

# Numerical integration: Introduction

Anne Kværnø, André Massing

Sep 8, 2021

## 1 Introduction

Imagine you want to compute the finite integral

$$I[f](a, b) = \int_a^b f(x) dx.$$

The "usual" way is to find a primitive function  $F$  (also known as the indefinite integral of  $f$ ) satisfying  $F'(x) = f(x)$  and then to compute

$$\int_a^b f(x) dx = F(b) - F(a).$$

While there are many analytical integration techniques and extensive tables to determine definite integral for many integrands, more often than not it may not be feasible or possible to compute the integral. For instance, what about

$$f(x) = \frac{\log(2 + \sin(1/2 - \sqrt{(x)})^6)}{\log(\pi + \arctan(\sqrt{1 - \exp(-2x - \sin(x))})})?}$$

Finding the corresponding primitive is highly likely a hopeless endeavor. And sometimes there even exist innocent looking functions like  $e^{-x^2}$  for which there is no primitive function which can be expressed as a composition of standard functions such as  $\sin, \cos$ , etc.

**Definition 1.1.** *Quadrature rule.*

A **numerical quadrature** or a **quadrature rule** is a formula for approximating such definite integrals  $I[f](a, b)$ . Quadrature rules are usually of the form

$$Q[f](a, b) = \sum_{i=0}^n w_i f(x_i),$$

where  $x_i, w_i$  for  $i = 0, 1, \dots, n$  are respectively the *nodes/points* and the *weights* of the quadrature rule. To emphasize that a quadrature rule is defined by some given quadrature points  $\{x_i\}_{i=0}^n$  and weights  $\{w_i\}_{i=0}^n$ , we sometimes might write

$$Q[f](\{x_i\}_{i=0}^n, \{w_i\}_{i=0}^n) = \sum_{i=0}^n w_i f(x_i).$$

If the function  $f$  is given from the context, we will for simplicity denote the integral and the quadrature simply as  $I(a, b)$  and  $Q(a, b)$ .

**Example 1.1.** *Quadrature rules from previous math courses.*

The [trapezoidal rule](#), the [midpoint rule](#) and [Simpson's rule](#) known from previous courses are all examples of numerical quadratures, and we quickly review them here.

