MA378 Chapter 3: Numerical Integration

Any question marked with a $\star$ may feature on the class test and/or Assignment 2, and so won't be covered in tutorials.

Exercise 1.1 ($\star$)**.** (*For simplicity, you may assume that the quadrature rule is integrating* f *on the interval* $[-1, 1]$.) Let $q_0, q_1, \dots, q_N$ be the quadrature weights for the Newton-Cotes rule $Q_N(f)$. Show that $q_i = q_{N-i}$ for $i = 0, \dots N$.

Answer: There are a few possible ways of answering this one. Here is one. Recall that $q_i = \int_{-1}^{1} L_i(x)dx$, where L_i is the ith Lagrange polynomial associated with the points $-1 = x_0 < x_1 < \cdots < x_n = 1$. That is, $L_i(x)$ and $L_{n-i}(x)$ are the unique polynomials of degree n with the properties that

$$L_i(x_j) = \begin{cases} 1 & x_j = x_i \\ 0 & x_j \neq x_i, \end{cases} \qquad \text{and} \qquad L_{n-i}(x_j) = \begin{cases} 1 & x_j = x_{n-i} \\ 0 & x_j \neq x_{n-i}. \end{cases}$$

Since the x_i are uniformly spaced on $[-1, 1]$ we can see that $x_i = -x_{n-i}$. Therefore, $L_{n-i}(-x_j) = \begin{cases} 1 & x_j = -x_{n-i} = x_i \\ 0 & x_j \neq -x_{n-i} = x_i. \end{cases}$. Thus $L_{n-i}(x) = L_i(-x)$. With the substitution $y = -x$, we can see that $q_{n-i} = \int_{-1}^{1} L_{n-i}(x)dx = \int_{-1}^{1} L_i(-x)dx = -\int_{1}^{-1} L_i(y)dy = \int_{-1}^{1} L_i(y)dy = q_i$ (note the change in the limits of integration). So $q_i = q_{n-i}$.

Exercise 1.2. Show that $\sum_{i=0}^{n} q_i = b - a$.

Exercise 2.1. Deduce the 4-point Newton-Cotes Rule for estimating the integral $\int_0^1 f(x)dx$:

$$Q_3(f) = q_0 f(x_0) + q_1 f(x_1) + q_2 f(x_2) + q_3 f(x_3).$$

Extend the rule to estimate the integral of functions over $[a, b]$.

Exercise 2.2. Prove the error bound given for the Trapezium rule. That is, show that

$$\left|\int_a^b f(x)dx - Q_1(f)\right| := \mathcal{E}_1 \leqslant \frac{(b-a)^3}{12} M_2.$$

Exercise 3.1. Explain clearly, with an example, why in general it is not true that $Q_n(f) \to \displaystyle\int_a^b f(x)dx$ as $n \to \infty$.

Exercise 3.2. (i) Deduce an error estimate for the Composite Trapezium Rule.

(ii) Taking $N = 10$, give an upper bound for the error in the Composite Trapezium Rule when approximating $\int_1^2 \ln(x)dx$.

(iii) What value of n would you have to take to ensure that the error was less that 10^{-5}?

Exercise 3.3. (i) Deduce the formula for the *composite Simpson's Rule*.

(ii) Derive an error estimate for the *composite Simpson's Rule*.

(iii) What value of N would you have to take to ensure that the error in the estimate of $\int_1^2 \ln(x)dx$ is less that 10^{-6}?

(iv) Denote the $(N+1)$-point Composite Simpson's Rule by $S_N(f) \approx \int_a^b f(x)dx$. Show that, for sufficiently smooth $f(x)$,

$$\lim_{n\to\infty} S_N(f) = \int_a^b f(x)dx.$$

Exercise 3.4. Determine the precision of the following schemes for estimating $\int_0^1 f(x)dx$.

(i) $Q(f) = f(\frac{1}{2})$.

> **Answer:** $Q(1) = 1 = I(1)$ and $Q(x) = 1/2 = I(x)$, but $Q(x^2)1/4 \neq I(x^2)$. So this method has precision 1. FYI, this is the so-called mid-point rule. It is the 1-point Gaussian Quadrature Rule.

(ii) $Q(f) = \frac{1}{4}f(0) + \frac{3}{4}f(\frac{2}{3})$.

> **Answer:** $Q(1) = 1 = I(1)$, $Q(x) = 1/2 = I(x)$, $Q(x^2)1/3 = I(x^2)$. But $Q(x^3) = 2/9 \neq I(x^3)$. So this method has precision 2.

