

Problem 1. Derive a Newton-Cotes formula for $\int_0^1 f(x) dx$ based on the nodes $\{0, 1/3, 2/3, 1\}$.

Solution. Our starting point is the Lagrange interpolation of the function $f(x)$, given by

$$f(x) \approx \sum_{i=0}^n f_i \ell_i(x), \quad (1)$$

where $f_i \equiv f(x_i)$ and

$$\ell_i(x) = \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \quad \text{for } i = 0, \dots, n. \quad (2)$$

Then, letting the *weights* w_i be given by

$$w_i := \int_a^b \ell_i(x) dx, \quad (3)$$

we have the **quadrature formula**

$$\int_a^b f(x) dx = \sum_{i=0}^n w_i f_i + \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\xi(x)) dx \quad (4)$$

where $\xi \in (a, b)$. This formula is of the form

$$\int_a^b f(x) dx = P + E,$$

where P is the *quadrature approximation*

$$P = \sum_{i=0}^n w_i f_i, \quad (5)$$

and E is the *error term*

$$E = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\xi(x)) dx. \quad (6)$$

If we let $n = 1$ in (4), the approximation is linear and we get the *Trapezoidal Rule*, while for $n = 2$ the approximation is quadratic and yields *Simpson's 1/3 rule*. Now, in our case, we have the four nodes $\{x_0 = 0, x_1 = 1/3, x_2 = 2/3, x_3 = 1\}$. A more accurate approximation to the integral of $f(x)$ over the interval $[0, 1]$ would entail a *composite* Newton-Cotes formula (for instance, break up the interval into four subintervals using the provided four nodes), but this problem is asking to write a generic, non-composite formula, so we will accomplish that by using $n = 3$ in (4) and get a cubic polynomial to integrate in place of $f(x)$:

$$\int_0^1 f(x) dx = \sum_{i=0}^3 w_i f_i + \frac{1}{4!} \int_0^1 \prod_{i=0}^3 (x - x_i) f^{(4)}(\xi(x)) dx.$$

Let's look at the approximation and error terms, one at a time. Starting with the approximation,

$$\begin{aligned} P &= w_0 f_0 + w_1 f_1 + w_2 f_2 + w_3 f_3 \\ &= \int_0^1 \frac{x - x_1}{x_0 - x_1} \frac{x - x_2}{x_0 - x_2} \frac{x - x_3}{x_0 - x_3} f_0 dx + \int_0^1 \frac{x - x_0}{x_1 - x_0} \frac{x - x_2}{x_1 - x_2} \frac{x - x_3}{x_1 - x_3} f_1 dx \\ &\quad + \int_0^1 \frac{x - x_0}{x_2 - x_0} \frac{x - x_1}{x_2 - x_1} \frac{x - x_3}{x_2 - x_3} f_2 dx + \int_0^1 \frac{x - x_0}{x_3 - x_0} \frac{x - x_1}{x_3 - x_1} \frac{x - x_2}{x_3 - x_2} f_3 dx. \end{aligned} \quad (7)$$

Instead of looking for a tricky change of variables here or just doing a straightforward, but LONG antiderivation, we make our lives easier by summoning Mathematica to the rescue:

```
1 Integrate[(x - x1)/(x0 - x1) * (x - x2)/(x0 - x2) * (x - x3)/(x0 - x3),
2 {x, a, b}] /. {x0 -> 0, x1 -> 1/3, x2 -> 2/3, x3 -> 1}
3 Integrate[(x - x0)/(x1 - x0) * (x - x2)/(x1 - x2) * (x - x3)/(x1 - x3),
4 {x, a, b}] /. {x0 -> 0, x1 -> 1/3, x2 -> 2/3, x3 -> 1}
5 Integrate[(x - x0)/(x2 - x0) * (x - x1)/(x2 - x1) * (x - x3)/(x2 - x3),
6 {x, a, b}] /. {x0 -> 0, x1 -> 1/3, x2 -> 2/3, x3 -> 1}
7 Integrate[(x - x0)/(x3 - x0) * (x - x1)/(x3 - x1) * (x - x2)/(x3 - x2),
8 {x, a, b}] /. {x0 -> 0, x1 -> 1/3, x2 -> 2/3, x3 -> 1}
```

The above yields

$$\begin{aligned} & -\frac{3}{8} \left(\frac{8a}{3} - \frac{22a^2}{3} + 8a^3 - 3a^4 + b \left(-\frac{8}{3} + \frac{22b}{3} - 8b^2 + 3b^3 \right) \right) \\ & \frac{9}{8} \left(-4a^2 + \frac{20a^3}{3} - 3a^4 + b(4b - \frac{20b^2}{3} + 3b^3) \right) \\ & -\frac{9}{8} \left(-2a^2 + \frac{16a^3}{3} - 3a^4 + b(2b - \frac{16b^2}{3} + 3b^3) \right) \\ & \frac{3}{8} \left(-\frac{4a^2}{3} + 4a^3 - 3a^4 + b(\frac{4b}{3} - 4b^2 + 3b^3) \right) \end{aligned}$$

That shows the result for a general $[a, b]$, but it simplifies greatly once we substitute actual values... In our case, with $a = 0$, $b = 1$, the results simplify to

$$\{w_0, w_1, w_2, w_3\} = \left\{ \frac{1}{8}, \frac{3}{8}, \frac{3}{8}, \frac{1}{8} \right\},$$

so that all the weights add up to 1. Hence, the quadrature approximation is

$$P = \sum_{i=0}^3 w_i f_i = \frac{1}{8} (f_0 + 3f_1 + 3f_2 + f_3). \quad (8)$$

In fact, for a general $[a, b]$, this result takes the form

$$P = \sum_{i=0}^3 w_i f_i = \frac{b-a}{8} (f_0 + 3f_1 + 3f_2 + f_3). \quad (9)$$

Moreover, can also rewrite this in terms of $h = x_{i+1} - x_i$. Since there are four interpolating nodes in the interval $[a, b]$ in this approach, $[a, b]$ splits into three subintervals $\{[a = x_0, x_1], [x_1, x_2], [x_2, x_3 = b]\}$. Thus, $h = (b - a)/3$, and we have

$$P = \sum_{i=0}^3 w_i f_i = \frac{3h}{8} (f_0 + 3f_1 + 3f_2 + f_3). \quad (10)$$

(Whence the name for this approach: *Simpson's 3/8 rule*.)

