Numerical Analysis
Lecture 5

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Introduction

Numerical integration formulas or quadrature formulas are methods for the approximate evaluation of definite integrals. Such formulas are needed when the primitive cannot be expressed in terms of elementary functions of for which the integrand is available only at discrete points. Examples include

$$\int_0^\pi \cos(x^2)\,dx$$

as well as

$$\int_1^{2000} \exp(\sin(\cos(\sinh(\cosh(\tan(\log(x))))))) \,dx$$

The calculation of surface areas can be traced back to the Greeks, Babylonians and Egyptians but it is again Newton who had the idea of interpolating functions and then integrating the interpolating polynomial, leading to what is known today as the Newton-Cotes quadrature. Gauss noticed that non-equidistant points lead to more accurate approximations.

Quadrature

The most common approach at approximating the definite integral

$$I_{[a,b]} = \int_a^b f(x)\,dx$$

is to rely on a weighted sum S_{n+1} of the form

$$S_{n+1}(f) = \sum_{k=0}^{n} w_k f(x_k)$$

and based on the $(n+1)$ distinct quadrature points $x_0, x_1, \ldots, x_n \in [a, b]$ and weights $w_0, \ldots, w_n \in \mathbb{R}$. For simplicity, we will choose evenly spaced points so that $x_{i+1} - x_i = h$ for all i and some $h > 0$. Since polynomials are easy to integrate, it seems like a good idea to first approximate f with an interpolating polynomial p and then integrate this polynomial. I.e.

$$\int_a^b f(x)\, dx \approx \int_a^b \Phi_n f\, dx = \int_a^b p_n\, dx = \sum_{k=0}^{n} w_k f(x_k)$$

where $\Phi_n : C[a, b] \to \mathbb{P}_n$ denotes the (polynomial) interpolation operator with interpolation points $x_0, x_1, \ldots, x_n$.

Note that this is equivalent to the finite difference approximation where we used $f'(x) \approx p'(x)$.

Recall that the order n Lagrange interpolation polynomial for f at the points $x_0, x_1, \ldots, x_n$ is defined as

$$p_n(x) = \sum_{k=0}^{n} \ell_k(x) f(x_k) = \Phi_n f$$

where the polynomials $\ell_k(x)$ are defined as

$$\ell_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i}$$

Substituting this approximation for f in the integral, we get

$$\begin{aligned}
\int_a^b f(x)\, dx &\approx \int_a^b \sum_{k=0}^{n} \ell_k(x) f(x_k)\, dx \\
&= \sum_{k=0}^{n} f(x_k) \int_a^b \ell_k(x)\, dx \\
&= \sum_{k=0}^{n} f(x_k) w_k
\end{aligned}$$

The values w_k, $k = 0, 1, \ldots, n$ are referred to as the quadrature weights.

Definition 1. *The quadrature rule obtained from the Lagrange polynomials of degree n is known as Newton-Cotes formula of order n (defined on $n+1$ points).*

Newton-Cotes formulas are called "closed" if the end points a and b are used as first and last quadrature points. In this case, the rule is thus defined based on a step $h = \frac{b-a}{n}$ and interpolation points $x_k = a + kh$, $k = 0, \dots, n$.

Conversely, Newton-Cotes formulas are called "open" if they do not include the endpoints a and b but place the first and last points so that they are at a distance h from the endpoints a and b. In this case, we thus define $h = \frac{b-a}{n+2}$ and define the interpolation points as $x_k = a + (k+1)h$, for $k = 0, 1, \dots, n$.

We will discuss four particular instances of Newton-Cotes quadratures.