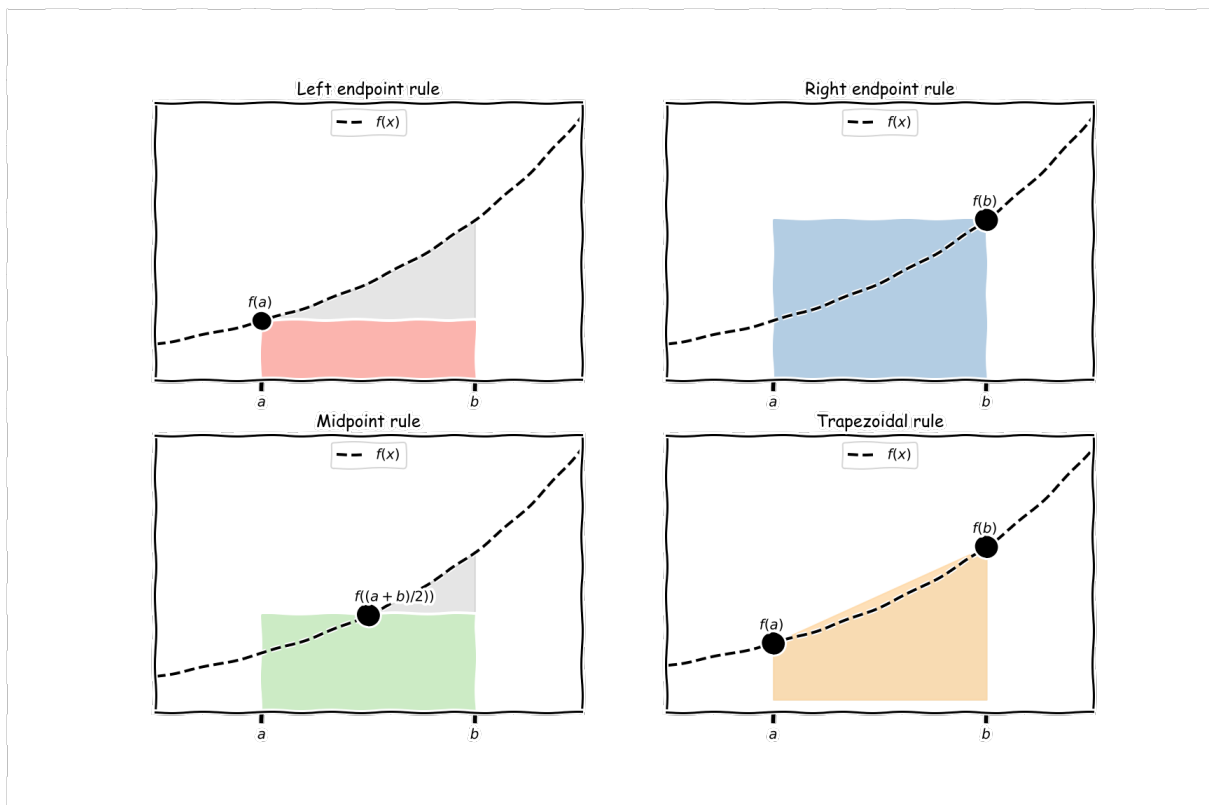


Figure 1: Classical quadrature rules.

- **Left and right endpoint rule** are among the simplest possible quadrature rule defined by

$$QL[f](a, b) := f(a)(b - a) \quad \text{and} \quad QR[f](a, b) := f(b)(b - a)$$

respectively. The (single) quadrature point for  $QL[\cdot]$  and  $QR[\cdot]$  is given by  $x_0 = a$  and  $x_0 = b$  respectively, and both use the corresponding weight  $w_0 = b - a$ .

- **Midpoint rule** is the quadrature rule defined by

$$Q[f](a, b) := (b - a)f\left(\frac{a + b}{2}\right).$$

The node is given by the midpoint,  $x_0 = \frac{a+b}{2}$  with the corresponding weight  $w_0 = b - a$ .

- **Trapezoidal rule** is given by

$$Q[f](a, b) := (b - a) \left( \frac{f(a) + f(b)}{2} \right)$$

and thus the nodes are defined by  $x_0 = a$ ,  $x_1 = b$  with corresponding weights  $w_0 = w_1 = \frac{1}{2}$ .

- Finally, **Simpson's rule** which you know from M1, is defined as follows:

$$Q[f](a, b) = \frac{b - a}{6} \left( f(a) + 4f\left(\frac{a + b}{2}\right) + f(b) \right),$$

which we identify as quadrature rule with 3 points  $x_0 = a$ ,  $x_1 = \frac{a+b}{2}$ ,  $x_2 = b$  and corresponding weights  $w_0 = w_2 = \frac{b-a}{6}$  and  $w_1 = \frac{4(b-a)}{6}$ .

In this note we will see how quadrature rules can be constructed from integration of interpolation polynomials. We will demonstrate how to do error analysis and how to find error estimates. In the sequel, we will use material from *Preliminaries*, section 3.2, 4 and 5.

## 2 Quadrature based on polynomial interpolation.

This section relies on the content of the note on polynomial interpolation, in particular the section on Lagrange polynomials.

Choose  $n + 1$  distinct nodes  $x_i$ ,  $i = 0, \dots, n$  in the interval  $[a, b]$ , and let  $p_n(x)$  be the interpolation polynomial satisfying the interpolation condition

$$p_n(x_i) = f(x_i), \quad i = 0, 1, \dots, n.$$

We will then use  $\int_a^b p_n(x) dx$  as an approximation to  $\int_a^b f(x) dx$ . By using the Lagrange form of the polynomial

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

with the cardinal functions  $\ell_i(x)$  given by

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

the following quadrature formula is obtained

$$I[f](a, b) \approx Q[f](a, b) = \int_a^b p_n(x) dx = \sum_{i=0}^n f(x_i) \int_a^b \ell_i(x) dx = \sum_{i=0}^n w_i f(x_i) = Q(a, b),$$

where the weights in the quadrature are simply the integral of the cardinal functions over the interval

$$w_i = \int_a^b \ell_i(x) dx \quad \text{for } i = 0, \dots, n.$$

Let us derive three schemes for integration over the interval  $[0, 1]$ , which we will finally apply to the integral

$$I(0, 1) = \int_0^1 \cos\left(\frac{\pi}{2}x\right) dx = \frac{2}{\pi} = 0.636619\dots$$

