Solutions_3

January 27, 2016

1 Exercise 5.2.3

Apply composite Simpson's rule with m = 1, 2, 4 panels to approximate the integrals:

(a)
$$\int_0^1 x^2 dx = \frac{1}{3}$$
, (b) $\int_0^{\pi/2} \cos(x) dx = 1$, (c) $\int_0^1 e^x dx = e - 1$,

and report the errors.

Solution

(a) $f(x) = x^2$.

For m = 1 we put h = (1 - 0)/2 = 1/2, $x_0 = 0$, $x_1 = 1/2$, $x_2 = 1$; $y_0 = f(x_0) = 0$, $y_1 = f(x_1) = 1/4$, $y_2 = f(x_2) = 1$. The approximation is then $I \approx h/3(y_0 + 4y_1 + y_2) = (0 + 4 * 1/4 + 1)/6 = 1/3$. The error is thus 0.

For m = 2 we have h = (1 - 0)/4 = 1/4, $(x_0, x_1, \dots, x_4) = (0, 1/4, 1/2, 3/4, 1)$, $(y_0, y_1, \dots, y_4) = (0, 1/16, 1/4, 9/16, 1)$. The approximation is then $I \approx h/3(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4) = (0 + 4 \cdot 1/16 + 2 \cdot 1/4 + 4 \cdot 9/16 + 1)/12 = (1/4 + 2/4 + 9/4 + 4/4)/12 = 16/(3 \cdot 4 \cdot 4) = 1/3$. The error is thus 0.

One could continue with m = 3, but the error has to be zero. Indeed, Simpson's rule is based on quadratic interpolation polynomials, which means that x^2 will be represented exactly by the interpolating polynomial and the quadrature will be exact.

(b) $f(x) = \cos(x)$

For m = 1 we put $h = (\pi/2 - 0)/2 = \pi/4$, $x_0 = 0$, $x_1 = \pi/4$, $x_2 = \pi/2$; $y_0 = f(x_0) = 1$, $y_1 = f(x_1) = 1/\sqrt{2}$, $y_2 = f(x_2) = 0$. The approximation is then $I \approx h/3(y_0 + 4y_1 + y_2) = (1 + 4/\sqrt{2} + 0) \cdot \pi/12 \approx 1.00227$. The error is thus ≈ 0.00227 .

For m = 2, $h = \pi/8$, $(x_0, \ldots, x_4) = (0, \pi/8, \pi/4, 3\pi/8, \pi/2)$, $(y_0, \ldots, y_4) \approx (1, 0.9238795, 1/\sqrt{2}, 0.38268343, 0)$. $I \approx h/3(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4) \approx 1.000135$, giving the error ≈ 0.000135 .

For m = 3, $h = \pi/6$, $I \approx 1.00002631$, error ≈ 0.00002631 .

(c) $f(x) = \exp(x)$

For m = 1 we put h = (1 - 0)/2 = 1/2, $x_0 = 0$, $x_1 = 1/2$, $x_2 = 1$; $y_0 = f(x_0) = 1$, $y_1 = f(x_1) = e^{1/2}$, $y_2 = f(x_2) = e$. The approximation is then $I \approx h/3(y_0 + 4y_1 + y_2) = (1 + 4\sqrt{e} + e)/6 \approx 1.71886115$. The error is thus $\approx 1.71886115 - e + 1 \approx 5.79 \cdot 10^{-4}$.

For m = 2, h = 1/4, $(x_0, \ldots, x_4) = (0, 1/4, 1/2, 3/4, 1)$, $\ldots I \approx h/3(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4) \approx 1.71831884192175$, giving the error $\approx 3.70 \cdot 10^{-5}$.

For $m = 3, h = 1/6, I \approx 1.71828916992083$, error $\approx 7.34 \cdot 10^{-6}$.

2 Exercise 5.2.11

Find the degree of precision of the following approximation for $\int_{-1}^{1} f(x) dx$:

First of all, let us evaluate the integral of a monomial x^n , $n \ge 0$:

$$\int_{-1}^{1} x^{n} \, \mathrm{d}x = \left[\frac{x^{n+1}}{n+1}\right]_{x=-1}^{x=1} = \begin{cases} 0, & \text{for odd } n, \\ 2/(n+1), & \text{for even } n. \end{cases}$$

(a) f(1) + f(-1): Let us apply the quadrature to the monomial $x^n, n \ge 0$:

$$1^{n} + (-1)^{n} = \begin{cases} 0, & \text{for odd } n, \\ 2, & \text{for even } n, \end{cases}$$

Therefore the quadrature agrees with the integral for n = 0, 1 (and all odd n), and its degree of precision is 1. (One could also observe that this is trapezoid quadrature on [-1, 1], which is known to be exact for polynomials up to degree 1.)