- The closed Newton-Cotes quadrature defined on $n+1 = 1$ point (order 0) is known as the left endpoint rule and given by the approximation

$$\int_a^b f(x)\,dx \approx (b-a)f(a)$$

- Similarly, the (order 0) open rule defined on $n+1$ point is known as the midpoint rule. The approximation in this case is given by $\int_a^b f(x)\,dx \approx (b-a)f\left(\frac{a+b}{2}\right)$

- The Newton-Cotes formula of order $n = 1$ is known as the trapezoidal rule. In this case, we have $x_0 = a$, $x_1 = b$, the Lagrange polynomial of order 1 is given by

$$\begin{aligned}
p_1(x) &= \ell_0(x)f(x_0) + \ell_1(x)f(x_1) \\
&= \frac{x-b}{a-b}f(a) + \frac{x-a}{b-a}f(b) \\
&= \frac{1}{b-a}\left[-(x-b)f(a) + (x-a)f(b)\right]
\end{aligned}$$

  Substituting this interpolating polynomial for f in the integral, we get

$$\begin{aligned}
\int_a^b f(x)\,dx &\approx \frac{1}{b-a}\left[f(b)\frac{(x-a)^2}{2} - \frac{(x-b)^2}{2}f(a)\right]_a^b \\
&\approx \frac{(b-a)f(b)}{2} + \frac{(b-a)f(a)}{2} \\
&= \frac{(b-a)}{2}\left(f(b) + f(a)\right) \\
&= \frac{h}{2}\left[f(x_0) + f(x_1)\right]
\end{aligned}$$

- The Newton-Cotes quadrature formula of order $n = 2$ was already known to Kepler in 1612 and Cavalieri in 1639 and is called Simpson's rule as it was rediscovered by Simpson in 1743. The quadrature points are now defined as $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$. And the quadrature weights are computed as

$$
\begin{aligned}
w_0 &= \int_a^b \ell_0(x)\, dx = \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\, dx \\
&= \frac{1}{(x_0-x_1)(x_0-x_2)} \left| \frac{x^3}{3} - (x_1+x_2)\frac{x^2}{2} + x_1x_2x \right|_a^b \\
&= \frac{1}{(x_0-x_1)(x_0-x_2)} \left(\frac{b^3}{3} - \left(\frac{a+3b}{2}\right)\frac{b^2}{2} + b\left(\frac{ab+b^2}{2}\right)\right) \\
&- \frac{1}{(x_0-x_1)(x_0-x_2)} \left(\frac{b^3}{12} - \frac{a^3}{3} - \left(\frac{a+3b}{2}\right)\frac{a^2}{2} + a\left(\frac{ab+b^2}{2}\right)\right) \\
&= \frac{2}{(a-b)^2}\left(\frac{b^3}{12} - \frac{a^3}{12} + \frac{ab^2}{4} - \frac{2ab^2}{4} + \frac{a^2b}{4}\right) \\
&= \frac{1}{6(a-b)^2}(b-a)^3 \\
&= \frac{b-a}{6}
\end{aligned}
$$

Similarly we can obtain $w_1 = \frac{4}{6}(b-a)$ as well as $w_2 = w_0$ by symmetry. Combining those weights, we get

$$
\int_a^b f(x)\, dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]
$$

One way to compare quadrature rules is to determine the highest degree polynomial that the rule integrates exactly (we call this the degree of precision of the rule). The degree of precision of the rule is obiously always at least equal to the order of the rule. However, it can sometimes be larger as shown by the following examples. Let us consider the midpoint rule first. As we will see, this rule integrates a linear function exactly but cannot integrate a quadratic polynomial

$$
\int_a^b (p_0 + p_1x)\ dx = \left| p_0x + p_1\frac{x^2}{2}\right|_a^b = p_0(b-a) + \frac{p_1}{2}(b^2-a^2)
$$

$$
\begin{aligned}
\int_a^b \left(p_0 + p_1x + p_2x^2\right)\ dx &= \left| p_0 + p_1\frac{x^2}{2} + p_2\frac{x^3}{3}\right|_a^b \\
&= p_0\,(b-a) + p_1\left(\frac{b^2-a^2}{2}\right) + p_2\left(\frac{b^3-a^3}{3}\right)
\end{aligned}
$$

Applying the midpoint rule to the degree-1 polynomial, we get

$$
\begin{aligned}
\int_a^b (p_0 + p_1x)\ dx \approx (b-a)f\left(\frac{a+b}{2}\right) &= (b-a)\left(p_0 + p_1\left(\frac{a+b}{2}\right)\right) \\
&= (b-a)p_0 + p_1\left(\frac{b^2-a^2}{2}\right)
\end{aligned}
$$

