Numerical Analysis
Problem Sheet 2

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1. Newton-Cotes Quadrature: Find the integral approximation to

$$\int_0^1 \frac{1}{x+1}\, dx$$

using the Trapezium Rule and Simpson's Rule.

Answer

Using the Trapezium Rule:

$$\int_0^1 \frac{1}{x+1}\, dx \approx \frac{1-0}{2}\left(\frac{1}{0+1} + \frac{1}{1+1}\right) = \frac{3}{4}$$

Using Simpson's Rule:

$$\int_0^1 \frac{1}{x+1}\, dx \approx \frac{\frac{1}{2}-0}{3}\left(\frac{1}{0+1} + \frac{4}{\frac{1}{2}+1} + \frac{1}{1+1}\right) = \frac{25}{36}$$

2. Explicitly derive Simpson's Rule from its definition in terms of the quadratic Lagrange Interpolating Polynomial.

Answer

$$\begin{aligned} & \int_{x_0}^{x_2} f(x)dx \\ \approx \; & f(x_0)\int_{x_0}^{x_2} \tfrac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx + f(x_1)\int_{x_0}^{x_2} \tfrac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}dx + f(x_2)\int_{x_0}^{x_2} \tfrac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx \end{aligned}$$

We note that $x_i = x_0 + ih$. Using this and the substitution $x = x_0 + th$, we observe that $x - x_i = (t-i)h$ and rewrite as follows:

$$\begin{aligned} & h\left(f(x_0)\int_0^2 \tfrac{(t-1)(t-2)h^2}{2h^2}dt + f(x_1)\int_0^2 \tfrac{(t-0)(t-2)h^2}{-h^2}dt + \int_0^2 \tfrac{(t-0)(t-1)h^2}{2h^2}dt\right) \\ = \; & h\left(\tfrac{f(x_0)}{2}\int_0^2 (t-1)(t-2)dt + \tfrac{f(x_1)}{-1}\int_0^2 t(t-2)dt + \tfrac{f(x_2)}{2}\int_0^2 t(t-1)dt\right) \\ = \; & h\left(\tfrac{f(x_0)}{2}\left[\tfrac{1}{3}t^3 - \tfrac{3}{2}t^2 + 2t\right]_0^2 + \tfrac{f(x_1)}{-1}\left[\tfrac{1}{3}t^3 - t^2\right]_0^2 + \tfrac{f(x_2)}{2}\left[\tfrac{1}{3}t^3 - \tfrac{1}{2}t^2\right]_0^2\right) \\ = \; & h\left(\tfrac{f(x_0)}{2}\left(\tfrac{2}{3}\right) + \tfrac{f(x_1)}{-1}\left(-\tfrac{4}{3}\right) + \tfrac{f(x_2)}{2}\left(\tfrac{2}{3}\right)\right) \\ = \; & \tfrac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) \;\square \end{aligned}$$

3. Find the Newton-Cotes quadrature rule based on exact integration of the cubic Lagrange Interpolating Polynomial. (Hint: You may find it helpful to consider symmetries and the substitution $x = x_0 + th$.)

Answer

We calculate as follows:

$$\begin{aligned}
& \int_{x_0}^{x_3} f(x)dx \\
\approx \quad & f(x_0)\int_{x_0}^{x_3} \tfrac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}dx + f(x_1)\int_{x_0}^{x_3} \tfrac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}dx + \\
& f(x_2)\int_{x_0}^{x_3} \tfrac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}dx + f(x_3)\int_{x_0}^{x_3} \tfrac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}dx \\
= \quad & h\left(f(x_0)\int_0^3 \tfrac{(t-1)(t-2)(t-3)h^3}{-6h^3}\ dt + f(x_1)\int_0^3 \tfrac{t(t-2)(t-3)}{2}\ dt + \zeta\right)
\end{aligned}$$

where here ζ represents the symmetric bit we've left out. Continuing:

$$\begin{aligned}
= \quad & h\left(\tfrac{f(x_0)}{-6}\left[\tfrac{1}{4}t^4 - 2t^3 + \tfrac{11}{2}t^2 - 6t\right]_0^3 + \tfrac{f(x_1)}{2}\left[\tfrac{1}{4}t^4 - \tfrac{5}{3}t^3 + 3t^2\right]_0^3 + \zeta\right) \\
= \quad & h\left(\tfrac{f(x_0)}{-6}\left(-\tfrac{9}{4}\right) + \tfrac{f(x_1)}{2}\left(\tfrac{9}{4}\right) + \zeta\right) \\
= \quad & \tfrac{3h}{8}(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3))
\end{aligned}$$