(b) 2/3[f(-1) + f(0) + f(1)]. We check the quadrature on monomials of increasing degree:

$$2/3[(-1)^n + 0^n + (-1)^n] = \begin{cases} 2, & \text{for } n = 0, \\ 0, & \text{for odd } n, \\ 4/3, & \text{for even } n > 0 \end{cases}$$

which agrees with the integral for n = 0, 1 (and odd n). Thus degree of precision is 1. (c) We check the quadrature on monomials of increasing degree:

$$[(-1/\sqrt{3})^n + (1/\sqrt{3})^n] = \begin{cases} 0, & \text{for odd } n, \\ 2/3^{n/2}, & \text{for even } n, \end{cases}$$

which agrees with the integral for n = 0, 1, 2, 3 (and odd n). Thus degree of precision is 3. (This is an example of Gaussian quadrature, which are exact for polynomials of degree up to 2n - 1 when n points are used.)

3 Exercise 5.2.16

Use the fact that the error term of Boole's Rule (see Exercise 5.2.15) is proportional to $f^{(6)}(c)$ to find the exact error term.

Solution

We apply the quadrature to the monomial x^6 , for which $f^{(6)}(c) \equiv 6!$, for all c. Thus

$$\int_{0}^{4h} x^{6} dx = \left[\frac{x^{7}}{7}\right]_{x=0}^{x=4h} = \frac{4^{7}h^{7}}{7} = \frac{2h}{45}(7 \cdot 0^{6} + 32 \cdot h^{6} + 12 \cdot (2h)^{6} + 32 \cdot (3h)^{6} + 7 \cdot (4h)^{6}) + C6!$$

and we are interested in finding C.

```
In [1]: from sympy import *
    init_printing()
    h,C=symbols('h C')
    integral = (4*h)**7/7
    quadrature = 2*h/45*(32*h**6 + 12*(2*h)**6 + 32*(3*h)**6 + 7*(4*h)**6)
    simplify(integral-quadrature)
```

Out[1]:

$$-\frac{128h^7}{21}$$

Thus $C = -128h^7/(21 \cdot 6!) = -8h^7/945$

4 Exercise 5.4.1

Apply Adaptive Quadrature by hand, using the Trapezoid Rule with tolerance TOL = 0.05 to approximate the integrals. Find the approximation error.

Solution

(a) In this case, $f(x) = x^2$, $a_0 = 0$, $b_0 = 1$.

We begin with n = 1 interval, $a = a_0$, $b = b_0$. We will use S[a, b] to denote the Trapezoid quadrature applied on the interval [a, b].

 $\begin{aligned} c &= (a+b)/2, \ S[a,b] = (0^2+1^2)/2 = 1/2, \ S[a,c] = (0^2+(1/2)^2)/4 = 1/16, \ S[c,b] = ((1/2)^2+1^2)/4 = 5/16. \\ |S[a,b] - S[a,c] - S[c,b]| &= 1/8 = 0.125 < 3 \cdot 0.05 \cdot ((b-a)/(b_0-a_0)) = 0.15. \\ \text{Thus we stop with the approximation } S[a,c] + S[c,b] = 3/8 = 0.375 \text{ and an error estimate } -(S[a,b] - S[a,c] - S[c,b])/3 = -1/24 \approx -0.0417. \end{aligned}$

The actual integration error is $\int_0^1 x^2 - 3/8 = 1/3 - 3/8 = -1/24$. Our estimate is exact because f'' is constant in this case, thus the approximate equation (5.38) in the book is actually exact.

(b) $f(x) = \cos(x), a_0 = 0, b_0 = \pi/2.$

$$\begin{split} S[0,\pi/2] &= (1+0)/2 = 1/2, \ S[0,\pi/4] = (1+1/\sqrt{2})/4 \approx 0.42678, \ S[\pi/4,\pi,2] = (1/\sqrt{2}+0)/4 \approx 0.17678. \\ |S[a,b] - S[a,c] - S[c,b]| &= |1/4 - 1/(2\sqrt{2})| \approx 0.104 < 3 \cdot 0.05 \cdot 1 = 0.15. \\ \text{Thus we stop with the approximation} \\ S[a,c] + S[c,b] &= 1/4 + 1/(2\sqrt{2}) \approx 0.60355 \text{ and an error estimate} - (S[a,b] - S[a,c] - S[c,b])/3 = 1/(6\sqrt{2}) - 1/12 \approx 0.0345, \\ \text{whereas the actual integration error is } \int_{0}^{\pi/2} \cos(x) - 1/4 - 1/(2\sqrt{2}) = 1 - 1/4 - 1/(2\sqrt{2}) \approx 0.396. \end{split}$$

 $1/12 \approx 0.0345$, whereas the actual integration error is $\int_0^{\pi/2} \cos(x) - 1/4 - 1/(2\sqrt{2}) = 1 - 1/4 - 1/(2\sqrt{2}) \approx 0.396$. Thus the adaptive quadrature underestimates the error in this case. The problem is the assumption made in equation (5.38) is not realistic in this case.