Similarly, for the degree-2 polynomial

$$\begin{aligned}\int_a^b \left(p_0 + p_1 x + p_2 x^2\right)\,dx &= p_0\,(b-a) + p_1\left(\frac{b^2-a^2}{2}\right) + p_2\left(\frac{b^3-a^3}{3}\right)\\ &\neq (b-a)\left(p_0 + p_1\left(\frac{a+b}{2}\right) + p_2\left(\frac{a+b}{2}\right)^2\right)\end{aligned}$$

Let us now consider the trapezoidal rule. As this rule has 2 quadrature points whereas the Midpoint rule only has one, we might think that the degree of precision of this rule would be higher. Applying the rule to the degree-1 and degree-2 polynomials however shows a different reality.

For degree-1 polynomials, we indeed have

$$\begin{aligned}\int_a^b (p_0 + p_1 x)\,dx &= (b-a)\left[\frac{(p_0 + p_1 a) + (p_0 + p_1 b)}{2}\right]\\ &= (b-a)p_0 + \frac{b^2-a^2}{2}p_1\end{aligned}$$

For degree-2 polynomials, the rule again gives

$$\begin{aligned}&(b-a)\left[\frac{p_0 + p_1 a + p_2 a^2 + p_0 + p_1 b + p_2 b^2}{2}\right]\\ &= (b-a)p_0 + \frac{p_1}{2}(b^2-a^2) + \frac{(b-a)(a^2+b^2)p_2}{2}\end{aligned}$$

While the integral gives

$$\int_a^b \left(p_0 + p_1 x + p_2 x^2\right)\,dx = p_0\,(b-a) + p_1\left(\frac{b^2-a^2}{2}\right) + p_2\left(\frac{b^3-a^3}{3}\right)$$

In a similar manner, we can show that Simpson's rule integrate polynomials of degree at most 3 exactly.

For the Newton-Cotes quadratures, our observations can in fact be summarized more generally as follows:

- For any even n, the Newton-Cotes quadrature of order n (i.e. defined on $n+1$ points) has degree of precision $n+1$
- For every odd n, the Newton-Cotes quadrature of order n (defined on $n+1$ points) has degree of precision n

Error estimates

In the previous section, we have discussed the precision of the Newton-Cotes quadratures based on the highest degree of the polynomial for which the quadrature was equal to the integral.

In this section, we will derive estimates on the error made by the quadrature for general functions. One of the simplest approach at deriving error bounds on quadratures is to rely on the interpolation error.

As an example, let us consider the trapezoidal rule. In this case and for the interval $[a, b]$, integrating the interpolating polynomial gives us the estimate

$$\int_a^b f(x)\, dx \approx \frac{f(a) + f(b)}{2} h$$

From our bound on the interpolation error, recall that we have

$$f(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a} + \frac{(x-a)(x-b)}{2} f''(\xi), \quad \text{where } \xi \in [a, b]$$

Substituting this in the integral, we get

$$\begin{aligned}
&\int_a^b \frac{(x-a)(x-b)}{2} f''(\xi)\, dx = f''(\xi) \left| \frac{x^3}{6} - (a+b)\frac{x^2}{4} + ab\frac{x}{2} \right|_a^b \\
&= f''(\xi) \left(\frac{ab^2}{4} - \frac{a^2 b}{4} - \frac{b^3}{12} + \frac{a^3}{12} \right) \\
&= -\frac{f''(\xi)}{12} (b-a)^3
\end{aligned}$$

From which we can thus write

$$\left| \int_a^b f(x)\, dx - \frac{f(a) + f(b)}{2} h \right| \leq \sup_{\xi \in [a,b]} \frac{f''(\xi)}{12} h^3, \quad h \in [a, b]$$

