, thus re-using the computed function values. Since the error of the midpoint rule is known to be

$$\frac{(b_k - a_k)^3}{24} f^{(2)}(\xi), \quad \xi \in [a_k, b_k], \tag{2.15}$$

the local integration error can be estimated by computing the second divided difference of $f(x)$ over the three values of $f(x)$ in the center of the sub-intervals, $f_1$, $f_2$ and $f_3$:

$$\frac{(b_k - a_k)^3}{24} f^{(2)}(\xi) \approx (f_1 - 2f_2 + f_3) \frac{2(b_k - a_k)^3}{3(b_k - a_k + h_c)^2} \tag{2.16}$$

Gallaher, however, uses the expression

$$\varepsilon = 14.6 \left| f_1 - 2f_2 + f_3 \right| \frac{b_k - a_k - h_c}{2} \sqrt{3}^d . \tag{2.17}$$

In which the constant 14.6 is determined empirically.

Gallaher shows that this error estimate works well for a number of integrands and gives a justification for using $\sqrt{3}^d$ as opposed to $3^d$ as a scaling factor, stating:

> *"The assumption here is that error contributed by the individual panels is random and not additive, thus the error from three panels is assumed to be $\sqrt{3}$ (not 3) times the error of one panel."*

similar to the derivation in Section 2.4.

## 2.7 Lyness' `SQUANK` Integrator

In 1969, Lyness [61] publishes the first rigorous analysis of McKeeman's adaptive integrator (see Section 2.3). He suggests using the absolute local error instead of the globally relative local error, bisection instead of trisection and includes the resulting factor of 15 in the error estimate[6]:

$$\varepsilon_k = \left| \mathsf{S}^{(1)}[a_k, b_k] - \mathsf{S}^{(2)}[a_k, b_k] \right| \frac{2^d}{15} \tag{2.18}$$

He further suggests using Romberg extrapolation to compute the five-node Newton-Cotes formula from the two Simpson's approximations[7]:

$$\mathsf{NC}_5^{(1)}[a, b] = \frac{1}{15} \left( 16 \mathsf{S}^{(2)}[a, b] - \mathsf{S}^{(1)}[a, b] \right) . \tag{2.19}$$

[6]Note that McKeeman's original error estimate was off by a factor of 80 (see Equation 2.7). The factor of 15 comes from using bisection instead of trisection.

[7]Interestingly enough, this was already suggested by Villars in 1956 [100] and implemented in Henriksson in 1961 [45], but apparently subsequently forgotten.

This is a departure from previous methods, in which the error estimate and the integral approximation were of the same degree, making it impracticable to relate the error estimate to the integral approximation without making additional assumptions on the smoothness of the integrand.

Note that although Lyness mentions McKeeman's [70] use of the scaling $\sqrt{3}^d$ as opposed to $3^d$ and notes that it "*evidently gives better results*", he himself uses the stricter scaling $2^d$. By using an *absolute* local error he avoids the problems encountered by Kuncir's error estimate (see Section 2.2, Equation 2.4), yet the depth-dependent scaling still makes the algorithm vulnerable to problems such as shown in Equation 2.8 and Equation 2.9.

Lyness later implements these improvements in the algorithm SQUANK [62], in which he also includes a guard for round-off errors: Lyness starts by showing that the un-scaled error estimate

$$\mathsf{S}^{(1)}[a,b] - \mathsf{S}^{(2)}[a,b] = \frac{(b-a)^5}{3072} f^{(4)}(\xi), \quad \xi \in [a,b] \tag{2.20}$$

should decrease by a factor of 16 after subdivision for constant $f^{(4)}(x)$, $x \in [a,b]$, *i.e.*

$$\frac{\mathsf{S}^{(1)}[a,\frac{a+b}{2}] - \mathsf{S}^{(2)}[a,\frac{a+b}{2}]}{\mathsf{S}^{(1)}[a,b] - \mathsf{S}^{(2)}[a,b]} = \frac{\mathsf{S}^{(1)}[\frac{a+b}{2},b] - \mathsf{S}^{(2)}[\frac{a+b}{2},b]}{\mathsf{S}^{(1)}[a,b] - \mathsf{S}^{(2)}[a,b]} = \frac{1}{16}.$$

If $f^{(4)}(x)$ is of constant sign for $x \in [a,b]$, then the un-scaled error measure should at least *decrease* after subdivision. Therefore, if this estimate *increases* after subdivision, Lyness assumes that one of the following has happened:

1. There is a zero of $f^{(4)}(x)$ in the interval an the error estimate is therefore not valid,

2. The error estimate is seriously affected by rounding errors in the integrand.

The first case is regarded by Lyness to be rare enough to be safely ignored. Therefore, if the error estimate increases after subdivision, significant round-off error is assumed and the tolerance is adjusted accordingly. If in latter intervals the error is smaller than the required tolerance, the tolerance is re-adjusted until the original tolerance is met. If this is not possible, then the user is informed that something may have gone horribly wrong.

It should be noted that this noise detection does not take discontinuities or singularities into account. These may have the same effect on consecutive error estimates (*i.e.* the estimate increases after subdivision), yet will be treated as noise in the integrand.

In a 1975 paper, Malcolm and Simpson [66] present a *global* version of `SQUANK` called `SQUAGE` (Simpson's Quadrature Used Adaptively Global Error) along the lines of Algorithm 2, yet without the noise detection described above. They use the same error estimate (Equation 2.18), albeit neglect to apply the Romberg extrapolation[8] and use $\mathsf{S}^{(2)}[a_k, b_k]$ to approximate the integral. Their results show that for the same quadrature rule and local error estimate, the global, non-recursive approach (Algorithm 2) is more efficient in terms of required function evaluations than the local, recursive approach (Algorithm 1), but at the expense of larger memory requirements.

In 1977, Forsythe, Malcolm and Moler [29] publish the recursive quadrature routine `QUANC8`, which uses essentially the same basic error estimate as Lyness (Equation 2.18), yet using Newton-Cotes rules over 9 points, resulting in a different scaling factor:

$$\varepsilon_k = \left| \mathsf{NC}_9^{(1)}[a_k, b_k] - \mathsf{NC}_9^{(2)}[a_k, b_k] \right| \frac{2^d}{1023}. \tag{2.21}$$

Analogously to Equation 2.19, the two quadrature rules are combined using Romberg extrapolation to compute an approximation of degree 11:

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{1}{1023}\left(1024\mathsf{NC}_9^{(2)}[a,b] - \mathsf{NC}_9^{(1)}[a,b]\right)$$

which is used as the approximation to the integral. This routine was integrated into MATLAB as `quad8`, albeit without the Romberg extrapolation, and has since been replaced by `quadl` (see Section 2.20).

[8]In their paper, Malcolm and Simpson state (erroneously) that Lyness' `SQUANK` uses $\mathsf{S}^{(2)}[a, b]$ as its approximation to the integral and, as their results suggest, $\mathsf{S}^{(2)}[a, b]$ was also used in their implementation thereof. This omission, however, has no influence on their results or the conclusions they draw in their paper.

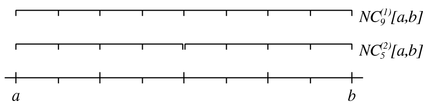


**Figure 2.6:** O'Hara and Smith's first error estimate computes the difference between a 9-point Newton-Cotes rule ($NC_9^{(1)}[a,b]$) and two 5-point Newton-Cotes rules ($NC_5^{(2)}[a,b]$).

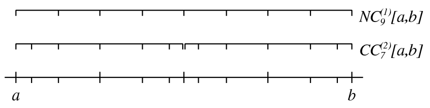


**Figure 2.7:** O'Hara and Smith's [77] second error estimate computes the difference between a 9-point Newton-Cotes rule ($\mathsf{NC}_9^{(1)}[a,b]$) and two 7-point Clenshaw-Curtis rules ($\mathsf{CC}_7^{(2)}[a,b]$).

## 2.8 O'Hara and Smith's Clenshaw-Curtis Quadrature

In 1969, O'Hara and Smith [77] publish a recursive adaptive quadrature routine based on Clenshaw-Curtis quadrature rules [10]. Their algorithm uses a cascade of error estimates. First, the error estimate

$$\varepsilon_k^{(1)} = \left|\mathsf{NC}_9^{(1)}[a_k,b_k] - \mathsf{NC}_5^{(2)}[a_k,b_k]\right| \tag{2.22}$$

is computed using 9 equidistant function evaluations in the interval (see Figure 2.6). This and subsequent error estimates are compared with a local tolerance $\tau_k$, which will be explained later on.

If the requested tolerance is not met, the interval is sub-divided. Otherwise, a second error estimate is computed using

$$\varepsilon_k^{(2)} = \left|\mathsf{NC}_9^{(1)}[a_k,b_k] - \mathsf{CC}_7^{(2)}[a_k,b_k]\right| \tag{2.23}$$

where $\mathsf{CC}_7^{(2)}[a,b]$ is the Clenshaw-Curtis rule over 7 points applied over 2 sub-intervals of $[a,b]$. The evaluation of this rule requires the evaluation of only 4 additional function values since the points $a + \frac{1}{4}(b-a)$ and

$b - \frac{1}{4}(b-a)$ in the Clenshaw-Curtis rule overlap with already evaluated points in the Newton-Cotes rule (see Figure 2.7).

If this error estimate is larger than the required tolerance, the interval is subdivided. Otherwise, a final, third error estimate is computed using

$$\varepsilon_k^{(3)} = \frac{32}{(6^2-9)(6^2-1)} \left[ \left| {\sum_{i=1}^{7}}'' (-1)^{i-1} f_{l,i} \right| + \left| {\sum_{i=1}^{7}}'' (-1)^{i-1} f_{r,i} \right| \right] \qquad (2.24)$$

where $\Sigma''$ denotes a sum in which first and last terms are halved and where the $f_{l,i}$ and $f_{r,i}$ are the values of the integrand evaluated at the nodes of the 7-point Clenshaw-Curtis quadrature rules over the left and right halves of the interval respectively. These sums are, as we will see later (Equation 2.28), the approximated Chebyshev coefficients $\tilde{c}_6$ of the integrand over the left and right half of the interval.

If this third error estimate is also below the prescribed tolerance, then $\mathsf{CC}_7^{(2)}[a_k, b_k]$ is used as an approximation to the integral. Otherwise, the interval is bisected.

The scaled tolerance $\tau_k$ is computed and updated such that it represents one tenth of the global tolerance $\tau$ minus the accumulated error estimates of the previously converged intervals. That is, as the algorithm recurs towards the leftmost interval, $\tau_1$ is simply $0.1\tau$. Once the leftmost interval has converged, with an estimated error $\varepsilon_1$, the $\tau_2$ of the next interval is set to $0.1(\tau - \varepsilon_1)$. For the $k$th interval, this can be written recursively as

$$\tau_k = 0.1 \left( \tau - \sum_{i=1}^{k-1} \varepsilon_i \right). \qquad (2.25)$$

Assuming that $\varepsilon_k \leq \tau_k$, the local tolerance in the $k$th interval is bounded by

$$\left( \frac{9}{10} \right)^{k-1} \frac{\tau}{10} \leq \tau_k \leq 0.1\tau.$$

Using this scheme, the global error estimate after processing $k$ intervals should be bounded by

$$\varepsilon \leq \sum_{i=1}^{k} \tau_i = \left( 1 - \left( \frac{9}{10} \right)^k \right) \tau.$$

note that as $k \to \infty$, the error estimate becomes more and more restrictive. This can become a problem if we have a singularity at the right end of the interval and can lead the algorithm to fail. In general, this type of local tolerance is problematic since it requires the algorithm to allot a certain part of the error tolerance before knowing how the rest of the function will or may behave. This allocation can be either overly generous (*i.e.* for a singularity/discontinuity on the right) or overly restrictive (*i.e.* for a singularity/discontinuity on the left).

The first two error estimates (Equation 2.22 and Equation 2.23) are similar to those used by Kuncir, McKeeman and Lyness, yet differ in that the difference between estimates of *different degree* are computed, *i.e.* they use the difference between a rule of degree 9 and one of degree 5 or one of degree 7 respectively. It is therefore no longer possible to formulate the error estimate as a multiple of the actual error for "sufficiently smooth" integrands without making additional assumptions on the integrand itself.

The third error estimate (Equation 2.24) is derived by O'Hara and Smith in [76] based on the error estimation used by Clenshaw and Curtis in [10]. Consider, as is done in [10], that the function $f(x)$ in $x \in [a,b]$ has a Chebyshev expansion

$$f\left(\frac{a+b}{2} + \frac{b-a}{2}x\right) = {\sum_{i=0}^{\infty}}' c_i T_i(x), \quad x \in [-1,1] \tag{2.26}$$

in the interval $[a,b]$, where $\Sigma'$ denotes a sum in which first term is halved and the $T_i(x)$ are the Chebyshev polynomials satisfying

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x).$$

The integral of $f(x)$ can therefore be written as

$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x &= (b-a){\sum_{i=0}^{\infty}}' c_i \int_{-1}^{1} T_i(x)\,\mathrm{d}x \\ &= (b-a)\left[c_0 - \frac{2}{3}c_2 - \frac{2}{15}c_4 - \dots \right. \\ &\qquad \left. - \frac{2}{(2i-1)(2i+1)}c_{2i} - \dots\right].\end{aligned} \tag{2.27}$$

The coefficients $c_i$ are unknown, yet they can be approximated using

$$\tilde{c}_i = \frac{2}{n} \sum_{j=0}^{n}{}'' f(x_j) \cos \frac{\pi i j}{n} \tag{2.28}$$

where the $x_j$, $j = 0 \dots n$ are the $n+1$ Chebyshev nodes in $[a, b]$:

$$x_j = a + \frac{(b-a)}{2} \left( \cos \frac{\pi j}{n} + 1 \right).$$

Inserting the expansion in Equation 2.26 into Equation 2.28 and using the orthogonality of the Chebyshev polynomials, the approximate coefficients can be expressed, for even $n$, as

$$\tilde{c}_i = c_i + c_{2n-i} + c_{2n+i} + c_{4n-i} + c_{4n+i} + \dots \tag{2.29}$$

Using the $n+1$ approximated coefficients $\tilde{c}_i$, and integrating over the Chebyshev polynomials as in Equation 2.27, we can approximate the integral as we did in Equation 2.27, which is what the $n+1$ point Clenshaw-Curtis rule computes:

$$\mathsf{CC}^{(1)}_{n+1}[a, b] = (b-a) \left[ \tilde{c}_0 - \frac{2}{3}\tilde{c}_2 - \frac{2}{15}\tilde{c}_4 - \dots - \frac{2}{(n-1)(n+1)}\tilde{c}_n \right] \tag{2.30}$$

for even $n$. Now, inserting Equation 2.29 into Equation 2.30 and subtracting it from Equation 2.27, assuming that the coefficients $c_i$ may be neglected for $i \geq 3n$, we can compute

$$\begin{aligned} \int_a^b f(x)\,\mathrm{d}x - \mathsf{CC}^{(1)}_{n+1}[a, b] = \\ (b-a) \Bigg[ -2c_{2n} + \frac{2}{3}(c_{2n-2} + c_{2n+2}) + \dots \\ + \quad \frac{2}{(n-3)(n-1)}(c_{n+2} + c_{3n-2}) \\ - \quad \sum_{i=1}^{n-1} \frac{2c_{n+2i}}{(n+2i-1)(n+2i+1)} \Bigg] \end{aligned} \tag{2.31}$$

as is done in [10]. O'Hara and Smith, however, collect the terms in Equation 2.31 and write

$$\begin{aligned} &\int_a^b f(x)\,\mathrm{d}x - \mathsf{CC}^{(1)}_{n+1}[a,b] = \\ &\quad (b-a)\left[\frac{16n}{(n^2-1)(n^2-9)}c_{n+2} + \frac{32n}{(n^2-9)(n^2-25)}c_{n+4} + \dots \right. \\ &+ \quad \frac{16(n/2-1)n}{3(2n-1)(2n-3)}c_{2n-2} - \left(2 + \frac{2}{4n^2-1}\right)c_{2n} \\ &+ \quad \left.\left(\frac{2}{3} - \frac{2}{(2n+1)(2n+3)}\right)c_{2n+2} + \dots\right]. \end{aligned} \tag{2.32}$$

They note that for most regular functions, the magnitude of the coefficients $c_i$ of its Chebyshev series fall to zero exponentially as $i \to \infty$ and therefore, the first term in Equation 2.32 is often larger than the sum of the following terms.

They find that if they define the higher-order $|c_{2i}|$, $i > n+1$ in terms of $|c_{n+2}|$ using the recurrence relation $|c_{i+2}| = K_n|c_i|$, then they can define $K_n$ for different $n$ such that the first term of Equation 2.32 dominates the series. For the 7-point Clenshaw-Curtis rule, this value is $K_6 = 0.12$. If the relation $|c_{i+2}| \leq K_n|c_i|$ holds, then the error is bounded by twice the first term of Equation 2.32

$$\left|\int_a^b f(x)\,\mathrm{d}x - \mathsf{CC}^{(1)}_{n+1}[a,b]\right| \leq (b-a)\frac{32n}{(n^2-1)(n^2-9)}|c_{n+2}|.$$

However, we do not know $c_{n+2}$, yet since we assume that the magnitude of the coefficients decays, we can assume that

$$|c_{n+2}| < |c_n| \approx \frac{1}{2}|\tilde{c}_n|$$

and use $\frac{1}{2}|\tilde{c}_n|$. Since $|c_n|$ might be "*accidentally small*", they suggest, in [76], as an error estimate

$$\varepsilon = (b-a)\frac{16n}{(n^2-1)(n^2-9)}\max\left\{|\tilde{c}_n|, 2K_n|\tilde{c}_{n-2}|, 2K_n^2|\tilde{c}_{n-4}|\right\}. \tag{2.33}$$

In their algorithm, however, since after passing the first two error estimates the function is assumed to be sufficiently smooth, the third error estimate Equation 2.24 uses only $|\tilde{c}_n|$ instead of $\max\{\cdots\}$.

## 2.9 De Boor's `CADRE` Error Estimator

In 1971, de Boor [14] publishes the integration subroutine `CADRE`. The algorithm, which follows the scheme in Algorithm 1, generates a Romberg T-table [3] with

$$T_{\ell,i} = T_{\ell,i-1} + \frac{T_{\ell,i-1} - T_{\ell-1,i-1}}{4^i - 1} \tag{2.34}$$

in every interval. The entries of the T-table are equivalent to quadratures of the type

$$T_{\ell,i} = \frac{1}{b-a} Q_{2i+1}^{(2^{\ell-i})}[a,b]. \tag{2.35}$$

The entries in the T-table are used to decide whether to extend the table or bisect the interval[9]. After adding each $\ell$th row to the table, the decision is made as follows:

1. If $\ell = 1$ and $T_{1,0} = T_{0,0}$, assume that the integrand is a straight line. This is verified by evaluating the integrand at four random[10] points in the interval. If the computed values differ from the expected value by more than $\varepsilon_{\mathsf{mach}}|\hat{I}_k|$, where $|\hat{I}_k|$ is the approximation $T_{\ell,1}$ computed over the absolute function values, then the interval is bisected. Otherwise $T_{\ell,0}$ is returned as an approximation of the integral.

2. If $\ell > 1$, the ratios
$$R_i = \frac{T_{\ell-1,i} - T_{\ell-2,i}}{T_{\ell,i} - T_{\ell-1,i}} \tag{2.36}$$
for $i = 0 \dots \ell - 2$ are computed.

3. If $R_0 = 4 \pm 0.15$, the function is assumed to be sufficiently smooth and "*cautious extrapolation*" is attempted: $(b_k - a_k)T_{\ell,i}$ is used as an approximation to the integral for the smallest $i \leq \ell$ for which
$$\varepsilon_k = \left| (b_k - a_k) \frac{T_{\ell,i-1} - T_{\ell-1,i-1}}{4^i - 1} \right| \tag{2.37}$$

[9]Thus making it the first doubly-adaptive quadrature algorithm known to the author, although this title is usually bestowed upon other authors, *e.g.* Cools and Haegmans by [21] or Oliver by [24].

[10]The "random" points are hard-coded as [0.71420053, 0.34662815, 0.843751, 0.12633046] for the interval $[0, 1]$.

is smaller than the local tolerance $\tau_k$.

4. If $R_0 = 2 \pm 0.01$, the integrand is assumed to have a jump discontinuity and the error is bounded by the difference between the two previous estimates, $T_{\ell,0}$ and $T_{\ell-1,0}$. If $\tau_k < |T_{\ell,0} - T_{\ell-1,0}|$ the interval is bisected. Otherwise, $T_{\ell,0}$ is returned as an approximation to the integral.

5. If $R_0$ is within 10% of the $R_0$ computed at the previous level $\ell - 1$ and $R_0 \in (1, 4)$, assume that the interval has an integrable singularity of the type
$$f(x) = (x - \xi)^\alpha g(x) \tag{2.38}$$
where $\xi$ is near the edges of $[a_k, b_k]$ and $\alpha \in (-1, 1)$. If this is the case, $R_0$ should be $\approx 2^{\alpha+1}$. The exponent $\alpha$ (or rather, the value $2^{\alpha+1}$) is estimated from successive $R_i$ and used to recompute the T-table where "*cautious extrapolation*" is attempted as above, yet interleaving the recursion
$$T_{\ell,i} = T_{\ell,i-1} + \frac{T_{\ell,i-1} - T_{\ell-1,i-1}}{2^{\alpha+i} - 1} \tag{2.39}$$
where necessary. As with above, the first entry to satisfy the error requirement is returned as an approximation to the integral. If no such estimate is found, the interval is bisected.

6. If the previous tests have failed, the "*noise level*" of the integrand in the interval is approximated by evaluating the function at four "random" nodes inside the interval and comparing the functions values to the line through the endpoints of the interval. If each of these differences is smaller than the required tolerance the last estimate of the integrand considered ($T_{\ell,i}$) is returned.

7. Otherwise, if $\ell < 5$ or the rate of decrease of the error computed from the last two T-table rows indicates that the scheme will converge for $\ell < 10$, another row is added to the table.

8. Otherwise, the interval is bisected.

The local tolerance $\tau_k$ for each $k$th interval is computed as
$$\tau_k = \max\left\{(b_k - a_k)\varepsilon_{\mathsf{mach}}|T_{\ell,1}|, 2^{-d}\max\left\{\tau_{\mathsf{abs}}, \tau_{\mathsf{rel}}\left|\hat{I}\right|\right\}\right\} \tag{2.40}$$

where $\tau_{\mathsf{abs}}$ and $\tau_{\mathsf{rel}}$ are the absolute and relative error requirements given by the user and $\hat{I}$ is the current approximation to the *global* integral. This local tolerance, which is scaled with $2^{-d}$ where $d$ is the recursion depth, is in essence the strict tolerance first used by Kuncir (see Section 2.2), yet with a guard for error estimates below machine precision relative to the *local* integral itself, similar to that of McKeeman (see Section 2.4).

The rationale for using the ratios $R_i$ (Equation 2.36) is based on the observation that, given the correspondence in Equation 2.35, the error of each entry of the T-table is, for sufficiently smooth integrands,

$$\frac{1}{b-a}\int_a^b f(x)\,\mathrm{d}x - T_{\ell,i} \approx \kappa_i \left(2^{-(\ell-i)}\right)^{2i+2}. \tag{2.41}$$

The ratio $R_i$ can therefore be re-written as

$$\begin{aligned} R_i &= \frac{\kappa_i \left(2^{-(\ell-i-1)}\right)^{2i+2} - \kappa_i \left(2^{-(\ell-2-i)}\right)^{2i+2}}{\kappa_i \left(2^{-(\ell-i)}\right)^{2i+2} - \kappa_i \left(2^{-(\ell-1-i)}\right)^{2i+2}} \\ &= \frac{2^{2i+2} - 4^{2i+2}}{1 - 2^{2i+2}} \\ &= 4^{i+1}. \end{aligned} \tag{2.42}$$

If this condition is actually satisfied (approximately), then de Boor considers it safe to assume that the difference between the two approximations $T_{\ell,i-1}$ and $T_{\ell,i}$ is a good bound for the error of $T_{\ell,i}$, as is computed in Equation 2.37[11].

Assuming that the integrand does have the form described in Equation 2.38, with $\alpha \in (-1,1)$ then, as Lyness and Ninham [65] have shown, assuming $f(x)$ is $2k+1$ times continuously differentiable,

$$\frac{1}{b-a}\int_a^b f(x)\,\mathrm{d}x - T_{\ell,0} = \sum_{1\leq i\leq 2k+1-\alpha} A_i h^{i+\alpha} + \sum_{i=1}^{k} B_i h^{2i} + \mathcal{O}(h^{2k+1}), \quad h = 2^{-\ell}. \tag{2.43}$$

[11]Remember that $T_{\ell,i} = T_{\ell,i-1} + (T_{\ell,i-1} - T_{\ell-1,i-1})/(4^i - 1)$.

Thus, when constructing the T-table, we need to eliminate not only the terms in $h^{2i}$, as is usually done, but also the terms in $h^{i+\alpha}$, using

$$T_{\ell,i} = T_{\ell,i-1} + \frac{T_{\ell,i-1} - T_{\ell-1,i-1}}{2^{i+\alpha} - 1} \tag{2.44}$$

interleaved with the "normal" recurrence relation (Equation 2.34). As with the "normal" T-table, the error estimate is computed as in Equation 2.37 as the difference between the last two elements in this "special" T-table.

Another interesting feature of this algorithm is that it returns, along with the integral and error estimates, a value `IFLAG` which can have any of the following values (and their descriptions from [14]):

`1`: "*All is well,*"

`2`: "*One or more singularities were successfully handled,*"

`3`: "*In one or more sub-intervals the local estimate was accepted merely because the error estimate was small, even though no regular behavior could be recognized,*"

`4`: "*Failure, overflow of stack,*"

`5`: "*Failure, too small a sub-interval is required, which may be due to too much noise in the function relative to the given error requirement or due to a plain ornery integrand.*"

Regarding these values, de Boor himself states:

> "*A very cautious man would accept* `CADRE` *[the returned value of the integral] only if* `IFLAG` *is 1 or 2. The merely reasonable man would keep the faith even if* `IFLAG` *is 3. The adventurous man is quite often right in accepting* `CADRE` *even if* `IFLAG` *is 4 or 5.*"

## 2.10 Rowland and Varol's Modified Exit Procedure

In 1972, Rowland and Varol [88] publish an error estimator based on Simpson's compound rule. In their paper, they show that the "*stopping* *inequality*"

$$\left|\mathsf{S}^{(m)}[a,b] - \mathsf{S}^{(2m)}[a,b]\right| \geq \left|\mathsf{S}^{(2m)}[a,b] - \int_a^b f(x)\,\mathrm{d}x\right|$$

as it is used by Lyness with $m = 1$ (see Section 2.7) is valid if $f^{(4)}(x)$ is of constant sign for $x \in [a,b]$. They also show that under certain conditions there exists an integer $m_0$ such that the inequality is valid for all $m \geq m_0$. Similarly to de Boor (see Section 2.9), they note that for the compound Simpson's rule

$$\frac{\mathsf{S}^{(m)}[a,b] - \mathsf{S}^{(2m)}[a,b]}{\mathsf{S}^{(2m)}[a,b] - \mathsf{S}^{(4m)}[a,b]} \approx 2^{2q} \tag{2.45}$$

holds, where usually $q = 2$. This condition is used to test if $m$ is indeed large enough, much in the same way as de Boor's `CADRE` does (Equation 2.36 in Section 2.9) to test for regularity. If this condition is more or less satisfied[12] for any given $m$, then they suggest using

$$\varepsilon_k = \frac{\left(\mathsf{S}^{(2m)}[a_k,b_k] - \mathsf{S}^{(4m)}[a_k,b_k]\right)^2}{\left|\mathsf{S}^{(m)}[a_k,b_k] - \mathsf{S}^{(2m)}[a_k,b_k]\right|}. \tag{2.46}$$

This error estimate can be interpreted as follows: Let us assume that

$$e_m = \left|\mathsf{S}^{(m)}[a,b] - \mathsf{S}^{(2m)}[a,b]\right| \tag{2.47}$$

is, for a sufficiently smooth integrand or sufficiently large $m$, an estimate of the error of $\mathsf{S}^{(m)}[a,b]$. This error estimate is in itself somewhat impracticable, since to compute it, one has to evaluate the more precise compound rule $\mathsf{S}^{(2m)}[a,b]$, and if we are to compute this rule, we would rather use it instead of $\mathsf{S}^{(m)}[a,b]$ as our estimate to the integral. If we assume, however, that the error estimates decrease at a constant rate[13] $r$ such that

$$\begin{aligned} e_{2m} &= r e_m \\ r &= \frac{e_{2m}}{e_m}, \end{aligned} \tag{2.48}$$

[12]Since their paper does not include an implementation, no specification is given to how close to a power of two this ratio has to be.

[13]If the error of the compound rule behaves as in Equation 1.2, then this assumption is indeed valid.

then we can *extrapolate* the error of $S^{(4m)}[a,b]$ using

$$\begin{aligned} e_{4m} &= re_{2m} \\ &= \frac{e_{2m}^2}{e_m} \end{aligned} \tag{2.49}$$

which is exactly what is computed in Equation 2.46.

This error estimate can also be explained in terms of the Romberg T-table, where $\mathsf{S}^{(m)}[a,b]$, $\mathsf{S}^{(2m)}[a,b]$ and $\mathsf{S}^{(4m)}[a,b]$ are the last three entries in the second column, $T_{\ell-2,1}$, $T_{\ell-1,1}$ and $T_{\ell,1}$. If we assume that the relation in Equation 2.45 holds with $q=2$, then the error estimate is equivalent to

$$\varepsilon_k = \frac{1}{16}\left|T_{\ell,1} - T_{\ell-1,1}\right|,$$

which, except for a constant factor of $\frac{16}{15}$, is the same error estimate used by de Boor for regular integrands (see Section 2.9, Equation 2.37).

The main differences between both algorithms are that

1. Rowland and Varol only consider the second column of the Romberg T-table,
2. `CADRE` tests for singularities and discontinuities explicitly, whereas Rowland and Varol's error estimate tries to catch them implicitly by extrapolating the convergence rate directly (see Equation 2.45).

A similar approach is taken by Venter and Laurie [99], where instead of using compound Simpson's rules of increasing multiplicity, they used a sequence of stratified quadrature rules, described by Laurie in [58]. In their algorithm, the sequence of quadratures

$$Q_1[a,b], Q_3[a,b], Q_7[a,b], \dots, Q_{2^i-1}[a,b]$$

is computed and the differences

$$E_i = \left|Q_{2^i-1}[a,b] - Q_{2^{i+1}-1}[a,b]\right|$$

are used to extrapolate the error of the highest-order ($i$th) quadrature rule:

$$\varepsilon_k = \frac{E_{i-1}^2}{E_{i-2}}. \tag{2.50}$$

The resulting algorithm, which is implemented as an adaptation of QUADPACK's `QAG` (see Section 2.17), follows the global scheme in Algorithm 2. The interval is bisected if $i = 8$ or the ratio

$$\texttt{hint} = \frac{E_{i-1}}{E_{i-2}} \tag{2.51}$$

is larger than 0.1, an empirically determined threshold.

In [98], Venter notes that the error estimates usually converge *faster* than linearly. If we assume that the error of the $i$th quadrature rule behaves as

$$Q_{2^i-1}[a,b] - \int_a^b f(x)\,\mathrm{d}x \approx \kappa_{2^i}(b-a)^{2^i+1}$$

and that the coefficients $\kappa_{2^i}$ are of more or less the same magnitude, then the successive error estimates can be expected to decrease as

$$\frac{E_i}{E_{i-1}} \sim 2^{-(i+1)}.$$

A similar approach, yet using nested Clenshaw-Curtis rules, had already been suggested in 1992 by Pérez-Jordá *et al.* [81]. They use the same extrapolation as Venter and Laurie Equation 2.50, yet the errors $E_{i-1}$ and $E_{i-2}$ are approximated using

$$E_{i-1} = \left|Q_{2^i-1}[a,b] - Q_{2^{i-1}-1}[a,b]\right| \tag{2.52}$$

$$E_{i-2} = \left|Q_{2^i-1}[a,b] - Q_{2^{i-2}-1}[a,b]\right| \tag{2.53}$$

resulting in the error estimate

$$\varepsilon = \frac{(Q_{2^i-1}[a,b] - Q_{2^{i-1}-1}[a,b])^2}{\left|Q_{2^i-1}[a,b] - Q_{2^{i-2}-1}[a,b]\right|}.$$

Since their algorithm is non-adaptive, though, it is only mentioned in passing.

## 2.11 Oliver's Doubly-Adaptive Quadrature Routine

In 1972, Oliver [79] presents a recursive doubly-adaptive Clenshaw-Curtis quadrature routine using an extension of the error estimate of O'Hara and

Smith (see Section 2.8). The quadrature routine is doubly adaptive in the sense that for each interval after the application of an $(n+1)$-point Clenshaw-Curtis rule, the algorithm make a decision whether to double the order of the quadrature rule to $2n+1$ points or to subdivide the interval.

Instead of assuming a constant $K_n$ such that

$$|c_{i+2}| \leq K_n\,|c_i|$$

where the $c_i$ are the Chebyshev coefficients (see Equation 2.26) of the integrand, as do O'Hara and Smith, such that the first term in the error expansion (Equation 2.32) dominates the sum of all following terms, Oliver approximates the smallest rate of decrease of the coefficients as

$$K = \max\left\{\left|\frac{\tilde{c}_n}{\tilde{c}_{n-2}}\right|, \left|\frac{\tilde{c}_{n-2}}{\tilde{c}_{n-4}}\right|, \left|\frac{\tilde{c}_{n-4}}{\tilde{c}_{n-6}}\right|\right\} \tag{2.54}$$

where the $\tilde{c}_i$ are the computed Chebyshev coefficients (see Equation 2.28).

He also pre-computes a number of convergence rates $K_n(\sigma)$, which are the rates of decay required such that, for $n$ coefficients, $\sigma$ times the first term of the error expansion in Equation 2.32 dominates the sum of the remaining terms. If $K$ is less than any $K_n(\sigma)$ for $\sigma = 2$, 4, 8 or 16, then the error estimate

$$\varepsilon_k = \sigma\frac{16n}{(n^2-1)(n^2-9)}\max\left\{K|\tilde{c}_n|, K^2|\tilde{c}_{n-2}|, K^3|\tilde{c}_{n-4}|\right\}, \tag{2.55}$$

which is consistent with Equation 2.33 by O'Hara and Smith, is used.

If $K \leq K_n(16)$, then $\varepsilon_k$ Equation 2.55 is used as an error estimate. Otherwise, since the previous extrapolations might have been unreliable, the difference between the two previous estimates

$$\left|\mathsf{CC}^{(1)}_{n+1}[a,b] - \mathsf{CC}^{(1)}_{n/2+1}[a,b]\right|$$

is used. If this estimate does not exist (*i.e.* we have just started on this interval), then the interval is immediately subdivided.

The error estimate is compared to the required local tolerance

$$\tau_k = \left(\tau - \sum_{i=1}^{k-1}\varepsilon_i\right)\max\left\{\frac{2(b_k-a_k)}{b-a_k}, 0.1\right\} \tag{2.56}$$

which is similar to the local tolerance of O'Hara and Smith (Equation 2.25), yet with a relaxation when the interval is larger than one tenth of the remaining integration interval.

If $\varepsilon_k$ exceeds the required local tolerance $\tau_k$, the computed rate of decrease $K$ is compared to a pre-computed limit $K_n^*$. This limit is defined by Oliver in [78] as the rate of decrease of the Chebyshev coefficients as of which it is preferable to subdivide the interval as opposed to doubling the order of the quadrature rule. Therefore, if $K > K_n^*$, the interval is subdivided, otherwise the order of the Clenshaw-Curtis quadrature rule is doubled.

## 2.12 Gauss-Kronrod Type Error Estimators

In 1973 both Patterson [80] and Piessens [82] publish adaptive quadrature routines based on Gauss quadrature rules and their Kronrod extensions [54].

Piessens' algorithm computes both a $n$-point Gauss quadrature $\mathsf{G}_n[a,b]$ of degree $2n-1$ and its $2n+1$-point Kronrod extension $\mathsf{K}_{2n+1}[a,b]$ of degree $3n+1$. The Kronrod extension is used as an approximation to the integral and an the error estimate

$$\varepsilon_k = \left|\mathsf{G}_n[a_k,b_k] - \mathsf{K}_{2n+1}[a_k,b_k]\right| \tag{2.57}$$

is computed. Notice the absence of a scaling factor relative to the recursion depth: it is not necessary since this is the first algorithm published adhering to the heap-based scheme shown in Algorithm 2. The global error is computed as the sum of the local errors $\varepsilon_k$ and subdivision of the interval with the largest local error estimate continues until the sum of the local error estimates (hence the global error estimate) is below the required tolerance. This avoids any problems related to having to estimate a local tolerance, such as those observed in Equation 2.8 and Equation 2.9.

Patterson's integrator takes a different approach, starting with a 3-point Gauss quadrature rule and successively extending it using the Kronrod scheme [54] to 7, 15, 31, 63, 127 and 255 nodes, resulting in quadrature rules of degree 5, 11, 23, 47, 95, 191 and 383 respectively, until the difference between two successive estimates is below the required local tolerance:

$$\varepsilon_k = \left|\mathsf{K}_n[a_k, b_k] - \mathsf{K}_{2n+1}[a_k, b_k]\right| / \left|\hat{I}\right| \tag{2.58}$$

where $\mathsf{K}_n[a,b]$ is the Kronrod extension over $n$ nodes and $\mathsf{K}_{2n+1}[a,b]$ its extension over $2n+1$ nodes. $\hat{I}$ is an initial approximation of the global integral generated by applying successive Kronrod extensions to the whole interval before subdividing.

The interval is only subdivided if the error estimate for the highest-degree rule is larger than the requested tolerance. Since it is not possible to re-use points after subdivision of the interval, subdivision itself is regarded as a "rescue operation" to be used only as a last resort.

Notice here also the lack of a scaling factor relative to the recursion depth, although, as opposed to Piessens' algorithm, this algorithm works recursively (as in Algorithm 1). If many subdivisions occur, then the sum of the local error estimates, each smaller the global tolerance, may not necessarily be itself smaller than the global tolerance. The sum of the local error estimates is therefore also returned such that the user may himself/herself verify the quality of the integration.

In both algorithms the error is approximated using quadrature rules of different degree, ss with the estimator of O'Hara and Smith (see Section 2.8), thus rendering an analytical interpretation somewhat difficult.

## 2.13 The `SNIFF` Error Estimator

In 1978, Garribba *et al.* [35] publish `SNIFF`, a Self-tuning Numerical Integrator For analytical Functions. Their algorithm is one of the few exceptions which differs, in its general structure, from both Algorithm 1 and Algorithm 2: Since it is based on Gauss-Legendre quadrature rules, and therefore no function evaluations can be recycled upon interval subdivision, the authors decided on a scheme along the lines of Algorithm 3, similar to the algorithm of Morrin (see Section 2.1).

The interval subdivision works by first considering the entire interval $[a,b]$ and computing the integral and the error estimate. If the requested tolerance is not satisfied, the interval is reduced by

$$[a_{k+1}, b_{k+1}] = [a_k, a_k + h_k], \quad h_k = \frac{b_k - a_k}{m_k}$$

where $m_k$ is chosen dynamically, as we will see later. Once an interval $[a_k, b_k]$ has converged, the next interval is chosen as

$$[a_{k+1}, b_{k+1}] = [b_k, \min\{b_k + h_k, b\}], \quad h_k = \frac{b_k - a_k}{m_k}$$

where, since the $k$th interval was accepted, $m_k \leq 1$.

For the error estimate, they start by noting that for any integration rule $Q_n$ of degree $n$, the error can be written as

$$Q_n^{(1)}[a,b] - \int_a^b f(x)\,\mathrm{d}x = K_n (b-a)^{n+2} f^{(n+1)}(\xi), \quad \xi \in [a,b] \tag{2.59}$$

where the constant $K_n$ depends on the type an number of nodes of the quadrature rule $Q_n^{(1)}[a,b]$.

If the interval is subdivided into $m$ sub-intervals of equal width, this estimate becomes

$$Q_n^{(m)}[a,b] - \int_a^b f(x)\,\mathrm{d}x \approx K_n \frac{(b-a)^{n+2}}{m^{n+2}} \bar{f}^{(n+1)}$$

where $\bar{f}^{(n+1)}$ is the average of the $m$ $n+1$st derivatives $f^{(n+1)}(\xi_i)$, $\xi_k \in [a+(i-1)h, a+ih]$, $h = (b-a)/m$ from the errors of each of the $m$ panels of $Q_n^{(m)}[a,b]$. They combine these two estimates for $m=1$ and $m=2$, as is done in Romberg extrapolation, to approximate the value

$$\kappa_n := \frac{2^{n+2}\left(Q_n^{(1)}[a,b] - Q_n^{(2)}[a,b]\right)}{2^{n+2}-1} \approx K_n (b-a)^{n+2} \bar{f}^{(n+1)}. \tag{2.60}$$

The resulting value $\kappa_n$ can then be used to represent the error of any compound rule of multiplicity $m$:

$$Q_n^{(m)}[a,b] - \int_a^b f(x)\,\mathrm{d}x \approx \kappa_n m^{-(n+2)}. \tag{2.61}$$

Given the representation of the locally relative error of the $k$th interval

$$\left| Q_n^{(m)}[a_k, b_k] - \int_{a_k}^{b_k} f(x)\,\mathrm{d}x \right| \leq \tau_k \left| \int_{a_k}^{b_k} f(x)\,\mathrm{d}x \right| \tag{2.62}$$

where $\tau_k$ is the required tolerance for that interval, they insert Equation 2.61 into the left hand side of Equation 2.62 and $\int_a^b f(x)\,\mathrm{d}x \approx Q_n^{(1)} - \kappa_n$ into its right hand side and solve for $m$, resulting in

$$\frac{2^{n+2}\left| Q_n^{(2)}[a_k, b_k] - Q_n^{(1)}[a_k, b_k] \right|}{\tau_k \left| 2^{n+2} Q_n^{(2)}[a_k, b_k] - Q_n^{(1)}[a_k, b_k] \right|} \leq m^{n+2} \tag{2.63}$$

Using this relation, they compute the number of intervals $m_k$ in which they should subdivide the domain such that the relative tolerance $\tau_k$ should be satisfied:

$$m_k = \left( \frac{2^{n+2}\left| Q_n^{(2)}[a_k, b_k] - Q_n^{(1)}[a_k, b_k] \right|}{\tau_k \left| 2^{n+2} Q_n^{(2)}[a_k, b_k] - Q_n^{(1)}[a_k, b_k] \right|} \right)^{1/(n+2)}.$$

If $m_k \leq 1$, then the interval is sufficiently converged and no further subdivision is needed. We can re-formulate this condition as an error estimate for the quadrature rule $Q_n^{(2)}$ from Equation 2.61:

$$\varepsilon_k = \frac{\left| Q_n^{(2)}[a_k, b_k] - Q_n^{(1)}[a_k, b_k] \right|}{2^{n+2} - 1} \tag{2.64}$$

according to which, if it is larger than $\tau_k$, the interval will be subdivided into $m_k$ sub-intervals. This is similar to the error estimate of de Boor for the entries of the Romberg T-table (see Section 2.9, Equation 2.37).

The local tolerance $\tau_k$ for the $k$th interval is computed from the global relative tolerance $\tau$ as

$$\tau_k = \tau \max\left\{ 1, \left| \frac{\hat{I}_k}{Q_n^{(2)}[a_k, b_k]} \right| \right\} \left| \frac{(b_k - a_k)}{(b - a)} \right| \tag{2.65}$$

where $\hat{I}_k$ is the running estimate of the global integral at the time that the $k$th interval is inspected. The factor $\hat{I}_k / Q_n^{(2)}[a_k, b_k]$ basically converts the relative tolerance into an absolute tolerance and the factor $(b_k - a_k)/(b-a)$ scales the local tolerance relative to the interval width. If we assume that the cumulative estimates $\hat{I}_k$ are correct, then the sum of the tolerances is equal to $\tau \left| \int_a^b f(x)\,\mathrm{d}x \right|$. This is, in essence, the same as using a *globally relative* local tolerance and scaling the local error with $m$ after each subdivision into $m$ sub-intervals, as is done by McKeeman (see Section 2.4) and therefore shares the same problems as shown in Equation 2.8.

## 2.14 De Doncker's Adaptive Extrapolation Algorithm

The probably most well-known quadrature algorithm using non-linear extrapolation is published by de Doncker in 1978 [15]. The main idea of the algorithm is similar to that of the Romberg scheme: Given a basic quadrature rule $Q_n[a,b]$, the sequence

$$Q_n^{(1)}[a,b], Q_n^{(2)}[a,b], Q_n^{(4)}[a,b], \dots, Q_n^{(2^i)}[a,b], \dots \tag{2.66}$$

converges exponentially[14], for large enough $i$, towards $\int_a^b f(x)\,\mathrm{d}x$.

In Romberg's scheme, $Q_n^{(m)}[a,b] = T^{(m)}[a,b]$, the trapezoidal rule, and the limit of the sequence is extrapolated linearly using the the Romberg T-table. De Doncker's algorithm, however, differs in two main points:

1. The 21-point Gauss-Kronrod rule is used as the basic rule $Q_n^{(m)}[a,b]$ instead of the trapezoidal rule,

2. The non-linear $\epsilon$-Algorithm [102] is used to extrapolate the limit of the sequence instead of the Romberg T-table.

The $\epsilon$-Algorithm computes a sequence of approximations using the recursion

$$\epsilon_k^{(j)} = \epsilon_{k-2}^{(j+1)} + \left( \epsilon_{k-1}^{(j+1)} - \epsilon_{k-1}^{(j)} \right)^{-1}$$

[14]If we assume that the error of each quadrature behaves as in Equation 1.2, then the error decreases by a factor of $2^{-(n+2)}$ every time $m$ is doubled.

where $\epsilon_0^{(j)} = Q_n^{(2^j)}[a,b]$, $j = 0 \ldots i$ are the initial approximations to the integral and $\epsilon_j^{(-1)} = 0$. This recursion is usually represented and stored in an epsilon-table

$$\begin{array}{cccccc}
 & \epsilon_0^{(0)} & & & & \\
\epsilon_{-1}^{(1)} & & \epsilon_1^{(0)} & & & \\
 & \epsilon_0^{(1)} & & \epsilon_2^{(0)} & & \\
\epsilon_{-1}^{(2)} & & \epsilon_1^{(1)} & & \epsilon_3^{(0)} & \\
 & \epsilon_0^{(2)} & & \epsilon_2^{(1)} & & \ddots \\
\epsilon_{-1}^{(3)} & & \epsilon_1^{(2)} & & \ddots & \\
 & \epsilon_0^{(3)} & & \ddots & & \\
\epsilon_{-1}^{(4)} & \vdots & \ddots & & &
\end{array}$$

in which the even columns $\epsilon_{2i}^{(j)}$ represent the faster converging sequences. The last entry in the rightmost even column is then used as an estimate for the sequence limit, in this case $I_i$.

The use of the Gauss-Kronrod rule for adaptive quadrature is not new, as it was first introduced by Piessens in 1973 (see Section 2.12) and the use of the $\epsilon$-Algorithm instead of the Romberg T-table was already tested by Kahaner in 1972 [50]. The combination of both, however, with the following modification, is novel.

The algorithm, as described thus far, is not yet adaptive. The main (and new) innovation is that instead of using $Q_n^{(m)}[a,b]$, de Doncker uses *approximations* $\tilde{Q}_n^{(m)}[a,b]$. Each approximation $\tilde{Q}_n^{(m)}[a,b]$ is computed by iteratively picking out the sub-interval of width greater than $h = (b-a)/m$ with the largest local error estimate

$$\varepsilon_k = |\mathsf{G}_{10}[a_k,b_k] - \mathsf{K}_{21}[a_k,b_k]| \tag{2.67}$$

which is the same local error estimate as first used by Piessens (see Section 2.12), and subdividing it until:

1. The sum of the local error estimates $\varepsilon_k$ of all intervals of width larger than $h$ is smaller than the required tolerance or

2. There are no more intervals of width larger than $h$ left to subdivide.

In the first case, the error induced by *not* subdividing the intervals larger than $h$ is below the required global tolerance $\tau$ and thus so should

$$\left|\tilde{Q}_n^{(m)}[a,b] - Q_n^{(m)}[a,b]\right| < \tau.$$

In the second case, all intervals are of the width $h$ and therefore $\tilde{Q}_n^{(m)}[a,b] = Q_n^{(m)}[a,b]$.

In her original paper, de Doncker does not give any details on how the $\epsilon$-Algorithm is applied or how the global error is estimated. The algorithm, however, was later packaged as `QAGS` in QUADPACK. In that implementation, the local error estimate (Equation 2.67) is replaced by the local error estimator used in the other QUADPACK-routines (see Section 2.17, Equation 2.97). Furthermore, to avoid problems in the extrapolation due to bad initial estimates, the error

$$e_k^{(j)} = \left|\epsilon_{k-2}^{(j)} - \epsilon_{k-2}^{(j+1)}\right| + \left|\epsilon_{k-2}^{(j+1)} - \epsilon_{k-2}^{(j+2)}\right| + \left|\epsilon_{k-2}^{(j+2)} - \epsilon_{k}^{(j)}\right| \tag{2.68}$$

is computed for every entry $\epsilon_k^{(j)}$ and the element at the bottom of the even column with the smallest $e_k^{(j)}$ is used as the extrapolated value $I_i$. A global error estimate is computed for the extrapolated $I_i$ using

$$\varepsilon_i = |I_i - I_{i-1}| + |I_i - I_{i-2}| + |I_i - I_{i-3}| \tag{2.69}$$

where $I_{i-1}$, $I_{i-2}$ and $I_{i-3}$ are the previous three estimates of the global integral.

In 1983, Kahaner and Stoer [51] publish a similar algorithm which, in contrast to de Doncker's, uses the trapezoidal rule $T^{(m)}[a,b]$ as a basic rule and constructs a Romberg T-table [3] from the successive estimates, yet as with de Doncker's algorithm, it only sub-divides the intervals selectively and uses the last element $T_{i,i}$ of the T-table as the estimate $I$.

Kahaner and Stoer refer to de Doncker and note that both her use of a higher-order rule for $Q_n^{(m)}[a,b]$ and the use of the $\epsilon$-Algorithm for extrapolation of both $I$ and the error are much better choices.

Kahaner and Stoer suggest computing a conservative estimate of the error from the last three elements in the T-table:

$$\varepsilon = |T_{i,i} - T_{i,i-1}| + |T_{i,i} - T_{i-1,i-1}|\,. \tag{2.70}$$

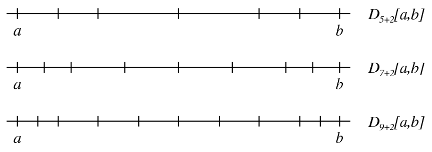


**Figure 2.8:** Ninomiya's error estimate approximates the $6th$, 8th and 10th derivative using 7, 9 and 11 points respectively.

No specific mention is made of how the error is approximated when using the $\epsilon$-Algorithm, yet we may assume that again the difference between the final and the last two estimates is used. Note that the three last estimates are the last three elements in the *even* columns of the $\epsilon$-table.

## 2.15 Ninomiya's Improved Adaptive Quadrature Method

In a 1980 paper [74], Ninomiya presents a recursive adaptive quadrature routine based on closed Newton-Cotes rules. He uses rules with $2n+1$ nodes (results are given for 5, 7 and 9 points) and notes that these have an error of the form

$$\mathsf{NC}_{2n-1}[a,b] - \int_a^b f(x)\,\mathrm{d}x = K_{2n+1}(b-a)^{2n+1} f^{(2n)}(\xi), \quad \xi \in [a,b].$$

Instead of using the same quadrature rule on two or more sub-intervals to approximate the error as in Kuncir's and Lyness' error estimates, he adds two nodes in the center of the leftmost and the rightmost intervals. This choice is made

> "*taking account of the excellent properties of interpolation based on zeros of Chebyshev or Legendre polynomials which have high densities near the ends of [the] interval.*"

Using $5+2$, $7+2$ and $9+2$ point stencils (Figure 2.8), he computes the error estimators

$$D_{5+2}[a,b] \approx \frac{(b-a)^7}{15\,120} f^{(6)}(\xi), \quad \xi \in [a,b] \tag{2.71}$$

$$D_{7+2}[a,b] \approx \frac{(b-a)^9}{1\,020\,600} f^{(8)}(\xi), \quad \xi \in [a,b] \tag{2.72}$$

$$D_{9+2}[a,b] \approx \frac{37(b-a)^{11}}{3\,066\,102\,400} f^{(10)}(\xi), \quad \xi \in [a,b], \tag{2.73}$$

which approximate the analytical error of the Newton-Cotes rules over 5, 7 and 9 points respectively. The weights of these estimators are pre-computed by solving a Vandermonde-like system of linear equations.

The error term is later subtracted from the initial estimate of the integral, resulting in a higher-degree estimate. The function values at the points added near the ends of the intervals are not used for the approximation of the integral itself. They can, however, be re-used if the interval needs to be sub-divided.

The resulting error estimate for the $k$th interval using $2n+1$ points is approximated using

$$\varepsilon_k = |D_{2n+3}[a_k,b_k]| \frac{(b-a)}{(b_k-a_k)} \left( \log_2 \frac{(b-a)}{(b_k-a_k)} \right)^{-1}. \tag{2.74}$$

The interval-dependent scaling factor is proposed as an alternative to scaling by $2^d$. Ninomiya states that

> "*Unfortunately, no adequate analytical or statistical theory concerning the application of the new method has been conceived as yet.*"

However, since bisection is used, the width of the $k$th interval can be written as

$$(b_k - a_k) = 2^{-d}(b-a) \tag{2.75}$$

where $d$ is the depth of the $k$th subdivision (in a recursive scheme). Re-inserting this into Equation 2.74, we obtain

$$\varepsilon_k = |D_{2n+3}[a_k,b_k]| \frac{2^d}{d}, \tag{2.76}$$

which lies asymptotically below the $2^d$ first used by Kuncir (Section 2.2), yet larger than the $\sqrt{2}^d$ introduced by McKeeman (Section 2.4). This scaling is therefore also vulnerable to the problems described in Equation 2.8 and Equation 2.9.

## 2.16 Laurie's Sharper Error Estimate

In 1983, Laurie publishes a sharper error estimate [56] based on two quadrature rules $Q_\alpha[a,b]$ and $Q_\beta[a,b]$ of degree $\alpha$ and $\beta$ respectively, where $\alpha > \beta$, or $\alpha = \beta$ and $Q_\alpha[a,b]$ is assumed to be more precise than $Q_\beta[a,b]$. Laurie states that whereas the difference of the two rules is generally a good approximation to the error of $Q_\beta[a,b]$, it is a severe overestimate of the error of $Q_\alpha[a,b]$. He therefore proposes, as an error estimate for the more precise $Q_\alpha[a,b]$, which is usually used as an approximation to the integral, the extrapolated error estimate

$$\varepsilon_k = \frac{\left(Q_\alpha^{(2)} - Q_\beta^{(2)}\right)\left(Q_\alpha^{(2)} - Q_\alpha^{(1)}\right)}{Q_\beta^{(2)} - Q_\beta^{(1)} - Q_\alpha^{(2)} + Q_\alpha^{(1)}} \tag{2.77}$$

where the ranges $[a_k, b_k]$ are omitted for simplicity.

He shows that this error estimate is valid when

$$\left|Q_\alpha^{(2)} - Q_\alpha^{(1)}\right| < \left|Q_\beta^{(2)} - Q_\beta^{(1)}\right|, \tag{2.78}$$

which can be checked for in practice, and when

$$0 \leq \frac{Q_\alpha^{(2)} - I}{Q_\alpha^{(1)} - I} \leq \frac{Q_\beta^{(2)} - I}{Q_\beta^{(1)} - I} < 1 \tag{2.79}$$

which is impossible to verify since the exact integral $I = \int_a^b f(x)\,\mathrm{d}x$ must be known. These two conditions imply that the error of $Q_\alpha[a,b]$ is smaller than and decreases at a faster rate than that of $Q_\beta[a,b]$.

Laurie suggests a weaker condition that can be checked in practice, namely replacing $I$ by $Q_\alpha^{(2)}[a_k,b_k] + \varepsilon_k$ in Equation 2.79, resulting in

$$0 \leq \frac{Q_\alpha^{(2)} - Q_\beta^{(2)}}{Q_\alpha^{(1)} - Q_\beta^{(1)}} < 1. \tag{2.80}$$

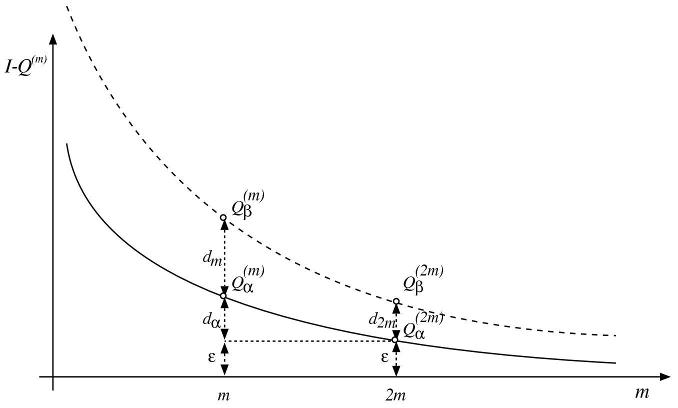


**Figure 2.9:** The error of the quadrature rules $Q_\alpha^{(m)}$ (solid curve) and $Q_\beta^{(m)}$ (dotted curve) as a function of the number of panels or subdivisions $m$.

Espelid and Sørevik [25] show, however, that this weaker condition is often satisfied when Equation 2.79 is not, which can lead to bad error estimates[15].

The error estimate itself, based on these assumptions, is best explained graphically (see Fig. 2.9). The errors of both rules $Q_\alpha^{(m)}[a,b]$ and $Q_\beta^{(m)}[a,b]$ are assumed to decrease exponentially with the increasing number of panels or subdivisions $m$:

$$Q_\alpha^{(m)} - I = \kappa_\alpha \left(\frac{b-a}{m}\right)^{\alpha+2} f^{(\alpha+1)}(\xi_\alpha), \quad \xi_\alpha \in [a,b], \tag{2.81}$$

$$Q_\beta^{(m)} - I = \kappa_\beta \left(\frac{b-a}{m}\right)^{\beta+2} f^{(\beta+1)}(\xi_\beta), \quad \xi_\beta \in [a,b], \tag{2.82}$$

where we will assume that $f^{(\alpha+1)}(x)$ and $f^{(\beta+1)}(x)$ are constant. Under this assumption, we can verify that Equation 2.79 holds for $\beta \leq \alpha$ by

[15]Espelid and Sørevik show that this is the case when using the 10-point Gauss rule and its 21-point Kronrod extension for $Q_\beta^{(1)}$ and $Q_\alpha^{(1)}$ respectively and integrating $\int_1^2 0.1/(0.01+(x-\lambda)^2)\,\mathrm{d}x$ for $1 \leq \lambda \leq 2$.

inserting Equation 2.81 and Equation 2.82 therein:

$$\begin{array}{rcl}
\frac{\kappa_\alpha \left(\frac{b-a}{2m}\right)^{\alpha+2} f^{(\alpha+1)}(\xi_\alpha)}{\kappa_\beta \left(\frac{b-a}{2m}\right)^{\beta+2} f^{(\beta+1)}(\xi_\beta)} & \leq & \frac{\kappa_\alpha \left(\frac{b-a}{m}\right)^{\alpha+2} f^{(\alpha+1)}(\xi_\alpha)}{\kappa_\beta \left(\frac{b-a}{m}\right)^{\beta+2} f^{(\beta+1)}(\xi_\beta)} \\
\frac{2^{-(\alpha+2)} \left(\frac{b-a}{m}\right)^{\alpha+2}}{2^{-(\beta+2)} \left(\frac{b-a}{m}\right)^{\beta+2}} & \leq & \frac{\left(\frac{b-a}{m}\right)^{\alpha+2}}{\left(\frac{b-a}{m}\right)^{\beta+2}} \\
\frac{2^{-(\alpha+2)}}{2^{-(\beta+2)}} & \leq & 1 \\
2^{\beta-\alpha} & \leq & 1, \quad \beta \leq \alpha.
\end{array}$$

We then define the distances

$$d_\alpha = Q_\alpha^{(m)} - Q_\alpha^{(2m)} \tag{2.83}$$
$$d_m = Q_\beta^{(m)} - Q_\alpha^{(m)} \tag{2.84}$$
$$d_{2m} = Q_\beta^{(2m)} - Q_\alpha^{(2m)} \tag{2.85}$$
$$\varepsilon = Q_\alpha^{(2m)} - I \tag{2.86}$$

as they are shown in Figure 2.9. Using these differences, we can re-write the terms in Equation 2.79 as

$$Q_\alpha^{(2m)} - I = \varepsilon \tag{2.87}$$
$$Q_\beta^{(2m)} - I = \varepsilon + d_{2m} \tag{2.88}$$
$$Q_\alpha^{(m)} - I = \varepsilon + d_\alpha \tag{2.89}$$
$$Q_\beta^{(m)} - I = \varepsilon + d_\alpha + d_m. \tag{2.90}$$

Re-inserting these terms into Equation 2.79, we obtain

$$\begin{array}{rcl}
\frac{\varepsilon}{\varepsilon + d_\alpha} & \geq & \frac{\varepsilon + d_{2m}}{\varepsilon + d_\alpha + d_m} \\
\varepsilon(\varepsilon + d_\alpha + d_m) & \geq & (\varepsilon + d_{2m})(\varepsilon + d_\alpha) \\
\varepsilon(d_m + d_\alpha) & \geq & d_\alpha d_{2m} + \varepsilon(d_\alpha + d_{2m}) \\
\varepsilon & \leq & \frac{d_\alpha d_{2m}}{d_{2m} - d_m}.
\end{array} \tag{2.91}$$

Re-inserting Equation 2.83–Equation 2.85, we see that this bound is identical to the error estimate proposed by Laurie in Equation 2.77.

