3.3 Iterated Quadratures; Romberg's Method

3.3.1 Richardson Extrapolation

Extrapolation is a method for generating high-accuracy numerical schemes using low-order formulas. The most widely used is *Richardson extrapolation*.

Consider the integral

$$I := \int_a^b f(x)\,dx$$

and a numerical integration scheme

$$I \;\approx\; I_n,$$

for which we have an asymptotic error formula of the form

$$I - I_n \;\approx\; \frac{c}{n^p}, \tag{3.1}$$

where c depends on a, b and the derivatives of a certain order of the function f on $[a, b]$. The difficulty in using this estimate is not knowing the value of the constant c. We can obtain a computable estimate of the error without needing to know c explicitly. We write (3.1) for a larger n:

$$I - I_{2n} \;\approx\; \frac{c}{(2n)^p} \;=\; \frac{c}{2^p n^p} \tag{3.2}$$

and eliminate the unknown c from relations (3.1)-(3.2). We obtain

$$I - I_n \;\approx\; 2^p\big(I - I_{2n}\big),$$

and then the approximation

$$I \;\approx\; \frac{2^p I_{2n} - I_n}{2^p - 1} \;=\; I_{2n} + \frac{I_{2n} - I_n}{2^p - 1} \;\overset{\text{not}}{=}\; R_{2n}, \tag{3.3}$$

called **Richardson's extrapolation formula**. From this, we can get another error estimate for I_{2n},

$$I - I_{2n} \;\approx\; \frac{I_{2n} - I_n}{2^p - 1}, \tag{3.4}$$

called **Richardson's error estimate**. The term R_{2n} is an improved estimate of I, based on using

I_n, I_{2n}, p and the assumption (3.1). It is a more accurate approximation to I than is I_{2n}. How much more accurate it is depends on the validity of (3.1)–(3.2).

Example 3.1. Let us consider a few simple Newton-Cotes formulas.

Solution. For the composite trapezoidal rule, if f has continuous second order derivatives on $[a, b]$, we have

$$\int_a^b f(x)dx \;=\; \frac{b-a}{n}\Big[f(a)+f(b)+\sum_{i=1}^{n-1} f\Big(a+\frac{b-a}{n}i\Big)\Big] - \frac{(b-a)^3}{12n^2}f''(\xi) \;=\; T_n + \frac{c}{n^2},$$

hence, $p = 2$. Using Richardson extrapolation, we get

$$I \;\approx\; \frac{4T_{2n}-T_n}{3} \;=\; T_{2n} + \frac{1}{3}\big(T_{2n}-T_n\big) \tag{3.5}$$

and the error formula

$$I - T_{2n} \;\approx\; \frac{1}{3}\big(T_{2n}-T_n\big). \tag{3.6}$$

With Simpson's repeated rule, if f has continuous fourth order derivatives on $[a, b]$ and $f_j = f\Big(a + \frac{b-a}{2n}j\Big)$, $j = \overline{0, 2n}$, we have

$$\int_a^b f(x)dx \;=\; \frac{b-a}{6n}\Big[f(a)+f(b)+4\sum_{i=1}^{n} f_{2i-1} + 2\sum_{i=1}^{n-1} f_{2i}\Big] - \frac{(b-a)^5}{2880n^4}f^{(4)}(\xi) \;=\; S_n + \frac{c}{n^4},$$

so in this case, $p = 4$. With Richardson extrapolation, we obtain

$$I \;\approx\; \frac{16S_{2n}-S_n}{15} \;=\; S_{2n} + \frac{1}{15}\big(S_{2n}-S_n\big) \tag{3.7}$$

and the error

$$I - S_{2n} \;\approx\; \frac{1}{15}\big(S_{2n}-S_n\big). \tag{3.8}$$

■

Example 3.2. Consider again the problem in Example 3.8 in Lecture 9: the approximation of the integral

$$I = \int_0^1 e^{-x^2} dx = 0.746824132812427,$$

using the composite trapezoidal rule.

Solution. Last time we obtained the values

n	Approx. value T_n	Error	Ratio
2	0.7313702518	$1.55e-2$	
4	0.7429840978	$3.84e-3$	4.02
8	0.7458656148	$9.59e-4$	4.01
16	0.7465845968	$2.40e-4$	4.00
32	0.7467642547	$5.99e-5$	4.00

Table 1: Approximations and errors for repeated trapezoidal rule, Example 3.2

We have

$$\begin{aligned} T_2 &= 0.7313702518, \\ T_4 &= 0.7429840978. \end{aligned}$$

By (3.5), we get the approximation

$$I \approx R_4 = \frac{1}{3}\big(4T_4 - T_2\big) = 0.7468553798,$$

with absolute error

$$0.0000312 = 3.12e-5.$$

Notice in Table 1 that the error of R_4 is smaller than that of T_{32}, so R_4 (after only 2 steps) gives a better approximation of I than T_{32}, obtained after 5 steps!