A similar idea can be used for Simpson's rule. Using the expression of the interpolation error, we get

$$\begin{aligned}
\int_a^b f(x)\, dx &= \int_a^b \left[\frac{(x-b)(x-\left(\frac{a+b}{2}\right))}{(a-b)\left(a-\left(\frac{a+b}{2}\right)\right)} f(a) + \ldots + f(b) \frac{(x-a)(x-\left(\frac{a+b}{2}\right))}{(b-a)(b-\left(\frac{a+b}{2}\right))} \right] dx \\
&= \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2} + f(b) \right) \right] + \int_a^b \frac{f^{(3)}(\xi)}{6} \pi_3(x)\, dx \\
&= \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2} + f(b) \right) \right] \\
&+ \int_a^b \frac{f^{(3)}(\xi)}{6} (x-a) \left(x - \left(\frac{a+b}{2} \right) \right) (x-b)\, dx \\
&= \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2} \right) + f(b) \right] + \frac{f^{(3)}(\xi)}{6} h^4 C
\end{aligned}$$

where C is an absolute constant. In this case, it is however possible to do better as we will see. Recall that it was stated above that the Newton-Cotes quadrature of order n could perfectly integrate any polynomial of order $n+1$ for any even n and any polynomial of order n for odd n.

In the case of even n, we will see that it is possible to improve the bound by relying on the fact that a tighter interpolation error can be obtained for even functions.

Let us go back to the derivation of the interpolation error for Lagrange polynomials. We consider the case $n+1=3$ (equivalent to Simpson's rule) although the reasoning holds for any even n. Now assuming that $f(x)$ is an even function with respect to the center of the interval $[a,b]$ (i.e. $f\left(\left(\frac{a+b}{2}\right)+t\right)=f\left(\left(\frac{a+b}{2}\right)-t\right)$ for $t\in\left[-\frac{(b-a)}{2},\frac{b-a}{2}\right]$)

Let us define $\tilde{\pi}_4(x)$ as

$$\tilde{\pi}_4(x)=\left(x-\frac{a+b}{2}\right)^2(x-a)(x-b)$$

and consider the function $\varphi(y)$ defined as

$$\varphi(y)=f(y)-p_2(y)-\frac{f(x)-p_2(x)}{\tilde{\pi}_4(x)}\tilde{\pi}_4(y),\quad x\neq a,b,\left(\frac{a+b}{2}\right)$$

Obviously we have $\varphi(x)=0$, for all x. The function $\varphi(y)$ vanishes at $a,b,\left(\frac{a+b}{2}\right)$ as well as $x\neq\frac{a+b}{2}$. In accordance with Rolle's theorem, the derivative must therefore vanish on at least 3 points interlacing the roots of $\varphi(y)$ but since $\varphi(y)$ is even with respect to $\left(\frac{a+b}{2}\right)$, $\varphi'(y)$ must also vanish at $\left(\frac{a+b}{2}\right)$. As a result $\varphi'(y)$ vanishes on at least 4 points including $\left(\frac{a+b}{2}\right)$. Applying Rolle's theorem to $\varphi'(y)$, we conclude that $\varphi''(y)$ must vanish on at least 3 points and continuing like this up to $\varphi^{(4)}(y)$, we get that there must exist a $\xi\in(a,b)$ such that $\varphi^{(4)}(\xi)=0$. This in particular implies

$$\frac{f^{(4)}(\xi)\tilde{\pi}_4(x)}{4!}=(f(x)-p_2(x))$$

Now note that for any given function f, decomposing f into its even and odd parts with respect to $\frac{a+b}{2}$, i.e.

$$f_{\text{even}}\left(\frac{a+b}{2}+t\right)=f_{\text{even}}\left(\frac{a+b}{2}-t\right),\quad t\in\left[-\frac{a+b}{2},\frac{a+b}{2}\right]\tag{1}$$

$$f_{\text{odd}}\left(\frac{a+b}{2}+t\right)=-f_{\text{odd}}\left(\frac{a+b}{2}-t\right),\quad t\in\left[-\frac{a+b}{2},\frac{a+b}{2}\right]\tag{2}$$

we can write

$$\begin{aligned}I_{\text{Simpson}}[f]&=\frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]\\&=\frac{b-a}{6}\left[f_{\text{even}}(a)+f_{\text{odd}}(a)+4f_{\text{even}}\left(\frac{a+b}{2}\right)\right.\\&\left.+4f_{\text{odd}}\left(\frac{a+b}{2}\right)+f_{\text{even}}(b)+f_{\text{odd}}(b)\right]\\&=\frac{b-a}{6}\left[f_{\text{even}}(a)+f_{\text{even}}(b)+4f_{\text{even}}\left(\frac{a+b}{2}\right)\right]\end{aligned}$$