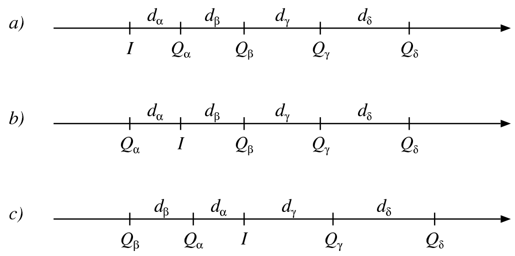


**Figure 2.10:** Different configurations of the four estimates $Q_\alpha$, $Q_\beta$, $Q_\gamma$ and $Q_\delta$ around the exact integral $I$.

This error estimate was tested both by Laurie himself in 1985 [57] and by Espelid and Sørevik in 1989 [25]. Laurie notes that while the error estimates are more accurate than other linear estimators, some reliability is lost, whereas Espelid and Sørevik show that when the error estimate is used in QUADPACK's `QAG`, the results can be catastrophic. In both cases, however, it is not specified if the conditions in Equation 2.78 and Equation 2.80 are tested for and if so, what is done if they fail.

In 1991, Favati, Lotti and Romani [27] publish a similar error estimator, based on four quadratures $Q_\alpha[a,b]$, $Q_\beta[a,b]$, $Q_\gamma[a,b]$ and $Q_\delta[a,b]$ of degree $\alpha > \beta > \gamma > \delta$ that satisfy

$$|I - Q_\alpha| \leq |I - Q_\delta| \tag{2.92}$$

$$|I - Q_\alpha| \leq |I - Q_\gamma| \tag{2.93}$$

$$|I - Q_\alpha| \leq |I - Q_\beta| \tag{2.94}$$

and the relation

$$\frac{|I - Q_\alpha|}{|I - Q_\gamma|} \leq \frac{|I - Q_\beta|}{|I - Q_\delta|}. \tag{2.95}$$

For any ordering of the four estimates $Q_\alpha$, $Q_\beta$, $Q_\gamma$ and $Q_\delta$ around the exact integral $I$, we can define the distances $d_\alpha$, $d_\beta$, $d_\gamma$ and $d_\delta$. Note that the definition of the distances depends on the configuration of the estimates around $I$ (see Fig. 2.10). The algorithm therefore first makes a decision as to which configuration is actually correct based on the differences between the actual estimates. Based on this decision, it computes the $d_\alpha$, $d_\beta$, $d_\gamma$ and $d_\delta$ or bounds them using Equation 2.92–

Equation 2.94 and inserts them into Equation 2.95 to extract an upper bound for $d_\alpha = |I - Q_\alpha|$, *i.e.* for the setup in Fig. 2.10a, and only for that setup, where $I < Q_\alpha < Q_\beta < Q_\gamma < Q_\delta$,

$$\begin{aligned}
\frac{d_\alpha}{d_\alpha + d_\beta + d_\gamma} &\leq \frac{d_\alpha + d_\beta}{d_\alpha + d_\beta + d_\gamma + d_\delta} \\
d_\alpha d_\delta &\leq d_\alpha d_\beta + d_\beta^2 + d_\beta d_\gamma \\
d_\alpha &\leq \frac{d_\beta^2 + d_\beta d_\gamma}{d_\delta - d_\beta} \qquad (2.96)
\end{aligned}$$

where

$$d_\beta = Q_\beta - Q_\alpha, \quad d_\gamma = Q_\gamma - Q_\beta, \quad d_\delta = Q_\delta - Q_\gamma.$$

Favati *et al.* test this algorithm on a number of integrands and show that the milder condition in Equation 2.95, which does not require successive estimates to decrease monotonically, is satisfied more often than that of Laurie in Equation 2.79.

## 2.17 QUADPACK's `QAG` Adaptive Quadrature Subroutine

In 1983, the most widely-used "commercial strength" quadrature subroutine library QUADPACK is published by Piessens *et al.* [83]. The general adaptive quadrature subroutine `QAG` is an extension of Piessens' integrator (see Section 2.12), yet with a slight modification to the local error estimate

$$\varepsilon_k = \tilde{I}_k \min \left\{ 1, \left( 200 \frac{|\mathsf{G}_n[a_k, b_k] - \mathsf{K}_{2n+1}[a_k, b_k]|}{\tilde{I}_k} \right)^{3/2} \right\} \qquad (2.97)$$

where the default value of $n$ is 10 and the value

$$\tilde{I}_k = \int_{a_k}^{b_k} \left| f(x) - \frac{\mathsf{K}_{2n+1}[a_k, b_k]}{b_k - a_k} \right| \mathrm{d}x,$$

which is also evaluated using the $K_{2n+1}[a, b]$ rule, is used, as described by Krommer and Überhuber [53], as "*a measure for the smoothness of f on* $[a, b]$".

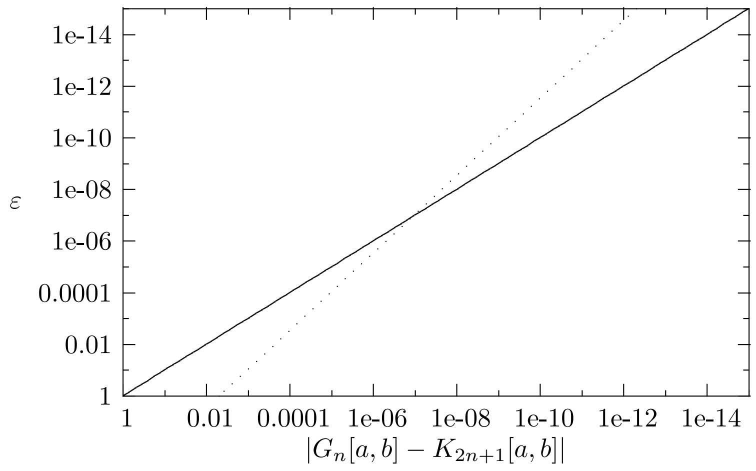


**Figure 2.11:** The error measure $(200\,|\mathsf{G}_n[a,b] - \mathsf{K}_{2n+1}[a,b]|)^{3/2}$ (dashed line) plotted as a function of $|\mathsf{G}_n[a,b] - \mathsf{K}_{2n+1}[a,b]|$.

As with Piessens' original error estimate (see Section 2.12), this estimate is also used in a non-recursive scheme as in Algorithm 2, hence the absence of a depth-dependent scaling factor and the problems involved therewith.

The error measure

$$(200 \times |\mathsf{G}_n[a_k,b_k] - \mathsf{K}_{2n+1}[a_k,b_k]|)^{3/2}$$

is best explained graphically, as is done in Piessens *et al.* (Figure 2.11). The exponent $\frac{3}{2}$ is determined experimentally and scales the error exponentially, with a break-even point at $1.25 \times 10^{-6}$ which is approximately relative machine precision for IEEE 754 32-bit floating point arithmetic. The scaling makes the estimate overly pessimistic for error estimates larger than $1.25 \times 10^{-6}$ and overly optimistic for error estimates below that threshold.

This measure is further divided by $\sqrt{\tilde{I}_k}$. Krommer and Überhuber explain this as follows:

*"If this ratio is small, the difference between the two quadra-*

> *ture formulas is small compared to the variation of $f$ on $[a, b]$;* i.e. *, the discretization of $f$ in the quadrature formulas $\mathsf{G}_n$ and $\mathsf{K}_{2n+1}$ is fine with respect to its variation. In this case, $\mathsf{K}_{2n+1}$ can indeed be expected to yield a better approximation for $If$ than $\mathsf{G}_n$."*

Unfortunately, no further analysis is given in either [83] or [53].

Although difficult to interpret mathematically, this error estimate works well in practice. As Favati *et al.* [26] have pointed out, its tendency to over-estimate the error guard it from bad estimates on highly fluctuating, discontinuous or otherwise tricky integrands.

This local error estimate is re-used by Favati *et al.* [26], yet using pairs of "recursive monotone stable" (RMS) nested quadrature rules presented in [27], which allow for function evaluations to be re-used after bisection. The algorithm (using `KEY=2` as described in [26]) is doubly-adaptive in the sense that it tries up to 4 rules of increasing degree before deciding to bisect the interval. They show this to be substantially more efficient than the original `QAG`'s use of Gauss-Kronrod rules of a fixed order.

Hasegawa *et al.* [42] extend this approach by choosing bisection over increasing the degree of the quadrature rule when the ratio of two successive error estimates is larger than an empirically determined constant (as is suggested by Venter and Laurie in [99], see Section 2.10). They also use an interval-dependent scaling factor for the tolerance (their algorithm is recursive, not global as in QUADPACK's `QAG`) based on Ninomiya's quadrature method (see Section 2.15, Equation 2.74), replacing the $\log(\cdot)$ by a $\sqrt{\cdot}$:

$$\tau_k = \tau \frac{(b_k - a_k)}{(b - a)} \sqrt{\frac{(b - a)}{(b_k - a_k)}}$$

which, using the same analysis as in Equation 2.75, is equivalent to

$$\begin{aligned} \tau_k &= \tau \frac{2^{-d}(b - a)}{(b - a)} \sqrt{\frac{(b - a)}{2^{-d}(b - a)}} \\ &= \frac{\tau}{\sqrt{2}^d} \end{aligned} \tag{2.98}$$

which is the same as the local scaling introduced by McKeeman (see

Section 2.4) and hence also shares the same problems (see Equation 2.8 and Equation 2.9).

## 2.18 Berntsen and Espelid's Improved Error Estimate

In 1984 Berntsen and Espelid [4] suggest that instead of using the difference between a Gauss quadrature rule over $n$ points and its Kronrod extension over $2n+1$ points, one could directly use a Gauss quadrature rule over $2n+1$ points for the estimate of the integral. To estimate the error of this rule of degree $4n+1$, they suggest removing one of the points and creating a new interpolatory quadrature rule $Q_{2n-1}[a,b]$ of degree $2n-1$ over the remaining $2n$ points:

$$\varepsilon_k = \left| \mathsf{G}_{2n+1}[a_k,b_k] - Q_{2n-1}[a_k,b_k] \right|. \tag{2.99}$$

Since the degree of the rule $Q_{2n-1}[a,b]$ is the same as that of the Gauss quadrature rule $\mathsf{G}_n[a,b]$ used by Piessens (see Section 2.12), the error estimate is 0 for functions of up to the same algebraic degree of precision, yet the final estimate is $n$ degrees higher: $4n+1$ for $\mathsf{G}_{2n+1}[a,b]$ vs. $3n+1$ for $\mathsf{K}_{2n+1}[a,b]$. A further advantage is the relative ease with which the weights of the rule $Q_{2n-1}[a,b]$ can be computed, as opposed to the effort required for the nodes and weights of the Kronrod extension.

## 2.19 Berntsen and Espelid's Null Rules

In a 1991 paper, Berntsen and Espelid [5] present an error estimator based on sequences of null rules.

Introduced by Lyness in 1965 [60], a null rule $N_n^{(k)}$ of degree $k$ is defined as a set of weights $u_i^{(k)}$ over the $n$ nodes $x_i$, $i = 1 \dots n$ such that

$$N_n^{(k)}[a,b] = \sum_{i=1}^{n} u_i^{(k)} x_i^j = \left\{ \begin{array}{ll} 0, & j \leq k \\ \neq 0 & j = k+1 \end{array} \right., \tag{2.100}$$

*i.e.* the rule evaluates all polynomials of degree $j \leq k$ to 0 and the $(k+1)$st monomial to some non-zero value.

The null rules themselves can be constructed by solving a Vandermonde-like system of equations, which is under-determined for $k < n - 1$:

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \\ x_1^2 & x_2^2 & \dots & x_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{k+1} & x_2^{k+1} & \dots & x_n^{k+1} \end{pmatrix} \begin{pmatrix} u_1^{(k)} \\ u_2^{(k)} \\ \vdots \\ u_n^{(k)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \tag{2.101}$$

Berntsen and Espelid compute a sequence of *orthogonal* null rules of decreasing degree. Two rules $N_n^{(j)}$ and $N_n^{(k)}$ are orthogonal if

$$\sum_{i=1}^{n} u_i^{(j)} u_i^{(k)} = 0.$$

The null rules are further normalized such that they are "equally strong", that is, given the weights $w_i$ of the underlying interpolatory quadrature rule $Q_n$ over the same nodes $x_i$, $i = 1 \dots n$, for any null rule $N_n^{(k)}$,

$$\sum_{i=1}^{n} \left(u_i^{(k)}\right)^2 = \sum_{i=1}^{n} w_i^2. \tag{2.102}$$

This set of orthogonal null rules $N_n^{(n-1)}$, $N_n^{(n-2)}$, ..., $N_n^{(0)}$ thus forms an orthogonal vector basis $S_n$ in $\mathbb{R}^n$.

Applying the null rules to the integrand $f(x)$:

$$e_k := N_n^{(k)}[a,b] = \sum_{i=1}^{n} u_i^{(k)} f(x_i), \quad k = 0 \dots n-1, \tag{2.103}$$

we obtain the *coefficients of the interpolation*[16] $e_k$ of the integrand $f(x)$ onto $S_n$. Since the basis $S_n$ is orthogonal, we can write

$$f(x_i) = \frac{1}{\sum_{k=1}^{n} w_k^2} \sum_{k=0}^{n-1} e_k u_i^{(k)}, \quad i = 1 \dots n. \tag{2.104}$$

[16]Let $p_k(x)$, $k = 0 \dots n-1$ be the polynomials of increasing degree $k$ orthogonal with respect to the discrete scalar product

$$(f, g) = \sum_{i=1}^{n} f(x_i) g(x_i),$$

This connection between null rules, interpolation and orthogonal polynomials was already made by Laurie in [59], in which he also suggests different types of coefficients constructed using non-linear combinations of null rules.

The scaling of the null rules to match the "strength" of the quadrature rule, described in detail in [18], has no effect either on the basis or the interpolation itself. Any different scaling would result in a constant scaling of the coefficients $e_k$.

Following Berntsen and Espelid, to avoid "phase effects" as described in [63], the values are then paired as

$$E_k = \left(e_{2k}^2 + e_{2k+1}^2\right)^{1/2}, \quad k = 0 \dots n/2 - 1. \tag{2.105}$$

and the ratio of these pairs is computed

$$r_k = \frac{E_k}{E_{k+1}}, \quad k = 0 \dots n/2 - 2 \tag{2.106}$$

and the largest of the last $K$ ratios

$$r_{\mathsf{max}} = \max_k r_k,$$

is taken as an estimate of the convergence rate of the coefficients. If this ratio is larger than 1, then the function is assumed to be "*non-asymptotic*" in the interval and the largest $E_k$ is used as a local error estimate.

If $r_{\mathsf{max}}$ is below 1 yet still above some critical value $r_{\mathsf{critical}}$, the function is assumed to be "*weakly asymptotic*" and the value of the next-highest coefficient $E_{n/2+1}$ — and thus the local error — is estimated using

$$\varepsilon_k = 10 r_{\mathsf{max}} E_{n/2-1} \tag{2.107}$$

that interpolate the weights of the respective null rules, such that

$$p_k(x_i) = u_i^{(k)}, \quad i = 1 \dots n$$

then the coefficients $e_k$ computed in Equation 2.103 are also the coefficients of interpolation of the integrand at the nodes of the quadrature rule such that

$$f(x_i) = \sum_{k=0}^{n-1} e_k p_k(x_i), \quad i = 1 \dots n.$$

Finally, if $r_{\mathsf{max}}$ is below the critical ratio, then the function is assumed to be "*strongly asymptotic*" and the error is estimated using

$$\varepsilon_k = 10 r_{\mathsf{critical}}^{1-\alpha} r_{\mathsf{max}}^{\alpha} E_{n/2-1}. \tag{2.108}$$

where $\alpha \geq 1$ is chosen to reflect, as Berntsen and Espelid state, "*the degree of optimism we want to put into this algorithm.*"

In summary we can say that the coefficients of the polynomial interpolating the integrand at the nodes of the quadrature rule, relative to some discretely orthogonal basis, are computed (Equation 2.103) and paired (Equation 2.105). The monotonic decrease of these pairs ($r_{\mathsf{max}} < 1$) is used as an indicator for the asymptoticity of the function in the interval. If the function is deemed sufficiently asymptotic, the ratio of decrease of the coefficient pairs is used to extrapolate the magnitude of the next coefficient pair, which is used as an error estimate.

Berntsen and Espelid implement and test this error estimate using, as basic quadrature rules, 21-point Gauss, Lobatto, Gauss-Kronrod and Clenshaw-Curtis rules as well as 61-point Gauss and Gauss-Kronrod rules, and later in `DQAINT` [19], based on QUADPACK's `QAG` (see Section 2.17), using as a basic quadrature rule the Gauss, Gauss-Lobatto and Gauss-Kronrod rules over 21 nodes with the constants

$$r_{\mathsf{critical}} = 1/4 \tag{2.109}$$
$$\alpha = (d-(n-4))/4 \tag{2.110}$$
$$K = 3, \tag{2.111}$$

where $d$ is the degree of the underlying quadrature rule.

In [20] and [21], Espelid implements this error estimate in four adaptive quadrature routines based on Newton-Cotes rules. The first of these routines, `modsim`, is an adaptation of Gander and Gautschi's recursive `adaptsim` (see Section 2.20) and uses the 5-point Newton-Cotes rule $\mathsf{NC}_5^{(1)}[a,b]$ over which the last 4 null rules are computed. Due to the small number of points, the null rules are not paired as in Equation 2.105 and their ratios are computed directly. As with `adaptsim`, the global tolerance is also used as the local tolerance (*i.e.* the error estimate is not scaled by a depth-dependent factor), meaning that for a large number of intervals, the global error may be above the required tolerance, even if the tolerance is satisfied in all local intervals.

The second routine, `modlob`, differs only in that it uses the 7-point Kronrod extension of a 4-point Gauss-Lobatto rule used by Gander and Gautschi's `adaptlob` [34] (see Section 2.20). Here too only the last 4 null rules are computed and the resulting values are not paired.

The third routine, `coteda`, uses what Espelid terms a "*doubly adaptive*"[17] strategy of first applying a 5-point Newton-Cotes rule and estimating the error as in `modsim` above and, if the requested tolerance is not satisfied, extending it to a 9-point Newton-Cotes rule. The error of the 9-point rule is computed using the last 8 null rules and by pairing the coefficients as in Equation 2.105. If this second error estimate is above the requested tolerance, then the interval is subdivided. Here too the global tolerance is used in every subinterval.

The fourth and last routine, `coteglob`, is a global (as in Algorithm 2) version of `coteda` and was added to illustrate the difference between local and global strategies, reinforcing the conclusions by Malcolm and Simpson [66].

In [22] and [24] this global doubly adaptive strategy is extended to four Newton-Cotes rules over 5, 9, 17 and 33 equidistant points. The error estimates for the 5 and 9 point rules are computed as above and for the 17 and 33 point rules, 15 null rules are computed and grouped into triplets instead of pairs:

$$E_k = \left(e_{3k}^2 + e_{3k+1}^2 + e_{3k+2}^2\right)^{1/2}, k = 0 \dots (n-1)/3.$$

As opposed to the previous doubly adaptive integrators, the interval is subdivided if, for a rule over $2n-1$ points, the error estimate over that rule is larger than the sum of the errors of the $n$ point rule over the left and right half-intervals.

Some details must be observed regarding the order of the null rules used: For the 5 and 9 point stencils, the normal Newton-Cotes rules are used,

[17]The term "doubly adaptive" may be somewhat abusive in this context since, in fact, only two successive quadrature rules are applied and the decision to bisect is only taken *after* the highest-order rule has failed, as opposed to Oliver's doubly-adaptive quadrature (Section 2.11), where, for every interval, the decision to subdivide *or* increase the degree of the quadrature rule is evaluated. Interestingly enough, Espelid credits Cools and Haegmans [11] with having published the first doubly-adaptive strategy, although they were preceded by de Boor in 1971 (Section 2.9), Oliver in 1972 (Section 2.11) and Patterson in 1973 (Section 2.12) — an error he corrects (somewhat) in [24] by attributing the first publication to Oliver in 1972.

yet for the 17 and 33 point stencils, the Newton-Cotes rules are numerically unstable. Therefore, rules of degree 13, 15 and 17 (for the 17 point stencil) and 21, 23 and 27 (for the 33 point stencil) are constructed such as to minimize truncation errors (*i.e.* the sum of squares of the quadrature weights). The degrees of these rules, however, are well below the degree of the moments that the null rules approximate over the same points. Espelid treats this problem by choosing $\alpha$ "*to fit the order of the actual rule used, the order of* $r_{\mathsf{max}}$ *and of* $E_{n/3+2}$."

In [23], Espelid compares these routines to QUADPACK's `QAG` and concludes that they are generally more efficient.

## 2.20 Gander and Gautschi's Revisited Adaptive Quadrature

In a 2001 paper, Gander and Gautschi [34] present two recursive adaptive quadrature routines. The first of these routines, `adaptsim` is quite similar to Lyness' `SQUANK` (see Section 2.7). It computes the approximations $\mathsf{S}^{(1)}[a,b]$ and $\mathsf{S}^{(2)}[a,b]$ and uses them to extrapolate $\mathsf{NC}_5^{(1)}[a,b]$ as in Equation 2.19. The *globally relative* local error estimate, however, is then computed as

$$\varepsilon_k = \left|\mathsf{NC}_5^{(1)}[a_k,b_k] - \mathsf{S}^{(2)}[a_k,b_k]\right| / |\hat{I}| \tag{2.112}$$

where $\hat{I}$ is a rough approximation to the global integral computed over a set of random nodes (if this approximation yields 0, then $b-a$ is used instead to avoid division by zero). If the tolerance is met, the approximation $\mathsf{NC}_5^{(1)}[a_k,b_k]$ is used for the integral, otherwise, the interval is bisected, re-using all evaluations of the integrand.

To guard against machine-dependent problems and to prevent the algorithm from trying to achieve spurious accuracy, *i.e.* when the local interval is less than $\varepsilon_{\mathsf{mach}}\hat{I}$, the termination criterion

$$\frac{\tau}{\varepsilon_{\mathsf{mach}}}\hat{I} + \left(\mathsf{NC}_5^{(1)}[a_k,b_k] - \mathsf{S}^{(2)}[a_k,b_k]\right) = \frac{\tau}{\varepsilon_{\mathsf{mach}}}\hat{I} \tag{2.113}$$

where $\varepsilon_{\mathsf{mach}}$ is the machine precision, is used. This termination criterion exploits the fact that if the error estimate is below tolerance, it will be canceled-out in the addition.

In order to avoid cases in which the error estimate will not converge (as, for example, Equation 2.8), the algorithm computes the midpoint of the interval $m = (a_k + b_k)/2$ and checks if

$$(a_k < m) \ \wedge \ (m < b_k).$$

If this condition is not satisfied then there is no machine number between $a$ and $b$ and further bisection is neither reasonable nor possible. In such a case, the recursion is aborted and an error message is issued that the requested tolerance may not have been met.

The second routine, `adaptlob`, uses a 4-point Gauss-Lobatto rule $\mathsf{GL}_4^{(1)}[a,b]$ and its 7-point Kronrod extension $\mathsf{K}_7^{(1)}[a,b]$. The globally relative local error is computed, analogously to Equation 2.112, as

$$\varepsilon_k = \left| \mathsf{GL}_4^{(1)}[a_k,b_k] - \mathsf{K}_7^{(1)}[a_k,b_k] \right| / |\hat{I}| \tag{2.114}$$

and evaluated using the same scheme as in Equation 2.113. If the tolerance is met, the approximation $\mathsf{K}_7^{(1)}[a,b]$ is used for the integral. Otherwise, the interval is divided into the 6 sub-intervals between the nodes of the Kronrod extension, thus re-using all evaluations of the integrand.

Note that although both algorithms are recursive as per Algorithm 1, the error estimates are not subject to a depth-dependent scaling factor. The error estimates of both algorithms thus suffer from a common problem already discussed in the context of Patterson's integrator (see Section 2.12), namely that the sum of the local error estimates, which are each below the required tolerance, is not guaranteed to be itself below the required tolerance. This, however, also avoids the problems related to using such a scaling factor, as seen in Equation 2.8 and Equation 2.9.

These two algorithms, with modifications (*i.e.* a cap on the number of function evaluations and on the recursion depth and an absolute tolerance requirement), have been added to MATLAB [67] as of release 6.5 as the standard integrators `quad` and `quadl`.

# Chapter 3

# Function Representation

## 3.1 Function Representation using Orthogonal Polynomials

In most quadrature algorithms, the integrand is not explicitly represented, except through different approximations $Q_n^{(m)}$ of its integral. The *differences* between these different approximations are used to extrapolate information on the integrand, such as higher derivatives, used to approximate the quadrature error.

Some authors such as Gallaher (see Section 2.6) or Ninomiya (see Section 2.15) use additional nodes to numerically approximate the higher derivative directly using divided differences, thus supplying additional information on the integrand $f(x)$.

Other authors such as O'Hara and Smith (see Section 2.8), Oliver (see Section 2.11) and Berntsen and Espelid (see Section 2.19) compute some of the higher-order coefficients of the function relative to some orthogonal base, thus further characterizing the integrand.

In all these cases, however, the characterization is not complete and in most cases only implicit. In the following, we will attempt to characterize the integrand as completely as possible.

Before further characterizing the integrand, we note that for every interpolatory quadrature rule, we are in fact computing an interpolation polynomial $g_n(x)$ of degree $n$ such that

$$g_n(x_i) = f(x_i), \quad i = 0 \ldots n,$$

and evaluating the integral thereof

$$Q_n[a,b] = \int_a^b g_n(x)\,\mathrm{d}x.$$

This equivalence is easily demonstrated, as is done in many textbooks in numerical analysis ([94, 90, 38, 91, 84] to name a few), by constructing the interpolation $g_n(x)$ using Lagrange polynomials

$$g_n(x) = \sum_{i=0}^{n} \ell_i(x) f(x_i)$$

and integrating $g_n(x)$

$$\begin{aligned} \int_a^b g_n(x)\,\mathrm{d}x &= \int_a^b \sum_{i=0}^{n} \ell_i(x) f(x_i)\,\mathrm{d}x \\ &= \sum_{i=0}^{n} f(x_i) \int_a^b \ell_i(x)\,\mathrm{d}x \end{aligned}$$

to obtain the weights of the quadrature rule from Equation 1.1 with

$$w_i = \int_a^b \ell_i(x)\,\mathrm{d}x.$$

Since any polynomial interpolation of degree $n$ over $n+1$ distinct points is uniquely determined, it does not matter how we represent $g_n(x)$ – its integral will always be identical to the result of the interpolatory quadrature rule $Q_n[a,b]$ over the same nodes.

In the following, we will represent $g_n(x)$ as a weighted sum of orthogonal polynomials:

$$g_n(x) = \sum_{i=0}^{n} c_i p_i(x) \tag{3.1}$$

where the $p_i(x)$, $i = 0 \ldots n$ are polynomials of degree $i$ which are orthonormal with respect to some product

$$(p_i, p_j) = \begin{cases} 0 & i \neq j, \\ 1 & i = j. \end{cases}$$

We will use the coefficients $\mathbf{c} = (c_0, c_1, \ldots, c_n)^\mathsf{T}$ as our representation of $g_n(x)$.

Furthermore, for notational simplicity, we will assume that the integrand has been transformed from the interval $[a, b]$ to the interval $[-1, 1]$. The polynomial $g_n(x)$ interpolates the integrand $f(x)$ at the nodes $x_i \in [-1, 1]$:

$$g_n(x_i) = f(x_i), \quad i = 0 \ldots n.$$

In the following, we will use the orthonormal Legendre polynomials, which are orthogonal with respect to the product

$$(p_i, p_j) = \int_{-1}^{1} p_i(x) p_j(x) \, \mathrm{d}x,$$

and satisfy the three-term recurrence relation

$$\alpha_k p_{k+1}(x) = (x + \beta_k) p_k(x) - \gamma_k p_{k-1}(x)$$

with the coefficients

$$\alpha_k = \sqrt{\frac{(k+1)^2}{(2k+1)(2k+3)}}, \quad \beta_k = 0, \quad \gamma_0 = \sqrt{2}, \quad \gamma_k = \sqrt{\frac{k^2}{4k^2 - 1}}.$$

Note that although we will use the orthonormal Legendre polynomials, the following derivations will still be valid for any set of polynomials orthonormal with respect to the product

$$(p_i, p_j) = \int_{-1}^{1} p_i(x) p_j(x) w(x) \, \mathrm{d}x \qquad (3.2)$$

for any measure $w(x)$ positive on $[-1, 1]$. The resulting norms will, however, also all be defined with respect to the measure $w(x)$.

The representation of $g_n(x)$ using orthogonal polynomials (Equation 3.1) has some interesting properties. First of all, it is simple to evaluate the integral of $g_n(x)$ using

$$\begin{aligned}\int_{-1}^{1} g_n(x)\,\mathrm{d}x &= \int_{-1}^{1} \sum_{i=0}^{n} c_i p_i(x)\,\mathrm{d}x \\ &= \sum_{i=0}^{n} c_i \underbrace{\int_{-1}^{1} p_i(x)\,\mathrm{d}x}_{=\omega_i} \\ &= \boldsymbol{\omega}^{\mathsf{T}}\mathbf{c}\end{aligned}$$

where the weights $\boldsymbol{\omega}^{\mathsf{T}}$ can be pre-computed and applied much in the same way as the weights of a quadrature rule. Note that for the normalized Legendre polynomials used herein, $\boldsymbol{\omega}^{\mathsf{T}} = (1/\sqrt{2}, 0, \ldots, 0)$.

We can also evaluate the $L_2$-norm of $g_n(x)$ quite efficiently using Parseval's theorem:

$$\left[\int_{-1}^{1} g_n^2(x)\,\mathrm{d}x\right]^{1/2} = \left[\sum_{i=0}^{n} c_i^2\right]^{1/2} = \|\mathbf{c}\|_2.$$

In the following, we will use $\|\cdot\|$ to denote the 2-norm[1].

A final useful feature is that, given the coefficients of $g_n(x)$ on $[a, b]$, we can construct upper-triangular matrices

$$T_{i,j}^{(\ell)} = \int_{-1}^{1} p_i(x) p_j((x-1)/2)\,\mathrm{d}x, \quad i = 0 \ldots n,\ j \geq i$$

and

$$T_{i,j}^{(r)} = \int_{-1}^{1} p_i(x) p_j((x+1)/2)\,\mathrm{d}x, \quad i = 0 \ldots n,\ j \geq i$$

such that

$$\mathbf{c}^{(\ell)} = \mathbf{T}^{(\ell)}\mathbf{c} \quad \text{and} \quad \mathbf{c}^{(r)} = \mathbf{T}^{(r)}\mathbf{c} \tag{3.3}$$

are the coefficients of $g_n(x)$ on the intervals $[a, \frac{a+b}{2}]$ and $[\frac{a+b}{2}, b]$ respectively. If $\mathbf{c}$ are the coefficients of any given polynomial $g_n(x)$ on the interval $[a, b]$, then $\mathbf{c}^{(\ell)}$, as computed in Equation 3.3, are the coefficients of a

[1]Note that if we use different orthonormal polynomials with respect to some measure $w(x)$, we would obtain the $L_2$-norm with respect to that measure.

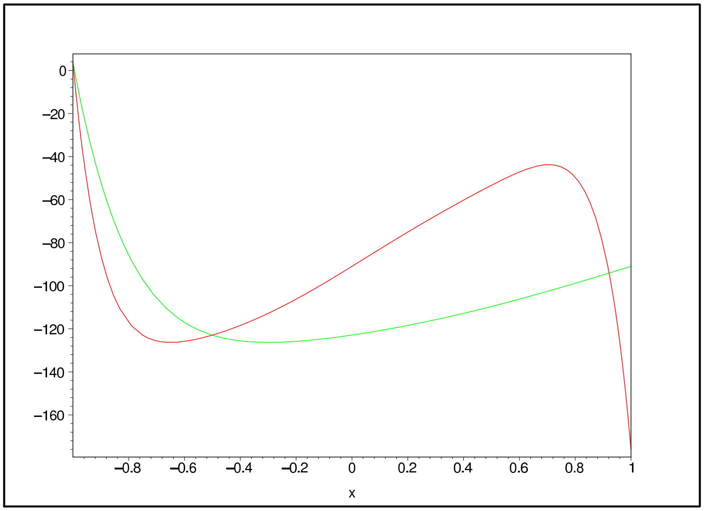


**Figure 3.1:** The interpolation polynomial $g_n(x)$ (red) and the polynomial $g_n^{(\ell)}(x)$ resulting from shifting its coefficients to the left half-interval as per Equation 3.3 (green). The polynomial $g_n^{(\ell)}(x)$ matches the left half of $g_n(x)$.

polynomial $g_n^{(\ell)}(x)$ matching $g_n(x)$ on the left half-interval $[a, (a+b)/2]$ such that

$$g_n^{(\ell)}(x) = g_n\left(\frac{x-1}{2}\right), \quad x \in [-1, 1]$$

as is shown in Figure 3.1. The coefficients $\mathbf{c}^{(\ell)}$ can be useful if, after bisecting an interval, we want to re-use, inside one of the sub-intervals, the interpolation computed over the entire original interval.

These matrices depend only on the polynomials $p_i(x)$ and can therefore be pre-computed for any set of nodes.

## 3.2 Interpolation Algorithms

In many applications, we need to compute polynomial interpolations of data or functions. In practical terms, this means that given $n+1$ function values $f_i$ at the $n+1$ nodes $x_i$, $i = 0 \ldots n$, we want to construct a polynomial $g_n(x)$ of degree $n$ such that

$$g_n(x_i) = f_i, \quad i = 0 \ldots n. \tag{3.4}$$

That is, the polynomial $g_n(x)$ interpolates the $n+1$ function values $f_i$ at the nodes $x_i$.

There are many ways in which $g_n(x)$ can be represented. The most common thereof, which is often used as an introduction to interpolation in many textbooks ([94, 90, 38, 91, 84] to name a few), is the interpolation using Lagrange polynomials:

$$g_n(x) = \sum_{i=0}^{n} f_i \ell_i(x) \tag{3.5}$$

where the Lagrange polynomials are defined as

$$\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}. \tag{3.6}$$

These polynomials satisfy, by construction,

$$\ell_i(x_j) = \left\{ \begin{array}{ll} 0 & i \neq j \\ 1 & i = j \end{array} \right. \tag{3.7}$$

such that the condition in Equation 3.4 is also satisfied.

Although the representation with Lagrange polynomials is usually only considered as a didactical example, since its definition is also an algorithm for its construction, a more useful and computationally efficient variant thereof called *barycentric interpolation* [6] is still used in practical applications (*e.g.* see [2]).

Another representation constructs $g_n(x)$ using the Newton polynomials

$$\pi_i(x) = \prod_{j=0}^{i-1} (x - x_j). \tag{3.8}$$

The coefficients $a_i$ of the interpolation

$$g_n(x) = \sum_{i=0}^{n} a_i \pi_i(x) \tag{3.9}$$

are computed from the divided differences

$$a_i = f[x_0, \ldots, x_i]. \tag{3.10}$$

As with the Lagrange interpolation, Equation 3.4 is satisfied by construction. One advantage of this representation is that it can be easily extended, *i.e.* additional nodes and function values added, since, unlike the Lagrange interpolation, the first $k$ polynomials and coefficients depend only on the first $k$ nodes and function values.

Yet another common representation for $g_n(x)$ uses monomials:

$$g_n(x) = \sum_{i=0}^{n} b_i x^i. \tag{3.11}$$

Unlike the representation with Lagrange or Newton polynomials, the interpolation property is not guaranteed by construction and the coefficients $b_i$ must be computed such that Equation 3.4 is satisfied. These constraints themselves form a system of $n+1$ linear equations which can be solved for the $n+1$ coefficients $b_i$

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \ldots & x_0^n \\ 1 & x_1 & x_1^2 & \ldots & x_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \ldots & x_n^n \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}. \tag{3.12}$$

The matrix in Equation 3.12 is called the *Vandermonde* matrix and the system of equations can be solved naively using Gaussian elimination at a cost in $\mathcal{O}(n^3)$, which is not especially economical. Furthermore, as Gautschi shows in [36], for some common node distributions, the condition number of the Vandermonde matrix grows exponentially with the matrix dimension, making a precise numerical computation of the coefficients impossible already for moderate $n$.

A final representation, which will be the main focus of this paper, is the linear combination of polynomials

$$g_n(x) = \sum_{i=0}^{n} c_i p_i(x) \tag{3.13}$$

where the polynomials $p_i(x)$ of degree $i$ can be constructed using a three-term recurrence relation, which we will write as[2]

$$\alpha_k p_{k+1}(x) = x p_k(x) + \beta_k p_k(x) - \gamma_k p_{k-1}(x), \tag{3.14}$$

with

$$p_0(x) = 1, \quad p_{-1}(x) = 0.$$

Examples of such polynomials are the Legendre polynomials $P_k(x)$ with

$$\alpha_k = \frac{k}{2k-1}, \quad \beta_k = 0, \quad \gamma_k = \frac{k-1}{2k-1} \tag{3.15}$$

which are orthogonal with respect to the scalar product

$$(f, g) = \int_{-1}^{1} f(x) g(x) \, \mathrm{d}x$$

or the Chebyshev polynomials $T_k(x)$ with

$$\alpha_0 = 1, \quad \alpha_k = \frac{1}{2}, \quad \beta_k = 0, \quad \gamma_k = \frac{1}{2} \tag{3.16}$$

which satisfy the trigonometric identity

$$T_k(\cos\theta) = \cos(k\theta)$$

in $[-1, 1]$ and whose properties, such as the minimal infinity-norm, have led to their wide use in interpolation and approximation applications [2, 86].

As with the coefficients of the monomials, the coefficients $c_i$ of Equation 3.13 can be computed solving the system of linear equations

$$\begin{pmatrix} p_0(x_0) & p_1(x_0) & \dots & p_n(x_0) \\ p_0(x_1) & p_1(x_1) & \dots & p_n(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ p_0(x_n) & p_1(x_n) & \dots & p_n(x_n) \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix} \tag{3.17}$$

[2]Gautschi [39] and Higham [46] use different recurrence relations which can both be transformed to the representation used herein.

which can be written as

$$\mathbf{P}^{(n)}\mathbf{c}^{(n)} = \mathbf{f}^{(n)}. \tag{3.18}$$

The matrix $\mathbf{P}^{(n)}$ is a *Vandermonde-like* matrix and the system of equations can be solved naively in $\mathcal{O}(n^3)$ using Gaussian elimination. As with the computation of the monomial coefficients, the matrix may be ill-conditioned [37].

Note that the previously described Newton polynomials also satisfy a three-term recurrence relation with

$$\alpha_k = 1, \quad \beta_k = -x_{k-1}, \quad \gamma_k = 0$$

as do the monomials, with

$$\alpha_k = 1, \quad \beta_k = 0, \quad \gamma_k = 0. \tag{3.19}$$

Creating the matrix $\mathbf{P}^{(n)}$ using the Newton polynomials results in a lower-triangular matrix since, by the definition in Equation 3.8, $\pi_k(x_i) = 0$ for all $i < k$. Solving this lower-triangular system using back-substitution results in the divided differences for the coefficients $d_i$ (see Equation 3.10). This computation is straight-forward and can be done in $\mathcal{O}(n^2)$, which is a further advantage of using Newton polynomials.

If the nodes $x_i$ are distinct then the polynomial that interpolates the $f_i$ at these nodes is unique and all these representations – Equation 3.5, Equation 3.9, Equation 3.11 and Equation 3.13 – are different representations of the same polynomial. It therefore seems intuitive that it should be possible to convert the coefficients of one representation to those of another. In [31], such a connection is made and a set of elegant basis transformations for moving between Lagrange, monomial, Newton and (discrete) orthogonal polynomial interpolations is given.

This was already done implicitly by Björck and Pereyra in [7], where an algorithm is presented to compute the monomial coefficients of an interpolation, without having to solve the expensive and unstable Vandermonde system using Gaussian elimination, by computing first the coefficients of a Newton interpolation and then converting these to monomial coefficients. This approach was later extended by Higham in [46] to compute the coefficients for any polynomial basis satisfying a three-term recurrence relation.

In Section 3.2.1, we will re-formulate the algorithms of Björck and Pereyra and of Higham and extend them to facilitate the *downdate* of an interpolation, *i.e.* the removal of a node. In Section 3.2.2 we present a new algorithm for the construction of interpolations of the type of Equation 3.13 based on a successive decomposition of the Vandermonde-like matrix in Equation 3.17. Finally, in Section 3.2.3, we will present results regarding the efficiency and stability of the two algorithms.

### 3.2.1 A Modification of Björck and Pereyra's and of Higham's Algorithms Allowing Downdates

In [7], Björck and Pereyra present an algorithm which exploits the recursive definition of the Newton polynomials

$$\pi_k(x) = (x - x_{k-1})\pi_{k-1}(x). \tag{3.20}$$

They note that given the Newton interpolation coefficients $a_i$, the interpolation polynomial can be constructed using Horner's scheme:

$$q_n(x) = a_n, \quad q_k(x) = (x - x_k)q_{k+1}(x) + a_k, \quad k = n-1 \ldots 0 \tag{3.21}$$

where the interpolation polynomial is $g_n(x) = q_0(x)$.
They also note that given a monomial representation for $q_k(x)$, such as

$$q_k(x) = \sum_{i=0}^{n-k} b_i^{(k)} x^i$$

the polynomial $q_{k-1}(x)$ can then be constructed, following the recursion in Equation 3.21, as

$$\begin{aligned}
q_{k-1}(x) &= (x - x_{k-1})q_k(x) + a_{k-1} \\
&= (x - x_{k-1}) \sum_{i=0}^{n-k} b_i^{(k)} x^i + a_{k-1} \\
&= \sum_{i=1}^{n-k+1} b_{i-1}^{(k)} x^i - x_{k-1} \sum_{i=0}^{n-k} b_i^{(k)} x^i + a_{k-1} \\
&= b_{n-k}^{(k)} x^{n-k+1} + \sum_{i=1}^{n-k} (b_{i-1}^{(k)} - x_{k-1} b_i^{(k)}) x^i \\
&\quad + b_0^{(k-1)} + a_{k-1}. \qquad (3.22)
\end{aligned}$$

From Equation 3.22 we can then extract the new coefficients $b_i^{(k-1)}$:

$$b_i^{(k-1)} = \begin{cases} b_{i-1}^{(k)} & i = n-k+1 \\ b_{i-1}^{(k)} - x_{k-1} b_i^{(k)}, & 1 \leq i \leq n-k \\ b_0^{(k)} + a_{k-1}, & i = 0. \end{cases} \qquad (3.23)$$

In [46], Higham uses the same approach, yet represents the Newton polynomials as a linear combination of polynomials satisfying a three-term recurrence relation as shown in Equation 3.13. Using such a representation

$$q_k(x) = \sum_{i=0}^{n-k} c_i^{(k)} p_i(x) \qquad (3.24)$$

he computes $q_{k-1}(x)$ by expanding the recursion in Equation 3.21 using the representation Equation 3.24 and the recurrence relation in Equation 3.14:

$$
\begin{aligned}
q_{k-1}(x) &= (x - x_{k-1}) \sum_{i=0}^{n-k} c_i^{(k)} p_i(x) + a_{k-1} \\
&= \sum_{i=0}^{n-k} c_i^{(k)} x p_i(x) - x_{k-1} \sum_{i=0}^{n-k} c_i^{(k)} p_i(x) + a_{k-1} \\
&= \sum_{i=0}^{n-k} c_i^{(k)} \left(\alpha_i p_{i+1}(x) - \beta_i p_i(x) + \gamma_i p_{i-1}(x)\right) \\
&\quad -x_{k-1} \sum_{i=0}^{n-k} c_i^{(k)} p_i(x) + a_{k-1}. \qquad (3.25)
\end{aligned}
$$

Expanding Equation 3.25 for the individual $p_k(x)$, and keeping in mind that $p_{-1}(x) = 0$, we obtain

$$
\begin{aligned}
q_{k-1}(x) &= \sum_{i=1}^{n-k+1} c_{i-1}^{(k)} \alpha_{i-1} p_i(x) - \sum_{i=0}^{n-k} c_i^{(k)} \left(x_{k-1} + \beta_i\right) p_i(x) \\
&\quad + \sum_{i=0}^{n-k-1} c_{i+1}^{(k)} \gamma_{i+1} p_i(x) + a_{k-1}. \qquad (3.26)
\end{aligned}
$$

By shifting the sums in Equation 3.26 and re-grouping around the individual $p_k(x)$ we finally obtain

$$
\begin{aligned}
q_{k-1}(x) &= c_{n-k}^{(k)} \alpha_{n-k} p_{n-k+1}(x) \\
&\quad + \left(c_{n-k-1}^{(k)} \alpha_{n-k-1} - c_{n-k}^{(k)} (x_{k-1} + \beta_{n-k})\right) p_{n-k}(x) \\
&\quad + \sum_{i=1}^{n-k-1} \left(c_{i-1}^{(k)} \alpha_{i-1} - c_i^{(k)} (x_{k-1} + \beta_i) + c_{i+1}^{(k)} \gamma_{i+1}\right) p_i(x) \\
&\quad -c_0^{(k)} (x_{k-1} + \beta_0) + c_1^{(k)} \gamma_1 + a_{k-1}. \qquad (3.27)
\end{aligned}
$$

Higham then extracts the new coefficients $c_i^{(k-1)}$ from Equation 3.27 as:

$$c_i^{(k-1)} = \begin{cases} c_{i-1}^{(k)}\alpha_{i-1}, & i = n-k+1 \\ c_{o-1}^{(k)}\alpha_{i-1} - c_i^{(k)}(x_{k-1}+\beta_i), & i = n-k \\ c_{i-1}^{(k)}\alpha_{i-1} - c_i^{(k)}(x_{k-1}+\beta_i) + c_{i+1}^{(k)}\gamma_{i+1}, & 1 \leq i < n-k \\ -c_0^{(k)}(x_{k-1}+\beta_0) + c_1^{(k)}\gamma_1 + a_{k-1} & i = 0 \end{cases} \tag{3.28}$$

In both algorithms, the interpolating polynomial is constructed by first computing the $a_i$, $i = 0 \ldots n$ and, starting with $q_n(x) = a_n$, and hence $c_0^{(n)} = a_n$ or $b_0^{(n)} = a_n$, and successively updating the coefficients per Equation 3.28 and Equation 3.23.

Alternatively, we could use the same approach to compute the coefficients of the Newton polynomials themselves

$$\pi_k(x) = \sum_{i=0}^{k} \eta_i^{(k)} p_i(x).$$

Expanding the recurrence relation in Equation 3.20 analogously to Equation 3.27, we obtain

$$\begin{aligned} \pi_{k+1}(x) &= \eta_k^{(k)}\alpha_k p_{k+1}(x) + \left(\eta_{k-1}^{(k)}\alpha_{k-1} - \eta_k^{(k)}(x_k+\beta_k)\right) p_k(x) \\ &\quad + \sum_{i=1}^{k-1}\left(\eta_{i-1}^{(k)}\alpha_{i-1} - \eta_i^{(k)}(x_k+\beta_i) + \eta_{i+1}^{(k)}\gamma_{i+1}\right) p_i(x) \\ &\quad - \eta_0^{(k)}(x_k+\beta_0) + \eta_1^{(k)}\gamma_1. \end{aligned} \tag{3.29}$$

We initialize with $\eta_0^{(0)} = 1$ and use

$$\eta_i^{(k+1)} = \begin{cases} \eta_{i-1}^{(k)}\alpha_{i-1}, & i = k+1 \\ \eta_{i-1}^{(k)}\alpha_{i-1} - \eta_i^{(k)}(x_k+\beta_i), & i = k \\ \eta_{i-1}^{(k)}\alpha_{i-1} - \eta_i^{(k)}(x_k+\beta_i) + \eta_{i+1}^{(k)}\gamma_{i+1}, & 1 \leq i < k \\ -\eta_0^{(k)}(x_k+\beta_0) + \eta_1^{(k)}\gamma_1 & i = 0 \end{cases} \tag{3.30}$$

to compute the coefficients for $\pi_k(x)$, $k = 1 \ldots n$. Alongside this computation, we can also compute the coefficients of a sequence of polynomial

$g_k(x)$ of increasing degree $k$

$$g_k(x) = \sum_{i=0}^{k} c_i^{(k)} p_i(x)$$

initializing with $c_0^{(0)} = a_0$, where the $a_i$ are still the Newton coefficients computed and used above. The subsequent coefficients $c_i^{(k)}$, $k = 1 \ldots n$ are computed using

$$c_i^{(k)} = \begin{cases} \eta_i^{(k)} a_k, & i = k \\ c_i^{(k-1)} + \eta_i^{(k)} a_k & 0 \leq i < k. \end{cases} \tag{3.31}$$

This *incremental* construction of the coefficients, which is equivalent to effecting the summation of the weighted Newton polynomials in Equation 3.9 and referred to by Björck and Pereyra as the “progressive algorithm”, can be used to efficiently update an interpolation. If the coefficients $\eta_i^{(n)}$ and $c_i^{(n)}$ are stored and a new node $x_{n+1}$ and function value $f_{n+1}$ are added to the data, a new coefficient $a_{n+1}$ can be computed per Equation 3.10. The coefficients $\eta_i^{(n+1)}$ are then computed per Equation 3.30 and, finally, the $c_i^{(n)}$ are updated per Equation 3.31, resulting in the coefficients $c_i^{(n+1)}$ of the updated interpolation polynomial $g_{n+1}(x)$.

We can re-write the recursion for the coefficients $\eta_i^{(k)}$ of the Newton polynomials in matrix-vector notation as

$$\left(\mathbf{T}^{(k+1)} - \underline{\mathbf{I}}_0 x_k\right) \boldsymbol{\eta}^{(k)} = \boldsymbol{\eta}^{(k+1)}$$

where $\mathbf{T}^{(k+1)}$ is the $(k+2) \times (k+1)$ tri-diagonal matrix

$$\mathbf{T}^{(k+1)} = \begin{pmatrix} -\beta_0 & \gamma_1 & & & \\ \alpha_0 & -\beta_1 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_{k-2} & -\beta_{k-1} & \gamma_k \\ & & & \alpha_{k-1} & -\beta_k \\ & & & & \alpha_k \end{pmatrix}$$

and $\underline{\mathbf{I}}_0 x_k$ is a $(k+2) \times (k+1)$ matrix with $x_k$ in the diagonal and zeros

**Algorithm 4** Incremental construction of $g_n(x)$

```
1: $c_0^{(0)} \leftarrow f_0$                                                   $(init\ \mathbf{c}^{(0)})$
2: $\eta_0^{(1)} \leftarrow -x_0 - \beta_0,\ \eta_1^{(1)} \leftarrow \alpha_0$                              $(init\ \boldsymbol{\eta}^{(1)})$
3: for $k = 1 \dots n$ do
4:     $v_0 \leftarrow 0,\ v_1 \leftarrow x_k$                                          $(init\ \mathbf{v})$
5:     for $i = 2 \dots k$ do
6:         $v_i \leftarrow ((x_k + \beta_{i-1})v_{i-1} - \gamma_{i-1}v_{i-2}) / \alpha_{i-1}$        $(compute\ the\ v_i)$
7:     end for
8:     $g_k \leftarrow \mathbf{v}(0:k-1)^\mathsf{T}\mathbf{c}^{(k-1)}$                          $(compute\ g_{k-1}(x_k))$
9:     $\pi_k \leftarrow \mathbf{v}^\mathsf{T}\eta^{(k)}$                                    $(compute\ \pi_k(x_k))$
10:    $a_k \leftarrow (f_k - g_k)/\pi_k$                        $(compute\ a_k,\ Equation\ 3.32)$
11:    $\mathbf{c}^{(k)} \leftarrow [\mathbf{c}^{(k-1)}; 0] + a_k\boldsymbol{\eta}^{(k)}$        $(compute\ the\ new\ \mathbf{c}^{(k)},\ Equation\ 3.31)$
12:    $\boldsymbol{\eta}^{(k+1)} \leftarrow [0; \underline{\alpha}(0:k).*\boldsymbol{\eta}^{(k)}] - [(x_k + \underline{\beta}(0:k)).*\boldsymbol{\eta}^{(k)}; 0]+$
           $[\underline{\gamma}(1:k).*\boldsymbol{\eta}^{(k)}(1:k); 0; 0]$
                                         $(compute\ the\ new\ \boldsymbol{\eta}^{(k+1)},\ Equation\ 3.30)$
13: end for
```

elsewhere

$$\underline{\mathbf{I}}_0 x_k = \begin{pmatrix} x_k & & & \\ & x_k & & \\ & & \ddots & \\ & & & x_k \\ 0 & 0 & \dots & 0 \end{pmatrix}.$$

The vectors $\boldsymbol{\eta}^{(k)} = (\eta_0^{(k)}, \eta_1^{(k)}, \dots, \eta_k^{(k)})^\mathsf{T}$ and $\boldsymbol{\eta}^{(k+1)} = (\eta_0^{(k+1)}, \eta_1^{(k+1)}, \dots, \eta_{k+1}^{(k+1)})^\mathsf{T}$ contain the coefficients of the $k$th and $(k+1)$st Newton polynomial.

Given the vector of coefficients $\mathbf{c}^{(n)} = (c_0^{(n)}, c_1^{(n)}, \dots, c_n^{(n)})^\mathsf{T}$ of an interpolation polynomial $g_n(x)$ of degree $n$ and the vector of coefficients $\boldsymbol{\eta}^{(n+1)}$ of the $(n+1)$st Newton polynomial over the $n+1$ nodes, we can *update* the interpolation, *i.e.* add a new node $x_{n+1}$ and function value $f_{n+1}$, as follows: We first compute the new Newton interpolation coefficient $a_k$ using the divided differences as in Equation 3.10 or, alternatively, by evaluating

$$a_{n+1} = \frac{f_{n+1} - g_n(x_{n+1})}{\pi_{n+1}(x_{n+1})} \tag{3.32}$$

using the coefficients and the three-term recurrence relation to evaluate both $g_n(x_{n+1})$ and $\pi_{n+1}(x_{n+1})$. The coefficient $a_{n+1}$ is chosen such that the new interpolation constraint

$$g_{n+1}(x_{n+1}) = g_n(x_{n+1}) + a_{n+1}\pi_{n+1}(x_{n+1}) = f_{n+1}$$

is satisfied by construction. Note that since $\pi_{n+1}(x_i) = 0$ for $i = 0 \dots n$, the addition of any multiple of $\pi_{n+1}(x)$ to $g_n(x)$ does not affect the interpolation at the other nodes at all.

This expression for $a_{n+1}$ is used instead of the divided difference since we have not explicitly stored the previous $a_i$, $i = 0 \dots n$, which are needed for the recursive computation of the latter.

We then update the coefficients of the interpolating polynomial

$$\mathbf{c}^{(n+1)} = \begin{pmatrix} \mathbf{c}^{(n)} \\ 0 \end{pmatrix} + a_{n+1}\boldsymbol{\eta}^{(n+1)} \tag{3.33}$$

and then the coefficients of the Newton polynomial

$$\boldsymbol{\eta}^{(n+2)} = \left(\mathbf{T}^{(n+2)} - \underline{\mathbf{I}}_0 x_{n+1}\right)\boldsymbol{\eta}^{(n+1)} \tag{3.34}$$

such that it is ready for further updates. Starting with $\eta_0^{(0)} = 1$ and $n = 0$, this update can be used to construct $g_n(x)$ by adding each $x_i$ and $f_i$, $i = 0 \dots n$, successively.

The complete algorithm is shown in Algorithm 4. The addition of each $n$th node requires $\mathcal{O}(n)$ operations, resulting in a total of $\mathcal{O}(n^2)$ operations for the construction of an $n$-node interpolation.

This is essentially the progressive algorithm of Björck and Pereyra, yet instead of storing the Newton coefficients $a_i$, we store the coefficients $\eta_i^{(n+1)}$ of the last Newton polynomial. This new representation offers no obvious advantage for the update, other than that it can be easily *reversed*:

Given an interpolation over a set of $n + 1$ nodes $x_i$ and function values $f_i$, $i = 0 \dots n$ defined by the coefficients $c_i^{(n)}$ and given the coefficients $\eta_i^{(n+1)}$ of the $(n + 1)st$ Newton polynomial over the same nodes, we can *downdate* the interpolation, *i.e.* remove the function value $f_j$ at the node $x_j$. The resulting polynomial of degree $n - 1$ will still interpolate the remaining $n$ nodes.

We begin by removing the root $x_j$ from the $(n+1)$st Newton polynomial by solving

$$\left(\mathbf{T}^{(n+1)} - \underline{\mathbf{I}}_0 x_j\right) \boldsymbol{\eta}^{(n)} = \boldsymbol{\eta}^{(n+1)}$$

for the vector of coefficients $\boldsymbol{\eta}^{(n)}$. If $x_j$ is a root of $\pi_{n+1}(x)$, the system is over-determined yet has a unique solution[3]. We can therefore remove the first row of $(\mathbf{T}^{(n+1)} - \underline{\mathbf{I}}_0 x_j)$ and the first entry of $\boldsymbol{\eta}^{(n+1)}$, resulting in the upper-tridiagonal system of linear equations

$$\begin{pmatrix} \alpha_0 & -(x_j+\beta_1) & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_{n-2} & -(x_j+\beta_{n-1}) & \gamma_n \\ & & & \alpha_{n-1} & -(x_j+\beta_n) \\ & & & & \alpha_n \end{pmatrix} \begin{pmatrix} \eta_0^{(n)} \\ \eta_1^{(n)} \\ \vdots \\ \eta_n^{(n)} \end{pmatrix} = \begin{pmatrix} \eta_1^{(n+1)} \\ \eta_2^{(n+1)} \\ \vdots \\ \eta_{n+1}^{(n+1)} \end{pmatrix} \tag{3.35}$$

which can be conveniently solved in $\mathcal{O}(n)$ using back-substitution.

Once we have our downdated $\boldsymbol{\eta}^{(n)}$, and thus the downdated Newton polynomial $\pi_n(x)$, we can downdate the coefficients of $g_n(x)$ by computing

$$g_{n-1}(x) = g_n(x) - a_j^\star \pi_n(x)$$

where the Newton coefficient $a_j^\star$ would need to be re-computed from the divided difference over all nodes *except* $x_j$. We can avoid this computation by noting that $g_{n-1}(x)$ has to be of degree $n-1$ and therefore the highest coefficient of $g_n(x)$, $c_n^{(n)}$, must disappear. This is the case when

$$c_n^{(n-1)} = c_n^{(n)} - a_j^\star \eta_n^{(n)} = 0$$

and therefore

$$a_j^\star = \frac{c_n^{(n)}}{\eta_n^{(n)}}.$$

Using this $a_j^\star$, we can the compute the coefficients of $g_{n-1}(x)$ as

$$c_i^{(n-1)} = c_i^{(n)} - \frac{c_n^{(n)}}{\eta_n^{(n)}} \eta_i^{(n)}, \quad i = 1 \dots n-1. \tag{3.36}$$

[3]Note that the $n \times (n+1)$ matrix $\left(\mathbf{T}^{(n+1)} - \underline{\mathbf{I}}_0 x_j\right)^\mathsf{T}$ has rank $n$ and the null space $\mathbf{p}(x_j) = (p_0(x_j), p_1(x_j), \dots, p_{n+1}(x_j))^\mathsf{T}$ since for $\mathbf{v} = \left(\mathbf{T}^{(n+1)} - \underline{\mathbf{I}}_0 x_j\right)^\mathsf{T} \mathbf{p}(x_j)$, $v_i = \alpha_i p_{i+1}(x_j) - (x_j + \beta_i) p_i(x_j) + \gamma_i p_{i-1}(x_j) = 0$ by the definition in Equation 3.14 and the right-hand side $\boldsymbol{\eta}^{(n+1)}$ is consistent.

The whole process is shown in Algorithm 5. The downdate of an $n$-node interpolation requires $\mathcal{O}(n)$ operations.