Now, let us estimate the error in T_4 using Richardson extrapolation. By (3.6), we have

$$I - T_4 \approx \frac{1}{3}\big(T_4 - T_2\big) = 0.00387.$$

The actual error in T_4 is 0.00384, so we obtained a very accurate error estimate.

■

Remark 3.3. Richardson's extrapolation and error estimation are not always as accurate as this example might suggest, but it is usually a fairly accurate procedure. The main assumption that must be satisfied is (3.1), with a known p. And the extrapolation itself provides a way of testing whether this assumption is valid for the actual values of I_n being used: Continue the ideas in (3.1)–(3.3) and write successively

$$\begin{aligned} I - I_n &\approx 2^p\big(I - I_{2n}\big), \\ I - I_{2n} &\approx 2^p\big(I - I_{4n}\big). \end{aligned}$$

We get

$$\begin{aligned} I_{2n} - I_n &= \big(I - I_n\big) - \big(I - I_{2n}\big) \\ &\approx 2^p\big(I - I_{2n}\big) - \big(I - I_{2n}\big) \;=\; (2^p - 1)\big(I - I_{2n}\big). \end{aligned}$$

Similarly, we have

$$\begin{aligned} I_{4n} - I_{2n} &= \big(I - I_{2n}\big) - \big(I - I_{4n}\big) \\ &\approx \big(I - I_{2n}\big) - 2^{-p}\big(I - I_{2n}\big) \;=\; (1 - 2^{-p})\big(I - I_{2n}\big). \end{aligned}$$

Then,

$$\frac{I_{2n} - I_n}{I_{4n} - I_{2n}} \;\approx\; \frac{2^p - 1}{1 - \dfrac{1}{2^p}} \;=\; 2^p.$$

We obtained the (computable) estimate

$$2^p \;\approx\; \frac{I_{2n} - I_n}{I_{4n} - I_{2n}},$$

or

$$p \;\approx\; \log_2\left(\frac{I_{2n} - I_n}{I_{4n} - I_{2n}}\right) \;=\; \frac{1}{\ln 2}\;\ln\left(\frac{I_{2n} - I_n}{I_{4n} - I_{2n}}\right). \tag{3.9}$$

This gives a practical means of checking/finding the value of p in (3.1), using three successive values I_n, I_{2n}, I_{4n}.

Example 3.4. Let us use the approximations in Table 1 to estimate the value of p for which

$$I - T_n \approx \frac{c}{n^p}.$$

Solution. We use (3.9).
For $n = 1$, we get the estimate

$$p_1 = \log_2 \left(\frac{T_4 - T_2}{T_8 - I_4} \right) = 2.0109.$$

If we use $n = 2$, we have

$$p_2 = \log_2 \left(\frac{T_8 - T_4}{T_{16} - I_8} \right) = 2.0028.$$

And, finally, if $n = 4$, we obtain

$$p_3 = \log_2 \left(\frac{T_{16} - T_8}{T_{32} - I_{16}} \right) = 2.0007.$$

We see that the estimates converge to $p = 2$, which is consistent with the theoretical value determined for the composite trapezoidal rule.

■

3.3.2 Iterated Quadratures; Romberg's Method

Just like in the case of Lagrange interpolation, we want algorithms for which it is easy to go from one step (iteration) to the next, by using previously computed values of the function.

One drawback of adaptive quadratures is that they compute repeatedly the function values at the nodes and when such an algorithm is executed, there is an extra computational cost due to recursion. *Iterated quadratures* overcome this shortcoming. They apply at the first step a composite quadrature rule and then divide the interval into equal parts using at each step the previously computed approximations. **Romberg's method** is such an iterative algorithm, starting with the composite trapezoidal (or midpoint) rule and then improving the convergence by using Richardson extrapolation.

The initial approximations are obtained by applying either the trapezoid or midpoint rule with $n_k = 2^{k-1}$, $k \in \mathbb{N}$. Then the value of the step h_k is

$$h_k = \frac{b - a}{n_k} = \frac{b - a}{2^{k-1}}.$$

With these notations, we have (for the trapezium rule)

$$\int_a^b f(x)dx \;=\; \frac{h_k}{2}\Big[f(a)+f(b)+2\sum_{i=1}^{2^{k-1}-1} f\big(a+ih_k\big)\Big] - \frac{b-a}{12}h_k^2 f''(\xi_k),\ \xi_k\in[a,b].$$

Denote by $R_{k,1}$ the approximation above, i.e.,

$$\begin{aligned}
R_{1,1} &= \frac{h_1}{2}\Big[f(a)+f(b)\Big] \;=\; \frac{b-a}{2}\Big[f(a)+f(b)\Big],\\
R_{2,1} &= \frac{h_2}{2}\Big[f(a)+f(b)+2f\big(a+h_2\big)\Big]\\
&= \frac{b-a}{4}\Big[f(a)+f(b)+2f\Big(a+\frac{1}{2}h_1\Big)\Big]\\
&= \frac{1}{2}\Big[\frac{b-a}{2}\Big(f(a)+f(b)\Big)+(b-a)f\Big(a+\frac{1}{2}h_1\Big)\Big]\\
&= \frac{1}{2}\Big[R_{1,1}+h_1 f\Big(a+\frac{1}{2}h_1\Big)\Big]\\
&\dots\\
R_{k,1} &= \frac{1}{2}\Big[R_{k-1,1}+h_{k-1}\sum_{i=1}^{2^{k-2}} f\Big(a+\big(i-\frac{1}{2}\big)h_{k-1}\Big)\Big],\ k=\overline{2,n}.
\end{aligned} \tag{3.10}$$