Similarly, for the error term,

$$\begin{aligned} & \text{Integrate}[\\ & \quad 1/4! * \text{Product}[x - \text{Subscript}[x, i], \{i, 0, 3\}], \{x, 0, 1\}] \\ & \quad /. \{\text{Subscript}[x, 0] \rightarrow 0, \text{Subscript}[x, 1] \rightarrow 1/3, \\ & \quad \text{Subscript}[x, 2] \rightarrow 2/3, \text{Subscript}[x, 3] \rightarrow 1\} \end{aligned}$$

which yields $-1/6480$. Hence,

$$\begin{aligned} E &= \frac{1}{4!} \int_0^1 \prod_{i=0}^3 (x - x_i) f^{(4)}(\xi(x)) dx \\ &= -\frac{1}{6480} f^{(4)}(\xi(x)). \end{aligned} \quad (11)$$

Note that here we were able to pull the factor $f^{(4)}(\xi(x))$ out of the integral because $\prod_{i=0}^3 (x - x_i)$ is a fourth-order polynomial which does not change sign in the entire interval $[0, 1]$; thus we were able to use the following theorem:

Weighted Mean Value Theorem for Integrals

Suppose that f is continuous on $[a, b]$. Let g be another function such that its Riemann integral exists, and g does not change sign on $[a, b]$. Then, there exists a number $c \in (a, b)$ that satisfies

$$\int_a^b f(x)g(x) dx = f(c) \int_a^b g(x) dx. \quad (12)$$

The error term (11) generalizes to any interval $[a, b]$, by using $h = (b - a)/3$ as before:

$$E = -\frac{3}{80} h^5 f^{(4)}(\xi(x)). \quad \square \quad (13)$$



Problem 2. Apply the composite Simpson's rule with $m = 4$ to the integral $\int_0^\pi x \cos x \, dx$.

Solution. In Simpson's (1/3) composite rule, an integral

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

is approximated by partitioning the interval $[a, b]$ into N evenly spaced segments $a = x_0 < x_1 < \dots < x_N = b$ with spacing $h \equiv (b - a)/N$, and then putting

$$I \approx \frac{h}{3} \left[f_0 + 4 \sum_{\substack{i=1 \\ i \text{ is odd}}}^{N-1} f_i + 2 \sum_{\substack{i=2 \\ i \text{ is even}}}^{N-2} f_i + f_N \right]. \quad (14)$$

(Note that N must be even in order for (14) to work.) In the case at hand, x and $\cos x$ have the same sign on the whole interval $[0, \pi]$, so we may exploit this symmetry and integrate instead the function $f(x) = 2x \cos x$ on the interval $[a, b] = [0, \pi/2]$. In this interval we must work with $m = 4$ panels (subintervals) and, moreover, Simpson's 1/3 rule uses three neighboring points, so each of these panels contain two further sub-subintervals. That makes a total of $N = 2 \times 4 = 8$ evenly spaced segments, and thus $h = (\pi/2 - 0)/8 = \pi/16$. Thus our nine nodes are

$$\left\{ x_0 = 0, x_1 = \frac{\pi}{16}, x_2 = \frac{\pi}{8}, x_3 = \frac{3\pi}{16}, x_4 = \frac{\pi}{4}, x_5 = \frac{5\pi}{16}, x_6 = \frac{3\pi}{8}, x_7 = \frac{7\pi}{16}, x_8 = \frac{\pi}{2} \right\}.$$

Evaluating $f(x) = 2x \cos x$ at these nodes,

```
1 In[1]:= Table[2*i*Cos[i], {i, 0, Pi/2, Pi/16}]
2
3 Out[1]= {0, 1/8 \[Pi] Cos[\[Pi]/16], 1/4 \[Pi] Cos[\[Pi]/8],
4 3/8 \[Pi] Cos[(3 \[Pi])/16], \[Pi]/(2 Sqrt[2])},
5 5/8 \[Pi] Sin[(3 \[Pi])/16], 3/4 \[Pi] Sin[\[Pi]/8],
6 7/8 \[Pi] Sin[\[Pi]/16], 0}
```

We plug these values back into (14),

$$\begin{aligned} \int_0^\pi x \cos x \, dx &= 2 \int_0^{\pi/2} x \cos x \, dx \\ &\approx \frac{\pi}{16 \cdot 3} \left[0 + 4 \left(\frac{\pi}{8} \cos \frac{\pi}{16} + \frac{3\pi}{8} \cos \frac{3\pi}{16} + \frac{5\pi}{8} \sin \frac{3\pi}{16} + \frac{7\pi}{8} \sin \frac{\pi}{16} \right) \right. \\ &\quad \left. + 2 \left(\frac{\pi}{4} \cos \frac{\pi}{8} + \frac{\sqrt{2}\pi}{4} + \frac{3\pi}{4} \sin \frac{\pi}{8} \right) + 0 \right] \\ &= \frac{\pi}{48} \left[\frac{\pi}{2} \cos \frac{\pi}{16} + \frac{3\pi}{2} \cos \frac{3\pi}{16} + \frac{5\pi}{2} \sin \frac{3\pi}{16} + \frac{7\pi}{2} \sin \frac{\pi}{16} + \frac{\pi}{2} \cos \frac{\pi}{8} + \frac{\sqrt{2}\pi}{2} + \frac{3\pi}{2} \sin \frac{\pi}{8} \right] \\ &= 1.14167. \end{aligned}$$

The error term is given by

$$-\frac{h^5}{90} f^{(4)}(\xi) = -\frac{\pi^5}{94371840} f^{(4)}(\xi),$$

for some $\xi \in (0, \pi/2)$. □



Problem 3. Develop a composite version of the following formula and give the error term

$$\int_{x_0}^{x_4} f(x) \, dx = \frac{4h}{3} [2f(x_1) - f(x_2) + 2f(x_3)] + \frac{14h^2}{45} f^{(4)}(c), \quad (15)$$

where

$$h = \frac{x_4 - x_0}{4}, \quad x_1 = x_0 + h, \quad x_2 = x_0 + 2h, \quad x_3 = x_0 + 3h, \quad \text{and} \quad c \in (x_0, x_4).$$

