1 Numerical Integration

1.1 Introduction

We want to approximate the integral

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

where we are given a, b and the function f as a subroutine which can evaluate $f(x)$ for any given x.

We want to evaluate f at points $x_1, \dots, x_n$ and construct out of the function values an approximation Q which should be close to the exact integral I.

We can do this using interpolation:

- construct the interpolating polynomial $p(x)$
- let $Q := \int_a^b f(x)dx$
- by writing Q in terms of the function values we obtain a quadrature rule of the form

$$Q = w_1 f(x_1) + \cdots + w_n f(x_n)$$

In the special case that the function $f(x)$ is a polynomial of degree$\leq n-1$ we obtain $p(x) = f(x)$ since the interpolating polynomial is unique, and hence $Q = I$. Therefore the quadrature rule is exact for all polynomials of degree$\leq n-1$.

1.2 Midpoint Rule, Trapezoid Rule, Simpson Rule

We consider some special cases with $n = 1, 2, 3$ points:

Midpoint Rule: Let $n = 1$ and pick the midpoint $x_1 := (a+b)/2$. Then $p(x) = f(x_1)$ (constant function) and

$$\boxed{Q^{\text{Midpt}} = (b-a)f(x_1)}$$

Trapezoid Rule: Let $n = 2$ and pick the endpoints: $x_1 := a$, $x_2 := b$. Then $p(x)$ is a linear function and Q is the area of the trapezoid:

$$\boxed{Q^{\text{Trap}} = (b-a)\frac{f(a)+f(b)}{2}}$$

Simpson Rule: Let $n = 3$ and pick the endpoints and midpoint: $x_1 := a$, $x_2 := (a+b)/2$, $x_3 := b$. Then $p(x)$ is a quadratic function and we obtain

$$\boxed{Q^{\text{Simpson}} = (b-a)\frac{f(x_1)+4f(x_2)+f(x_3)}{6}.}$$

Proof: Let us consider the interval $[a,b] = [-r,r]$ where $r = (b-a)/2$. We know that

$$Q = \int_a^b p(x)dx = w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3)$$

and we want to find w_1, w_2, w_3. We also know that we must have $Q = I$ for $f(x) = 1$, $f(x) = x$, $f(x) = x^2$ yielding the equations

$$\begin{aligned} w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1 &= \int_{-r}^{r} 1 dx = 2r \\ w_1 \cdot (-r) + w_2 \cdot 0 + w_3 \cdot r &= \int_{-r}^{r} x dx = 0 \\ w_1 \cdot r^2 + w_2 \cdot 0 + w_3 \cdot r^2 &= \int_{-r}^{r} x^2 dx = \tfrac{2}{3} r^3 \end{aligned}$$

Solving this system for w_1, w_2, w_3 yields $w_1 = w_3 = \frac{r}{3}$, $w_2 = \frac{4}{3}r$.

The midpoint rule is guaranteed to be exact for polynomials of degree 0. But actually it is also exact for all polynomials of degree 1: On the interval $[-r,r]$ consider $f(x) = c_0 + c_1 x$. Then the term c_0 is exactly integrated by the midpoint rule. For the term $c_1 \cdot x$ the exact integral is zero, and the midpoint rule also gives zero for this term.

The Simpson rule is guaranteed to be exact for polynomials of degree≤ 2. But actually it is also exact for all polynomials of degree≤ 3: On the interval $[-r,r]$ consider $f(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3$. Then the term $c_0 + c_1 x + c_2 x^2$ is exactly integrated by the Simpson rule. For the term $c_3 \cdot x^3$ the exact integral is zero, and the Simpson rule also gives zero for this term.

1.3 Errors for the Midpoint Rule, Trapezoid Rule, Simpson Rule

Note that we have for the quadrature error

$$I - Q = \int_a^b (f(x) - p(x))\,dx$$

and we know for the interpolating polynomial that

$$|f(x) - p(x)| \leq \frac{1}{n!}\left(\max_{t\in[a,b]}\left|f^{(n)}(x)\right|\right)|(x-x_1)\cdots(x-x_n)|$$

yielding

$$|I - Q| \leq \frac{1}{n!}\left(\max_{t\in[a,b]}\left|f^{(n)}(x)\right|\right)\cdot\int_a^b |(x-x_1)\cdots(x-x_n)|\,dx. \tag{1}$$