Since $h_k=\dfrac{1}{2}h_{k-1}$, each successive level of improvement increases the order of the error term from $O(h^{2k-2})$ to $O(h^{2k})$, so by

$$O(h^2) \;=\; O\Big(\frac{1}{n^2}\Big).$$

Then we can use Richardson extrapolation with $p=2$, by eliminating the term in h_k^2 from the approximation of I by $R_{k-1,1}$ and $R_{k,1}$, respectively. We obtain

$$I \;=\; \frac{4R_{k,1}-R_{k-1,1}}{3}+O(h_k^4)$$

and define

$$R_{k,2} \;=\; \frac{4R_{k,1}-R_{k-1,1}}{3}. \tag{3.11}$$

We apply Richardson extrapolation to these values, too. In general, if $f \in C^{2n+2}[a,b]$, then, for $k = \overline{1,n}$, we can write

$$\int_a^b f(x)dx \;=\; \frac{h_k}{2}\left[f(a)+f(b)+2\sum_{i=1}^{2^{k-1}-1} f\big(a+ih_k\big)\right]+\sum_{i=1}^{k} K_i h_k^{2i} + O(h_k^{2k+2}),$$

where K_i does not depend on h_k.

Successively eliminating the powers of h from the relation above, we get

$$R_{k,j} \;=\; \frac{4^{j-1}R_{k,j-1}-R_{k-1,j-1}}{4^{j-1}-1},\; k=\overline{2,n},\; j=\overline{2,k}. \tag{3.12}$$

The computations can be arranged in a table (from (3.10) and (3.12)):

$$\begin{array}{lllll}
R_{1,1} & & & & \\
R_{2,1} & R_{2,2} & & & \\
R_{3,1} & R_{3,2} & R_{3,3} & & \\
\vdots & \vdots & \vdots & \ddots & \\
R_{n,1} & R_{n,2} & R_{n,3} & \dots & R_{n,n}
\end{array}$$

If the sequence $\{R_{n,1}\}_n$ (which is just the repeated trapezium rule) converges, so does $\{R_{n,n}\}_n$, but at a *faster* rate. We can use the stopping criterion

$$|R_{n-1,n-1}-R_{n,n}| \;<\; \varepsilon.$$

Remark 3.5. The second column in Romberg's method corresponds to Simpson's composite rule. We introduce the notation

$$S_{k,1} \;=\; R_{k,2}.$$

Then, the values in the third column are

$$R_{k,3} \;=\; \frac{4^2R_{k,2}-R_{k-1,2}}{4^2-1} \;=\; \frac{16S_{k,1}-S_{k-1,1}}{15},$$

which is Richardson's extrapolation for Simpson's rule. The relation

$$S_{k,1} \;=\; \frac{16S_{k,1}-S_{k-1,1}}{15} \tag{3.13}$$

is at the core of a well-known (and oftenly used) adaptive quadrature algorithm (due to Gander and Gautschi).

Example 3.6. Approximate the integral

$$I = \int_0^\pi \sin x \, dx$$

with precision $\varepsilon = 10^{-1}$, using Romberg's method, .

Solution. The exact value of the integral is

$$I = -\cos x \Big|_0^\pi = 2.$$

Using the repeated trapezoidal rule with $n_1 = 2^0, h_1 = \pi$ (i.e. nodes $x_0 = 0, x_1 = \pi$) and $n_2 = 2^1, h_2 = \pi/2$ (so nodes $x_0 = 0, x_1 = \pi/2, x_2 = \pi$), we get

$$\begin{aligned}
R_{1,1} &= \frac{\pi}{2}(\sin 0 + \sin \pi) = 0, \\
R_{2,1} &= \frac{1}{2}\Big[R_{1,1} + h_1 f\Big(a + \frac{1}{2}h_1\Big)\Big] = \frac{1}{2}\Big(0 + \pi \sin\frac{\pi}{2}\Big) = \frac{\pi}{2} = 1.5708.
\end{aligned}$$

