TMA205 Differential Equations and Scientific Computing for Kb2, part A

QUADRATURE (1D)

To compute the L_2-projection of a given function and, as we will see later, to compute the Finite Element approximation of the solution to a differential equation, it is necessary to compute certain integrals.

To compute these integrals we often use *quadrature*, i.e., *numerical integration*. One reason for this is that it might be impossible to compute some of the integrals analytically. Another reason is that it increases the *generality*, since the same algorithm can be used for different data. For example, computing the L_2-projections of two different functions (defined on an interval) using quadrature to compute the integrals works in exactly the same way: you only need to evaluate the (different) integrands at some specific quadrature points (for instance the mid-points of the sub-intervals in a given partition of the interval). To compute the integrals analytically, on the other hand, requires different techniques for different integrands.

In these notes, we will present some different quadrature rules, some of which you already know from *Analysis and Linear Algebra K Kf Kb, part B*, and briefly discuss their accuracy.

1. General

Let $f : [a, b] \to \mathbb{R}$ be a given Lipschitz continuous function and let $a = x_0 < x_1 < \ldots < x_N = b$ be a partition of the interval $[a, b]$ into N sub-intervals of length $h_i = x_i - x_{i-1}$. We now seek to *approximate* the integral

$$\int_a^b f(x)\,dx, \tag{1}$$

but since

$$\int_a^b f(x)\,dx = \sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} f(x)\,dx, \tag{2}$$

we begin by approximating

$$\int_{x_{i-1}}^{x_i} f(x)\,dx, \tag{3}$$

and we then obtain an approximation of (1) by adding the approximations of (3) for each sub-interval.

2. Quadrature rules on one sub-interval

We now present some different *quadrature rules* for approximating (3), and begin with the:

2.1. Mid-point rule.

The *mid-point rule* reads as follows:

$$\boxed{\int_{x_{i-1}}^{x_i} f(x)\,dx \approx f(\frac{x_{i-1}+x_i}{2})\,h_i} \tag{4}$$

Since $f(\frac{x_{i-1}+x_i}{2})\,h_i$ is the *area of a rectangle* with sides h_i and $f(\frac{x_{i-1}+x_i}{2})$, (4) can be thought of as approximating the area under $f(x)$ by the area under the *constant* function $\pi_0 f(x) \equiv f(\frac{x_{i-1}+x_i}{2})$ that interpolates (i.e., agrees with the value of) $f(x)$ at the mid-point of the interval:

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$$\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \int_{x_{i-1}}^{x_i} \pi_0 f(x)\,dx = f\Big(\frac{x_{i-1}+x_i}{2}\Big)\, h_i.$$

See Figure 1.

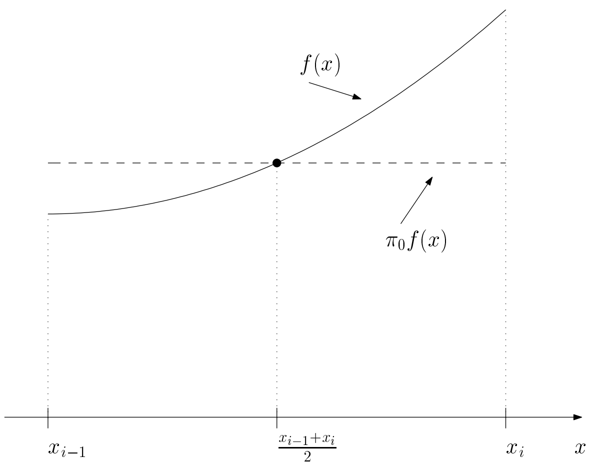

FIGURE 1. Mid-point rule.

For the *mid-point rule*, we have the following *estimate of the quadrature error* that we state without proof:

$$\boxed{\Big|\int_{x_{i-1}}^{x_i} f(x)\,dx - f\Big(\frac{x_{i-1}+x_i}{2}\Big)\, h_i\Big| \le \frac{h_i^3}{24} \max_{y\in[x_{i-1},\,x_i]} |f''(y)|} \tag{5}$$

2.2. **Trapezoidal rule.**

The *trapezoidal rule* reads as follows:

$$\boxed{\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \frac{f(x_{i-1})+f(x_i)}{2}\, h_i} \tag{6}$$

Since $\frac{f(x_{i-1})+f(x_i)}{2}\, h_i$ is the *area of a trapezoid* with sides $f(x_{i-1})$ and $f(x_i)$, and altitude h_i, (6) can be thought of as approximating the area under $f(x)$ by the area under the *linear* interpolant $\pi_1 f(x)$ that agrees with the values of $f(x)$ at the end-points of the interval:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \int_{x_{i-1}}^{x_i} \pi_1 f(x)\,dx = \frac{f(x_{i-1})+f(x_i)}{2}\, h_i.$$

See Figure 2.