Error for Trapezoid Rule: Here we need to compute $\int_a^b |(x-a)(x-b)|\,dx$. Let us consider the interval $[a,b] = [-r,r]$:

$$\int_a^b |(x-a)(x-b)|\,dx = \int_{-r}^r |(x+r)(x-r)|\,dx = \int_{-r}^r (r^2 - x^2)dx = \left[r^2 x - \tfrac{1}{3}x^3\right]_{-r}^r = \frac{4}{3}r^3$$

As $r = (b-a)/2$ and $n = 2$ the formula (1) becomes

$$\boxed{\left|I - Q^{\text{Trap}}\right| \leq \frac{(b-a)^3}{12}\cdot\max_{t\in[a,b]}\left|f''(x)\right|}$$

Error for Midpoint Rule: We want to exploit that the Midpoint Rule is exact for polynomials of degree 1 and consider the interpolating polynomial $\tilde{p}(x)$ which interpolates f at the nodes x_1, x_1 (which is the tangent line):

$$\tilde{p}(x) = f[x_0] + f[x_0,x_0](x-x_0) = p(x) + f[x_0,x_0](x-x_0)$$
$$\int_a^b \tilde{p}(x)dx = \int_a^b p(x)dx + f[x_0,x_0]\cdot\int_a^b (x-x_0)dx = Q + 0$$

Hence we have using the interpolation error for $\tilde{p}(x)$

$$|I-Q| = \left|\int_a^b (f(x) - \tilde{p}(x))\,dx\right| \leq \frac{1}{2!}\left(\max_{t\in[a,b]}\left|f''(x)\right|\right)\cdot\underbrace{\int_a^b |(x-x_1)(x-x_1)|\,dx}_{\left[\frac{1}{3}(x-x_1)^3\right]_a^b = \frac{2}{3}\left(\frac{b-a}{2}\right)^3}$$

yielding

$$\boxed{\left|I - Q^{\text{Midpt}}\right| \leq \frac{(b-a)^3}{24}\cdot\max_{t\in[a,b]}\left|f''(x)\right|}$$

Error for Simpson Rule: We want to exploit that the Simpson Rule is exact for polynomials of degree 3 and consider the interpolating polynomial $\tilde{p}(x)$ which interpolates f at the nodes x_1, x_2, x_3, x_2 (which also has the correct slope in the midpoint):

$$\tilde{p}(x) = p(x) + f[x_1,x_2,x_3,x_2](x-x_1)(x-x_2)(x-x_3)$$

$$\int_a^b \tilde{p}(x)dx = \int_a^b p(x)dx + f[x_1,x_2,x_3,x_2]\cdot\int_a^b (x-x_1)(x-x_2)(x-x_3)dx = Q+0$$

since the function $(x-x_1)(x-x_2)(x-x_3)$ is antisymmetric with respect to the midpoint x_2. Hence we have using the interpolation error for $\tilde{p}(x)$

$$|I-Q| = \left|\int_a^b (f(x)-\tilde{p}(x))\,dx\right| \le \frac{1}{4!}\left(\max_{t\in[a,b]}\left|f^{(4)}(x)\right|\right)\cdot\int_a^b \left|(x-x_1)(x-x_2)^2(x-x_3)\right|dx.$$

We consider the interval $[a,b]=[-r,r]$ with $r=(b-a)/2$. Then we have for the integral

$$\int_a^b \left|(x-x_1)(x-x_2)^2(x-x_3)\right|dx = \int_{-r}^r \left|(x+r)x^2(x-r)\right|dx = \int_{-r}^r (r^2-x^2)x^2\,dx = \left[r^2\frac{x^3}{3}-\frac{r^5}{5}\right]_{-r}^r = \frac{4}{15}r^5$$

yielding

$$\boxed{\left|I-Q^{\text{Simpson}}\right| \le \frac{(b-a)^5}{90\cdot 32}\cdot\max_{t\in[a,b]}\left|f^{(4)}(x)\right|.}$$

1.4 Higher Order Rules

It is tempting to construct rules with higher $n=3,4,5,\ldots$ which use an interpolating polynomial of degree $n-1$.

For equidistant nodes we have already seen that interpolating polynomials of large degree will have very large oscillations, and may not even converge to the function for $n\to\infty$. For the integral $Q=\int_a^b p(x)dx$ things are not quite as bad since integrating over the oscillations cancels out some of the errors. However, for larger values of n some of the "weights" w_j will become negative, and $\left|w_j\right|$ will increase with increasing n. This means that in machine arithmetic there will be substantial subtractive cancellation.

For interpolation we have seen that one can avoid these problems by carefully placing the nodes in a nonuniform way so that they are more closely clustered together at the endpoints. For interpolation a good choice are the so-called Chebyshev nodes (which are the zeros of Chebyshev polynomials).

