Numerical Methods for Partial Differential Equations - Exercise 1

(1) In 1225, Leonardo of Pisa (also known as Fibonacci) was requested to solve a collection of mathematical problems in order to justify his fame and prestige in the court of Federico II. One of the proposed problems can be formulated as the solution of a third degree polynomial equation

$$f(x) := x^3 + 2x^2 + 10x - 20 = 0 \qquad (1)$$

Note that the solution of cubic equations was an extremely difficult problem in the 13th century. Here iterative methods are considered for the solution of equation (1)

Compute the unique real root of (1) with 4 iterations of Newton's method with the initial approximation $x^0 = \sqrt[3]{20}$ (which is obtained neglecting the monomials with $x$ and $x^2$ in front of the monomial with $x^3$). Plot the convergence graphic. Does Newton's method behave as expected?

Solution

- When using Newton method, we can write

$$x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)}$$

Find derivative of function $f(x)$

$$f'(x) = 3x^2 + 4x + 10$$

Iteration 1 with given $x^0 = 20^{1/3} = 2.714418$

$$x^1 = 20^{1/3} - \frac{(20^{1/3})^3 + 2(20^{1/3})^2 + 10(20^{1/3}) - 20}{3(20^{1/3})^2 + 4(20^{1/3}) + 10} = 1.739592$$

Iteration 2

$$x^2 = 1.739592 - \frac{(1.739592)^3 + 2(1.739592)^2 + 10(1.739592) - 20}{3(1.739592)^2 + 4(1.739592) + 10} = 1.404967$$

Iteration 3

$$x^3 = 1.404967 - \frac{(1.404967)^3 + 2(1.404967)^2 + 10(1.404967) - 20}{3(1.404967)^2 + 4(1.404967) + 10} = 1.369183$$

Iteration 4

$$x^4 = 1.369183 - \frac{(1.369183)^3 + 2(1.369183)^2 + 10(1.369183) - 20}{3(1.369183)^2 + 4(1.369183) + 10} = 1.368808$$

The real root for this polynomial equation is 1.368808 same as the number got from Newton's method. And from the convergence graphic, it shows the quadratic convergence as expected since the initial approximation is near the root.


Convergence in x
Relative error in x
Iterations
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5

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(5) We are interested in the definition of third-order numerical quadratures in interval $(0,1)$

a) Determine the minimum number of integration points, and specify the integration points and weights

b) Is it possible to obtain a third-order quadrature with the following four integration points: $x_0 = 1/4$, $x_1 = 1/2$, $x_2 = 3/4$ and $x_3 = 1$? If it is possible, compute the corresponding weights; otherwise, justify why not.

Solution (a)

For Gauss quadrature, quadrature has order $2n+1$

Therefore, for a third-order quadrature, $n=1$

Imposing the Gauss quadrature

$$\int_{-1}^{1} f(z)\,dz \simeq \sum_{i=0}^{i=n} w_i f(z_i)$$

But we are interested in interval $(0,1)$, then we need to convert the limits of integration yielding.

$$\int_a^b F(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} F\left(\frac{b-a}{2}z + \frac{b+a}{2}\right)dz$$

$$\simeq \frac{b-a}{2}\sum_{i=0}^{n} w_i F\left(\frac{b-a}{2}z_i + \frac{b+a}{2}\right)$$

For interval $(0,1)$ and a third-order quadrature

$$\int_0^1 F(x)\,dx \simeq \frac{1}{2}\sum_{i=0}^{1} w_i F\left(\frac{1}{2}z_i + \frac{1}{2}\right) = \frac{1}{2}w_0 F\left(\frac{1}{2}z_0 + \frac{1}{2}\right) + \frac{1}{2}w_1 F\left(\frac{1}{2}z_1 + \frac{1}{2}\right)$$

From the Gauss-Legendre table when $n=1$: $w_0 = w_1 = 1$, $z_0 = -\sqrt{3}/3$, $z_1 = \sqrt{3}/3$

For interval $(0,1)$; integration points are $z_0' = \frac{1}{2}\left(-\frac{\sqrt{3}}{3}\right) + \frac{1}{2} = 0.21132$

$$z_1' = \frac{1}{2}\left(\frac{\sqrt{3}}{3}\right) + \frac{1}{2} = 0.78868$$

weights are $w_0' = \frac{1}{2}w_0 = 0.5$

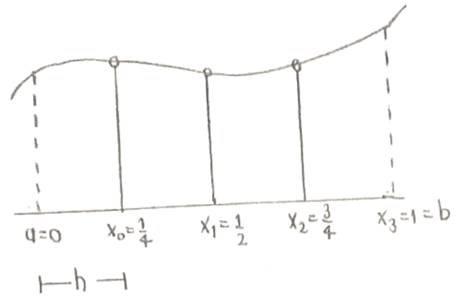
$$w_1' = \frac{1}{2}w_1 = 0.5$$

solution (a) - cont.