**Example 2.1.** *The trapezoidal rule revisited.*

Let  $x_0 = 0$  and  $x_1 = 1$ . The cardinal functions and thus the weights are given by

$$\begin{aligned} \ell_0(x) &= 1 - x, & w_0 &= \int_0^1 (1 - x) dx = 1/2 \\ \ell_1(x) &= x, & w_1 &= \int_0^1 x dx = 1/2 \end{aligned}$$

and the corresponding quadrature rule is the trapezoidal rule (usually denoted by  $T$ ) recalled in Example 1.1 with  $[a, b] = [0, 1]$ :

$$T(0, 1) = \frac{1}{2} [f(0) + f(1)].$$

**Example 2.2.** *Gauß-Legendre quadrature for  $n = 2$ .*

Let  $x_0 = 1/2 + \sqrt{3}/6$  and  $x_1 = 1/2 - \sqrt{3}/6$ . Then

$$\begin{aligned} \ell_0(x) &= -\sqrt{3}x + \frac{1 + \sqrt{3}}{2}, & w_0 &= \int_0^1 \ell_0(x) dx = 1/2, \\ \ell_1(x) &= \sqrt{3}x + \frac{1 - \sqrt{3}}{2}, & w_1 &= \int_0^1 \ell_1(x) dx = 1/2. \end{aligned}$$

The quadrature rule is

$$Q(0,1) = \frac{1}{2} \left[ f\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right) + f\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right) \right].$$

**Example 2.3.** *Simpson's rule revisited.*

We construct Simpson's rule on the interval  $[0, 1]$  by choosing the nodes  $x_0 = 0$ ,  $x_1 = 0.5$  and  $x_2 = 1$ . The corresponding cardinal functions are

$$\ell_0 = 2(x - 0.5)(x - 1) \quad \ell_1(x) = 4x(1 - x) \quad \ell_2(x) = 2x(x - 0.5)$$

which gives the weights

$$w_0 = \int_0^1 \ell_0(x) dx = \frac{1}{6}, \quad w_1 = \int_0^1 \ell_1(x) dx = \frac{4}{6}, \quad w_2 = \int_0^1 \ell_2(x) dx = \frac{1}{6}$$

such that

$$\int_0^1 f(x) dx \approx \int_0^1 p_2(x) dx = \sum_{i=0}^2 w_i f(x_i) = \frac{1}{6} [ f(0) + 4f(0.5) + f(1) ].$$

## Exercise 1: Accuracy of some quadrature rules

Use the QR function

```
def QR(f, xq, wq):
    """ Computes an approximation of the integral f
    for a given quadrature rule.

    Input:
    f: integrand
    xq: quadrature nodes
    wq: quadrature weights
    """
    n = len(xq)
    if (n != len(wq)):
        raise RuntimeError("Error: Need same number of quadrature nodes and weights!")
    return np.array(wq)@f(np.array(xq))
```

to compute an approximate value of integral

$$I(0,1) = \int_0^1 \cos\left(\frac{\pi}{2}x\right) dx = \frac{2}{\pi} = 0.636619\dots$$

using the quadrature rules from Example 2.1-2.3. Tabulate the corresponding quadrature errors  $I(0,1) - Q(0,1)$ .

**Solution.** The trapezoidal rule applied to the function  $f(x) = \cos(\pi x/2)$  gives

$$T(0,1) = \frac{1}{2} \left[ \cos(0) + \cos\left(\frac{\pi}{2}\right) \right] = \frac{1}{2},$$

and the error is

$$I(0,1) - T(0,1) = \frac{2}{\pi} - \frac{1}{2} = 0.138\dots$$

The Gauß-Legendre quadrature with two points applied to  $f(x) = \cos(\pi x/2)$  is given by

$$Q(0,1) = \frac{1}{2} \left[ \cos\left(\frac{\pi}{2}x_0\right) + \cos\left(\frac{\pi}{2}x_1\right) \right] = 0.635647\dots$$

with an error

$$I(0,1) - Q(0,1) = 9.72 \dots \cdot 10^{-4}.$$

Simpson's rule applied to  $f(x) = \cos(\pi x/2)$  gives

$$Q(0,1) = 0.6380712 \dots$$

with an error

$$I(0,1) - Q(0,1) = -1.45 \dots \cdot 10^{-3}.$$

**Remarks.** We observe that with the same number of quadrature points, the Gauß-Legendre quadrature gives a much more accurate answer than the trapezoidal rule. So the choice of nodes clearly matters. Simpson's rule gives very similar results to Gauß-Legendre quadrature, but it uses 3 instead of 2 quadrature nodes. The quadrature rules which are based on polynomial interpolation and *equidistributed quadrature nodes* go under the name **Newton Cotes formulas**.

We observe that with the same number of quadrature points, the Gauß-Legendre quadrature gives a much more accurate answer than the trapezoidal rule. So the choice of nodes clearly matters. Simpson's rule gives very similar results to Gauß-Legendre quadrature, but it uses 3 instead of 2 quadrature nodes.

### 3 Degree of exactness and an estimate of the quadrature error

Motivated by the previous examples, we now take a closer look at how to assess the quality of a method. We start with the following definition.