4. Noting that for $b > a$, and any function f continuous on $[a, b]$

$$min_{x\in[a,b]}\ f(x) \leq \frac{1}{b-a}\int_a^b f(x)\ dx \leq max_{x\in[a,b]}\ f(x),$$

use the Intermediate Value Theorem to show that $\exists\eta \in (a, b)$ satisfying

$$\int_a^b f(x)\ dx = (b-a)f(\eta).$$

Thus if $G'(x) = g(x) \geq 0$ for $x \in [a, b]$, prove that

$$\int_a^b f(x)g(x)dx = f(\eta)\int_a^b g(x)dx$$

for some $\eta \in (a, b)$. [Note $dG = G'(x)\ dx$.]

Answer

(a) Using the Intermediate Value Theorem,[1] we obtain that

$$\exists\eta \in [a, b] \cdot f(\eta) = \frac{1}{b-a}\int_a^b f(x)\ dx$$

This almost gives us what we need immediately (just multiply both sides by $b - a$), but note that so far we only have that $\eta \in [a, b]$, not that $\eta \in (a, b)$. So why is it the case that there exists such an η such that $\eta \neq a$ and $\eta \neq b$?

[1] As stated on p.419 of Süli and Mayers.

Well, if we look at

$$\frac{1}{b-a}\int_a^b f(x)\ dx$$

we notice that this is (in a sense) the 'average' value of $f(x)$ on the closed interval. This leads us to one of two possibilities. Calling the average avg, we have that either:

i. $\forall x \in [a,b] \cdot f(x) = avg$, in which case since $b > a$, $\exists \eta \cdot a < \eta < b\ and\ f(\eta) = avg$

ii. $\exists \phi \in [a,b] \cdot f(\phi) < avg$ and $\exists \psi \in [a,b] \cdot f(\psi) > avg$ (intuitively, all this is saying is that if we add a lot of things up and take their average and they're not all equal, then there must have been at least one of them below the average and at least one above it), in which case since f is continuous on $[a,b]$, $\exists \eta \cdot \phi < \eta < \psi$ and $f(\eta) = avg$

In both of these cases, η is strictly between the two endpoints a and b, so we have the result we wanted, namely that $\eta \in (a,b)$.

(b) This second bit is essentially a proof of the Integral Mean Value Theorem.[2] The proof goes as follows: f is continuous on $[a,b]$ and therefore bounded on $[a,b]$, i.e.

$$\exists m, M \cdot m \leq f(x) \leq M, \quad x \in [a,b]$$

Now since $g(x) \geq 0$ for $x \in [a,b]$ and hence for $x \in (a,b)$:

$$\begin{aligned} mg(x) \leq f(x)g(x) \leq Mg(x), \quad x \in (a,b) \\ m\int_a^b g(x)\ dx \leq \int_a^b f(x)g(x)\ dx \leq M\int_a^b g(x)\ dx, \quad x \in (a,b) \end{aligned}$$

Suppose $\int_a^b g(x)\ dx = 0$. Then we have that $0 \leq \int_a^b f(x)g(x)\ dx \leq 0$, i.e. that $\int_a^b f(x)g(x)\ dx = 0$, in which case the theorem is trivially true: we can pick any value of $\eta \in (a,b)$ we like since $0 \equiv f(\eta) \times 0$.

If $\int_a^b g(x)\ dx \neq 0$, then we can divide through by it, giving:

$$m \leq \frac{\int_a^b f(x)g(x)\ dx}{\int_a^b g(x)\ dx} \leq M, \quad x \in (a,b)$$

So by the Intermediate Value Theorem there is some $\eta \in (a,b)$ s.t.

$$f(\eta) = \frac{\int_a^b f(x)g(x)\ dx}{\int_a^b g(x)\ dx}$$

Whence:

$$\int_a^b f(x)g(x)dx = f(\eta)\int_a^b g(x)dx$$

[2]As stated on p.420 of Süli and Mayers.