Moreover, in the case of odd $n+1$, the integral reduces to

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_a^b f_{\text{even}}(x)\,dx + \int_a^b f_{\text{odd}}(x)\,dx \\ &= \int_a^b f_{\text{even}}(x)\,dx\end{aligned}$$

so in particular, the error ε

$$\varepsilon = \int_a^b f(x)\,dx - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

in the case of odd $n+1$ quadratures can be defined from the even part of f solely

$$\varepsilon = \int_a^b f_{\text{even}}(x)\,dx - \frac{b-a}{6}\left[f_{\text{even}}(a) + f_{\text{even}}(b) + 4f_{\text{even}}\left(\frac{a+b}{2}\right)\right]$$

yet from our previous discussion, we can express this last quantity as

$$f_{\text{even}}(x) - p_{\text{even}}(x) = \frac{f_{\text{even}}^{(4)}(\xi)\tilde{\pi}_4(x)}{4!}$$

To conclude with use the fact that for any function f, we can express f_{even} as $f_{\text{even}}(x) = \frac{f\left(\frac{a+b}{2}+t\right)+f\left(\frac{a+b}{2}-t\right)}{2}$. In particular, we can thus write

$$\left|\frac{f_{\text{even}}^{(4)}(\xi)\tilde{\pi}_4(x)}{4!}\right| \leq \frac{1}{2}\left|\frac{f^{(4)}(\xi)+f^{(4)}(-\xi)}{4!}\tilde{\pi}_4(x)\right|$$

from this we can finally conclude

$$\begin{aligned}\int_a^b f(x)\,dx &= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2} + f(b)\right) + f(b)\right] + \int_a^b \frac{f^{(4)}(\xi)+f^{(4)}(-\xi)}{2\cdot 4!}\tilde{\pi}_4(x)\,dx \\ &= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{f^{(4)}(\xi)+f^{(4)}(-\xi)}{2\cdot 4!}\frac{(b-a)^5}{120}\end{aligned}$$

The $(b-a)^5$ coming from the fact that $\tilde{\pi}_4(x)$ is a degree 4 polynomial.

Composite rules

In order to improve the accuracy of our estimates, instead of increasing the order of quadrature, it is often more convenient to consider composite formulas which are obtained by subdividing the original interval of integration $[a,b]$ and by applying a simpler quadrature formula to each of the subintervals. I.e. for a step size $h = (b-a)/n$, we consider the subdivision

$$\int_a^b f(x)\,dx = \sum_{k=0}^{n-1}\int_{x_k}^{x_{k+1}} f(x)\,dx \tag{3}$$

where $x_k = a + kh = a + \frac{k}{n}(b-a)$, $k = 0, 1, \ldots, n$. From this we derive the (refined) approximation

$$\int_a^b f(x)\,dx = \sum_{k=0}^{n-1} (x_{k+1} - x_k) \frac{[f(x_{k+1}) + f(x_k)]}{2}$$

Two of the most popular composite formulas are the composite formulas derived from the Trapezoidal rule and Simpson's rule. Those two rules are recalled below.