(iii) $Q(f) = \frac{3}{2}f(\frac{1}{3}) - 2f(\frac{1}{2}) + \frac{3}{2}f(\frac{2}{3})$.

> **Answer:** $Q(x^k) = 1/(k+1) = I(x^k)$, for $k = 0, 1, 2, 3$. But $Q(x^4) = 41/216 \neq I(x^4)$. So $Q(\cdot)$ has precision 3.

Exercise 3.5 ($\star$). Consider the rule:

$$R(f) = q_0 f\big(\frac{1}{3}\big) - f\big(\frac{1}{2}\big) + q_2 f\big(\frac{3}{4}\big)$$

for approximating $\int_0^1 f(x)dx$.

(a) Determine values of q_0 and q_2 that ensure this rule has precision 2.

> **Answer:** (a) We need to find q_0 and q_2 so that $R(f) = \int_0^1 p_2(x)dx$ where p_2 is any polynomial of degree 2. Since that space of polynomials is spanned by the set $\{1, x, x^2\}$, we take q_0 and q_2 to satisfy the equations $q_0 - 1 + q_2 = 1$, $q_0/2 - 1/2 + q_2(3/4) = 1/2$, and $q_0/9 - 1/4 + q_2(9/16) = 1/3$. These equations are not linearly independent (since there are only two unknowns. Solving any pair of them should give $q_0 = 6/5$ and $q_2 = 4/5$. So $R(f) = \frac{6}{5}f\big(\frac{1}{3}\big) - f\big(\frac{1}{2}\big) + \frac{4}{5}f\big(\frac{3}{4}\big)$.

(b) What is the maximum precision of $R(\cdot)$ with the values of q_1 and q_2 that you have determined?

> **Answer:** (b) Could this method be exact for some higher degree polynomials? Checking with $f(x) = x^3$, we should find that $R(x^3) = 37/144 \neq \int_0^1 x^4 dx$. So the precision is at most 2.

(c) Why is this not, strictly speaking, a Newton-Cotes rule?

> **Answer:** (c) Either one of the following reasons would suffice: the limits of integration are not included as quadrature points, and the points are not equally spaced.

Exercise 4.1. Use a change of variables, as we did with the Trapezium rule, to show that the rule for approximating $\int_0^1 f(x)dx$ is

$$G_1(f) = \frac{1}{2}\Big(f(\frac{1}{2} - \frac{1}{2\sqrt{3}}) + f(\frac{1}{2} + \frac{1}{2\sqrt{3}})\Big).$$

More generally, extend the rule to an arbitrary interval $[a, b]$.

Exercise 4.2. Use $G_1(x)$ to estimate $\int_1^2 \ln(x)dx$. How does this compare with the Trapezium and Simpson's Rule?

Exercise 4.3. Derive a 3-point Gaussian Quadrature Rule to estimate $\int_{-1}^1 f(x)dx$. *Hint:* $x_1 = 0$.

Answer: The method is $G_2(f) := w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2)$, and, since it has 6 degrees of freedom, it should be exact for each of the polynomials in $\{1, x, x^2, x^3, x^4, x^5\}$. These 6 polynomials will lead to 6 (nonlinear) equations. However, since we know that $x_1 = 0$, we need only 5. In any case the equations are

(i) $w_0 + w_1 + w_2 = 2$	(ii) $w_0 x_0 + w_2 x_2 = 0$	(iii) $w_0 x_0^2 + w_2 x_2^2 = 2/3$
(iv) $w_0 x_0^3 + w_2 x_2^3 = 0$	(v) $w_0 x_0^4 + w_2 x_2^4 = 2/5$	(vi) $w_0 x_0^5 + w_2 x_2^5 = 0$

(ii) Gives that $w_0 x_0 = -w_2 x_2$. Substitute this into (iv) to get that $(-w_2 x_2)x_0^2 - w_2 x_2^3 = 0$. Since $x_2 \neq 0$, and $w_2 \neq 0$, we can deduce that $x_0^2 = x_2^2$. So $x_0 = -x_2$, because $x_0 < x_2$. Again using (ii) we get $w_0 = w_2$. Next use (iii) to see that $w_0 x_0^2 = 1/3$, and (v) to give $w_0 x_0^4 = 1/5$. Combining those leads to $x_0 2 = 3/5$. So now we have that $x_0 = -\sqrt{3/5}$ and $x_1 = \sqrt{3/5}$. Reusing $w_0 x_0^2 = 1/3$, we have that $w_0 = 5/9 = w_2$. Finally, (i) gives $w_1 = 8/9$. That is, the method is

$$G_2(f) = \frac{5}{9} f(-\sqrt{\frac{3}{5}}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{\frac{3}{5}}).$$

Exercise 5.1. $\mathcal{P}_n$, the space of polynomials of degree (at most) n forms a vector space. Is it true that the space of *monic* polynomials of degree n forms a vector space?