**Algorithm 5** Remove a function value $f_j$ at the node $x_j$ from the interpolation given by the coefficients $\mathbf{c}^{(n)}$

```
1: $\eta_n^{(n)} \leftarrow \eta_{n+1}^{(n+1)}/\alpha_n$    (*compute $\boldsymbol{\eta}^{(n)}$ from $\boldsymbol{\eta}^{(n+1)}$*)
2: $\eta_{n-1}^{(n)} \leftarrow \left(\eta_n^{(n+1)} + (x_j+\beta_n)\eta_n^{(n)}\right)/\alpha_{n-1}$
3: **for** $i = n-2 \dots 0$ **do**
4:     $\eta_i^{(n)} \leftarrow \left(\eta_{i+1}^{(n+1)} + (x_j+\beta_{i+1})\eta_{i+1}^{(n)} - \gamma_{i+2}\eta_{i+2}^{(n)}\right)/\alpha_i$
5: **end for**
6: $a_j \leftarrow c_n^{(n)}/\eta_n^{(n)}$    (*compute the coefficient $a_j$*)
7: $\mathbf{c}^{(n-1)} \leftarrow \mathbf{c}^{(n)} - a_j\boldsymbol{\eta}^{(n)}$    (*compute the new coefficients $\mathbf{c}^{(n-1)}$*)
```

## 3.2.2 A New Algorithm for the Construction of Interpolations

Returning to the representation in Equation 3.17, we can try to solve the Vandermonde-like system of linear equations directly. The matrix has some special characteristics which can be exploited to achieve better performance and stability than when using Gaussian elimination or even the algorithms of Björck and Pereyra, Higham or the one described in the previous section.

We start by de-composing the $(n+1)\times(n+1)$ Vandermonde-like matrix $\mathbf{P}^{(n)}$ as follows:

$$\mathbf{P}^{(n)} = \left(\begin{array}{c|c} \mathbf{P}^{(n-1)} & \mathbf{p}^{(n)} \\ \hline \mathbf{q}^{\mathsf{T}} & p_n(x_n) \end{array}\right).$$

The sub-matrix $\mathbf{P}^{(n-1)}$ is a Vandermonde-like matrix analogous to $\mathbf{P}^{(n)}$. The column $\mathbf{p}^{(n)}$ contains the $n$th polynomial evaluated at the nodes $x_i$,

$i = 0 \ldots n-1$

$$\mathbf{p}^{(n)} = \begin{pmatrix} p_n(x_0) \\ p_n(x_1) \\ \vdots \\ p_n(x_{n-1}) \end{pmatrix}$$

and the vector $\mathbf{q}^\mathsf{T}$ contains the first $0 \ldots n-1$ polynomials evaluated at the node $x_n$

$$\mathbf{q}^\mathsf{T} = (p_0(x_n), p_1(x_n), \ldots, p_{n-1}(x_n)).$$

Inserting this into the product in Equation 3.18, we obtain

$$\left(\begin{array}{c|c} \mathbf{P}^{(n-1)} & \mathbf{p}^{(n)} \\ \hline \mathbf{q}^\mathsf{T} & p_n(x_n) \end{array}\right) \left(\begin{array}{c} \mathbf{c}^{(n-1)} \\ \hline c_n \end{array}\right) = \left(\begin{array}{c} \mathbf{f}^{(n-1)} \\ \hline f_n \end{array}\right)$$

which, when applied, results in the equations

$$\begin{aligned} \mathbf{P}^{(n-1)}\mathbf{c}^{(n-1)} + \mathbf{p}^{(n)}c_n &= \mathbf{f}^{(n-1)} \\ \mathbf{q}^\mathsf{T}\mathbf{c}^{(n-1)} + p_n(x_n)c_n &= f_n. \end{aligned} \tag{3.37}$$

where the vectors $\mathbf{c}^{(n-1)} = (c_0, c_1, \ldots, c_{n-1})^\mathsf{T}$ and $\mathbf{f}^{(n-1)} = (f_0, f_1, \ldots, f_{n-1})^\mathsf{T}$ contain the first $n$ coefficients or function values respectively.

Before solving Equation 3.37, we note that the matrix $\mathbf{P}^{(n-1)}$ contains the first $0 \ldots n-1$ polynomials evaluated at the same $n$ nodes each. Similarly, $\mathbf{q}^\mathsf{T}$ contains the same polynomials evaluated at the node $x_n$. Since the polynomials in the columns are of degree $< n$ and they are evaluated at $n$ points, $\mathbf{P}^{(n-1)}$ actually contains enough data to extrapolate the values of these polynomials at $x_n$. Using the Lagrange interpolation described in Equation 3.5, we can write

$$\begin{aligned} p_i(x_n) &= \sum_{j=0}^{n-1} \ell_j^{(n)}(x_n) p_i(x_j) \\ q_i &= \sum_{j=0}^{n-1} \ell_j^{(n)}(x_n) P_{j,i}^{(n-1)} \end{aligned} \tag{3.38}$$

where the $\ell_j^{(n)}(x)$ are the Lagrange polynomials over the first $n$ nodes $x_i$, $i = 0 \dots n-1$. We write Equation 3.38 as

$$\mathbf{q}^\mathsf{T} = \underline{\ell}^{(n)} \mathbf{P}^{(n-1)} \tag{3.39}$$

where the entries of the $1 \times n$ vector $\underline{\ell}^{(n)}$ are

$$\ell_i^{(n)} = \ell_i(x_n).$$

The entries of $\underline{\ell}^{(n)}$ can be computed recursively. Using the definition in Equation 3.6, we can write the individual $\ell_i^{(n)}$ as

$$\ell_i^{(n)} = \prod_{\substack{j=0 \\ j \neq i}}^{n-1} \frac{x_n - x_j}{x_i - x_j}.$$

If we define

$$w_n = \prod_{j=0}^{n-1} (x_n - x_j)$$

we can re-write $\ell_i^{(n)}$ as

$$\ell_i^{(n)} = \frac{w_n}{x_n - x_i} \left[ \prod_{\substack{j=0 \\ j \neq i}}^{n-1} (x_i - x_j) \right]^{-1}. \tag{3.40}$$

We can extract the product on the right-hand side using the previous $\ell_i^{(n-1)}$ and $w_{n-1}$ over the first $0 \dots n-2$ nodes:

$$\begin{aligned} \ell_i^{(n-1)} &= \frac{w_{n-1}}{x_{n-1} - x_i} \left[ \prod_{\substack{j=0 \\ j \neq i}}^{n-2} (x_i - x_j) \right]^{-1} \\ \left[ \prod_{\substack{j=0 \\ j \neq i}}^{n-2} (x_i - x_j) \right]^{-1} &= \frac{\ell_i^{(n-1)}}{w_{n-1}} (x_{n-1} - x_i) \end{aligned}$$

which, re-inserted into Equation 3.40, gives

$$\begin{aligned} \ell_i^{(n)} &= \frac{w_n}{x_n - x_i} \frac{\ell_i^{(n-1)}}{w_{n-1}} \frac{x_{n-1} - x_i}{x_i - x_{n-1}} \\ &= -\frac{\ell_i^{(n-1)}}{x_n - x_i} \frac{w_n}{w_{n-1}} \end{aligned} \tag{3.41}$$

for all $i < n-1$. We then compute the last entry $i = n-1$ using

$$\ell_{n-1}^{(n)} = \frac{w_n}{w_{n-1}(x_n - x_{n-1})}. \tag{3.42}$$

Therefore, starting with $\ell_0^{(1)} = 1$, we can construct all the $\underline{\ell}^{(k)}$, $k = 2 \dots n$ successively. Since, given $\underline{\ell}^{(k)}$, $k = 1 \dots n$ the construction of each additional $\underline{\ell}^{(n+1)}$ requires $\mathcal{O}(n)$ operations, the construction of all the $\underline{\ell}^{(k)}$, $k = 1 \dots n$ requires a total of $\mathcal{O}(n^2)$ operations.

Returning to the Vandermonde-like matrix, inserting Equation 3.39 into Equation 3.37, we obtain

$$\begin{aligned} \mathbf{P}^{(n-1)}\mathbf{c}^{(n-1)} + \mathbf{p}^{(n)}c_n &= \mathbf{f}^{(n-1)} \\ \underline{\ell}^{(n)}\mathbf{P}^{(n-1)}\mathbf{c}^{(n-1)} + p_n(x_n)c_n &= f_n. \end{aligned} \tag{3.43}$$

Multiplying the first line in Equation 3.43 with $\underline{\ell}^{(n)}$ from the left we obtain

$$\begin{aligned} \underline{\ell}^{(n)}\mathbf{P}^{(n-1)}\mathbf{c}^{(n-1)} + \underline{\ell}^{(n)}\mathbf{p}^{(n)}c_n &= \underline{\ell}^{(n)}\mathbf{f}^{(n-1)} \\ \underline{\ell}^{(n)}\mathbf{P}^{(n-1)}\mathbf{c}^{(n-1)} + p_n(x_n)c_n &= f_n. \end{aligned} \tag{3.44}$$

and subtracting the bottom equation from the top one we obtain

$$\underline{\ell}^{(n)}\mathbf{p}^{(n)}c_n - p_n(x_n)c_n = \underline{\ell}^{(n)}\mathbf{f}^{(n-1)} - f_n$$

from which we can finally isolate the coefficient $c_n$:

$$c_n = \frac{\underline{\ell}^{(n)}\mathbf{f}^{(n-1)} - f_n}{\underline{\ell}^{(n)}\mathbf{p}^{(n)} - p_n(x_n)}. \tag{3.45}$$

Having computed $c_n$, we can now re-insert it into the first Equation in Equation 3.43, resulting in the new system

$$\mathbf{P}^{(n-1)}\mathbf{c}^{(n-1)} = \mathbf{f}^{(n-1)} - \mathbf{p}^{(n)}c_n \tag{3.46}$$

in the remaining coefficients $\mathbf{c}^{(n-1)}$.

Applying this computation recursively to $\mathbf{P}^{(n)}$, $\mathbf{P}^{(n-1)}$, ..., $\mathbf{P}^{(1)}$ we can compute the interpolation coefficients $\mathbf{c}^{(n)}$. The final coefficient $c_0$ can be computed as

$$c_0 = f_0 / P^{(0)}_{1,1}.$$

The complete algorithm is shown in Algorithm 6. Since the construction of the $\underline{\ell}^{(k)}$, $k = 1 \dots n$ requires $\mathcal{O}(n^2)$ operations (for each $\underline{\ell}^{(k)}$, $\mathcal{O}(k)$ operations are required to compute $w_k$ and $\mathcal{O}(k)$ are required to compute the new entries) and the evaluation of Equation 3.45 requires $\mathcal{O}(k)$ operations for each $c_k$, $k = n \dots 0$, the total cost of the algorithm is in $\mathcal{O}(n^2)$ operations.

**Algorithm 6** Direct construction of $g_n(x)$

```
1: $\mathbf{p}^{(0)} \leftarrow 0$, $\mathbf{p}^{(1)} \leftarrow \mathbf{x}$    ($\textit{init } \mathbf{P}^{(n)}$)
2: for $i = 2 \dots n$ do
3:     $\mathbf{p}^{(i)} \leftarrow \left( (\mathbf{x} + \beta_{i-1}) .* \mathbf{p}^{(i-1)} - \gamma_{i-1}\mathbf{p}^{(i-2)} \right) / \alpha_{i-1}$    ($\textit{fill } \mathbf{P}^{(n)}$)
4: end for
5: $\ell^{(1)}_0 \leftarrow 1$, $w_1 = x_1 - x_0$    ($\textit{init } \ell^{(1)}_0 \textit{ and } w_1$)
6: for $i = 2 \dots n$ do
7:     $w_i \leftarrow 1$    ($\textit{construct } w_i$)
8:     for $j = 0 \dots i-1$ do
9:         $w_i \leftarrow w_i(x_i - x_j)$
10:    end for
11:    for $j = 0 \dots i-2$ do
12:        $\ell^{(i)}_j \leftarrow -\frac{\ell^{(i-1)}_j}{x_i - x_j} \frac{w_i}{w_{i-1}}$    ($\textit{compute the } \ell^{(i)}_j\textit{, Equation 3.41}$)
13:    end for
14:    $\ell^{(i)}_{i-1} \leftarrow \frac{w_i}{w_{i-1}(x_i - x_{i-1})}$    ($\textit{compute } \ell^{(i)}_{i-1}\textit{, Equation 3.42}$)
15: end for
16: for $i = n \dots 1$ do
17:    $c_i \leftarrow \frac{\underline{\ell}^{(i)}\mathbf{f}(0{:}i-1) - f_i}{\underline{\ell}^{(i)}\mathbf{p}^{(i-1)}(0{:}i-1) - p_i(x_i)}$    ($\textit{compute coefficient } c_i\textit{, Equation 3.45}$)
18:    $\mathbf{f} \leftarrow \mathbf{f} - c_i\mathbf{p}^{(i)}$    ($\textit{update the right-hand side } \mathbf{f}$)
19: end for
20: $c_0 \leftarrow f_0 / \mathbf{p}^{(0)}(0)$    ($\textit{compute the final } c_0$)
```

Note that, as opposed to the incremental Algorithm 4 presented in Section 2.1, this algorithm can not be extended to update or downdate an interpolation. It has an advantage, however, when multiple right-hand sides, *i.e.* interpolations over the same set of nodes, are to be computed. In such a case, the vectors $\underline{\ell}^{(k)}$, $k = 1 \dots n$ only need to be computed once (Lines 5 to 15 of Algorithm 6). For any new vector $\mathbf{f}$, only the Lines 16 to 20 need to be re-evaluated.

### 3.2.3 Numerical Tests

To assess the stability of the two new interpolation routines described herein, we will follow the methodology used by Higham in [46]. Higham defines a set of interpolations consisting of all combinations of the nodes

$$\begin{array}{llll}
\text{A1:} & x_i = & -\cos(i\pi/n), & \text{(extrema of } T_n(x)) \\
\text{A2:} & x_i = & -\cos\left[(i+\tfrac{1}{2})\pi/(n+1)\right], & \text{(zeros of } T_{n+1}(x)) \\
\text{A3:} & x_i = & -1+2i/n, & \text{(equidistant on } [-1,1]) \\
\text{A4:} & x_i = & i/n, & \text{(equidistant on } [0,1])
\end{array}$$

with the right-hand sides

$$\begin{array}{lrcl}
\text{F1:} & f_i & = & (-1)^i, \\
\text{F2:} & f & = & [1,0,\dots,0]^\mathsf{T} \\
\text{F3:} & f_i & = & 1/(1+25x_i^2)
\end{array}$$

for $i = 0 \dots n$.

To avoid instabilities caused by unfortunate orderings of the nodes $x_i$, the nodes and corresponding function values were re-ordered according to the same permutation that would be produced by Gaussian elimination with partial pivoting applied to the Vandermonde-like matrix as described by Higham in [47]. This ordering is optimal for the Björck-Pereyra and Higham algorithms and produces good results for the new algorithms described in the previous two sections.

For each combination of nodes and right-hand sides, we compute, following Higham, the coefficients $\mathbf{c}$ for the Chebyshev base (see Equation 3.16) using for $n = 5$, 10, 20 and 30 and compute the quantities

$$\text{ERR} = \frac{\|\mathbf{c} - \mathbf{c}^\star\|_2}{u\|\mathbf{c}^\star\|_2}, \quad \text{RES} = \frac{\|\mathbf{f} - \mathbf{Pc}\|_2}{u\|\mathbf{c}^\star\|_2},$$

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 0.00 | 0.50 | 2.00 | 3.94 | **3.20** | **4.30** | 0.00 | 0.50 | 0.00 | 0.72 |
| 10 | 3.20 | 5.32 | **1.20e1** | **2.79e1** | 7.76 | $2.21e1$ | 2.26 | 7.00 | 0.00 | 2.47 |
| 20 | 7.28 | $2.16e1$ | **1.61e2** | **5.27e2** | 8.92 | $3.64e1$ | 9.14 | $2.60e1$ | 0.00 | $3.40e1$ |
| 30 | 2.61 | $1.03e1$ | **6.72e2** | **2.65e3** | $2.08e1$ | $1.11e2$ | 3.51 | $1.60e1$ | 0.00 | $8.76e1$ |

**Table 3.1:** Results for problem A1/F1.

where $\mathbf{c}^\star$ is the exact solution and $u$ is the unit roundoff [4] as defined in [41, Section 2.4.2].

Results were computed using Gaussian elimination (GE[5]), Higham's extension of the algorithm of Björck and Pereyra (BP/H[6]), the incremental Algorithm 4 (INCR) and the direct Algorithm 6 (DIRECT). The exact values were computed in Maple [9] with 50 decimal digits of precision using the `interp` function therein.

Results were also computed for the interpolation downdate (DEL) described in Algorithm 5. Starting from $\mathbf{c}^\star$ and $\boldsymbol{\eta}^\star$, the exact coefficients for the interpolation $g_n(x)$ and the Newton polynomial $\pi_{n+1}(x)$ respectively, we compute the coefficients $\mathbf{c}^{(n-1)}$ and $\boldsymbol{\eta}^{(n)}$ for $g_{n-1}(x)$ and $\pi_n(x)$, resulting from the removal of the rightmost function value $f_k$ at $x_k$, $k = \arg\max_i x_i$. The exact coefficients $\hat{\mathbf{c}}^\star$ *after* deletion were computed and used to compute the quantities ERR and RES.

The results are shown in Tables 3.1 to 3.12. For each $n$, the largest values for ERR and RES are highlighted. For the problem sets over the nodes A1 and A2 (Tables 3.1 to 3.6), the condition of the Vandermonde-like matrix is always $\leq 2$ [37], resulting in very small errors for Gaussian elimination. The Björck-Pereyra/Higham generates larger residuals than both the incremental and direct algorithms for both sets of nodes. The values for ERR, however, are usually within the same order of magnitude for the three algorithms.

[4]All results were computed using IEEE 754 double-precision arithmetic and hence $u \approx 2.2 \times 10^{-16}$.

[5]For the tests in this section, Matlab's backslash-operator, which uses partial pivoting, was used. In cases where the matrix is rank-deficient, a minimum-norm solution is returned.

[6]Algorithm 1 in [46] was implemented in Matlab.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 0.97 | 2.40 | **1.82** | **3.19** | 0.93 | 2.07 | 0.88 | 1.68 | 0.00 | 1.70 |
| 10 | 2.22 | 4.19 | **1.37e1** | **3.77e1** | 4.94 | 1.32e1 | 1.93 | 3.00 | 0.00 | 3.80 |
| 20 | 2.11e1 | 8.96 | **9.93e1** | **3.47e2** | 2.24e1 | 4.80e1 | 1.80e1 | 1.27e1 | 0.00 | 5.39e1 |
| 30 | 3.63e1 | 1.36e1 | **1.27e2** | **4.84e2** | 5.55e1 | 2.27e2 | 4.31e1 | 2.88e1 | 0.00 | 1.19e2 |

**Table 3.2:** Results for problem A1/F2.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 1.26 | 2.67 | 1.16 | 2.27 | 1.26 | 2.70 | **1.43** | **2.99** | 0.00 | 1.18 |
| 10 | 2.12 | 5.30 | **7.27** | **1.66e1** | 1.83 | 3.63 | 1.19 | 1.87 | 0.32 | 2.67 |
| 20 | 1.13 | 4.81 | **8.28** | **2.68e1** | 1.78 | 6.74 | 3.02 | 1.01e1 | 0.05 | 5.25 |
| 30 | 1.99 | 7.35 | **6.33** | **2.53e1** | 1.14 | 5.86 | 2.55 | 1.04e1 | 0.61 | 6.09 |

**Table 3.3:** Results for problem A1/F3.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 3.55 | 0.70 | **5.07** | **7.31** | 3.79 | 1.58 | 4.96 | 4.96 | 1.48 | 3.16 |
| 10 | 1.19e1 | 3.65 | **2.03e1** | **3.31e1** | 8.34 | 1.08e1 | 1.16e1 | 2.24 | 7.23 | 7.47 |
| 20 | 1.66e1 | 1.23e1 | 4.64e1 | **1.63e2** | **5.57e1** | 1.41e2 | 1.61e1 | 2.58 | 1.69e1 | 2.41e1 |
| 30 | 6.48e1 | 2.28e1 | **1.24e2** | **4.36e2** | 4.45e1 | 2.29e2 | 6.49e1 | 5.98 | 4.71e1 | 9.82e1 |

**Table 3.4:** Results for problem A2/F1.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 2.57 | 3.29 | **2.88** | **4.52** | 2.35 | 0.97 | 2.30 | 1.20 | 0.60 | 3.25 |
| 10 | 5.27 | 3.89 | **1.67e1** | **4.59e1** | 4.94 | 5.23 | 3.94 | 3.75 | 4.65 | 1.03e1 |
| 20 | 8.40 | 8.80 | **5.09e1** | **1.63e2** | 3.89e1 | 9.85e1 | 8.44 | 4.04 | 1.15e1 | 2.43e1 |
| 30 | 3.39e1 | 1.95e1 | **1.17e2** | **4.31e2** | 3.00e1 | 1.99e1 | 3.42e1 | 2.55e1 | 3.27e1 | 1.13e2 |

**Table 3.5:** Results for problem A2/F2.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | **1.44** | 0.11 | 1.40 | **1.71** | 1.17 | 1.45 | 1.12 | 1.67 | 0.00 | 2.76 |
| 10 | 2.73 | 3.22 | **6.06** | **1.14e1** | 2.86 | 3.75 | 3.64 | 6.34 | 6.56 | 7.47 |
| 20 | 1.52 | 5.59 | **7.34** | **2.42e1** | 2.06 | 6.34 | 3.92 | $1.34e1$ | $1.27e1$ | $1.81e1$ |
| 30 | 2.81 | $1.19e1$ | **7.24** | **3.08e1** | 1.65 | 6.07 | 2.79 | 9.46 | $1.41e1$ | $2.94e1$ |

**Table 3.6:** Results for problem A2/F3.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 1.41 | 0.58 | **6.12** | **1.01e1** | 2.04 | 0.97 | 1.48 | 0.73 | 0.60 | 0.78 |
| 10 | 2.99 | 2.50 | **1.18e1** | **2.00e1** | 2.16 | 1.52 | 2.62 | 3.11 | 0.50 | 1.42 |
| 20 | **2.26e3** | 4.85 | $2.01e1$ | **7.19e1** | $3.58e1$ | $1.02e1$ | $6.23e1$ | 3.97 | 0.55 | 2.77 |
| 30 | **1.39e6** | 9.51 | $3.90e1$ | **1.34e2** | $5.42e4$ | $2.60e1$ | $3.07e2$ | 7.33 | 0.55 | 2.20 |

**Table 3.7:** Results for problem A3/F1.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 1.02 | 1.98 | **2.19** | **3.53** | 0.69 | 0.80 | 0.73 | 1.40 | 0.40 | 0.86 |
| 10 | **4.91** | 7.58 | 3.83 | **1.03e1** | 1.05 | 1.82 | 1.61 | 2.46 | 0.47 | 0.85 |
| 20 | **3.65e3** | $1.07e1$ | 8.32 | **2.54e1** | $5.73e2$ | 2.94 | 1.29 | 4.25 | 0.63 | 2.26 |
| 30 | **4.02e5** | 9.93 | $3.23e1$ | **1.09e2** | $1.35e5$ | $1.25e1$ | 4.98 | 7.32 | 0.65 | 3.48 |

**Table 3.8:** Results for problem A3/F2.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | 1.48 | 0.86 | **1.87** | **1.98** | 1.78 | 1.89 | 1.38 | 0.36 | 0.00 | 2.23 |
| 10 | 2.31 | 3.28 | **8.96** | **2.76e1** | 2.00 | 2.97 | 3.27 | 3.80 | 0.45 | 1.12 |
| 20 | **2.30e3** | 5.53 | $3.81e1$ | **7.38e1** | $1.12e2$ | $1.24e1$ | $3.13e1$ | 5.11 | 0.47 | 3.39 |
| 30 | **1.39e6** | $1.10e1$ | $2.28e2$ | **1.88e2** | $5.29e4$ | $2.69e1$ | $2.41e2$ | 4.78 | 0.49 | 2.29 |

**Table 3.9:** Results for problem A3/F3.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | $2.01e2$ | 0.55 | 0.55 | **0.76** | **5.40e2** | 0.74 | $1.57e1$ | 0.48 | 3.06 | 3.80 |
| 10 | $2.49e4$ | 0.84 | 0.45 | 0.76 | **3.56e6** | **1.67** | $8.20e2$ | 0.60 | 1.94 | 3.55 |
| 20 | **2.77e15** | **2.53** | 1.87 | 1.69 | $5.08e14$ | 1.78 | $6.00e7$ | 1.63 | 5.93 | $1.41e1$ |
| 30 | $4.50e15$ | 0.00 | 4.44 | 1.16 | – | – | $3.47e11$ | 1.60 | 8.93 | $3.82e1$ |

**Table 3.10:** Results for problem A4/F1.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | $1.82e2$ | 0.48 | 0.55 | **0.65** | **3.64e2** | 0.37 | $1.12e1$ | 0.45 | 1.34 | 2.27 |
| 10 | $1.35e5$ | 0.63 | 0.40 | 0.85 | **3.77e6** | **1.55** | $6.28e2$ | 0.75 | 0.99 | 2.01 |
| 20 | **2.81e15** | **3.64** | 0.71 | 1.20 | $6.57e14$ | 0.93 | $4.05e7$ | 1.57 | 1.83 | 3.30 |
| 30 | $4.50e15$ | 0.00 | 0.40 | 1.27 | – | – | $1.37e11$ | 1.73 | 2.88 | $1.27e1$ |

**Table 3.11:** Results for problem A4/F2.

| | GE | | BP/H | | INCR | | DIRECT | | DEL | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | ERR | RES | ERR | RES | ERR | RES | ERR | RES | ERR | RES |
| 5 | $2.41e2$ | 0.23 | $3.96e1$ | 0.72 | **8.24e2** | **0.73** | 8.23 | 0.62 | 9.95 | $1.13e1$ |
| 10 | $3.79e5$ | **1.38** | $1.55e3$ | 0.88 | **4.94e6** | 1.35 | $3.04e2$ | 0.55 | 0.26 | 0.28 |
| 20 | **2.81e15** | **3.74** | $4.84e6$ | 1.21 | $9.48e14$ | 0.87 | $3.56e7$ | 1.03 | 1.45 | 2.58 |
| 30 | $4.50e15$ | 0.00 | $1.02e11$ | 1.47 | – | – | $1.18e11$ | 1.49 | 4.56 | $1.97e1$ |

**Table 3.12:** Results for problem A4/F3.

For the nodes A3 (Tables 3.7 to 3.9), the condition number of the Vandermonde-like matrix is $5.11e6$ for $n = 30$, resulting in the errors of approximately that magnitude when Gaussian elimination is used. In general, both the Björck-Pereyra/Higham and the direct algorithm generate smaller errors and residues than Gaussian elimination. The errors for the incremental algorithm are due to cancellation while evaluating $g_n(x_{n+1})$ for Equation 3.32, since the intermediate coefficients $\mathbf{c}^{(k)}$ are several orders of magnitude larger than the result[7].

Finally, the condition number of the Vandermonde-like matrix for the nodes A4 is $4.26e16$ for $n = 30$, making it numerically singular and thus resulting in the complete failure of Gaussian elimination. Note that since in such cases Matlab's backslash-operator computes the minimum norm solution, the resulting residual error RES is quite small. For the first two right-hand sides F1 and F2, the Björck-Pereyra/Higham algorithm performs significantly better than the two new algorithms, since the magnitude of the intermediate coefficients does not vary significantly. For the right-hand side F3, however, the errors are larger, caused by truncation in computing the Newton coefficients $a_i$. The incremental algorithm fails completely for all right-hand sides since the intermediate and final coefficients $\mathbf{c}^{(k)}$, $k \leq n$ are more than ten orders of magnitude larger than the function values[8] and the numerical condition of $g_n(x_{n+1})$ in Equation 3.32 exceeds machine precision, resulting in numerical overflow. These relatively large coefficients also cause problems for the direct algorithm when evaluating the right-hand side of Equation 3.46, where the original function values are clobbered by the subtraction of the much larger $\mathbf{p}^{(n)} c_n$.

The errors and residuals for the downdate algorithm are shown in the rightmost columns of Tables 3.1 to 3.12. In general the errors and residues of the downdate are relatively small for all test cases. The larger values, *e.g.* for A2/F2, are due to cancellation in the final subtraction in Algorithm 5, Line 7.

[7] In [46], Higham shows that the coefficients can be written as the weighted sum of any of the intermediate coefficients $c_i^{(n)} = \sum_j \mu_j c_j^{(k)}$, where the $\mu_j$ depend only on the nodes and the coefficients of the three-term recurrence relation. If the $\mu_j$ are $\mathcal{O}(1)$ and the intermediate $c_j^{(k)}$ are much larger than the $c_i^{(n)}$, then cancellation is likely to occur in the above sum.

[8] $\|\mathbf{c}^\star\| = 2.23e13$ for F3 and $n = 30$.

# Chapter 4

# Error Estimation

In this chapter we will start by discussing the different types of error estimators used in the adaptive quadrature algorithms discussed in Chapter 2. We will divide these error estimators using the explicit representation of the integrand described in Chapter 3, in two distinct categories and discuss their common features and shortcomings (Section 4.1).

We then derive two new error estimators based on using the $L_2$-norms of the interpolating polynomials on which each quadrature rule is based (Section 4.2).

Finally, the most prominent error estimators from Chapter 2, as well as the two new estimates presented here are tested against a set of problematic integrands (Section 4.3) and the results of these tests are analyzed (Section 4.4).

## 4.1 Categories of Error Estimators

In the following, we will distinguish between *linear* and *non-linear* error estimates.

### 4.1.1 Linear Error Estimators

We can group the different linear error estimators from Chapter 2 in the following categories:

1. $\varepsilon \sim \left|Q_n^{(m_1)}[a,b] - Q_n^{(m_2)}[a,b]\right|$: Error estimators based on the difference between two estimates of the same degree yet of different multiplicity (Kuncir [55], McKeeman [68, 71, 69], Lyness [61, 62], Malcolm and Simpson [66] and Forsythe *et al.* [29]).

2. $\varepsilon \sim |Q_{n_1}[a,b] - Q_{n_2}[a,b]|$: Error estimators based on the difference between two estimates of different degree (Patterson [80], Piessens *et al.* [82, 83], Hasegawa *et al.* [42], Berntsen and Espelid [4], Favati *et al.* [26] and Gander and Gautschi [34]).

3. $\varepsilon \sim \left|f^{(n)}(\xi)\right|$: Error estimators based on directly approximating the derivative in the analytic error term (Gallaher [30], Garribba *et al.* [35] and Ninomiya [74]).

4. $\varepsilon \sim |\tilde{c}_n|$: Error estimators based on the estimate of the highest-degree coefficient of the function relative to some orthogonal base (O'Hara and Smith [76, 77], Oliver [79], Berntsen and Espelid [5, 19, 20, 22, 23, 24]).

Already in 1985, Laurie [57] shows that the first three categories are, in essence, *identical*. Consider Kuncir's (see Section 2.2) error estimate from the **first** category,

$$\left|\mathsf{S}^{(1)}[a,b] - \mathsf{S}^{(2)}[a,b]\right|,$$

which can be viewed as a 5-point "rule" (or linear functional) over the nodes used by $\mathsf{S}^{(1)}[a,b]$ and $\mathsf{S}^{(2)}[a,b]$ (see Fig. 2.2).

Since both approximations evaluate polynomials of up to degree 3 exactly, their difference will be, when applied to polynomials of up to degree 3, zero. When applied to a polynomial of degree 4 or higher, the estimates will, in all but pathological cases, differ. This is, up to a constant factor, *exactly* what the 4*th divided difference* over the same 5 nodes computes:

It evaluates polynomials of up to degree 3 to zero and polynomials of degree 4 and higher in all but pathological cases to some non-zero value[1].

The same can be said of error estimates from the **second** category, such as the one used by Piessens (see Section 2.12)

$$|\mathsf{G}_n[a,b] - \mathsf{K}_{2n+1}[a,b]|$$

where the Gauss quadrature rule $\mathsf{G}_n[a,b]$ integrates all polynomials of degree up to $2n-1$ exactly and its Kronrod extension $\mathsf{K}_{2n+1}[a,b]$ integrates all polynomials of degree up to $3n+1$ exactly. Since the approximation computed by these rules differ only for polynomials of degree $2n$ and higher, the combined "rule" over the $2n+1$ points behaves just as the *$2n$th divided difference* would.

This same principle also applies to Berntsen and Espelid's (see Section 2.18) improved error estimate

$$|\mathsf{G}_{2n+1}[a,b] - Q_{2n-1}[a,b]|$$

where the interpolatory quadrature rule $Q_{2n-1}[a,b]$ over $2n$ points integrates all polynomials up to degree $2n-1$ exactly, making the difference to $\mathsf{G}_{2n+1}[a,b]$ zero for all polynomials up to degree $2n-1$ and non-zero for all non-pathological polynomials of degree $2n$ or higher, which is equivalent to the *$2n$th divided difference* over those same points.

In all these cases, the divided differences are *unique* (*i.e.* the $n$th difference over $n+1$ points), as are the quadrature rules. They therefore *differ only by a constant factor*. As a consequence, the first and second categories, in which the difference between two quadrature rules is used to approximate the error, are both equivalent to the **third** category, in which the lowest degree derivative of the error expansion are approximated explicitly.

Not all error estimators in these categories, though, are identical up to a constant factor to the highest-degree divided differences over the same points. McKeeman's error estimator (see Section 2.3), for instance, approximates a 4th divided difference over 7 points, which is neither unique nor of the highest-possible degree. The same can be said of Forsythe,

[1]Note that this is also, up to a constant factor, the definition of a null-rule, as used by Berntsen and Espelid (see Section 2.19). Lyness [60], who originally introduced the concept of null-rules, creates them explicitly from the difference of two quadrature rules, as is done in these error estimates implicitly.

Malcolm and Moler's `QUANC8` (see Section 2.7). Patterson's successive Kronrod extensions (see Section 2.12) are also an exception since the error estimates of the type

$$|\mathsf{K}_n[a,b] - \mathsf{K}_{2n+1}[a,b]|,$$

where $\mathsf{K}_n[a,b]$ integrates polynomials up to degree $(3n+1)/2$ exactly, compute only the $(3n-1)/2$th difference over $2n+1$ points, which is no longer unique. In general, though, we can say that in all these methods the approximated divided difference is of one degree higher than the degree of the lowest-degree rule in the pair used to compute it.

In the **fourth** and final category we again find finite differences, namely in Berntsen and Espelid's null rules (see Section 2.19), in which the coefficients $e_k$ relative to an orthogonal base are computed (see Equation 2.103). The highest-degree coefficient $e_{n-1}$, computed with the $(n-1)$st null rule over $n$ nodes is, as Berntsen and Espelid themselves note in [5], identical up to a constant factor to the $(n-1)$st divided difference over the same nodes. This value is combined with the $(n-2)$nd divided difference (see Equation 2.105), itself identical only up to a linear factor, to avoid phase effects, and used as an error estimate.

The same goes for the coefficients relative to *any* base computed over $n$ points, such as the coefficients $\tilde{c}_i$ of the Chebyshev polynomials used by O'Hara and Smith (see Section 2.8) and Oliver (see Section 2.11). The "rule" used to compute the highest-degree coefficients (Equation 2.24 and Equation 2.28) is identical up to a constant factor to the $n$th divided difference over the $n+1$ nodes used. While O'Hara and Smith use the highest-degree coefficient directly, Oliver uses $K^3|\tilde{c}_{n-4}|$ (see Equation 2.54 and Equation 2.55), which is related (*i.e.* no longer identical up to a constant factor) to the $(n-4)$th divided difference.

We therefore establish that *all* linear error estimators presented in this section are equivalent in that they all use one or more divided difference approximations of the higher derivatives of the integrand. The quality of the error estimate therefore depends on the quality of these approximations.

Using the difference of two interpolatory quadrature rules to compute the divided differences, as is done in the first two categories of error estimators, it is easy to show how problems can arise: Consider the case of the smooth function in Fig. 4.1, the integral of which is approximated

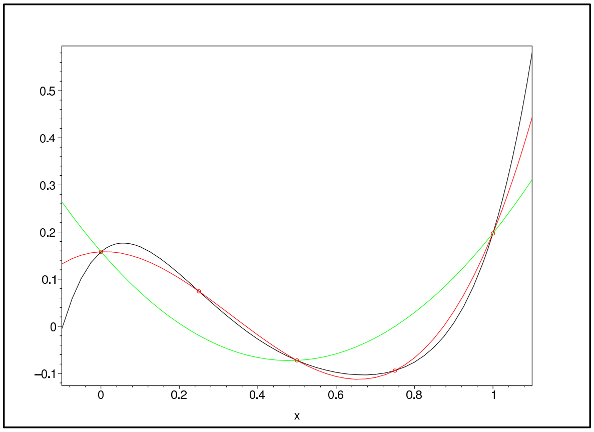


**Figure 4.1:** A smooth function (black) interpolated by $\tilde{f}_1(x)$ (green) using the nodes of $\mathsf{S}^{(1)}[a,b]$ and $\tilde{f}_2(x)$ (red) using the nodes of $\mathsf{S}^{(2)}[a,b]$.

over $[0,1]$ using both $\mathsf{S}^{(1)}[a,b]$ and $\mathsf{S}^{(2)}[a,b]$. Let $\tilde{f}_1(x)$ be the polynomial interpolated over the nodes of $\mathsf{S}^{(1)}[a,b]$ and $\tilde{f}_2(x)$ that interpolated over the nodes of $\mathsf{S}^{(2)}[a,b]$.

Although the interpolations $\tilde{f}_1(x)$ and $\tilde{f}_2(x)$ differ significantly, which is or should be a good indication that the degree of our quadrature rule is not sufficient, the integral of both $\tilde{f}_1(x)$ and $\tilde{f}_2(x)$ in $[0,1]$ is identical and the 4th divided difference over the nodes used, and thus the error estimate, gives 0.

In smooth functions, this type of problem may occur when the integrand is not "sufficiently smooth", *i.e.* the derivative in the error term is *not* more or less constant in the interval. This may seem like a rare occurrence, yet in discontinuous or otherwise non-smooth functions (*e.g.* Fig. 4.2), this type of problem can arise even for higher-degree quadrature rules.

The probability of such an unfortunate coincidence is rather small and decreases as the degree of the quadrature rules used in the difference increases. Another way of reducing this probability is to consider *more than one* derivative of the function, which is what the error estimators in the fourth category do rather explicitly: O'Hara and Smith (Section 2.8)

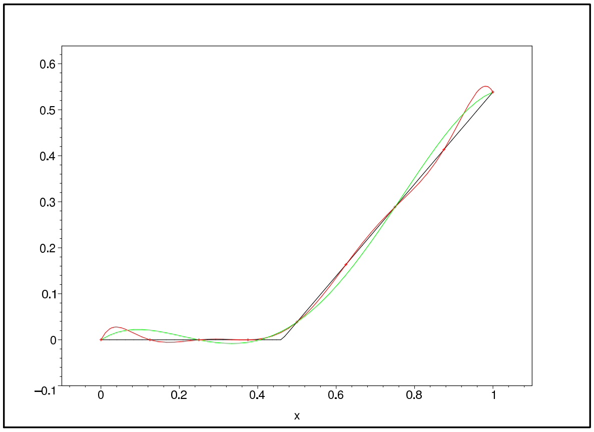


**Figure 4.2:** A non-smooth function (black) interpolated by $\tilde{f}_1(x)$ (green) using the nodes of $\mathsf{NC}_5^{(1)}[a,b]$ and $\tilde{f}_2(x)$ (red) using the nodes of $\mathsf{NC}_9^{(2)}[a,b]$.

effectively approximate three derivatives, Oliver (Section 2.11) computes the three highest-degree even Chebyshev coefficients and Berntsen and Espelid (Section 2.19) use a non-linear combination of higher-degree coefficients computed using null rules.

### 4.1.2 Non-Linear Error Estimators

Although most of the non-linear error estimators presented in Chapter 2 differ significantly in their approach, they all rely on the same basic principle, namely the assumption that, for any quadrature rule $Q^{(m)}[a,b]$, for sufficiently smooth $f(x)$ in the interval $x \in [a,b]$, the error can be written as

$$Q^{(m)}[a,b] - \int_a^b f(x)\,\mathrm{d}x \approx \kappa h^\alpha, \quad h = \frac{b-a}{m} \tag{4.1}$$

where $\kappa$ depends on the basic quadrature rule $Q$ and the higher derivatives of the integrand and $\alpha$ is the order of the error. In the most general case, Equation 4.1 has three unknowns, namely the actual integral $I = \int_a^b f(x)\,\mathrm{d}x$, the scaling $\kappa$ and the order $\alpha$ of the error. In many cases, the order $\alpha$ is assumed to be the order of the quadrature rule, but in the presence of singularities or discontinuities, this is not always the case. The three unknowns may be resolved using three successive approximations:

$$\begin{aligned} Q^{(m)} &= I + \kappa h^\alpha & (4.2) \\ Q^{(2m)} &= I + \kappa h^\alpha 2^{-\alpha} & (4.3) \\ Q^{(4m)} &= I + \kappa h^\alpha 4^{-\alpha} & (4.4) \end{aligned}$$

We can subtract Equation 4.2 from Equation 4.3 to isolate the error term

$$\begin{aligned} Q^{(m)} - Q^{(2m)} &= \kappa h^\alpha \left(1 - 2^{-\alpha}\right) \\ \kappa h^\alpha &= \frac{Q^{(m)} - Q^{(2m)}}{1 - 2^{-\alpha}} = \frac{2^\alpha \left(Q^{(m)} - Q^{(2m)}\right)}{2^\alpha - 1}. \qquad (4.5) \end{aligned}$$

Re-inserting this expression into Equation 4.3, we obtain

$$\begin{aligned} Q^{(2m)} &= I + \frac{2^\alpha \left(Q^{(m)} - Q^{(2m)}\right)}{2^\alpha - 1} 2^{-\alpha} \\ I &= Q^{(2m)} - \frac{Q^{(m)} - Q^{(2m)}}{2^\alpha - 1} \qquad (4.6) \end{aligned}$$

which is the linear extrapolation used in the Romberg T-table (for even integer values of $\alpha$) and also used by de Boor's `CADRE` (see Section 2.9, Equation 2.39), where the $Q^{(m)}$, $Q^{(2m)}$ and $Q^{(4m)}$ are the T-table entries $T_{\ell-2,i}$, $T_{\ell-1,i}$ and $T_{\ell,i}$ respectively, for an unknown $\alpha$.

Inserting Equation 4.5 into Equation 4.3 and Equation 4.4 and taking the difference of the two, we can extract

$$\begin{aligned} Q^{(2m)} - Q^{(4m)} &= \frac{2^\alpha \left(Q^{(m)} - Q^{(2m)}\right)}{2^\alpha - 1} \left(2^{-\alpha} - 4^{-\alpha}\right) \\ 2^\alpha &= \frac{Q^{(2m)} - Q^{(4m)}}{Q^{(m)} - Q^{(2m)}} \qquad (4.7) \end{aligned}$$

which is the ratio $R_i$ used by de Boor (Equation 2.36) to approximate the order of the error ($2^{\alpha+1}$ therein).

Inserting both Equation 4.5 and Equation 4.7 into the last estimate, Equation 4.4, we obtain

$$\begin{aligned}
I &= Q^{(4m)} - \frac{Q^{(m)} - Q^{(2m)}}{1 - \frac{Q^{(2m)}-Q^{(4m)}}{Q^{(m)}-Q^{(2m)}}} \left( \frac{Q^{(2m)} - Q^{(4m)}}{Q^{(m)} - Q^{(2m)}} \right)^2 \\
&= Q^{(4m)} - \frac{\left(Q^{(m)} - Q^{(2m)}\right)^2}{Q^{(m)} - 2Q^{(2m)} + Q^{(4m)}} \frac{\left(Q^{(2m)} - Q^{(4m)}\right)^2}{\left(Q^{(m)} - Q^{(2m)}\right)^2} \\
&= Q^{(4m)} - \frac{\left(Q^{(2m)} - Q^{(4m)}\right)^2}{Q^{(m)} - 2Q^{(2m)} + Q^{(4m)}} \qquad (4.8)
\end{aligned}$$

which is one step of the well-known Aitken $\Delta^2$-process [1], for accelerating the convergence of a sequence of linearly converging estimates, which, if Equation 4.1 holds, is what the individual $Q^{(m)}[a, b]$ are.

The approach taken by Rowland and Varol (see Section 2.10) is almost identical, except that, instead of using the exact integral, they use

$$\begin{aligned}
Q^{(m)} &= Q^{(2m)} + \kappa h^{\alpha} \qquad (4.9) \\
Q^{(2m)} &= Q^{(4m)} + \kappa h^{\alpha} 2^{-\alpha} \qquad (4.10) \\
Q^{(4m)} &= I + \kappa h^{\alpha} 4^{-\alpha} \qquad (4.11)
\end{aligned}$$

to solve for $\kappa h^{\alpha}$, $2^{-\alpha}$ and the exact integral $I$, resulting in their simpler error estimate (Equation 2.46).

In a similar vein, Laurie (see Section 2.16) uses the equations

$$\begin{aligned}
Q_{\alpha}^{(1)} &= I + \kappa_{\alpha}(b-a)^{\alpha+2} \\
Q_{\alpha}^{(2)} &= I + \kappa_{\alpha}(b-a)^{\alpha+2} 2^{-(\alpha+2)} \\
Q_{\beta}^{(1)} &= I + \kappa_{\beta}(b-a)^{\beta+2} \\
Q_{\beta}^{(2)} &= I + \kappa_{\beta}(b-a)^{\beta+2} 2^{-(\beta+2)} \qquad (4.12)
\end{aligned}$$

which are, however, under-determined, since there are 5 unknowns ($\kappa_{\alpha}$, $\kappa_{\beta}$, $\alpha$, $\beta$ and $I$) yet only four equations. To get a bound on the equation, Laurie therefore adds the conditions in Equation 2.78 and Equation 2.79, obtaining the inequality in Equation 2.77 from which he constructs his error estimate.

Similarly, Favati, Lotti and Romani use the equations

$$\begin{aligned} Q_\alpha &= I + \kappa_\alpha (b-a)^{\alpha+2} \\ Q_\beta &= I + \kappa_\beta (b-a)^{\beta+2} \\ Q_\gamma &= I + \kappa_\gamma (b-a)^{\gamma+2} \\ Q_\delta &= I + \kappa_\delta (b-a)^{\delta+2} \end{aligned} \tag{4.13}$$

which have 8 unknowns, and which can be solved together with the four conditions in Equation 2.92 to Equation 2.95.

Laurie and Venter's error estimator (see Section 2.10), is an exception: Although similar in form to that of Rowland and Varol, it does not follow the same approach, since the estimates

$$\begin{aligned} Q_1^{(1)} &= I + \kappa_1 (b-a)^3 \\ Q_3^{(1)} &= I + \kappa_3 (b-a)^5 \\ &\vdots \\ Q_{255}^{(1)} &= I + \kappa_{255} (b-a)^{257} \end{aligned} \tag{4.14}$$

form a set of $n$ equations in $n+1$ unknowns ($I$ and the $n$ different $\kappa_i$, assuming, for simplicity, that the actual order of the error is that of the quadrature rule) which can *not* be solved as above.

In summary, these methods, *i.e.* Romberg's method, the Aitken $\Delta^2$-process and Rowland and Varol's extrapolation, take a sequence of initial estimates $Q^{(m)}$, $Q^{(2m)}$, $Q^{(4m)}$, … and use them to create a sequence of *improved* estimates by removing the dominant error term as per Equation 4.1. These approaches can, of course, be re-applied to the resulting sequence, thus eliminating the next dominant error term, and so on. This is exactly what is done in the columns of the Romberg T-table and in successive re-applications of the Aitken $\Delta^2$-process.

In all these methods, the error estimate is taken to be *the difference between the last estimate and the extrapolated value of the integral.* In the case of de Boor's `CADRE`, this is the difference between the last two entries in the bottom row of the modified T-table, and for Rowland and Varol (Section 2.10), Laurie (Section 2.16) and Favati, Lotti and Romani (Section 2.16), this is $Q^{(4m)} - I$, $Q_\alpha^{(2)} - I$ and $Q_\alpha - I$ respectively.

Instead of successively and iteratively removing the dominant term in the error, we could also simply model the error directly as the sum of several powers

$$Q^{(m)} - I \approx \kappa_1 h^{\alpha_1} + \kappa_2 h^{\alpha_2} + \cdots + \kappa_N h^{\alpha_N}, \quad h = \frac{b-a}{m} \tag{4.15}$$

Since this equation has $2N+1$ unknowns (the $n$ constants $\kappa_i$, the $N$ exponents $\alpha_i$ and the exact integral $I$), we need $2N+1$ estimates to solve for them:

$$\begin{aligned}
Q^{(m)} &= I + \kappa_1 h^{\alpha_1} + \kappa_2 h^{\alpha_2} + \cdots + \kappa_N h^{\alpha_N} \qquad (4.16)\\
Q^{(2m)} &= I + \kappa_1 h^{\alpha_1} 2^{-\alpha_1} + \kappa_2 h^{\alpha_2} 2^{-\alpha_2} + \cdots + \kappa_N h^{\alpha_N} 2^{-\alpha_N}\\
Q^{(4m)} &= I + \kappa_1 h^{\alpha_1} 2^{-2\alpha_1} + \kappa_2 h^{\alpha_2} 2^{-2\alpha_2} + \cdots + \kappa_N h^{\alpha_N} 2^{-2\alpha_N}\\
Q^{(8m)} &= I + \kappa_1 h^{\alpha_1} 2^{-3\alpha_1} + \kappa_2 h^{\alpha_2} 2^{-3\alpha_2} + \cdots + \kappa_N h^{\alpha_N} 2^{-3\alpha_N}\\
&\vdots\\
Q^{(2^{2N} m)} &= I + \kappa_1 h^{\alpha_1} 2^{-2n\alpha_1} + \kappa_2 h^{\alpha_2} 2^{-2n\alpha_2} + \cdots + \kappa_N h^{\alpha_N} 2^{-2N\alpha_N}
\end{aligned}$$

This non-linear system of equations does not appear to be an easy thing to solve, yet in [50] Kahaner shows that, if we are only interested in $I$, this is *exactly* what the $\epsilon$-Algorithm [102] does. For an even number of approximations $2N$, the algorithm computes the same approximation as in Equation 4.15, yet only over the first $N-1$ terms, ignoring the first estimate $Q^{(m)}$.

Keeping Equation 4.15 in mind, de Doncker's error estimate (see Section 2.14, Equation 2.69) then reduces to

$$\varepsilon_i \approx 2 \left| \kappa_N h^{\alpha_N} \right|$$

for $N = \lfloor i/2 \rfloor$, assuming that, ideally, for all estimates the right-most even column of the epsilon-table was used.

Kahaner also shows that if such an expansion as per Equation 4.15 exists with more than one non-integer $\alpha_i$, then the Romberg T-table and the Aitken $\Delta^2$-process, applied iteratively, will insert spurious terms in the error expansion. Although both methods eventually converge to the correct result, they do so much more slowly than the $\epsilon$-Algorithm.

In summary, we can say that all the error estimators presented in Chapter 2 assume that the error of a quadrature rule $Q^{(m)}[a,b]$ behaves as

$$Q^{(m)} - I \approx \kappa_1 h^{\alpha_1} + \kappa_2 h^{\alpha_2} + \cdots + \kappa_N h^{\alpha_N}, \quad h = \frac{b-a}{m}. \tag{4.17}$$

The unknowns in this equation ($I = \int_a^b f(x)\,\mathrm{d}x$, $\kappa_i$ and $\alpha_i$) can be solved approximately using several approximations $Q_n^{(m)}$.

If the exponents $\alpha_i$ are known or assumed to be known, the resulting system is a *linear* system of equations. This is what Romberg's method computes quite explicitly and what many of the linear error estimators in Section 4.1.1 compute implicitly. If the exponents $\alpha_i$ are *not* known, the resulting system of equations is *non-linear* and can therefore only be solved for non-linearly.

The non-linear methods discussed here are therefore a conceptual extension of the linear error estimators presented earlier. As such, they are subject to the same problem of the difference between two estimates being accidentally small in cases where the assumptions in Equation 4.1 or Equation 4.17 do not actually hold, as is the case for singular or discontinuous integrands. The different error estimation techniques in this section differ only in the depth $N$ of the expansion and the use of additional constraints when the resulting system of equations is under-determined.

Although it is impossible to test if the assumptions on which these error estimates are based actually *hold*, it is possible to test if they are *plausible* This is done in most cases, yet as Espelid and Sørevik [25] show, these tests are not always adequate and their failure to detect a problem can lead to the catastrophic failures of the algorithm.

## 4.2 A New Error Estimator

Instead of constructing our error estimate from the difference between different estimates of the *integral* of the integrand, as is done in almost all the methods analyzed in Section 4.1, we will use the $L_2$-norm of the difference between the different *interpolations* of the integrand to construct:

$$\varepsilon = \sqrt{\int_{-1}^{1} \left[\hat{f}(x) - g_n(x)\right]^2 \mathrm{d}x} \tag{4.18}$$

where $\hat{f}(x)$ is the integrand $f(x)$ transformed from the interval $[a,b]$ to $[-1,1]$

$$\hat{f}(x) = f\left(\frac{a+b}{2} + \frac{b-a}{2}x\right)$$

and $g_n(x)$ is the interpolation polynomial of degree $n$ resulting from interpolating the integrand at the nodes of the quadrature rule:

$$g_n(x_i) = \hat{f}(x_i), \quad i = 0 \dots n.$$

The error estimate in Equation 4.18 is an approximation of the integration error of the interpolant $g_n(x)$

$$Q_n[-1,1] - \int_a^b \hat{f}(x)\,\mathrm{d}x = \int_{-1}^1 (g_n(x) - \hat{f}(x))\,\mathrm{d}x$$

and will only be zero if the interpolated integrand matches the integrand on the entire interval

$$g_n(x) = \hat{f}(x), \quad x \in [-1,1].$$

In such a case, the integral will also be computed exactly. The error Equation 4.18 is therefore, assuming we can evaluate Equation 4.18 reliably, not susceptible to “accidentally small” values.

Since we don’t know $f(x)$ explicitly, we cannot evaluate the right-hand side of Equation 4.18 exactly. In a first, naive approach, we could compute two interpolations $g^{(1)}_{n_1}(x)$ and $g^{(2)}_{n_2}(x)$ of different degree where $n_1 < n_2$. If we assume, similarly to Piessens’ and Patterson’s error estimates (see Section 2.12) in which the estimate from a higher-degree rule is used to estimate the error of a lower-degree rule, that $g^{(2)}_{n_2}(x)$ is a sufficiently precise approximation of the integrand

$$g^{(2)}_{n_2}(x) \approx f(x), \quad x \in [-1,1] \tag{4.19}$$

then we can approximate the error of the interpolation $g^{(1)}_{n_1}(x)$ as

$$\begin{aligned} \left[\int_{-1}^1 \left(f(x) - g^{(1)}_{n_1}(x)\right)^2 \mathrm{d}x\right]^{1/2} &\approx \left[\int_{-1}^1 \left(g^{(2)}_{n_2}(x) - g^{(1)}_{n_1}(x)\right)^2 \mathrm{d}x\right]^{1/2} \\ &\approx \|\mathbf{c}^{(2)} - \mathbf{c}^{(1)}\| \end{aligned}$$

where $\mathbf{c}^{(1)}$ and $\mathbf{c}^{(2)}$ are the vectors of the coefficients of $g^{(1)}_{n_1}(x)$ and $g^{(2)}_{n_2}(x)$ respectively and $c^{(1)}_i = 0$ where $i > n_1$. Our first, naive error estimate is hence

$$\varepsilon = (b-a)\|\mathbf{c}^{(1)} - \mathbf{c}^{(2)}\|. \tag{4.20}$$

This error estimate, however, is only valid for the lower-degree interpolation $g^{(1)}_{n_1}(x)$ and would over-estimate the error of the higher-degree interpolation $g^{(2)}_{n_2}(x)$ which we would use to compute the integral. For a more refined error estimate, we could consider the interpolation error

$$\hat{f}(x) - g_n(x) = \frac{\hat{f}^{(n+1)}(\xi_x)}{(n+1)!}\pi_{n+1}(x), \quad \xi_x \in [-1,1] \tag{4.21}$$

for any $n$ times continuously differentiable $f(x)$ where $\xi_x$ depends on $x$ and where $\pi_{n+1}(x)$ is the Newton polynomial over the $n+1$ nodes of the quadrature rule:

$$\pi_{n+1}(x) = \prod_{i=0}^{n}(x - x_i).$$

Taking the $L_2$-norm on both sides of Equation 4.21 we obtain

$$\varepsilon = \left[\int_{-1}^{1}\left(g_n(x) - \hat{f}(x)\right)^2 \mathrm{d}x\right]^{1/2} = \\ \left[\int_{-1}^{1}\left(\frac{\hat{f}^{(n+1)}(\xi_x)}{(n+1)!}\right)^2 \pi^2_{n+1}(x)\,\mathrm{d}x\right]^{1/2}.$$

Since $\pi^2_{n+1}(x)$ is, by definition, positive for any $x$, we can apply the mean value theorem of integration and extract the derivative resulting in

$$\varepsilon = \left[\int_{-1}^{1}\left(g_n(x) - \hat{f}(x)\right)^2 \mathrm{d}x\right]^{1/2} = \\ \left|\frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\right| \left[\int_{-1}^{1}\pi^2_{n+1}(x)\,\mathrm{d}x\right]^{1/2}, \quad \xi \in [-1,1]. \tag{4.22}$$

If we represent the polynomial $\pi_{n+1}(x)$ analogously to $g_n(x)$, as

$$\pi_{n+1}(x) = \sum_{k=0}^{n+1} b_k p_k(x), \tag{4.23}$$

then we can compute its $L_2$-norm as

$$\sqrt{\int_{-1}^{1} \pi_{n+1}^2(x)\,\mathrm{d}x} = \|\mathbf{b}\|$$

where $\mathbf{b}$ is the vector of the $n+2$ coefficients[2] $b_k$. Therefore, the terms on the right-hand side of Equation 4.22, only the $(n+1)$st derivative of the integrand is unknown.

Given two interpolations of the integrand, $g_n^{(1)}(x)$ and $g_n^{(2)}(x)$, of the same degree yet not over the same set of nodes, if we assume that the derivative $f^{(n+1)}(\xi)$ is constant for $\xi \in [a,b]$[3], we can extract the unknown derivative as follows:

$$\begin{aligned} g_n^{(1)}(x) - g_n^{(2)}(x) &= \hat{f}(x) + \frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\pi_{n+1}^{(1)}(x) - \hat{f}(x) - \frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\pi_{n+1}^{(2)}(x) \\ &= \frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\left(\pi_{n+1}^{(1)}(x) - \pi_{n+1}^{(2)}(x)\right) \end{aligned} \tag{4.24}$$

where $\pi_{n+1}^{(1)}(x)$ and $\pi_{n+1}^{(2)}(x)$ are the $(n+1)$st Newton polynomials over the $n+1$ nodes of $g_n^{(1)}(x)$ and $g_n^{(2)}(x)$ respectively. Taking the $L_2$-norm on both sides of (4.24), we obtain

$$\begin{aligned} \sqrt{\int_{-1}^{1}\left[g_n^{(1)}(x) - g_n^{(2)}(x)\right]^2 \mathrm{d}x} &= \left|\frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\right| \sqrt{\int_{-1}^{1}\left[\pi_{n+1}^{(1)}(x) - \pi_{n+1}^{(2)}(x)\right]^2 \mathrm{d}x} \\ \left\|\mathbf{c}^{(1)} - \mathbf{c}^{(2)}\right\| &= \left|\frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\right| \left\|\mathbf{b}^{(1)} - \mathbf{b}^{(2)}\right\| \\ \left|\frac{\hat{f}^{(n+1)}(\xi)}{(n+1)!}\right| &= \frac{\left\|\mathbf{c}^{(1)} - \mathbf{c}^{(2)}\right\|}{\left\|\mathbf{b}^{(1)} - \mathbf{b}^{(2)}\right\|} \end{aligned} \tag{4.25}$$

[2]In [46], Higham shows how the coefficients of a Newton-like polynomial can be computed relative to any orthogonal base.

[3]This assumption is a stronger form of the "sufficiently smooth" condition, which we will use only to construct the error estimator.

from which we can construct an error estimate for either interpolation

$$\begin{aligned}\sqrt{\int_{-1}^{1}\left[g_n^{(1)}(x)-\hat{f}(x)\right]^2\,\mathrm{d}x} &= \frac{\left\|\mathbf{c}^{(1)}-\mathbf{c}^{(2)}\right\|}{\left\|\mathbf{b}^{(1)}-\mathbf{b}^{(2)}\right\|}\|\mathbf{b}^{(1)}\| \\ \sqrt{\int_{-1}^{1}\left[g_n^{(2)}(x)-\hat{f}(x)\right]^2\,\mathrm{d}x} &= \frac{\left\|\mathbf{c}^{(1)}-\mathbf{c}^{(2)}\right\|}{\left\|\mathbf{b}^{(1)}-\mathbf{b}^{(2)}\right\|}\|\mathbf{b}^{(2)}\|. \qquad (4.26)\end{aligned}$$

For the interpolation $g_n^{(1)}(x)$, this gives us the refined error estimate

$$\varepsilon_2 = (b-a)\frac{\left\|\mathbf{c}^{(1)}-\mathbf{c}^{(2)}\right\|}{\left\|\mathbf{b}^{(1)}-\mathbf{b}^{(2)}\right\|}\|\mathbf{b}^{(1)}\| \qquad (4.27)$$

Note that for this estimate, we have made the assumption that the $n$th derivative is constant. We can't verify this directly, but we can verify if our computed $|\frac{f^{(n+1)}(\xi)}{(n+1)!}|$ (4.25) actually satisfies (4.21) for the nodes of the first interpolation by testing

$$\left|g_n^{(2)}(x_i)-\hat{f}(x_i)\right| \leq \vartheta_1\left|\frac{f^{(n)}(\xi)}{n!}\right|\left|\pi_{n+1}^{(2)}(x_i)\right|, \quad i=1\dots n \qquad (4.28)$$

where the $x_i$ are the nodes of the interpolation $g_n^{(1)}(x)$ and the value $\vartheta_1 \geq 1$ is an arbitrary relaxation parameter. If this condition is violated for any of the $x_i$, then we use, as in the naive error estimate (4.20), the un-scaled error estimate

$$\varepsilon = (b-a)\|\mathbf{c}^{(1)}-\mathbf{c}^{(2)}\|. \qquad (4.29)$$

In practice, we can implement this error estimator in a recursive adaptive quadrature by first computing the $n+1$ coefficients $c_k$ of $g_n(x)$ in the interval $[a,b]$. We also need the $n+2$ coefficients $b_k$ of the $(n+1)$st Newton polynomial over the nodes of the basic quadrature rule. If the same rule is used throughout the algorithm, then the $b_k$ can be pre-computed.