Solution. Let's extend the integral in (15) to a larger, general interval $[a, b] = [x_0, x_n]$, and let us use, say, m panels. In order to mimic Eq. (15), in each of these panels $[x_i, x_{i+4}]$ we want three interior nodes, besides the two panel endpoints x_i and x_{i+4} . So, we have

$$\int_{x_0}^{x_n} f(x) dx = \underbrace{\int_{x_0}^{x_4} f(x) dx}_{\text{1st panel}} + \cdots + \underbrace{\int_{x_{n-4}}^{x_n} f(x) dx}_{\text{mth panel}}.$$

Since we are using evenly spaced nodes, h remains unchanged for all i :

$$h := \frac{x_{i+4} - x_i}{4} \quad \text{for } i = 0, \dots, n-4.$$

Putting all this together, we get

$$\int_{x_0}^{x_n} f(x) dx = \frac{4h}{3} \left[2 \sum_{\substack{i=1 \\ i \text{ is odd}}}^{n-1} f_i - \sum_{i \in I} f_i \right] + \frac{14h^2}{45} \sum_{j=1}^m f^{(4)}(c_j), \quad (16)$$

where $I = \{2, 6, 10, \dots, n-2\}$ and c_j is located in the j^{th} panel. □



Problem 4. Show, by induction or otherwise, that for $0 \leq k \leq n$,

$$\frac{d^k}{dx^k} (1 - x^2)^n = (1 - x^2)^{n-k} q_k(x), \quad (17)$$

where q_k is a polynomial of degree k . Deduce that all the derivatives of the function $(1 - x^2)^n$ of order less than n vanish at $x = \pm 1$. Define

$$\psi_j(x) := \frac{d^j}{dx^j} (1 - x^2)^j, \quad (18)$$

and show by repeated integration by parts that

$$\int_{-1}^1 \psi_k(x) \psi_j(x) dx = 0, \quad 0 \leq k < j. \quad (19)$$

Hence obtain the expressions for the Legendre polynomials of degrees 0, 1, 2, and 3.

Solution. Let's show Eq. (17) by induction. For $k = 0$,

$$\frac{d^0}{dx^0} (1 - x^2)^n = (1 - x^2)^n = (1 - x^2)^{n-0} q_0(x) \quad \text{with } q_0(x) = 1. \quad \checkmark \quad (20a)$$

For $k = 1$,

$$\frac{d}{dx} (1 - x^2)^n = (1 - x^2)^{n-1} \cdot (-2nx) = (1 - x^2)^{n-1} q_1(x) \quad \text{with } q_1(x) = -2nx. \quad \checkmark \quad (20b)$$

Now assume (17) holds for any k ; then we show that it must hold for $k + 1$:

$$\begin{aligned} \frac{d^{k+1}}{dx^{k+1}} (1 - x^2)^n &= \frac{d^k}{dx^k} \left(\frac{d}{dx} (1 - x^2)^n \right) \\ &= \frac{d^k}{dx^k} \left((1 - x^2)^{n-1} q_1(x) \right) && \text{(By (20b))} \\ &= (1 - x^2)^{n-k-1} q_k(x) q_1(x) && \text{(By (17))} \\ &= (1 - x^2)^{n-(k+1)} q_{k+1}(x). \quad \checkmark \end{aligned}$$

On the last equality we used the fact that a degree- i polynomial multiplying a degree- j polynomial results in a degree- $(i + j)$ polynomial.

Now, it is obvious that plugging in $x = \pm 1$ will make all k -derivatives vanish, except when $k = n$, since in that case we have

$$\frac{d^n}{dx^n}(1-x^2)^n = (1-x^2)^{n-n} q_n(x) = q_n(x).$$

Integrating by parts now, we show the orthogonality condition (19). From the calculations above, note that for $k < j$, the k^{th} -derivative of $(1-x^2)^j$ is divisible by $(1-x^2)$; that is,

$$\frac{d^k}{dx^k}(1-x^2)^j = (1-x^2)^{j-k} q_k(x) = \frac{(1-x^2)^j}{(1-x^2)^k} q_k(x) \quad \text{for } k < j. \quad (21)$$

Note also that since $(1-x^2)^k$ is a polynomial of degree $2k$, its $(2k+1)^{\text{st}}$ derivative must vanish; i.e.,

$$\frac{d^{2k+1}}{dx^{2k+1}}(1-x^2)^k = 0. \quad (22)$$

(These last two expressions are crucial to our calculation below.) Now define the integration-by-parts variables $\{u, v\}$:

$$\begin{aligned} u &= \frac{d^k}{dx^k}(1-x^2)^k, & dv &= \frac{d^j}{dx^j}(1-x^2)^j dx, \\ du &= \frac{d^{k+1}}{dx^{k+1}}(1-x^2)^k dx, & v &= \frac{d^{j-1}}{dx^{j-1}}(1-x^2)^j. \end{aligned}$$

We are now ready to integrate:

$$\begin{aligned} \int_{-1}^1 \psi_k(x) \psi_j(x) dx &= \int_{-1}^1 \frac{d^k}{dx^k}(1-x^2)^k \frac{d^j}{dx^j}(1-x^2)^j dx \\ &= uv \Big|_{-1}^1 - \int_{-1}^1 v du \\ &= \underbrace{\left(\frac{d^k}{dx^k}(1-x^2)^k \frac{d^{j-1}}{dx^{j-1}}(1-x^2)^j \right) \Big|_{-1}^1}_{= 0 \text{ by (21)}} - \int_{-1}^1 \left(\frac{d^{j-1}}{dx^{j-1}}(1-x^2)^j \frac{d^{k+1}}{dx^{k+1}}(1-x^2)^k \right) dx \\ &= - \int_{-1}^1 \left(\frac{d^{j-1}}{dx^{j-1}}(1-x^2)^j \frac{d^{k+1}}{dx^{k+1}}(1-x^2)^k \right) dx. \end{aligned}$$

Repeating the integration $k+1$ times, we get

$$(-1)^{k+1} \int_{-1}^1 \left(\frac{d^{j-k-1}}{dx^{j-k-1}}(1-x^2)^j \frac{d^{2k+1}}{dx^{2k+1}}(1-x^2)^k \right) dx \stackrel{\text{by Eq. (22)}}{=} 0. \quad \square$$



Problem 5. For what value of α is the formula $\int_0^2 f(x) dx \approx f(\alpha) + f(2-\alpha)$ exact on Π_3 ?