For the *trapezoidal rule*, we have the following *estimate of the quadrature error*:

$$\boxed{\Big|\int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{f(x_{i-1})+f(x_i)}{2}\, h_i\Big| \le \frac{h_i^3}{12} \max_{y\in[x_{i-1},\,x_i]} |f''(y)|} \tag{7}$$

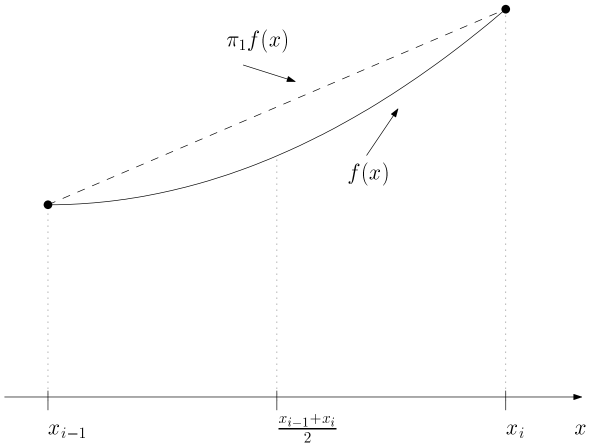

FIGURE 2. Trapezoidal rule.

2.3. **Simpson's rule.** *Simpson's rule* reads as follows:

$$\boxed{\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \frac{f(x_{i-1}) + 4f(\frac{x_{i-1}+x_i}{2}) + f(x_i)}{6}\,h_i} \tag{8}$$

To derive (8), one approximates the area under $f(x)$ by the area under the *quadratic* interpolant $\pi_2 f(x)$ that agrees with the values of $f(x)$ at the mid-point and the end-points of the interval:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \int_{x_{i-1}}^{x_i} \pi_2 f(x)\,dx = \ \dots\ = \frac{f(x_{i-1}) + 4f(\frac{x_{i-1}+x_i}{2}) + f(x_i)}{6}\,h_i.$$

See Figure 3.

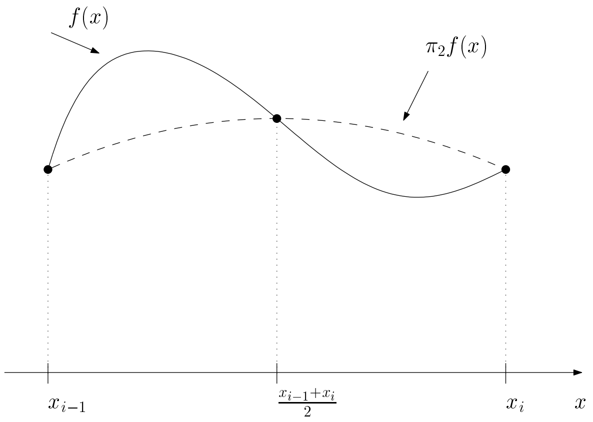

FIGURE 3. Simpson's rule.

For *Simpson's rule*, we have the following *estimate of the quadrature error*:

$$\boxed{\left|\int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{f(x_{i-1}) + 4f(\frac{x_{i-1}+x_i}{2}) + f(x_i)}{6}\,h_i\right| \le \frac{h_i^5}{2880} \max_{y\in[x_{i-1},\,x_i]} |f^{(4)}(y)|} \tag{9}$$

2.4. **Newton-Cotes Formulas.** The quadrature rules that have been presented so far (*mid-point rule*, *trapezoidal rule* and *Simpson's rule*) are examples of *Newton-Cotes formulas*. As we have seen, they can be derived by approximating the integrand with a polynomial interpolant and integrating this interpolant. (Since the *trapezoidal rule* and *Simpson's rule* use the values of the integrand at the end-points of the interval, these rules are called *Closed Newton-Cotes formulas*. The *mid-point rule* is accordingly called an *Open Newton-Cotes formula*.)

2.5. **Accuracy.** By construction, it is clear that the *mid-point rule* must be exact for constant polynomials, the *trapezoidal rule* for linear polynomials and *Simpson's rule* for quadratic polynomials.

From the error estimate (7) we see that for the *trapezoidal rule* this is indeed true: Since $|f''(y)|$ vanishes if f is a linear polynomial the *trapezoidal rule is exact for linear polynomials*.

From the error estimates (5) and (9), however, we see that the *mid-point rule* and *Simpson's rule* actually perform better than expected! These error estimates show that also the *mid-point rule is exact for linear polynomials* and that *Simpson's rule is exact for cubic polynomials*.

The reason we "win" extra accuracy for the *mid-point rule* and *Simpson's rule* can be understood by examining Figure 1 and Figure 3: Note how the interpolation error changes signs which leads to cancellation effects when integrating over the interval. In Figure 2, on the other hand, the sign of the interpolation error is constant and no "lucky" cancellation occurs.

To sum up: The *mid-point rule* and the *trapezoidal rule* are both exact for polynomials of degree less than or equal to one. *Simpson's rule* is exact for polynomials of degree less than or equal to three. Further, since the quadrature error for the *mid-point rule* and the *trapezoidal rule* is proportional to h_i^3 while the quadrature error for *Simpson's rule* is proportional to h_i^5, we expect the latter method to give more accurate approximations (provided the integrand is "smooth" enough, i.e., the higher derivatives do not become "too" large).