For third-order quadrature using Newton - Cotes, we need 4 integration points which depend on using the concept of closed or open quadrature. The integration points and weights are specified in the table below

| | Closed quadrature | | Open quadrature | |
|---|---|---|---|---|
| | Integration points | weights | Integration points | weights |
| $X_0$ | $0$ | $\frac{1}{8} = 0.125$ | $\frac{1}{5} = 0.2$ | $\frac{11}{24} = 0.4583$ |
| $X_1$ | $\frac{1}{3} = 0.33$ | $\frac{3}{8} = 0.375$ | $\frac{2}{5} = 0.4$ | $\frac{1}{24} = 0.0417$ |
| $X_2$ | $\frac{2}{3} = 0.67$ | $\frac{3}{8} = 0.375$ | $\frac{3}{5} = 0.6$ | $\frac{1}{24} = 0.0417$ |
| $X_3$ | $1$ | $\frac{1}{8} = 0.125$ | $\frac{4}{5} = 0.8$ | $\frac{11}{24} = 0.4583$ |

Solution (b) using Newton - Cotes because there are predetermined points




$x = x_0 + \alpha h \rightarrow dx = h d\alpha$

$h = \frac{1}{4}$

For third-order quadrature, we need $P_3(x)$

$$P_3(x) = f(x_0) + (x-x_0)\frac{\Delta f(x_0)}{h} + (x-x_0)(x-x_1)\frac{\Delta^2 f(x_0)}{2h^2} + (x-x_0)(x-x_1)(x-x_2)\frac{\Delta^3 f(x_0)}{3!h^3}$$

$$= f(x_0) + \frac{1}{h}(x-x_0)\left[f(x_1)-f(x_0)\right] + \frac{1}{2h^2}(x-x_0)(x-x_1)\left[\Delta f(x_1) - \Delta f(x_0)\right]$$

$$+ \frac{1}{6h^3}(x-x_0)(x-x_1)(x-x_2)\left[\Delta^2 f(x_1) - \Delta^2 f(x_0)\right]$$

$$= f(x_0) + \frac{1}{h}(x-x_0)\left[f(x_1)-f(x_0)\right] + \frac{1}{2h^2}(x-x_0)(x-x_1)\left[f(x_2)-f(x_1)-f(x_1)+f(x_0)\right]$$

$$+ \frac{1}{6h^3}(x-x_0)(x-x_1)(x-x_2)\left[(f(x_3)-2f(x_2)+f(x_1)) - (f(x_2)-2f(x_1)+f(x_0))\right]$$

$$= f(x_0) + \frac{1}{h}(x-x_0)\left[f(x_1)-f(x_0)\right] + \frac{1}{2h^2}(x-x_0)(x-x_1)\left[f(x_2)-2f(x_1)+f(x_0)\right]$$

$$+ \frac{1}{6h^3}(x-x_0)(x-x_1)(x-x_2)\left[f(x_3)-3f(x_2)+3f(x_1)-f(x_0)\right]$$

Replacing $x = x_0 + \alpha h$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$

$$P_3(x_0+\alpha h) = f(x_0) + \frac{1}{h}(x_0+\alpha h - x_0)\left[f(x_1)-f(x_0)\right] + \frac{1}{2h^2}(x_0+\alpha h-x_0)(x_0+\alpha h-x_0-h)\left[f(x_2)-2f(x_1)+f(x_0)\right]$$

$$+ \frac{1}{6h^3}(x_0+\alpha h-x_0)(x_0+\alpha h-x_0-h)(x_0+\alpha h-x_0-2h)\left[f(x_3)-3f(x_2)+3f(x_1)-f(x_0)\right]$$

$$= f(x_0) + \alpha\left(f(x_1)-f(x_0)\right) + \frac{1}{2}\alpha(\alpha-1)\left(f(x_2)-2f(x_1)+f(x_0)\right)$$

$$+ \frac{1}{6}\alpha(\alpha-1)(\alpha-2)\left(f(x_3)-3f(x_2)+3f(x_1)-f(x_0)\right)$$