For the first interval, no error estimate is computed. The interval is bisected and for the recursion on the left half of $[a,b]$, we compute

$$\mathbf{c}^{\mathsf{old}} = \mathbf{T}^{(\ell)}\mathbf{c}, \quad \mathbf{b}^{\mathsf{old}} = \mathbf{T}^{(\ell)}\mathbf{b}. \qquad (4.30)$$

Note that to compute $\mathbf{b}^{\mathsf{old}}$ we would actually need to extend $\mathbf{T}^{(\ell)}$ and, since $\mathbf{b}^{\mathsf{old}}$ and $\mathbf{b}$ are not in the same interval, we have to scale the coefficients of $\mathbf{b}^{\mathsf{old}}$ by $2^{n+2}$ so that Equation 4.21 holds for $g_n^{(2)}(x)$ in the sub-interval.

Inside the left sub-interval $[a, (a+b)/2]$, we then evaluate the new coefficients $\mathbf{c}$ and $\mathbf{b}$. Note that if the base quadrature rule is the same throughout the algorithm, this is the same vector $\mathbf{b}$ we used above.

Given the old and new coefficients, we then compute the error estimate

$$\varepsilon_2 = (b-a)\frac{\|\mathbf{c}-\mathbf{c}^{\mathsf{old}}\|}{\|\mathbf{b}-\mathbf{b}^{\mathsf{old}}\|}\|\mathbf{b}\| \tag{4.31}$$

which is then either compared to a local tolerance $\tau_k$ in the case of a purely recursive algorithm along the lines of Algorithm 1, or summed to compute a global error estimate in the case of a heap-based algorithm as per Algorithm 2.

## 4.3 Numerical Tests

In the following, we will compare the performance of some of the error estimation techniques discussed in Section 4.1, including the new error estimator presented in Section 4.2.

### 4.3.1 Methodology

Whereas other authors [8, 48, 49, 66, 87, 53] have focused on comparing different algorithms as a whole, using sets of functions chosen to best represent typical integrands, we will focus here only on the error estimators and integrands chosen such that they specifically should or should not cause the error estimator to fail.

For these test functions we will not consider the usual metrics of efficiency, *i.e.* number of function evaluations required for a given accuracy, but the number of *false negatives* and *false positives* for each error estimator when integrating functions which it should or should not integrate correctly, respectively.

We define a *false positive* as a returned error estimate which is *below* the required tolerance when the actual error is *above* the latter. Likewise, a *false negative* is a returned error estimate which is *above* the required tolerance when the actual error is *below* the latter.

In practical terms, false negatives are a sign that the error estimator is overly cautious and continues to refine the interval even though the required tolerance would already have been achieved. False positives, however, may cause the algorithm to fail completely: if the actual error in a sub-interval is larger than the global tolerance, no amount of excess precision in the other intervals will fix it and the result will be incorrect, save an identical false positive elsewhere of opposite sign.

The test integrands, along with an explanation of why they were chosen, are:

1. $p_n(x)$: The Chebyshev polynomial of degree $n$ in the interval $[-\alpha, \beta]$, where $\alpha$ and $\beta$ are chosen randomly in $(0, 1]$ and $n$ is the degree of the quadrature rule for which the error estimate is computed[4]. The polynomial is shifted by $+1$ to avoid an integral of zero.

   This function should, by design, be integrated exactly by all quadrature routines and hence any error estimate larger than the required tolerance is a false negative.

2. $p_{n+1}(x)$: Same as the function above, yet one degree above the degree of the quadrature rule.

   Although this integrand is, by design, beyond the degree of the quadrature rule, the error term (*i.e.* the $n + 1$st derivative) is constant and can be extrapolated reliably from the difference of two quadratures of degree $n$, *e.g.* as is done implicitly in `SQUANK` (see Section 2.7, Equation 2.20) or explicitly in Ninomiya's error estimator (see Section 2.15, Equation 2.73), thus providing an exact error estimate.

3. $p_{n+2}(x)$: Same as the function above, yet two degrees above the degree of the quadrature rule.

[4]For error estimates computed from the difference of two quadrature rules of different degree, the degree of the quadrature rule of lower degree is used since although the result rule of higher degree is effectively used for the returned integrand, the error estimate is usually understood to be that of the lower-degree rule.

By design, the $n+1$st derivative is linear in $x$ and changes sign at the origin, meaning that any attempt to extrapolate that derivative from two estimates of equal degree may fail, causing an incorrect error estimate unless this is specifically tested for, *e.g.* using the noise detection in `SQUANK` (see Section 2.7) or the decision process in `CADRE` (see Section 2.9).

4. $d_k(x)$: A function with a discontinuity at $x = \alpha$ in the $k$th derivative, where $\alpha$ is chosen randomly in the interval of integration $[-1, 1]$ for $k = 0, 1$ and 2:

$$d_0(x) = \begin{cases} 0 & x < \alpha \\ 1 & \text{otherwise} \end{cases} \tag{4.32}$$

$$d_1(x) = \max\{0, x-\alpha\} \tag{4.33}$$

$$d_2(x) = (\max\{0, x-\alpha\})^2 \tag{4.34}$$

Since all quadrature rules considered herein are interpolatory in nature and these integrands can not be reliably interpolated, these functions will only be correctly integrated by chance. The only exception is `CADRE` (see Section 2.9), which attempts to detect jump discontinuities explicitly.

5. $s(x)$: A function with an integrable singularity at $x = \alpha$, where $\alpha$ is chosen randomly in $(-1, 1)$:

$$s(x) = |x-\alpha|^{-1/2}$$

As with the previous set of functions, this function can not be reliably interpolated and an interpolatory quadrature rule will produce a correct result only by chance. The only exception is again `CADRE`, which treats such singularities explicitly when detected (see Section 2.9, Equation 2.38) in cases where $\alpha$ is near the edges of the domain.

These functions were tested for 10 000 realizations of the random parameters $\alpha$ and $\beta$ for each of the relative tolerances $\tau = 10^{-1}$, $10^{-3}$, $10^{-6}$, $10^{-9}$ and $10^{-12}$. Since most error estimators use absolute tolerances, the tolerance was set to the respective fraction of the integral. The following error estimators were implemented in Matlab [67] (see Appendix A) and tested:

1. Kuncir's error estimate (Section 2.2, Equation 2.1), where $n = 3$ is the degree of the composite Simpson rules used,
2. McKeeman's 1962 error estimate (Section 2.3, Equation 2.5), where $n = 3$ is the degree of the composite Simpson rules used,
3. McKeeman's 1963 variable-order error estimate with $n = 7$ (Section 2.5, Equation 2.14), which is also the degree of the composite Newton-Cotes rules used,
4. Gallaher's error estimate (Section 2.6, Equation 2.17), where $n = 2$ is the degree of the trapezoidal rule used,
5. Lyness' error estimate as implemented in `SQUANK` (Section 2.7, Equation 2.18), where $n = 3$ is the degree of the Simpson's rules used. Note that two levels of recursion are evaluated to check for noise and, if it is detected, $2\tau$ is returned,
6. O'Hara and Smith's error estimate (Section 2.8, Equation 2.22, Equation 2.23 and Equation 2.24), which, if implemented as described in their original manuscript, the algorithm only rarely gets past the first error estimate (Equation 2.22) and is therefore not suited for testing the more interesting, third error estimate (Equation 2.24). For this reason, the algorithm was implemented *without* the initial error estimate and hence $n = 6$,
7. Oliver's error estimate (Section 2.11, Equation 2.55), where $n = 9$ is the degree of the second-last Clenshaw-Curtis quadrature used and the first error estimate below tolerance is returned or $2\tau$ if the interval is to be subdivided,
8. Piessens' error estimate (Section 2.12, Equation 2.57), where $n = 19$ is the degree of the 10-point Gauss quadrature used,
9. Patterson's error estimate (Section 2.12, Equation 2.58), where $n = 191$ is the degree of the second-last quadrature rule used and the first error estimate below tolerance is returned or $2\tau$ if the error estimate for 255 nodes is still larger than tolerance. Since Patterson's original algorithm is known to be prone to rounding and truncation errors, the improved implementation by Krogh and Snyder [52] was used,

10. Garribba *et al.* 's `SNIFF` error estimate (Section 2.13, Equation 2.64) using a 6-point Gauss-Legendre quadrature rule with $n = 11$ as suggested in [35],

11. Ninomiya's error estimate (Section 2.15, Equation 2.73) using the 9-point quadrature rule with $n = 9$ and the 11-point error estimator,

12. QUADPACK's `QAG` error estimator (Section 2.17, Equation 2.97) using the 10-point Gauss quadrature rule with $n = 19$ and its 21-point Kronrod extension,

13. Berntsen and Espelid's error estimate (Section 2.18, Equation 2.99) using the 21-point Gauss quadrature rule and the 20-point interpolatory quadrature rule with $n = 19$ ,

14. Berntsen and Espelid's null-rule error estimate (Section 2.19, Equation 2.107 and Equation 2.108) using, as a basic quadrature rule, the 21-point Clenshaw-Curtis quadrature rule (the 21-point Gauss quadrature rule was also tried but left out since it produced worse results, *i.e.* more false positives) with $n = 21$ and values $K = 3$, $r_{\mathsf{critical}} = 1/4$ and $\alpha = 1/2$.

15. Gander and Gautschi's error estimate (Section 2.20, Equation 2.114) using the 4-point Gauss-Lobatto quadrature rule with $n = 5$ and its 7-point Kronrod extension,

16. De Boor's `CADRE` error estimate (Section 2.9, Equation 2.37) where the entire decision process was considered with a maximum T-table depth of 10 and thus $n = 17$

17. Rowland and Varol's error estimate (Section 2.10, Equation 2.46) with $m = 1$ and $n = 3$ from the underlying Simpson's rule,

18. Venter and Laurie's error estimate (Section 2.10, Equation 2.50) where $n = 19$ is the degree of the second-last stratified quadrature rule and where the algorithm decides to subdivide an error estimate of $2\tau$ is returned,

19. Laurie's sharper error estimate (Section 2.16, Equation 2.77) using the 10-point Gauss quadrature rule with $n = 19$ and its 21-point Kronrod extension for the two rules $Q_\beta$ and $Q_\alpha$ respectively, as suggested by Laurie himself in [57],

20. Favati, Lotti and Romani's error estimate (Section 2.16, Equation 2.96), using as quadrature rules the 7 and 10 point Gauss quadrature rules as well as their 15 and 21 point Kronrod extensions with $n = 21$ being the degree of the 15 point Kronrod extension,

21. Kahaner and Stoer's error estimate (Section 2.14, Equation 2.70) using, for simplicity, the full trapezoidal sums (*i.e.* bisecting all intervals) with a maximum depth of $i = 7$ and using the $\epsilon$-Algorithm to extrapolate the integral, where error estimate was computed from the difference between the final estimate and the previous two estimates, the lower of which has degree $n = 5$,

22. The new, trivial error estimate (Section 4.2, Equation 4.20) using the nodes of the $n = n_1 = 11$ and $n_2 = 21$-point Clenshaw-Curtis quadrature rules to compute the two interpolations $g^{(1)}_{n_1}(x)$ and $g^{(2)}_{n_2}(x)$ respectively.

23. The new, more refined error estimate (Section 4.2, Equation 4.27) using the nodes of an 11-point Clenshaw-Curtis quadrature rule with $n = 10$ and one level of recursion to obtain $\mathbf{c}^{\mathsf{old}}$, as well as 1.1 for the constant $\vartheta_1$ in Equation 4.28.

Not all error estimators described in the previous sections were included in this test. The error estimate of McKeeman and Tesler (Section 2.4) is identical to McKeeman's first error estimate (Section 2.3), differing only in how the local tolerance is adjusted after bisection. Forsythe, Malcolm and Moler's error estimate (Section 2.7) is also not included since it is only an extension of Lyness' error estimate. Favati *et al.* 's error estimate using recursively monotone stable rules (Section 2.17) is, in essence, identical to that of QUADPACK's `QAG`. The different variants of Berntsen and Espelid's null-rule based error estimate (Section 2.19) were condensed into the version used here since the error estimation procedure is in essence identical. Finally, de Doncker's error estimate (Section 2.14) was not included since it works pretty much in the same way as Kahaner and Stoer's variant with the $\epsilon$-Algorithm, yet requiring much fewer nodes. The local error estimates are provided by the same error estimate as QUADPACK's `QAG`, which is included in the test, and hence will be as reliable as the latter.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 65.67 (0/34.33) | 8.49 (0/21.14) | 0.38 (0/0.76) | 0.01 (0/0.02) | 0 (0/0.01) |
| $p_{n+2}(x)$ | 51.07 (0/48.93) | 8.44 (0/15.77) | 0.50 (0/1.07) | 0.03 (0/0.11) | 0.02 (0/0) |
| $d_0(x)$ | 16.58 (0/22.27) | 0 (0/0.35) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 44.92 (0/29.98) | 0.73 (0/1.59) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 54.30 (0/22.66) | 5.74 (0/7.16) | 0.22 (0/0.12) | 0.01 (0/0) | 0 (0/0) |
| $s(x)$ | 0 (33.05/17.11) | 0 (0.42/0.20) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.1:** Results for Kuncir's 1962 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 64.19 (0/35.81) | 8.06 (0/51.21) | 0.26 (0/2.19) | 0.01 (0/0.05) | 0 (0/0) |
| $p_{n+2}(x)$ | 49.14 (0/50.86) | 8.29 (0/37.35) | 0.45 (0/2.51) | 0.04 (0/0.15) | 0.01 (0/0) |
| $d_0(x)$ | 0 (0/53.59) | 0 (0/0.74) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 47.48 (0/35.05) | 0.90 (0/4.73) | 0 (0/0.01) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 54.57 (0/30.24) | 5.52 (0/28.66) | 0.17 (0/0.49) | 0.02 (0/0.02) | 0 (0/0) |
| $s(x)$ | 0.03 (21.61/23.13) | 0 (0.21/0.21) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.2:** Results for McKeeman's 1962 error estimate.

### 4.3.2 Results

The results of the tests described in Section 4.3.1 are shown in Tables 4.1 to 4.23. For each integrand and tolerance, the percentage of correct integrations is given (*i.e.* the error estimate and the actual error are both below the required tolerance), as well as, in brackets, the percentage of false positives and false negatives respectively.

The results for Kuncir's error estimate (Section 2.2) are summarized in Table 4.1. Despite the low degree of the quadrature rule and its simplicity, the error estimator performs rather well. The function $p_n(x)$ is integrated reliably as would be expected. For the higher-degree $p_{n+1}(x)$, the error estimate is exact save a constant factor of 15, resulting in about as many false negatives as correct predictions with no false positives. Surprisingly enough, the function $p_{n+2}(x)$ is also handled correctly, despite the zero in the $n+1$st derivative, causing no false positives. The discontinuous functions do not generate any false positives either and the error estimator returns positive results only for the lowest tolerances. Finally, the singularity is not detected for $\tau = 10^{-1}$ in more than a third of the cases, returning a false positive.

The results for McKeeman's 1962 error estimate (Section 2.3) are summarized in Table 4.2. As with Kuncir's error estimate, with which it is

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 93.20 (0/6.80) | 41.73 (0/58.27) | 8.07 (0/91.93) | 1.54 (0/62.01) | 0.31 (0/11.38) |
| $p_{n+2}(x)$ | 87.13 (0/12.87) | 33.28 (0/66.72) | 6.97 (0/93.03) | 1.25 (0/48.18) | 0.46 (0/9.99) |
| $d_0(x)$ | 56.53 (1.03/37.73) | 0.26 (3.56/4.84) | 0 (2.12/0) | 0 (2.11/0) | 0 (1.87/0) |
| $d_1(x)$ | 84.52 (0/12.91) | 4.65 (0.08/72.32) | 0 (0/0.23) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 82.86 (0/14.69) | 30.27 (0/58.70) | 0.32 (0/14.20) | 0.01 (0/0.25) | 0 (0/0) |
| $s(x)$ | 35.25 (0.39/55.61) | 0 (0.44/0.56) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.3:** Results for McKeeman's 1963 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 0 (0/0) | 0 (0/0) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $p_{n+2}(x)$ | 1.21 (0/47.06) | 0.07 (0/2.45) | 0 (0/0.02) | 0 (0/0) | 0 (0/0) |
| $d_0(x)$ | 18.32 (81.68/0) | 0.28 (99.72/0) | 0 (100/0) | 0 (100/0) | 0 (100/0) |
| $d_1(x)$ | 23.77 (76.23/0) | 3.20 (96.80/0) | 0.06 (99.94/0) | 0 (100/0) | 0 (100/0) |
| $d_2(x)$ | 0 (0/0) | 0 (0/0) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $s(x)$ | 0 (0/19.09) | 0 (0/0.18) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.4:** Results for Gallaher's 1967 error estimate.

almost identical, it integrates the function $p_n(x)$ exactly and returns no false positives for the functions $p_{n+1}(x)$ and $p_{n+2}(x)$, yet the rate of false negatives is slightly higher due to the larger constant factor of 80 vs. 15 in the error term (Equation 2.7). As with Kuncir's error estimator the discontinuities are handled properly and the singularity is not detected for low tolerances, albeit less often due to more conservative scaling factor of the error. The same conclusions are also valid for McKeeman's 1963 error estimate (Section 2.5, Table 4.3), which is even more conservative – the error is over-estimated by a factor of 5 764 800 – resulting in an even larger number of false negatives for the polynomials, and, interestingly enough, some false positives for the discontinuity $d_0(x)$.

The results for Gallaher's 1967 error estimate (Section 2.6) are summarized in Table 4.4. The results for $p_n(x)$ and $p_{n+1}(x)$ are correct as expected, despite the odd form of the second derivative (Equation 2.17), which does not compute the error term exactly. Although the algorithm correctly fails on the singularity $s(x)$, it does not detect the first two discontinuities $d_0(x)$ and $d_1(x)$, returning false positives in almost all cases. As for the second degree discontinuity $d_2(x)$, it is beyond the degree of the integrator and the error is thus predicted correctly. If the correct expression (Equation 2.16) with the same constant scaling of 14.1 is used, better results are obtained (not shown), yet with some (ca. 10%) false

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 83.59 (0/16.41) | 4.36 (0/95.64) | 0.24 (0/99.76) | 0 (0/100) |
| $p_{n+2}(x)$ | 100 (0/0) | 54.66 (0/45.34) | 3.41 (0/96.59) | 0.28 (0/99.72) | 0.01 (0/99.99) |
| $d_0(x)$ | 63.20 (33.91/0) | 0 (0/0.57) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 87.11 (7.66/0) | 6.89 (30.14/1.46) | 0 (0.04/0) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 85.57 (6.07/0) | 42.96 (16.35/0.85) | 0.50 (1.39/0.01) | 0.03 (0.04/0) | 0 (0/0) |
| $s(x)$ | 26.90 (70.92/0) | 0 (4.84/0.32) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.5:** Results for Lyness' 1969 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 86.69 (0/13.31) | 7.32 (0/92.68) | 0.21 (0/99.79) | 0 (0/100) |
| $p_{n+1}(x)$ | 100 (0/0) | 62.89 (0/37.11) | 8.88 (0/91.12) | 1.09 (0/98.91) | 0.19 (0/99.81) |
| $p_{n+2}(x)$ | 99.72 (0/0.28) | 49.87 (0/50.13) | 7.24 (0/46.45) | 0.70 (0/8.81) | 0.10 (0/1.70) |
| $d_0(x)$ | 24.79 (0/47.57) | 0 (0/1.16) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 76.59 (0.80/15.09) | 4.27 (1.36/21.91) | 0 (0/0.03) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 83.95 (0/11.31) | 24.42 (0/40.68) | 0.29 (0/1.80) | 0.01 (0/0.01) | 0 (0/0) |
| $s(x)$ | 5.02 (35.95/34.85) | 0 (0/0.29) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.6:** Results for O'Hara and Smith's 1969 error estimate.

positives for $d_2(x)$.

The results for Lyness' 1969 error estimate (Section 2.7) are summarized in Table 4.5. For the polynomials $p_{n+1}(x)$ and $p_{n+2}(x)$ the number of false negatives is almost 100% since although the error for the compound Simpson's rule of degree 3 is computed, the 5-point Newton-Cotes quadrature of degree 5 is returned as an the integral. The quadratures are therefore exact, but this is not recognized by the error estimate. Although the algorithm implicitly tests for noise or odd behavior in the integrand, it does not reliably catch the first or second degree discontinuities $d_1(x)$ and $d_2(x)$ or the singularity $s(x)$, producing a large number of false positives for moderate tolerances. Although this error estimator is in essence identical to that of Kuncir, it's exact scaling of the difference of the quadratures by 1/15 is what makes it fail more often for the discontinuities.

The results for O'Hara and Smith's 1969 error estimate (Section 2.8) are summarized in Table 4.6. The algorithm drastically over-predicts the error for the polynomial $p_n(x)$ since it's estimate uses the last coefficient of the integrand, which is large by construction, to infer the magnitude of the following coefficients, which are zero by construction. The errors for $p_{n+1}(x)$ and $p_{n+2}(x)$ are similarly over-predicted. The interpolations of the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ often have large higher-degree

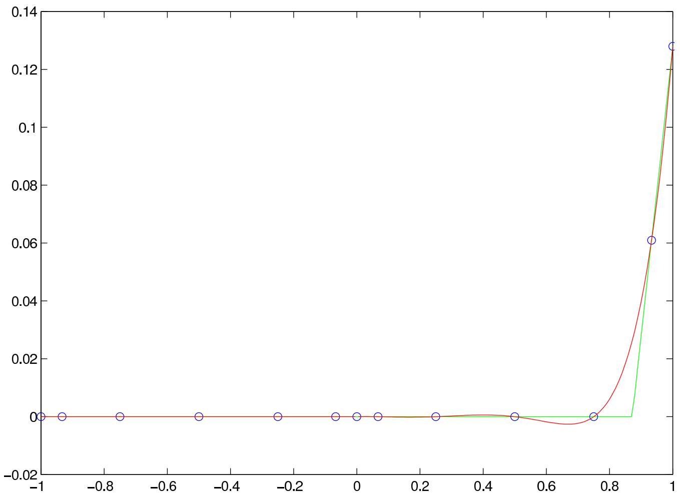


**Figure 4.3:** The polynomial interpolated by O'Hara and Smith's error estimate (red) for the discontinuous integrand $d_1(x)$ (green).

coefficients which are caught by the error estimate except for some cases in $d_1(x)$ in which the higher-degree Chebyshev coefficients are small and thus the interpolated integrand looks smooth, causing the error estimate to under-predict the error (see Fig. 4.3). Similarly, the error for singularity $s(x)$ is mis-predicted whenever the interpolation is *too* smooth (see Fig. 4.4).

The results for Oliver's 1972 error estimate (Section 2.11) are summarized in Table 4.7. Similarly to O'Hara and Smith's error estimator, the algorithm mis-predicts the errors for all three polynomials $p_n(x)$, $p_{n+1}(x)$

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 65.69 (2.40/31.91) | 22.20 (0.25/77.55) | 8.67 (0/91.33) | 2.77 (0/97.23) | 0.72 (0/99.28) |
| $p_{n+1}(x)$ | 55.07 (3.87/41.06) | 18.34 (0.22/69.25) | 6.03 (0/21.70) | 1.18 (0/5.57) | 0.23 (0/1.13) |
| $p_{n+2}(x)$ | 49.62 (5.79/44.59) | 14.93 (0.30/64.31) | 5.72 (0/18.04) | 1.52 (0/5.15) | 0.50 (0/1.58) |
| $d_0(x)$ | 20.44 (0/35.08) | 0 (0/0.64) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 71.27 (0.86/18.23) | 3.60 (6.96/10.86) | 0 (0/0.03) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 78.09 (0/16.14) | 23.55 (5.33/18.77) | 0.35 (0/0.90) | 0.01 (0/0.03) | 0 (0/0) |
| $s(x)$ | 2.06 (66.71/15.27) | 0 (0.60/0.23) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.7:** Results for Oliver's 1972 error estimate.

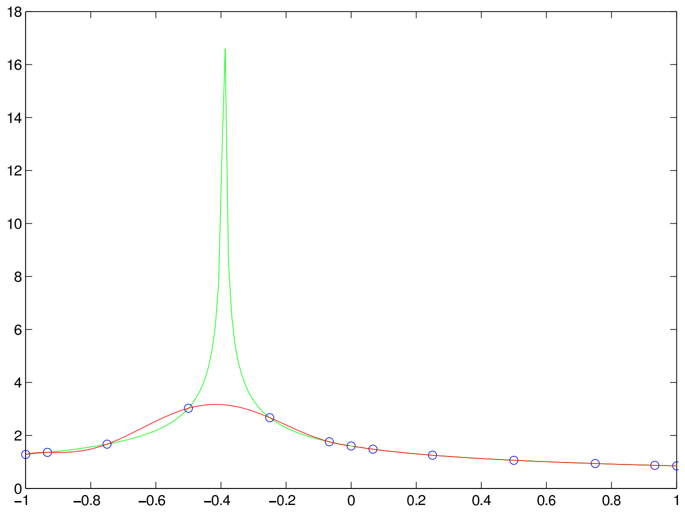


**Figure 4.4:** The polynomial interpolated by O'Hara and Smith's error estimate (red) for the singular integrand $s(x)$ (green).

and $p_{n+2}(x)$, due to the large higher-degree coefficients of the integrands. The false positives are cases where the doubly-adaptive algorithm exited after incorrectly predicting the error with a lower-order rule. This is also true for the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$, which are detected well by the higher-oder rules since the higher-degree Chebyshev coefficients become relatively large, yet fail when the error is mis-predicted by the lower-degree rules. The algorithm fails when integrating the singularity $s(x)$, since the coefficients of the interpolation often decay smoothly, misleading it to believe the integrand itself is smooth, similarly to O'Hara and Smith's error estimate (see Fig. 4.4).

The results for Piessens' 1973 error estimate (Section 2.12) are summarized in Table 4.8. As would be expected, the error estimate for the polynomial $p_n(x)$ is exact. For the higher-degree polynomials $p_{n+1}(x)$ and $p_{n+2}(x)$ the high number of false negatives is due to the higher-degree Kronrod extension being used as an approximation to the integral although the error is estimated for its underlying lower-degree Gauss rule. The error for the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ is approximated

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 98.02 (0/1.98) | 83.76 (0/16.24) | 52.05 (0/47.95) | 25.96 (0/74.04) | 12.69 (0/87.31) |
| $p_{n+2}(x)$ | 96.05 (0/3.95) | 76.82 (0/23.18) | 42.95 (0/57.05) | 21.48 (0/78.52) | 11.60 (0/88.40) |
| $d_0(x)$ | 63.54 (0.34/22.58) | 0.14 (0.27/2.21) | 0.01 (0.46/0) | 0 (0.39/0) | 0 (0.44/0) |
| $d_1(x)$ | 94.56 (0.21/4.21) | 18.19 (3.98/28.56) | 0.14 (0.32/0.16) | 0 (0.46/0) | 0 (0.40/0) |
| $d_2(x)$ | 95.70 (0.28/3.53) | 55.06 (0.40/27.79) | 1.18 (0.56/4.51) | 0.11 (0.44/0.01) | 0.01 (0.46/0) |
| $s(x)$ | 38.89 (25.21/23.75) | 0 (1.05/0.36) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.8:** Results for Piessens' 1973 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 42.37 (57.63/0) | 97.69 (2.31/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 43.24 (56.76/0) | 97.55 (2.45/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+2}(x)$ | 44.01 (55.99/0) | 97.90 (2.10/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $d_0(x)$ | 87.12 (12.88/0) | 0.10 (22.66/12.78) | 0 (22.27/0.01) | 0 (22.60/0) | 0 (22.68/0) |
| $d_1(x)$ | 88.99 (11.01/0) | 71.84 (28.16/0) | 0.14 (24.07/4.98) | 0 (21.89/0) | 0.01 (22.60/0) |
| $d_2(x)$ | 87.33 (12.67/0) | 88.28 (11.72/0) | 56.91 (12.46/25.98) | 0.72 (13.13/4.70) | 0.01 (12.85/0) |
| $s(x)$ | 20.31 (79.56/0.06) | 0 (9.73/1.16) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.9:** Results for Patterson's 1973 error estimate.

reliably in most cases due to the high degree of the quadrature rule, which more reliably interpolates the function. This, however, fails now and then due to accidentally small differences between the Gauss and Gauss-Kronrod rules, producing false positives. The singularity $s(x)$ produces many false positives at $\tau = 10^{-1}$ for the same reason (see Fig. 4.5).

Patterson's 1973 error estimate (Section 2.12), for which the results are summarized in Table 4.9, suffers from the same problems as Oliver's when using cascading error estimates. For the polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$ and in some cases the singularity $s(x)$ at moderate tolerances, the error estimator mis-predicts the errors using the lower-order quadrature rules, causing a large number of false positives. The exact predictions for higher tolerances for $p_{n+1}(x)$ and $p_{n+2}(x)$ are due to the relatively small contribution to the integral of the error term at such high degree ($n = 191$). The high number of false positives for the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ are caused when the discontinuity at $\alpha$ is outside of the first 7 quadrature nodes, making it practically undetectable. The remaining false positives when integrating the singularity $s(x)$ are due to the same accidentally small differences observed for Piessens' 1973 error estimate (see Fig. 4.5).

The results for Garribba *et al.* 's 1980 error estimate (Section 2.13) are summarized in Table 4.10. The error estimate is extremely precise for

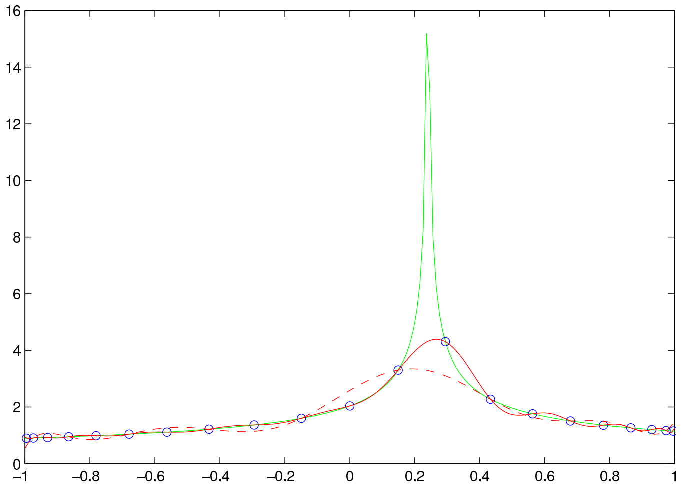


**Figure 4.5:** The integrands assumed by the Gauss (red dashed) and Gauss-Kronrod (red solid) quadratures in Piessens' 1973 error estimate for the singular integrand $s(x)$ (green).

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 100 (0/0) | 74.94 (0/0) | 26.16 (0/0) | 8.70 (0/0) |
| $p_{n+2}(x)$ | 100 (0/0) | 100 (0/0) | 63.34 (0/0) | 22.54 (0/0) | 7.47 (0/0) |
| $d_0(x)$ | 74.63 (25.37/0) | 1.26 (98.74/0) | 0 (6.69/0.01) | 0 (7.12/0) | 0 (6.72/0) |
| $d_1(x)$ | 93.09 (6.91/0) | 29.45 (70.55/0) | 0.15 (29.92/0.09) | 0.02 (3.75/0) | 0 (3.22/0) |
| $d_2(x)$ | 94.97 (5.03/0) | 66.17 (33.83/0) | 2.20 (56.55/0.03) | 0.18 (4.42/0.14) | 0.02 (3.63/0) |
| $s(x)$ | 40.88 (59.12/0) | 0.23 (99.30/0) | 0 (0.94/0) | 0 (0.01/0) | 0 (0/0) |

**Table 4.10:** Results for Garribba *et al.* 's 1978 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 90.28 (0/9.72) | 49.13 (0/50.87) | 11.90 (0/88.10) | 2.37 (0/97.63) | 0.40 (0/99.60) |
| $p_{n+2}(x)$ | 83.59 (0/16.41) | 38.58 (0/61.42) | 10.94 (0/89.06) | 3.06 (0/96.94) | 0.85 (0/99.15) |
| $d_0(x)$ | 23.84 (0.52/42.09) | 0 (0/1.02) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 73.27 (0.32/19.85) | 4.36 (1.79/14.75) | 0 (0/0.01) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 82.87 (0/9.71) | 21.25 (0.12/28.62) | 0.48 (0.08/0.15) | 0.01 (0.01/0) | 0 (0/0) |
| $s(x)$ | 4.30 (33.41/29.49) | 0 (0.53/0.27) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.11:** Results for Ninomiya's 1980 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 84.04 (0/15.96) | 70.01 (0/29.99) | 47.75 (0/52.25) | 30.61 (0/69.39) | 18.19 (0/81.81) |
| $p_{n+2}(x)$ | 76.68 (0/23.32) | 60.87 (0/39.13) | 38.91 (0/61.09) | 25.60 (0/74.40) | 16.22 (0/83.78) |
| $d_0(x)$ | 6.04 (0.32/79.64) | 0.11 (0.29/2.06) | 0 (0.49/0) | 0 (0.45/0) | 0 (0.38/0) |
| $d_1(x)$ | 22.50 (0.21/76.36) | 1.43 (0.35/44.96) | 0.12 (0.45/0.22) | 0.01 (0.52/0) | 0 (0.44/0) |
| $d_2(x)$ | 57.99 (0.18/41.19) | 15.36 (0.28/67.99) | 0.79 (0.30/5.23) | 0.09 (0.34/0) | 0.03 (0.48/0) |
| $s(x)$ | 0.26 (0.54/62.29) | 0 (0.03/0.35) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.12:** Results for Piessens *et al.* 's 1983 error estimate.

the polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$, generating no false negatives. The discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ and the singularity $s(x)$, however, are not well detected at all, resulting in many false positives over all tolerances since the underlying assumption of smoothness (Equation 2.59) is not valid for these functions.

The results for Ninomiya's 1980 error estimate (Section 2.15) are summarized in Table 4.11. The error for the polynomial $p_n(x)$ is correctly approximated. For $p_{n+1}(x)$, the large number of false positives is due to the subtraction of the (exact) error estimate from the approximation to the integral, thus returning an approximation of higher degree than the quadrature itself, and $p_{n+2}(x)$ causes no special difficulties. The discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ and the singularity $s(x)$ are integrated with a low number of false positives, even for moderate tolerances, due to the approximation of the derivative being "accidentally small".

Piessens *et al.* 's 1983 error estimate (Section 2.17) does a very good job over all functions (Table 4.12). The error estimate generates a high number of false negatives for the polynomials $p_{n+1}(x)$ and $p_{n+2}(x)$ since the quadrature rule used to approximate the integral is several degrees more exact then that for which the returned error estimate is computed. The few false positives are due to the error estimate's scaling of the error, causing it to under-predict the actual error and to cases where

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 98.62 (0/1.38) | 85.42 (0/14.58) | 52.85 (0/47.15) | 26.09 (0/73.91) | 13.52 (0/86.48) |
| $p_{n+2}(x)$ | 97.03 (0/2.97) | 78.10 (0/21.90) | 44.73 (0/55.27) | 22.57 (0/77.43) | 12.23 (0/87.77) |
| $d_0(x)$ | 66.48 (0.35/20.07) | 0.14 (0.63/2.06) | 0 (0.61/0) | 0 (0.59/0) | 0 (0.57/0) |
| $d_1(x)$ | 96.70 (0.32/2.08) | 20.73 (3.70/26.64) | 0.08 (0.53/0.08) | 0 (0.72/0) | 0 (0.72/0) |
| $d_2(x)$ | 97.66 (0.34/1.52) | 56.70 (0.75/26.47) | 2.05 (0.64/4.47) | 0.13 (0.48/0.01) | 0.01 (0.54/0) |
| $s(x)$ | 44.02 (24.34/19.57) | 0 (1.27/0.39) | 0 (0.01/0) | 0 (0/0) | 0 (0/0) |

**Table 4.13:** Results for Berntsen's 1984 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 51.98 (0/48.02) | 23.69 (0/76.31) | 8.15 (0/91.85) | 2.56 (0/97.44) | 0.97 (0/99.03) |
| $p_{n+1}(x)$ | 48.42 (0/51.58) | 21.97 (0/78.03) | 7.24 (0/78.24) | 2.13 (0/54.11) | 0.84 (0/29.48) |
| $p_{n+2}(x)$ | 43.89 (0/56.11) | 20.23 (0/79.77) | 6.77 (0/71.77) | 2.34 (0/45.22) | 0.73 (0/26.05) |
| $d_0(x)$ | 53.45 (0/31.20) | 0 (0/1.86) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 85.10 (0/13.32) | 3.76 (0/41.23) | 0 (0/0.26) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 90.18 (0/8.94) | 34.92 (0/47.13) | 0.27 (0/5.23) | 0 (0/0.11) | 0 (0/0) |
| $s(x)$ | 13.03 (28.88/45.80) | 0 (0/0.34) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.14:** Results for Berntsen and Espelid's 1991 error estimate.

the discontinuity at $\alpha$ was outside of the open nodes of the quadrature rule. The error estimates for the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ generate almost no false positives and the integration of the singularity $s(x)$ at $\tau = 10^{-1}$ generates less than 1% false positives for the same reasons as Piessens' 1973 error estimate (see Fig. 4.5).

Berntsen and Espelid's error estimate (Section 2.18), for which the results are summarized in Table 4.13, does as well on the polynomials $p_n(x)$, $p_{n+1}(s)$ and $p_{n+2}(x)$ as Piessens *et al.* 's, after which it is modelled. On the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$, however, it generates more false positives and does poorly on the singularity $s(x)$ for moderate tolerances. Since the two quadratures from which the error is computed differ by only a single node, the difference in the resulting interpolations will be small for functions which can *not* be interpolated reliably (see Fig. 4.6).

Berntsen and Espelid's null-rule error estimate (Section 2.19), for which the results are summarized in Table 4.14, suffers from the same problems as O'Hara and Smith's and Oliver's error estimates for the polynomial $p_n(x)$: Although the integration is exact, the coefficients $\tilde{c}_i$ increase towards $i = n$, leading the algorithm to believe that the $n+1$st coefficient will be large when it is, in fact, zero. This pessimistic approximation, however, works to their advantage for the remaining polynomials $p_{n+1}(x)$ and $p_{n+2}(x)$ as well as for the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$. The

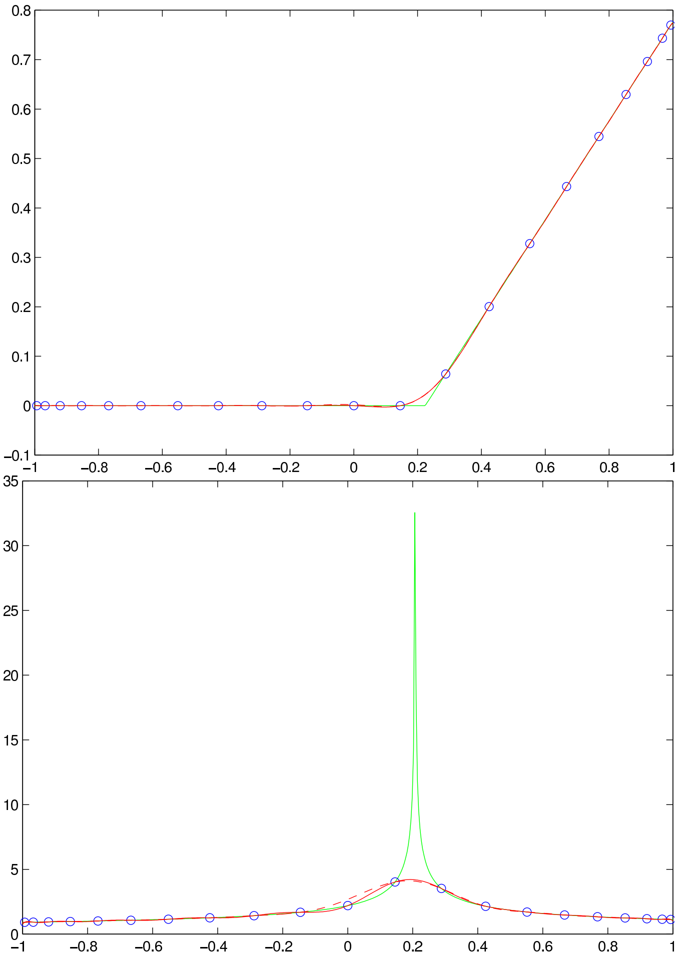


**Figure 4.6:** The integrands assumed by the quadrature rules $Q_{20}[a,b]$ (red dashed) and $G_{21}[a,b]$ (red solid) in Berntsen's 1984 error estimate for the discontinuous and singular integrands $d_1(x)$ and $s(x)$ respectively (green).

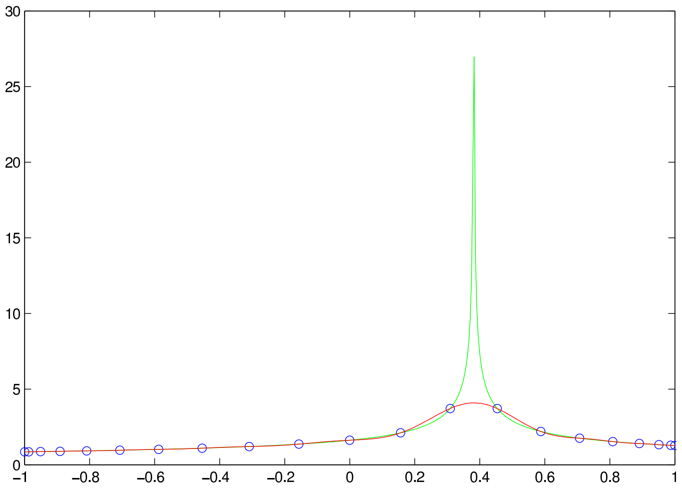


**Figure 4.7:** The integrand assumed by Berntsen and Espelid's 1991 error estimate (red) for the singular integrand $s(x)$ (green).

algorithm mis-predicts the error for the singularity $s(x)$ for the same reason as Oliver's algorithm, namely that the coefficients of the polynomial interpolation decrease smoothly, falsely indicating convergence (see Fig. 4.7).

The results for Gander and Gautschi's error estimate (Section 2.20) are summarized in Table 4.15. The algorithm performs well on the polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$, generating no false positives. The high number of false negatives for $p_{n+1}(x)$ and $p_{n+2}(x)$ are due to the higher degree of the estimate effectively returned. The error estimation

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 80.08 (0/19.92) | 17.69 (0/82.31) | 0.56 (0/99.44) | 0 (0/100) | 0 (0/99.99) |
| $p_{n+2}(x)$ | 68.15 (0/31.85) | 17.88 (0/82.12) | 2.46 (0/97.54) | 0.33 (0/99.67) | 0.08 (0/99.92) |
| $d_0(x)$ | 10.33 (0/39.32) | 0 (0/0.59) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 63.43 (2.32/23.63) | 0.70 (1.33/9.97) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 68.98 (0/19.77) | 8.69 (0.03/25.79) | 0.31 (0/0.13) | 0.02 (0/0.01) | 0 (0/0) |
| $s(x)$ | 0 (44.15/22.67) | 0 (0.50/0.22) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.15:** Results for Gander and Gautschi's 2001 error estimate.

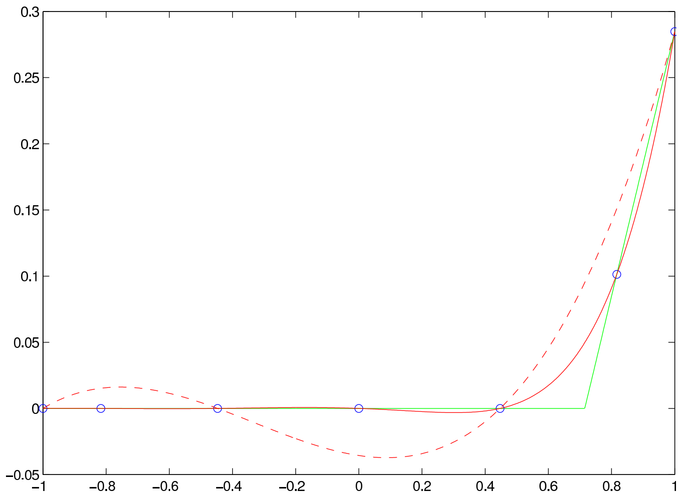


**Figure 4.8:** The integrands assumed by the Gauss-Lobatto (red dashed) and Gauss-Kronrod (red solid) quadrature rules in Gander and Gautschi's 2001 error estimate over the discontinuous integrand $d_1(x)$ (green).

returns some false positives for the discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$, as well as for the singularity $s(x)$, due to the difference between the two quadrature rules used being "accidentally small" (*e.g.* Fig. 4.8).

The results for de Boor's error estimate (Section 2.9), as shown in Table 4.16, are somewhat mixed. As with other doubly adaptive routines, it often fails to integrate the polynomial $p_n(x)$. Specifically, De Boor's error estimate fails because the ratio $R_i$ (Equation 2.36) is not close enough to 4 in the first few rows of the T-table and the algorithm therefore assumes that the integrand is not smooth enough. The false positives in all polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$ are caused by bad (*i.e.* "accidentally small") error estimates in the lower-degree rules. Otherwise, the jump discontinuity $d_0(x)$ is often detected as such and (correctly) treated explicitly. The algorithm, however, also treats $d_1(x)$ in the same way since the ratios $R_i$ also converge to $\approx 2$, resulting in a large number of false positives, since the error estimate assumes a jump in the 0th derivative. The third discontinuity $d_2(x)$ is only occasionally treated as a jump. In most cases it is treated as a normal, smooth function or in some cases as

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 25.73 (0.81/1.25) | 24.94 (1.90/0.04) | 23.78 (1.23/0) | 23.40 (1.23/0) | 23.26 (0.89/0) |
| $p_{n+1}(x)$ | 24.15 (1.04/1.38) | 23.20 (2.32/0.09) | 21.77 (0.76/0) | 21.16 (1.33/0) | 20.79 (1.05/0) |
| $p_{n+2}(x)$ | 21.80 (1.63/1.39) | 20.72 (1.95/0.08) | 19.54 (0.82/0) | 19.18 (1.46/0) | 18.92 (1.13/0) |
| $d_0(x)$ | 0 (0/57.95) | 0 (0/0.75) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 67.83 (0/4.92) | 3.83 (1.02/4.31) | 0 (0.32/0.02) | 0 (0.04/0) | 0 (0.02/0) |
| $d_2(x)$ | 48.85 (0/0) | 36.59 (12.60/0) | 2.87 (32.78/0) | 0.47 (35.38/0) | 0.09 (33.75/0) |
| $s(x)$ | 1.14 (3.54/0.71) | 0 (4.18/0) | 0 (0.03/0) | 0 (0/0) | 0 (0/0) |

**Table 4.16:** Results for De Boor's 1971 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 83.58 (0.94/0) | 3.98 (0.14/0) | 0.08 (0/0) | 0.01 (0/0) |
| $p_{n+2}(x)$ | 100 (0/0) | 71.14 (1.57/0) | 4.63 (0.06/0) | 0.36 (0/0) | 0.02 (0/0) |
| $d_0(x)$ | 40.85 (8.33/23.61) | 0 (0/0.90) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 80.23 (0.58/7.32) | 4.65 (12.12/5.35) | 0 (0.53/0) | 0 (0.01/0) | 0 (0/0) |
| $d_2(x)$ | 81.89 (0/7.15) | 36.63 (11.34/14.60) | 0.82 (2.54/0.12) | 0.03 (0.21/0.01) | 0 (0.01/0) |
| $s(x)$ | 5.85 (43.68/22.25) | 0 (7.42/0.24) | 0 (0.22/0) | 0 (0/0) | 0 (0/0) |

**Table 4.17:** Results for Rowland and Varol's 1972 error estimate.

a singularity, resulting in a large number of false positives. For the singularity $s(x)$, De Boor's special treatment for integrable singularities rarely kicks in and the algorithm usually aborts since the successive approximations do not seem to converge (*i.e.* the ratios $R_i$ are not $\approx 4$). When the singularity is detected, the extrapolation often returns an erroneous approximation of the error.

Rowland and Varol's error estimate (Section 2.10), for which the results are shown in Table 4.17, generates some false positives for the polynomials $p_{n+1}(x)$ and $p_{n+2}(x)$ where the error estimate was off by a small fraction due to "accidentally small" estimates by the lowest-degree rule. The discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ and the singularity $s(x)$ are not well detected since the integration error does not decay smoothly enough, *i.e.* the condition in Equation 2.45 is not valid, causing the error extrapolation to fail, resulting in a number of false positives for moderate tolerances. Note that better results may be achieved using larger values for $m$ making the observed problems more rare, yet not resolving them completely.

As with other doubly-adaptive quadratures, Venter and Laurie's error estimate (Section 2.10), for which the results are summarized in Table 4.18, fails to integrate $p_n(x)$ correctly due to bad error estimates using the lower-degree rules, resulting in either bad values of `hint` (Equa-

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 3.83 (6.17/36.23) | 2.44 (4.18/6.88) | 2.12 (0.05/1.57) | 0.40 (2.17/0.02) | 0 (1.69/0) |
| $p_{n+1}(x)$ | 3.81 (5.76/35.27) | 2.09 (3.89/5.97) | 2.02 (0.14/1.58) | 0.69 (1.66/0.01) | 0.02 (1.36/0) |
| $p_{n+2}(x)$ | 3.44 (5.72/33.32) | 2.28 (4.05/6.18) | 1.87 (0.19/1.39) | 0.86 (1.28/0.03) | 0 (1.54/0) |
| $d_0(x)$ | 0 (0/47.96) | 0 (0/0.58) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 25.86 (0/63.46) | 0.29 (13.26/12.85) | 0 (0.48/0.10) | 0 (0.02/0.01) | 0 (0/0) |
| $d_2(x)$ | 64.84 (0/26.22) | 34.51 (19.83/9.32) | 1.65 (12.77/1.02) | 0 (2.70/0.01) | 0 (1.53/0) |
| $s(x)$ | 0 (9.71/25.61) | 0 (6.81/0.34) | 0 (0.22/0) | 0 (0.01/0) | 0 (0/0) |

**Table 4.18:** Results for Venter and Laurie's 2002 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+2}(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $d_0(x)$ | 30.26 (0.09/62.46) | 0.12 (0.09/3.93) | 0 (0.18/0.01) | 0 (0.20/0) | 0 (0.24/0) |
| $d_1(x)$ | 36.78 (0.07/62.75) | 24.67 (3.78/48.51) | 0.25 (1.14/0.55) | 0 (0.41/0.01) | 0 (0.46/0) |
| $d_2(x)$ | 44.81 (0.11/54.70) | 40.21 (0.94/51.18) | 3.52 (4.74/15.25) | 0.14 (0.13/0.16) | 0.03 (0.32/0) |
| $s(x)$ | 25.01 (0.06/64.82) | 0 (4.52/0.52) | 0 (0.03/0) | 0 (0/0) | 0 (0/0) |

**Table 4.19:** Results for Laurie's 1983 error estimate.

tion 2.51) resulting in false negatives, or, less often, false convergence of the lower-degree rules used in the cascading error estimate, resulting in false positives. The use of `hint` guards the error estimate from making false assumptions on the discontinuity $d_0(x)$, yet not for $d_1(x)$ and $d_2(x)$ due to bogus convergence caused by "accidentally small" differences in the lower-degree rules, thus resulting in a large number of false positives. This works better, however, for the singularity $s(x)$, generating only few false positives.

The results for Laurie's error estimate (Section 2.16) are shown in Table 4.19. The error estimate is exact for the three polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$: even though the degree of the polynomials $p_{n+1}(x)$ and $p_{n+2}(x)$ is higher than the second-highest degree rule, the error of the highest-degree rule is correctly extrapolated as the polynomials are sufficiently smooth. Although these errors are themselves far below the required tolerance, they cause the original algorithm to fail when testing for the conditions in Equation 2.78 and Equation 2.80, where the difference between two otherwise exact quadrature rules becomes non-zero due to rounding and cancellation errors. This was partially amended by computing a somewhat arbitrary noise level

$$\varepsilon_{\mathsf{arb}} = 10\varepsilon_{\mathsf{mach}}(b-a)\max_i\{|f(x_i)|\} \tag{4.35}$$

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+2}(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $d_0(x)$ | 72.73 (3.65/13.16) | 0.21 (6.68/1.68) | 0 (0.23/0) | 0 (0.24/0) | 0 (0.18/0) |
| $d_1(x)$ | 86.79 (0/12.20) | 27.21 (9.03/18.60) | 0.10 (0.48/0.22) | 0.02 (0.25/0) | 0 (0.27/0) |
| $d_2(x)$ | 94.28 (0/4.64) | 68.74 (3.34/13.73) | 2.49 (2.80/3.70) | 0.03 (0.10/0.03) | 0 (0.13/0) |
| $s(x)$ | 41.45 (24.22/20.66) | 0 (2.72/0.34) | 0 (0.01/0) | 0 (0/0) | 0 (0/0) |

**Table 4.20:** Results for Favati *et al.* 's 1991 error estimate.

and truncating the moduli of the quadrature rules below it to zero. The discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ are not always detected since the condition in Equation 2.80 holds in some cases where the necessary condition in Equation 2.79 does not, resulting in some false positives over all tolerances and the error of the singularity $s(x)$ is, in most cases, extrapolated correctly.

The results for the error estimate of Favati *et al.* (Section 2.16) are shown in Table 4.20. This algorithm has a problem similar to that of Laurie's error estimate for integrands that are integrated exactly, *i.e.* the difference between two higher-order rules becomes zero or contains only noise, making the estimate fail. In their tests in [26], Favati *et al.* suggest avoiding this problem by aborting and bisecting the interval whenever $|Q_\alpha - Q_\beta|$, $|Q_\alpha - Q_\gamma|$ or $|Q_\alpha - Q_\delta|$ are below the required tolerance. This, however, would causes the algorithm to fail to converge for *any* integrand which can be integrated exactly by $Q_\beta$, which was not the case for any of their test integrands. This condition was therefore replaced with returning the result for $Q_\alpha$ if the error estimate $|Q_\alpha - Q_\beta|$ is below the noise level $\varepsilon_{\mathsf{arb}}$ defined in Equation 4.35. For the polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$, the noise exceeded this value only rarely, causing the occasional false negatives in these functions. The discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ and the singularity $s(x)$ were not always well detected since the conditions in Equation 2.92 to Equation 2.94 are not satisfied, resulting in a moderate number of false positives.

The result for Kahaner and Stoer's error estimate (Section 2.14), which are shown in Table 4.21, are somewhat mixed. The error estimator does a good job for the polynomials $p_n(x)$ The large number of false negatives for $p_{n+1}(x)$ and $p_{n+2}(x)$ is due to the algorithm returning a higher-degree estimate that the one for which the error estimate is computed. The results for the discontinuities, however, are not very encouraging. For

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 99.85 (0/0.15) | 37.83 (0/62.17) | 1.31 (0/98.69) | 0.05 (0/99.95) |
| $p_{n+2}(x)$ | 99.99 (0/0.01) | 99.64 (0/0.36) | 37.87 (0/62.13) | 4.11 (0/95.89) | 0.59 (0/99.35) |
| $d_0(x)$ | 57.55 (42.45/0) | 1.22 (98.78/0) | 0.01 (99.99/0) | 0 (100/0) | 0 (100/0) |
| $d_1(x)$ | 85.34 (13.84/0.22) | 30.37 (53.23/11.73) | 0.61 (67.36/0.41) | 0 (68.25/0) | 0 (67.71/0) |
| $d_2(x)$ | 87.84 (11.25/0.01) | 78.42 (10.90/9.58) | 5.96 (15.69/10.90) | 0.40 (16.59/0.27) | 0.02 (17.24/0.01) |
| $s(x)$ | 23.71 (3.03/35.37) | 0 (0.30/0.68) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.21:** Results for Kahaner and Stoer's 1983 error estimate.

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 89.78 (0/10.22) | 52.10 (0/47.90) | 14.80 (0/85.20) | 4.06 (0/95.94) | 1.12 (0/98.88) |
| $p_{n+2}(x)$ | 81.73 (0/18.27) | 40.76 (0/59.24) | 12.22 (0/87.78) | 4.52 (0/95.48) | 1.34 (0/98.66) |
| $d_0(x)$ | 0 (0/84.09) | 0 (0/2.31) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 66.03 (0/32.46) | 0.34 (0/44.30) | 0 (0/0.28) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 76.67 (0/22.50) | 16.19 (0/65.95) | 0.16 (0/5.34) | 0.01 (0/0.12) | 0 (0/0) |
| $s(x)$ | 0 (0/59.16) | 0 (0/0.39) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.22:** Results for the trivial error estimate in Equation 4.20.

the functions $d_0(x)$ and $d_1(x)$, the error estimator fails more often than not, resulting in many false positives. These false positives are due to false convergence in the $\epsilon$-Algorithm, whenever the difference between two estimates was accidentally small. The results for the singularity $s(x)$ are comparable to other methods.

The results for the *new* error estimates (Equation 4.20 and Equation 4.31) described in Section 4.2 are summarized in Tables 4.22 and 4.23. In both estimators, the polynomials $p_n(x)$, $p_{n+1}(x)$ and $p_{n+2}(x)$ don't cause any problems, except that the errors for the two higher-degree polynomials tend to be over-estimated as the computed $L_2$-norm is a somewhat pessimistic estimate of the integration error. The discontinuities $d_0(x)$, $d_1(x)$ and $d_2(x)$ are correctly detected and in many cases integrated correctly

| Function | $\tau = 10^{-1}$ | $\tau = 10^{-3}$ | $\tau = 10^{-6}$ | $\tau = 10^{-9}$ | $\tau = 10^{-12}$ |
|---|---|---|---|---|---|
| $p_n(x)$ | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) | 100 (0/0) |
| $p_{n+1}(x)$ | 100 (0/0) | 100 (0/0) | 58.76 (0/41.24) | 17.49 (0/82.51) | 5.15 (0/94.85) |
| $p_{n+2}(x)$ | 83.30 (0/16.70) | 58.78 (0/41.22) | 28.18 (0/71.08) | 9.05 (0/46.17) | 3.03 (0/14.26) |
| $d_0(x)$ | 0 (0/81.48) | 0 (0/2) | 0 (0/0) | 0 (0/0) | 0 (0/0) |
| $d_1(x)$ | 68.87 (0/27.89) | 0.40 (0/54.34) | 0 (0/0.10) | 0 (0/0) | 0 (0/0) |
| $d_2(x)$ | 82.21 (0/15.81) | 17.88 (0/58.11) | 0.22 (0/5.08) | 0 (0/0.07) | 0 (0/0) |
| $s(x)$ | 0 (0/59.19) | 0 (0/0.33) | 0 (0/0) | 0 (0/0) | 0 (0/0) |

**Table 4.23:** Results for the refined error estimate in Equation 4.27.

despite the pessimistic error estimate and the singularity $s(x)$ did not return a single false positive for either estimate. What is interesting about these error estimates is that they never under-estimated the error, resulting in no false positives at all.

### 4.3.3 Summary

From the descriptions of the behavior of the individual error estimators, we can extract some general observations:

1. The higher the degree of the quadrature rules used to compute a linear error estimate, the smaller the probability of an "accidentally small" error estimate (*e.g.* Gander and Gautschi's vs. Piessens *et al.* 's error estimators),

2. The higher the number of nodes by which two quadrature rules differ, the more sensitive the error estimate computed from their difference reacts to non-interpolable integrands (*e.g.* Berntsen and Espelid's 1984 error estimator vs. Piessens *et al.* 's),

3. Based on the two first observations, doubly-adaptive quadrature algorithms which rely on initial error estimates from lower-degree rules are only as reliable as the lowest-degree error estimate (*e.g.* Oliver's, de Boor's and Venter and Laurie's error estimators),

4. Error estimators using non-linear extrapolation usually rely more than the linear error estimates on assumptions which can not be verified, which are valid for *most* but not *all* (*e.g.* discontinuous or singular) integrands (*e.g.* Laurie's 1983 error estimator and de Boor's `CADRE`).

According to the results using the chosen test integrands, the best two error estimators appear to be that of Piessens *et al.* (Section 2.17) which is the error estimator for the adaptive routines in the popular integration library QUADPACK, and the two new error estimators presented herein (Section 4.2).