Definition 2 (Composite Trapezoidal rule)**.**

$$\int_a^b f(x)\,dx \approx h\left[\frac{1}{2}f(x_0) + f(x_1) + \ldots + f(x_{n-1}) + \frac{1}{2}f(x_n)\right] \tag{4}$$

The error for the Trapezoidal rule can be made arbitrarily small provided that the function is sufficiently regular, as indicated by the following theorem

Theorem 1. *Let $f : [a,b] \mapsto \mathbb{R}$, twice continuously differentiable. Let $I_h(f)$ denote the approximation of the integral $\int_a^b f(x)\,dx$ obtained from the composite Trapezium rule (4). The error made by this approximation obeys*

$$\int_a^b f(x)\,dx - I_h(f) = -\frac{(b-a)^3}{12n^2} \max_{\xi \in [a,b]} |f''(\xi)|$$

Proof. The result follows from the application of the error estimate for the simple Trapezium rule on each of the subintervals. I.e. recall that for an interval $[a,b]$, we have

$$\int_a^b f(x)\,dx - \frac{(b-a)}{2}[f(a) + f(b)] = -\frac{h^3}{12} f''(\xi)$$

Applying this to the subdivision (3) we get

$$\begin{aligned}
\left|\int_a^b f(x)\,dx - I_h(f)\right| &\leq \sum_{k=0}^{n-1} \left|\int_{x_k}^{x_{k+1}} f(x)\,dx - (x_{k+1} - x_k)\frac{[f(x_{k+1}) + f(x_k)]}{2}\right| \\
&\leq \sum_{k=0}^{n-1} \frac{(b-a)^3}{12n^3} \max_{\xi_k \in [x_k, x_{k+1}]} |f''(\xi_k)| \\
&\leq \frac{(b-a)^3}{12n^2} \max_{\xi \in [a,b]} |f''(\xi)|
\end{aligned}$$

□

A similar result can be derived for the composite Simpson's rule which is defined below.

Definition 3 (Composite Simpson's rule)**.**

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \right. \qquad (5)$$

$$\left. +2f(x_{2n-2}) + 4f(x_{2n-1}) + f(x_{2n})\right]$$

$$= \sum_{i=0}^{n-1} \frac{h}{3}\left[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})\right] \qquad (6)$$

The corresponding error estimate is summarized by Theorem 2 below.

Theorem 2. *Let $f : [a,b] \mapsto \mathbb{R}$, four times continuously differentiable. Let $I_h(f)$ denote the approximation of the integral $\int_a^b f(x)\,dx$ obtained from the composite Simpson's rule (6). The error made by this approximation obeys*

$$\left|\int_a^b f(x)\,dx - I_h(f)\right| \leq \frac{(b-a)^5}{2880n^4} \max_{\xi\in[a,b]} \left|f^{(4)}(\xi)\right|$$

Gauss quadrature

So far, we have considered quadrature formulas that were designed on $n+1$ points to perfectly integrate polynomials of degree at most n.

Unlike the polynomial interpolation problem, in which our only freedom was in the $n+1$ coefficients, a quadrature however relies on the $n+1$ quadrature weights w_k and the $n+1$ quadrature points x_k which we have so far consideresd as fixed and equispaced. In other words, provided that we can choose the quadrature points x_k, nothing should prevent us from requiring exact interpolation for polynomials of degrees larger than n. In particular, using $n+1$ quadrature weights and $n+1$ quadrature points, we should in theory be able to integrate polynomials of degree $2n+1$ (defined on $2n+2$ parameters) exactly. This is the idea behind Gauss quadrature formula. We will in fact generalize our original quadrature setting by considering general integrals of the form

$$\int_a^b w(x)f(x)\,dx$$

For which we will study approximations derived from interpolation polynomials. I.e. as in the $w(x) = 1$ setting, we look for a decomposition of the form

$$\int_a^b f(x)\,dx \approx \int_a^b w(x)(\Phi_n f)(x)\,dx$$

The meaning of the $w(x)$ will become clear later. For now, we summarize the above discussion through the following definition

Definition 4. *A quadrature formula*

$$\int_a^b w(x)f(x)\,dx \approx \sum_{k=0}^{n} a_k f(x_k)$$

with $n+1$ distinct quadrature points is called a Gaussian quadrature formula if it integrates all polynomials $p \in \mathbb{P}_{2n+1}$ exactly. I.e.

$$\sum_{k=0}^{n} a_k p(x_k) = \int_a^b w(x)p(x)\,dx \tag{7}$$

for all polynomials $p \in \mathbb{P}_{2n+1}$.