(c) In this case, $f(x) = \exp(x)$, $a_0 = 0$, $b_0 = 1$.

$$\begin{split} S[0,1] &= (1+e)/2 \approx 1.85914, \ S[0,0.5] = (1+\exp(0.5))/4 \approx 0.66218, \ S[0.5,1] = (\exp(0.5)+\exp(1))/4 \approx 1.09175. \ |S[a,b] - S[a,c] - S[c,b]| \approx 0.1052 < 3 \cdot 0.05 \cdot ((b-a)/(b_0-a_0)) = 0.15. \ \text{Thus we stop with the approximation } S[a,c] + S[c,b] \approx 1.75393 \ \text{and an error estimate } -(S[a,b] - S[a,c] - S[c,b])/3 = \approx -0.035. \end{split}$$

The actual integration error is $\int_0^1 \exp(x) - (S[a,c] + S[c,b]) \approx -0.036$. Our estimate is quite good in this case.

5 Exercise 5.4.4

Develop an Adaptive Quadrature method for rule (5.28).

Solution

Let c = (a+b)/2, h = b - a and apply the quadrature on [a, b], [a, c], and [c, b] (we use the same notation as in the book):

$$\int_{a}^{b} f(x) \, \mathrm{d}x = S[a, b] + \frac{14h^{5}}{45} f^{(4)}(c_{1}), \qquad c_{1} \in [a, b],$$

$$\int_{a}^{c} f(x) \, \mathrm{d}x + \int_{c}^{b} f(x) \, \mathrm{d}x = S[a, c] + S[c, b] + \frac{14(h/2)^{5}}{45} f^{(4)}(c_{2}) + \frac{14(h/2)^{5}}{45} f^{(4)}(c_{3}), \qquad c_{2} \in [a, c], c_{3} \in [c, b].$$

Further assuming that $f^{(4)}(c_1) \approx f^{(4)}(c_2) \approx f^{(4)}(c_3)$ we obtain:

$$\int_{a}^{b} f(x) \, \mathrm{d}x = S[a, b] + \frac{14h^{5}}{45} f^{(4)}(c_{1}),$$
$$\int_{a}^{c} f(x) \, \mathrm{d}x + \int_{c}^{b} f(x) \, \mathrm{d}x \approx S[a, c] + S[c, b] + \frac{1}{16} \frac{14h^{5}}{45} f^{(4)}(c_{1}).$$

We can now subtract the second equation from the first to obtain:

$$S[a,b] - S[a,c] - S[c,b] \approx 15 \frac{1}{16} \frac{14h^5}{45} f^{(4)}(c_1).$$

Thus the number S[a, b] - S[a, c] - S[c, b] gives an approximation to 15 times the error of the quadrature S[a, c] + S[c, b].

The rest is exactly the same as for other quadratures; one stops subdividing the interval when $|S[a, b] - S[a, c] - S[c, b]| < 15 \cdot TOL \cdot (b - a)/(b_{\text{orig}} - a_{\text{orig}})$ and returns S[a, c] + S[c, b] as the approximation of the integral over the interval [a,b].

6 Exercise 5.5.1

Approximate the integrals using n = 2 Gaussian Quadrature. Compare with the correct value and give the approximation error.

Solution

Gaussian Quadrature with n = 2 is defined by the points $x_{1,2} = \pm 1/\sqrt{3}$, $w_{1,2} = 1$.

```
In [2]: x1 = -1/sqrt(3)
    x2 = 1/sqrt(3)
    w1 = 1
    w2 = 1
    (a)
In [3]: from sympy import *
    init_printing()
    x=symbols('x')
    f=Lambda(x,x**3+2*x)
    # Exact integral
    integrate(f(x),(x,-1,1))
```

Out[3]:

0

Out[4]:

0

Thus the error is 0, which agrees with the theory for Gaussian Quadratures being exact for polynomials up to degree 2n - 1.