Integration using third-order quadrature

$a = x_0 - h$

$b = x_0 + 3h$

$$I \approx \int_a^b P_3(x)\,dx = h\int_{-1}^{3} P_3(x_0+\alpha h)\,d\alpha$$

$$= h\int_{-1}^{3}\left[\begin{gathered} f(x_0) + \alpha\left(f(x_1)-f(x_0)\right) + \frac{1}{2}\alpha(\alpha-1)\left(f(x_2)-2f(x_1)+f(x_0)\right) \\ + \frac{1}{6}\alpha(\alpha-1)(\alpha-2)\left(f(x_3)-3f(x_2)+3f(x_1)-f(x_0)\right)\end{gathered}\right] d\alpha$$

Solution (b) - cont.

$$I \approx \left[ \begin{array}{l} \left[\alpha f(x_0)\right]_{-1}^{3} + \left[\frac{1}{2}\alpha^2 (f(x_1) - f(x_0))\right]_{-1}^{3} + \left[\left(\frac{1}{6}\alpha^3 - \frac{1}{4}\alpha^2\right)\left(f(x_2) - 2f(x_1) + f(x_0)\right)\right]_{-1}^{3} \\ + \left[\left(\frac{1}{24}\alpha^4 - \frac{1}{6}\alpha^3 + \frac{1}{6}\alpha^2\right)\left(f(x_3) - 3f(x_2) + 3f(x_1) - f(x_0)\right)\right]_{-1}^{3} \end{array} \right] \times h$$

$$= \left(4f(x_0) + 4\left[f(x_1) - f(x_0)\right] + \frac{8}{3}\left[f(x_2) - 2f(x_1) + f(x_0)\right] + 0\left[f(x_3) - 3f(x_2) + 3f(x_1) - f(x_0)\right]\right) \times h.$$

$$= \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2)\right]$$

Using a third-order quadrature with four integration points: $x_0 = 1/4$, $x_1 = 1/2$, $x_2 = 3/4$, and $x_3 = 1$

turns out to be the same as a second-order quadrature with open ends.

Therefore, we can't obtain a third-order quadrature with the given integration points.

Numerical Methods for Partial Differential Equations - Exercise 1

(6) a) If $n+1$ points Gaussian quadrature is used for numerial integration state the order of the polynomial that is integrated exactly.

b) If $n=2$ is selected for Gaussian quadrature, which (if any) of the following integrals will be integrated exactly?

i) $\int_0^1 \sin x \, dx$ ii) $\int_0^1 x^3 \, dx$ iii) $\int_0^1 x^4 \, dx$ iv) $\int_0^1 x^{5.5} \, dx$

Solution

a) If $n+1$ points Gaussian quadrature is used, the polynomial of degree $n$ or less can be integrated exactly.

b) If $n=2$, then the polynomials of degree 5 or less can be integrated exactly. Therefore, $\int_0^1 x^3 dx$ and $\int_0^1 x^4 dx$ will be integrated exactly if $n=2$ for Gaussian quadrature.

Numerical Methods for Partial Differential Equations - Exercise 1

(7) Compute $\int_0^1 12x\,dx$ , $\int_0^1 (5x^3+2x)\,dx$ by hand calculation using

i) Trapezoidal rule over 2 uniform intervals

ii) Simpson's rule over 2 uniform intervals

Compute the error of both approximations. Are the methods behaving as expected?

Solution

The trapezoidal rule approximates the region under the graph of f(x) as a trapezoidal and calculate the trapezoidal area. So

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)\left[f(a)+f(b)\right]$$

compute $\int_0^1 12x\,dx$ using trapezoidal rule over 2 uniform intervels

$$\int_0^1 12x\,dx = \int_0^{1/2} 12x\,dx + \int_{1/2}^{1} 12x\,dx$$

$$\approx \frac{1}{2}\left(\frac{1}{2}\right)\left[12(0)+12\left(\frac{1}{2}\right)\right] + \frac{1}{2}\left(\frac{1}{2}\right)\left[12\left(\frac{1}{2}\right)+12(1)\right] = 6$$

compute $\int_0^1 (5x^3+2x)\,dx$ using trapezoidal rule over 2 uniform intervals

$$\int_0^1 (5x^3+2x)\,dx = \int_0^{1/2} (5x^3+2x)\,dx + \int_{1/2}^{1} (5x^3+2x)\,dx.$$