2.6. **Abscissas and Weights.** All the quadrature rules that we have met can be described in the following way:

$$\boxed{\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \left(\sum_{j=1}^{n} w_j\, f(q_j)\right) h_i} \tag{10}$$

The quadrature points q_j are called *abscissas* and w_j are *weight coefficients*. We summarize:

Mid-point rule: $n = 1$; $w_1 = 1$; $q_1 = (x_{i-1} + x_i)/2$
Trapezoidal rule: $n = 2$; $w_1 = w_2 = 1/2$; $q_1 = x_{i-1}$, $q_2 = x_i$
Simpsons's rule: $n = 3$; $w_1 = w_3 = 1/6$, $w_2 = 4/6$; $q_1 = x_{i-1}$, $q_2 = (x_{i-1}+x_i)/2$, $q_3 = x_i$

2.7. **Gaussian Quadrature.** A common property of the Newton-Cotes quadrature rules is that their abscissas are evenly distributed over the interval. One then chooses the weight coefficients in such a way as to obtain optimal accuracy. In *Gaussian Quadrature* we give ourselves the additional freedom to *choose also the location of the abscissas* which will no longer be equally spaced. Thus, we will have twice the number of degrees of freedom at our disposal to obtain optimal accuracy. We will not delve into how to choose abscissas and weights, merely give one example:

The *Gauss-Legendre 2-point rule* results by choosing (following the syntax in (10))

$$n = 2; \quad w_1 = w_2 = 1/2; \quad q_1 = \frac{x_{i-1} + x_i}{2} - \frac{\sqrt{3}}{6}\, h_i,\; q_2 = \frac{x_{i-1} + x_i}{2} + \frac{\sqrt{3}}{6}\, h_i;$$

and it thus reads as follows:

$$\boxed{\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \frac{f(q_1)+f(q_2)}{2}\,h_i} \tag{11}$$

See Figure 4.

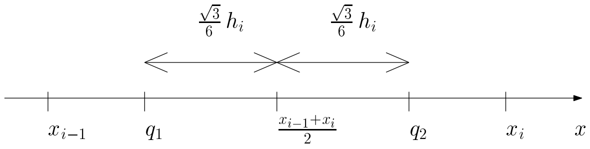

FIGURE 4. Abscissas ("Gauss-points") for the Gauss-Legendre 2-point rule.

For the *Gauss-Legendre 2-point rule*, we have the following *estimate of the quadrature error*:

$$\boxed{\left|\int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{f(q_1)+f(q_2)}{2}\,h_i\right| \le \frac{h_i^5}{4320}\max_{y\in[x_{i-1},\,x_i]}|f^{(4)}(y)|} \tag{12}$$

Note that the order of accuracy is the same as for *Simpson's rule* with only two quadrature points!

3. Quadrature on $[a,\, b]$

To extend the local results to $[a,\, b]$, we need only use (2) and add the contributions from the different sub-intervals. As an example we take the *trapezoidal rule*, for which we get using (6):

$$\int_a^b f(x)\,dx = \sum_{i=1}^N \int_{x_{i-1}}^{x_i} f(x)\,dx \approx \sum_{i=1}^N \frac{f(x_{i-1})+f(x_i)}{2}\,h_i \tag{13}$$

We conclude by deriving the corresponding *global* quadrature error estimate:

$$\left|\int_a^b f(x)\,dx - \sum_{i=1}^N \frac{f(x_{i-1})+f(x_i)}{2}\,h_i\right| = \left|\sum_{i=1}^N \int_{x_{i-1}}^{x_i} f(x)\,dx - \sum_{i=1}^N \frac{f(x_{i-1})+f(x_i)}{2}\,h_i\right| =$$

$$\left|\sum_{i=1}^N \left(\int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{f(x_{i-1})+f(x_i)}{2}\,h_i\right)\right| \le \{\text{ triangle inequality }\} \le$$

$$\sum_{i=1}^N \left|\int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{f(x_{i-1})+f(x_i)}{2}\,h_i\right| \le \ (7)\ \le$$

$$\sum_{i=1}^N \frac{h_i^3}{12}\max_{y\in[x_{i-1},\,x_i]}|f''(y)| = \{h(y)=h_i,\ \text{in } [x_{i-1},\,x_i]\} = \sum_{i=1}^N \frac{h_i}{12}\max_{y\in[x_{i-1},\,x_i]}|h(y)^2 f''(y)| \le$$

$$\sum_{i=1}^N \frac{h_i}{12}\max_{y\in[a,\,b]}|h(y)^2 f''(y)| = \frac{b-a}{12}||h^2 f''||_{L_\infty(a,\,b)}.$$

Note that we "lose" one power of h compared to the local estimate (7). The extension of the other quadrature rules to $[a,\, b]$ is analogous.