 $\frac{2}{5}$

```
(b)
```

```
In [5]: f=Lambda(x,x**4)
    # Exact integral
    integrate(f(x),(x,-1,1))
Out[5]:
In [6]: # Numerical quadrature
    f(x1)*w1 + f(x2)*w2
```

Out[6]:

 $\frac{2}{9}$

Out[7]:

0.1777777777777778

(c)

```
In [8]: f=Lambda(x,exp(x))
```

```
# Exact integral
integrate(f(x),(x,-1,1))
```

Out[8]:

 $-\frac{1}{e}+e$

```
In [9]: # Numerical quadrature
    f(x1)*w1 + f(x2)*w2
```

Out[9]:

$$e^{-\frac{\sqrt{3}}{3}} + e^{\frac{\sqrt{3}}{3}}$$

```
In [10]: # Approximation error
N(integrate(f(x),(x,-1,1))-(f(x1)*w1 + f(x2)*w2))
```

Out[10]:

0.00770629937787234

```
(d)
```

```
In [11]: f=Lambda(x,cos(pi*x))
```

```
# Exact integral
integrate(f(x),(x,-1,1))
```

Out[11]:

0

```
In [12]: # Numerical quadrature
    f(x1)*w1 + f(x2)*w2
```

Out[12]:

$$2\cos\left(\frac{\sqrt{3}\pi}{3}\right)$$

In [13]: # Approximation error N(0-2*cos(sqrt(3)*pi/3))

Out[13]:

7 Exercise 5.5.7

Show that the Legendre polynomials $p_1(x) = x$ and $p_2(x) = x^2 - 1/3$ are orthogonal on [-1, 1]. Solution $\int_{-1}^{1} p_1(x) p_2(x) dx = \int_{-1}^{1} (x^3 - x/3) dx = 0$ because $x^3 - x/3$ is an odd function.

8 Exercise 5.5.8

Compute Legendre polynomials up to degree 3.

Solution

Legendre polynomials are given by the expression

$$p_i(x) = \frac{1}{2^i i!} \frac{\mathrm{d}}{\mathrm{d}x^i} [(x^2 - 1)^i]$$

Thus

$$\begin{aligned} p_0(x) &= 1, \\ p_1(x) &= 1/2[(x^2 - 1)]' = x, \\ p_2(x) &= 1/(4 \cdot 2)[(x^2 - 1)^2]'' = 1/8[x^4 - 2x^2 + 1]'' = 1/8[12x^2 - 4] = 3/2(x^2 - 3), \\ p_3(x) &= 1/(8 \cdot 6)[(x^2 - 1)^3]''' = 1/48[x^6 - 3x^4 + 3x^2 - 1]''' = 1/48[120x^3 - 72x] = 5/2[x^3 - 3/5x]. \end{aligned}$$

9 Exercise 5.5.9

Verify the coefficients c_i and x_i in Table 5.1 for degree n = 3.

Solution

We have computed $p_3(x) = 5/2x(x^2 - 3/5)$ in Exercise 5.5.8. This immediatly implies that $p_3(0) = p_3(\pm\sqrt{3/5}) = 0$ confirming the roots listed in Table 5.1.

The coefficients c_i are obtained by integrating the Lagrange polynomials. For example,

$$L_2(x) = \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} = \frac{(x+\sqrt{3/5})(x-\sqrt{3/5})}{(0+\sqrt{3/5})(0-\sqrt{3/5})} = 1 - \frac{5}{3}x^2,$$

and therefore

$$c_2 = \int_{-1}^{1} [1 - 5/3x^2] \, \mathrm{d}x = [x - 5/9x^3]_{x=-1}^{x=1} = 2 - 10/9 = 8/9.$$

Similarly

$$L_{1,3}(x) = \frac{(x-0)(x \mp \sqrt{3/5})}{(\mp \sqrt{3/5} - 0)(\mp \sqrt{3/5} \mp \sqrt{3/5})} = \frac{x(x \mp \sqrt{3/5})}{2 \cdot 3/5}$$

and therefore

$$c_{1,3} = \frac{5}{6} \int_{-1}^{1} [x^2 \mp x\sqrt{3/5}] \, \mathrm{d}x = \frac{5}{6} [x^3/3 \mp \sqrt{3/5}x^2/2]_{x=-1}^{x=1} = \frac{5}{6} \frac{2}{3} = \frac{5}{9}.$$

10 Computer exercise 5.2.8

Answers:

- (a) 1.547866
- (b) 1.277978
- (c) 1.277978

11 Computer exercise 5.2.10

See the file uniform_refinement.m available on the wiki. Adapt the code to use Simpson's rule instead of Trapezoid.