Typical examples of Gaussian quadratures are given by

$$w(x) = 1, \quad w(x) = \sqrt{1-x^2}, \quad w(x) = \frac{1}{\sqrt{1-x^2}} \tag{8}$$

The key idea behind Gaussian quadrature formulas is that each choice for $w(x)$ comes with an associated family of orthogonal polynomials.

Lemma 3. *Given a weight function $w(x)$, there exists a unique sequence $(q_n)_n$ of polynomials of the form $q_0 = 1$, $q_n = x^n + r_{n-1}(x), \quad n = 1, \dots$ with $r_{n-1} \in \mathbb{P}_{n-1}$ satisfying*

$$\int_a^b w(x)q_n(x)q_m(x)\,dx = 0, \quad n \neq m$$

and $\mathbb{P}_n = span\{q_0, \dots, q_n\}$, $n = 0, 1, \dots$. Moreover, the unique Gaussian quadrature formula defined on $n+1$ points has quadrature points given by the zeros of q_{n+1}.

Deriving the quadrature weights and points can be done directly through (7), substituting polynomials of degree less than or equal to $2n+1$ and requiring an exact match between the integral and its approximation. However when the family of underlying orthogonal polynomials is known (which is the case for the weights functions given in (8) as we will see), and when the zeros of those polynomials are known, deriving the quadrature points and weights becomes a lot easier.

Consider the approximation of the integral $\int_0^1 f(x)\,dx$ on 2 points x_0, x_1. Deriving the Gauss quadrature requires the approximation $a_0 f(x_0) + a_1 f(x_1)$ to be exact for every polynomial up to degree $2n+1 = 3$ (i.e on $2n+2 = 4$ parameters). Concretely, considering separately the polynomials $p(x) = 1$, $p(x) = x$ and $p(x) = x^2$, we get the equations

$$1 = \int_0^1 1\ dx = a_0 + a_1 \tag{9}$$

$$\frac{1}{2} = \int_0^1 x\ dx = a_0 x_0 + a_1 x_1 \tag{10}$$

$$\frac{1}{3} = \int_0^1 x^2\ dx = a_0 x_0^2 + a_1 x_1^2 \tag{11}$$

$$\frac{1}{4} = \int_0^1 x^3\ dx = a_0 x_0^3 + a_1 x_1^3 \tag{12}$$

Because of the non-linear nature of the equations, the system (9) to (12) is not easy to solve. There are more efficient approaches however.

Instead of solving (9) to (12) explicitly, we can rely on the following property of the Gaussian quadrature which states that the quadrature points x_k correspond to the roots of the polynomial of degree $(n+1)$ orthogonal to every polynomial of $\mathbb{P}_n$.

Lemma 4. *Let $x_0, \ldots, x_n$ be the $n+1$ quadrature points of a Gaussian quadrature formula. We then have*

$$\int_a^b w(x) q_{n+1}(x) q(x)\ dx = 0 \tag{13}$$

for $q_{n+1}(x) = (x - x_0) \ldots (x - x_n)$ and all $q \in \mathbb{P}_n$

Applying the result of this lemma to our example, building a polynomial $q_2(x) = (x - x_0)(x - x_1) = x^2 + px + q$, and requiring the orthogonality of this polynomial with respect to the polynomials $p(x) = 1$ and $p(x) = x$, we have

$$\begin{aligned} &\int_0^1 x^2 + px + q\ dx = 0 \\ &\int_0^1 (x^2 + px + q) x\ dx = 0 \end{aligned} \qquad \iff \qquad \begin{aligned} &\frac{1}{3} + \frac{p}{2} + q = 0 \\ &\frac{1}{4} + \frac{p}{3} + \frac{q}{2} = 0 \end{aligned}$$

From those equations, we get

$$\begin{aligned} p &= -1 \\ q &= 1/6 \end{aligned}$$

Which together give $(x_0 + x_1) = 1$ and $x_0 x_1 = 1/6$ and hence $x_i = \frac{1 \pm \sqrt{2/6}}{2}$. Since x_0 and x_1 are undifferentiated, by symmetry we can choose any of the solutions

$$x_0 = \frac{1}{2} + \sqrt{\frac{1}{12}}, \quad x_1 = \frac{1}{2} - \sqrt{\frac{1}{12}}$$
$$x_0 = \frac{1}{2} - \sqrt{\frac{1}{12}}, \quad x_1 = \frac{1}{2} + \sqrt{\frac{1}{12}}$$

