Chapter 5

Numerical Differentiation and Integration

1. Let $f(x) = (x-1)e^x$ and take $h = 0.01$.
(a) Calculate approximation to $f'(2.3)$ using the two-point forward-difference formula. Also, compute the actual error and an error bound for you approximation.
(b) Solve part *(a)* using the two-point backward-difference formula.

two-point forward-difference formula: $f'(x_0) \approx \dfrac{f(x_0+h) - f(x_0)}{h} = D_h f(x_0).$

The error bound formula $\dfrac{h}{2}M,$ where $M = \max_{x_0 \le x \le x_1} |f''(x)|.$

Solution: (a) Given $f(x) = (x-1)e^x$ and $h = 0.01$, then using the two-point forward-difference formula with $x_0 = 2.3$, we have

$$f'(2.3) \approx \frac{f(2.3+h) - f(2.3)}{h}$$

Then for $h = 0.01$, we get

$$\begin{aligned} f'(2.3) &\approx \frac{f(2.31) - f(2.3)}{0.01} \\ &\approx \frac{(2.31-1)e^{2.31} - (2.3-1)e^{2.3}}{0.01} = 23.10591068 \end{aligned}$$

The actual error is

$$Error = f'(2.3) - 23.10591068 = 2.3e^{2.3} - 23.10591068 = -0.16529103$$

To find the error bound, we use the following formula

$$E_F(f,h) = -\frac{h}{2} f''(\eta(x)), \quad \text{where} \quad \eta(x) \in (x_0, x_0+h)$$

which can be written as

$$|E_F(f,h)| = \left| -\frac{0.01}{2} \right| |f''(\eta(x))|, \quad \text{for} \quad \eta \in (2.3, 2.31)$$

The second derivative $f''(x)$ of the function can be found as

$$f'(x) = xe^x, \quad \text{and} \quad f''(x) = (1+x)e^x$$

The value of the second derivative $f''(\eta(x))$ cannot be computed exactly because $\eta(x)$ is not known. But one can bound the error by computing the largest possible value for $|f''(\eta(x))|$. So bound $|f''|$ on $[2.3, 2.31]$ can be obtain

$$M = \max_{2.3 \le x \le 2.31} |(1+x)e^x| = 33.346346$$

at $x = 2.31$. Since $|f''(\eta(x))| \le M$, therefore, for $h = 0.01$, we have

$$|E_F(f,h)| \le \frac{0.01}{2} M = 0.005(33.346346) = 0.16673173$$

which is the possible maximum error in our approximation.

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two-point backward-difference formula: $$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}.$$

(b) Using the two-point backward-difference formula with $x_0 = 2.3$, we have

$$f'(2.3) \approx \frac{f(2.3) - f(2.3 - h)}{h}$$

Then for $h = 0.01$, we get

$$\begin{aligned} f'(2.3) &\approx \frac{f(2.3) - f(2.29)}{0.01} \\ &\approx \frac{(2.3 - 1)e^{2.3} - (2.29 - 1)e^{2.29}}{0.01} = 22.77675826 \end{aligned}$$

The actual error is

$$Error = f'(2.3) - 22.77675826 = 2.3e^{2.3} - 22.77675826 = 0.16386139$$

To find the error bound, we use the following formula

$$E_F(f, h) = -\frac{h}{2} f''(\eta(x)), \quad \text{where} \quad \eta(x) \in (x_0 - h, x_0)$$

which can be written as

$$|E_F(f, h)| = \left| -\frac{0.01}{2} \right| |f''(\eta(x))|, \quad \text{for} \quad \eta \in (2.29, 2.3)$$

The second derivative $f''(x)$ of the function can be found as

$$f'(x) = xe^x, \quad \text{and} \quad f''(x) = (1 + x)e^x$$

The value of the second derivative $f''(\eta(x))$ cannot be computed exactly because $\eta(x)$ is not known. But one can bound the error by computing the largest possible value for $|f''(\eta(x))|$. So bound $|f''|$ on $[2.29, 2.3]$ can be obtain

$$M = \max_{2.29 \leq x \leq 2.3} |(1 + x)e^x| = 32.9148021$$

at $x = 2.3$. Since $|f''(\eta(x))| \leq M$, therefore, for $h = 0.01$, we have

$$|E_F(f, h)| \leq \frac{0.01}{2} M = 0.005(32.9148021) = 0.16457401$$

which is the possible maximum error in our approximation.