Solution. The integration is exact, i.e.,

$$\int_0^2 f(x) dx = f(\alpha) + f(2-\alpha) \quad (23)$$

on Π_3 , whenever $f(x)$ is a polynomial of degree ≤ 3 (that is, the quadrature has degree of precision 3). Thus,

$$f(x) = A_0 + A_1x + A_2x^2 + A_3x^3 \quad (24)$$

for some undetermined coefficients $\{A_0, A_1, A_2, A_3\}$. Now, expanding the LHS of (23) with f given as in (24),

$$\begin{aligned} \int_0^2 f(x) dx &= \int_0^2 (A_0 + A_1x + A_2x^2 + A_3x^3) dx \\ &= \left(A_0x + \frac{x^2}{2}A_1 + \frac{x^3}{3}A_2 + \frac{x^4}{4}A_3 \right) \Big|_0^2 \\ &= 2A_0 + 2A_1 + \frac{8}{3}A_2 + 4A_3. \end{aligned} \quad (25)$$

On the other hand, expanding the RHS of (23) with f given as in (24),

$$\begin{aligned}
f(\alpha) + f(2 - \alpha) &= A_0 + A_0 + A_1(\alpha) + A_1(2 - \alpha) + A_2(\alpha^2) + A_2([2 - \alpha]^2) + A_3(\alpha^3) + A_3([2 - \alpha]^3) \\
&= 2A_0 + A_1(\alpha + 2 - \alpha) + A_2(\alpha^2 + (2 - \alpha)^2) + A_3(\alpha^3 + (2 - \alpha)^3) \\
&= 2A_0 + 2A_1 + A_2(\alpha^2 + 4 - 4\alpha + \alpha^2) + A_3(\alpha^3 - \alpha^3 + 6\alpha^2 - 12\alpha + 8) \\
&= 2A_0 + 2A_1 + (2\alpha^2 - 4\alpha + 4)A_2 + (6\alpha^2 - 12\alpha + 8)A_3.
\end{aligned} \tag{26}$$

Hence, comparing Eqs. (25) and (26), we see that in order for (23) to hold, the following equations must be satisfied

$$2\alpha^2 - 4\alpha + 4 = \frac{8}{3} \tag{27a}$$

$$6\alpha^2 - 12\alpha + 8 = 4. \tag{27b}$$

From either of these two equations we get $\alpha = 1 \pm \sqrt{3}/3$, so this is the value that satisfies Eq. (23) on Π_3 . \square



Problem 6. A quadrature formula on $[-1, 1]$ uses the quadrature points $x_0 = -\alpha$ and $x_1 = \alpha$, where $0 < \alpha \leq 1$:

$$\int_{-1}^1 f(x) dx \approx w_0 f(-\alpha) + w_1 f(\alpha). \tag{28}$$

The formula is required to be exact whenever f is a polynomial of degree 1. Show that $w_0 = w_1 = 1$, independent of the value of α . Show also that there is one particular value of α for which the formula is exact also for all polynomials of degree 2. Find this α , and show that, for this value, the formula is also exact for all polynomials of degree 3.

Proof. Assume that Eq. (28) is exact on Π_1 ; that is

$$\int_{-1}^1 f(x) dx = w_0 f(-\alpha) + w_1 f(\alpha) \tag{29}$$

on Π_1 . Then

$$f(x) = A_0 + A_1 x \tag{30}$$

for some undetermined coefficients $\{A_0, A_1\}$. Now, expanding the LHS of (29) with f given as in (30),

$$\begin{aligned}
\int_{-1}^1 f(x) dx &= \int_{-1}^1 (A_0 + A_1 x) dx \\
&= \left(A_0 x + \frac{x^2}{2} A_1 \right) \Big|_{-1}^1 \\
&= 2A_0.
\end{aligned} \tag{31}$$

On the other hand, expanding the RHS of (29) with f given as in (30),

$$\begin{aligned}
w_0 f(-\alpha) + w_1 f(\alpha) &= w_0 (A_0 + A_1(-\alpha)) + w_1 (A_0 + A_1(\alpha)) \\
&= (w_0 + w_1)A_0 + (w_1\alpha - w_0\alpha)A_1.
\end{aligned} \tag{32}$$

Thus we have the system

$$w_0 + w_1 = 2 \tag{33a}$$

$$-\alpha w_0 + \alpha w_1 = 0, \tag{33b}$$

from which we get $w_0 = w_1 = 1$, which is completely independent of α .

On Π_2 , on the other hand, the exactness of this quadrature will depend on a specific value of α ; we show this now. Let

$$f(x) = A_0 + A_1 x + A_2 x^2 \tag{34}$$

for some undetermined coefficients $\{A_0, A_1, A_2\}$. Now, expanding the LHS of (29) with f given as in (34),

$$\begin{aligned}\int_{-1}^1 f(x) dx &= \int_{-1}^1 (A_0 + A_1 x + A_2 x^2) dx \\ &= \left(A_0 x + \frac{x^2}{2} A_1 + \frac{x^3}{3} A_2 \right) \Big|_{-1}^1 \\ &= 2A_0 + \frac{2}{3} A_2.\end{aligned}\tag{35}$$

Expanding the RHS of (29) with f given as in (34),

$$\begin{aligned}w_0 f(-\alpha) + w_1 f(\alpha) &= w_0 (A_0 + A_1(-\alpha) + A_2(-\alpha)^2) + w_1 (A_0 + A_1\alpha + A_2\alpha^2) \\ &= (w_0 + w_1)A_0 + (w_1\alpha - w_0\alpha)A_1 + (w_0\alpha^2 + w_1\alpha^2)A_2.\end{aligned}\tag{36}$$