5. Using the Integral Mean Value Theorem, show that

$$\int_a^b f(x)\,dx - \frac{b-a}{2}\left[f(b)+f(a)\right] = -\frac{1}{12}(b-a)^3 f''(\eta) \text{ for some } \eta \in (a,b).$$

Hence show that the Trapezium Rule always overestimates integrals for functions satisfying $f''(x) \geq 0$. Explain geometrically why this is reasonable.

Answer

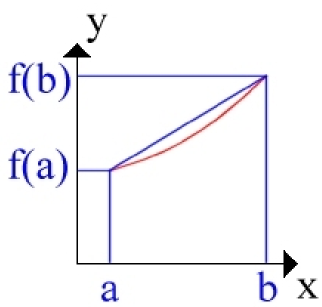
(a) TODO: I don't know how to do the 'show' part of this.

(b) Given the above, we have that:

$$\begin{aligned} \tfrac{b-a}{2}\left[f(b)+f(a)\right] &= \int_a^b f(x)\,dx + \tfrac{1}{12}(b-a)^3 f''(\eta) && \text{for some } \eta \in (a,b) \\ &\geq \int_a^b f(x)\,dx && \text{provided } f''(\eta) \geq 0 \end{aligned}$$

Now this is clearly true when $f''(x) \geq 0$, in other words the result of the Trapezium Rule (the left-hand side) always overestimates the true integral when $f''(x) \geq 0$.

(c) The diagram shows why this is geometrically reasonable (noting that functions with $f''(x) \geq 0$ slope upwards (well, not downwards, technically):



The Trapezium Rule calculates the area under the trapezium which is clearly more than the result of the integral which is the area under the red curve.

6. Show that Simpson's Rule *exactly* integrates any cubic polynomial on $[-1,1]$. By making the change of variables $t \leftrightarrow \frac{b+a+x(b-a)}{2}$ (or otherwise) show that Simpson's Rule *exactly* integrates any cubic polynomial on an arbitrary interval $[a,b]$.

Answer

(a) Firstly we integrate an arbitrary cubic polynomial on $[-1,1]$:

$$\begin{aligned} &\int_{-1}^{1} a_3x^3 + a_2x^2 + a_1x + a_0\,dx \\ =\ &\left[\tfrac{1}{4}a_3x^4 + \tfrac{1}{3}a_2x^3 + \tfrac{1}{2}a_1x^2 + a_0x\right]_{-1}^{1} \\ =\ &\left(\tfrac{1}{4}a_3 + \tfrac{1}{3}a_2 + \tfrac{1}{2}a_1 + a_0\right) - \left(\tfrac{1}{4}a_3 - \tfrac{1}{3}a_2 + \tfrac{1}{2}a_1 - a_0\right) \\ =\ &\tfrac{2}{3}a_2 + 2a_0 \end{aligned}$$

Then we evaluate the integral using Simpson's Rule, first noting that $x_0 = -1$, $x_1 = 0$, $x_2 = 1$ and $h = 1$:

$$
\begin{aligned}
& \tfrac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \\
= & \tfrac{1}{3}[(-a_3 + a_2 - a_1 + a_0) + 4a_0 + (a_3 + a_2 + a_1 + a_0)] \\
= & \tfrac{1}{3}[2a_2 + 6a_0] \\
= & \tfrac{2}{3}a_2 + 2a_0
\end{aligned}
$$

Since these are equal, Simpson's Rule exactly integrates any cubic polynomial on $[-1, 1]$.

(b) Suppose $f(t) = \sum_{i=0}^{3} c_i t^i$ and $g(x) = \sum_{i=0}^{3} c_i \left(\frac{b+a+x(b-a)}{2}\right)^i$. Clearly if $t = \frac{b+a+x(b-a)}{2}$ then $f(t) \equiv g(x)$. We calculate as follows:

$$
\begin{aligned}
& \int_a^b f(t)\ dt \\
= & \tfrac{b-a}{2}\int_{-1}^{1} g(x)\ dx && \{\text{since } dx = \tfrac{2}{b-a}\ dt\} \\
= & \tfrac{b-a}{2} \times \tfrac{1}{3}[g(-1) + 4g(0) + g(1)] && \{\text{from part (a)}\} \\
= & \tfrac{b-a}{6}\left[f(a) + 4f\left(\tfrac{b+a}{2}\right) + f(b)\right]
\end{aligned}
$$

This is what we wanted, since $\frac{b-a}{6}$ is indeed the required $\frac{h}{3}$ as $h = \frac{b-a}{2}$. So Simpson's Rule exactly integrates any cubic polynomial on an arbitrary interval $[a, b]$.