Exercise 5.2 ($\star$). (i) Using the Inner Product

$$(f, g) := \int_0^1 f(x)g(x)dx,$$

find $\widetilde{p}_0(x)$, $\widetilde{p}_1(x)$, $\widetilde{p}_2(x)$ and $\widetilde{p}_3(x)$.

Answer: We'll use Thm 5.12. Define

$$\alpha_{n+1} = \frac{(x\widetilde{p}_n, \widetilde{p}_n)}{(\widetilde{p}_n, \widetilde{p}_n)}, \quad \text{and} \quad \beta_{n+1} = \frac{(x\widetilde{p}_n, \widetilde{p}_{n-1})}{(\widetilde{p}_{n-1}, \widetilde{p}_{n-1})},$$

and

$$\widetilde{p}_0(x) \equiv 1, \widetilde{p}_1(x) = x - \alpha_1, \quad \text{and} \quad \widetilde{p}_{n+1}(x) = (x - \alpha_{n+1})\widetilde{p}_n(x) - \beta_{n+1}\widetilde{p}_{n-1}(x), \text{ for } n \geqslant 1.$$

- $n = 0$: $\alpha_1 = (x, 1)/(1, 1) = 1/2$ which gives that $\mathbf{\widetilde{p}_1 = x - 1/2}$;
- $n = 1$: $\alpha_2 = (1/24)/(1/12) = 1/2$ and $\beta_2 = (1/12)/1 = 1/12$, which gives that $\widetilde{p}_2 = (x-1/2)^2 - 12$. Can simplify as $\mathbf{\widetilde{p}_2(x) = x^2 - x + 1/6}$.
- $n = 2$: $\alpha_3 = (1/360)/(1/180) = 1/2$ and $\beta_3 = (1/180)/(1/12) = 1/15$, which gives that $\widetilde{p}_3 = (x - 1/2)\big((x-1/2)^2 - 1/12\big) - x/15 + 1/30$. Can simplify this as $\mathbf{\widetilde{p}_3(x) = x^3 - (3/2)x^2 + (3/5)x - 1/20}$.

(ii) Find the zeros of $\widetilde{p}_2(x)$ and call them x_0 and x_1. Construct a quadrature rule for $\displaystyle\int_0^1 f(x)dx$ taking these as the quadrature points, and the weights as the integrals to the corresponding Lagrange polynomials.

Answer: The zeros of $\widetilde{p}_2(x) = x^2 - x + 1/6$ are $x_0 = 1/2 - \sqrt{3}/6$ and $x_1 = 1/2 + \sqrt{3}/6$.
The associated Lagrange Polynomials are

- $L_0 = \frac{x-x_1}{x_0-x_1} = \frac{x-1/2-\sqrt{3}/6}{-\sqrt{3}/3} = -\sqrt{3}x + (1+\sqrt{3})/2$
- $L_1 = \frac{x-x_0}{x_1-x_0} = \frac{x-1/2+\sqrt{3}/6}{\sqrt{3}/3} = \sqrt{3}x + (1-\sqrt{3})/2$

With a little calculus we can see that $w_0 = \int_0^1 L_0(x)dx = \frac{1}{2}$ and $w_1 = \int_0^1 L_1(x)dx = \frac{1}{2}$. However, it is OK to derive the values of w_0 and w_1 using, e.g., undetermined coefficients.

Exercise 6.1. Give a complete proof of Theorem 6.1 (i.e., that $G_n(\cdot)$ has precision $2n+1$).

Exercise 6.2. Show that it is impossible to choose $n+1$ quadrature points and weights so that the $n+1$-point quadrature rule

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

has precision $2n+2$.

Hint: To show the method does not have precision $2n+2$, you just need to give a an example of a single polynomial p of degree exactly $2n+2$ for which $\int_a^b p(x)dx \neq \sum_{k=0}^{n} w_k f(x_k)$.