Thus we have the system

$$w_0 + w_1 = 2\tag{37a}$$

$$-\alpha w_0 + \alpha w_1 = 0\tag{37b}$$

$$\alpha^2 w_0 + \alpha^2 w_1 = \frac{2}{3},\tag{37c}$$

from which we get $w_0 = w_1 = 1$, but now

$$2\alpha^2 = \frac{2}{3} \implies \alpha = \pm \frac{\sqrt{3}}{3}.\tag{38}$$

Since $w_0 = w_1$, it's clear from (29) that it doesn't matter whether we use $+$ or $-$; thus set $\alpha = \sqrt{3}/3$. Then, in order for the quadrature to be exact on Π_3 , f must be of the form

$$f(x) = A_0 + A_1 x + A_2 x^2 + A_3 x^3.\tag{39}$$

Similarly as before, upon expanding the LHS of (29), with f now given as in (39), we end up with

$$\int_{-1}^1 f(x) dx = 2A_0 + \frac{2}{3} A_2.\tag{40}$$

So there is no change when compared to Π_2 . Also, expanding the RHS of (29) with f now given as in (39) and $\alpha = \sqrt{3}/3$, we get

$$\begin{aligned}w_0 f\left(-\frac{\sqrt{3}}{3}\right) + w_1 f\left(\frac{\sqrt{3}}{3}\right) &= w_0 \left(A_0 + A_1 \left(-\frac{\sqrt{3}}{3}\right) + A_2 \left(-\frac{\sqrt{3}}{3}\right)^2 + A_3 \left(-\frac{\sqrt{3}}{3}\right)^3 \right) \\ &\quad + w_1 \left(A_0 + A_1 \left(\frac{\sqrt{3}}{3}\right) + A_2 \left(\frac{\sqrt{3}}{3}\right)^2 + A_3 \left(\frac{\sqrt{3}}{3}\right)^3 \right) \\ &= (w_0 + w_1)A_0 + \left(w_1 \frac{\sqrt{3}}{3} - w_0 \frac{\sqrt{3}}{3} \right) A_1 + \left(w_0 \frac{1}{3} + w_1 \frac{1}{3} \right) A_2 \\ &\quad + \left(w_1 \frac{\sqrt{3}}{3} - w_0 \frac{\sqrt{3}}{3} \right) A_3.\end{aligned}\tag{41}$$

This yields the same system (37) that we saw for Π_2 . Hence, for the given value of $\alpha = \pm \sqrt{3}/3$ the quadrature (28) is also exact on Π_3 . \square



Problem 7. The function f has a continuous fourth derivative on the interval $[-1, 1]$. Construct the Hermite interpolation polynomial of degree 3 for f using the interpolation points $x_0 = -1$ and $x_1 = 1$. Deduce that

$$\int_{-1}^1 f(x) dx - [f(-1) + f(1)] = \frac{1}{3} [f'(-1) - f'(1)] + E,\tag{42}$$

where

$$|E| \leq \frac{2}{45} \max_{x \in [-1, 1]} |f^{(4)}(x)|.\tag{43}$$

Solution. We use the following important theorem:

Hermite Interpolation Theorem

Given $n + 1$ distinct nodes x_0, \dots, x_n and a differentiable function $f(x)$, there exists a unique polynomial $H_n \in \Pi_{2n+1}$ such that

$$H_n(x_i) = f(x_i), \quad H'_n(x_i) = f'(x_i), \quad 0 \leq i \leq n. \quad (44)$$

Defining

$$h_i(x) \equiv \ell_i^2(x) (1 - 2\ell'_i(x_i)) (x - x_i) \quad (45a)$$

$$\tilde{h}_i(x) \equiv \ell_i^2(x)(x - x_i), \quad (45b)$$

we get the **Hermitian polynomial**

$$H_n(x) = \sum_{i=0}^n (f(x_i)h_i(x) + f'(x_i)\tilde{h}_i(x)), \quad (46)$$

which does satisfy Eq. (44).

Proceeding to compute Eq. (46) by direct calculation is highly inefficient though. A more time-saving approach is to tabulate the method, similarly to how we did with the Newton's Divided Differences coefficients. In the cubic Hermite interpolation we only need two nodes $x_0 = a$ and $x_1 = b$. The algorithm is as follows: We set up the table

$$\begin{array}{c|ccc} a & f(a) & & \\ & f'(a) & & \\ a & f(a) & A & B \\ & & C & D \\ b & f(b) & & \\ & f'(b) & & \\ b & f(b) & & \end{array} \quad (47)$$

where A, B, C, D are calculated as usual in finite difference tables,

$$\begin{aligned} A &= \frac{f(b) - f(a)}{b - a}, & B &= \frac{A - f'(a)}{b - a}, \\ C &= \frac{f'(b) - A}{b - a}, & D &= \frac{C - B}{b - a}. \end{aligned}$$

Then the cubic Hermite polynomial is given by

$$H_1(x) = f(a) + f'(a)(x - a) + B(x - a)^2 + D(x - a)^2(x - b). \quad (48)$$

In the case at hand, we have $x_0 = -1$ and $x_1 = 1$. Thus,

$$\begin{array}{c|ccc} -1 & f(-1) & & \\ & f'(-1) & & \\ -1 & f(-1) & A & B \\ & & C & D \\ 1 & f(1) & & \\ & f'(1) & & \\ 1 & f(1) & & \end{array} \quad (49)$$

where

$$\begin{aligned} A &= \frac{f(1) - f(-1)}{2}, \\ B &= \frac{\frac{f(1) - f(-1)}{2} - f'(-1)}{2} = \frac{f(1) - f(-1) - 2f'(-1)}{4}, \\ C &= \frac{f'(1) - \frac{f(1) - f(-1)}{2}}{2} = \frac{2f'(1) - f(1) + f(-1)}{4}, \\ D &= \frac{\frac{2f'(1) - f(1) + f(-1)}{4} - \frac{f(1) - f(-1) - 2f'(-1)}{4}}{2} = \frac{f'(1) - f(1) + f'(-1) + f(-1)}{4}. \end{aligned}$$