The relatively few false positives returned by the QUADPACK error estimator may seem negligible in contrast with its efficiency (evidenced by the much smaller percentage of false negatives) compared to the new error estimate. We can verify this by evaluating the smooth integral

$$\int_1^2 \frac{0.1}{0.01 + (x - \lambda)^2} \, \mathrm{d}x$$

first suggested by Lyness in [63], for which compute 1 000 realizations of the parameter $\lambda \in [1, 2]$. We use both Piessens *et al.* 's error estimate with 10 and 21 point Gauss and Gauss-Kronrod rules respectively and the new error estimates using both a pair of 11 and 21-point Clenshaw-Curtis quadrature rules for the trivial error estimate and an 11-point Clenshaw-Curtis quadrature rule with $\vartheta_1 = 1.1$ for the more refined estimate, all within a recursive scheme such as in Algorithm 1 with $\tau' = \tau/\sqrt{2}$, to a relative precision of $\tau = 10^{-9}$. On average, Piessens *et al.* 's error estimate requires 157 function evaluations while the new error estimates require 379 and 330 evaluations respectively – roughly twice as many. Both methods integrate all realizations to the required tolerance.

If we consider, however, the Waldvogel[5] function

$$W(x) = \int_0^x \lfloor e^t \rfloor \, \mathrm{d}t$$

which we wish to evaluate to the relative precision $\tau = 10^{-9}$ for 1 000 realizations of $x \in [2.5, 3.5]$ using both the error estimates of Piessens *et al.* and our new error estimators as described above, we get very different results. While Piessens *et al.* 's error estimator fails in roughly three quarters of all cases (753 failures out of 1 000, see Fig. 4.9), usually missing a sub-interval containing one or more discontinuities and using, on average, 29 930 function evaluations, our new error estimators succeeds on every trial, using on average 31 439 and 29 529 function evaluations respectively. The cautious estimate, in this case, pays off.

## 4.4 Analysis

The reason in this increased reliability is best explained by considering, for any error estimator, the set of integrands for which it will *always* fail.

[5]This function was suggested to the author by Prof. Jörg Waldvogel.

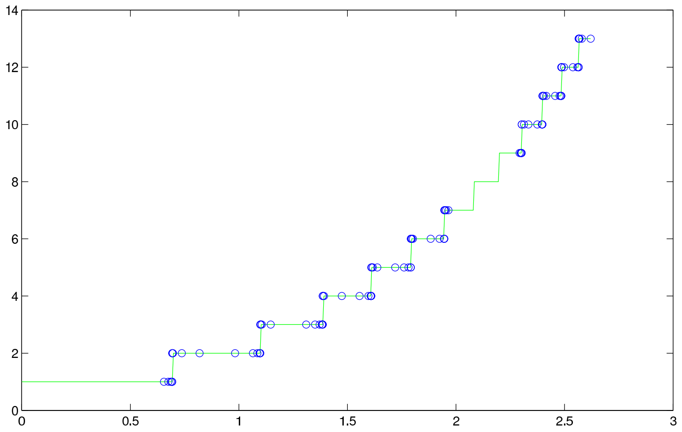


**Figure 4.9:** Piessens *et al.* 's error estimate used to evaluate one realization of the Waldvogel-function (green). The blue circles mark the edges of the sub-intervals. Note that the integrand is not well resolved near $\sim 2.1$.

Consider the polynomials orthogonal with respect to the discrete product

$$(p_i(x), p_j(x)) = \sum_{i=0}^{n} p_i(x_i) p_j(x_j), \quad 0 \leq i, j < n \tag{4.36}$$

where the $x_i$ are the nodes of the quadrature rule or the combined nodes of all the quadrature rules used in the computation of the error estimate in the interval. In the following, when we refer to a pair of functions being orthogonal, we understand them to be orthogonal with respect to the above product.

For any *linear* error estimate relying on the difference between two quadrature rules over the nodes $x_i$, the error estimate can be computed as

$$\varepsilon = \sum_{i=1}^{n} \eta_i f(x_i)$$

where the $\eta_i$ are the difference of the weights of the two quadrature rules used in the error estimate for each node[6]. Let $\eta(x)$ be the polynomial

[6]The $\eta_i$ are, incidentally, the weights of a null rule, such as they are constructed by Lyness in [60].

interpolating the $\eta_i$ at the nodes $x_i$, $i = 1 \dots n$. The error can then be computed as the product in Equation 4.36 applied to the integrand $f(x)$ and the polynomial $\eta(x)$:

$$\varepsilon = (\eta(x), f(x)) .$$

Therefore, if the integrand $f(x)$ is of algebraic degree *higher* than that of the quadrature rule used — and will therefore not be correctly integrated — and the integrand $f(x)$ is *orthogonal* to the polynomial $\eta(x)$, then the linear error estimate will be zero and therefore it will *fail*.

For the error estimate of O'Hara and Smith (Section 2.8), which uses more than one derivative, the error estimate fails when the integrand $f(x)$ is of higher algebraic degree than the basic quadrature rule and the coefficients $\tilde{c}_n$, $\tilde{c}_{n-2}$ and $\tilde{c}_{n-4}$ are zero (see Equation 2.33). This is the case when the integrand $f(x)$ is orthogonal to the Chebyshev polynomials $T_n(x)$, $T_{n-2}(x)$ and $T_{n-4}(x)$.

For the error estimate of Berntsen and Espelid (Section 2.19), the error estimate fails when the integrand $f(x)$ is of higher algebraic degree than the basic quadrature rule and the integrand $f(x)$ is orthogonal to the last $2(K-1)$ null rules[7].

For the non-linear error estimates discussed in Section 4.1.2, the error estimates will fail under similar circumstances: In de Boor's `CADRE` (see Section 2.9), it is sufficient that the difference between two neighboring entries in the T-table is zero for the error estimate to fail. For a T-table of depth $\ell$, this engenders $\mathcal{O}(\ell^2/2)$ different polynomials to which the integrand *may* be orthogonal to for the error estimate to fail.

In the case of Rowland and Varol's or Venter and Laurie's error estimates (see Section 2.10), a difference of zero between two consecutive pairs of rules is sufficient for the error estimate to fail and thus, as for the simple error estimators discussed above, for a sequence of $m$ rules, there are $m-1$ polynomials to which an integrand $f(x)$ *may* be orthogonal to for which the error estimator will always fail.

In Laurie's error estimate (see Section 2.16), either $Q_\alpha^{(2)} - Q_\beta^{(2)}$ or $Q_\alpha^{(2)} -$

[7]In Berntsen and Espelid's original error estimate 2 null-rules are used to compute each $E_k$ (see Equation 2.105) from which the $K$ ratios $r_k$ (see Equation 2.106) are computed. It is, however, only necessary that the nominators of the ratios be zero, hence only $2(K-1)$ null-rules need to be zero for the estimate to be zero.

$Q_\alpha^{(1)}$ need to be zero for the estimate to fail, resulting in two polynomials to which the integrand *may* be orthogonal to for the error estimate to fail. Similarly, for Favati *et al.* 's error estimate (see Section 2.16), there are three such polynomials.

Finally, for de Doncker's error estimate (see Section 2.14), the case is somewhat more complicated due to the global approach of the algorithm. Since it uses, locally, Piessens *et al.* 's local error estimate (see Section 2.17), it will fail whenever this estimate fails, making it vulnerable to the same family of integrands. Additionally, it will fail whenever the difference between two *global* estimates $\hat{Q}_n^{(m)}[a,b] - \hat{Q}^{(m-1)}[a,b]$ accidentally becomes zero, causing the algorithm to fail *globally.*

For both new error estimates presented here (Equation 4.20 and Equation 4.27), the matter is a bit more complicated. Given two interpolations $g_{n_1-1}^{(1)}(x)$ and $g_{n_2-1}^{(2)}(x)$, with $n_2 \geq n_1$, over the nodes $x_i^{(1)}$, $i = 1 \dots n_1 - 1$ and $x_i^{(2)}$, $i = 1 \dots n_2 - 1$ respectively, we define the joint set of $n_u$ nodes $x^{(u)} = x^{(1)} \cup x^{(2)}$ which we will use for the product in Equation 4.36. Given the inverse Vandermonde-like matrices $\mathbf{U}^{(1)} = (P^{(1)})^{-1}$ and $\mathbf{U}^{(2)} = (P^{(2)})^{-1}$ of size $n_1 \times n_1$ and $n_2 \times n_2$ used to compute the coefficients of $g_{n_1}^{(1)}(x)$ and $g_{n_2}^{(2)}(x)$, we can stretch them to size $n_2 \times n_u$ such that

$$\mathbf{c}^{(1)} = \tilde{\mathbf{U}}^{(1)}\mathbf{f}^{(u)}, \quad \mathbf{c}^{(2)} = \tilde{\mathbf{U}}^{(2)}\mathbf{f}^{(u)}$$

where $\tilde{\mathbf{U}}^{(1)}$ and $\tilde{\mathbf{U}}^{(2)}$ are the stretched matrices and $\mathbf{f}^{(u)}$ contains the integrand evaluated at the joint set of nodes $x^{(u)}$. For the error estimate $\|\mathbf{c}^{(1)} - \mathbf{c}^{(2)}\|$ to be zero, $\mathbf{f}^{(u)}$ must lie in the null-space of the $n_2 \times n_u$ matrix

$$\mathbf{U}^{(u)} = \left[\tilde{\mathbf{I}}^{(1)} - \tilde{\mathbf{U}}^{(2)}\right]$$

which has rank $r_u$ equal to the smaller of the number of nodes *not* shared by both $x^{(1)}$ and $x^{(2)}$, *i.e.* $x^{(u)} \backslash \{x^{(1)} \cap x^{(2)}\}$ or $n_2$. For the error estimate to be zero, the product $(\mathbf{P}^{(n)})^{-1}\mathbf{f}^{(u)}$ must be zero. This is the case when the integrand $f(x)$ is of algebraic degree $> n_2$ and orthogonal to the $r_u$ polynomials generated by interpolating the values of the first $r_u$ rows of $\mathbf{U}^{(u)}$ at the nodes $x^{(u)}$. If, additionally, the integrand is of degree $> n_2$, then both error estimates will fail.

The space of functions that will cause any of the error estimators presented here to fail is, in essence, infinite, yet for each type of error estimator, this infinite space is subject to different *restrictions*. For the simple **linear** error estimators which compute a *single* divided difference, the space is restricted by a *single* orthogonality restriction. In the case of error estimators such as O'Hara and Smith's or Berntsen and Espelid's, the space is restricted by *three or four*[8] orthogonality restrictions. Instead of being subject to *one or more* restrictions, the space of functions that will cause the **non-linear** error estimators discussed in Section 4.1.2 to fail is *larger* than that of the simple error estimators, since the integrand needs only to be orthogonal to *any* of a set of polynomials for the algorithm to fail. The set of functions for which they will fail is therefore the *union* of a set of functions, each subject to only *one* restriction. For our **new** error estimators, the number of restrictions depends on the number of nodes used. For the trivial error estimate (Equation 4.20), if the nodes $x^{(1)} \subset x^{(2)}$ and $n_2 \approx 2n_1$ (*i.e.* if Clenshaw-Curtis or Gauss-Kronrod rule pairs are used), the number of restrictions will be $\approx n_2/2$. For the more refined error estimate (Equation 4.27), if the basic rule does not re-use more than $\lceil n/2 \rceil$ of its $n$ nodes in each sub-interval, the number of restrictions will be at least $n-1$.

The new error estimates presented in Section 4.2 are therefore more reliable since the space of functions for which it will fail, albeit infinite, is *more restricted* than that of the other error estimators presented here. It is also interesting to note that if we were to *increase the degree* of the underlying quadrature rules in all our error estimates, the number of restrictions to the space of functions for which they will fail *would not grow*, whereas for our new error estimates, the number of restrictions *grows linearly* with the degree of the underlying quadrature rule.

[8]In Berntsen and Espelid's original error estimate, a constant $K = 3$ is used.

# Chapter 5

# Some Common Difficulties

## 5.1 Singularities and Non-Numerical Function Values

Since most adaptive quadrature algorithms are designed for general-purpose use, they will often be confronted with non-integrable integrands or integrands containing singularities or undefined values.

*Singularities* in the integrand can cause problems on two levels:

- The quadrature rule has to deal with a non-numerical value such as a NaN or $\pm$Inf,
- The integrand may not be as smooth and continuous as the algorithm might assume.

Such problems arise when integrating functions such as

$$\int_0^h x^\alpha \, \mathrm{d}x, \quad \alpha < 0$$

which have a singularity at $x = 0$, or when computing seemingly innocuous integrals such as

$$\int_0^h \frac{\sin x}{x}\,\mathrm{d}x$$

for which the integrand is undefined at $x = 0$, yet has a well-defined limit

$$\lim_{x\to 0} \frac{\sin x}{x} = 1.$$

In both cases problems *could* be avoided by either shifting the integration domain slightly or by modifying the integrand such as to catch the undefined cases and return a correct numerical result. This would, however, require some prior reflection and intervention by the user, which would defeat the purpose of a general-purpose quadrature algorithm.

Most algorithms deal with singularities by ignoring them, setting the offending value of the integrand to 0 [13, Section 2.12.7]. Another approach, taken by `quad` and `quadl` in Matlab, is to shift the edges of the domain by $\varepsilon_{\mathsf{mach}}$ if a non-numerical value is encountered there and to abort with a warning if a non-numerical value is encountered elsewhere in the interval. Since singularities may exist explicitly at the boundaries (*e.g.* integration of $x^\alpha$, $\alpha < 0$ in the range $[0, h]$), the explicit treatment of the boundaries is needed, whereas for arbitrary singularities within the interval, the probability of hitting them exactly is somewhat small.

QUADPACK's `QAG` and `QAGS` algorithms take a similar approach: since the nodes of the Gauss and Gauss-Lobatto quadrature rules used therein do not include the interval boundaries, non-numerical values at the interval boundaries will be implicitly avoided. If the algorithms has the misfortune of encountering such a value inside the interval, it aborts.

Our approach to treating singularities will be somewhat different: instead of setting non-numerical values to 0, we will simply *remove* that node from our interpolation of the integrand. This can be done rather efficiently by computing the interpolation as shown before using a function value of $f(x_j) = 0$ for the offending $j$th node and then *down-dating* (as opposed to up-dating) the interpolation, *i.e.* removing the $j$th node from the interpolation, resulting in an interpolation of degree $n - 1$:

$$g_{n-1}(x) = \sum_{i=0}^{n-1} c_i^{(n-1)} p_i(x)$$

which still interpolates the integrand at the remaining $n$ nodes.

The coefficients $c_i^{(n-1)}$ of $g_{n-1}(x)$ can be computed, as described in Section 3.2.1, using

$$c_i^{(n-1)} = c_i - \frac{c_n}{b_n^{(n-1)}} b_i^{(n-1)}, \quad i = 0 \dots n$$

where the $c_i$ are the computed coefficients of $g_n(x)$. The $b_i^{(n-1)}$ are the coefficients of the downdated Newton-polynomial computed by solving the upper-triangular system of equations

$$\begin{pmatrix} \alpha_0 & -(x_j+\beta_1) & \gamma_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \alpha_{n-2} & -(x_j+\beta_{n-1}) & \gamma_n & \\ & & & \alpha_{n-1} & -(x_j+\beta_n) & \\ & & & & \alpha_n & \end{pmatrix} \begin{pmatrix} b_0^{(n-1)} \\ b_1^{(n-1)} \\ \vdots \\ b_{n-1}^{(n-1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

using back-substitution, where the $b_i$ are the coefficients of the Newton polynomial over the nodes of the quadrature rule (Equation 4.23). $\alpha_i$, $\beta_i$ and $\gamma_i$ are the coefficients of the three-term recurrence relation satisfied by the polynomials of the orthogonal basis:

$$\alpha_k p_{k+1}(x) = (x + \beta_k)p_k(x) - \gamma_k p_{k-1}(x).$$

For the case of the normalized Legendre polynomials used here, the coefficients are

$$\alpha_k = \sqrt{\frac{(k+1)^2}{(2k+1)(2k+3)}}, \quad \beta_k = 0, \quad \gamma_0 = \sqrt{2}, \quad \gamma_k = \sqrt{\frac{k^2}{4k^2-1}}$$

The modified vectors $\mathbf{c}^{(n-1)}$ and $\mathbf{b}^{(n-1)}$ are then used in the same way as $\mathbf{c}$ and $\mathbf{b}$ respectively for the computation of the integral and of the error estimate.

## 5.2 Divergent Integrals

In the following, we will refer to *divergent integrals* as integrals which tend to $\pm\infty$ and thus cause most algorithms to either recurse infinitely or return an incorrect finite result. Divergent integrals are usually caught by limiting the recursion depth or the number of function evaluations artificially. Both approaches do not *per se* attempt to detect divergent behavior, and may therefore cause the algorithm to fail for complicated yet non-divergent integrals.

In [73], Ninham studied the approximation error when computing

$$\int_0^h x^\alpha \, \mathrm{d}x \tag{5.1}$$

using the trapezoidal rule. The integral exists for $\alpha > -1$ and is divergent otherwise. Following his analysis, we compute the refined error estimate described in Section 4.2 (Equation 4.29) for the intervals $[0, h]$ and $[0, h/2]$ using an 11-node Clenshaw-Curtis quadrature rule and removing the singular node at $x = 0$ as described above.

We note that as the algorithm recurses to the leftmost interval, the local error estimate as well as the computed integral itself remain constant for $\alpha = -1$ and *increase* for $\alpha < -1$. In Figure 5.1 we plot the ratio of the error estimate in the left sub-interval versus the error in the entire interval, $\varepsilon[0, h/2]/\varepsilon[0, h]$, over the parameter $\alpha$. For $\alpha = -1$ the ratio is 1 meaning that the error estimate of the leftmost interval remains constant even after halving the interval. For $\alpha < -1$, for which the integral diverges, the error estimate in the left half-interval is *larger* than the error estimate over the entire interval.

The rate at which the error decreases (or, in this case, increases) may be a good indicator for the convergence or divergence of the integral in Equation 5.1, where the singularity is at the boundary of the domain, yet it does not work as well for the shifted singularity

$$\int_0^h |x - \beta|^\alpha \, \mathrm{d}x, \quad \beta \in [0, h/2]. \tag{5.2}$$

Depending on the location of the singularity ($x = \beta$), the ratio of the error estimates over $[0, h]$ and $[0, h/2]$ varies widely for both $\alpha > -1$ and $\alpha \leq -1$ and can not be used to determine whether the integral diverges or not (see Figure 5.2).

In Figure 5.2 we have shaded the regions in which the ratio of the error estimates $\varepsilon[0, h/2]/\varepsilon[0, h] > 1$ for different values of $\alpha$ and the location of

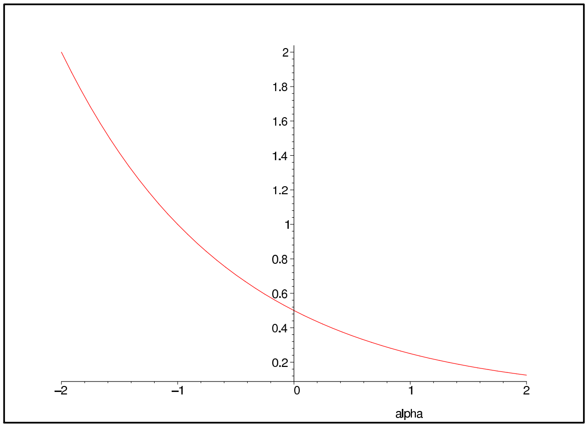


**Figure 5.1:** Ratio of the error estimates for $\int_0^h x^\alpha \, \mathrm{d}x$ for the intervals $[0, h/2]$ over $[0, h]$ for different $\alpha$. Note that the error grows (ratio $> 1$) for $\alpha < -1$, where the integral is divergent.

the singularity $\beta$. For this ratio to be a good indicator for the value of $\alpha$ (and hence the convergence/divergence of the integral), the shaded area should at least partially cover the lower half of the plot where $\alpha < -1$, which it does not.

A more reliable approach consists of comparing the computed *integral* in two successive intervals $[a, b]$ and $[a, (a + b)/2]$ or $[(a + b)/2, b]$. For the integrand in Equation 5.1, the integral in the left sub-interval $[0, h/2]$ is *larger* than that over the interval $[0, h]$ when $\alpha < -1$. For the integral in Equation 5.2 the ratio of the integrals in the intervals $[0, h]$ and $[0, h/2]$ is larger than 1 for *most* cases where $\alpha \leq -1$ (see Figure 5.3).

Although this relation (ratio $> 1 \Rightarrow \alpha < -1$), which is independent of the interval $h$, is not always correct, it can still be used as a statistical *hint* for the integrand's behavior during recursion. In the interval $-2 \leq \alpha \leq -1$ it is correct approximately two thirds of the time. We will therefore count the number of times that

$$\frac{Q_n[a, (a + b)/2]}{Q_n[a, b]} \geq 1 \quad \text{or} \quad \frac{Q_n[(a + b)/2, b]}{Q_n[a, b]} \geq 1 \tag{5.3}$$

during recursion. Note that since the integral tends to either $+\infty$ or $-\infty$,

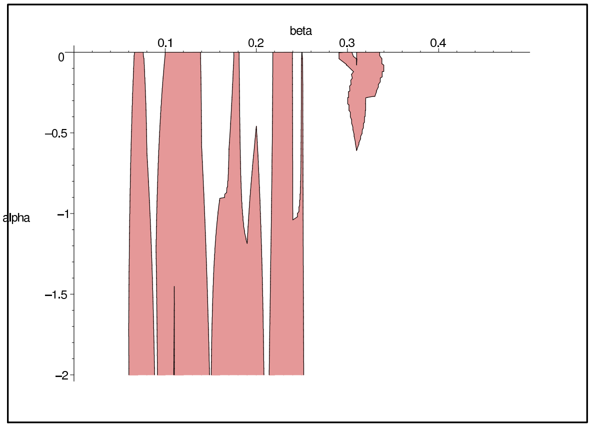


**Figure 5.2:** Contour of the ratio of the error estimates for $\int_0^h |x-\beta|^\alpha \,\mathrm{d}x$ over the intervals $[0,1]$ and $[0,1/2]$. The filled area represent the region in which this ratio is larger than 1.

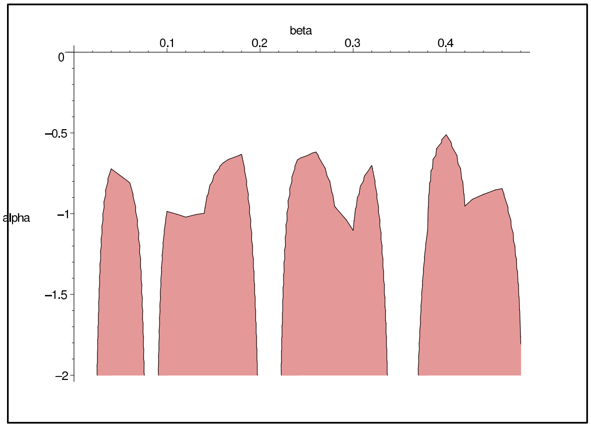


**Figure 5.3:** Contour of the ratio of the integral estimates for $\int_0^h |x-\beta|^\alpha \,\mathrm{d}x$ over the intervals $[0,1]$ and $[0,1/2]$. The filled area represent the region in which this ratio is larger than 1.

the integral approximations will be of the same sign and thus the sign of the ratios do not matter. If this count exceeds some maximum number and is more than half of the recursion depth – *i.e.* the ratio of integrals was larger than one over more than half of the subdivisions – then we declare the integral to be divergent and return an error or warning to the user to this effect.

This approach will not work for all types of divergent integrals. Consider the integral

$$\int_0^b \frac{\log(1/x)^{-1-\alpha}}{x}\,\mathrm{d}x \quad = \quad \frac{\log(1/b)^{-\alpha}}{\alpha}, \quad b < 1$$

which does not exist for $\alpha = 0$. As opposed to singularities of the type in Equation 5.2, however, the ratios in Equation 5.3 are all $< 1$ although the integral goes to $\infty$. Such singularities could, in theory, be caught by checking the convergence of the sequence of estimates

$$Q[0,h],\ Q[0,h/2],\ Q[0,h/4],\ \ldots$$

yet for each type of convergence test it would be possible to create families of integrals for which such a test would fail.

# Chapter 6

# The Quadrature Algorithms

## 6.1 Design Considerations

Although the main foci of this thesis are function representation (see Chapter 3), error estimation (see Chapter 4) and the treatment of singular or divergent integrals (see Chapter 5), there are a number of implementation details that have to be considered before implementing these new features in an adaptive quadrature algorithm.

In 1975, Rice [85] describes several common components of quadrature algorithms:

- "*Interval Processor Components*": The basic quadrature rule or set of rules and the associated error estimator,
- "*Bound Estimator Components*": Effectively the distribution of the global tolerance over the sub-intervals,
- "*Special Behaviour Components*": Possible detection of noise, discontinuities and singularities,
- "*Interval Collection Management Components*": The order in which intervals are processed,

Arguing that there are several different possibilities for the implementation of each component, he concludes that there are possibly "*1 to 10 million*" potentially interesting combinations thereof worth studying.

Since we want to test the new error estimates and the treatment of non-numerical values of the integrand and divergent integrals, we will not test the several million alternatives, but make some common design decision based both on published results and our own observations.

### 6.1.1 Recursive vs. Heap Structure

The main difference between the general Algorithms presented in Chapter 1, Algorithm 1 and Algorithm 2, is in the strategy they use to select the next interval for processing.

Rice calls this process the "*interval collection management component*" and specifies four types of such components:

- **Stack**: The intervals are generated and traversed *depth-first* from left to right (see Figure 6.1). This can be done either implicitly using recursion as in Algorithm 1 or explicitly as is done in McKeeman and Tesler's integrator (see Section 2.4).

- **Heap**: The intervals are sorted by decreasing error estimate and the interval with the largest error estimate is processed, as is done in Algorithm 2.

- **Queue**: A FIFO-queue of all intervals is maintained and processed in-order. This is equivalent to a *breadth-first* traversal of the intervals.

- **Boxes**: The intervals are grouped into boxes for different ranges of the error estimate. Intervals are selected as with the queue, yet no sorted structure is preserved.

The *stack* has the advantage that it is relatively simple to implement in programming environments where recursion is permitted and that it does not require that we store data for more intervals than the maximum recursion depth.

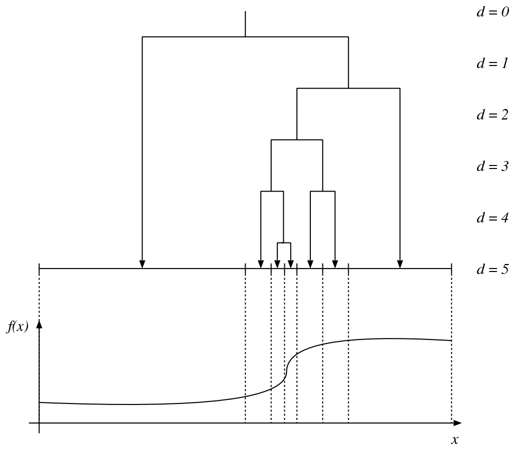


**Figure 6.1:** The intervals generated during adaptive quadrature.

It also has the disadvantage that during recursion, the algorithm must allocate a portion of the allowed total error to each interval. This is usually done by selecting a local tolerance $\tau_k$ such that

$$\tau_k = \tau \frac{b_k - a_k}{b - a} \quad \text{or} \quad \tau_k = \tau 2^{-d/2}.$$

In the former case, we can guarantee that the sum of the local errors will be below the global tolerance. In the latter case we guarantee that, when using bisection, the sum of the local errors will have the same *variance* as the global error (see Section 2.4). Different variations of how the local tolerance can be allocated can be found in O'Hara and Smith's integrator (see Section 2.8), Oliver's integrator (see Section 2.11), Garribba *et al.* 's integrator (see Section 2.13) or Ninomiya's integrator (see Section 2.15).

In Equation 2.8 and Equation 2.9 we saw how this could go wrong, causing the algorithm to fail to converge even for simple integrands. This problem is inherent to stack-based algorithms and can only be alleviated therein by using a less strict (or no) local tolerance such as is done by Patterson (see Section 2.12) or Gander and Gautschi (see Section 2.20). These approaches, however, do not guarantee that the sum of the error estimates will be below the global tolerance.

The *queue*, traverses the tree in Figure 6.1 *breadth-first* and requires only as much memory as the maximum number of intervals at any recursion level. In [92], Shapiro implements an adaptive quadrature based on Forsythe, Malcolm and Moler's `QUANC8` (see Section 2.7) using a queue and notes that whereas the stack, queue and heap all generate and traverse the same tree of intervals (see Figure 6.1), and therefore generate the same result, the queue generates better results than the stack when the number of allowed function evaluations is limited, *i.e.* when the algorithm is terminated before reaching the required tolerance, and is more efficient in terms of memory requirements and maintenance than the heap.

The queue, however, has the same problem as the stack in that we must also decide, at each recursion level, which intervals to discard. Although this decision can be made considering *all* the intervals at a given recursion depth, the allocation of error or tolerance is made nonetheless, which may cause the algorithm to fail to converge. Shapiro, for example, discards an interval only when the error estimate is less than the local tolerance

$$\tau_k = \tau \frac{b_k - a_k}{b - a}.$$

This is equivalent to the scaling of the local tolerance used by Kuncir (see Section 2.2) and by McKeeman (see Section 2.3) and thus, as with McKeeman's algorithm, the queue-based algorithm will *also* fail to converge for the left-most interval of the problems in Equation 2.8 and Equation 2.9. This problem arises whenever we have to discard an interval and can therefore only be avoided if we do not discard *any* intervals. This is essentially what both the *heap* and the *boxes* do. The only difference between the two is that the boxes sort the intervals with a larger granularity.

The main drawback of such an approach is of course that the heap or the boxes grow with every interval subdivision. The resulting memory requirements and the overhead to manage the heap or boxes make these approaches somewhat less attractive than the stack or queue. The first algorithm using a heap only appeared in 1973 (see Section 2.12), when computer memories were less restricted, making such an approach practicable.

The use of a heap was shown, in a direct comparison by Malcolm and Simpson [66], to be more efficient than the use of a stack since the error in intervals that may not have reached the local tolerance requirements used by the stack can be compensated for by intervals who's error estimates are well below the local requirements, thus requiring no further refinement.

For the algorithms presented herein, we will use, in principle, a heap to store the intervals and select the interval with the largest error estimate for further processing. To avoid the heap growing indefinitely, we will remove the following intervals:

- Intervals who's width no longer contains sufficient machine numbers such that the nodes of the quadrature are distinct,
- Intervals who's error estimate is smaller than the precision of the computation of the integral,
- The interval with the smallest error estimate if the heap exceeds a pre-determined size.

The first condition is detected when sub-dividing an integral by verifying that

$$\tilde{x}_0 < \tilde{x}_1 \quad \wedge \quad \tilde{x}_{n-1} < \tilde{x}_n, \quad \tilde{x}_i = \frac{a+b}{2} + \frac{b-a}{2} x_i, \quad x_i \in [-1, 1]$$

*i.e.* by verifying that the nodes of the quadrature rule in the integration interval $[a, b]$ are indeed distinct.

The second condition is verified by testing if

$$\varepsilon < |q| \, \mathrm{cond}(\mathbf{P}^{-1}) \, \varepsilon_{\mathsf{mach}}$$

where $\varepsilon_{\mathsf{mach}}$ is the machine epsilon, $\varepsilon$ and $q$ are the computed error estimate and integral respectively and $\mathbf{P}^{-1}$ is the inverse Vandermonde-like matrix used to compute the coefficients from which the integral is computed.

The final condition is verified by keeping tabs not only on the interval with the *largest* error estimate, but also on the interval with the *smallest*. If the heap grows beyond a maximum size, the interval with the smallest error is dropped.

In any case, every time an interval is dropped, its approximation to the integral and the integration error are stored in the excess variables $q_{\mathsf{xs}}$ and

$\varepsilon_{\mathsf{xs}}$ respectively. The total integral and error estimate are then computed as

$$q_{\mathsf{tot}} = \sum_{k \in H} q_k + q_{\mathsf{xs}}, \quad \varepsilon_{\mathsf{tot}} = \sum_{k \in H} \varepsilon_k + \varepsilon_{\mathsf{xs}}$$

where $\sum_{k \in H}$ is the summation over all elements of the heap. The algorithms terminate if either $\varepsilon_{\mathsf{tot}} < \tau$ or, if $\varepsilon_{\mathsf{xs}} > \tau$ and thus the required tolerance can not be achieved, if $\sum_k \varepsilon_k < \tau$.

Since we need to keep tabs of both the intervals with the minimum and maximum error estimate, we only maintain a heap *in principle*. In practice, we maintain an unsorted array of intervals which is searched linearly for the maximum and minimum elements in each iteration. This has the advantage that the sums in Equation 6.1.1 can be computed in every iteration, thus avoiding truncation and cancellation problems that would arise when updating $q_{\mathsf{tot}}$ and $\varepsilon_{\mathsf{tot}}$.

### 6.1.2 The Choice of the Basic Rule

Most of the algorithms presented in Chapter 2 differ principally in the type of basic quadrature rule (or rules) used to compute both the integral and the error approximation. The most commonly used types of rules are:

- **Newton-Cotes** quadrature rules with $x_i = -1 + 2i/n$, $i = 0 \dots n$,
- **Recursively Monotone Stable** (RMS) quadrature rules where the distances between the nodes are all integer multiples of the smallest distance and where all the nodes can be re-used after bisection,
- **Clenshaw-Curtis** type quadrature rules where the nodes are either the roots or the extrema of a Chebyshev polynomial in either $[-1, 1]$ or $(-1, 1)$,
- **Gauss** or **Gauss-Lobatto** quadrature rules and their **Kronrod** extensions where the nodes $x_i$, $i = 0 \dots n$ are the roots of the $n + 1$st orthogonal polynomial relative to some measure.

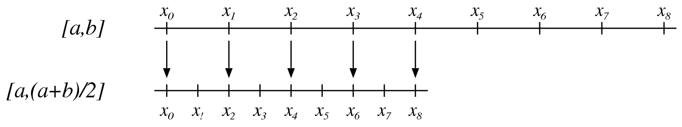

[a,b]
[a,(a+b)/2]
$x_0$ $x_1$ $x_2$ $x_3$ $x_4$ $x_5$ $x_6$ $x_7$ $x_8$
$x_0$ $x_1$ $x_2$ $x_3$ $x_4$ $x_5$ $x_6$ $x_7$ $x_8$

**Figure 6.2:** Re-use of nodes for a 9-point Newton Cotes rule after bisection.

The **Newton-Cotes rules** have the advantage that the nodes can easily be re-used after doubling $n$ or bisecting or otherwise sub-dividing the interval (see Figure 6.2).

The main disadvantage of Newton-Cotes rules is that they are numerically unstable: the 9-point Newton-Cotes quadrature rule and *all* rules with more than 11 nodes contain one or more negative weights, which can lead to cancellation when evaluating the quadrature rule. As the number of nodes $n$ grows, the condition number of the rule, as defined by Engels [17], grows to $\infty$:

$$\lim_{n\to\infty}\sum_{i=0}^{n}|w_i^{(n)}| = \infty.$$

Newton-Cotes rules are therefore only used in adaptive schemes for small $n$.

A compromise between the re-usability of the nodes and the condition number of the resulting rule is achieved with the **RMS rules** described by Favati *et al.* [26]. All the nodes of each RMS rule can be re-used after bisection (see Figure 6.3) or when increasing the multiplicity or degree of a rule within the same interval *and* the weights of the resulting quadrature rules are always positive and hence the rules are numerically stable.

Favati *et al.* identify 74 such rules for several odd $n$ up to $n = 249$. The rules can not be constructed on the fly and are generated by an exhaustive search and tabulated for latter use.

The **Clenshaw-Curtis type rules** were first introduced by Fejér in 1933 [28] and popularized by Clenshaw and Curtis in 1960 [10]. These rules

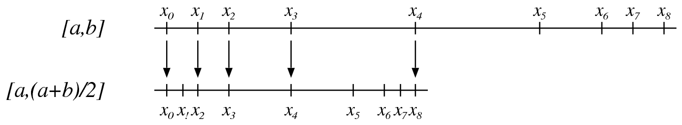


**Figure 6.3:** Re-use of nodes for a 9-point RMS rule after bisection.

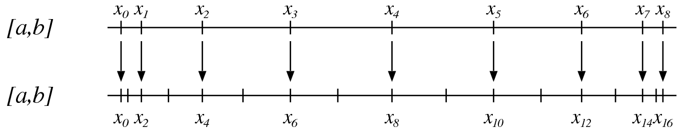


**Figure 6.4:** Re-use of nodes for a 9-point Clenshaw-Curtis rule in the 17-point Clenshaw-Curtis rule.

exist in three variants

$$\begin{aligned}
\text{Clenshaw-Curtis rule: } x_i &= -\cos\left(\frac{i\pi}{n}\right) \\
\text{Fejér's ``first rule'': } x_i &= -\cos\left(\frac{(i+1/2)\pi}{n+1}\right) \\
\text{Fejér's ``second rule'': } x_i &= -\cos\left(\frac{(i+1)\pi}{n+2}\right)
\end{aligned}$$

for $i = 0 \ldots n$. The quadrature rules, which are studied extensively in [75], all have positive weights and are numerically stable.

The weights of the Clenshaw-Curtis rules can be constructed efficiently using the Fast Fourier Transform [40, 101]. Although the nodes can generally not be re-used after bisection[1], the nodes can be re-used if the rule over $2n + 1$ points in the same interval is also computed (see Figure 6.4).

Finally, **Gauss quadrature rules**, which are used in most quadrature applications today, offer a degree of $2n + 1$ while requiring only $n + 1$ nodes. Although the nodes of the rules can not be re-used after bisection and are not part of any higher-degree Gauss quadrature rule, the rules can

[1]exceptions include the edge nodes in the Clenshaw-Curtis rule for even $n$ or the central nodes when $n$ is a multiple of 6.

be extended using Kronrod extensions [54], in which a Gauss quadrature rule over $n+1$ points is extended by $n+2$ points resulting in a quadrature rule of degree $3n+2$. The weights of the Gauss quadrature rules and those of their Kronrod extensions are always positive and thus the rules are numerically stable [39, Theorem 1.46].

The advantage in the degree of precision of Gauss quadrature rules over Clenshaw-Curtis quadrature rules is, however, as is shown by Trefethen in [95], does not translate into a corresponding advantage in the rate of convergence for functions which are not analytic in a large neighborhood around the interval of integration.

Since, in the algorithms presented here, we will not just evaluate a quadrature rule, but compute an interpolation, we are much more interested in the *interpolatory* characteristics of the nodes. In this vein, the nodes of Fejér's first rule are most interesting since given the interpolation error

$$f(x) - g_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x - x_i), \quad \xi \in [a,b] \tag{6.1}$$

for $f(x)$ $n+1$ times continuously differentiable in $[a,b]$, the nodes, which are the roots of the $n$th Chebyshev polynomial, *minimize the maximum* of the monic polynomial given by the product on the left hand side:

$$\prod_{i=0}^{n}(x - x_i) = \frac{1}{2^n}T_{n+1}(x).$$

The nodes of Fejér's first (and second) rule have one major disadvantage: the rules are "open" and thus the domain boundaries $\pm 1$ are not included in the quadrature rule. As seen in Section 4.3, certain features of the integrand near the boundaries could thus be missed. This is, of course, an advantage if we can not deal with singularities or non-numerical function values which often appear at the interval edges, but, as we will see later, we will deal with such problems differently.

For the nodes of the Clenshaw-Curtis quadrature rule, the polynomial in the interpolation error Equation 6.1 is no longer minimal, but can be represented as

$$C_n(x) = \prod_{i=0}^{n}\left(x - \cos\left(\frac{i\pi}{n}\right)\right) = \frac{1}{2^n}\left(T_{n+1}(x) - T_{n-1}(x)\right)$$

where $T_k(x)$ is the $k$th Chebyshev polynomial of the first kind[2]. Since for all Chebyshev polynomials, $T_k(x) \in [-1, 1]$ for all $k > 0$ and $x \in [-1, 1]$, this monic polynomial is *at most* twice as large as the one resulting from the nodes of Fejér's first rule

$$\prod_{i=0}^{n} \left( x - \cos\left( \frac{(i + 1/2)\pi}{n + 1} \right) \right) = \frac{1}{2^n} T_{n+1}(x).$$

The interpolation error over the nodes of the Clenshaw-Curtis rule therefore converges at the same *rate* as the error over the (optimal) nodes of Fejér's first rule.

For the nodes of the Gauss quadrature rule, the polynomial on the right hand side of Equation 6.1 is the monic $n + 1$st Legendre polynomial. Since the Legendre polynomials of degree $n \geq 1$ have a maximum of 1 at $x = 1$ and a leading coefficient $k_n = (2n!)/(2^n n!^2)$ [39, p. 27], the monic Legendre polynomials of degree $n \geq 1$ have a maximum value of $(2^n n!^2)/(2n!)$ at $x = 1$, which decays at a *slower* rate than do the maxima of the monic polynomials over the Fejér or Clenshaw-Curtis rules (see Figure 6.5).

[2] This can easily be shown by considering that $U_{n-1}(x)$, the Chebyshev polynomial of the second kind, has its roots at the nodes of Fejér's second rule. This rule can be extended to a Clenshaw-Curtis rule by adding the roots at $x = \pm 1$. The polynomial with the added roots can be written as

$$C_n(x) = (x + 1)(x - 1)U_{n-1}(x) = x^2 U_{n-1}(x) - U_{n-1}(x).$$

Using the relations

$$\begin{aligned} T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) \\ 2T_{n+1}(x) &= U_{n+1}(x) - U_{n-1}(x) \\ xU_n(x) &= U_{n+1}(x) - T_{n+1}(x) \end{aligned}$$

we can re-write $C_n(x)$ as

$$\begin{aligned} C_n(x) &= x(U_n(x) - T_n(x)) - U_{n-1}(x) \\ &= U_{n+1}(x) - U_{n-1}(x) - T_{n+1}(x) - xT_n(x) \\ &= T_{n+1}(x) - \frac{1}{2}(T_{n+1}(x) + T_{n-1}(x)) \\ &= \frac{1}{2}\left(T_{n+1}(x) - T_{n-1}(x)\right). \end{aligned}$$

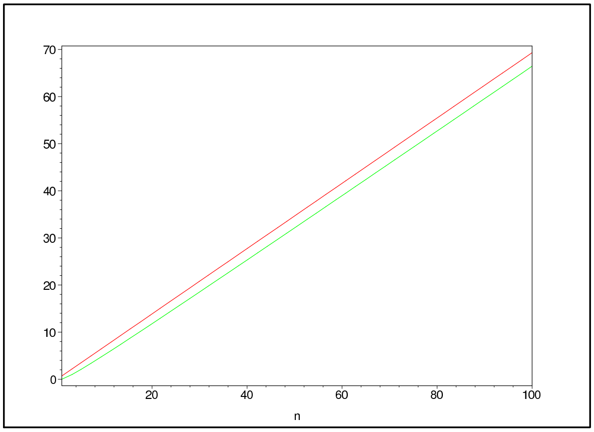


**Figure 6.5:** $-\ln$ of the maximum value of the $n$th monic Chebyshev (red) and Legendre (green) polynomials.

Finally, the interpolatory qualities of the equidistant nodes of the Newton-Cotes quadrature rules are undisputedly sub-optimal, as first noted by Runge in 1901 [89]. Henrici also shows in [44, Chapter 5.5] that the condition of the interpolation becomes exceedingly bad for large $n$ (*i.e.* small changes in the data may cause large changes in the interpolant) and Turetskii [97] (referenced in [96]) shows that the Lebesgue constant for an interpolation over the nodes of an $n+1$ point Newton-Cotes rule grows exponentially as

$$\Lambda_n \sim \frac{2^{n+1}}{n \log n}$$

for $n \to \infty$, *e.g.* that the norm of the difference between the constructed interpolation and the optimal interpolation grows exponentially with increasing $n$.

For the nodes of Clenshaw-Curtis type rules and the Gauss quadrature rules, the resulting Vandermonde-like matrix Equation 3.17 is well-conditioned even for large $n$ (see Figure 6.6). Therefore, for such cases, we do not need to apply any of the special algorithms described in Section 3.2 to compute the coordinates since, for a fixed set of nodes, we can pre-compute the inverse of the Vandermonde-like matrix and compute

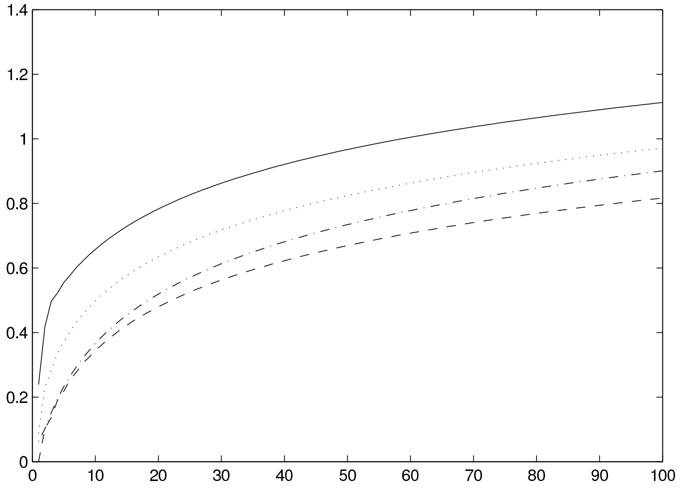


**Figure 6.6:** $\log_{10}$ of the condition number with respect to the 2-norm of the $(n+1) \times (n+1)$ Vandermonde-like matrix for the orthonormal Legendre polynomials over the nodes of the Clenshaw-Curtis rule (—), Fejér's first rule $(\cdots)$, Fejér's second rule (–·–) and the Gauss-Legendre quadrature rule (– –).

the coefficients, using the notation in Section 3.2, with

$$\mathbf{c} = \mathbf{P}^{-1}\mathbf{f}.$$

## 6.1.3 Handling Non-Numerical Function Values

Since most adaptive quadrature algorithms are designed for general-purpose use, they will often be confronted with integrands containing singularities or undefined values. As we have seen in Section 5.1, these function values can be removed from our interpolation of the integrand by *down-dating* the interpolation.

This is done as is shown in Algorithm 7. If, when evaluating the integrand, a non-numerical value is encountered, the function values is set to zero and the index of the node is stored in nans (Line 4). The coefficients of the interpolation are then computed for those function values (Line 6). For each index in nans, first the coefficients $\mathbf{b}$ of the Newton polynomial over the nodes of the quadrature rule are down-dated as per Equation 3.35 (Line 8) where the upper-triangular matrix $U_i^{-1}$ does not need to be inverted explicitly (see Algorithm 5). The downdated $\mathbf{b}$ is then in turn used to downdate the interpolation coefficients $\mathbf{c}$ as per Equation 3.36 (Line 9).

**Algorithm 7** Interpolation downdate procedure

```
 1: nans ← $\{\}$                                    (initialize nans)
 2: for $i = 0 \dots n$ do
 3:     $f_i \leftarrow f((a+b)/2 + x_i(b-a)/2)$    (evaluate the integrand at the nodes)
 4:     if $f_i \in \{\mathsf{NaN}, \mathsf{Inf}\}$ then $f_i \leftarrow 0$, nans ← nans $\cup \{i\}$ end if
          (if the result is non-numerical, set the node to zero and remember it)
 5: end for
 6: $\mathbf{c} \leftarrow \mathbf{P}^{-1}\mathbf{f}$            (compute the initial interpolation coefficients)
 7: for $i \in$ nans do
 8:     $\mathbf{b} \leftarrow \mathbf{U}_i^{-1}\mathbf{b}$        (downdate the coefficients of the Newton polynomial)
 9:     $\mathbf{c} \leftarrow \mathbf{c} - \frac{c_n}{b_n}\mathbf{b}$         (downdate the coefficients of the interpolation)
10:     $n \leftarrow n - 1$                                 (decrement the degree)
11: end for
```

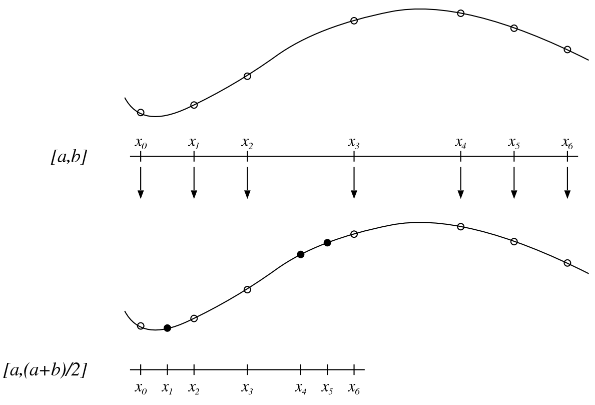

[a,b]
$x_0$ $x_1$ $x_2$ $x_3$ $x_4$ $x_5$ $x_6$
[a,(a+b)/2]
$x_0$ $x_1$ $x_2$ $x_3$ $x_4$ $x_5$ $x_6$

**Figure 6.7:** An interpolation is computed over the nodes of the quadrature rule in the interval $[a, b]$. After bisection, this interpolation is extended by the function values of the new nodes of the same rule in the sub-interval (filled dots).

## 6.2 An Adaptive Quadrature Algorithm using Interpolation Updates

The main idea behind this quadrature algorithm is that instead of applying a new quadrature rule in each interval, and thus ignoring information from previous intervals, we could simply *extend* the interpolation computed in the previous interval by *updating* the interpolation with new points inside the sub-interval, as shown in Figure 6.7.

For this algorithm we will use the 9-point RMS rule as described in [26] since for the $n + 1$ point rule we only need to evaluate an additional $n/2$ function values in each sub-interval. The interpolatory qualities of these nodes, while not optimal, are sufficiently good, since the polynomial in the right hand side of the interpolation error Equation 6.1 is at most $\sim 4$ times that of the optimal set of nodes. Finally, the condition number for the Vandermonde-like matrix for the orthonormal Legendre polynomials at the 9 RMS-nodes is only 8.46.

Given the coefficients $\mathbf{c}^{\mathsf{old}}$ and $\mathbf{b}^{\mathsf{old}}$ from the previous level of recursion as computed by Equation 4.30 (see Section 4.2), we can use Algorithm 4 to update the interpolation using the function values at the new nodes inside the sub-interval, resulting in the new coefficients $\mathbf{c}$ and $\mathbf{b}$ of degree $n/2$ higher than the original interpolation. Given these two approximations of different degree, we can compute the naive error estimate in Equation 4.20.

The interpolation update and the error estimate only make sense if the integrand is sufficiently smooth inside the entire interval from which the interpolation nodes are taken. This can not be tested in practice, but we can test that

$$\frac{\|\mathbf{c} - \mathbf{c}^{\mathsf{old}}\|}{\|\mathbf{c}\|} < \mathsf{hint} \tag{6.2}$$

*i.e.* that the change in the interpolation coefficients is relatively small when the degree is increased. This is analogous to the hint used by Venter and Laurie in [99]. If Equation 6.2 does *not* hold, we assume that the integrand is not sufficiently smooth and restart the interpolation using only the nodes and function values inside the current interval.

To avoid problems with loss of precision when updating the interpolation, we will also only allow the polynomial to grow up to a maximum degree $n_{\mathsf{max}}$. If the degree exceeds $n_{\mathsf{max}}$, we restart the interpolation using only the nodes and function values inside the current interval.

The entire algorithm is shown in Algorithm 8. In Line 1 the integrand is evaluated for the initial RMS rule and in Line 2 the initial interpolation coefficients are computed. The heap $H$ is initialized in Line 5 with this data and $\mathbf{b}_{\mathsf{def}}$, the pre-computed coefficients of the Newton polynomial over the nodes of the quadrature rule. While the sum of the error estimates in the heap is larger than the required tolerance $\tau$ (Line 7), the interval with the largest error estimate is popped from the heap (Lines 8 and 9). In each sub-interval, the coefficients of both the interpolation (Line 12) and the Newton polynomial (Line 13) are transformed to the sub-interval as described in Equation 3.3. The coefficients are then updated using the new nodes in the sub-interval as described in Section 3.2.1 (Lines 15 to 24), skipping non-numerical function values when encountered (Line 17). If the degree of the resulting interpolation is too high or the change in coefficients was too large, suggesting that the integrand is not sufficiently smooth, the interpolation is re-computed only on the nodes within the sub-interval (Lines 25 to 27). Note that we don't simply evaluate $\mathbf{c} = \mathbf{P}^{-1}\mathbf{f}$, but instead apply Algorithm 7. The estimates for the integral (Line 28) and the integration error (Line 29) are then computed and the algorithm tests for divergence of the integral (Lines 30 and 31). In Line 33, the new interval is returned to the heap unless its error is too small or the interval can no longer be sub-divided, in which case its estimates for the integral and error are stored in the excess variables $q_{\mathsf{xs}}$ and $\varepsilon_{\mathsf{xs}}$ and the interval is discarded (Line 35).

## 6.3 A Doubly-Adaptive Quadrature Algorithm using the Naive Error Estimate

In this algorithm we will use the naive error estimate described in Section 4.2 (Equation 4.20) within a doubly adaptive scheme. Although in Chapter 4 we observed that doubly-adaptive quadrature algorithms are only as good as the initial error estimates for the lowest-degree rule, we trust that our error estimate is sufficiently robust and will not cause the entire algorithm to fail.

In a scheme similar to that used in [99], we will compute interpolations over $n + 1$ and $2n + 1$ Clenshaw-Curtis nodes and use them to compute the naive error estimate in Equation 4.20. The interval is sub-divided, as in Algorithm 8, if the relative difference between the two approximations is larger than some value $\mathsf{hint}$ (see Equation 6.2) or if the degree $n$ has reached some maximum value. Otherwise, $n$ is doubled.

We use $d_{\mathsf{max}} + 1$ rules of degree $n_i = 2n_{i-1}$ starting at some initial degree $n_0$ The interpolations are computed using the pre-computed inverse Vandermonde-like matrices $(\mathbf{P}^{(i)})^{-1}$, $i = 0 \dots d_{\mathsf{max}}$.