**Definition 3.1.** *The degree of exactness.*

A numerical quadrature has degree of exactness  $d$  if  $Q[p](a,b) = I[p](a,b)$  for all  $p \in \mathbb{P}_d$  and there is at least one  $p \in \mathbb{P}_{d+1}$  such that  $Q[p](a,b) \neq I[p](a,b)$ .

Since both integrals and quadratures are linear in the integrand  $f$ , the degree of exactness is  $d$  if

$$\begin{aligned} I[x^j](a,b) &= Q[x^j](a,b), & j = 0, 1, \dots, d, \\ I[x^{d+1}](a,b) &\neq Q[x^{d+1}](a,b). \end{aligned}$$

**Observation:** All quadratures constructed from Lagrange interpolation polynomials in  $n+1$  distinct nodes will automatically have a degree of exactness of at least  $n$ . This follows immediately from the fact that the interpolation polynomial  $p_n \in \mathbb{P}_n$  of any polynomial  $q \in \mathbb{P}_n$  is just the original polynomial  $q$  itself.

#### Exercise 2: Degree of exactness for some quadrature rules

- What is the degree of exactness for the left and right endpoint rule from Example 1.1?
- What is the degree of exactness for the trapezoidal and midpoint rule from Example 1.1?
- What is the degree of exactness for Gauß-Legendre quadrature for 2 points from Example 2.2?
- What is the degree of exactness for Simpson's rule from Example 2.3?

**Hint.** You can do this either using pen and paper (boring!) or numerically (more fun!), using the code from Example 1. If you decide to code, the following overview might be helpful:

$$EL[f](0,1) = 1 \cdot f(0), \quad ER[f](0,1) = 1 \cdot f(1),$$

$$M(0,1) = 1 \cdot f\left(\frac{1}{2}\right), \quad T(0,1) = \frac{1}{2}[f(0) + f(1)].$$

$$GL(0,1) = \frac{1}{2} \left[ f \left( \frac{1}{2} - \frac{\sqrt{3}}{6} \right) + f \left( \frac{1}{2} + \frac{\sqrt{3}}{6} \right) \right], \quad S(0,1) = \frac{1}{6} [f(0) + 4f(0.5) + f(1)].$$

### 3.1 Estimates for the quadrature error

**Theorem 3.1.** *Error estimate for quadrature rule with degree of exactness  $n$ .*

Assume that  $f \in C^{n+1}(a, b)$  and let  $Q[\cdot](\{x_i\}_{i=0}^n, \{w_i\}_{i=0}^n)$  be a quadrature rule which has degree of exactness  $n$ . Then the quadrature error  $|I[f] - Q[f]|$  can be estimated by

$$|I[f] - Q[f]| \leq \frac{M}{(n+1)!} \int_a^b \prod_{i=0}^n |x - x_i| dx$$

where  $M = \max_{\xi \in [a,b]} |f^{n+1}(\xi)|$ .

**Proof.** Let  $p_n \in \mathbb{P}_n$  be the interpolation polynomial satisfying  $p_n(x_i) = f(x_i)$  for  $i = 0, \dots, n$ . Thanks to the error estimate for the interpolation error, we know that

$$f(x) - p_n(x) = \frac{f^{n+1}(\xi(x))}{(n+1)!} \prod_{k=0}^n (x - x_k).$$

for some  $\xi(x) \in (a, b)$ . Since  $Q(a, b)$  has degree of exactness  $n$  we have  $I[p_n] = Q[p_n] = Q[f]$  and thus

$$\begin{aligned} |I[f] - Q[f]| &= |I[f] - I[p_n]| \leq \int_a^b |f(x) - p_n(x)| dx \\ &= \int_a^b \left| \frac{f^{n+1}(\xi(x))}{(n+1)!} \prod_{k=0}^n (x - x_k) \right| dx \leq \frac{M}{(n+1)!} \int_a^b \prod_{k=0}^n |x - x_k| dx, \end{aligned}$$

which concludes the proof.

The previous theorem often The advantage of the previous theorem is that it is easy to prove. On downside is that the provided estimate can be rather crude, and often sharper estimates can be established. We give two examples here of some sharper estimates (but without proof).

**Theorem 3.2.** *Error estimate for the trapezoidal rule.*

For the trapezoidal rule, there is a  $\xi \in (a, b)$  such that

$$I[f] - Q[f] = \frac{(b-a)^3}{12} f''(\xi).$$

**Theorem 3.3.** *Error estimate for Simpson's rule.*

For Simpson's rule, there is a  $\xi \in (a, b)$  such that

$$I[f] - Q[f] = -\frac{(b-a)^5}{2880} f^4(\xi).$$