This choice of nodes is also useful for numerical integration. Instead of the zeros of Chebyshev polynomials one can also choose the extrema of Chebyshev polynomials, and in this case there is an efficient algorithm to compute Q (*Clenshaw-Curtis quadrature*).

Another choice are the so-called Gauss nodes for *Gaussian quadrature*. These nodes are also more closely clustered near the endpoints, but they are chosen to maximize the polynomial degree for which the rule is exact.

1.5 Composite Rules

For a practical integration problem it is better to increase the accuracy by first subdividing the interval into smaller subintervals with a partition

$$a = x_0 < x_1 < \cdots < x_{N-1} < x_N = b$$

and interval sizes

$$h_j := x_j - x_{j-1}.$$

Then we apply one of the basic rules (midpoint, trapezoid or Simpson rule) on each subinterval and add everything together. This is called a *composite rule*. For example, the **composite trapezoid rule** is defined by

$$\boxed{Q_N^{\text{Trap}} := Q_{[x_0,x_1]}^{\text{Trap}} + \cdots + Q_{[x_{N-1},x_N]}^{\text{Trap}}}$$

where $Q_{[x_{j-1},x_j]}^{\text{Trap}} = h_j\frac{1}{2}\left(f(x_{j-1})+f(x_j)\right)$. Similarly we can define the composite midpoint rule and the composite Simpson rule.

Work: For the composite trapezoid rule with N subintervals we use $N+1$ function evaluations.
For the composite midpoint rule with N subintervals we use N function evaluations.
For the composite Simpson rule with N subintervals we use $2N+1$ function evaluations.

1.6 Error for Composite Rules

The error of the composite trapezoid rule is the sum of the errors on each subinterval:

$$I - Q_N^{\text{Trap}} = \sum_{j=1}^{N} \left(I_{[x_{j-1},x_j]} - Q_{[x_{j-1},x_j]}^{\text{Trap}} \right) \le \sum_{j=1}^{N} \left| I_{[x_{j-1},x_j]} - Q_{[x_{j-1},x_j]}^{\text{Trap}} \right|$$

$$\left| I - Q_N^{\text{Trap}} \right| \le \sum_{j=1}^{N} \left| I_{[x_{j-1},x_j]} - Q_{[x_{j-1},x_j]}^{\text{Trap}} \right| \le \sum_{j=1}^{N} \frac{1}{12} \left(\max_{[x_{j-1},x_j]} \left| f''(t) \right| \right) h_j^3$$

Similarly we can obtain estimates for the composite midpoint rule and the composite Simpson rule.

1.7 Subintervals of equal size

The simplest choice is to choose all subintervals of the same size $h = (b-a)/N$. In this case we obtain for the composite trapezoid rule

$$\left| I - Q_N^{\text{Trap}} \right| \le \sum_{j=1}^{N} \frac{1}{12} \left(\max_{[x_{j-1},x_j]} \left| f''(t) \right| \right) h^3 \le \frac{1}{12} \left(\max_{[a,b]} \left| f''(t) \right| \right) h^3 \left(\sum_{j=1}^{N} 1 \right)$$

$$\boxed{\left| I - Q_N^{\text{Trap}} \right| \le \frac{1}{12} \cdot \frac{(b-a)^3}{N^2} \cdot \max_{[a,b]} \left| f''(t) \right|}$$

If $f''(x)$ is continuous for $x \in [a,b]$ we therefore obtain with $C = \frac{(b-a)^3}{12} \cdot \max_{[a,b]} |f''(t)|$ that

$$\left| I - Q_N^{\text{Trap}} \right| \le \frac{C}{N^2}.$$

This shows that the error tends to zero as $N \to \infty$.

Similarly we obtain for the composite midpoint rule

$$\boxed{\left| I - Q_N^{\text{Midpt}} \right| \le \frac{1}{24} \cdot \frac{(b-a)^3}{N^2} \cdot \max_{[a,b]} \left| f''(t) \right|}$$

where we also have $\left| I - Q_N^{\text{Midpt}} \right| \le \frac{C}{N^2}$.

For the composite Simpson rule we obtain in the same way

$$\boxed{\left| I - Q_N^{\text{Simpson}} \right| \le \frac{1}{90 \cdot 32} \cdot \frac{(b-a)^5}{N^4} \cdot \max_{[a,b]} \left| f^{(4)}(t) \right|}$$

In this case we have $\left| I - Q_N^{\text{Simpson}} \right| \le \frac{C}{N^4}$, so the composite Simpson rule will converge faster than the composite trapezoid or midpoint rule.