The algorithm is shown in Algorithm 9. In Lines 1 to 4, the coefficients of the two highest-degree rules are computed and used to approximate the initial integral and error estimate. In Line 5 the heap $H$ is initialized with this interval data. The algorithm then loops until the sum of the errors over all the intervals is below the required tolerance (Line 7). At the top of the loop, the interval with the largest error is selected (Line 8). If the error in this interval is below the numerical accuracy available for the rule used or the interval is too small (*i.e.* the space between the first two or last two nodes is zeros, Line 11), the interval is dropped and its

**Algorithm 8** int_update $(f, a, b, \tau)$

```
1: for $i = 0 \dots n_{\mathsf{init}}$ do $f_i \leftarrow f\left((a+b)/2 - x_i(a-b)/2\right)$ end for
                                   ($evaluate the integrand at the nodes x_i$)
2: $\mathbf{c} \leftarrow \mathbf{P}^{-1}\mathbf{f}$                    (compute the interpolation coefficients)
3: $q_0 \leftarrow (b-a)c_0/\sqrt{2}$                    (approximate the integral)
4: $\varepsilon_0 \leftarrow \infty$                    (start with a pessimistic error estimate)
5: $H \leftarrow \{[a, b, \mathbf{c}, \mathbf{b}_{\mathsf{def}}, q_0, \varepsilon_0, n_{\mathsf{init}}, 0]\}$                    (init the heap with the first interval)
6: $\varepsilon_{\mathsf{xs}} \leftarrow 0,\ q_{\mathsf{xs}} \leftarrow 0$                    (init the excess error and integral)
7: while $\sum_{\varepsilon_i \in H} \varepsilon_i > \tau$ do
8:     $k \leftarrow \arg\max_k \varepsilon_k$                    (get the index of the interval with the largest error)
9:     $H \leftarrow H \setminus \{[a_k, b_k, \mathbf{c}^{\mathsf{old}}, \mathbf{b}^{\mathsf{old}}, n_{\mathsf{old}}, q_k, \varepsilon_k, n_{\mathsf{div}}^{\mathsf{old}}]\}$                    (remove the kth interval)
10:    $h \leftarrow (b_k - a_k)/2,\ m \leftarrow (b_k + a_k)/2$                    (get the interval dimensions)
11:    for $\mathsf{half} \in \{\mathsf{left}, \mathsf{right}\}$ do
12:        $\mathbf{c}_{\mathsf{old}}^{\mathsf{half}} = \mathbf{T}^{\mathsf{half}}\mathbf{c}^{\mathsf{old}},\ \mathbf{c}_{\mathsf{half}} \leftarrow \mathbf{c}_{\mathsf{old}}^{\mathsf{half}}$                    (transform c from the previous level)
13:        $\mathbf{b}_{\mathsf{old}}^{\mathsf{half}} = \mathbf{T}^{\mathsf{half}}\mathbf{b}^{\mathsf{old}},\ \mathbf{b}_{\mathsf{half}} \leftarrow \mathbf{b}_{\mathsf{old}}^{\mathsf{half}}$                    (transform b from the previous level)
14:        $n_{\mathsf{half}} \leftarrow n_{\mathsf{old}}$                    (inherit the degree of the previous level)
15:        for $i = 1 \dots n_{\mathsf{init}}/2$ do
16:            $f_i \leftarrow f(m + h x_i^{\mathsf{half}})$                    (evaluate the integrand)
17:            if $f_i \notin \{\mathsf{NaN}, \pm\mathsf{Inf}\}$ then
18:                $v_0 \leftarrow 1, v_1 \leftarrow x_i^{\mathsf{half}}$                    (evaluate the polynomials at $x_i^{\mathsf{half}}$)
19:                for $j = 1 \dots n_{\mathsf{half}}$ do $v_j \leftarrow (x_i^{\mathsf{half}} - \beta_j)v_{j-1} - \gamma_j v_{j-2}$ end for
20:                $\mathbf{c}_{\mathsf{half}} \leftarrow \mathbf{c}_{\mathsf{half}} + \frac{\mathbf{v}^{\mathsf{T}}\mathbf{c}_{\mathsf{half}} - f_i}{\mathbf{v}^{\mathsf{T}}\mathbf{b}_{\mathsf{half}}}\mathbf{b}_{\mathsf{half}}$                    (update c as per Equation 3.33)
21:                $\mathbf{b}_{\mathsf{half}} \leftarrow (\mathbf{T} - \underline{\mathbf{I}}x_i^{\mathsf{half}})\mathbf{b}_{\mathsf{half}}$                    (update b as per Equation 3.34)
22:                $n_{\mathsf{half}} \leftarrow n_{\mathsf{half}} + 1$                    (increase the degree)
23:            end if
24:        end for
25:        if $n_{\mathsf{half}} > n_{\mathsf{max}} \vee \frac{\|\mathbf{c}_{\mathsf{half}} - \mathbf{c}_{\mathsf{old}}\|}{\|\mathbf{c}_{\mathsf{half}}\|} > \mathsf{hint}$ then
26:            $\mathbf{c}_{\mathsf{half}} \leftarrow \mathbf{P}^{-1}\mathbf{f}_{\mathsf{half}},\ \mathbf{b}_{\mathsf{half}} \leftarrow \mathbf{b}_{\mathsf{def}},\ n_{\mathsf{half}} \leftarrow n_{\mathsf{init}}$                    (reset the interpolation)
27:        end if
28:        $q_{\mathsf{half}} \leftarrow h c_0^{\mathsf{half}}/\sqrt{2}$                    (approximate the new integral)
29:        $\varepsilon_{\mathsf{half}} \leftarrow h\|\mathbf{c}_{\mathsf{half}} - \mathbf{c}_{\mathsf{old}}\|$                    (approximate the new error)
30:        if $q_{\mathsf{half}} \geq q_k^{(0)}$ then $n_{\mathsf{div}}^{\mathsf{half}} \leftarrow n_{\mathsf{div}}^{\mathsf{old}} + 1$ else $n_{\mathsf{div}}^{\mathsf{half}} \leftarrow n_{\mathsf{div}}^{\mathsf{old}}$ end if
31:        if $n_{\mathsf{div}}^{\mathsf{half}} > n_{\mathsf{divmax}} \wedge 2n_{\mathsf{div}}^{\mathsf{half}} > \text{rec. depth}$ then return error end if
                                   (abort on divergence)
32:        if $\varepsilon_k < |q_k|\varepsilon_{\mathsf{mach}}\mathrm{cond}(\mathbf{P}) \vee \text{interval too small}$ then
33:            $H \leftarrow H \cup \{[a_{k+1}, b_{k+1}, \mathbf{c}_{\mathsf{half}}, \mathbf{b}_{\mathsf{half}}, q_{\mathsf{half}}, \varepsilon_{\mathsf{half}}, n_{\mathsf{div}}^{\mathsf{half}}]\}$
                                   (push the new interval back on the heap)
34:        else
35:            $\varepsilon_{\mathsf{xs}} \leftarrow \varepsilon_{\mathsf{xs}} + \varepsilon_k,\ q_{\mathsf{xs}} \leftarrow q_{\mathsf{xs}} + q_k$                    (collect the excess error and integral)
36:        end if
37:    end for
38: end while
39: return $q_{\mathsf{xs}} + \sum_{q_i \in H} q_i,\ \varepsilon_{\mathsf{xs}} + \sum_{\varepsilon_i \in H} \varepsilon_i$                    (return the integral and the error)
```

**Algorithm 9** int_naive $(f, a, b, \tau)$

```
1: for $i = 0 \dots n_{d_{\mathsf{max}}}$ do $f_i \leftarrow f\left((a+b)/2 - (a-b)x_i^{(m)}/2\right)$ end for
                                  ($\textit{evaluate the integrand at the nodes}$ $x_i^{(m)}$)
2: $\mathbf{c}^{(d_{\mathsf{max}}-1)} \leftarrow (\mathbf{P}^{(d_{\mathsf{max}}-1)})^{-1}\mathbf{f}[1:2:n_m+1]$, $\mathbf{c}^{(d_{\mathsf{max}})} \leftarrow (\mathbf{P}^{(d_{\mathsf{max}})})^{-1}\mathbf{f}$
                                  (compute the interpolation coefficients)
3: $q_0 \leftarrow (b-a)c_0^{(d_{\mathsf{max}})}/\sqrt{2}$          (approximate the integral)
4: $\varepsilon_0 \leftarrow (b-a)\|\mathbf{c}^{(d_{\mathsf{max}})} - \mathbf{c}^{(d_{\mathsf{max}}-1)}\|$          (approximate the error)
5: $H \leftarrow \{[a, b, \mathbf{c}^{(d_{\mathsf{max}})}, q_0, \varepsilon_0, d_{\mathsf{max}}, 0]\}$          (init the heap with the first interval)
6: $\varepsilon_{\mathsf{xs}} \leftarrow 0$, $q_{\mathsf{xs}} \leftarrow 0$          (init the excess error and integral)
7: while $\sum_{\varepsilon_i \in H} \varepsilon_i > \tau$ do
8:     $k \leftarrow \arg\max_k \varepsilon_k$          (get the index of the interval with the largest error)
9:     $m \leftarrow (a+b)/2$, $h \leftarrow (b-a)/2$          (get dimensions of the interval)
10:    split $\leftarrow$ false          (init split)
11:    if $\varepsilon_k < |q_k|\varepsilon_{\mathsf{mach}}\mathrm{cond}(\mathbf{P}^{(d_k)}) \vee$ interval too small then
12:        $\varepsilon_{\mathsf{xs}} \leftarrow \varepsilon_{\mathsf{xs}} + \varepsilon_k$, $q_{\mathsf{xs}} \leftarrow q_{\mathsf{xs}} + q_k$          (collect the excess error and integral)
13:        $H \leftarrow H \setminus \{[a_k, b_k, \mathbf{c}^{\mathsf{old}}, q_k, \varepsilon_k, d_k]\}$          (remove the $k$th interval)
14:    else if $d_k < d_{\mathsf{max}}$ then
15:        $d_k \leftarrow d_k + 1$          (increase the degree in this interval)
16:        for $i = 0 \dots n_{d_k}$ do $f_i \leftarrow f(m + hx_i^{(d_k)}/2)$ end for
                                  (evaluate the integrand at the nodes $x_i^{(d_k)}$)
17:        $\mathbf{c}^{(d_k)} = (\mathbf{P}^{(d_k)})^{-1}\mathbf{f}$          (compute the new interpolation coefficients)
18:        $q_k \leftarrow (b_k - a_k)c_0^{(d_k)}/\sqrt{2}$          (approximate the new integral)
19:        $\varepsilon_k \leftarrow (b_k - a_k)\|\mathbf{c}^{(d_k)} - \mathbf{c}^{\mathsf{old}}\|$          (approximate the new error)
20:        split $\leftarrow \frac{\|\mathbf{c}^{(d_k)} - \mathbf{c}^{\mathsf{old}}\|}{\|\mathbf{c}^{(d_k)}\|} >$ hint          (check change in the coefficients)
21:    else
22:        split $\leftarrow$ true          (split the interval if we are already at highest-degree rule)
23:    end if
24:    if split then
25:        $H \leftarrow H \setminus \{[a_k, b_k, \mathbf{c}^{\mathsf{old}}, q_k, \varepsilon_k, d_k, n_{\mathsf{div}}^{\mathsf{old}}]\}$          (remove the $k$th interval)
26:        for $i = 0 \dots n_0$ do
27:            $f_i^{\mathsf{left}} \leftarrow f\left((a+m)/2 + hx_i^{(0)}/2\right)$, $f_i^{\mathsf{right}} \leftarrow f\left((m+b)/2 + hx_i^{(0)}/2\right)$
                      (evaluate the integrand at the nodes $x_i^0$ in the sub-intervals)
28:        end for
29:        for half $\in$ {left, right} do
30:            $\mathbf{c}^{\mathsf{half}} = (\mathbf{P}^{(0)})^{-1}\mathbf{f}^{\mathsf{half}}$          (compute the new interpolation coefficients)
31:            $q_{\mathsf{half}} \leftarrow hc_0^{\mathsf{half}}/\sqrt{2}$          (approximate the new integral)
32:            if $q_{\mathsf{half}} \geq q_k^{(0)}$ then $n_{\mathsf{div}}^{\mathsf{half}} \leftarrow n_{\mathsf{div}}^{\mathsf{old}} + 1$ else $n_{\mathsf{div}}^{\mathsf{half}} \leftarrow n_{\mathsf{div}}^{\mathsf{old}}$ end if
33:            if $n_{\mathsf{div}}^{\mathsf{half}} > n_{\mathsf{divmax}} \wedge 2n_{\mathsf{div}}^{\mathsf{half}} >$ rec. depth then return error end if
                                  (abort on divergence)
34:            $\varepsilon_{\mathsf{half}} \leftarrow h\|\mathbf{c}^{\mathsf{half}} - \mathbf{T}^{\mathsf{half}}\mathbf{c}^{\mathsf{old}}\|$          (approximate the new error)
35:        end for
36:        $H \leftarrow H \cup \{[a_k, m, \mathbf{c}^{\mathsf{left}}, q_{\mathsf{left}}, \varepsilon_{\mathsf{left}}, 0, n_{\mathsf{div}}^{\mathsf{left}}], [m, b_k, \mathbf{c}^{\mathsf{right}}, q_{\mathsf{right}}, \varepsilon_{\mathsf{right}}, 0, n_{\mathsf{div}}^{\mathsf{right}}]\}$
                                  (push the new intervals back on the heap)
37:    end if
38: end while
39: return $q_{\mathsf{xs}} + \sum_{q_i \in H} q_i$, $\varepsilon_{\mathsf{xs}} + \sum_{\varepsilon_i \in H} \varepsilon_i$          (return the integral and the error)
```

error and integral are accumulated in the excess variables $\varepsilon_{\mathsf{xs}}$ and $q_{\mathsf{xs}}$ (Line 12). If the selected interval has not already used the highest-degree rule (Line 14), the coefficients of the next-higher degree rule are computed and the integral and error estimate are updated (Lines 15 to 19). The interval is bisected if either the highest-degree rule has already been applied or if when increasing the degree of the rule the coefficients change too much (Line 20). For the two new sub-intervals, the coefficients for the lowest-degree rule are computed (Line 30) and used to approximate the integral (Line 31). The number of times the integral increases over the sub-interval is counted in the variables $n_{\mathsf{div}}$ (Line 32) and if they exceed $n_{\mathsf{divmax}}$ and half of the recursion depth of that interval, the algorithm aborts (Line 33) as per Section 5.1. Note that since the test in Equation 4.28 requires that both estimates be of the same degree, we will use, for the estimate $q_k^{(0)}$ from the parent interval, the estimate which was computed for the 0th rule. The error estimate for the new interval is computed by transforming the interpolation coefficients from the parent interval using Equation 3.3 and using its difference to the interpolation in the new interval (Line 34). When the sum of the errors falls below the required tolerance, the algorithm returns its approximations to the integral and the integration error (Line 39).

## 6.4 An Adaptive Quadrature Algorithm using the Refined Error Estimate

In this algorithm, we will use the refined error estimate from Section 4.2, Equation 4.27. The error estimate is computed from the transformed coefficients from the previous level of recursion and the coefficients computed in the current interval. Since both interpolations are of the same degree, $\varepsilon_2$ from Equation 4.27 can be computed.

We use the Clenshaw-Curtis quadrature rules since they are closed (*i.e.* the end-points are included) and have good interpolation properties as described in Section 6.1.2.

The algorithm is shown in Algorithm 10. In Lines 1 to 5 an initial estimate is computed and used to initialize the heap $H$. The error estimate is set to $\infty$ since it can not be estimated (Line 4). While the sum of error estimates is below the required tolerance, the algorithm selects the

**Algorithm 10** int_refined $(f, a, b, \tau)$

```
1: for $i = 0 \dots n$ do $f_i \leftarrow f\left((a+b)/2 + x_i(b-a)/2\right)$ end for
                                   (evaluate the integrand at the nodes $x_i$)
2: $\mathbf{c} \leftarrow \mathbf{P}^{-1}\mathbf{f}$,
                                   (compute the interpolation coefficients)
3: $q_0 \leftarrow (b-a)c_0^{(d_{\mathsf{max}})}/\sqrt{2}$          (approximate the integral)
4: $\varepsilon_0 \leftarrow \infty$          (start with a somewhat negative appreciation of the error)
5: $H \leftarrow \{[a, b, \mathbf{c}, \mathbf{b}, 0, q_0, \varepsilon_0, 0]\}$          (init the heap with the first interval)
6: $\varepsilon_{\mathsf{xs}} \leftarrow 0,\ q_{\mathsf{xs}} \leftarrow 0$          (init the excess error and integral)
7: while $\sum_{\varepsilon_i \in H} \varepsilon_i > \tau$ do
8:     $k \leftarrow \arg\max_k \varepsilon_k$          (get the index of the interval with the largest error)
9:     $H \leftarrow H \setminus \{[a_k, b_k, \mathbf{c}^{\mathsf{old}}, \mathbf{b}^{\mathsf{old}}, f_{\mathsf{old}}^{(n+1)}, q_k, \varepsilon_k, n_{\mathsf{div}}^{\mathsf{old}}]\}$          (remove the kth interval)
10:    if $\varepsilon_k < |q_k|\varepsilon_{\mathsf{mach}}\mathrm{cond}(\mathbf{P}) \vee$ interval too small then
11:        $\varepsilon_{\mathsf{xs}} \leftarrow \varepsilon_{\mathsf{xs}} + \varepsilon_k,\ q_{\mathsf{xs}} \leftarrow q_{\mathsf{xs}} + q_k$          (collect the excess error and integral)
12:    else
13:        $m \leftarrow (a+b)/2,\ h \leftarrow (b-a)/2$
14:        for $i = 0 \dots n$ do
15:            $f_i^{\mathsf{left}} \leftarrow f\left((a+m)/2 + hx_i/2\right),\ f_i^{\mathsf{right}} \leftarrow f\left((m+b)/2 + hx_i/2\right)$
                                   (evaluate the integrand at the nodes $x_i$ in the sub-intervals)
16:        end for
17:        for half $\in$ {left, right} do
18:            $\mathbf{c}^{\mathsf{half}} = (\mathbf{P})^{-1}\mathbf{f}^{\mathsf{half}}$          (compute the new interpolation coefficients)
19:            $q_{\mathsf{half}} \leftarrow hc_0^{\mathsf{half}}/\sqrt{2}$          (approximate the new integral)
20:            if $q_{\mathsf{half}} \geq q_k$ then $n_{\mathsf{div}}^{\mathsf{half}} \leftarrow n_{\mathsf{div}}^{\mathsf{old}} + 1$ else $n_{\mathsf{div}}^{\mathsf{half}} \leftarrow n_{\mathsf{div}}^{\mathsf{old}}$ end if
21:            if $n_{\mathsf{div}}^{\mathsf{half}} > n_{\mathsf{divmax}} \wedge 2n_{\mathsf{div}}^{\mathsf{half}} >$ rec. depth then return error end if
                                   (abort on divergence)
22:            $f_{\mathsf{half}}^{(n+1)} \leftarrow \frac{\|\mathbf{c}^{\mathsf{half}} - \mathbf{T}^{(\mathsf{half})}\mathbf{c}^{\mathsf{old}}\|}{\|\mathbf{b}^{\mathsf{half}} - \mathbf{T}^{(\mathsf{half})}\mathbf{b}^{\mathsf{old}}\|}$          (approximate the higher derivative)
23:            if $\max\left\{\left|\mathbf{P}\mathbf{c}^{\mathsf{old}} - \mathbf{f}^{\mathsf{half}}\right| - \vartheta_1 f_{\mathsf{half}}^{(n+1)}\left|\mathbf{P}\mathbf{b}^{\mathsf{old}}\right|\right\} > 0$ then
24:                $\varepsilon_{\mathsf{half}} \leftarrow h\|\mathbf{c}^{\mathsf{half}} - \mathbf{c}^{\mathsf{old}}\|$          (compute the un-scaled error)
25:            else
26:                $\varepsilon_{\mathsf{half}} \leftarrow hf_{\mathsf{half}}^{(n+1)}\|\mathbf{b}^{\mathsf{half}}\|$
                                   (compute the extrapolated error (Equation 4.31))
27:            end if
28:        end for
29:        $H \leftarrow H \cup \{[a_k, m, \mathbf{c}^{\mathsf{left}}, \mathbf{b}^{\mathsf{left}}, f_{\mathsf{left}}^{(n+1)}, q_{\mathsf{left}}, \varepsilon_{\mathsf{left}}, n_{\mathsf{div}}^{\mathsf{left}}], \dots$
                   $[m, b_k, \mathbf{c}^{\mathsf{right}}, \mathbf{b}^{\mathsf{right}}, f_{\mathsf{right}}^{(n+1)}, q_{\mathsf{right}}, \varepsilon_{\mathsf{right}}, n_{\mathsf{div}}^{\mathsf{left}}]\}$
                                   (push the new intervals back on the heap)
30:    end if
31: end while
32: return $q_{\mathsf{xs}} + \sum_{q_i \in H} q_i, \varepsilon_{\mathsf{xs}} + \sum_{\varepsilon_i \in H} \varepsilon_i$          (return the integral and the error)
```

interval with the largest error estimate (Line 8) and removes it from the heap (Line 9). As with the previous algorithm, if the error estimate is smaller than the numerical precision of the integral or the interval is too small, the interval is dropped (Line 10) and its error and integral estimates stored in the excess variables $\varepsilon_{\mathsf{xs}}$ and $q_{\mathsf{xs}}$ (Line 11). The algorithm then computes the new coefficients for each sub-intervals (Line 18), as well as their integral approximation (Line 19). If the integral over the sub-interval is larger than over the previous interval, the variable $n_{\mathsf{div}}$ is increased (Line 20) and if it exceeds $n_{\mathsf{divmax}}$ and half of the recursion depth, the algorithm aborts with an error (Line 21). In Line 23 the algorithm tests whether the conditions laid out in Equation 4.28 for the approximation of the $n+1$st derivative hold. If they do not, the un-scaled error estimate is returned (Line 24), otherwise, the scaled estimate is returned (Line 26). Finally, both sub-intervals are returned to the heap (Line 29). Once the required tolerance is met, the algorithm returns its approximations to the integral and the integration error (Line 32).

## 6.5 Numerical Tests

In the following, we will test the three algorithms described in earlier against the following routines:

- `quadl`, MATLAB's adaptive quadrature routine [67], based on Gander and Gautschi's `adaptlob` (see Section 2.20). This algorithm uses a 4-point Gauss-Lobatto quadrature rule and its 7-point Kronrod extension.

- `DQAGS`, QUADPACK's [83] adaptive quadrature routine based on de Doncker's adaptive extrapolation algorithm (see Section 2.14) using a 10-point Gauss quadrature rule and its 21-point Kronrod extension as well as the $\epsilon$-Algorithm to extrapolate the integral and error estimate. The routine is called through the GNU Octave [16] package's `quad` routine.

- `da2glob` from [24], which uses a doubly-adaptive strategy over Newton-Cotes rules of degree 5, 9, 17 and 27 using the null rule error estimator described in Section 2.19.

| | `quadl` | | | `DQAGS` | | | `da2glob` | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ |
| Eqn (6.3) | 406 (1) | 594 | 95 | 926 | 74 | 454 | 977 | 23 | 95 |
| Eqn (6.4) | 894 | 106 | 117 | 959 | 41 | 398 | 1000 | 0 | 59 |
| Eqn (6.5) | 868 | 132 | 45 | 998 | 2 | 179 | 1000 | 0 | 29 |
| Eqn (6.6) | 359 | 641 | 89 | 782 | 218 (49) | 482 | 882 | 118 | 136 |
| Eqn (6.7) | 303 | 697 | 308 | 969 | 31 (4) | 1692 | 997 | 3 | 480 |
| Eqn (6.8) | 994 | 6 | 746 | 1000 | 0 | 446 | 1000 | 0 | 523 |

| | Algorithm 10 | | | Algorithm 9 | | | Algorithm 8 | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ |
| Eqn (6.3) | 1000 | 0 | 358 | 1000 | 0 | 280 | 990 | 10 | 211 |
| Eqn (6.4) | 1000 | 0 | 308 | 1000 (1) | 0 | 175 | 1000 | 0 | 188 |
| Eqn (6.5) | 1000 | 0 | 100 | 1000 | 0 | 112 | 1000 | 0 | 67 |
| Eqn (6.6) | 1000 | 0 | 500 | 1000 | 0 | 342 | 1000 | 0 | 283 |
| Eqn (6.7) | 1000 | 0 | 1431 | 997 | 3 | 976 | 989 | 11 | 820 |
| Eqn (6.8) | 1000 | 0 | 685 | 1000 | 0 | 873 | 1000 | 0 | 562 |

**Table 6.1:** Results of the Lyness-Kaganove tests for $\tau = 10^{-3}$.

| | `quadl` | | | `DQAGS` | | | `da2glob` | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ |
| Eqn (6.3) | 398 | 602 | 368 | 908 | 92 | 1093 | 993 (7) | 7 | 298 |
| Eqn (6.4) | 886 | 114 | 236 | 915 | 85 | 788 | 1000 | 0 | 100 |
| Eqn (6.5) | 770 | 230 | 103 | 985 | 15 | 365 | 1000 | 0 | 58 |
| Eqn (6.6) | 992 | 8 | 481 | 925 (1) | 75 (75) | 700 | 1000 | 0 | 290 |
| Eqn (6.7) | 982 | 18 | 1297 | 998 | 2 (2) | 2031 | 1000 | 0 | 870 |
| Eqn (6.8) | 998 | 2 (2) | 2029 | 1000 | 0 | 577 | 1000 (1) | 0 | 695 |

| | Algorithm 10 | | | Algorithm 9 | | | Algorithm 8 | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ | ✓ | ✗ | $n_{\mathsf{eval}}$ |
| Eqn (6.3) | 1000 | 0 | 993 | 1000 | 0 | 866 | 1000 | 0 | 684 |
| Eqn (6.4) | 1000 | 0 | 627 | 1000 | 0 | 315 | 1000 | 0 | 414 |
| Eqn (6.5) | 1000 | 0 | 256 | 1000 | 0 | 313 | 1000 | 0 | 205 |
| Eqn (6.6) | 1000 | 0 | 766 | 1000 | 0 | 614 | 1000 | 0 | 488 |
| Eqn (6.7) | 1000 | 0 | 2258 | 1000 | 0 | 1811 | 1000 | 0 | 1483 |
| Eqn (6.8) | 1000 | 0 | 1188 | 1000 | 0 | 1196 | 1000 | 0 | 906 |

**Table 6.2:** Results of the Lyness-Kaganove tests for $\tau = 10^{-6}$.

| | quadl | | | DQAGS | | | da2glob | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ |
| Eqn (6.3) | 367 | 633 (31) | 1051 | 748 (68) | 252 (151) | 1784 | 874 (222) | 126 (125) | 627 |
| Eqn (6.4) | 886 | 114 | 356 | 869 | 131 (4) | 1167 | 1000 | 0 | 141 |
| Eqn (6.5) | 780 | 220 | 184 | 979 | 21 | 567 | 1000 | 0 | 93 |
| Eqn (6.6) | 999 | 1 | 1211 | 924 | 76 (76) | 824 | 1000 | 0 | 474 |
| Eqn (6.7) | 998 | 2 | 3336 | 998 | 2 (2) | 2449 | 1000 | 0 | 1431 |
| Eqn (6.8) | 959 | 41 (41) | 5186 | 1000 (2) | 0 | 737 | 998 (63) | 2 (2) | 799 |

| | Algorithm 10 | | | Algorithm 9 | | | Algorithm 8 | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ |
| Eqn (6.3) | 900 (154) | 100 (100) | 2005 | 910 (26) | 90 (88) | 1849 | 916 (155) | 84 (84) | 1487 |
| Eqn (6.4) | 1000 | 0 | 946 | 1000 | 0 | 460 | 1000 | 0 | 725 |
| Eqn (6.5) | 1000 | 0 | 415 | 1000 | 0 | 520 | 1000 | 0 | 407 |
| Eqn (6.6) | 1000 | 0 | 1294 | 1000 | 0 | 1077 | 1000 | 0 | 898 |
| Eqn (6.7) | 1000 | 0 | 3853 | 1000 | 0 | 3254 | 1000 | 0 | 2730 |
| Eqn (6.8) | 1000 (3) | 0 | 2025 | 1000 (2) | 0 | 1393 | 1000 (6) | 0 | 1480 |

**Table 6.3:** Results of the Lyness-Kaganove tests for $\tau = 10^{-9}$.

| | `quadl` | | | `DQAGS` | | | `da2glob` | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ |
| Eqn (6.3) | 261 | 739 (375) | 2843 | 473 (110) | 527 (493) | 2632 | 494 (267) | 506 (506) | 1068 |
| Eqn (6.4) | 879 (1) | 121 | 488.10 | 828 (4) | 172 (23) | 1533.59 | 1000 (2) | 0 | 184 |
| Eqn (6.5) | 795 | 205 | 315 | 962 | 38 | 766 | 1000 | 0 | 133 |
| Eqn (6.6) | 928 | 72 | 3217 | 866 | 134 (76) | 995 | 996 (765) | 4 (4) | 710 |
| Eqn (6.7) | 741 | 259 (259) | 8697 | 998 | 2 (2) | 2988 | 1000 (849) | 0 | 2068 |
| Eqn (6.8) | 249 | 751 (751) | 9601 | 962 (546) | 38 (38) | 1213 | 548 (548) | 452 (452) | 894 |

| | Algorithm 10 | | | Algorithm 9 | | | Algorithm 8 | | |
|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ | ✓ | ✗ | $n_{\text{eval}}$ |
| Eqn (6.3) | 566 (165) | 434 (434) | 9016 | 568 (103) | 432 (432) | 8593 | 601 (216) | 399 (399) | 2716 |
| Eqn (6.4) | 1000 (4) | 0 | 1264 | 1000 | 0 | 606 | 1000 (9) | 0 | 1140 |
| Eqn (6.5) | 1000 | 0 | 574 | 1000 | 0 | 736 | 1000 (2) | 0 | 650 |
| Eqn (6.6) | 1000 (596) | 0 | 10547 | 1000 (426) | 0 | 18000 | 1000 | 0 | 1608 |
| Eqn (6.7) | 1000 (382) | 0 | 9267 | 1000 (326) | 0 | 12835 | 1000 (12) | 0 | 4968 |
| Eqn (6.8) | 992 (644) | 8 (8) | 9039 | 994 (474) | 6 (6) | 20098 | 990 (889) | 10 (10) | 14689 |

**Table 6.4:** Results of the Lyness-Kaganove tests for $\tau = 10^{-12}$.

| $f(x)$ | quadl | DQAGS | da2glob | Algorithm 10 | Algorithm 9 | Algorithm 8 |
|---|---|---|---|---|---|---|
| Eqn (6.3) | 8.22 (86.37) | 138.57 (304.55) | 42.93 (447.35) | 32.30 (90.01) | 32.40 (115.66) | 40.76 (192.31) |
| Eqn (6.4) | 11.83 (100.97) | 130.20 (327.03) | 35.58 (596.84) | 28.34 (91.87) | 25.95 (147.97) | 42.93 (227.95) |
| Eqn (6.5) | 4.99 (109.92) | 76.16 (424.25) | 11.44 (392.45) | 8.21 (81.98) | 8.15 (72.28) | 14.03 (207.66) |
| Eqn (6.6) | 8.26 (92.12) | 180.08 (373.35) | 57.05 (417.98) | 54.31 (108.45) | 49.36 (144.27) | 57.78 (203.83) |
| Eqn (6.7) | 47.77 (154.72) | 1152.31 (680.94) | 186.14 (387.28) | 172.28 (120.39) | 193.79 (198.48) | 243.97 (297.34) |
| Eqn (6.8) | 64.38 (86.28) | 152.31 (341.18) | 116.72 (223.02) | 56.95 (83.04) | 84.49 (96.70) | 100.19 (178.10) |

| $f(x)$ | quadl | DQAGS | da2glob | Algorithm 10 | Algorithm 9 | Algorithm 8 |
|---|---|---|---|---|---|---|
| Eqn (6.3) | 27.41 (74.33) | 312.34 (285.65) | 76.48 (256.27) | 82.18 (82.69) | 69.93 (80.68) | 111.51 (162.85) |
| Eqn (6.4) | 18.55 (78.54) | 243.77 (309.09) | 48.41 (483.53) | 59.72 (95.13) | 47.14 (149.30) | 73.38 (176.84) |
| Eqn (6.5) | 9.96 (96.28) | 116.52 (318.67) | 27.31 (470.00) | 20.87 (81.46) | 25.62 (81.67) | 40.78 (198.89) |
| Eqn (6.6) | 43.85 (91.02) | 256.97 (366.67) | 78.52 (270.28) | 74.85 (97.72) | 58.91 (95.82) | 92.14 (188.79) |
| Eqn (6.7) | 203.37 (156.73) | 1377.19 (678.02) | 245.73 (282.45) | 277.88 (123.03) | 278.27 (153.59) | 452.17 (304.82) |
| Eqn (6.8) | 181.70 (89.53) | 207.11 (358.81) | 147.93 (212.84) | 98.24 (82.66) | 95.76 (80.04) | 172.44 (190.27) |

| $f(x)$ | quadl | DQAGS | da2glob | Algorithm 10 | Algorithm 9 | Algorithm 8 |
|---|---|---|---|---|---|---|
| Eqn (6.3) | 76.71 (72.97) | 514.15 (288.07) | 128.97 (205.56) | 151.80 (75.69) | 133.07 (71.95) | 261.73 (176.01) |
| Eqn (6.4) | 27.23 (76.37) | 355.91 (304.85) | 58.81 (414.71) | 85.18 (90.04) | 56.71 (123.12) | 124.43 (171.43) |
| Eqn (6.5) | 14.57 (78.77) | 170.05 (299.75) | 41.12 (438.68) | 36.73 (88.49) | 46.99 (90.28) | 70.63 (173.31) |
| Eqn (6.6) | 118.38 (97.68) | 293.45 (356.00) | 103.70 (218.40) | 113.45 (87.65) | 80.29 (74.54) | 168.15 (187.16) |
| Eqn (6.7) | 509.40 (152.70) | 1620.46 (661.45) | 306.04 (213.76) | 488.79 (126.84) | 425.67 (130.79) | 863.07 (316.13) |
| Eqn (6.8) | 469.28 (90.48) | 263.71 (357.60) | 153.95 (192.47) | 168.82 (83.33) | 113.38 (81.39) | 306.77 (207.14) |

| $f(x)$ | quadl | DQAGS | da2glob | Algorithm 10 | Algorithm 9 | Algorithm 8 |
|---|---|---|---|---|---|---|
| Eqn (6.3) | 207.77 (73.07) | 757.52 (287.80) | 165.00 (154.44) | 755.60 (83.81) | 800.29 (93.13) | 535.59 (197.15) |
| Eqn (6.4) | 35.95 (73.65) | 455.38 (296.94) | 65.30 (354.06) | 100.82 (79.75) | 68.09 (112.29) | 190.77 (167.27) |
| Eqn (6.5) | 24.05 (76.16) | 228.15 (297.47) | 42.37 (317.11) | 47.29 (82.34) | 57.66 (78.33) | 98.66 (151.58) |
| Eqn (6.6) | 277.48 (86.25) | 349.05 (350.78) | 120.99 (170.25) | 999.03 (94.72) | 2168.54 (120.47) | 308.72 (191.95) |
| Eqn (6.7) | 1257.42 (144.57) | 1856.19 (621.07) | 342.83 (165.75) | 1180.90 (127.43) | 1917.43 (149.39) | 1616.21 (325.29) |
| Eqn (6.8) | 793.89 (82.68) | 399.50 (329.29) | 153.20 (171.20) | 797.74 (88.25) | 2282.50 (113.57) | 4022.79 (273.85) |

**Table 6.5:** Average time in milliseconds per run and, in brackets, microseconds per evaluation of the integrand for the Lyness-Kaganove tests for $\tau = 10^{-3}, 10^{-6}, 10^{-9}$ and $10^{-12}$.

The three new algorithms were implemented in the MATLAB programming language and are listed in Appendix B.

Over the years, several authors have specified sets of test functions to evaluate the performance and reliability of quadrature routines. In the following, we will use, with some minor modifications, the test "families" suggested by Lyness and Kaganove [64] and the "battery" of functions compiled by Gander and Gautschi [33], which are an extension of the set proposed by Kahaner [49].

The function families used for the Lyness-Kaganove test are

$$\int_0^1 |x-\lambda|^\alpha \,\mathrm{d}x, \qquad \lambda \in [0,1],\ \alpha \in [-0.5,0] \tag{6.3}$$

$$\int_0^1 (x>\lambda)e^{\alpha x} \,\mathrm{d}x, \qquad \lambda \in [0,1],\ \alpha \in [0,1] \tag{6.4}$$

$$\int_0^1 \exp(-\alpha|x-\lambda|) \,\mathrm{d}x, \qquad \lambda \in [0,1],\ \alpha \in [0,4] \tag{6.5}$$

$$\int_1^2 10^\alpha/((x-\lambda)^2+10^\alpha) \,\mathrm{d}x, \qquad \lambda \in [1,2], \alpha \in [-6,-3] \tag{6.6}$$

$$\int_1^2 \sum_{i=1}^4 10^\alpha/((x-\lambda_i)^2+10^\alpha) \,\mathrm{d}x, \qquad \lambda_i \in [1,2], \alpha \in [-5,-3] \tag{6.7}$$

$$\int_0^1 2\beta(x-\lambda)\cos(\beta(x-\lambda)^2) \,\mathrm{d}x, \qquad \lambda \in [0,1],\ \alpha \in [1.8,2], \tag{6.8}$$

$$\beta = 10^\alpha / \max\{\lambda^2,(1-\lambda)^2\}$$

where the Boolean expressions are evaluated to 0 or 1. The integrals were evaluated to relative precisions of $\tau = 10^{-3}$, $10^{-6}$, $10^{-9}$ and $10^{-12}$ for 1 000 realizations of the random parameters $\lambda$ and $\alpha$. The results of these tests are shown in Tables 6.1 to 6.4. For each function, the number of correct and incorrect integrations is given with, in brackets, the number of cases each in which a warning (either explicit or if an error estimate larger than the requested tolerance is returned) was issued.

The functions used for the "battery" test are

$$\begin{aligned}
f_1 &= \int_0^1 e^x \,\mathrm{d}x \\
f_2 &= \int_0^1 H(x-0.3)\,\mathrm{d}x \\
f_3 &= \int_0^1 x^{1/2}\,\mathrm{d}x \\
f_4 &= \int_{-1}^1 (\tfrac{23}{25}\cosh(x) - \cos(x))\,\mathrm{d}x \\
f_5 &= \int_{-1}^1 (x^4 + x^2 + 0.9)^{-1}\,\mathrm{d}x \\
f_6 &= \int_0^1 x^{3/2}\,\mathrm{d}x \\
f_7 &= \int_0^1 x^{-1/2}\,\mathrm{d}x \\
f_8 &= \int_0^1 (1+x^4)^{-1}\,\mathrm{d}x \\
f_9 &= \int_0^1 2(2+\sin(10\pi x))^{-1}\,\mathrm{d}x \\
f_{10} &= \int_0^1 (1+x)^{-1}\,\mathrm{d}x \\
f_{11} &= \int_0^1 (1+e^x)^{-1}\,\mathrm{d}x \\
f_{12} &= \int_0^1 x(e^x-1)^{-1}\,\mathrm{d}x \\
f_{13} &= \int_{0.1}^1 \sin(100\pi x)/(\pi x)\,\mathrm{d}x \\
f_{14} &= \int_0^{10} \sqrt{50}e^{-50\pi x^2}\,\mathrm{d}x \\
f_{15} &= \int_0^{10} 25e^{-25x}\,\mathrm{d}x \\
f_{16} &= \int_0^{10} 50(\pi(2500x^2+1))^{-1}\,\mathrm{d}x \\
f_{17} &= \int_{0.01}^1 50(\sin(50\pi x)/(50\pi x))^2\,\mathrm{d}x \\
f_{18} &= \int_0^\pi \cos(\cos(x)+3\sin(x)+2\cos(2x)+3\cos(3x))\,\mathrm{d}x \\
f_{19} &= \int_0^1 \log(x)\,\mathrm{d}x \\
f_{20} &= \int_{-1}^1 (1.005+x^2)^{-1}\,\mathrm{d}x \\
f_{21} &= \int_0^1 \sum_{i=1}^3 \left[\cosh(20^i(x-2i/10))\right]^{-1}\,\mathrm{d}x \\
f_{22} &= \int_0^1 4\pi^2 x\sin(20\pi x)\cos(2\pi x)\,\mathrm{d}x \\
f_{23} &= \int_0^1 (1+(230x-30)^2)^{-1}\,\mathrm{d}x \\
f_{24} &= \int_0^3 \lfloor e^x \rfloor\,\mathrm{d}x \\
f_{25} &= \int_0^5 (x+1)(x<1)+(3-x)(1\le x\le 3)+2(x>3)\,\mathrm{d}x
\end{aligned}$$

where the Boolean expressions in $f_2$ and $f_{25}$ evaluate to 0 or 1. The functions are taken from [33] with the following modifications:

- No special treatment is given to the case $x = 0$ in $f_{12}$, allowing the integrand to return NaN.
- $f_{13}$ and $f_{17}$ are integrated from 0 to 1 as opposed to 0.1 to one and 0.01 to 1 respectively, allowing the integrand to return NaN for $x = 0$.
- No special treatment of $x < 10^{-15}$ in $f_{19}$ allowing the integrand to return $-$Inf.
- $f_{24}$ was suggested by J. Waldvogel as a simple test function with multiple discontinuities.
- $f_{25}$ was introduced in [33], yet not used in the battery test therein.

The rationale for the modifications of $f_{12}$, $f_{13}$, $f_{17}$ and $f_{19}$ is that we can't, on one hand, assume that the user was smart or diligent enough to remove the non-numerical values in his or her integrand, and on the other hand assume that he or she would still resort to a general-purpose quadrature routine to integrate it. Any general purpose quadrature routine should be robust enough to deal with any function, provided by either careful or careless users.

The changes have little effect on `quadl` and `DQAGS` since, as mentioned in Section 5.1, the former shifts the integration boundaries by $\varepsilon_{\mathsf{mach}}$ if a non-numerical value is encountered on the edges of the integration domain and the latter uses Gauss and Gauss-Kronrod quadrature rules which do not contain the end-points and thus avoid the NaN returned at $x = 0$ for $f_{12}$, $f_{13}$ and $f_{17}$ and the Inf at $x = 0$ in $f_{19}$. `da2glob`, however, only deals with $\pm$Inf explicitly, replacing such values with zero. To be able to deal with $f_{12}$, $f_{13}$ and $f_{17}$, the algorithm was modified to treat NaN in the same way as Inf.

The battery functions were integrated for the relative tolerances $\tau = 10^{-3}$, $10^{-6}$, $10^{-9}$ and $10^{-12}$. The results are summarized in Table 6.6, where the number of function evaluations for each combination of integrand, integrator and tolerance are given. If integration was unsuccessful, the number is stricken through. If the number of evaluations was the lowest for the given integrand and tolerance, it is shown in bold face.

| | $\tau = 10^{-3}$ | | | | | | $\tau = 10^{-6}$ | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | `quadl` | `DQAGS` | `da2glob` | Alg. 10 | Alg. 9 | Alg. 8 | `quadl` | `DQAGS` | `da2glob` | Alg. 10 | Alg. 9 | Alg. 8 |
| $f_1$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **9** | 27 | 33 | 17 |
| $f_2$ | 108 | 357 | **61** | 283 | 161 | 185 | 198 | 357 | **101** | 603 | 301 | 409 |
| $f_3$ | 48 | 105 | **25** | 107 | 101 | 49 | 108 | 231 | **65** | 315 | 429 | 177 |
| $f_4$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **9** | 27 | 33 | 17 |
| $f_5$ | 18 | 21 | **17** | 27 | 33 | 25 | 48 | **21** | 33 | 59 | 95 | 65 |
| $f_6$ | 18 | 21 | **9** | 27 | 33 | 17 | 48 | 105 | **41** | 123 | 159 | 65 |
| $f_7$ | 289 | 231 | **121** | 411 | 269 | 329 | 439 | **231** | 285 | 1035 | 709 | 673 |
| $f_8$ | 18 | 21 | **17** | 27 | 33 | **17** | **18** | 21 | 25 | 43 | 33 | 33 |
| $f_9$ | 198 | 315 | **121** | 251 | 261 | 201 | 468 | 399 | **233** | 411 | 587 | 417 |
| $f_{10}$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **17** | 27 | 33 | **17** |
| $f_{11}$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **9** | 27 | 33 | 17 |
| $f_{12}$ | 19 | 21 | 49 | 59 | 47 | **17** | 19 | 21 | 105 | 59 | 55 | **17** |
| $f_{13}$ | ~~589~~ | **651** | 929 | 891 | 1403 | 1129 | 1519 | **1323** | 1469 | 1611 | 2347 | 2153 |
| $f_{14}$ | 78 | 231 | **45** | 187 | 151 | 105 | 138 | 231 | **65** | 203 | 183 | 137 |
| $f_{15}$ | 78 | 147 | **41** | 187 | 135 | 97 | 168 | 189 | **69** | 219 | 159 | 113 |
| $f_{16}$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **9** | 27 | 33 | 17 |
| $f_{17}$ | **79** | 483 | 325 | 603 | 903 | 649 | ~~949~~ | **777** | 1065 | 1179 | 1491 | 1457 |
| $f_{18}$ | 108 | 105 | **73** | 123 | 145 | 105 | 228 | 147 | **129** | 187 | 209 | 193 |
| $f_{19}$ | 109 | 231 | **65** | 155 | 255 | 177 | 229 | 231 | **145** | 475 | 717 | 513 |
| $f_{20}$ | 18 | 21 | **17** | 27 | 33 | **17** | 48 | **21** | 33 | 59 | 33 | 65 |
| $f_{21}$ | ~~138~~ | ~~273~~ | ~~85~~ | ~~235~~ | ~~203~~ | ~~137~~ | ~~348~~ | ~~357~~ | ~~185~~ | ~~347~~ | ~~391~~ | ~~273~~ |
| $f_{22}$ | 228 | **147** | 241 | 235 | 371 | 257 | 888 | 315 | **305** | 379 | 627 | 449 |
| $f_{23}$ | 108 | 273 | **93** | 299 | 191 | 161 | 258 | 399 | **161** | 411 | 365 | 281 |
| $f_{24}$ | ~~138~~ | 1911 | ~~453~~ | 3227 | 4515 | **1905** | ~~1878~~ | ~~8211~~ | ~~857~~ | 9163 | 11433 | **6793** |
| $f_{25}$ | 108 | 567 | **81** | 379 | 277 | 225 | 348 | 819 | **149** | 859 | 593 | 569 |

**Table 6.6:** Results of battery test for $\tau = 10^{-3}$ and $10^{-6}$. For each test, the best result (least function evaluations) is in bold and unsuccessful runs are stricken through.

| | $\tau = 10^{-9}$ | | | | | | $\tau = 10^{-12}$ | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $f(x)$ | `quadl` | `DQAGS` | `da2glob` | Alg. 10 | Alg. 9 | Alg. 8 | `quadl` | `DQAGS` | `da2glob` | Alg. 10 | Alg. 9 | Alg. 8 |
| $f_1$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **17** | 27 | 33 | 33 |
| $f_2$ | 318 | 357 | **141** | 923 | 441 | 681 | 408 | 357 | **181** | 1243 | 581 | 1097 |
| $f_3$ | 258 | 231 | **137** | 523 | 799 | 393 | ~~618~~ | **231** | 241 | 827 | 1191 | 721 |
| $f_4$ | **18** | 21 | 25 | 27 | 33 | 33 | 48 | **21** | 33 | 27 | 33 | 33 |
| $f_5$ | **48** | 63 | 65 | 59 | 95 | 97 | 168 | **63** | 65 | 123 | 219 | 129 |
| $f_6$ | 108 | 189 | **73** | 251 | 359 | 169 | 288 | 189 | **137** | 427 | 607 | 337 |
| $f_7$ | ~~889~~ | **231** | 581 | 1867 | 1409 | 1281 | ~~2429~~ | **231** | 965 | 3291 | 2179 | 2209 |
| $f_8$ | 48 | **21** | 33 | 59 | 95 | 65 | 138 | 63 | **49** | 123 | 95 | 89 |
| $f_9$ | 1038 | 567 | **401** | 891 | 991 | 769 | 2808 | 735 | **577** | 1387 | 1425 | 1449 |
| $f_{10}$ | 48 | 21 | **17** | 59 | 33 | 33 | 48 | **21** | 33 | 75 | 33 | 65 |
| $f_{11}$ | 18 | 21 | **9** | 27 | 33 | 17 | 48 | 21 | **17** | 43 | 33 | 33 |
| $f_{12}$ | 19 | 21 | 217 | 59 | 63 | **17** | **19** | 21 | 557 | 59 | 63 | 33 |
| $f_{13}$ | 4879 | **1323** | 1913 | 2939 | 2459 | 2993 | ~~10039~~ | **1323** | 2233 | 5019 | 2521 | 6081 |
| $f_{14}$ | 228 | 273 | **105** | 315 | 225 | 185 | 588 | 273 | **153** | 379 | 369 | 345 |
| $f_{15}$ | 288 | 189 | **101** | 283 | 191 | 161 | 708 | 231 | **145** | 379 | 277 | 337 |
| $f_{16}$ | 18 | 21 | **9** | 27 | 33 | 17 | 18 | 21 | **9** | 27 | 33 | 17 |
| $f_{17}$ | 2839 | **1323** | 1725 | 2107 | 2419 | 2849 | 6469 | **1323** | 2077 | 3387 | 2451 | 3681 |
| $f_{18}$ | 738 | 189 | **185** | 379 | 395 | 257 | 1758 | **273** | **273** | 731 | 581 | 593 |
| $f_{19}$ | ~~499~~ | **231** | 285 | 875 | 1323 | 1033 | 1369 | **231** | 449 | 1563 | 1943 | 1833 |
| $f_{20}$ | **48** | 63 | 65 | 91 | 95 | 73 | 168 | **63** | 65 | 187 | 219 | 129 |
| $f_{21}$ | **1158** | ~~441~~ | ~~273~~ | 1179 | ~~653~~ | ~~521~~ | 2748 | ~~525~~ | **649** | 1771 | 1839 | ~~1025~~ |
| $f_{22}$ | 2508 | **315** | 385 | 699 | 627 | 513 | 5568 | **315** | 513 | 1291 | 627 | 2249 |
| $f_{23}$ | 588 | 441 | **241** | 699 | 569 | 497 | 1608 | 483 | **401** | 1083 | 957 | 865 |
| $f_{24}$ | ~~3738~~ | ~~12285~~ | ~~1301~~ | 15275 | 18503 | **14537** | ~~5538~~ | ~~16359~~ | ~~1745~~ | 21147 | 25191 | **20001** |
| $f_{25}$ | 528 | 819 | **201** | 1339 | 933 | 1041 | 678 | 819 | **269** | 1803 | 1253 | 1617 |

**Table 6.6:** Results of battery test for $\tau = 10^{-9}$ and $10^{-12}$. For each test, the best result (least function evaluations) is in bold and unsuccessful runs are stricken through.

Finally, the integrators were tested on the problem

$$\int_0^1 |x - \lambda|^\alpha \, \mathrm{d}x, \quad \lambda \in [0, 1]$$

for 100 realizations of the random parameter $\lambda$ and different values of $\alpha$ for a relative[3] tolerance $\tau = 10^{-6}$. Since for *alpha* $\leq -1$, the integral diverges and can not be computed numerically, we are interested in the warnings or errors returned by the different quadrature routines. The results are shown in Table 6.7. For each integrator we give the number of successes and failures as well as, in brackets, the number of times each possible error or warning was returned. The different errors, for each integrator, are:

- `quadl`: (Min/Max/Inf)
  - Min: Minimum step size reached; singularity possible.
  - Max: Maximum function count exceeded; singularity likely.
  - Inf: Infinite or Not-a-Number function value encountered.
- `DQAGS`: ($\text{ier}_1$/$\text{ier}_2$/$\text{ier}_3$/$\text{ier}_4$/$\text{ier}_5$)
  - $\text{ier}_1$: Maximum number of subdivisions allowed has been achieved.
  - $\text{ier}_2$: The occurrence of roundoff error was detected, preventing the requested tolerance from being achieved. The error may be under-estimated.
  - $\text{ier}_3$: Extremely bad integrand behavior somewhere in the interval.
  - $\text{ier}_4$: The algorithm won't converge due to roundoff error detected in the extrapolation table. It is presumed that the requested tolerance cannot be achieved, and that the returned result is the best which can be obtained.
  - $\text{ier}_5$: The integral is probably divergent or slowly convergent.
- `da2glob`: (noise/min/max/sing)
  - noise: The requested tolerance is below the noise level of the problem. Required tolerance may not be met.

[3]For $\alpha \leq -1$ an *absolute* tolerance of $\tau = 10^{-6}$ was used.

  - min: Interval too small. Required tolerance may not be met.
  - max: Maximum number of function evaluations. Required tolerance may not be met.
  - sing: Singularity probably detected. Required tolerance may not be met.

- Algorithms 8, 9 and 10: (err/div)
  - err: The final error estimate is larger than the required tolerance.
  - div: The integral is divergent.

Thus, the results for `DQAGS` at $\alpha = -0.8$ should be read as the algorithm returning 146 correct and 854 false results (requested tolerance not satisfied) and having returned the error $\text{ier}_3$ (bad integrand behavior) 58 times and the error $\text{ier}_5$ (probably divergent integral) 4 times.

## 6.6 Results

As can be seen from the results in Tables 6.1 to 6.4, all three algorithms are clearly more reliable than `quadl` and `DQAGS`. MATLAB's `quadl` performs best for high precision requirements (small tolerances, best results for $\tau = 10^{-9}$), yet still fails often without warning. QUADPACK's `DQAGS` does better for low precision requirements (large tolerances, best results for $\tau = 10^{-3}$), yet also fails often, more often than not with a warning.

Espelid's `da2glob` does significantly better, with only a few failures at $\tau = 10^{-3}$ (without warning) and a large number of failures for Equation 6.8 at $\tau = 10^{-12}$, albeit all of them with prior warning. The former are due to the error estimate not detecting specific features of the integrand due to the interpolating polynomial looking smooth, when it is, in fact, singular (see Figure 6.8). The latter were due to the integral estimates being affected by noise (most often in the 17-point rule), which was, in all cases, detected and warned against by the algorithm.

The new algorithms fail only for (6.3) at higher precisions since the integral becomes numerically impossible to evaluate (there are not sufficient machine numbers near the singularity to properly resolve the integrand),

| $\alpha$ | `quadl` | `DQAGS` | `da2glob` | Algorithm 10 | Algorithm 9 | Algorithm 8 |
|---|---|---|---|---|---|---|
| $\alpha = -0.1$ | 48 / 52 (0/0/0) | 96 / 4 (0/0/0/0/0) | 98 / 2 (0/0/0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) |
| $\alpha = -0.2$ | 44 / 56 (0/0/0) | 93 / 7 (0/0/0/0/0) | 100 / 0 (0/0/0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) |
| $\alpha = -0.3$ | 36 / 64 (0/0/0) | 86 / 14 (0/0/0/0/0) | 98 / 2 (0/0/0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) |
| $\alpha = -0.4$ | 31 / 69 (0/0/0) | 83 / 17 (0/0/0/0/0) | 100 / 0 (0/0/0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) |
| $\alpha = -0.5$ | 22 / 78 (0/0/0) | 72 / 28 (0/0/0/0/0) | 98 / 2 (0/0/0/28) | 100 / 0 (0/0) | 100 / 0 (0/0) | 100 / 0 (0/0) |
| $\alpha = -0.6$ | 10 / 90 (0/0/0) | 46 / 54 (0/0/39/0/9) | 100 / 0 (0/0/0/94) | 100 / 0 (82/0) | 100 / 0 (0/0) | 100 / 0 (80/0) |
| $\alpha = -0.7$ | 0 / 100 (0/0/44) | 0 / 100 (0/0/77/0/19) | 0 / 100 (0/0/0/100) | 0 / 100 (99/0) | 0 / 100 (99/0) | 0 / 100 (100/0) |
| $\alpha = -0.8$ | 0 / 100 (2/0/90) | 0 / 100 (0/0/73/1/26) | 0 / 100 (0/0/0/100) | 0 / 100 (100/0) | 0 / 100 (99/1) | 0 / 100 (100/0) |
| $\alpha = -0.9$ | 0 / 100 (1/0/98) | 0 / 100 (0/0/76/1/23) | 0 / 100 (0/0/0/100) | 0 / 100 (94/6) | 0 / 100 (88/12) | 0 / 100 (100/0) |
| $\alpha = -1.0$ | 0 / 100 (1/0/99) | 0 / 100 (0/0/55/5/40) | 0 / 100 (0/0/0/100) | 0 / 100 (25/75) | 0 / 100 (54/46) | 0 / 100 (100/0) |
| $\alpha = -1.1$ | 0 / 100 (1/0/99) | 0 / 100 (0/0/36/5/59) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (7/93) | 0 / 100 (56/44) |
| $\alpha = -1.2$ | 0 / 100 (0/90/10) | 0 / 100 (0/0/3/7/90) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (1/99) | 0 / 100 (25/75) |
| $\alpha = -1.3$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/1/6/93) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (1/99) | 0 / 100 (18/82) |
| $\alpha = -1.4$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/15/85) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (14/86) |
| $\alpha = -1.5$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/26/74) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (6/94) |
| $\alpha = -1.6$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/28/72) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (2/98) |
| $\alpha = -1.7$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/32/68) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (2/98) |
| $\alpha = -1.8$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/35/65) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (2/98) |
| $\alpha = -1.9$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/38/62) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (2/98) |
| $\alpha = -2.0$ | 0 / 100 (0/100/0) | 0 / 100 (0/0/0/44/56) | 0 / 100 (0/0/0/100) | 0 / 100 (0/100) | 0 / 100 (0/100) | 0 / 100 (2/98) |

**Table 6.7:** Results of computing $\int_0^1 |x - \lambda|^\alpha \, \mathrm{d}x$ for 100 realizations of $\lambda \in [0, 1]$ for different $\alpha$. The numbers are the number of correct and incorrect integrations as well as the number of times (in brackets) the different errors or warnings of each algorithm were returned.

for which a warning is issued. This problem is shared by the other integrators as well.

Algorithm 8 and Algorithm 9 also fail a few times when integrating Equation 6.7 at $\tau = 10^{-3}$. In all such cases, one of the peaks was simply missed completely by the lower-degree rules, giving the appearance of a flat curve.

Algorithm 8 also failed a few times to evaluate Equation 6.3 for $\tau = 10^{-3}$. These were cases where the assumption of the naive error estimate (see Equation 4.19) does not hold and although the resulting error estimate is large, it is just below the required tolerance.

All three algorithms also failed a few times on Equation 6.8 in cases where the resulting integral was several orders of magnitude smaller than the function values themselves, making the required tolerance practically un-attainable.

Whereas the new algorithms out-perform the others in terms of reliability, they do so at a cost of a higher number of function evaluations. On average, Algorithm 8 and Algorithm 9 require about *twice as many* function evaluations as `da2glob`, whereas Algorithm 10 requires roughly *six times* as many.

This trend is also visible in the results of the "battery" test (Table 6.6). The new algorithms all fail on $f_{21}$ for all but the highest and second-highest tolerances respectively, since the third peak at $x = 0.6$ is missed completely. Espelid's also does quite well, failing on $f_{21}$ at the same tolerances and for the same reasons as the new algorithms and on $f_{24}$ for $\tau < 10^{-3}$, using, however, in almost all cases, less function evaluations than the new algorithms.

It is interesting to note that `quadl`, `DAQGS` and `da2glob` all failed to integrate $f_{24}$ for tolerances $\tau < 10^{-3}$. A closer look at the intervals that caused each algorithm to fail (see Figure 6.9) reveals that in all cases, multiple discontinuities in the same interval caused the error estimate to be accidentally small, leading the algorithms to erroneously assume convergence. This is not a particularity of the interval chosen: if we integrate

$$\int_0^\lambda \lfloor e^x \rfloor \, \mathrm{d}x, \quad \lambda \in [2.5, 3.5]$$

for 1 000 realizations of the random parameter $\lambda$ for $\tau = 10^{-6}$ using these

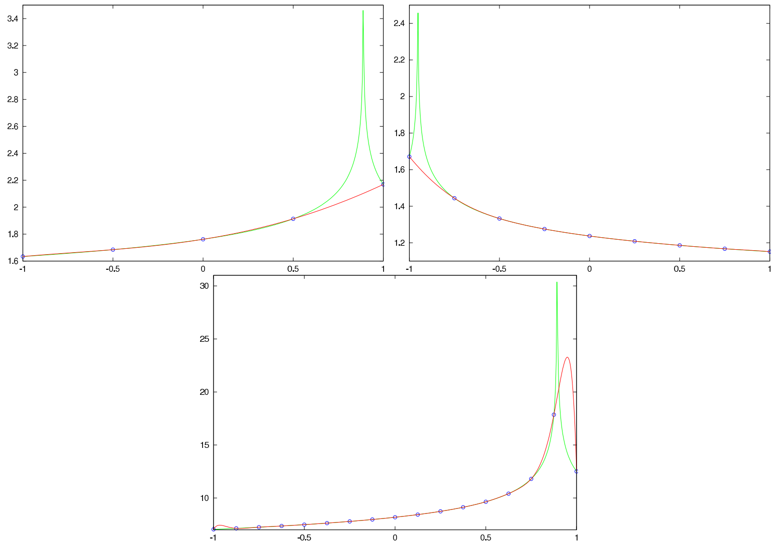


**Figure 6.8:** Some cases in which the 5, 9 and 17-point rules used in `da2glob` fail to detect a singularity (green). The assumed integrand (red) is sufficiently smooth such that its higher-degree coefficients, from which the error estimate is computed, are near zero.

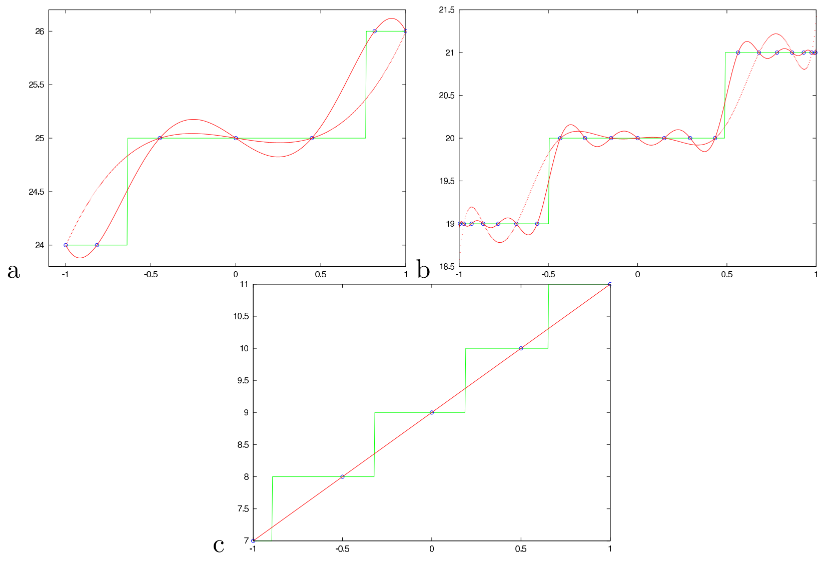


**Figure 6.9:** Intervals in which the error estimates of `quadl` (a), `DQAGS` (b) and `da2glob` (c) failed for $f_{24}$. The interpolatory polynomials used to compute the error estimates are shown in red.

three integrators, they fail on 894, 945 and 816 of the cases respectively. All three new algorithms succeed in all cases.

In the final test evaluating divergent integrals, (Table 6.7), `quadl` fails to distinguish between divergent and non-divergent integrals, reporting that a non-numerical value was encountered for $-1.1 \leq \alpha \leq -0.7$ and then aborting after the maximum 10 000 function evaluations[4] for $\alpha < 1.1$. For $\alpha < -1.0$, `DQAGS` reports the integral to be either subject to too much rounding error or divergent. The latter correct result was returned in more than half of the cases tested. In most cases where $\alpha < -0.6$, `da2glob` aborted, reporting that a singularity had probably been detected. This warning was usually accompanied by other warnings that the minimum interval size or the noise level had been reached (not shown).

[4]This termination criterion had been disabled for the previous tests.

For $\alpha = -0.8$, Algorithm 10 fails with a warning that the required tolerance was not met and as of $\alpha < -1.1$ both Algorithm 10 and Algorithm 9 abort, correctly, after deciding that the integral is divergent. Algorithm 8 is less successfull, reliably detecting the divergence only for $\alpha < -1.3$.

# Chapter 7

# Conclusions

In Chapter 3, we presented two new algorithms for the construction of polynomial interpolations. The first algorithm (Algorithm 4) offers no substantial improvement over that of Björck-Pereyra/Higham except that it can be easily downdated. The second algorithm, which does not allow for updates or downdates, is slightly more stable than the other algorithms tested and is more efficient when multiple right-hand sides need to be computed over the same set of nodes.

In Chapter 4, we presented two new error estimates. Over the set of problems treated therein, neither error estimate produced any false negative results, as opposed to the error estimators collected from Chapter 2.

In Chapter 6 we presented three new adaptive quadrature algorithms using the function representation discussed in Chapter 3, the error estimates described in Chapter 4 and the treatment of non-numerical function values and divergent integrals described in Chapter 5.

We conclude that the new algorithms presented in Chapter 6 are *more reliable* than MATLAB's `quadl`, QUADPACK's `DQAGS` and Espelid's `da2glob`. This increased reliability comes at a cost of a two to six times higher number of function evaluations required for complicated integrands.

The tradeoff between reliability and efficiency should, however, be of little concern in the context of automatic or general-purpose quadrature routines. Most modifications which increase efficiency usually rely on making certain assumptions on the integrand, *e.g.* smoothness, continuity, non-singularity, monotonically decaying coefficients, etc... If, however, the user knows enough about his or her integrand as to know that these assumptions are indeed valid and therefore that the algorithm will not fail, then he or she knows enough about the integrand as to *not* have to use a general-purpose quadrature routine and, if efficiency is crucial, should consider integrating it by a specialized routine or even analytically.

By making any assumptions for the user, we would be making two mistakes:

1. The increase in efficiency would *reward* users who, despite knowing enough about their integrand to trust the quadrature rule, have not made the effort to look for or implement a specialized routine,

2. The decrease in reliability *punishes* users who have turned to a general-purpose quadrature routine because they knowingly *can not* make any assumptions regarding their integrand.

It is for this reason that we should have no qualms whatsoever about sacrificing a bit of efficiency on certain integrands for much more reliability on tricky integrands of which we know, and can therefore assume, nothing.