Richardson extrapolation is next:

$$R_{2,2} = \frac{4R_{2,1} - R_{1,1}}{3} = \frac{2\pi}{3} = 2.0944.$$

We have

$$|R_{2,2} - R_{1,1}| = 2.0944 > 0.1,$$

so we continue. We compute

$$\begin{aligned}
R_{3,1} &= \frac{1}{2}\Big[R_{2,1} + h_2\Big[f\Big(a + \frac{1}{2}h_2\Big) + f\Big(a + \frac{3}{2}h_2\Big)\Big]\Big] \\
&= \frac{1}{2}\Big[R_{2,1} + \frac{\pi}{2}\Big(\sin\frac{\pi}{4} + \sin\frac{3\pi}{4}\Big)\Big] = 1.8961, \\
R_{3,2} &= \frac{4R_{3,1} - R_{2,1}}{3} = 2.0046, \\
R_{3,3} &= \frac{16R_{3,2} - R_{2,2}}{15} = 1.9986
\end{aligned}$$

and

$$|R_{3,3} - R_{2,2}| \;=\; 0.0958 \;<\; 0.1.$$

Hence, we obtained the approximation

$$I \;\approx\; R_{3,3} \;=\; 1.9986,$$

(with an error of $1.4e - 3$), which is obviously better than the trapezoidal rule with $n = 4$, $R_{3,1}$ (with the error of 0.1039). Also, it is more accurate than Simpson's approximation with 4 nodes, $I \approx 2.005$ (with error $5e - 3$).

In fact, for this example, the algorithm converges very fast, as seen below:

$$\begin{array}{llll} 0 & & & \\ 1.5708 & 2.0944 & & \\ 1.8961 & 2.0046 & 1.9986 & \\ 1.9742 & 2.0003 & 2.0000 & 2.0000 \end{array}$$

■

3.4 Weighted Gaussian Quadratures

The numerical methods studied so far were based on integrating linear and quadratic interpolating polynomials, and the resulting formulas were applied on subdivisions of ever smaller subintervals. In this section, we consider a numerical method that is based on the *exact integration* of polynomials of increasing degree; no subdivision of the integration interval is used. The motivation of this approach is the following: if we have a numerical integration formula to integrate low- to moderate-degree polynomials *exactly*, then the hope is that the same formula will integrate other functions $f(x)$ *almost exactly*, if $f(x)$ is well approximable by such polynomials.

3.4.1 General Framework

Definition 3.7. *An interpolatory formula of the form*

$$\int_a^b w(x)f(x)\,dx \;=\; \sum_{k=1}^{m} A_k f(x_k) + R_m(f) \tag{3.14}$$

is called ***(weighted) Gaussian quadrature*** *if it has maximum degree of precision,* $d = 2m - 1$.

The function $w : (a, b) \to \mathbb{R}_+$ is a *weight function*, a function for which the *moments*

$$\mu_j = \int_a^b w(x) x^j \, dx \tag{3.15}$$

exist and are finite for each $j \in \mathbb{N}$. The purpose of a weight function is to "absorb" some singularities of the integrand.

We want to determine the coefficients A_k and the nodes x_k such that

$$R_m(e_0) = R_m(e_1) = \ldots = R_m(e_{2m-1}) = 0. \tag{3.16}$$

Let us start with a simple example. Consider the integral

$$\int_{-1}^{1} f(x) \, dx. \tag{3.17}$$

So, in this case, $w(x) \equiv 1$.

Case $m = 1$.

We seek a numerical integration formula

$$\int_{-1}^{1} f(x) \, dx \approx A_1 f(x_1).$$

From the first two relations in (3.16), we get

$$\begin{aligned} A_1 &= 2, \\ A_1 x_1 &= 0, \end{aligned}$$

and, thus, the formula

$$\int_{-1}^{1} f(x) \, dx \approx 2 f(0),$$

which is the midpoint (rectangle) rule. Recall that the rectangle rule had indeed the maximum degree of precision possible with just one node, $d = 1$.

Case $m = 2$.

Now, we want a quadrature of the form

$$\int_{-1}^{1} f(x)\,dx \;\approx\; A_1 f(x_1) + A_2 f(x_2),$$

with 4 unknowns, which are determined from the first 4 relations (3.16). This leads to the system

$$\begin{array}{rcl} A_1 + A_2 & = & 2 \\ A_1 x_1 + A_2 x_2 & = & 0 \\ A_1 x_1^2 + A_2 x_2^2 & = & \frac{2}{3} \\ A_1 x_1^3 + A_2 x_2^3 & = & 0 \end{array} \tag{3.18}$$

with solution

$$A_1 \;=\; A_2 \;=\; 1,\; x_1 \;=\; -\frac{\sqrt{3}}{3},\; x_2 \;=\; \frac{\sqrt{3}}{3}. \tag{3.19}$$

Hence, we found the quadrature formula

$$\int_{-1}^{1} f(x)\,dx \;\approx\; f\Big(-\frac{\sqrt{3}}{3}\Big) + f\Big(\frac{\sqrt{3}}{3}\Big). \tag{3.20}$$

Being exact for the monomials $1, x, x^2$ and x^3, this formula will be exact for *all* polynomials of degree ≤ 3. Hence, its degree of exactness is $d = 3$. Compare this with Simpson's rule, which uses *three* nodes to attain the same degree of precision.

General case $m > 2$.