Hence, plugging back into Eq. (48)

$$H_1(x) = f(-1) + f'(-1)(x+1) + \frac{f(1) - f(-1) - 2f'(-1)}{4}(x+1)^2 + \frac{f'(1) - f(1) + f'(-1) + f(-1)}{4}(x+1)^2(x-1). \quad (50)$$

Integrating this expression

```

1 In[1] :=
2 h[x_] :=
3   f[-1] + f'[-1]*(x + 1) + (f[1] - f[-1] - 2 f'[-1])/4*(x + 1)^2
4   + (f'[1] + f'[-1] - f[1] + f[-1])/4*(x + 1)^2*(x - 1);
5
6 Integrate[h[x], {x, -1, 1}]
7
8 Out[2]= f[-1] + f[1] + 1/3 Derivative[1][f][-1] - Derivative[1][f][1]/3

```

Thus we have found

$$\int_{-1}^1 H_1(x) dx = f(1) + f(-1) + \frac{1}{3}[f'(-1) - f'(1)]. \quad (51)$$

We now use the Gaussian formula with error term, for a Hermite polynomial $H(x)$,

$$\int_a^b w(x) [f(x) - H(x)] dx = \int_a^b w(x) \frac{f^{(2n+2)}(\xi(x))}{(2n+2)!} \psi_n^2(x) dx, \quad (52)$$

where $\xi \in [a, b]$ and

$$\psi_n = \prod_{i=0}^n (x - x_i).$$

In our case we have ($w(x) = 1$ and $[a, b] = [-1, 1]$). Thus, putting together all our results, we have

$$\begin{aligned}
\int_{-1}^1 (f(x) - H_1(x)) dx &= \int_{-1}^1 f(x) dx - f(1) - f(-1) - \frac{1}{3}[f'(-1) - f'(1)] \\
&= \int_{-1}^1 \frac{f^{(4)}(\xi(x))}{4!} \psi_1^2(x) dx \\
&= \frac{f^{(4)}(\xi(x))}{24} \int_{-1}^1 [(x+1)^2 (x-1)^2] dx \\
&= \frac{f^{(4)}(\xi(x))}{24} \cdot \frac{16}{25} \\
&= \frac{2}{45} f^{(4)}(\xi(x)) \leq \frac{2}{45} \max_{x \in [-1, 1]} |f^{(4)}(x)|.
\end{aligned}$$

The last inequality holds because $\xi \in [-1, 1]$. On the third equality we were able to pull the $f^{(4)}(\xi)$ out of the integral by applying the Weighted Mean Value Theorem for Integrals, which we previously used on Problem 1 (c.f., Eq. (12)). Hence, we have shown that Eq. (42) holds. \square



Problem 8. Approximate the integral $\int_{-1}^1 \cos(\pi x) dx$ using $n = 3$ Gaussian Quadrature.¹

Proof. For $n = 3$ Gaussian Quadrature we need to use as nodes the three roots of the degree-3 Legendre polynomial

$$\begin{aligned}
p_3(x) &= \frac{1}{2^3 3!} \frac{d^3}{dx^3} [(x^2 - 1)^3] \\
&= \frac{1}{48} (120x^3 - 72x) \\
&= x \left(\frac{5}{2}x^2 - \frac{3}{2} \right).
\end{aligned} \quad (53)$$

¹For this problem I switch to indexing starting at 1 in order to avoid confusion, since in my convention this problem is actually asking for $n = 2$ Gaussian Quadrature.

So one root is 0, and as for the other two,

$$\frac{5}{2}x^2 - \frac{3}{2} = 0 \implies x = \pm\sqrt{\frac{3}{5}}.$$

So the three roots are

$$x_1 = -\sqrt{\frac{3}{5}}, \quad x_2 = 0, \quad x_3 = \sqrt{\frac{3}{5}}.$$

Now we Lagrange-interpolate the function $f(x) = \cos(\pi x)$ as usual,

$$\cos(\pi x) \approx \sum_{i=1}^3 \cos(\pi x_i) \ell_i(x), \quad (54)$$

except that now the Lagrange polynomials ℓ_i are applied on the Legendre roots we have just found. Start with ℓ_1 :

$$\begin{aligned} \ell_1(x) &= \frac{x - x_2}{x_1 - x_2} \frac{x - x_3}{x_1 - x_3} \\ &= \frac{x - 0}{-\sqrt{\frac{3}{5}} - 0} \frac{x - \sqrt{\frac{3}{5}}}{-\sqrt{\frac{3}{5}} - \sqrt{\frac{3}{5}}} \\ &= \frac{5}{6}x \left(x - \sqrt{\frac{3}{5}} \right). \end{aligned} \quad (55)$$

Integrating, we get the first coefficient

$$c_1 = \int_{-1}^1 \ell_1(x) dx = \int_{-1}^1 \left[\frac{5}{6}x \left(x - \sqrt{\frac{3}{5}} \right) \right] dx = \frac{5}{9}.$$

An identical calculation shows that the remaining two coefficients are $c_2 = 8/9$ and $c_3 = c_1 = 5/9$. Hence, putting it all together and integrating Eq. (54), we get we have the quadrature

$$\begin{aligned} \int_{-1}^1 \cos(\pi x) dx &= \sum_{i=1}^3 c_i \cos(\pi x_i) \\ &= \frac{5}{9} \cdot \cos\left(-\sqrt{\frac{3}{5}}\pi\right) + \frac{8}{9} \cdot 1 + \frac{5}{9} \cdot \cos\left(\sqrt{\frac{3}{5}}\pi\right) \\ &\approx 0.045. \end{aligned} \quad \square$$

Problem 9. Show how the Gaussian quadrature rule

$$\int_{-1}^1 f(x) dx \approx \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right) \quad (56)$$

can be used for $\int_a^b f(x) dx$. Apply this result to evaluate $\int_0^{\pi/2} x dx$.