# Appendix A

# Error Estimators in Matlab

## A.1 Kuncir's 1962 Error Estimate

```
function [ int , err ] = est_kuncir1962 ( f , a , b , tol )

    % the nodes
    xi = a + (b-a)*[ 0.0 0.25 0.5 0.75 1 ]';

    % get the function values
    fx = f(xi);

    % compute the simpson's rules
    s1 = (b-a) * [ 1 0 4 0 1 ] * fx / 6;
    s2 = (b-a) * [ 1 4 2 4 1 ] * fx / 12;

    % compute the integral
    int = s2;

    % compute the error estimate
    err = abs( s1 - s2 );

end
```

## A.2 McKeeman's 1962 Error Estimate

```
function [ int , err ] = est_mckeeman1962 ( f , a , b , tol )

    % the nodes
    xi = a + (b-a)*[ 0 1/6 1/3 1/2 2/3 5/6 1 ]';

    % get the function values
    fx = f(xi);
    % compute the simpson's rules
    s1 = (b-a) * [ 1 0 0  4 0 0 1 ] * fx / 6;
    s2 = (b-a) * [ 1 4 2 4 2 4 1 ] * fx / 18;

    % compute the integral
    int = s2;

    % compute the error estimate
    err = abs( s1 - s2 );

end
```

## A.3 McKeeman's 1963 Error Estimate

```
function [ int , err ] = est_mckeeman1963_7 ( f , a , b , tol )

    % the nodes
    xi = a + (b-a)*linspace(0,1,50)';

    % get the function values
    fx = f(xi);

    % compute the simpson's rules
    w = [ 751/17280, 3577/17280, 49/640, 2989/17280, ...
          2989/17280, 49/640, 3577/17280, 751/17280 ];
    s1 = (b-a) * w * fx(1:7:50);
    w = [ w(1:end-1) w(1)*2 w(2:end-1) w(1)*2 w(2:end-1) ...
          w(1)*2 w(2:end-1) w(1)*2 w(2:end-1) w(1)*2 ...
          w(2:end-1) w(1)*2 w(2:end) ];
    s2 = (b-a) * w * fx / sum(w);

    % compute the integral
    int = s2;

    % compute the error estimate
    err = abs( s1 - s2 );

end
```

## A.4 Gallaher's 1967 Error Estimate

```
function [ int , err ] = est_gallaher1967 ( f , a , b , tol )

    % the nodes
    h = (1/6 + rand(1)/3) * (b - a);
    xi = (b+a)/2 - [ h/2 0 -h/2 ]';

    % get the function values
    fx = f(xi);

    % compute the integral
    int = (fx(1) + fx(3)) * (b-a-h) / 2 + fx(2)*h;

    % compute the error estimate
    err = 14.6 * abs(f(1)-2*f(2)+f(3)) * (b - a - h) / 2;

end
```

## A.5 Lyness' 1969 Error Estimate

```
function [ int , err ] = est_lyness1969 ( f , a , b , tol )
```

```
    % the nodes
    xi = a + (b-a)*[ 0 1/8 1/4 3/8 1/2 5/8 3/4 7/8 1 ]';

    % get the function values
    fx = f(xi);

    % compute the 'old' simpson's rules
    s1 = (b-a) * [ 1 0 0 0 4 0 0 0 1 ] * fx / 6;
    s2 = (b-a) * [ 1 0 4 0 2 0 4 0 1 ] * fx / 12;

    % compute the 'old' error estimate
    err_old = abs( s1 - s2 ) / 15;

    % get the int and err left and right...
    s1_left = (b-a) * [ 1 0 4 0 1 0 0 0 0 ] * fx / 12;
    s2_left = (b-a) * [ 1 4 2 4 1 0 0 0 0 ] * fx / 24;
    int_left = (16*s2_left - s1_left) / 15;
    err_left = abs(s1_left - s2_left) / 15;
    s1_right = (b-a) * [ 0 0 0 0 1 0 4 0 1 ] * fx / 12;
    s2_right = (b-a) * [ 0 0 0 0 1 4 2 4 1 ] * fx / 24;
    int_right = (16*s2_right - s1_right) / 15;
    err_right = abs(s1_right - s2_right) / 15;

    % the integral
    int = int_left + int_right;

    % the noise-protected err
    if err_old > tol % && (err_old < err_left || err_old < err_right)
        err = err_old;
    else
        err = err_left + err_right;
    end;

end
```

## A.6 O'Hara and Smith's 1969 Error Estimate

```
function [ int , err ] = est_ohara1969 ( f , a , b , tol )

    % evaluate the nodes
    xi = a + (b-a) * linspace(0,1,9)';
    fx = f(xi);

    % compute nc9 and nc5_2
    nc9 = (b-a) * [ 989 5888 -928 10496 -4540 10496 -928 5888 989 ] * fx / 28350;
    nc5_2 = (b-a) * [ 7 32 12 32 14 32 12 32 7 ] * fx / 180;

    % compute err_1
    int = nc9;
    err = abs(nc9 - nc5_2);
    if err > tol, return; end;

    % evaluate cc7_2
    xi = a + (b-a) * ([ (cos( [6:-1:0]'/6*pi )-1)/2 ; (cos( [5:-1:0]'/6*pi )+1)/2 ] + 1)/2;
    fx = f(xi);
    cc7_2 = (b-a) * [ 0.028571428571428571425 0.25396825396825396823 0.45714285714285714282 ...
        0.52063492063492063487 0.45714285714285714282 0.25396825396825396823 ...
        2*0.028571428571428571425 0.25396825396825396823 0.45714285714285714282 ...
        0.52063492063492063487 0.45714285714285714282 0.25396825396825396823 ...
        0.028571428571428571425 ] * fx / 4;

    % test err_2
    int = cc7_2;
    err = abs(nc9 - cc7_2);
    if err > tol, return; end;

    % evaluate err_3
    err = (b-a) * 32 / 945 * (abs([ 1/2 -1 1 -1 1 -1 1/2 ] * fx(1:7)) + ...
          abs([ 1/2 -1 1 -1 1 -1 1/2 ] * fx(7:13)));

end
```

## A.7 De Boor's 1971 Error Estimate

```
function [ int , err ] = est_deboor1971 ( f , a , b , tol )

    % allocate the T-table
    T = zeros(10);
    R = zeros(10);

    % fill-in the first entry
    T(1,1) = (f(a) + f(b)) / 2;

    % main loop...
    for l=2:10

        % compute T(l,1)
        T(l,1) = [1/2 ones(1,2^(l-1)-1) 1/2 ] * f(linspace(a,b,2^(l-1)+1)') / 2^(l-1);

        % line?
        if l==2 && T(1,1) == T(2,1)
            int = T(2,1);
            xi = [0.71420053 , 0.34662815 , 0.843751 , 0.12633046]';
            fa = f(a); fb = f(b);
            fxi = f(a + (b-a)*xi);
            for i=1:4
                if abs(fxi(i) - (fa + xi(i)*(fb - fa))) > eps * (abs(fa) + abs(fb))/2
                    err = 2*tol;
                    return;
                end;
            end;
            err = 0;
            return;
        end;

        % fill in the rest of the row
        for i=2:l
            T(l,i) = T(l,i-1) + (T(l,i-1) - T(l-1,i-1)) / (4^(i-1) - 1);
        end;

        % compute the R_i
        for i=1:l-2
            R(i) = (T(l-1,i) - T(l-2,i)) / (T(l,i) - T(l-1,i));
        end;

        % if "sufficiently smooth"...
        if abs(R(1)-4) <= 0.15
            for i=2:l
                int = (b-a) * T(l,i);
                err = (b-a) * abs(T(l,i) - T(l,i-1));
                if err < tol, return; end;
            end

        % jump discontinuity?
        elseif abs(R(1)-2) <= 0.01
            int = (b-a) * T(l,1);
            err = (b-a) * abs(T(l,1) - T(l-1,1));
            return;

        % other singularity?
        elseif l > 2 && abs((R(1)-R_old)/R(1)) <= 0.1
            if R(1) < 1.1
                int = (b-a) * T(l,1);
                err = 2 * tol;
                return;
            end;
            if R(1) > 4.5, continue; end;
            for i=2:l-1
                for j=i+1:l
```

```
                    T(j,i) = T(j,i-1) - (T(j-1,i-1) - T(j,i-1))^2 / ...
                            (T(j-1,i-1) - 2*T(j-1,i-1) + T(j,i-1));
                end;
            end;
            int = (b-a) * T(l,l-1);
            err = (b-a) * abs( T(l,l-1) - T(l,l-2) );
            return;

        % too many rows?
        elseif l == 6
            int = T(l,l);
            err = 2*tol;
            return;

        end;

        % remember the last ratio
        R_old = R(1);

    end;

    % if we've landed here, then we have failed...
    int = T(1,1);
    err = 2*tol;

end
```

## A.8 Oliver's 1972 Error Estimate

```
function [ int , err ] = est_oliver1972 ( f , a , b , tol )

    % degree to begin with
    n = 4; j = 1; j_max = 2;

    % table of convergence rates
    Kn = [ 0.272 0.606 0.811 0.908 0.455
           0.144 0.257 0.376 0.511 0.550
           0.243 0.366 0.449 0.522 0.667
           0.283 0.468 0.565 0.624 0.780
           0.290 0.494 0.634 0.714 0.855
           0.292 0.499 0.644 0.745 0.0 ];

    % main loop
    while (1)

        % construct the nodes and get the function values
        xi = a + (b-a) * (cos([n:-1:0]/n*pi)' + 1) / 2;
        fx = f(xi);

        % compute the coefficients (brute-force vandermonde)
        xi = cos([n:-1:0]/n*pi)';
        V = [ ones(size(xi)) , xi ];
        for i = 2:n
            V = [ V , 2 * xi .* V(:,end) - V(:,end-1) ];
        end;
        c = V \ fx;

        % approximate the integral
        int = 2*c(1);
        for i=3:2:n+1
            int = int - 2 * c(i) / (i - 2) / i;
        end;
        int = int / 2 * (b - a);

        % get the convergence rate of the coeffs
        if j > 1
            if c(n-1) == 0, c(n-1) = eps * int; end;
            if c(n-3) == 0, c(n-3) = eps * int; end;
            if c(n-5) == 0, c(n-5) = eps * int; end;
            K = max( abs( [ c(n+1)/c(n-1) , c(n-1)/c(n-3) , c(n-3)/c(n-5) ] ) );
            An2 = K^3 * abs(c(n-3));
        else
            if c(n-1) == 0, c(n-1) = eps * int; end;
            if c(n-3) == 0, c(n-3) = eps * int; end;
            K = max( abs( [ c(n+1)/c(n-1) , c(n-1)/c(n-3) ] ) );
            An2 = K^2 * abs(c(n-1));
        end

        % find sigma such that K < Kn(j,sigma)
        sigma = 1;
        while sigma < 5 && K > Kn(j,sigma), sigma = sigma + 1; end;

        % do we have a sigma and thus an error estimate?
        if sigma < 5
            sigma = 2^sigma;
            err = (b-a) * sigma * 16*n / (n^2 - 1) / (n^2 - 9) * An2;
            if j > 1, err = min( err , abs(int - int_old) ); end;
            if err < tol || j == j_max, return; end;
        elseif j > 1
            err = abs(int - int_old);
            if err < tol || j == j_max, return; end;
        end;

        % otherwise split
        int_old = int;
        n = 2 * n; j = j + 1;

    end % while

end
```

## A.9 Rowland and Varol's 1972 Error Estimate

```
function [ int , err ] = est_rowland1972 ( f , a , b , tol )

    % the nodes
    xi = a + (b-a)*linspace(0,1,9)';

    % get the function values
    fx = f(xi);

    % compute the simpson's rules
    s1 = (b-a) * [ 1 0 0 0 4 0 0 0 1 ] * fx / 6;
    s2 = (b-a) * [ 1 0 4 0 2 0 4 0 1 ] * fx / 12;
    s4 = (b-a) * [ 1 4 2 4 2 4 2 4 1 ] * fx / 24;

    % compute the integral
    int = s4;

    % compute the error estimate
    if s1 ~= s2
        err = (s2 - s4)^2 / abs( s1 - s2 );
    else
        err = abs(s2 - s4);
    end;

end
```

## A.10 Garribba *et al.* 's 1978 Error Estimate

```
function [ int , err ] = est_garribba1978 ( f , a , b , tol )
```

```
    % the nodes and weights
    xi =[-0.93246951420315202781, -0.66120938646626451366, ...
        -0.23861918608319690863, 0.23861918608319690863, 0.66120938646626451366, ...
        0.93246951420315202781]';
    w = [0.17132449237917034513, 0.36076157304813860846, 0.46791393457269104698, ...
        0.46791393457269104752, 0.36076157304813860751, 0.17132449237917034507];

    % get the function values
    fx = f(a + (b-a) * (xi + 1)/2);
    fl = f(a + (b-a) * (xi + 1)/4);
    fr = f(a + (b-a) * (xi + 3)/4);

    % compute both quadratures
    q1 = (b-a) * w * fx / sum(w);
    q2 = (b-a) * w * (fl + fr) / sum(w) / 2;

    % compute the integral
    int = q2;

    % compute the error estimate
    err = abs( q1 - q2 ) / (2^12 - 1);

end
```

## A.11 Piessens' 1979 Error Estimate

```
function [ int , err ] = est_piessens1979 ( f , a , b , tol )

    % the nodes
    xi = [ 0.9956571630258081e+00,     0.9739065285171717e+00, ...
           0.9301574913557082e+00,     0.8650633666889845e+00, ...
           0.7808177265864169e+00,     0.6794095682990244e+00, ...
           0.5627571346686047e+00,     0.4333953941292472e+00, ...
           0.2943928627014602e+00,     0.1488743389816312e+00, ...
           0.0000000000000000e+00 ]';
    xi = [ xi ; -xi(end-1:-1:1) ];

    % get the function values
    fx = f(a + (b-a) * (xi + 1)/2);

    % the weights
    w =  [ 0.6667134430868814e-01,     0.1494513491505806e+00, ...
           0.2190863625159820e+00,     0.2692667193099964e+00, ...
           0.2955242247147529e+00 ];
    w = [ w , w(end:-1:1) ] / 2;
    wk = [ 0.1169463886737187e-01,     0.3255816230796473e-01, ...
           0.5475589657435200e-01,     0.7503967481091995e-01, ...
           0.9312545458369761e-01,     0.1093871588022976e+00, ...
           0.1234919762620659e+00,     0.1347092173114733e+00, ...
           0.1427759385770601e+00,     0.1477391049013385e+00, ...
           0.1494455540029169e+00 ];
    wk = [ wk , wk(end-1:-1:1) ] / 2;

    % compute the quadratures
    g = (b-a) * w * fx(2:2:end-1);
    gk = (b-a) * wk * fx;

    % compute the integral
    int = gk;

    % compute the error estimate
    err = abs( g - gk );

end
```

## A.12 Patterson's 1979 Error Estimate

```
function [ int , err ] = est_patterson1979 ( f , a , b , tol )
%
%   Shameles Matlab translation of Krogh and Van Snyder since
%   Patterson's original algorithm is numerically unstable

    % *****     Data Statements     ***********************************

      fl = [ 0 , 2, 3, 5, 9,12,14, 1];
      fh = [ 0 , 2, 4, 8,16,17,17, 0];
      kl = [ 1, 1, 1, 1, 1, 3, 5, 9, 5, 9,12];
      kh = [ 1, 2, 4, 8,16, 3, 6,17, 5, 9,17];
      kx = [ 0, 1, 2, 3, 4, 5,       8,      11];

    % init P for efficiency
      P = zeros(305,1);

    % In the comments below, F(K,I) refers to the function value
    % computed for the I'th node of the K'th formula.  The abscissae and
    % weights are stored in order according to the distance from the
    % boundary of the region, not from the center.  Since we store
    % 1 - |abscissa|, the first "node" coefficient for each formula is
    % the smallest.

    % Corrections, nodes and weights for the 3-point formula.

    % Correction for F(1,1).
      P(  1) = -.11111111111111111111e+00;
    % Node and weight for F(2,1).
      P(  2) = +.22540333075851662296e+00; P(  3) = +.55555555555555555556e+00;

    % Corrections, nodes and weights for the 7-point formula.

    % Corrections for F(1,1) and F(2,1).
      P(  4) = +.647209421402969791e-02; P(  5) = -.928968790944433705e-02;
    % Nodes and weights for F(3,1-2)
      P(  6) = +.39508731291979716579e-01; P(  7) = +.10465622602646726519e+00;
      P(  8) = +.56575625065319744200e+00; P(  9) = +.40139741477596222291e+00;

    % Corrections, nodes and weights for the 15-point formula.

    % Corrections for F(1,1), F(2,1), F(3,1-2).
      P( 10) = +.5223046896961622e-04; P( 11) = +.17121030961750000e-03;
      P( 12) = -.724830016153892898e-03; P( 13) = -.7017801099209042e-04;
    % Nodes and weights for F(4,1-4).
      P( 14) = +.61680367872449777899e-02; P( 15) = +.17001719629940260339e-01;
      P( 16) = +.11154076712774300110e+00; P( 17) = +.92927195315124537686e-01;
      P( 18) = +.37889705326277359705e+00; P( 19) = +.17151190913639138079e+00;
      P( 20) = +.77661331357103311837e+00; P( 21) = +.21915685840158749640e+00;

    % Corrections, nodes and weights for the 31-point formula.

    % Corrections for F(1,1), F(2,1), F(3,1-2), F(4,1-4).
      P( 22) = +.682166534792e-08; P( 23) = +.12667409859336e-06;
      P( 24) = +.59565976367837165e-05; P( 25) = +.1392330106826e-07;
      P( 26) = -.6629407564902392e-04; P( 27) = -.704395804282302e-06;
      P( 28) = -.34518205339241e-07; P( 29) = -.814486910996e-08;
    % Nodes and weights for F(5,1-8).
      P( 30) = +.90187503233240234038e-03; P( 31) = +.25447807915618744154e-02;
      P( 32) = +.18468850446259893130e-01; P( 33) = +.16446049854387810934e-01;
      P( 34) = +.70345142570259943330e-01; P( 35) = +.35957103307129322097e-01;
      P( 36) = +.16327406183113126449e+00; P( 37) = +.56979509494123357412e-01;
      P( 38) = +.29750379350847292139e+00; P( 39) = +.76879620499003531043e-01;
      P( 40) = +.46868025635562437602e+00; P( 41) = +.93627109981264473617e-01;
      P( 42) = +.66886460674202316691e+00; P( 43) = +.10566989358023480974e+00;
      P( 44) = +.88751105686681337425e+00; P( 45) = +.11195687302095345688e+00;

    % Corrections, nodes and weights for the 63-point formula.

    % Corrections for F(1,1), F(2,1), F(3,1-2), F(4,1-4), F(5,1-8).
      P( 46) = +.371583e-15; P( 47) = +.21237877e-12;
      P( 48) = +.10522629388435e-08; P( 49) = +.1748029e-14;
      P( 50) = +.3475718983017160e-06; P( 51) = +.90312761725e-11;
      P( 52) = +.12558916e-13; P( 53) = +.54591e-15;
      P( 54) = -.72338395508691963e-05; P( 55) = -.169699579757977e-07;
      P( 56) = -.854363907155e-10; P( 57) = -.12281300930e-11;
```

```
  P( 58) = -.462334825e-13; P( 59) = -.42244055e-14;
  P( 60) = -.88501e-15; P( 61) = -.40904e-15;
% Nodes and weights for F(6,1-16).
  P( 62) = +.127111879642388 06027e-03; P( 63) = +.36322148184553065969e-03;
  P( 64) = +.27937406277780409196e-02; P( 65) = +.25790497946856882724e-02;
  P( 66) = +.11315242452570520059e-01; P( 67) = +.61155068221172463397e-02;
  P( 68) = +.27817125251418203419e-01; P( 69) = +.10498246909621321898e-01;
  P( 70) = +.53657141626597094849e-01; P( 71) = +.15406750466559497802e-01;
  P( 72) = +.89628843042995707499e-01; P( 73) = +.20594233915912711149e-01;
  P( 74) = +.13609206180630952284e+00; P( 75) = +.25869679327214746911e-01;
  P( 76) = +.19305946804978238813e+00; P( 77) = +.31073551111687964880e-01;
  P( 78) = +.26024395564730524132e+00; P( 79) = +.36064432780782572640e-01;
  P( 80) = +.33709033997521940454e+00; P( 81) = +.40715510116944318934e-01;
  P( 82) = +.42280428994795418516e+00; P( 83) = +.44914531653632197414e-01;
  P( 84) = +.51638197305415897244e+00; P( 85) = +.48564330406673198716e-01;
  P( 86) = +.61664067580126965307e+00; P( 87) = +.51583253952048458777e-01;
  P( 88) = +.72225017797817568492e+00; P( 89) = +.53905499335266063927e-01;
  P( 90) = +.83176474844779253501e+00; P( 91) = +.55481404356559363988e-01;
  P( 92) = +.94365568695340721002e+00; P( 93) = +.56277699831254301273e-01;

% Corrections, nodes and weights for the 127-point formula.

% Corrections for F(3,1), F(4,1-2), F(5,1-3), F(6,1-6).
  P( 94) = +.1041098e-15; P( 95) = +.249472054598e-10;
  P( 96) = +.55e-20; P( 97) = +.290412475995385e-07;
  P( 98) = +.367282126e-13; P( 99) = +.5568e-18;
  P(100) = -.871176477376972025e-06; P(101) = -.8147324267441e-09;
  P(102) = -.8830920337e-12; P(103) = -.18018239e-14;
  P(104) = -.70528e-17; P(105) = -.506e-19;
% Nodes and weights for F(7,1-32).
  P(106) = +.17569645108401419961e-04; P(107) = +.50536095207862517625e-04;
  P(108) = +.40120032808931675009e-03; P(109) = +.37774664632698466027e-03;
  P(110) = +.16833646815926074696e-02; P(111) = +.93836984854238150079e-03;
  P(112) = +.42758953015928114900e-02; P(113) = +.16811428654214699063e-02;
  P(114) = +.85042788218938676006e-02; P(115) = +.25687649437940203731e-02;
  P(116) = +.14628500401479628890e-01; P(117) = +.35728927835172996494e-02;
  P(118) = +.22858485360294285840e-01; P(119) = +.46710503721143217474e-02;
  P(120) = +.33362148441583432910e-01; P(121) = +.58434498758356395076e-02;
  P(122) = +.46269993574238863589e-01; P(123) = +.70724899954335554680e-02;
  P(124) = +.61679602220407116350e-01; P(125) = +.83428387539681577056e-02;
  P(126) = +.79659974529987579270e-01; P(127) = +.96411777297025366953e-02;
  P(128) = +.10025510022305996335e+00; P(129) = +.10955733387837901648e-01;
  P(130) = +.12348658551529473026e+00; P(131) = +.12275830560082770087e-01;
  P(132) = +.14935550523164972024e+00; P(133) = +.13591571009765546790e-01;
  P(134) = +.17784374563501959262e+00; P(135) = +.14893641664815182035e-01;
  P(136) = +.20891506620015163857e+00; P(137) = +.16173218729577719942e-01;
  P(138) = +.24251603361948636206e+00; P(139) = +.17421930159464173747e-01;
  P(140) = +.27857691462990108452e+00; P(141) = +.18631848256138790186e-01;
  P(142) = +.31701256890892077191e+00; P(143) = +.19795495048097499488e-01;
  P(144) = +.35772335749024048622e+00; P(145) = +.20905851445812023852e-01;
  P(146) = +.40059606975775710702e+00; P(147) = +.21956366305317824939e-01;
  P(148) = +.44550486736806745112e+00; P(149) = +.22940964229387748761e-01;
  P(150) = +.49231224246628339785e+00; P(151) = +.23854052106038540080e-01;
  P(152) = +.54086998801016766712e+00; P(153) = +.24690524744487676909e-01;
  P(154) = +.59102017877011132759e+00; P(155) = +.25445769965464765813e-01;
  P(156) = +.64259616216846784762e+00; P(157) = +.26115673376706097680e-01;
  P(158) = +.69542355844328595666e+00; P(159) = +.26696622927450359906e-01;
  P(160) = +.74932126969651682339e+00; P(161) = +.27185513229624791819e-01;
  P(162) = +.80410249728889984607e+00; P(163) = +.27579749566481873035e-01;
  P(164) = +.85957576684743982540e+00; P(165) = +.27877251476613701609e-01;
  P(166) = +.91554595991628911629e+00; P(167) = +.28076455793817246607e-01;
  P(168) = +.97181535105025430566e+00; P(169) = +.28176319033016602131e-01;

% Corrections, nodes and weights for the 255-point formula.

% Corrections for F(4,1), F(5,1), F(6,1-2), F(7,1-4).
  P(170) = +.3326e-18; P(171) = +.114094770478e-11;
  P(172) = +.2952436056970351e-08; P(173) = +.51608328e-15;
  P(174) = -.110177219650597323e-06; P(175) = -.58656987416475e-10;
  P(176) = -.23340340645e-13; P(177) = -.1248950e-16;
% Nodes and weights for F(8,1-64).
  P(178) = +.24036202515353807630e-05; P(179) = +.69379364324108267170e-05;
  P(180) = +.56003792945624240417e-04; P(181) = +.53275293669780613125e-04;
  P(182) = +.23950907556795267013e-03; P(183) = +.13575491094922871973e-03;
  P(184) = +.61966197497641806982e-03; P(185) = +.24921240048299729402e-03;
```

```
    P(186) = +.12543855319048853002e-02; P(187) = +.38974528447328229322e-03;
    P(188) = +.21946455040427254399e-02; P(189) = +.55429531493037471492e-03;
    P(190) = +.34858540851097261500e-02; P(191) = +.74028280424450333046e-03;
    P(192) = +.51684971993789994803e-02; P(193) = +.94536151685852538246e-03;
    P(194) = +.72786557172113846706e-02; P(195) = +.11674841174299594077e-02;
    P(196) = +.98486295992298408193e-02; P(197) = +.14049079956551446427e-02;
    P(198) = +.12907472045965932809e-01; P(199) = +.16561127281544526052e-02;
    P(200) = +.16481342421367271240e-01; P(201) = +.19197129710138724125e-02;
    P(202) = +.20593718329137316189e-01; P(203) = +.21944069253638388388e-02;
    P(204) = +.25265540247597332240e-01; P(205) = +.24789582266575679307e-02;
    P(206) = +.30515340497540768229e-01; P(207) = +.27721957645934509940e-02;
    P(208) = +.36359378430187867480e-01; P(209) = +.30730184347025783234e-02;
    P(210) = +.42811783890139037259e-01; P(211) = +.33803979910869203823e-02;
    P(212) = +.49884702478705123440e-01; P(213) = +.36933779170256508183e-02;
    P(214) = +.57588434808916940190e-01; P(215) = +.40110687240750233989e-02;
    P(216) = +.65931563842274211999e-01; P(217) = +.43326409680929828545e-02;
    P(218) = +.74921067092924347640e-01; P(219) = +.46573172997568547773e-02;
    P(220) = +.84562412844234959360e-01; P(221) = +.49843645647655386012e-02;
    P(222) = +.94859641186738404810e-01; P(223) = +.53130866051870565663e-02;
    P(224) = +.10581543166444097714e+00; P(225) = +.56428181013844441585e-02;
    P(226) = +.11743115975265809315e+00; P(227) = +.59729195655081658049e-02;
    P(228) = +.12970694445188609414e+00; P(229) = +.63027734490857587172e-02;
    P(230) = +.14264168911376784347e+00; P(231) = +.66317812429018878941e-02;
    P(232) = +.15623311732729139895e+00; P(233) = +.69593614093904229394e-02;
    P(234) = +.17047780536259859981e+00; P(235) = +.72849479805538070639e-02;
    P(236) = +.18537121234486258656e+00; P(237) = +.76079896657190565832e-02;
    P(238) = +.20090770903915859819e+00; P(239) = +.79279493342948491103e-02;
    P(240) = +.21708060588171698360e+00; P(241) = +.82443037630328680306e-02;
    P(242) = +.23388218069623990928e+00; P(243) = +.85565435613076896192e-02;
    P(244) = +.25130370638306339718e+00; P(245) = +.88641732094824942641e-02;
    P(246) = +.26933547875781873867e+00; P(247) = +.91667111635607884067e-02;
    P(248) = +.28796684463774796540e+00; P(249) = +.94636899938300652943e-02;
    P(250) = +.30718623022088529711e+00; P(251) = +.97546565363174114611e-02;
    P(252) = +.32698116976958152079e+00; P(253) = +.10039172044056840798e-01;
    P(254) = +.34733833458998250389e+00; P(255) = +.10316812330947621682e-01;
    P(256) = +.36824356228880576959e+00; P(257) = +.10587167904885197931e-01;
    P(258) = +.38968188628481359983e+00; P(259) = +.10849844089337314099e-01;
    P(260) = +.41163756555233745857e+00; P(261) = +.11104461134006926537e-01;
    P(262) = +.43409411457634557737e+00; P(263) = +.11350654315980596602e-01;
    P(264) = +.45703433350168850951e+00; P(265) = +.11588074033043952568e-01;
    P(266) = +.48044033846254297801e+00; P(267) = +.11816385890830235763e-01;
    P(268) = +.50429359208123853983e+00; P(269) = +.12035270785279562630e-01;
    P(270) = +.52857493412834112307e+00; P(271) = +.12244424981611985899e-01;
    P(272) = +.55326461233797152625e+00; P(273) = +.12443560190714035263e-01;
    P(274) = +.57834231337383669993e+00; P(275) = +.12632403643542078765e-01;
    P(276) = +.60378719394238406082e+00; P(277) = +.12810698163877361967e-01;
    P(278) = +.62957791204992176986e+00; P(279) = +.12978202239537399286e-01;
    P(280) = +.65569265840056197721e+00; P(281) = +.13134690091960152836e-01;
    P(282) = +.68210918793152331682e+00; P(283) = +.13279951743930530650e-01;
    P(284) = +.70880485148175331803e+00; P(285) = +.13413793085110098513e-01;
    P(286) = +.73575662758907323806e+00; P(287) = +.13536035934956213614e-01;
    P(288) = +.76294115441017027278e+00; P(289) = +.13646518102571291428e-01;
    P(290) = +.79033476175681880523e+00; P(291) = +.13745093443001896632e-01;
    P(292) = +.81791350324074780175e+00; P(293) = +.13831631909506428676e-01;
    P(294) = +.84565318851862189130e+00; P(295) = +.13906019601325461264e-01;
    P(296) = +.87352941562769803314e+00; P(297) = +.13968158806516938516e-01;
    P(298) = +.90151760340188079791e+00; P(299) = +.14017968039456608810e-01;
    P(300) = +.92959302395714482093e+00; P(301) = +.14055382072649964277e-01;
    P(302) = +.95773083523463639678e+00; P(303) = +.14080351962553661325e-01;
    P(304) = +.98590611358921753738e+00; P(305) = +.14092845069160408355e-01;

  % *****     Executable Statements     ******************************

    icheck=0;
    delta=b-a;
    diff=0.5*delta;
    ip=1;
    jh=0;

  % Apply 1-point Gauss formula (Midpoint rule).

    fncval=f(a+diff);
  % Don't write "0.5*(b+a)" above if the radix of arithmetic isn't 2.
    npts=1;
    work(1)=fncval;
```

```
      acum=fncval*delta;
      result(1)=acum;

      for k = 2:8

    %   Go on to the next formula.

        pacum=acum;
        acum=0.0;

    %   Compute contribution to current estimate due to function
    %   values used in previous formulae.

        for kk = kx(k-1)+1 : kx(k)
          for j = kl(kk) : kh(kk)
            acum=acum+(P(ip)*work(j));
            ip=ip+1;
          end;
        end;

    %   Compute contribution from new function values.

        jl=jh+1;
        jh=jl+jl-1;
        j1=fl(k);
        j2=fh(k);
        for j = jl:jh
          x=P(ip)*diff;
          fncval=f(a+x)+f(b-x);
          npts=npts+2;
          acum=acum+(P(ip+1)*fncval);
          if (j1 <= j2)
            work(j1)=fncval;
            j1=j1+1;
          end
          ip=ip+2;
        end;
        acum=(diff)*acum+0.5*pacum;
        result(k)=acum;
        err = abs(result(k)-result(k-1));
        int = result(k);
        if (err <= tol)
            return;
        end;
      end; % for k=2:8
```

## A.13 Ninomiya's 1980 Error Estimate

```
function [ int , err ] = est_ninomiya1980 ( f , a , b , tol )

    % the nodes
    xi = linspace(0,1,9)';
    xi = a + (b - a) * sort( [ xi ; (xi(1)+xi(2))/2 ; (xi(end)+xi(end-1))/2 ] );

    % get the function values
    fx = f(xi);

    % compute the quadrature and the difference
    err = 4736 * (b-a) / 2 / 468242775 * [ 3003 -16384 27720 -38220 56056 -64350 ...
        56056 -38220 27720 -16384 3003 ] * fx;
    int = (b-a) * [ 989 0 5888 -928 10496 -4540 10496 -928 5888 0 989 ] * fx / 28350 - err;
    err = abs(err);

end
```

## A.14 Piessens *et al.* 's 1983 Error Estimate

```
function [ int , err ] = est_piessens1983 ( f , a , b , tol )

    % the nodes
    xi = [ 0.9956571630258081e+00,     0.9739065285171717e+00, ...
           0.9301574913557082e+00,     0.8650633666889845e+00, ...
           0.7808177265864169e+00,     0.6794095682990244e+00, ...
           0.5627571346686047e+00,     0.4333953941292472e+00, ...
           0.2943928627014602e+00,     0.1488743389816312e+00, ...
           0.0000000000000000e+00 ]';
    xi = [ xi ; -xi(end-1:-1:1) ];

    % get the function values
    fx = f(a + (b-a) * (xi + 1)/2);

    % the weights
    w =  [ 0.6667134430868814e-01,     0.1494513491505806e+00, ...
           0.2190863625159820e+00,     0.2692667193099964e+00, ...
           0.2955242247147529e+00 ];
    w = [ w , w(end:-1:1) ] / 2;
    wk = [ 0.1169463886737187e-01,     0.3255816230796473e-01, ...
           0.5475589657435200e-01,     0.7503967481091995e-01, ...
           0.9312545458369761e-01,     0.1093871588022976e+00, ...
           0.1234919762620659e+00,     0.1347092173114733e+00, ...
           0.1427759385770601e+00,     0.1477391049013385e+00, ...
           0.1494455540029169e+00 ];
    wk = [ wk , wk(end-1:-1:1) ] / 2;

    % compute the quadratures
    g = (b-a) * w * fx(2:2:end-1);
    gk = (b-a) * wk * fx;
    ik = (b-a) * wk * abs(fx - gk/(b-a));

    % compute the integral
    int = gk;

    % compute the error estimate
    if abs(ik) > 0
        err = ik * min( 1 , (200 * abs(g - gk) / ik)^(3/2) );
    else
        err = 0;
    end

end
```

## A.15 Laurie's 1983 Error Estimate

```
function [ int , err ] = est_laurie1983 ( f , a , b , tol )
%
%   Introduced "myeps" to avoid spurious failue due to
%   noise in the quadratures.

    % the nodes
    xi = [ 0.9956571630258081e+00,     0.9739065285171717e+00, ...
           0.9301574913557082e+00,     0.8650633666889845e+00, ...
           0.7808177265864169e+00,     0.6794095682990244e+00, ...
           0.5627571346686047e+00,     0.4333953941292472e+00, ...
           0.2943928627014602e+00,     0.1488743389816312e+00, ...
           0.0000000000000000e+00 ]';
    xi = [ -xi ; xi(end-1:-1:1) ];

    % get the function values
    fx = f(a + (b-a) * (xi + 1)/2);

    % the weights
    w =  [ 0.6667134430868814e-01,     0.1494513491505806e+00, ...
           0.2190863625159820e+00,     0.2692667193099964e+00, ...
           0.2955242247147529e+00 ];
    w = [ w , w(end:-1:1) ] / 2;
    wk = [ 0.1169463886737187e-01,     0.3255816230796473e-01, ...
           0.5475589657435200e-01,     0.7503967481091995e-01, ...
           0.9312545458369761e-01,     0.1093871588022976e+00, ...
```

```
            0.1234919762620659e+00,     0.1347092173114733e+00, ...
            0.1427759385770601e+00,     0.1477391049013385e+00, ...
            0.1494455540029169e+00 ];
    wk = [ wk , wk(end-1:-1:1) ] / 2;

    % compute the quadratures
    qb1 = (b-a) * w * fx(2:2:end-1);
    qa1 = (b-a) * wk * fx;

    % get the double-nodes
    xi2 = [ (xi - 1)/2 ; (xi + 1)/2 ];
    fx2 = f(a + (b-a)*(xi2+1)/2);

    % compute the double quadratures
    qb2 = (b-a) * [ w , w ] * fx2([ 2:2:20 , 23:2:41 ]') / 2;
    qa2 = (b-a) * [ wk , wk ] * fx2 / 2;

    % the integral
    int = qa2;

    % test the conditions
    qab1 = qa1 - qb1; qaa = qa2 - qa1;
    qab2 = qa2 - qb2; qbb = qb2 - qb1;

    % set some noise limits
    noise = 21 * eps * (b-a) * max(abs(fx));
    if abs(qab1) <= noise, qab1 = 0; end;
    if abs(qab2) <= noise, qab2 = 0; end;
    if abs(qaa) <= noise, qaa = 0; end;
    if abs(qbb) <= noise, qbb = 0; end;

    if (qab1 == 0 || (0 <= qab2/qab1 && qab2/qab1 <= 1)) && ...
        (qaa == 0 || abs(qaa) <= abs(qbb))
        if qaa == 0
            err = 0;
        else
            err = abs( qab2 * qaa / (qbb - qaa) );
        end;
    else
        err = 2 * tol;
    end;

end
```

## A.16 Kahaner and Stoer's 1983 Error Estimate

```
function [ int , err ] = est_kahaner1983 ( f , a , b , tol )
%
%   Modified epsilon-algorithm slightly such that it abandons if
%   two successive column entries are identical (or almost).

    % the nodes and function values
    n = 7;
    xi = a + (b-a) * linspace(0,1,2^(n-1) + 1)';
    fx = f(xi);

    % construct the basic quadratures
    for i=1:n
        q(i) = (b-a) * [ 1/2 ones(1,2^(i-1)-1) 1/2 ] * fx(1:2^(n-i):2^(n-1)+1) / 2^(i-1);
    end;

    % init the eps-table
    e = zeros(n);
    e(:,1) = q(:);
    for i=1:n-1
        e(i,2) = 1.0 / (e(i+1,1) - e(i,1));
    end;
    for k=3:n
```

```
        for i=1:n-k+1
            d = e(i+1,k-1) - e(i,k-1);
            if d == 0 || abs(2 * d / (e(i+1,k-1) + e(i,k-1))) < max(abs(fx))*eps*(b-a)*10
                int = e(1+1,k-1);
                if d == 0
                    err = 0.0;
                else
                    err = tol * abs(d / (e(i+1,k-1) + e(i,k-1)));
                end;
                return;
            end;
            e(i,k) = e(i+1,k-2) + 1.0 / d;
        end;
    end;

    % the integral is the last entry in the rightmost odd column
    k = mod(n,2);
    int = e(2-k,n-1+k);
    int_prev1 = e(1+2*k,n-1-k);
    int_prev2 = e(4-k*2,n-3+k);
    err = abs(int - int_prev1) + abs(int - int_prev2);

end
```

## A.17 Berntsen and Espelid's 1984 Error Estimate

```
function [ int , err ] = est_berntsen1984 ( f , a , b , tol )

    % the nodes
    xi21 = [-0.993752170620389500260242035938, -0.967226838566306294316622214908, ...
        -0.920099334150400828790187133715, -0.853363364583317283647250638588, ...
        -0.768439963475677908615877851306, -0.667138804197412319305966669990, ...
        -0.551618835887219807059018796724, -0.424342120207438783573668888544, ...
        -0.288021316802401096600792516065, -0.145561854160895090937030982339, 0., ...
        0.145561854160895090937030982339, 0.288021316802401096600792516065, ...
        0.424342120207438783573668888544, 0.551618835887219807059018796724, ...
        0.667138804197412319305966669990, 0.768439963475677908615877851306, ...
        0.853363364583317283647250638588, 0.920099334150400828790187133715, ...
        0.967226838566306294316622214908, 0.993752170620389500260242035938]';

    % weights
    w21 = [0.0160172282577743333242187078818, 0.0369537897708524937998313495754, ...
        0.0571344254268572082833743308836, 0.0761001136283793020169811548244, ...
        0.0934444234560338615532228314058, 0.108797299167148377663350290783, ...
        0.121831416053728534195322926580, 0.132268938633337461781132575048, ...
        0.139887394791073154722007273919, 0.144524403989970059063948267891, ...
        0.146081133649690427191905279357, 0.144524403989970059063810750568, ...
        0.139887394791073154722088567485, 0.132268938633337461781231504338, ...
        0.121831416053728534195305122553, 0.108797299167148377663477278496, ...
        0.0934444234560338615533044174841, 0.0761001136283793020170415377821, ...
        0.0571344254268572082836554562868, 0.0369537897708524937999293341024, ...
        0.0160172282577743333242239053239];
    w20 = [0.0106185068786295819657339016891, 0.0556095497747986766747966146793, ...
        0.0213509066165672182894520098703, 0.131065748488434560353592700481, ...
        0.0186790125246841257874886375194, 0.202709839222086678141907431408, ...
        0.0105576177287917472191747007450, 0.258136954188164115974337527090, ...
        0.00299435192317801232423909724150, 0.288277512654665283269117549094, ...
        0.288277512654665283269107675162, 0.00299435192317801232422502623669, ...
        0.258136954188164115974416663785, 0.0105576177287917472193162480098, ...
        0.202709839222086678141844327320, 0.0186790125246841257874671063730, ...
        0.131065748488434560353692369995, 0.0213509066165672182893290880775, ...
        0.0556095497747986766748067438711, 0.0106185068786295819657745168233];

    % compute stuff
    fx = f(xi21);
    g21 = (b-a) * w21 * fx / sum(w21);
    q20 = (b-a) * w20 * fx([1:10,12:21]) / sum(w20);
    % the integral
    int = g21;

    % the error
    err = abs( g21 - q20 );

end
```

## A.18 Berntsen and Espelid's 1991 Error Estimate

```
function [ int , err ] = est_berntsen1991 ( f , a , b , tol )

    % some constants
    r_crit = 1/4;
    alpha = (21 - (2*10 - 3)) / 4;
    K = 3;

    % the nodes and function values
    xi = -cos( [0:20] / 20 * pi )';
    fx = f(a + (b-a) * (xi + 1) / 2);

    % legendre base...
    N = [ ones(21,1) , xi ];
    for i=3:21, N(:,i) = 2*xi.*N(:,i-1)-N(:,i-2); end;
    [ N , r ] = qr(N);
    N = N';

    w = [.25062656641604010e-2, .23978647239640935e-1, .48754129106911638e-1, ...
         .71202738820962617e-1, .92397630395614637e-1, .11102364439825740, ...
         .12711755339015786, .13992786619265645, .14941903247367981, ...
         .15512023618056280, .15710451227479091, .15512023618056280, ...
         .14941903247367981, .13992786619265645, .12711755339015786, ...
         .11102364439825740, .92397630395614637e-1, .71202738820962617e-1, ...
         .48754129106911638e-1, .23978647239640935e-1, .25062656641604010e-2];
    N = N * norm(w);

    % compute the coefficients
    int = (b-a) * w * fx / sum(w);
    e = N * fx;
    E = sqrt(e(2:2:20).^2 + e(3:2:21).^2);
    r = E(end-K:end-1) ./ max(E(end-K+1:end),eps);
    r_max = max(r);

    % so many decisions...
    if r_max > 1
        err = max(E(end-K:end));
    elseif r_max > r_crit;
        err = 10 * r_max * E(end);
    else
        err = 10 * r_crit^(1-alpha) * r_max^alpha * E(end);
    end

end
```

## A.19 Favati *et al.* 's 1991 Error Estimate

```
function [ int , err ] = est_favati1991 ( f , a , b , tol )

    % nodes and weights
    xi15 = [ -0.99145537112081263 -0.94910791234275852 -0.86486442335976907 ...
        -0.74153118559939443 -0.58608723546769113 -0.40584515137739716 -0.20778495500789846 ...
        0.0000000000000000 0.20778495500789846 0.40584515137739716 0.58608723546769113 ...
        0.74153118559939443 0.86486442335976907 0.94910791234275852 0.99145537112081263 ]';
    w7 = [  0.12948496616886969 0.27970539148927666 0.38183005050511894 ...
```

```
        0.41795918367346938 0.38183005050511894 0.27970539148927666 0.12948496616886969 ];
    w15 = [  0.02293532201052922 0.06309209262997855 0.10479001032225018 ...
        0.14065325971552591 0.16900472663926790 0.19035057806478540 0.20443294007529889 ...
        0.20948214108472782 0.20443294007529889 0.19035057806478540 0.16900472663926790 ...
        0.14065325971552591 0.10479001032225018 0.06309209262997855 0.02293532201052922 ];
    xi21 = [  -0.99565716302580808 ...
        -0.97390652851717172 -0.93015749135570822 -0.86506336668898451 -0.78081772658641689 ...
        -0.67940956829902440 -0.56275713466860468 -0.43339539412924719 -0.29439286270146019 ...
        -0.14887433898163121 0.00000000000000000 0.14887433898163121 0.29439286270146019 ...
        0.43339539412924719 0.56275713466860468 0.67940956829902440 0.78081772658641689 ...
        0.86506336668898451 0.93015749135570822 0.97390652851717172 0.99565716302580808 ]';
    w10 = [ 0.06667134430868813 0.14945134915058059 ...
        0.21908636251598204 0.26926671930999635 0.29552422471475287 0.29552422471475287 ...
        0.26926671930999635 0.21908636251598204 0.14945134915058059 0.06667134430868813 ];
    w21 = [ 0.01169463886737187 ...
        0.03255816230796472 0.05475589657435199 0.07503967481091995 0.09312545458369760 ...
        0.10938715880229764 0.12349197626206585 0.13470921731147332 0.14277593857706008 ...
        0.14773910490133849 0.14944555400291690 0.14773910490133849 0.14277593857706008 ...
        0.13470921731147332 0.12349197626206585 0.10938715880229764 0.09312545458369760 ...
        0.07503967481091995 0.05475589657435199 0.03255816230796472 0.01169463886737187 ];

    % get the function values
    fx15 = f(a + (b-a) * (xi15 + 1)/2);
    fx21 = f(a + (b-a) * (xi21 + 1)/2);

    % compute the four quadratures
    q7 = (b-a) * w7 * fx15(2:2:14) / sum(w7);
    q10 = (b-a) * w10 * fx21(2:2:20) / sum(w10);
    q15 = (b-a) * w15 * fx15 / sum(w15);
    q21 = (b-a) * w21 * fx21 / sum(w21);

    % if the difference between the last two estimates is noise,
    % just split.
    if abs(q21-q15) < 100 * (b-a) * eps * max(abs(fx21))
        int = q21;
        err = abs(q21-q15);
        return;
    end;

    % compute the bounds
    b1 = (q7 - q21) / (q15 - q21);
    b2 = (q10 - q21) / (q15 - q21);
    if 1 - b1 + b2 == 0, s0 = inf;
    else s0 = b2 / ( 1 - b1 + b2 );
    end;
    delta = (1 + b1 + b2)^2 - 8*b2;
    s1 = (1 + b1 + b2 - sqrt(delta)) / 4;
    s2 = (1 + b1 + b2 + sqrt(delta)) / 4;
    if b1 > 1 + b2 && b2 > 0
        alpha = s0; beta = min([ b2/2 , 1/2 , s1 ]);
    elseif b1 > 0 && b1 <= 1 + b2 && b2 < 0
        alpha = max(b2/2,s1); beta = min(b1/2,1/2);
    elseif b1 > 0 && b1 > 1 + b2 && b2 < 0
        alpha = max(b2/2,s1); beta = min([b1/2,1/2,s0]);
    elseif b1 < 0 && b1 < 1 + b2 && b2 < 0
        alpha = max([b1/2,b2/2,s0]); beta = min(1/2,s2);
    elseif b1 < 0 && b1 >= 1 + b2 && b2 < 0
        alpha = max(b1/2,b2/2); beta = min(1/2,s2);
    elseif b1 < 0 && b2 > 0
        alpha = b1/2; beta = min([1/2,b2/2,s0]);
    else
        int = q21;
        err = 2*tol;
        return;
    end;

    % compute the error bound an the integral
    int = q21;
    err = max( abs(alpha) , abs(beta) ) * abs(q15 - q21);

end
```

## A.20 Gander and Gautschi's 2001 Error Estimate

```
function [ int , err ] = est_gander2001 ( f , a , b , tol )

    % the nodes and function values
    c = (a + b)/2;
    h = (b - a)/2;
    alpha = sqrt(2/3);
    beta = 1/sqrt(5);
    xi = a + (b-a)*([-1 c-alpha*h c-beta*h c c+beta*h c+alpha*h 1]' + 1) / 2;
    fx = f(xi);

    % compute the rules
    gl = (b-a) * [1 5 5 1] * fx(1:2:7) / 12;
    gk = (b-a) * [77 432 625 672 625 432 77] * fx / 2940;

    % the int and the error
    int = gk;
    err = abs( gl - gk );

end
```

## A.21 Venter and Laurie's 2002 Error Estimate

```
function [ int , err ] = est_venter2002 ( f , a , b , tol )

    % the nodes and weigths
    xi = [ 0.0 0.8164965809277260 0.4744811695891284 0.9744079242540920 ...
        0.2467208395344672 0.6676815505186759 0.9176634454676027 0.9967032921348130 ...
        0.1245872428182431 0.3640598996653803 0.5761686879241989 0.7479928493493064 ...
        0.8729905887501410 0.9511171199458969 0.9890095712955333 0.9995868407682468 ]';
    w = [ 0.15625e-1/2 0.78125e-2 0.1329095288597234e-1 0.2334047114027659e-2 ...
        0.1501395420099286e-1 0.1075598273807455e-1 0.4865753315451455e-2 0.6143097454811318e-3 ...
        0.1547045578486217e-1 0.1427638731917522e-1 0.1210082672197449e-1 0.9309261194540840e-2 ...
        0.6314881366348385e-2 0.3519722515847501e-2 0.1353274640802211e-2 0.1551904564491656e-3 ]';

    % get the function values
    fx = [ f(a + (b-a) * (xi + 1)/2) f(a + (b-a) * (-xi + 1)/2) ]';

    % compute the quadrature rules
    for i=1:5
        q(i) = (b-a) * 2^(8-i) * sum( fx(:,1:2^(i-1)) * w(1:2^(i-1)) ) / 2;
    end;

    % compute the error estimates
    E = max( abs( q(2:end) - q(1:end-1) ) , 2.2e-16 );
    hint = E(2:end) ./ E(1:end-1);
    eps = hint .* E(2:end);

    % loop...
    for i=1:length(eps)
        if hint(i) > 0.1
            err = 2*tol;
            int = q(i+2);
            % disp('bail hint...');
            return;
        elseif eps(i) < tol
            err = eps(i);
            int = q(i+2);
            % disp('bail conv...');
            return;
        end;
    end;
    % ran out of quadratures
    err = 2*tol;
    int = q(end);

end
```

## A.22 The New Trivial Error Estimate

```
function [ int , err ] = est_gonnet2008b ( f , a , b , tol )

    % the nodes and function values
    n = 10;
    xi_1 = -cos([0:n]/n*pi)';
    xi_2 = -cos([0:2*n]/2/n*pi)';
    fx = f(a + (b-a)*(xi_2 + 1)/2);

    % compute the coefficients
    V_1 = [ ones(size(xi_1)) xi_1 ];
    for i=3:n+1
        V_1 = [ V_1 , ((2*i-3) / (i-1) * xi_1 .* V_1(:,i-1) - (i-2) / (i-1) * V_1(:,i-2)) ];
    end;
    V_2 = [ ones(size(xi_2)) xi_2 ];
    for i=3:2*n+1
        V_2 = [ V_2 , ((2*i-3) / (i-1) * xi_2 .* V_2(:,i-1) - (i-2) / (i-1) * V_2(:,i-2)) ];
    end;
    for i=1:n+1, V_1(:,i) = V_1(:,i) * sqrt(4*i-2)/2; end;
    for i=1:2*n+1, V_2(:,i) = V_2(:,i) * sqrt(4*i-2)/2; end;
    c_1 = V_1 \ fx([1:2:2*n+1]);
    c_2 = V_2 \ fx;

    % compute the integral
    w = [ 1/sqrt(2) , zeros(1,2*n) ];
    int = (b-a) * w * c_2;

    % compute the errors left and right
    scale = 0.00097458556689523308842;
    c_diff = norm([c_1;zeros(n,1)]-c_2);
    err = (b-a) * c_diff;

end
```

## A.23 The New Refined Error Estimate

```
function [ int , err ] = est_gonnet2008 ( f , a , b , tol )

    % the nodes and function values
    n = 10;
    xi = -cos([0:n]/n*pi)';
    xil = (xi - 1)/2; xir = (xi + 1)/2;
    fx = f(a + (b-a)*(xi + 1)/2);
    fxl = f(a + (b-a)*(xil+1)/2);
    fxr = f(a + (b-a)*(xir+1)/2);

    % compute the coefficients
    V = [ ones(size(xi)) xi ];
    Vl = [ ones(size(xi)) xil ]; Vr = [ ones(size(xi)) xir ];
    for i=3:n+2
        V = [ V , ((2*i-3) / (i-1) * xi .* V(:,i-1) - (i-2) / (i-1) * V(:,i-2)) ];
        Vl = [ Vl , ((2*i-3) / (i-1) * xil .* Vl(:,i-1) - (i-2) / (i-1) * Vl(:,i-2)) ];
        Vr = [ Vr , ((2*i-3) / (i-1) * xir .* Vr(:,i-1) - (i-2) / (i-1) * Vr(:,i-2)) ];
    end;
    for i=1:n+2
        V(:,i) = V(:,i) * sqrt(4*i-2)/2;
        Vl(:,i) = Vl(:,i) * sqrt(4*i-2)/2;
```

```
            Vr(:,i) = Vr(:,i) * sqrt(4*i-2)/2;
        end;
        c_old = V(:,1:n+1) \ fx;
        c_left = V(:,1:n+1) \ fxl;
        c_right = V(:,1:n+1) \ fxr;

        % shift matrix
        T_left = V(:,1:n+1) \ Vl(:,1:n+1);
        T_right = V(:,1:n+1) \ Vr(:,1:n+1);

        % compute the integral
        w = [ 1/sqrt(2) , zeros(1,n) ];
        int = (b-a) * w * (c_left + c_right) / 2;

        % compute the errors left and right
        b_old = [0., .1062084505244398872914101554 56e-4, 0., ...
            .2271305231870350977068612042 96e-4, 0., .5818880429155495585247887545 54e-4, ...
            0., .3346672959803132367207928892 10e-3, 0., ...
            -.1301559109423132468162631382 78e-2, 0., ...
            .8561027177820947428577968724 76e-3]';
        b_left = 2^(n+1) * [.2762135864009951267190798289 71e-3, ...
            .4996576554922274497624390769 73e-3, .5234346802369847210040730149 10e-3, ...
            .2578742618612802055750399170 99e-3, -.7483429034160827009611833127 97e-3, ...
            -.9176699834696952207096935814 07e-3, .5495009802501479949746753579 71e-3, ...
            .3000600294606954616883339296 27e-3, -.2766784927768361196821577660 61e-3, ...
            .7610434734053716458128667387 09e-4, -.9186910571689206374201861321 98e-5, ...
            .4180189051670384486610336291 39e-6]';
        b_right = 2^(n+1) * [-.2762135864009951267190798289 71e-3, ...
            .4996576554922274497624390769 73e-3, -.5234346802369847210040730149 10e-3, ...
            .2578742618612802055750399170 99e-3, .7483429034160827009611833127 97e-3, ...
            -.9176699834696952207096935814 07e-3, -.5495009802501479949746753579 71e-3, ...
            .3000600294606954616883339296 27e-3, .2766784927768361196821577660 61e-3, ...
            .7610434734053716458128667387 09e-4, .9186910571689206374201861321 98e-5, ...
            .4180189051670384486610336291 39e-6]';
        scale = norm(b_old) / norm((b_old - b_left));
        fn_left = norm(c_left - T_left*c_old) / norm((b_old - b_left));
        fn_right = norm(c_right - T_right*c_old) / norm((b_old - b_right));
        err_left = (b-a)/2 * fn_left * norm(b_old);
        if max(abs(V(:,1:n+1) * T_left * c_old - fxl)(2:end-1) - ...
            1.1 * fn_left * abs( V * b_left )(2:end-1)) > cond(V)*eps*norm(c_old)
            err_left = (b-a)/2 * norm(c_left - T_left*c_old);
        else
            err_left = (b-a)/2 * fn_left * norm(b_old);
        end;
        if max(abs(V(:,1:n+1) * T_right * c_old - fxr)(2:end-1) - ...
            1.1 * fn_right * abs( V * b_right )(2:end-1)) > cond(V)*eps*norm(c_old)
            err_right = (b-a)/2 * norm(c_right - T_right*c_old);
        else
            err_right = (b-a)/2 * fn_right * norm(b_old);
        end;
        err = err_left + err_right;

    end
```