We seek now the formula

$$\int_{-1}^{1} f(x)\,dx \;\approx\; \sum_{k=1}^{m} A_k f(x_k),$$

which has $2m$ unspecified parameters, the nodes $x_1, \ldots, x_m$, and the coefficients $A_1, \ldots, A_m$. They are found by forcing the integration formula to be exact for the $2m$ monomials $1, x, x^2, \ldots, x^{2m-1}$. In turn, this forces the quadrature formula to be exact for *all* polynomials of degree $2m - 1$. This leads to the following system of $2m$ nonlinear equations in $2m$ unknowns:

$$
\begin{array}{rcl}
A_1 + A_2 + \cdots + A_{2m-1} & = & 2 \\
A_1 x_1 + A_2 x_2 + \cdots + A_{2m-1} x_{2m-1} & = & 0 \\
A_1 x_1^2 + A_2 x_2^2 + \cdots + A_{2m-1} x_{2m-1}^2 & = & \dfrac{2}{3} \\
A_1 x_1^3 + A_2 x_2^3 + \cdots + A_{2m-1} x_{2m-1}^3 & = & 0 \\
& \cdots & \cdots \\
A_1 x_1^{2m-2} + A_2 x_2^{2m-2} + \cdots + A_{2m-1} x_{2m-1}^{2m-2} & = & \dfrac{2}{2m-1} \\
A_1 x_1^{2m-1} + A_2 x_2^{2m-1} + \cdots + A_{2m-1} x_{2m-1}^{2m-1} & = & 0.
\end{array}
\tag{3.21}
$$

Example 3.8. Consider again the integral in Example 3.2,

$$
I = \int_0^1 e^{-x^2} dx = 0.746824132812427.
$$

Solution. The linear change of variables

$$
x = \frac{b + a + t(b-a)}{2} \tag{3.22}
$$

maps the interval $[-1, 1]$ to $[a, b]$. So, with the substitution

$$
x = \frac{1+t}{2}, \quad t = 2x - 1,
$$

we get

$$
I = \frac{1}{2} \int_{-1}^{1} e^{-\frac{1}{4}(1+t)^2} \, dt.
$$

We apply Gaussian quadratures to the above integral. The errors are given in Table 2.
Comparing these with the ones given by the composite trapezoid or Simpson's rules (even with extrapolation), we see that these approximations are much more accurate, with fewer nodes.

■

m	Error
2	$2.29e-4$
3	$9.55e-6$
4	$3.35e-7$
5	$6.05e-9$
6	$7.77e-11$
7	$7.89e-13$

Table 2: Gaussian quadratures errors, Example 3.8

Gaussian quadrature formulas for a general weight function w can be found completely similarly. From relations (3.16), we obtain the system

$$\begin{aligned} A_1 + A_2 + \cdots + A_{2m-1} &= \mu_0 \\ A_1 x_1 + A_2 x_2 + \cdots + A_{2m-1} x_{2m-1} &= \mu_1 \\ A_1 x_1^2 + A_2 x_2^2 + \cdots + A_{2m-1} x_{2m-1}^2 &= \mu_2 \\ \cdots \quad & \cdots \\ A_1 x_1^{2m-1} + A_2 x_2^{2m-1} + \cdots + A_{2m-1} x_{2m-1}^{2m-1} &= \mu_{2m-1}. \end{aligned} \tag{3.23}$$

Example 3.9. Find a Gaussian quadrature formula with 1 node, on the interval $[0,1]$, with respect to the weight function $w(x) = \dfrac{1}{\sqrt{x}}$.

Solution. First off, let us notice that the function $w(x) = \dfrac{1}{\sqrt{x}}$ *is* indeed a weight function on $[0,1]$, since the moments

$$\mu_j = \int_0^1 \frac{1}{\sqrt{x}} x^j \, dx = \int_0^1 x^{j-\frac{1}{2}} \, dx = \frac{1}{j+\frac{1}{2}} x^{j+\frac{1}{2}} \Big|_0^1 = \frac{2}{2j+1}$$

exist and are finite for every $j \in \mathbb{N}$.
We want a formula of the form

$$\int_0^1 \frac{f(x)}{\sqrt{x}} \, dx \approx A_1 f(x_1),$$

having the maximum degree of precision possible, i.e., $d = 1$.

Forcing equality for $e_0(x) = 1$ and $e_1(x) = x$ leads to the system

$$\begin{aligned} A_1 &= 2, \\ A_1 x_1 &= \frac{2}{3}, \end{aligned}$$

with solution $A_1 = 2, x_1 = \dfrac{1}{3}$. We obtain the formula

$$\int_0^1 \frac{f(x)}{\sqrt{x}}\, dx \approx 2f\Big(\frac{1}{3}\Big),$$

with degree of precision $d = 1$.

■

Example 3.10. Determine a Gaussian quadrature formula with 2 nodes, with respect to the weight function $w(x) = e^{-x}$ on the interval $[0, \infty)$.