7. Estimate how many equal length intervals $[0, 2]$ should be broken into in order that $f(x)$ be integrated with an accuracy of 10^{-5} using the Composite Simpson Rule if

$$\max_{x\in[0,2]} \left|f^{IV}(x)\right| = 1.$$

[M] Check how accurate or how pessimistic this estimate is by using the MATLAB function $adaptive\_simpson$ for the function $f(x) = cos(x)$ which you can define in MATLAB with $f = inline('cos(x)')$. $adaptive\_simpson$ can be downloaded from the course website at http://web.comlab.ox.ac.uk/internal/courses/materials05-06/na/. $help\ adaptive\_simpson$ will describe what data you have to enter.

Hence

$f = inline('cos(x)')$
$adaptive\_simpson(f, 0, 2, 6, 1.e-5)$

will be all that is required here. $sin(2)$ will evaluate the analytical (exact) value of the integral in this case: to see more decimal places so that you can compare use $format\ long$ ($format\ short$ will revert to displaying fewer decimal places).

Answer

We calculate as follows:

$$
\begin{aligned}
& \left|\tfrac{(x_{2n}-x_0)}{45}h^4 f^{IV}(\zeta)\right| && \zeta \in (0, 2) \\
\leq & \left|\tfrac{(x_{2n}-x_0)}{45}h^4\right| && \{\text{given by the question information}\} \\
= & \tfrac{2h^4}{45} \leq 10^{-5} && \{\text{note that } h^4 \geq 0\} \\
\Leftrightarrow & \ h^4 \leq \tfrac{45\times10^{-5}}{2} \\
\Leftrightarrow & \ 4\ln h \leq \ln\tfrac{45\times10^{-5}}{2} \\
\Leftrightarrow & \ h \leq e^{\frac{1}{4}\ln\frac{45\times10^{-5}}{2}} = 0.1225 \text{ (4SF)}
\end{aligned}
$$

So we need to break $[0, 2]$ into $\frac{2}{0.1225}$ intervals, i.e. just over 16 intervals (16.33 to 2DP if we're being precise). Thus it's not surprising that MATLAB needs 5 iterations, since $2^4 = 16$ and we need slightly more than 16 intervals.

8. [M] Apply *adaptive_simpson* (see information in question 7 above) for the following functions:

   (a)
   $$\int_0^{\pi/2} \cos x \; dx$$
   (Note that *pi* in MATLAB is what you would expect it to be!)

   (b)
   $$\int_{-1}^{1} |x| \; dx$$
   (see *help abs*)

   (c)
   $$\int_{-1}^{3/2} |x| \; dx$$

   (d)
   $$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \; dx \text{ approximated by } \int_{-5}^{5} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \; dx$$
   (since $e^{-25} \leq 10^{-10}$). [Recall the Normal distribution from probability.]
   Note MATLAB for the integrand here is
   $exp(-x*x/2)/sqrt(2*pi)$

   Comment on what you observe in each case, in particular relating what you see to the theory covered in lectures.

Answer

(a) MATLAB Results:

```
adaptive_simpson(f, 0, pi/2, 6, 1.e-5)
Step 1 integral is 1.0022798775, with error estimate 1.0023.
Step 2 integral is 1.0001345850, with error estimate 0.0021453.
Step 3 integral is 1.0000082955, with error estimate 0.00012629.
Successful termination at iteration 4:
The integral is 1.0000005167, with error estimate 7.7788e-006.
ans = 1.00000051668471
```

Observations:

To get an error of less than 10^{-5} here, we calculate that:

$$\begin{aligned}
& \left|\frac{(x_{2n}-x_0)}{45} h^4 f^{IV}(\zeta)\right| \\
= & \left|\frac{\frac{\pi}{2}}{45} h^4 \cos(\zeta)\right| && \{\text{since } \tfrac{d^4(\cos x)}{dx^4} = \cos x\} \\
= & \left|\frac{\pi}{90} h^4 \cos(\zeta)\right| \\
\leq & \frac{\pi}{90} h^4 && \{\text{since } |\cos x| \leq 1 \text{ and } h^4 \geq 0\} \\
\leq & 10^{-5}
\end{aligned}$$

So:

$$h^4 \leq \frac{90\times 10^{-5}}{\pi}$$
$$\Leftrightarrow \quad 4\ln h \leq \ln \frac{90\times 10^{-5}}{\pi}$$
$$\Leftrightarrow \quad h \leq e^{\frac{1}{4}\ln\frac{90\times 10^{-5}}{\pi}} = 0.1301 \text{ (4SF)}$$

Now our i^{th} try for h is $\frac{\frac{\pi}{2}-0}{2^i}$ = $\frac{\pi}{2^{i+1}}$. We want the smallest i such that this is less than or equal to 0.1301, which in this case turns out to be 4. This is the number of iterations that MATLAB needed to perform (as indeed it did in this case, as we can see above).

(b) MATLAB Results:

```
g = inline('abs(x)')
adaptive_simpson(g, -1, 1, 6, 1.e-5)
Step 1 integral is 0.6666666667, with error estimate 0.66667.
Step 2 integral is 1.0000000000, with error estimate 0.33333.
Successful termination at iteration 3:
The integral is 1.0000000000, with error estimate 0.
ans = 1
```

Observations:

TODO: I'm not sure what to observe here.

(c) MATLAB Results:

```
adaptive_simpson(g, -1, 1.5, 15, 1.e-5)
Step 1 integral is 1.4583333333, with error estimate 1.4583.
Step 2 integral is 1.6666666667, with error estimate 0.20833.
Step 3 integral is 1.6145833333, with error estimate 0.052083.
Step 4 integral is 1.6276041667, with error estimate 0.013021.
Step 5 integral is 1.6243489583, with error estimate 0.0032552.
Step 6 integral is 1.6251627604, with error estimate 0.0008138.
Step 7 integral is 1.6249593099, with error estimate 0.00020345.
Step 8 integral is 1.6250101725, with error estimate 5.0863e-005.
Step 9 integral is 1.6249974569, with error estimate 1.2716e-005.
Successful termination at iteration 10:
The integral is 1.6250006358, with error estimate 3.1789e-006.
ans = 1.62500063578288
```

Observations:

TODO: Likewise.

(d) MATLAB Results:

```
h = inline('exp(-x*x/2)/sqrt(2*pi)', 'x')
adaptive_simpson(h,-5,5,15,1.e-5)
Step 1 integral is 2.6596201584, with error estimate 2.6596.
Step 2 integral is 0.7817616152, with error estimate 1.8779.
Step 3 integral is 0.9716725770, with error estimate 0.18991.
Step 4 integral is 0.9999971150, with error estimate 0.028325.
Successful termination at iteration 5:
The integral is 0.9999994125, with error estimate 2.2975e-006.
ans = 0.99999941250045
```

Observations:

TODO: Likewise.

9. If $x_0, x_1, ..., x_n$ are distinct real values, then by considering the Lagrange Interpolating Polynomial in the form $p_n = a_0 + a_1 x + ... + a_n x^n$ or otherwise, prove that the square matrix

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix}$$

is non-singular.

Answer

Given points $(x_0, f_0), ..., (x_n, f_n)$, we know that we can fit a unique polynomial $p_n \in \Pi_n$ to them s.t. for $0 \leq i \leq n$, $p_n(x_i) = f_i$. In other words, there are unique coefficients $a_0, ..., a_n$ s.t. $\sum_{j=0}^{n} a_j x_i^j = f_i$. Thus if we write the matrix equation

$$\underbrace{\begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix}}_{M} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}$$

then we know it has a unique solution. Now it's a theorem that if an equation of the form $A\mathbf{x} = \mathbf{b}$ has a unique solution for each $\mathbf{b}$ then A is invertible. So M, in this case, is invertible and hence non-singular.