Solution. This is the same $n = 3$ Gaussian quadrature that we derived on the previous problem. If the quadrature is to take place on a more general interval $[a, b]$, the problem needs to be translated back to $[-1, 1]$. Using the substitution

$$t = \frac{2x - (b + a)}{b - a}, \quad (57)$$

a Gaussian quadrature rule of the form

$$\int_{-1}^1 f(t) dt \approx \sum_{i=0}^n A_i f(t_i) \quad (58)$$

can be used over the interval $[a, b]$; i.e.,

$$\int_a^b f(x) dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{(b-a)t+b+a}{2}\right) dt. \quad (59)$$

For this problem we have $[a, b] = [0, \pi/2]$. Hence, plugging into (59),

$$\begin{aligned} \int_0^{\pi/2} x dx &= \frac{\pi/2 - 0}{2} \int_{-1}^1 f\left(\frac{(\pi/2 - 0)t + \pi/2 + 0}{2}\right) dt \\ &= \frac{\pi}{4} \int_{-1}^1 f\left(\frac{\pi}{4}t + \frac{\pi}{4}\right) dt \\ &= \frac{\pi}{4} \left[\frac{5}{9} f\left(\frac{\pi}{4} - \frac{\pi}{4}\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f\left(\frac{\pi}{4}\right) + \frac{5}{9} f\left(\frac{\pi}{4}\sqrt{\frac{3}{5}} + \frac{\pi}{4}\right) \right]. \end{aligned} \quad \text{(Using (58))} \quad (60)$$

Then, since $f(x) = x$ in this case,

$$\begin{aligned} \int_0^{\pi/2} x dx &= \frac{\pi}{4} \left[\frac{5}{9} \left(\frac{\pi}{4} - \frac{\pi}{4}\sqrt{\frac{3}{5}} \right) + \frac{8}{9} \left(\frac{\pi}{4} \right) + \frac{5}{9} \left(\frac{\pi}{4}\sqrt{\frac{3}{5}} + \frac{\pi}{4} \right) \right] \\ &= \frac{\pi^2}{8} \approx 1.2337. \end{aligned} \quad \square$$



Problem 10. Solve the following:

- a) Find $\{p_0, p_1, p_2\}$ such that p_i is polynomial of degree i and this set is orthogonal on $[0, \infty)$ with weight function $w(x) = e^{-x}$.
- b) Determine the nodes and the weights in the two-node Gaussian Quadrature formula:

$$\int_0^\infty f(x)e^{-x} dx = w_1 f(x_1) + w_2 f(x_2). \quad (61)$$

Solution to a). We need to find a set of polynomials that are w -orthogonal on $[0, \infty)$, with $w(x) = e^{-x}$; that is, we need to find a set $\{p_k\}$ that satisfies

$$\int_0^\infty e^{-x} p_i(x) p_j(x) dx = 0 \quad i \neq j. \quad (62)$$

In general, constructing a set of orthogonal polynomials entails using a Gram-Schmidt algorithm (c.f., (67)); we use this approach on the next problem. For this particular weight function $w(x) = e^{-x}$, however, the set of polynomials that satisfy Eq. (62) are well known; they go by the name of *Laguerre polynomials*, and can be easily derived from their *Rodrigues representation*

$$p_k(x) = \frac{e^x}{k!} \frac{d^k}{dx^k} (x^k e^{-x}). \quad (63)$$

For $k = 0, 1, 2$, we have

$$p_0(x) = 1, \quad (64a)$$

$$p_1(x) = 1 - x, \quad (64b)$$

$$p_2(x) = \frac{1}{2}(x^2 - 4x + 2). \quad (64c)$$

It can be easily checked that these polynomials are indeed w -orthogonal (with $w(x) = e^{-x}$, of course) in the non-negative real line $[0, \infty)$ by just plugging them into Eq. (62) and making sure the integrals do vanish. \square

Solution to b). Just as in the case of a unit weight function the Gauss nodes were roots of the Legendre polynomial, in the case of the nontrivial weight function $w(x) = e^{-x}$ the nodes are the Laguerre roots. Thus, for the two-node Gaussian Quadrature, the nodes are the two roots of the degree-2 Laguerre polynomial

$$\frac{1}{2}(x^2 - 4x + 2) = 0 \quad \implies \quad x = 2 \pm \sqrt{2}.$$

Thus the two Gauss nodes are

$$x_1 = 2 - \sqrt{2}, \quad x_2 = 2 + \sqrt{2}.$$

As for the weights, they are calculated as before; start with the Lagrange polynomials

$$\ell_1 = \frac{x - x_2}{x_1 - x_2} = \frac{x - 2 - \sqrt{2}}{-2\sqrt{2}};$$

$$\ell_2 = \frac{x - x_1}{x_2 - x_1} = \frac{x - 2 + \sqrt{2}}{2\sqrt{2}}.$$

Then, integrating, we get

$$w_1 = \int_0^\infty e^{-x} \frac{x - 2 - \sqrt{2}}{-2\sqrt{2}} dx = \frac{1}{4}(2 + \sqrt{2});$$

$$w_2 = \int_0^\infty e^{-x} \frac{x - 2 + \sqrt{2}}{2\sqrt{2}} dx = \frac{1}{4}(2 - \sqrt{2}).$$

Thus, we have

$$\int_0^\infty f(x)e^{-x} dx = \frac{2 + \sqrt{2}}{4} f(2 - \sqrt{2}) + \frac{2 - \sqrt{2}}{4} f(2 + \sqrt{2}). \quad \square$$



Problem 11. Solve the following:

- a) Construct orthogonal polynomials of degrees 0, 1, and 2 on the interval $(0, 1)$ with the weight function $w(x) = -\log x$.
- b) Determine the quadrature points and weights for the weight function $w: x \mapsto -\log x$ on the interval $(0, 1)$, for $n = 1$.