Solution. To compute the moments, recall *Euler's Gamma function* $\Gamma : (0, \infty) \to (0, \infty)$,

$$\Gamma(a) = \int_0^\infty x^{a-1} e^{-x}\, dx, \ \ \Gamma(n+1) = n!, \ \ n \in \mathbb{N}.$$

Then the moments are

$$\mu_j = \int_0^\infty e^{-x} x^j\, dx = \int_0^\infty x^{(j+1)-1} e^{-x}\, dx = \Gamma(j+1) = j!, \ j \in \mathbb{N}.$$

A quadrature formula with 2 nodes is of the form

$$\int_0^\infty e^{-x} f(x)\, dx \approx A_1 f(x_1) + A_2 f(x_2).$$

The nodes and coefficients are determined by having the formula above be exact for $1, x, x^2$ and x^3, i.e. from the equations

$$\begin{aligned} A_1 + A_2 &= 1, \\ A_1 x_1 + A_2 x_2 &= 1, \end{aligned}$$

$$
\begin{aligned}
A_1 x_1^2 + A_2 x_2^2 &= 2, \\
A_1 x_1^3 + A_2 x_2^3 &= 6.
\end{aligned}
$$

The solution of the system above is

$$A_1 \;=\; \frac{2+\sqrt{2}}{4},\; A_2 \;=\; \frac{2-\sqrt{2}}{4},\; x_1 \;=\; 2-\sqrt{2},\; x_2 \;=\; 2+\sqrt{2}$$

and yields the numerical integration formula

$$\int_0^\infty e^{-x} f(x)\,dx \;\approx\; \frac{2+\sqrt{2}}{4} f\big(2-\sqrt{2}\big) \;+\; \frac{2-\sqrt{2}}{4} f\big(2+\sqrt{2}\big),$$

with degree of exactness $d = 3$.

■

We see from these examples that solving the system (3.23) is *not* an easy task, even for a small number of nodes. This system is not linear in the nodes. It is linear in the coefficients, but with a Vandermonde system matrix, which is known to have *conditioning* (stability) problems. Even when a solution can be found (numerically), it is possible that some of the nodes are complex, or have values outside the interval $[a, b]$. Which is why we use another approach, one that involves *orthogonal polynomials*.

3.4.2 Orthogonal Polynomials

The use of orthogonal polynomials is justified by the following result.

Theorem 3.11. *Let* $u(x) = (x - x_1)(x - x_2)\dots(x - x_m)$. *Then, the quadrature formula* (3.14) *is exact for all polynomials* $p \in \mathbb{P}_{2m-1}$ *if and only if* u *is orthogonal to the set* $\mathbb{P}_{m-1},\ u \perp \mathbb{P}_{m-1}$, *with respect to the inner product*

$$< f, g >_w \;=\; \int_a^b w(x) f(x) g(x)\,dx. \tag{3.24}$$

Proof. "⇒" Let $p \in \mathbb{P}_{m-1}$. Since u has degree m, it follows that $up \in \mathbb{P}_{2m-1}$, so formula (3.14) is exact for up, i.e.,

$$\int_a^b w(x)u(x)p(x)\,dx \;=\; \sum_{k=1}^{m} A_k u(x_k)p(x_k) \;=\; 0,$$

because $u(x_k) = 0, \forall k = \overline{1,m}$. Hence, $u \perp p$ and, further, $u \perp \mathbb{P}_{m-1}$.

"$\Leftarrow$" Let $f \in \mathbb{P}_{2m-1}$, arbitrary. By the division algorithm, there exist $q, r \in \mathbb{P}_{m-1}$ such that $f = uq + r$. Thus, we have

$$\int_a^b w(x)f(x)\,dx \;=\; \int_a^b w(x)u(x)q(x)\,dx + \int_a^b w(x)r(x)\,dx \;=\; 0 + \int_a^b w(x)r(x)\,dx,$$

since $u \perp q$.

Now, formula (3.14) is an interpolatory one, and as such, has degree of exactness at least $d = m-1$. Since $r \in \mathbb{P}_{m-1}$, we have

$$\int_a^b w(x)r(x)\,dx \;=\; \sum_{k=1}^{m} A_k r(x_k).$$

But for any $k = \overline{1,m}$, $f(x_k) \;=\; u(x_k)q(x_k) + r(x_k) \;=\; r(x_k)$ and, thus,

$$\int_a^b w(x)f(x)\,dx \;=\; \sum_{k=1}^{m} A_k f(x_k),$$

i.e. formula (3.14) is exact for every $f \in \mathbb{P}_{2m-1}$. $\square$

Remark 3.12. So we now know that the nodes of a Gaussian quadrature are the roots of a polynomial orthogonal to $\mathbb{P}_{m-1}$ with respect to the weight w. Such families of orthogonal polynomials have been studied extensively. Table 3 contains such examples. A few immediate conclusions:

1. A first consequence is the fact that all the nodes in (3.14) are real, distinct and interior to the interval (a, b).

2. Another consequence: the nodes can be obtained from the equation

$$u(x) = \begin{vmatrix} \mu_0 & \mu_1 & \dots & \mu_m \\ \mu_1 & \mu_2 & \dots & \mu_{m+1} \\ \vdots & & & \\ \mu_{m+1} & \mu_{m+2} & \dots & \mu_{2m-1} \\ 1 & x & \dots & x^m \end{vmatrix} = 0. \tag{3.25}$$

