3 Exercise 3

3.1 Task 1

(a) The analytical solutions are

$$I = \int_0^4 (x^4 - 1)dx = \int_0^4 x^4 dx - \int_0^4 1dx = \frac{4^5 - 0^5}{5} - (4 - 0) = 200.8 \text{ and}$$

$$I = \int_0^\pi \sin^2(x)dx = \frac{1}{2}[\pi - \sin(\pi)\cos(\pi)] - \frac{1}{2}[0 - \sin(0)\cos(0)] = \frac{\pi}{2} \approx 1.57.$$

The numerical solution is calculated using the approximation

$$I = \int_{x^L}^{x^R} f(x)dx \approx \frac{x^R - x^L}{2} \sum_i h_i f(x_i), \tag{3.1}$$

with the vertices x^L and x^R (L and R stand here for “left” and “right”, not exponents), weighting factors h_i defined by the quadrature formula, and integration points x_i (which are not necessarily at the vertices!). Values of the function f at the integration points are used for approximation of the integral. The sum $\sum_i h_i = 2$ for all quadrature formulas (see Table 3.1 below) explains the factor 1/2 before the sum in eq. (3.1). (Why?) The number of integration points (maximum value of the positive integer i) and corresponding weighting factors depend on the particular quadrature formula.

The integration points x_i are given above in global coordinates (on the x-axis), while the quadrature formulas are defined universally (regardless of the particular geometry) in local coordinates (on the r-axis for $r \in [-1, +1]$). Transformation from local to global coordinates is in general

$$x_i = x(r_i) = \sum_j \mathcal{N}^j(r_i)x^j, \tag{3.2}$$

where $\mathcal{N}^j$ denotes a shape function associated with vertex j. Note that the upper index j and the sum run over the vertices, while the lower index i and the sum in eq. (3.1) run over the integration points. Here, $j = L, R$ for the two vertices, so eq. (3.2) becomes

$$x_i = \mathcal{N}^L(r_i)x^L + \mathcal{N}^R(r_i)x^R \tag{3.3}$$

and we use a simple linear transformation (linear shape functions, because coordinates are “trivial” linear functions of themselves, $f(x_i) = x_i$),

$$\mathcal{N}^L(r_i) = \frac{1}{2}(1 - r_i) \quad \text{and} \quad \mathcal{N}^R(r_i) = \frac{1}{2}(1 + r_i). \tag{3.4}$$

As expected, $\mathcal{N}^L(-1) = \mathcal{N}^R(+1) = 1$, while $\mathcal{N}^R(-1) = \mathcal{N}^L(+1) = 0$, so r^L transforms to x^L and r^R transforms to x^R.

Table 3.1: Integration points and weighting factors for quadrature formulas.

Quadrature formula	r_i	h_i
trapezoidal rule	-1 1	1 1
Simpson's rule	-1 0 1	1/3 4/3 1/3
Simpson's 3/8 rule	-1 -1/3 1/3 1	1/4 3/4 3/4 1/4
Gaussian (1 int. point)	0	2
Gaussian (2 int. points)	$-1/\sqrt{3}$ $1/\sqrt{3}$	1 1
Gaussian (3 int. points)	$-\sqrt{3/5}$ 0 $\sqrt{3/5}$	5/9 8/9 5/9

The integration points in local coordinates (r_i) and weighting factors (h_i) are listed in Table 3.1 for several quadrature formulas.

(b) For the given integral,

$$f(x) = x^4 - 1, \quad x^L = 0, \quad x^R = 4.$$

For the trapezoidal rule (see Table 3.1),

$$r_1 = -1, \quad r_2 = 1, \quad h_1 = 1, \quad h_2 = 1.$$

Equations (3.1), (3.3), and (3.4) give then

$$\begin{aligned} I &\approx \frac{4-0}{2} \sum_{i=1}^{2} h_i f\left(\frac{0}{2}(1 - r_i) + \frac{4}{2}(1 + r_i)\right) = 2 \sum_{i=1}^{2} h_i f\left(2(1 + r_i)\right) \\ &= 2[1 \cdot f\left(2(1 + (-1))\right) + 1 \cdot f\left(2(1 + (+1))\right)] = 2[f(0) + f(4)] \\ &= 2[0^4 - 1 + 4^4 - 1] = 508. \end{aligned}$$

This is much larger than the exact solution, 200.8, because the large change with x of the fourth-order function $x^4 - 1$ over the interval $[0, 4]$ cannot be captured well with only two integration points in the interval.

Draw the function $f(x) = x^4 - 1$ in the interval $[0, 4]$. Where are the integration points on the x-axis? What are the values of $f(x_i)$ at these points which lead to the large error? Which integration points could give a better estimation?

(d) Why does the Gaussian quadrature with three integration points give the accurate result for $f(x) = x^4 - 1$? What is its order of accuracy? Why does the Gaussian quadrature with only one integration point underestimate the value by far, while the trapezoidal rule overestimates it?

Why is the estimated value obtained with the trapezoidal rule equal to zero for $f(x) = \sin^2(x)$ and to π with the Gaussian quadrature with one integration point? Why does not any of the quadrature formulas give the exact solution?