# Appendix B

# Algorithms in Matlab

## B.1 An Adaptive Quadrature Algorithm using Interpolation Updates

```
function [ int , err , nr_points ] = int_gonnet2008d ( f , a , b , tol )
%INT_GONNET2008D  evaluates an integral using adaptive quadrature. The
%   algorithm uses a 9-point RMS quadrature rule as a basic stencil
%   and extends an interpolation of the integrand generated in the
%   previous level of recursion by adding the new nodes in the interval.
%   If a maximum number of nodes has been reached or the change in the
%   interpolation is too large, the interpolation is reset. The error
%   estimate is computed from the L2-norm of the difference between two
%   successive interpolations.
%
%   INT = INT_GONNET2008D ( F , A , B , TOL ) approximates the integral
%   of F in the interval [A,B] up to the relative tolerance TOL. The
%   integrand F should accept a vector argument and return a vector
%   result containing the integrand evaluated at each element of the
%   argument.
%
%   [INT,ERR,NR_POINTS] = INT_GONNET2008D ( F , A , B , TOL ) returns
%   ERR, an estimate of the absolute integration error as well as
%   NR_POINTS, the number of function values for which the integrand
%   was evaluated. The value of ERR may be larger than the requested
%   tolerance, indicating that the integration may have failed.
%
%   INT_GONNET2008D halts with a warning if the integral is or appears
%   to be divergent.
%
%   Reference: "Adaptive Quadrature Re-Revisited", P. Gonnet, PhD Thesis,
%       submitted 2008.

   % declare persistent variables
   persistent n_init n_max xi b_init V Vx xx Vinv Vcond T_left T_right w ...
      alpha beta gamma T_incr xi_left xi_right sel_left sel_right

   % have the persistent variables been declared already?
   if ~exist('w') || isempty(w)

      % the nodes and function values
```

```
        n_init = 8;
        n_max = 20;
        % xi = linspace(-1,1,n_init+1)';
        xi = [ -1, -7/8, -3/4, -1/2, 0, 1/2, 3/4, 7/8, 1 ]';
        xi_left = [ 2 6 7 8 ]; sel_left = [ 1 1 2 3 4 4 4 4 5 ];
        xi_right = [ 2 3 4 8 ]; sel_right = [ 5 5 5 5 6 7 8 8 9 ];

        % the initial vector b
        b_init = [ 0., 0.0016413188422920629082, 0., -0.0053032949213072811071, 0., ...
          0.0062061518050860500735, 0., -0.0062710590362925230324, 0., ...
          0.0034165926622357227290 , zeros(1,n_max-n_init) ]';

        % compute the vandermonde-like matrix
        V = [ ones(size(xi)) xi ];
        xx = linspace(-1,1,200)'; Vx = [ ones(size(xx)) xx ];
        for i=3:n_max+2
           V = [ V , ((2*i-3) / (i-1) * xi .* V(:,i-1) - (i-2) / (i-1) * V(:,i-2)) ];
           Vx = [ Vx , ((2*i-3) / (i-1) * xx .* Vx(:,i-1) - (i-2) / (i-1) * Vx(:,i-2)) ];
        end;
        for i=1:n_max+2
           V(:,i) = V(:,i) * sqrt(4*i-2)/2;
           Vx(:,i) = Vx(:,i) * sqrt(4*i-2)/2;
        end;
        Vinv = inv(V(:,1:n_init+1));
        Vcond = cond(V);

        % shift matrices
        T_left = [ ... ];
        T_right = [ ... ];
        T_left = T_left(1:n_max+2,1:n_max+2);
        T_right = T_right(1:n_max+2,1:n_max+2);

        % the coefficient matrix (not explicit)
        k = [0:n_max+1]';
        alpha = sqrt( (k+1).^2 ./ (2*k+1) ./ (2*k+3) );
        beta = 0 * k;
        gamma = [ sqrt(2) ; sqrt( k(2:end).^2 ./ (4*k(2:end).^2 - 1) ) ];
        T_incr = diag(alpha(1:end-1),-1) - diag(beta) + diag(gamma(2:end),1);

        % compute the integral
        w = [ sqrt(2) , zeros(1,n_max) ] / 2; % legendre

     end; % if exist('w')

     % create the original datatype
     ivals = struct( ...
        'a', [], 'b',[], 'n', [], 'n_old', [], ...
        'c', [], 'c_old', [], ...
        'b_new', [], 'b_old', [], ...
        'fx', [], ...
        'int', [], ...
        'err', [], ...
        'tol', [], ...
        'depth', [], ...
        'ndiv' , [] );

     % compute the first interval
     points = a + (b-a) * (xi + 1) / 2;
     fx = f(points); nans = [];
     for i=1:length(fx), if ~isfinite(fx(i)), nans = [ i , nans ]; fx(i) = 0.0; end; end;
     c_new = [ Vinv * fx ; zeros(n_max-n_init,1) ];
     b_new = b_init; n = n_init;
     for i=1:length(nans)
        b_new(1:end-1) = (T_incr(2:end,1:end-1) - diag(ones(n_max,1)*xi(nans(i)),1)) \ b_new(2:end);
        b_new(end) = 0; c_new = c_new - c_new(n+1) / b_new(n+1) * b_new(1:end-1);
        n = n - 1;
     end;
     ivals(1).fx = fx;
     ivals(1).c = c_new;
     ivals(1).c_old = c_new;
     ivals(1).a = a; ivals(1).b = b; ivals(1).n = n_init;
     ivals(1).int = (b-a) * w * ivals(1).c;
     ivals(1).b_new = b_new;
     ivals(1).err = abs((b-a) * norm(ivals(1).c));
     ivals(1).tol = tol;
```

```
    ivals(1).depth = 1;
    ivals(1).ndiv = 0;

    % init some globals
    int = ivals(1).int; err = ivals(1).err; nr_ivals = 1;
    int_final = 0; err_final = 0; err_excess = 0;
    i_max = 1; nr_points = n_init+1;
    ndiv_max = 20; theta_1 = 0.1;

    % main loop
    while true

       % compute the left interval
       a_left = ivals(i_max).a; b_left = (ivals(i_max).a + ivals(i_max).b)/2;
       h_left = b_left - a_left;
       points_left = a_left + h_left * (xi + 1) / 2;
       fx_left = ivals(i_max).fx(sel_left);
       fx_left(xi_left) = f(points_left(xi_left));
       n_left = ivals(i_max).n;
       b_old = T_left * ivals(i_max).b_new;
       c_old = T_left(1:n_max+1,1:n_max+1) * ivals(i_max).c;
       nr_points = nr_points + n_init/2;
       if (n_left + n_init/2 <= n_max)
          b_new = b_old; c_left = c_old;
          for i=xi_left
             if ~isfinite(fx_left(i)), continue; end;
             g_k = V(i,1:n_left+1) * c_left(1:n_left+1);
             p_k = V(i,1:n_left+2) * b_new(1:n_left+2);
             a_k = (fx_left(i) - g_k) / p_k;
             n_left = n_left + 1;
             c_left = c_left + a_k * b_new(1:end-1);
             b_new = (T_incr - diag(xi(i)*ones(n_max+2,1))) * b_new;

          end;
          nc = norm(c_left);
       end;
       if n_left == ivals(i_max).n || ( nc > 0 && norm(c_left - c_old) / nc > theta_1 )

          nans = [];
          for i=1:length(fx_left), if ~isfinite(fx_left(i)), fx_left(i) = 0.0; nans = [ i , nans ]; end; end;
          c_left = [ Vinv * fx_left ; zeros(n_max-n_init,1) ];
          b_new = b_init;
          n_left = n_init;
          for i=nans
             b_new(1:end-1) = (T_incr(2:end,1:end-1) - diag(ones(n_max,1)*xi(i),1)) \ b_new(2:end);
             b_new(end) = 0; c_left = c_left - c_left(n_left+1) / b_new(n_left+1) * b_new(1:end-1);
             n_left = n_left - 1;
             fx_left(i) = NaN;
          end;
       end;
       int_left = h_left * w(1:n_left+1) * c_left(1:n_left+1);
       err_left = h_left * norm(c_left - c_old);
       if abs(ivals(i_max).int) > 0 && ...
          int_left / ivals(i_max).int > 1
          ndiv_left = ivals(i_max).ndiv + 1;
       else
          ndiv_left = ivals(i_max).ndiv;
       end;
       if ndiv_left > ndiv_max && 2*ndiv_right > ivals(i_max).depth
          warning(sprintf('possibly␣divergent␣integral␣in␣the␣interval␣[%e,%e]!',a_left,b_left));
          int = sign(int) * Inf;
          return;
       end;
       if points_left(end) <= points_left(end-1) || ...
          err_left < abs(int_left) * Vcond * eps
          err_excess = err_excess + err_left;
          int_final = int_final + int_left;

       else
          nr_ivals = nr_ivals + 1;
          ivals(nr_ivals).c = c_left;
          ivals(nr_ivals).c_old = c_old;
          ivals(nr_ivals).a = a_left; ivals(nr_ivals).b = b_left;
          ivals(nr_ivals).fx = fx_left;
          ivals(nr_ivals).b_new = b_new;
```

```
         ivals(nr_ivals).b_old = b_old;
         ivals(nr_ivals).n = n_left;
         ivals(nr_ivals).n_old = ivals(i_max).n;
         ivals(nr_ivals).int = int_left;
         ivals(nr_ivals).err = err_left;
         ivals(nr_ivals).tol = ivals(i_max).tol / sqrt(2);
         ivals(nr_ivals).depth = ivals(i_max).depth + 1;
         ivals(nr_ivals).ndiv = ndiv_left;
      end;


      % compute the right interval
      a_right = (ivals(i_max).a + ivals(i_max).b)/2; b_right = ivals(i_max).b;
      h_right = b_right - a_right;
      points_right = a_right + h_right * (xi + 1) / 2;
      fx_right = ivals(i_max).fx(sel_right);
      fx_right(xi_right) = f(points_right(xi_right));
      nr_points = nr_points + n_init/2;
      n_right = ivals(i_max).n;
      b_old = T_right * ivals(i_max).b_new;
      c_old = T_right(1:n_max+1,1:n_max+1) * ivals(i_max).c;
      if (n_right + n_init/2 <= n_max)
         b_new = b_old; c_right = c_old;
         for i=xi_right
            if ~isfinite(fx_right(i)), continue; end;
            g_k = V(i,1:n_right+1) * c_right(1:n_right+1);
            p_k = V(i,1:n_right+2) * b_new(1:n_right+2);
            a_k = (fx_right(i) - g_k) / p_k;
            n_right = n_right + 1;
            c_right = c_right + a_k * b_new(1:end-1);
            b_new = (T_incr - diag(xi(i)*ones(n_max+2,1))) * b_new;
         end;
         nc = norm(c_right);
      end;
      if n_right == ivals(i_max).n || ( nc > 0 && norm(c_right - c_old) / nc > theta_1 )
         fx = f(points_right); nans = [];
         for i=1:length(fx), if ~isfinite(fx(i)), fx(i) = 0.0; nans = [ i , nans ]; end; end;
         c_right = [ Vinv * fx ; zeros(n_max-n_init,1) ];
         b_new = b_init;
         n_right = n_init;
         for i=nans
            b_new(1:end-1) = (T_incr(2:end,1:end-1) - diag(ones(n_max,1)*xi(i),1)) \ b_new(2:end);
            b_new(end) = 0; c_right = c_right - c_right(n_right+1) / b_new(n_right+1) * b_new(1:end-1);
            n_right = n_right - 1;
            fx_right(i) = NaN;
         end;
      end;
      int_right = h_right * w(1:n_right+1) * c_right(1:n_right+1);
      err_right = h_right * norm(c_right - c_old);
      if abs(ivals(i_max).int) > 0 && ...
         int_right / ivals(i_max).int > 1
         ndiv_right = ivals(i_max).ndiv + 1;
      else
         ndiv_right = ivals(i_max).ndiv;
      end;
      if ndiv_right > ndiv_max && 2*ndiv_right > ivals(i_max).depth
         warning(sprintf('possibly␣divergent␣integral␣in␣the␣interval␣[%e,%e]!',a_right,b_right));
         int = sign(int) * Inf;
         return;
      end;
      if points_right(end) <= points_right(end-1) || ...
         err_right < abs(int_right) * Vcond * eps
         err_excess = err_excess + err_right;
         int_final = int_final + int_right;
      else
         nr_ivals = nr_ivals + 1;
         ivals(nr_ivals).c = c_right;
         ivals(nr_ivals).c_old = c_old;
         ivals(nr_ivals).a = a_right; ivals(nr_ivals).b = b_right;
         ivals(nr_ivals).fx = fx_right;
         ivals(nr_ivals).b_new = b_new;
         ivals(nr_ivals).b_old = b_old;
         ivals(nr_ivals).int = int_right;
         ivals(nr_ivals).n = n_right;
         ivals(nr_ivals).n_old = ivals(i_max).n;
```

```
            ivals(nr_ivals).err = err_right;
            ivals(nr_ivals).tol = ivals(i_max).tol / sqrt(2);
            ivals(nr_ivals).depth = ivals(i_max).depth + 1;
            ivals(nr_ivals).ndiv = ndiv_right;
         end;

         % copy last interval into i_max
         ivals(i_max) = ivals(nr_ivals);
         nr_ivals = nr_ivals - 1;

         % compute the running err and new max
         i_max = 1; i_min = 1; err = err_final; int = int_final;
         for i=1:nr_ivals
            if ivals(i).err > ivals(i_max).err, i_max = i;
            elseif ivals(i).err < ivals(i_min).err, i_min = i; end;
            err = err + ivals(i).err;
            int = int + ivals(i).int;
         end;

         % nuke smallest element if stack is larger than 500
         if nr_ivals > 500
            err_final = err_final + ivals(i_min).err;
            int_final = int_final + ivals(i_min).int;
            ivals(i_min) = ivals(nr_ivals);
            if i_max == nr_ivals, i_max = i_min; end;
            nr_ivals = nr_ivals - 1;
         end;

         % are we there yet?
         if err < abs(int) * tol || ...
            (err_final > abs(int) * tol && err - err_final < abs(int) * tol) || ...
            nr_ivals == 0
            break;
         end;

      end; % main loop

      % clean-up and tabulate
      err = err + err_excess;

end
```

## B.2 A Doubly-Adaptive Quadrature Algorithm using the Naive Error Estimate

```
function [ int , err , nr_points ] = int_gonnet2008c ( f , a , b , tol )
%INT_GONNET2008C  evaluates an integral using adaptive quadrature. The
%   algorithm uses Clenshaw-Curtis quadrature rules of increasing
%   degree in each interval and bisects the interval if either the
%   function does not appear to be smooth or a rule of maximum
%   degree has been reached. The error estimate is computed from the
%   L2-norm of the difference between two successive interpolations
%   of the integrand over the nodes of the respective quadrature rules.
%
%   INT = INT_GONNET2008C ( F , A , B , TOL ) approximates the integral
%   of F in the interval [A,B] up to the relative tolerance TOL. The
%   integrand F should accept a vector argument and return a vector
%   result containing the integrand evaluated at each element of the
%   argument.
%
%   [INT,ERR,NR_POINTS] = INT_GONNET2008C ( F , A , B , TOL ) returns
%   ERR, an estimate of the absolute integration error as well as
%   NR_POINTS, the number of function values for which the integrand
%   was evaluated. The value of ERR may be larger than the requested
%   tolerance, indicating that the integration may have failed.
%
```

```
%    INT_GONNET2008C halts with a warning if the integral is or appears
%    to be divergent.
%
%    Reference: "Adaptive Quadrature Re-Revisited", P. Gonnet, submitted
%          to ACM Transactions on Mathematical Software, 2008.

   % declare persistent variables
   persistent n xi_1 xi_2 xi_3 xi_4 b_1_def b_2_def b_3_def b_4_def ...
      V_1 V_2 V_3 V_4 V_1_inv V_2_inv V_3_inv V_4_inv xx Vcond T_left T_right w U

   % have the persistent variables been declared already?
   if ~exist('U') || isempty(U)

      % the nodes and newton polynomials
      n = [4,8,16,32];
      xi_1 = -cos([0:n(1)]/n(1)*pi)';
      xi_2 = -cos([0:n(2)]/n(2)*pi)';
      xi_3 = -cos([0:n(3)]/n(3)*pi)';
      xi_4 = -cos([0:n(4)]/n(4)*pi)';
      b_1_def = [0., .233284737407921723637836578544e-1, 0., ...
         -.831479419283098085685277496071e-1, 0.,0.0541462136776153483932540272848 ]';
      b_2_def = [0., .883654308363339862264532494396e-4, 0., ...
         .238811521522368331303214066075e-3, 0., .135365534194038370983135068211e-2, ...
         0., -.520710690438660595086839959882e-2, 0.,0.00341659266223572272892690737979 ]';
      b_3_def = [0., .379785635776247894184454273159e-7, 0., ...
         .655473977795402040043020497901e-7, 0., .103479954638984842226816620692e-6, ...
         0., .173700624961660596894381303819e-6, 0., .337719613424065357737699682062e-6, ...
         0., .877423283550614343733565759649e-6, 0., .515657204371051131603503471028e-5, ...
         0.,-.203244736027387801432055290742e-4, 0.,0.0000134265158311651777460545854542 ]';
      b_4_def = [0., .703046511513775683031092069125e-13, 0., ...
         .110617117381148770138566741591e-12, 0., .146334657087392356024202217074e-12, ...
         0., .184948444492681259461791759092e-12, 0., .231429962470609662207589449428e-12, ...
         0., .291520062115989014852816512412e-12, 0., .373653379768759953435020783965e-12, ...
         0., .491840460397998449461993671859e-12, 0., .671514395653454630785723660045e-12, ...
         0., .963162916392726862525650710866e-12, 0., .147853378943890691325323722031e-11, ...
         0., .250420145651013003355273649380e-11, 0., .495516257435784759806147914867e-11, ...
         0., .130927034711760871648068641267e-10, 0., .779528640561654357271364483150e-10, ...
         0., -.309866395328070487426324760520e-9, 0., .205572320292667201732878773151e-9]';

      % compute the coefficients
      V_1 = [ ones(size(xi_1)) xi_1 ];
      V_2 = [ ones(size(xi_2)) xi_2 ];
      V_3 = [ ones(size(xi_3)) xi_3 ];
      V_4 = [ ones(size(xi_4)) xi_4 ];
      xil = (xi_4 - 1) / 2; xir = (xi_4 + 1) / 2;
      Vl = [ ones(size(xil)) xil ]; Vr = [ ones(size(xir)) xir ];
      xx = linspace(-1,1,500)'; Vx = [ ones(size(xx)) xx ];
      for i=3:n(1)+1
         V_1 = [ V_1 , ((2*i-3) / (i-1) * xi_1 .* V_1(:,i-1) - (i-2) / (i-1) * V_1(:,i-2)) ];
      end;
      for i=3:n(2)+1
         V_2 = [ V_2 , ((2*i-3) / (i-1) * xi_2 .* V_2(:,i-1) - (i-2) / (i-1) * V_2(:,i-2)) ];
      end;
      for i=3:n(3)+1
         V_3 = [ V_3 , ((2*i-3) / (i-1) * xi_3 .* V_3(:,i-1) - (i-2) / (i-1) * V_3(:,i-2)) ];
      end;
      for i=3:n(4)+1
         V_4 = [ V_4 , ((2*i-3) / (i-1) * xi_4 .* V_4(:,i-1) - (i-2) / (i-1) * V_4(:,i-2)) ];
         Vx = [ Vx , ((2*i-3) / (i-1) * xx .* Vx(:,i-1) - (i-2) / (i-1) * Vx(:,i-2)) ];
         Vl = [ Vl , ((2*i-3) / (i-1) * xil .* Vl(:,i-1) - (i-2) / (i-1) * Vl(:,i-2)) ];
         Vr = [ Vr , ((2*i-3) / (i-1) * xir .* Vr(:,i-1) - (i-2) / (i-1) * Vr(:,i-2)) ];
      end;
      for i=1:n(1)+1, V_1(:,i) = V_1(:,i) * sqrt(4*i-2)/2; end;
      for i=1:n(2)+1, V_2(:,i) = V_2(:,i) * sqrt(4*i-2)/2; end;
      for i=1:n(3)+1, V_3(:,i) = V_3(:,i) * sqrt(4*i-2)/2; end;
      for i=1:n(4)+1
         V_4(:,i) = V_4(:,i) * sqrt(4*i-2)/2;
         Vx(:,i) = Vx(:,i) * sqrt(4*i-2)/2;
         Vl(:,i) = Vl(:,i) * sqrt(4*i-2)/2;
         Vr(:,i) = Vr(:,i) * sqrt(4*i-2)/2;
      end;
      V_1_inv = inv(V_1); V_2_inv = inv(V_2); V_3_inv = inv(V_3); V_4_inv = inv(V_4);
      Vcond = [ cond(V_1) , cond(V_2) , cond(V_3) , cond(V_4) ];

      % shift matrix
```

```
        T_left = V_4_inv * Vl;
        T_right = V_4_inv * Vr;

        % compute the integral
        % w := [ seq( int(T(k,x),x=-1..1) , k=0..n ) ];
        w = [ sqrt(2) , zeros(1,n(4)) ] / 2; % legendre

        % set-up the downdate matrix
        k = [0:n(4)]';
        U = diag(sqrt((k+1).^2 ./ (2*k+1) ./ (2*k+3))) + diag(sqrt(k(3:end).^2 ./ (4*k(3:end).^2-1)),2);

    end; % if exist('n')

    % create the original datatype
    ivals = struct( ...
        'a', [], 'b',[], ...
        'c', [], 'c_old', [], ...
        'fx', [], ...
        'int', [], ...
        'err', [], ...
        'tol', [], ...
        'depth', [], ...
        'rdepth', [], ...
        'ndiv', [] );

    % compute the first interval
    points = (a+b)/2 + (b-a) * xi_4 / 2;
    fx = f(points); nans = [];
    for i=1:length(fx), if ~isfinite(fx(i)), nans = [ i , nans ]; fx(i) = 0.0; end; end;
    ivals(1).c = zeros(n(4)+1,4);
    ivals(1).c(1:n(4)+1,4) = V_4_inv * fx;
    ivals(1).c(1:n(3)+1,3) = V_3_inv * fx([1:2:n(4)+1]);
    for i=nans, fx(i) = NaN; end;
    ivals(1).fx = fx;
    ivals(1).c_old = zeros(size(fx));
    ivals(1).a = a; ivals(1).b = b;
    ivals(1).int = (b-a) * w * ivals(1).c(:,4);
    c_diff = norm(ivals(1).c(:,4) - ivals(1).c(:,3));
    ivals(1).err = (b-a) * c_diff;
    if c_diff / norm(ivals(1).c(:,4)) > 0.1
        ivals(1).err = max( ivals(1).err , (b-a) * norm(ivals(1).c(:,4)) );
    end;
    ivals(1).tol = tol;
    ivals(1).depth = 4;
    ivals(1).ndiv = 0;
    ivals(1).rdepth = 1;

    % init some globals
    int = ivals(1).int; err = ivals(1).err; nr_ivals = 1;
    int_final = 0; err_final = 0; err_excess = 0;
    i_max = 1; nr_points = n(4)+1;
    ndiv_max = 20;

    % do we even need to go this way?
    if err < int * tol, return; end;

    % main loop
    while true

        % get some global data
        a = ivals(i_max).a; b = ivals(i_max).b;
        depth = ivals(i_max).depth;
        split = 0;

        % depth of the old interval
        if depth == 1
            points = (a+b)/2 + (b-a)*xi_2/2;
            fx(1:2:n(2)+1) = ivals(i_max).fx;
            fx(2:2:n(2)) = f(points(2:2:n(2)));
            fx = fx(1:n(2)+1);
            nans = [];
            for i=1:length(fx), if ~isfinite(fx(i)), fx(i) = 0.0; nans = [ i , nans ]; end; end;
            c_new = V_2_inv * fx;
            if length(nans) > 0
                b_new = b_2_def; n_new = n(2);
                for i=nans
                    b_new(1:end-1) = (U(1:n(2)+1,1:n(2)+1) - diag(ones(n(2),1)*xi_2(i),1)) \ b_new(2:end);
                    b_new(end) = 0; c_new = c_new - c_new(n_new+1) / b_new(n_new+1) * b_new(1:end-1);
                    n_new = n_new - 1; fx(i) = NaN;
                end;
            end;
            ivals(i_max).fx = fx;
            nc = norm(c_new);
            nr_points = nr_points + n(2)-n(1);
            ivals(i_max).c(1:n(2)+1,2) = c_new;
            c_diff = norm(ivals(i_max).c(:,1) - ivals(i_max).c(:,2));
            ivals(i_max).err = (b-a) * c_diff;
            int_old = ivals(i_max).int; ivals(i_max).int = (b-a) * w(1) * c_new(1);
            if nc > 0 && c_diff / nc > 0.1
                split = 1;
            else
                ivals(i_max).depth = 2;
            end;
        elseif depth == 2
            points = (a+b)/2 + (b-a)*xi_3/2;
            fx(1:2:n(3)+1) = ivals(i_max).fx;
            fx(2:2:n(3)) = f(points(2:2:n(3)));
            fx = fx(1:n(3)+1);
            nans = [];
            for i=1:length(fx), if ~isfinite(fx(i)), fx(i) = 0.0; nans = [ i , nans ]; end; end;
            c_new = V_3_inv * fx;
            if length(nans) > 0
                b_new = b_3_def; n_new = n(3);
                for i=nans
                    b_new(1:end-1) = (U(1:n(3)+1,1:n(3)+1) - diag(ones(n(3),1)*xi_3(i),1)) \ b_new(2:end);
                    b_new(end) = 0; c_new = c_new - c_new(n_new+1) / b_new(n_new+1) * b_new(1:end-1);
                    n_new = n_new - 1; fx(i) = NaN;
                end;
            end;
            ivals(i_max).fx = fx;
            nc = norm(c_new);
            nr_points = nr_points + n(3)-n(2);
            ivals(i_max).c(1:n(3)+1,3) = c_new;
            c_diff = norm(ivals(i_max).c(:,2) - ivals(i_max).c(:,3));
            ivals(i_max).err = (b-a) * c_diff;
            int_old = ivals(i_max).int; ivals(i_max).int = (b-a) * w(1) * c_new(1);
            if nc > 0 && c_diff / nc > 0.1
                split = 1;
            else
                ivals(i_max).depth = 3;
            end;
        elseif depth == 3
            points = (a+b)/2 + (b-a)*xi_4/2;
            fx(1:2:n(4)+1) = ivals(i_max).fx;
            fx(2:2:n(4)) = f(points(2:2:n(4)));
            fx = fx(1:n(4)+1);
            nans = [];
            for i=1:length(fx), if ~isfinite(fx(i)), fx(i) = 0.0; nans = [ i , nans ]; end; end;
            c_new = V_4_inv * fx;
            if length(nans) > 0
                b_new = b_4_def; n_new = n(4);
                for i=nans
                    b_new(1:end-1) = (U(1:n(4)+1,1:n(4)+1) - diag(ones(n(4),1)*xi_4(i),1)) \ b_new(2:end);
                    b_new(end) = 0; c_new = c_new - c_new(n_new+1) / b_new(n_new+1) * b_new(1:end-1);
                    n_new = n_new - 1; fx(i) = NaN;
                end;
            end;
            ivals(i_max).fx = fx;
            nc = norm(c_new);
            nr_points = nr_points + n(4)-n(3);
            ivals(i_max).c(:,4) = c_new;
            c_diff = norm(ivals(i_max).c(:,3) - ivals(i_max).c(:,4));
            ivals(i_max).err = (b-a) * c_diff;
            int_old = ivals(i_max).int; ivals(i_max).int = (b-a) * w(1) * c_new(1);
            if nc > 0 && c_diff / nc > 0.1
                split = 1;
            else
                ivals(i_max).depth = 4;
            end;
        else
```

```
   split = 1;
end;

% can we safely ignore this interval?
if points(2) <= points(1) || points(end) <= points(end-1) || ...
   ivals(i_max).err < abs(ivals(i_max).int) * eps * Vcond(ivals(i_max).depth)

   err_final = err_final + ivals(i_max).err;
   int_final = int_final + ivals(i_max).int;
   ivals(i_max) = ivals(nr_ivals);
   nr_ivals = nr_ivals - 1;
elseif split
   m = (a + b) / 2;
   nr_ivals = nr_ivals + 1;
   ivals(nr_ivals).a = a; ivals(nr_ivals).b = m;
   ivals(nr_ivals).tol = ivals(i_max).tol / sqrt(2);
   ivals(nr_ivals).depth = 1; ivals(nr_ivals).rdepth = ivals(i_max).rdepth + 1;
   ivals(nr_ivals).c = zeros(n(4)+1,4);
   fx = [ ivals(i_max).fx(1) ; f((a+m)/2+(m-a)*xi_1(2:end-1)/2) ; ivals(i_max).fx((end+1)/2) ];
   nr_points = nr_points + n(1)-1; nans = [];
   for i=1:length(fx), if ~isfinite(fx(i)), fx(i) = 0.0; nans = [ i , nans ]; end; end;
   c_new = V_1_inv * fx;
   if length(nans) > 0
      b_new = b_1_def; n_new = n(1);
      for i=nans
         b_new(1:end-1) = (U(1:n(1)+1,1:n(1)+1) - diag(ones(n(1),1)*xi_1(i),1)) \ b_new(2:end);
         b_new(end) = 0; c_new = c_new - c_new(n_new+1) / b_new(n_new+1) * b_new(1:end-1);
         n_new = n_new - 1; fx(i) = NaN;
      end;
   end;
   ivals(nr_ivals).fx = fx;
   ivals(nr_ivals).c(1:n(1)+1,1) = c_new; nc = norm(c_new);
   ivals(nr_ivals).c_old = T_left * ivals(i_max).c(:,depth);
   c_diff = norm(ivals(nr_ivals).c(:,1) - ivals(nr_ivals).c_old);
   ivals(nr_ivals).err = (m - a) * c_diff;
   ivals(nr_ivals).int = (m - a) * ivals(nr_ivals).c(1,1) * w(1);
   ivals(nr_ivals).ndiv = ivals(i_max).ndiv + ...
      (abs(ivals(i_max).c(1,1)) > 0 && ivals(nr_ivals).c(1,1) / ivals(i_max).c(1,1) > 2);
   if ivals(nr_ivals).ndiv > ndiv_max && 2*ivals(nr_ivals).ndiv > ivals(nr_ivals).rdepth
      warning(sprintf('possibly␣divergent␣integral␣in␣the␣interval␣[%e,%e]!␣(h=%e)',a,m,m-a));
      int = sign(int) * Inf;
      return;
   end;
   nr_ivals = nr_ivals + 1;
   ivals(nr_ivals).a = m; ivals(nr_ivals).b = b;
   ivals(nr_ivals).tol = ivals(i_max).tol / sqrt(2);
   ivals(nr_ivals).depth = 1; ivals(nr_ivals).rdepth = ivals(i_max).rdepth + 1;
   ivals(nr_ivals).c = zeros(n(4)+1,4);
   fx = [ ivals(i_max).fx((end+1)/2) ; f((m+b)/2+(b-m)*xi_1(2:end-1)/2) ; ivals(i_max).fx(end) ];
   nr_points = nr_points + n(1)-1; nans = [];
   for i=1:length(fx), if ~isfinite(fx(i)), fx(i) = 0.0; nans = [ i , nans ]; end; end;
   c_new = V_1_inv * fx;
   if length(nans) > 0
      b_new = b_1_def; n_new = n(1);
      for i=nans
         b_new(1:end-1) = (U(1:n(1)+1,1:n(1)+1) - diag(ones(n(1),1)*xi_1(i),1)) \ b_new(2:end);
         b_new(end) = 0; c_new = c_new - c_new(n_new+1) / b_new(n_new+1) * b_new(1:end-1);
         n_new = n_new - 1; fx(i) = NaN;
      end;
   end;
   ivals(nr_ivals).fx = fx;
   ivals(nr_ivals).c(1:n(1)+1,1) = c_new; nc = norm(c_new);
   ivals(nr_ivals).c_old = T_right * ivals(i_max).c(:,depth);
   c_diff = norm(ivals(nr_ivals).c(:,1) - ivals(nr_ivals).c_old);
   ivals(nr_ivals).err = (b - m) * c_diff;
   ivals(nr_ivals).int = (b - m) * ivals(nr_ivals).c(1,1) * w(1);
   ivals(nr_ivals).ndiv = ivals(i_max).ndiv + ...
      (abs(ivals(i_max).c(1,1)) > 0 && ivals(nr_ivals).c(1,1) / ivals(i_max).c(1,1) > 2);
   if ivals(nr_ivals).ndiv > ndiv_max && 2*ivals(nr_ivals).ndiv > ivals(nr_ivals).rdepth
      warning(sprintf('possibly␣divergent␣integral␣in␣the␣interval␣[%e,%e]!␣(h=%e)',m,b,b-m));
      int = sign(int) * Inf;
      return;
   end;
   ivals(i_max) = ivals(nr_ivals);
   nr_ivals = nr_ivals - 1;
```

```
        end;

        % compute the running err and new max
        i_max = 1; i_min = 1; err = err_final; int = int_final;
        for i=1:nr_ivals
           if ivals(i).err > ivals(i_max).err, i_max = i;
           elseif ivals(i).err < ivals(i_min).err, i_min = i; end;
           err = err + ivals(i).err;
           int = int + ivals(i).int;
        end;

        % nuke smallest element if stack is larger than 500
        if nr_ivals > 200
           err_final = err_final + ivals(i_min).err;
           int_final = int_final + ivals(i_min).int;
           ivals(i_min) = ivals(nr_ivals);
           if i_max == nr_ivals, i_max = i_min; end;
           nr_ivals = nr_ivals - 1;
        end;

        % get up and leave?
        if err < abs(int) * tol || ...
           (err_final > abs(int) * tol && err - err_final < abs(int) * tol) || ...
           nr_ivals == 0
           break;
        end;

     end; % main loop

     % clean-up and tabulate
     err = err + err_excess;

  end
```

## B.3 An Adaptive Quadrature Algorithm using the Refined Error Estimate

```
function [ int , err , nr_points ] = int_gonnet2008b ( f , a , b , tol )
%INT_GONNET2008B  evaluates an integral using adaptive quadrature. The
%   algorithm is based on a 10-point Clenshaw-Curtis rule and the error
%   is extrapolated from the L2-norm of the difference between two
%   successive interpolations of the integrand over the nodes of the
%   respective quadrature rules.
%
%   INT = INT_GONNET2008B ( F , A , B , TOL ) approximates the integral
%   of F in the interval [A,B] up to the relative tolerance TOL. The
%   integrand F should accept a vector argument and return a vector
%   result containing the integrand evaluated at each element of the
%   argument.
%
%   [INT,ERR,NR_POINTS] = INT_GONNET2008B ( F , A , B , TOL ) returns
%   ERR, an estimate of the absolute integration error as well as
%   NR_POINTS, the number of function values for which the integrand
%   was evaluated. The value of ERR may be larger than the requested
%   tolerance, indicating that the integration may have failed.
%
%   INT_GONNET2008B halts with a warning if the integral is or appears
%   to be divergent.
%
%   Reference: "Adaptive Quadrature Re-Revisited", P. Gonnet, submitted
%       to ACM Transactions on Mathematical Software, 2008.

   % declare persistent variables
   persistent n xi b_def b_def_left b_def_right V Vx xx Vinv Vcond Tleft Tright w

   % have the persistent variables been declared already?
   if ~exist('w') || isempty(w)

      % the nodes and function values
```

```
        n = 10;
        xi = -cos([0:n]/n*pi)';
        b_def = [0., .106208450524439887291410155456e-4, 0., ...
           .227130523187035097706861204296e-4, 0., .581888042915549558524788754554e-4, ...
           0., .334667295980313236720792889210e-3, 0., -.130155910942313246816263138278e-2, 0., ...
           .856102717782094742857796872476e-3]';
        b_def_left = 2^(n+1) * [.276213586400995126719079828971e-3, ...
           .499657655492227449762439076973e-3, .523434680236984721004073014910e-3, ...
           .257874261861280205575039917099e-3, -.748342903416082700961183312797e-3, ...
           -.917669983469695220709693581407e-3, .549500980250147994974675357971e-3, ...
           .300060029460695461688333929627e-3, -.276678492776836119682157766061e-3, ...
           .761043473405371645812866738709e-4, -.918691057168920637420186132198e-5, ...
           .418018905167038448661033629139e-6]';
        b_def_right = 2^(n+1) * [-.276213586400995126719079828971e-3, ...
           .499657655492227449762439076973e-3, -.523434680236984721004073014910e-3, ...
           .257874261861280205575039917099e-3, .748342903416082700961183312797e-3, ...
           -.917669983469695220709693581407e-3, -.549500980250147994974675357971e-3, ...
           .300060029460695461688333929627e-3, .276678492776836119682157766061e-3, ...
           .761043473405371645812866738709e-4, .918691057168920637420186132198e-5, ...
           .418018905167038448661033629139e-6]';

        % compute the coefficients
        V = [ ones(size(xi)) xi ];
        xil = (xi - 1) / 2; xir = (xi + 1) / 2;
        Vl = [ ones(size(xil)) xil ]; Vr = [ ones(size(xir)) xir ];
        xx = linspace(-1,1,200)'; Vx = [ ones(size(xx)) xx ];
        for i=3:n+2
           V = [ V , ((2*i-3) / (i-1) * xi .* V(:,i-1) - (i-2) / (i-1) * V(:,i-2)) ];
           Vx = [ Vx , ((2*i-3) / (i-1) * xx .* Vx(:,i-1) - (i-2) / (i-1) * Vx(:,i-2)) ];
           Vl = [ Vl , ((2*i-3) / (i-1) * xil .* Vl(:,i-1) - (i-2) / (i-1) * Vl(:,i-2)) ];
           Vr = [ Vr , ((2*i-3) / (i-1) * xir .* Vr(:,i-1) - (i-2) / (i-1) * Vr(:,i-2)) ];
        end;
        for i=1:n+2
           V(:,i) = V(:,i) * sqrt(4*i-2)/2;
           Vx(:,i) = Vx(:,i) * sqrt(4*i-2)/2;
           Vl(:,i) = Vl(:,i) * sqrt(4*i-2)/2;
           Vr(:,i) = Vr(:,i) * sqrt(4*i-2)/2;
        end;
        Vinv = inv(V(:,1:n+1));
        Vcond = cond(V);

        % shift matrix
        Tleft = V(:,1:n+1) \ Vl(:,1:n+1);
        Tright = V(:,1:n+1) \ Vr(:,1:n+1);

        % compute the integral
        w = [ sqrt(2) , zeros(1,n) ] / 2; % legendre

     end; % if exist('w')

     % create the original datatype
     ivals = struct( ...
        'a', [], 'b',[], ...
        'fx', [], ...
        'c', [], 'c_old', [], ...
        'b_new', [], 'b_old', [], ...
        'fn', [], 'fn_old', [], ...
        'int', [], ...
        'err', [], ...
        'tol', [], ...
        'depth', [], ...
        'ndiv' , [] );
     ivals_new = ivals;

     % compute the first interval
     points = a + (b-a) * (xi + 1) / 2;
     fx = f(points); nans = [];
     for i=1:length(fx), if ~isfinite(fx(i)), nans = [i,nans]; fx(i) = 0.0; end; end;
     ivals(1).c = Vinv * fx;
     for i=nans, fx(i) = NaN; end;
     ivals(1).fx = fx;
     ivals(1).c_old = zeros(size(fx));
     ivals(1).a = a; ivals(1).b = b;
     ivals(1).int = (b-a) * w * ivals(1).c;
     ivals(1).b_new = b_def;
```

```
    ivals(1).fn = 0;
    ivals(1).err = abs((b-a) * norm(ivals(1).c));
    ivals(1).tol = tol;
    ivals(1).depth = 1;
    ivals(1).ndiv = 0;

    % init some globals
    int = ivals(1).int; err = ivals(1).err; nr_ivals = 1;
    int_final = 0; err_final = 0; err_excess = 0;
    i_max = 1; nr_points = n+1;
    ndiv_max = 20; theta_1 = 1.1;

    % main loop
    while true

        % compute the left interval
        a_left = ivals(i_max).a; b_left = (ivals(i_max).a + ivals(i_max).b)/2;
        h_left = b_left - a_left;
        points_left = a_left + h_left * (xi + 1) / 2;
        nr_points = nr_points + n-2;
        fx_left = [ ivals(i_max).fx(1) ; f(points_left(2:end-1)) ; ivals(i_max).fx(n/2+1) ];
        nans = [];
        for i=1:length(fx_left), if ~isfinite(fx_left(i)), nans = [ nans , i ]; fx_left(i) = 0.0; end; end;
        c_left = Vinv * fx_left;
        if length(nans) > 0
            k = [0:length(xi)-1]';
            U = diag(sqrt((k+1).^2 ./ (2*k+1) ./ (2*k+3))) + diag(sqrt(k(3:end).^2 ./ (4*k(3:end).^2-1)),2);
            b_new_left = b_def; n_left = n;
            for i=nans
                b_new_left(1:end-1) = (U - diag(ones(length(xi)-1,1)*xi(i),1)) \ b_new_left(2:end);
                b_new_left(end) = 0;
                c_left = c_left - c_left(n_left+1) / b_new_left(n_left+1) * b_new_left(1:end-1);
                n_left = n_left - 1; fx_left(i) = NaN;
            end;
        else
            b_new_left = b_def;
        end;
        nc_left = norm(c_left);
        c_old_left = Tleft * ivals(i_max).c;
        c_diff = norm(c_left - c_old_left);
        if ivals(i_max).b_new(end) == 0, b_old_left =  2^(n+1) * [ Tleft * ivals(i_max).b_new(1:end-1) ; 0 ];
        else b_old_left = b_def_left; end;
        fn_left = c_diff / norm(b_old_left - b_new_left);
        int_left = h_left * w * c_left;
        if abs(ivals(i_max).int) > 0 && int_left / ivals(i_max).int > 1
            ndiv_left = ivals(i_max).ndiv + 1;
        else
            ndiv_left = ivals(i_max).ndiv;
        end;
        if ndiv_left > ndiv_max && 2*ndiv_right > ivals(i_max).depth
            warning(sprintf('possibly␣divergent␣integral␣in␣the␣interval␣[%e,%e]!',a_left,b_left));
            int = sign(int) * Inf;
            return;
        end;
        absVcmf = abs(V(:,1:n+1) * c_old_left - fx_left);
        absVb = abs( V * b_old_left );
        if max(absVcmf(2:end-1) - theta_1 * fn_left * absVb(2:end-1)) > eps*Vcond*nc_left
            err_left = h_left * c_diff;
        else
            err_left = abs( h_left * fn_left * norm(b_new_left) );
        end;

        % store the left interval
        if points_left(end) <= points_left(end-1) || ...
            err_left < abs(int_left) * Vcond * eps
            % disp(sprintf('excess: %e (eps=%e,h=%e)',err_left,nc_left * Vcond * eps,b_left - a_left));
            err_excess = err_excess + err_left;
            int_final = int_final + int_left;
        else % if err_left > abs(int) * ivals(i_max).tol / sqrt(2)
            nr_ivals = nr_ivals + 1;
            ivals(nr_ivals).c = c_left;
            ivals(nr_ivals).fx = fx_left;
            ivals(nr_ivals).c_old = c_old_left;
            ivals(nr_ivals).a = a_left; ivals(nr_ivals).b = b_left;
            ivals(nr_ivals).b_new = b_new_left;
```

```
   ivals(nr_ivals).b_old = b_old_left;
   ivals(nr_ivals).fn = fn_left;
   ivals(nr_ivals).fn_old = ivals(i_max).fn;
   ivals(nr_ivals).int = int_left;
   ivals(nr_ivals).err = err_left;
   ivals(nr_ivals).tol = ivals(i_max).tol / sqrt(2);
   ivals(nr_ivals).depth = ivals(i_max).depth + 1;
   ivals(nr_ivals).ndiv = ndiv_left;
end;

% compute the right interval
a_right = (ivals(i_max).a + ivals(i_max).b)/2; b_right = ivals(i_max).b;
h_right = b_right - a_right;
points_right = a_right + h_right * (xi + 1) / 2;
nr_points = nr_points + n-2;
fx_right = [ ivals(i_max).fx(n/2+1) ; f(points_right(2:end-1)) ; ivals(i_max).fx(end) ];
nans = [];
for i=1:length(fx_right), if ~isfinite(fx_right(i)), nans = [ nans , i ]; fx_right(i) = 0.0; end; end;
c_right = Vinv * fx_right;
if length(nans) > 0
   k = [0:length(xi)-1]';
   U = diag(sqrt((k+1).^2 ./ (2*k+1) ./ (2*k+3))) + diag(sqrt(k(3:end).^2 ./ (4*k(3:end).^2-1)),2);
   b_new_right = b_def; n_right = n;
   for i=nans
      b_new_right(1:end-1) = (U - diag(ones(length(xi)-1,1)*xi(i),1)) \ b_new_right(2:end);
      b_new_right(end) = 0;
      c_right = c_right - c_right(n_right+1) / b_new_right(n_right+1) * b_new_right(1:end-1);
      n_right = n_right - 1; fx_right(i) = NaN;
   end;
else
   b_new_right = b_def;
end;
nc_right = norm(c_right);
c_old_right = Tright * ivals(i_max).c;
c_diff = norm(c_right - c_old_right);
if ivals(i_max).b_new(end) == 0, b_old_right = 2^(n+1) * [ Tright * ivals(i_max).b_new(1:end-1) ; 0 ];
else b_old_right = b_def_right; end;
fn_right = c_diff / norm(b_old_right - b_new_right);
int_right = h_right * w * c_right;
if abs(ivals(i_max).int) > 0 && int_right / ivals(i_max).int > 1
   ndiv_right = ivals(i_max).ndiv + 1;
else
   ndiv_right = ivals(i_max).ndiv;
end;
if ndiv_right > ndiv_max && 2*ndiv_right > ivals(i_max).depth
   warning(sprintf('possibly␣divergent␣integral␣in␣the␣interval␣[%e,%e]!',a_right,b_right));
   int = sign(int) * Inf;
   return;
end;
absVcmf = abs(V(:,1:n+1) * c_old_right - fx_right);
absVb = abs( V * b_old_right );
if max(absVcmf(2:end-1) - theta_1 * fn_right * absVb(2:end-1)) > eps*Vcond*nc_left
   err_right = h_right * c_diff;
else
   err_right = abs( h_right * fn_right * norm(b_new_right) );
end;

% store the right interval
if points_right(end) <= points_right(end-1) || ...
   err_right < abs(int_right) * Vcond * eps
   % disp(sprintf('excess: %e (eps=%e,h=%e)',err_right,nc_right * Vcond * eps,b_right - a_right));
   err_excess = err_excess + err_right;
   int_final = int_final + int_right;
else % if err_right > abs(int) * ivals(i_max).tol / sqrt(2)
   nr_ivals = nr_ivals + 1;
   ivals(nr_ivals).c = c_right;
   ivals(nr_ivals).fx = fx_right;
   ivals(nr_ivals).c_old = c_old_right;
   ivals(nr_ivals).a = a_right; ivals(nr_ivals).b = b_right;
   ivals(nr_ivals).b_new = b_new_right;
   ivals(nr_ivals).b_old = b_old_right;
   ivals(nr_ivals).fn = fn_right;
   ivals(nr_ivals).fn_old = ivals(i_max).fn;
   ivals(nr_ivals).int = int_right;
   ivals(nr_ivals).err = err_right;
```

```
            ivals(nr_ivals).tol = ivals(i_max).tol / sqrt(2);
            ivals(nr_ivals).depth = ivals(i_max).depth + 1;
            ivals(nr_ivals).ndiv = ndiv_right;
         end;

         % copy last interval into i_max
         ivals(i_max) = ivals(nr_ivals);
         nr_ivals = nr_ivals - 1;

         % compute the running err and new max
         i_max = 1; i_min = 1; err = err_final; int = int_final;
         for i=1:nr_ivals
            if ivals(i).err > ivals(i_max).err, i_max = i;
            elseif ivals(i).err < ivals(i_min).err, i_min = i; end;
            err = err + ivals(i).err;
            int = int + ivals(i).int;
         end;

         % nuke smallest element if stack is larger than 500
         if nr_ivals > 200
            err_final = err_final + ivals(i_min).err;
            int_final = int_final + ivals(i_min).int;
            ivals(i_min) = ivals(nr_ivals);
            if i_max == nr_ivals, i_max = i_min; end;
            nr_ivals = nr_ivals - 1;
         end;

         % are we done yet?
         if err < abs(int) * tol || ...
            (err_final > abs(int) * tol && err - err_final < abs(int) * tol) || ...
            nr_ivals == 0
            break;
         end;

      end; % main loop

      % clean-up and tabulate
      err = err + err_excess;

   end
```

# Bibliography

[1] A. Aitken. On Bernoulli's numerical solution of algebraic equations. *Proceedings of the Royal Society of Edinburgh*, 46:289–305, 1926.

[2] Z. Balles and L. N. Trefethen. An extensions of MATLAB to continuous functions and operators. *SIAM Journal of Scientific Computing*, 25(5):1743–1770, 2004.

[3] F. L. Bauer, H. Rutishauser, and E. Stiefel. New aspects in numerical quadrature. In N. C. Metropolis, A. H. Taub, J. Todd, and C. B. Tompkins, editors, *Experimental Arithmetic, High Speed Computing and Mathematics*, pages 199–217, Providence, RI, 1963. American Mathematical Society.

[4] J. Berntsen and T. O. Espelid. On the use of Gauss quadrature in adaptive automatic integration schemes. *BIT Numerical Mathematics*, 24:239–242, 1984.

[5] J. Berntsen and T. O. Espelid. Error estimation in automatic quadrature routines. *ACM Transactions on Mathematical Software*, 17(2):233–252, 1991.

[6] J. P. Berrut and L. N. Trefethen. Barycentric Lagrange interpolation. *SIAM Review*, 46(3):501–517, 2004.

[7] Å. Björck and V. Pereyra. Solution of Vandermonde systems of equations. *Mathematics of Computation*, 24(112):893–903, 1970.

[8] J. Casaletto, M. Pickett, and J. Rice. A comparison of some numerical integration programs. *SIGNUM Newsletter*, 4(3):30–40, 1969.

[9] B. Char, K. Geddes, and G. Gonnet. The Maple symbolic computation system. *SIGSAM Bull.*, 17(3-4):31–42, 1983.

[10] C. W. Clenshaw and A. R. Curtis. A method for numerical integration on an automatic computer. *Numerische Mathematik*, 2:197–205, 1960.

[11] R. Cools and A. Haegemans. CUBPACK: Progress report. In T. O. Espelid and A. Genz, editors, *Numerical Integration*, pages 305–315. Kluwer Academic Publishers, Netherlands, 1992.

[12] P. J. Davis and P. Rabinowitz. *Numerical Integration.* Blaisdell Publishing Company, Waltham, Massachusetts, 1967.

[13] P. J. Davis and P. Rabinowitz. *Numerical Integration, 2nd Edition.* Blaisdell Publishing Company, Waltham, Massachusetts, 1984.

[14] C. de Boor. CADRE: An algorithm for numerical quadrature. In J. R. Rice, editor, *Mathematical Software*, pages 201–209. Academic Press, New York and London, 1971.

[15] E. de Doncker. An adaptive extrapolation algorithm for automatic integration. *SIGNUM Newsletter*, 13(2):12–18, 1978.

[16] J. W. Eaton. *GNU Octave Manual.* Network Theory Limited, 2002.

[17] H. Engels. *Numerical quadrature and cubature.* Academic Press, London, New York, 1980.

[18] T. O. Espelid. Integration rules, null rules and error estimation. Technical Report 22, Department of Informatics, University of Bergen, Norway, December 1988.

[19] T. O. Espelid. DQUAINT: An algorithm for adaptive quadrature over a collection of finite intervals. In T. O. Espelid and A. Genz, editors, *Numerical Integration*, pages 341–342. Kluwer Academic Publishers, Netherlands, 1992.

[20] T. O. Espelid. Doubly adaptive quadrature routines based on Newton-Cotes rules. Technical Report 229, Department of Informatics, University of Bergen, Norway, May 2002.

[21] T. O. Espelid. Doubly adaptive quadrature routines based on Newton-Cotes rules. *BIT Numerical Mathematics*, 43:319–337, 2003.

[22] T. O. Espelid. Extended doubly adaptive quadrature routines. Technical Report 266, Department of Informatics, University of Bergen, Norway, February 2004.

[23] T. O. Espelid. A test of QUADPACK and four doubly adaptive quadrature routines. Technical Report 281, Department of Informatics, University of Bergen, Norway, October 2004.

[24] T. O. Espelid. Algorithm 868: Globally doubly adaptive quadrature – reliable Matlab codes. *ACM Transactions on Mathematical Software*, 33(3):Article 21, 2007.

[25] T. O. Espelid and T. Sørevik. A discussion of a new error estimate for adaptive quadrature. *BIT Numerical Mathematics*, 29:293–294, 1989.

[26] P. Favati, G. Lotti, and F. Romani. Interpolatory integration formulas for optimal composition. *ACM Transactions on Mathematical Software*, 17(2):207–217, 1991.

[27] P. Favati, G. Lotti, and F. Romani. Local error estimates in quadrature. *BIT Numerical Mathematics*, 31:102–111, 1991.

[28] L. Fejér. Mechanische Quadraturen mit positiven Cotesschen Zahlen. *Mathematische Zeitschrift*, 37:287–309, 1933.

[29] G. E. Forsythe, M. A. Malcolm, and C. B. Moler. *Computer Methods for Mathematical Computations*. Prentice-Hall, Inc., Englewood Cliffs, N.J. 07632, 1977.

[30] L. J. Gallaher. Algorithm 303: An adaptive quadrature procedure with random panel sizes. *Communications of the ACM*, 10(6):373–374, 1967.

[31] W. Gander. Change of basis in polynomial interpolation. *Numerical Linear Algebra with Applications*, 12(8):769–778, 2005.

[32] W. Gander. Generating numerical algorithms using a computer algebra system. *BIT Numerical Mathematics*, 46:491–504, 2006.

[33] W. Gander and W. Gautschi. Adaptive quadrature — revisited. Technical Report 306, Department of Computer Science, ETH Zurich, Switzerland, 1998.

[34] W. Gander and W. Gautschi. Adaptive quadrature — revisited. *BIT*, 40(1):84–101, 2001.

[35] S. Garribba, L. Quartapelle, and G. Reina. SNIFF: Efficient self-tuning algorithm for numerical integration. *Computing*, 20:363–375, 1978.

[36] W. Gautschi. Norm estimates for inverses of Vandermonde matrices. *Numerische Mathematik*, 23:337–347, 1975.

[37] W. Gautschi. The condition of Vandermonde-like matrices involving orthogonal polynomials. *Linear Algebra and its Applications*, 52–53:293–300, 1983.

[38] W. Gautschi. *Numerical Analysis, An Introduction.* Birkhäuser Verlag, Boston, Basel and Stuttgart, 1997.

[39] W. Gautschi. *Orthogonal Polynomials: Computation and Approximation.* Oxford University Press, Great Clarendon Street, Oxford OX2 6DP, 2004.

[40] W. M. Gentleman. Implementing Clenshaw-Curtis quadrature I and II. *Communications of the ACM*, 15(5):337–346, 1972.

[41] G. H. Golub and C. F. Van Loan. *Matrix Computations.* John Hopkins University Press, Baltimore, Maryland, third edition, 1996.

[42] T. Hasegawa, S. Hibino, Y. Hosoda, and I. Ninomiya. An extended doubly-adaptive quadrature method based on the combination of the Ninomiya and the FLR schemes. *Numerical Algorithms*, 45(1–4):101–112, 2007.

[43] P. Henrici. *Elements of numerical analysis.* John Wiley & Sons Inc., New York, 1964.

[44] P. Henrici. *Essentials of Numerical Analysis, with Pocket Calculator Demonstrations.* John Wiley & Sons, Inc., New York, 1982.

[45] S. Henriksson. Contribution no. 2: Simpson numerical integration with variable length of step. *BIT Numerical Mathematics*, 1:290, 1961.

[46] N. J. Higham. Fast solution of Vandermonde-like systems involving orthogonal polynomials. *IMA Journal of Numerical Analysis*, 8:473–486, 1988.

[47] N. J. Higham. Stability analysis of algorithms for solving confluent Vandermonde-like systems. *SIAM Journal on Matrix Analysis and Applications*, 11(1):23–41, 1990.

[48] K. E. Hillstrom. Comparison of several adaptive Newton-Cotes quadrature routines in evaluating definite integrals with peaked integrands. *Communications of the ACM*, 13(6):362–365, 1970.

[49] D. K. Kahaner. 5.15 Comparison of numerical quadrature formulas. In J. R. Rice, editor, *Mathematical Software*, pages 229–259. Academic Press, New York and London, 1971.

[50] D. K. Kahaner. Numberical quadrature by the $\varepsilon$-algorithm. *Mathematics of Computation*, 26(119):689–693, 1972.

[51] D. K. Kahaner and J. Stoer. Extrapolated adaptive quadrature. *SIAM Journal on Scientific and Statistical Computing*, 4(1):31–44, 1983.

[52] F. T. Krogh and W. Van Snyder. Algorithm 699: A new representation of Patterson's quadrature formulae. *ACM Transactions on Mathematical Software*, 17(4):457–461, 1991.

[53] A. R. Krommer and C. W. Überhuber. *Computational Integration.* SIAM, Philadelphia, 1998.

[54] A. S. Kronrod. *Nodes and Weights of Quadrature Formulas — Authorized Translation from the Russian.* Consultants Bureau, New York, 1965.

[55] G. F. Kuncir. Algorithm 103: Simpson's rule integrator. *Communications of the ACM*, 5(6):347, 1962.

[56] D. P. Laurie. Sharper error estimates in adaptive quadrature. *BIT Numerical Mathematics*, 23:258–261, 1983.

[57] D. P. Laurie. Practical error estimation in numerical integration. *Journal of Computational and Applied Mathematics*, 12–13:425–431, 1985.

[58] D. P. Laurie. Stratified sequences of nested quadrature formulas. *Quaestiones Mathematicae*, 15:364–384, 1992.

[59] D. P. Laurie. Null rules and orthogonal expansions. In *Approximation and computation (West Lafayette, IN, 1993)*, volume 119 of *Internat. Ser. Numer. Math.*, pages 359–370. Birkhäuser Boston, Boston, MA, 1994.

[60] J. N. Lyness. Symmetric integration rules for hypercubes III: Construction of integration rules using null rules. *Mathematics of Computation*, 19:625–637, 1965.

[61] J. N. Lyness. Notes on the adaptive Simpson quadrature routine. *Journal of the ACM*, 16(3):483–495, 1969.

[62] J. N. Lyness. Algorithm 379: SQUANK (Simpson Quadrature Used Adaptively – Noise Killed). *Communications of the ACM*, 13(4):260–262, 1970.

[63] J. N. Lyness and J. J. Kaganove. Comments on the nature of automatic quadrature routines. *ACM Transactions on Mathematical Software*, 2(1):170–177, 1976.

[64] J. N. Lyness and J. J. Kaganove. A technique for comparing automatic quadrature routines. *The Computer Journal*, 20(2):170–177, 1977.

[65] J. N. Lyness and B. W. Ninham. Numerical quadraure and asymptotic expansions. *Mathematics of Computation*, 21:162–178, 1967.

[66] M. A. Malcolm and R. B. Simpson. Local versus global strategies for adaptive quadrature. *ACM Transactions on Mathematical Software*, 1(2):129–146, 1975.

[67] The Mathworks, Cochituate Place, 24 Prime Park Way, Natick, MA, USA. *MATLAB 6.5 Release Notes*, 2003.

[68] W. M. McKeeman. Algorithm 145: Adaptive numerical integration by Simpson's rule. *Communications of the ACM*, 5(12):604, 1962.

[69] W. M. McKeeman. Algorithm 198: Adaptive integration and multiple integration. *Communications of the ACM*, 6(8):443–444, 1963.

[70] W. M. McKeeman. Certification of algorithm 145: Adaptive numerical integration by Simpson's rule. *Communications of the ACM*, 6(4):167–168, 1963.

[71] W. M. McKeeman and L. Tesler. Algorithm 182: Nonrecursive adaptive integration. *Communications of the ACM*, 6(6):315, 1963.

[72] H. Morrin. Integration subroutine – fixed point. Technical Report 701 Note #28, U.S. Naval Ordnance Test Station, China Lake, California, March 1955.

[73] B. W. Ninham. Generalised functions and divergent integrals. *Numerische Mathematik*, 8:444–457, 1966.

[74] I. Ninomiya. Improvements of adaptive Newton-Cotes quadrature methods. *Journal of Information Processing*, 3(3):162–170, 1980.

[75] S. E. Notaris. Interpolatory quadrature formulae with Chebyshev abscissae. *Journal of Computational and Applied Mathematics*, 133:507–517, 2001.

[76] H. O'Hara and F. J. Smith. Error estimation in Clenshaw-Curtis quadrature formula. *Computer Journal*, 11(2):213–219, 1968.

[77] H. O'Hara and F. J. Smith. The evaluation of definite integrals by interval subdivision. *The Computer Journal*, 12(2):179–182, 1969.

[78] J. Oliver. A practical strategy for the Clenshaw-Curtis quadrature method. *Journal of the Institute of Mathematics and its Applications*, 8:53–56, 1971.

[79] J. Oliver. A doubly-adaptive Clenshaw-Curtis quadrature method. *The Computer Journal*, 15(2):141–147, 1972.

[80] T. N. L. Patterson. Algorithm 468: Algorithm for automatic numerical integration over a finite interval. *Communications of the ACM*, 16(11):694–699, 1973.

[81] J. M. Pérez-Jordá, E. San-Fabián, and F. Moscardó. A simple, reliable and efficient scheme for automatic numerical integration. *Computer Physics Communications*, 70:271–284, 1992.

[82] R. Piessens. An algorithm for automatic integration. *Angewandte Informatik*, 9:399–401, 1973.

[83] R. Piessens, E. de Doncker-Kapenga, C. W. Überhuber, and D. K. Kahaner. *QUADPACK A Subroutine Package for Automatic Integration.* Springer-Verlag, Berlin, 1983.

[84] A. Ralston and P. Rabinowitz. *A first course in Numerical Analysis.* McGraw-Hill Inc., New York, 1978.

[85] J. R. Rice. A metalgorithm for adaptive quadrature. *Journal of the ACM*, 22(1):61–82, 1975.

[86] T. J. Rivlin. *Chebyshev Polynomials: From Approximation Theory to Algebra and Number Theory.* John Wiley & Sons, Inc., New York, Chichester, Brisbane, Toronto, Singapore, 1990.

[87] I. Robinson. A comparison of numerical integration programs. *Journal of Computational and Applied Mathematics*, 5(3):207–223, 1979.

[88] J. H. Rowland and Y. L. Varol. Exit criteria for Simpson's compound rule. *Mathematics of Computation*, 26(119):699–703, 1972.

[89] C. Runge. Über empirische Funktionen und die Interpolation zwischen äquidistanten Ordinaten. *Zeitschrift für Mathematik und Physik*, 46:224–243, 1901.

[90] H. Rutishauser. *Vorlesungen über numerische Mathematik, Band 1.* Birkhäuser Verlag, Basel and Stuttgart, 1976.

[91] H. R. Schwarz. *Numerische Mathematik.* B. G. Teubner, Stuttgart, fourth edition, 1997. With a contribution by Jörg Waldvogel.

[92] H. D. Shapiro. Increasing robustness in global adaptive quadrature through interval selection heuristics. *ACM Transactions on Mathematical Software*, 10(2):117–139, 1984.

[93] R. D. Skeel and J. B. Keiper. *Elementary Numerical Computing with Mathematica.* McGraw-Hill, Inc., New York, 1993.

[94] E. Stiefel. *Einführung in die numerische Mathematik.* B. G. Teubner Verlagsgesellschaft, Stuttgart, 1961.

[95] L. N. Trefethen. Is Gauss quadrature better than Clenshaw–Curtis? *SIAM Review*, 50(1):67–87, 2008.

[96] L. N. Trefethen and J. A. C. Weideman. Two results on polynomial interpolation in equally spaced points. *Journal of Approximation Theory*, 65:247–260, 1991.

[97] A. H. Turetskii. The bounding of polynomials prescribed at equally distributed points (in Russian). *Proc. Pedag. Inst. Vitebsk*, 3:117–127, 1940.

[98] A. Venter. *Aanpasbare Numeriese Integrasie (Adaptive Numerical Integration).* PhD thesis, Potchefstroom Univeristy for Christian Higher Education, 1995.

[99] A. Venter and D. P. Laurie. A doubly adaptive integration algorithm using stratified rules. *BIT Numerical Mathematics*, 42(1):183–193, 2002.

[100] D. S. Villars. Use of the IBM 701 computer for quantum mechanical calculations II. overlap integral. Technical Report 5257, U.S. Naval Ordnance Test Station, China Lake, California, August 1956.

[101] J. Waldvogel. Fast construction of the Fejér and Clenshaw-Curtis quadrature rules. *BIT Numerical Mathematics*, 46:195–202, 2006.

[102] P. Wynn. On a device for computing the $e_m(s_n)$ transformation. *Mathematical Tables and Other Aids to Computation*, 10(54):91–96, 1956.

# Index

# Curriculum Vitae

## Personal Information

| | |
|---|---|
| Name | Pedro Gonnet |
| Birth | January 6, 1978 in Montevideo, Uruguay |
| Nationalities | Swiss, Canadian and Uruguayan |
| Languages | English, German French and Spanish |

## Education

| | |
|---|---|
| 2009 | PhD in Computer Science, ETH Zurich |
| 2003 | Diploma in Computer Science with a minor (Nebenfach) in Biochemistry, ETH Zurich |
| 1996 | Matura Type C, MNG Rämibḧl, Zurich |

## Academic Positions

| | |
|---|---|
| since 08.2005 | Research Assistant in the Group of Prof.W.Gander, Institute of Computational Science, Department of Computer Science, ETH Zurich |
| 02.2002 – 08.2005 | Research Assistant in the Group of Prof.P.Koumoutsakos, Institute of Computational Science, Department of Computer Science, ETH Zurich |

## Work Experience

| | |
|---|---|
| 08.2001 – 02.2002 | Researcher at GeneBio S.A.. Geneva, Switzerland |
| 09.1998 – 08.2001 | Teaching Assistant (Hilfsassistent) for the Dept. of Computer Science, ETH Zurich |
| 08.1998 – 02.1999 | Programmer for GlobalNet Communications, Dbendorf, Switzerland |
| 02.1997 – 08.1997 | Programmer for SoftPoint, Montevideo, Uruguay |
| 02.1996 – 02.1997 | Layouter for DAZ – Die Andere Zeitung, Zurich, Switzerland |

## Other Activities

| | |
|---|---|
| Referee | Journal of Computational Physics; Bioinformatics; Journal of Computational Chemistry; Journal of Bioinformatics and Computational Biology |
| Teaching Assistant | Informatik I, II, III and IV; Information Systems; Introduction to Computational Science; Computational Science; Software for Numerical Linear Algebra; Parallel Numerical Computing |