3. Recall that there exists a linear recurrence relation between 3 consecutive monic orthogonal polynomials on the interval $[a, b]$ with respect to the weight w:

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t),\ k = 0, 1, \dots,\ \pi_{-1}(t) = 0,\ \pi_0(t) = 1, \tag{3.26}$$

where

$$\alpha_k = \frac{< t\pi_k, \pi_k >}{||\pi_k||^2},\ k = 0, 1, \dots,\ \beta_k = \frac{||\pi_k||^2}{||\pi_{k-1}||^2},\ k = 1, 2, \dots,\ \beta_0 = \mu_0. \tag{3.27}$$

Name	**Notation**	**Polynomial**	**Weight fn.**	**Interval**	$\boldsymbol{\alpha_k}$	$\boldsymbol{\beta_k}$
Legendre	l_m	$\left[(x^2-1)^m\right]^{(m)}$	1	$[-1, 1]$	0	$\beta_0 = 2$, $\beta_k = (4 - k^{-2})^{-1}, k \geq 1$
Chebyshev 1^{st}	T_m	$\cos(m \arccos x)$	$(1-x^2)^{-\frac{1}{2}}$	$[-1, 1]$	0	$\beta_0 = \pi$, $\beta_1 = \frac{1}{2}$, $\beta_k = \frac{1}{4}, k \geq 2$
Chebyshev 2^{nd}	Q_m	$\dfrac{\sin[(m+1)\arccos x]}{\sqrt{1-x^2}}$	$(1-x^2)^{\frac{1}{2}}$	$[-1, 1]$	0	$\beta_0 = \frac{\pi}{2}$, $\beta_k = \frac{1}{4}, k \geq 1$
Laguerre	L_m^a	$x^{-a}e^x\left(x^{m+a}e^{-x}\right)^{(m)}$	$x^a e^{-x},\ a > -1$	$[0, \infty)$	$2k + a + 1$	$\beta_0 = \Gamma(1 + a)$, $\beta_k = k(k + a), k \geq 1$
Hermite	H_m	$(-1)^m e^{x^2}\left(e^{-x^2}\right)^{(m)}$	e^{-x^2}	$\mathbb{R}$	0	$\beta_0 = \sqrt{\pi}$, $\beta_k = \frac{k}{2}, k \geq 1$

Table 3: Orthogonal polynomials and recurrence coefficients

Example 3.13. Let us revisit some previous examples.

Solution. For the weight function $w \equiv 1$, we can now solve system (3.18) (a 2-point formula) much easier. We know that the nodes are the roots of the Legendre polynomial

$$l_2(x) = \left[(x^2-1)^2\right]'' = \left[x^4 - 2x^2 + 1\right]'' = \left[4x^3 - 4x\right]' = 4(3x^2 - 1),$$

i.e. $\pm\frac{\sqrt{3}}{3}$. Then the coefficients $A_0 = A_1 = 1$ are immediately found.

In Example 3.10, the nodes are the roots of the Laguerre polynomial (with $a = 0$)

$$L_2^0(x) \;=\; e^x\left[x^2e^{-x}\right]'' \;=\; e^x\left[(2x-x^2)e^{-x}\right]' \;=\; x^2-4x+2,$$

so, $2\pm\sqrt{2}$. Alternatively, by (3.25),

$$u(x) \;=\; \begin{vmatrix} \mu_0 & \mu_1 & \mu_2 \\ \mu_1 & \mu_2 & \mu_3 \\ 1 & x & x^2 \end{vmatrix} \;=\; \begin{vmatrix} 1 & 1 & 2 \\ 1 & 2 & 6 \\ 1 & x & x^2 \end{vmatrix} \;=\; (2x^2-6x)-(x^2-6)+2(x-2) \;=\; x^2-4x+2.$$

Once the nodes are known, the coefficients can be easily found to be $A_{1,2} \;=\; \frac{2\mp\sqrt{2}}{4}$.

$\blacksquare$

Other properties of Gaussian quadratures:

Proposition 3.14. *The coefficients $A_k, k=\overline{1,m}$ in* (3.14) *are all positive.*

Regarding the convergence of Gaussian quadratures, we have:

Theorem 3.15. *If $[a,b]$ is bounded and $f\in C[a,b]$, then the Gaussian formula* (3.14) *converges, $R_m(f)\to 0,\ m\to\infty$.*

The proof is based on Weierstrass' theorem.

For the remainder of the quadrature formula, the following holds:

Proposition 3.16. *If $f\in C^{2m}[a,b]$, then there exists $\xi\in(a,b)$ such that*

$$R_m(f) \;=\; \frac{f^{(2m)}(\xi)}{(2m)!}\int_a^b w(x)u^2(x)\,dx. \tag{3.28}$$

The proof is based on writing the Hermite interpolation polynomial at the double nodes $x_1,\dots,x_m$, multiplying it by the weight function and integrating.

Example 3.17. Find the error in the Gauss-Legendre and Gauss-Laguerre quadrature formulas with 2 nodes.