Substituting those solutions in (9)-(10), we finally get the equations

$$\begin{aligned} a_0 + a_1 &= 1 \\ a_0 x_0 + a_1 x_1 &= \frac{a_0 + a_1}{2} + a_0 \frac{1}{\sqrt{12}} - a_1 \frac{1}{\sqrt{12}} = 1/2 \end{aligned}$$

We now introduce the orthogonal polynomials associated to the weight functions (8).

Example 1 (Gauss-Chebyshev)**.** *We start by considering the weight function* $w(x) = \frac{1}{\sqrt{1-x^2}}$ *on* $[-1, 1]$*. In this case the quadrature points are given by the zeros of the Chebyshev polynomials*

$$T_n(x) = \cos(n \arccos x)$$

which are defined as $x_k = \cos\left(\frac{2k+1}{2n}\pi\right)$*,* $k = 0, \dots, n$*. Given those points, the quadrature weights can be derived by using the fact that the quadrature must be exact for degree* n *polynomials (which includes Chebyshev polynomials of degree at most* n*). In the case of the Chebyshev polynomials, requiring exact integration gives the constraint*

$$\sum_{k=0}^{n} a_k T_m(x_k) = \int_{-1}^{1} \frac{T_m(x)}{\sqrt{1-x^2}}\, dx, \quad m = 0, \dots, n$$

The integral on the right can be solved by noting that the Chebyshev polynomial is multiplied by the derivative of the arccos. From this, we then derive $a_k = \pi/(n+1)$*,* $k = 0, \dots, n$*, and the Gauss-Chebyshev quadrature on* $n+1$ *points can be defined as*

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\, dx \approx \frac{\pi}{n+1} \sum_{k=0}^{n} f\left(\cos\left(\frac{2k+1}{2(n+1)}\pi\right)\right) \tag{14}$$

Note that we did not put any contraint on the function f appearing in (14). As a result, nothing prevents us from deriving an approximation for the integral of any function g by simply setting $f(x) = g(x)\sqrt{1-x^2}$.

Example 2 (Gauss-Legendre)**.** *If we consider the weight function $w(x) = 1$, the family of orthogonal polynomials is now given by the family of Legendre polynomials,*

$$L_n(x) \equiv \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2 - 1)^n$$

Clearly we have $L_n \in \mathbb{P}_n$. The n zeros of those polynomials define the Gauss-Legendre quadrature. Unlike the Gauss-Chebyshev setting discussed in Example 1, it is difficult to write down the zeros of the Legendre polynomials explicitly. For this reason, in these notes, we restrict to the cases $n = 1, 2$. In this setting, the Legendre polynomials are given by

$$q_0(x) = 1, \quad q_1(x) = x, \quad q_2(x) = x^2 - \frac{1}{3}$$

In the case $n = 1$, we have $x = 0$ and w_1 can be estimated by exact integration of the degree 0 polynomial $p(x) = 1$, i.e. $w_1 = \int_{-1}^{1} 1 \; dx = 2$. For the degree-2 rule, using the Legendre polynomial of degree 2, we find the zeros $x_1 = -\frac{1}{\sqrt{3}}$, $x_2 = \frac{1}{\sqrt{3}}$. Again, relying on the fact that the rule must be exact for polynomials of degree at most $2n + 1$, we have

$$w_1 + w_2 = \int_{-1}^{1} dx = 2 \tag{15}$$

$$w_1 x_1 + w_2 x_2 = \int_{-1}^{1} x \; dx = 0 \tag{16}$$

which gives $w_1 = w_2 = 1$. The final Gauss-Legendre quadrature of order 2 can finally read as

$$\int_{-1}^{1} f(x) \; dx \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

References

[1] Rainer Kress, *Numerical Analysis*, Springer, Graduate Texts in Mathematics, 1997.