Solution to a). The general procedure for orthogonalizing polynomials is given by the Gram-Schmidt recurrence relation

$$p_{-1}(x) \equiv 0 \tag{67a}$$

$$p_0(x) \equiv 1 \tag{67b}$$

$$p_{i+1}(x) = (x - a_i)p_i(x) - b_i p_{i-1}(x) \quad i = 0, \dots, n, \tag{67c}$$

where

$$a_i = \frac{\langle x p_i, p_i \rangle}{\langle p_i, p_i \rangle} \quad i = 0, \dots, n, \tag{68a}$$

$$b_i = \frac{\langle p_i, p_i \rangle}{\langle p_{i-1}, p_{i-1} \rangle} \quad i = 1, \dots, n, \tag{68b}$$

$$b_0 = \text{constant (can be set to 0)}. \tag{68c}$$

We could then divide each p_i by $\langle p_i, p_i \rangle^2$ if we wanted to normalize, but this is not necessary in our case; we are merely after an orthogonal set of polynomials. In the case at hand we want the first three w -orthogonal polynomials

$$p_0(x) = 1, \tag{69a}$$

$$p_1(x) = (x - a_0)p_0(x) = x - a_0 = x - \frac{\int_0^1 x(-\log x) dx}{\int_0^1 (-\log x) dx} = x - \frac{1}{4}, \tag{69b}$$

$$\begin{aligned} p_2(x) &= (x - a_1)p_1(x) - b_1 p_0(x) \\ &= \left[x - \frac{\int_0^1 x(-\log x) \left(x - \frac{1}{4}\right)^2 dx}{\int_0^1 (-\log x) \left(x - \frac{1}{4}\right)^2 dx} \right] \left[x - \frac{1}{4} \right] - \frac{\int_0^1 (-\log x) \left(x - \frac{1}{4}\right)^2 dx}{\int_0^1 (-\log x) dx} \\ &= \left[x - \frac{\frac{13}{576}}{\frac{7}{144}} \right] \left[x - \frac{1}{4} \right] - \frac{7}{144} \\ &= x^2 - \frac{5}{7}x + \frac{17}{252}. \end{aligned} \tag{69c}$$

A quick check to make sure that these three polynomials are indeed w -orthogonal:

```

1 In[1]:=
2 Integrate[(-Log[x])*(17/252 - (5 x)/7 + x^2)*(x - 1/4), {x, 0, 1}]
3 Integrate[(-Log[x])*1*(x - 1/4), {x, 0, 1}]
4 Integrate[(-Log[x])*(17/252 - (5 x)/7 + x^2)*1, {x, 0, 1}]
5
6 Out[1]= 0
7 Out[2]= 0
8 Out[3]= 0

```

□

Solution to b). For $n = 1$ the only Gauss node is the single root of p_1 , namely $x_0 = 1/4$. Since we only have one node, the Lagrange polynomial $\ell_0 = 1$, and thus the (single) weight is

$$w_0 = \int_0^1 (-\log x) \ell_0 dx = \int_0^1 (-\log x) dx = 1.$$

□



Problem 12. Find weights w_0, w_1, w_2 and nodes $x_0, x_1, x_2 \in [-1, 1]$ such that the quadrature

$$\int_{-1}^1 f(x) dx \approx \sum_i w_i f(x_i)$$

integrates all quintic polynomials exactly.

Solution. This is yet again the $n = 3$ Gaussian Quadrature rule that we found earlier (c.f. (56)),

$$\int_{-1}^1 f(x) dx \approx \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right).$$

Whence the weights and nodes are

$$\{w_0, w_1, w_2\} = \left\{\frac{5}{9}, \frac{8}{9}, \frac{5}{9}\right\} \quad (70a)$$

$$\{x_0, x_1, x_2\} = \left\{-\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}\right\}. \quad (70b)$$

However, previously we saw that the rule is exact for polynomials up to degree three (as is expected from $n = 3$ Gaussian Quadrature). This time we will show that the rule is, in fact, exact for quintic polynomials as well, which was not expected. Let

$$f(x) = A_0 + A_1x + A_2x^2 + A_3x^3 + A_4x^4 + A_5x^5. \quad (71)$$

Then, expanding the LHS of (56) with f given as in (71),

$$\begin{aligned} \int_{-1}^1 f(x) dx &= \int_{-1}^1 (A_0 + A_1x + A_2x^2 + A_3x^3 + A_4x^4 + A_5x^5) dx \\ &= \left(A_0x + \frac{x^2}{2}A_1 + \frac{x^3}{3}A_2 + \frac{x^4}{4}A_3 + \frac{x^5}{5}A_4 + \frac{x^6}{6}A_5 \right) \Big|_{-1}^1 \\ &= 2A_0 + \frac{2}{3}A_2 + \frac{2}{5}A_4. \end{aligned} \quad (72)$$

On the other hand, consider the RHS of (56), term by term, with f given as in (71),

$$\begin{aligned} \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) &= \frac{5}{9} \left[A_0 + A_1 \left(-\sqrt{\frac{3}{5}}\right) + A_2 \left(-\sqrt{\frac{3}{5}}\right)^2 + A_3 \left(-\sqrt{\frac{3}{5}}\right)^3 + A_4 \left(-\sqrt{\frac{3}{5}}\right)^4 + A_5 \left(-\sqrt{\frac{3}{5}}\right)^5 \right] \\ &= \frac{5}{9} \left[A_0 - \sqrt{\frac{3}{5}}A_1 + \frac{3}{5}A_2 - \frac{3}{5}\sqrt{\frac{3}{5}}A_3 + \frac{9}{25}A_4 - \frac{9}{25}\sqrt{\frac{3}{5}}A_5 \right]. \end{aligned} \quad (73)$$

Similarly,

$$\frac{8}{9} f(0) = \frac{8}{9} A_0, \quad (74)$$

and

$$\frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right) = \frac{5}{9} \left[A_0 + \sqrt{\frac{3}{5}} A_1 + \frac{3}{5} A_2 + \frac{3}{5} \sqrt{\frac{3}{5}} A_3 + \frac{9}{25} A_4 + \frac{9}{25} \sqrt{\frac{3}{5}} A_5 \right] \quad (75)$$

Thus, adding Eqs. (73)–(75), we get

$$\begin{aligned} \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right) &= \frac{5}{9} \left[2A_0 + \frac{6}{5} A_2 + \frac{18}{25} A_4 \right] + \frac{8}{9} A_0 \\ &= 2A_0 + \frac{2}{3} A_2 + \frac{2}{5} A_4. \end{aligned} \quad (76)$$

We see that this result coincides with (72). Thus we have proven that the $n = 3$ Gaussian quadrature given by Eq. (56) is, in fact, exact for quintic polynomials. \square