Solution. We have the 2-point numerical integration formula (3.20) (Gauss-Legendre):

$$\int_{-1}^{1} f(x)\,dx \;=\; f\Big(-\frac{\sqrt{3}}{3}\Big) + f\Big(\frac{\sqrt{3}}{3}\Big) + R_2(f),$$

with $u(x) \;=\; \Big(x + \frac{\sqrt{3}}{3}\Big)\Big(x - \frac{\sqrt{3}}{3}\Big) \;=\; x^2 - \frac{1}{3}$. If $f \in C^4[-1,1]$, for some $\xi \in (-1,1)$, we have

$$\begin{aligned} R_2(f) \;&=\; \frac{f^{(\mathrm{iv})}(\xi)}{4!}\int_{-1}^{1} u^2(x)\,dx \;=\; \frac{f^{(\mathrm{iv})}(\xi)}{4!}\int_{-1}^{1}\Big(x^4 - \frac{2}{3}x^2 + \frac{1}{9}\Big)\,dx \\ &=\; 2\,\frac{f^{(\mathrm{iv})}(\xi)}{24}\int_{0}^{1}\Big(x^4 - \frac{2}{3}x^2 + \frac{1}{9}\Big)\,dx \;=\; \frac{f^{(\mathrm{iv})}(\xi)}{12}\Big(\frac{1}{5}x^5 - \frac{2}{9}x^3 + \frac{1}{9}x\Big)\Big|_0^1 \;=\; \frac{1}{135}f^{(\mathrm{iv})}(\xi). \end{aligned}$$

For the 2-point Gauss-Laguerre quadrature

$$\int_{0}^{\infty} e^{-x} f(x)\,dx \;=\; \frac{2+\sqrt{2}}{4}f\big(2-\sqrt{2}\big) \;+\; \frac{2-\sqrt{2}}{4}f\big(2+\sqrt{2}\big) + R_2(f),$$

again, assuming $f \in C^4[0,\infty)$, there exists $\xi > 0$ such that the remainder is expressed as

$$\begin{aligned} R_2(f) \;&=\; \frac{f^{(\mathrm{iv})}(\xi)}{4!}\int_{0}^{\infty} e^{-x}u^2(x)\,dx \;=\; \frac{f^{(\mathrm{iv})}(\xi)}{24}\int_{0}^{\infty} e^{-x}\Big(\big(x-2\big)^2 - 2\Big)^2\,dx \\ &=\; \frac{f^{(\mathrm{iv})}(\xi)}{24}\int_{0}^{\infty} e^{-x}\big(x^2 - 4x + 2\big)^2\,dx \\ &=\; \frac{f^{(\mathrm{iv})}(\xi)}{24}\int_{0}^{\infty} e^{-x}\big(x^4 - 8x^3 + 20x^2 - 16x + 4\big)\,dx \\ &=\; \frac{f^{(\mathrm{iv})}(\xi)}{24}\Big(\Gamma(5) - 8\,\Gamma(4) + 20\,\Gamma(3) - 16\,\Gamma(2) + 4\,\Gamma(1)\Big) \\ &=\; \frac{f^{(\mathrm{iv})}(\xi)}{24}\big(4! - 8\cdot 3! + 20\cdot 2! - 16\cdot 1! + 4\cdot 0!\big) \;=\; \frac{1}{6}f^{(\mathrm{iv})}(\xi). \end{aligned}$$

■

Now we have better procedures for finding the nodes of a Gaussian quadrature formula (orthogonal polynomials are implemented in most mathematical software, for Matlab, see https://www.mathworks.com/matlabcentral/fileexchange/69956-orthogonalpolynomials). But system (3.23) is still a Vandermonde system in the coefficients. So, for an efficient implementation, we can still improve computations. For that, we will make use of the recurrence relation and the parameters in (3.26)–(3.27). With these, we define

$$J_m(w) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{m-1}} \\ 0 & & & \sqrt{\beta_{m-1}} & \alpha_{m-1} \end{bmatrix}, \tag{3.29}$$

called the **Jacobi matrix** of order m for the weight function w on the interval $[a, b]$. The following holds:

Theorem 3.18. *The nodes* $\{x_k\}_{k=1}^m$ *of the Gaussian formula* (3.14) *are the eigenvalues of* J_m*,*

$$J_m v_k = x_k v_k, \; v_k^T v_k = 1, \; k = 1, \ldots, m, \tag{3.30}$$

while the coefficients $\{A_k\}_{k=1}^m$ *are given by*

$$A_k = \beta_0 v_{k,1}^2, \; k = 1, \ldots, m, \tag{3.31}$$

where $v_{k,1}$ *is the first component of the normalized* ($||v_k|| = 1$) *eigenvector associated with the eigenvalue* x_k*.*

This is easily proved by writing the recurrence relation (3.26) in matrix (vector) form.

Remark 3.19. Thus, the problem of determining a Gauss numerical integration formula is now reduced to that of finding e-values and e-vectors for a *symmetric* and *tridiagonal* matrix. This problem has been studied extensively in linear algebra, there is a vast literature on it and there are many very efficient methods for solving it.