$$\approx \frac{1}{2}\left(\frac{1}{2}\right)\left[(5(0)^3+2(0))+(5(1/2)^3+2(1/2))\right]$$

$$+\frac{1}{2}\left(\frac{1}{2}\right)\left[(5(1/2)^3+2(1/2))+(5(1)^3+2(1))\right]$$

$$\approx 2.5625$$

The approximation using Simpson's rule can be written as

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

compute $\int_0^1 12x\,dx$ using Simpson's rule over 2 uniform intervals

$$\int_0^1 12x\,dx = \int_0^{1/2} 12x\,dx + \int_{1/2}^1 12x\,dx$$

$$\approx \frac{(1/2)}{6}\left[12(0) + 4(12)(1/4) + 12(1/2)\right] + \frac{(1/2)}{6}\left[12(1/2) + 4(12)(3/4) + 12(1)\right] = 6$$

Compute $\int_0^1 (5x^3 + 2x)\,dx$ using Simpson's rule over 2 uniform intervals

$$\int_0^1 (5x^3 + 2x)\,dx = \int_0^{1/2} (5x^3 + 2x)\,dx + \int_{1/2}^1 (5x^3 + 2x)\,dx$$

$$\approx \frac{(1/2)}{6}\left[\left(5(0)^3 + 2(0)\right) + 4\times\left(5(1/4)^3 + 2(1/4)\right) + \left(5(1/2)^3 + 2(1/2)\right)\right]$$

$$+ \frac{(1/2)}{6}\left[\left(5(1/2)^3 + 2(1/2)\right) + 4\times\left(5(3/4)^3 + 2(3/4)\right) + \left(5(1)^3 + 2(1)\right)\right]$$

$$\approx 2.25$$

Comparing between the exact integration and approximation using trapezoidal rule and Simpson's rule

| | | | | error | |
|---|---|---|---|---|---|
| problems | exact | trapezoidal | Simpson | exact vs trapezoidal | exact vs Simpson |
| $\int_0^1 12x\,dx$ | 6 | 6 | 6 | 0 | 0 |
| $\int_0^1 (5x^3 + 2x)\,dx$ | 2.25 | 2.5625 | 2.25 | $\frac{2.5625 - 2.25}{2.25} = 0.14$ | 0 |

The trapezoidal rule gives error when approximating the integration of $(5x^3+2x)$ as expected since it is using linear approximation. while Simpson's rule gives no error as expected since it uses quadratic polynomials to approximate functions and can give exact results when approximating the integration of polynomials up to cubic degree.

Numerical Methods for Partial Differential Equations - Exercise 1

(10) Perform the numerical integration of

$$\int_0^1 \int_0^1 (9x^3 + 8x^2)(y^3 + y)\,dx\,dy$$

using Simpson's rule in each direction. Is the approximation behaving as expected?

solution

The approximation using Simpson's rule, can be written as

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

When applying Simpson's rule to x-direction, treat $(y^3+y)$ as constant A

$$\int_0^1 A \int_0^1 (9x^3 + 8x^2)\,dx\,dy \approx \int_0^1 A \times \frac{1}{6}\left[0 + 4\left(9(1/2)^3 + 8(1/2)^2\right) + (9+8)\right] dy$$

$$= \int_0^1 \frac{59}{12} A\,dy = \frac{59}{12}\int_0^1 (y^3 + y)\,dy$$

Now applying Simpson's rule to y-direction

$$\frac{59}{12}\int_0^1 (y^3+y)\,dy \approx \frac{59}{12} \times \frac{1}{6}\left[0 + 4\left((1/2)^3 + (1/2)\right) + (1+1)\right] = \frac{59}{16}$$

Exact integration

$$\int_0^1\int_0^1 (9x^3 + 8x^2)(y^3+y)\,dx\,dy = \int_0^1 (y^3+y)\int_0^1 (9x^3+8x^2)\,dx\,dy$$

$$= \int_0^1 (y^3+y)\left[\frac{9}{4}x^4 + \frac{8}{3}x^3\right]_0^1 dy = \frac{59}{12}\int_0^1 (y^3+y)\,dy$$

$$= \frac{59}{12}\left[\frac{1}{4}y^4 + \frac{1}{2}y^2\right]_0^1 = \frac{59}{16}$$

The approximation is behaving as expected giving the exact result since Simpson's rule uses quadratic polynomials to approximate functions and can give exact results when approximating the integration of polynomials up to cubic degree which is the highest degree in both x- and y- direction.