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5. Use the three-point central-difference formula to compute the approximate value for $f'(5)$ with $f(x) = (x^2+1)\ln x$, and $h = 0.05$. Compute the actual error and the error bound for you approximation.

three-point central-difference formula (second-order)

$$f'(x_1) \approx \frac{f(x_1+h) - f(x_1-h)}{2h} = D_h f(x_1).$$

The error bound formula of central difference three-point formula $\frac{h^2}{6}M,$ where

$$M = \max_{x_0 \le x \le x_2} |f'''(x)|.$$

Solution: Given $f(x) = (x^2+1)\ln x$ and $x_1 = 5, h = 0.05$, then using the three-point formula, we have

$$f'(5) \approx \frac{f(5+0.05) - f(5-0.05)}{2(0.05)} = \frac{f(5.05) - f(4.95)}{0.1}$$

Then

$$\begin{aligned} f'(5) &\approx \frac{[(5.05)^2+1]\ln(5.05) - [(4.95)^2+1]\ln(4.95)}{0.1} \\ &\approx \frac{42.917837 - 40.788382}{0.1} = 21.294553 \end{aligned}$$

The actual error is

$$Error = f'(5) - 21.294553 = 21.294379 - 21.294553 = -0.000174$$

To compute the error bound for the approximation, we use the formula

$$E_C(f,h) = -\frac{(0.05)^2}{6} f'''(\eta(x_1)), \quad \text{for} \quad \eta(x_1) \in (4.95, 5.05)$$

or

$$|E_C(f,h)| = \Big| -\frac{(0.05)^2}{6} \Big| |f'''(\eta(x_1))|, \quad \text{for} \quad \eta(x_1) \in (4.95, 5.05)$$

The third derivative $f'''(x)$ of the function can be found as

$$f'(x) = 2x\ln x + (x^2+1)/x, \;\; f''(x) = 2\ln x - (x^2+1)/x^2 - 4, \;\; f'''(x) = 2(x^2+1)/x^3$$

The value of the third derivative $f'''(\eta(x_1))$ cannot be computed exactly because $\eta(x_1)$ is not known. But one can bound the error by computing the largest possible value for $|f'''(\eta(x_1))|$. So bound $|f'''|$ on $[4.95, 5.05]$ can be obtain

$$M = \max_{4.95 \le x \le 5.05} |2(x^2+1)/x^3| = 0.4205302$$

at $x = 4.95$. Since $|f''(\eta(x))| \le M$, therefore, for $h = 0.1$, we have

$$|E_F(f,h)| \le \frac{(0.05)^2}{6} M = 0.00042(0.4205302) = 0.000175$$

which is the possible maximum error in our approximation.

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20. Let $f(x) = x + \ln(x+2)$, with $h = 0.1$. Use the three-point formula to approximate $f''(2)$. Find error bound for your approximation and compare the actual error to the bound.

three-point central-difference formula

$$f''(x_1) \approx \frac{f(x_1 - h) - 2f(x_1) + f(x_1 + h)}{h^2} = D_h^2 f(x_1),$$

Error Bound for Three Point Central Difference Formula

$$E(f)| \leq \frac{h^2}{12} M, \quad M = \max_{a \leq x \leq b} |f^{(4)}(x)|.$$

Solution: Given $f(x) = x + \ln(x+2)$, $x_1 = 2$, $h = 0.1$, then using three-point formula for finding the approximation of $f''(2)$, we have

$$f''(2) \approx \frac{f(2+0.1) - 2f(2) + f(2-0.1)}{(0.1)^2}$$

or

$$\begin{aligned} f''(2) &\approx \frac{f(2.1) - 2f(2) + f(1.9)}{0.01} \\ &\approx \frac{(2.1 + \ln(4.1)) - 2(2 + \ln(4.0)) + (1.9 + \ln(3.9))}{0.01} \\ &\approx \frac{3.5109870 - 6.7725887 + 3.2609766}{0.01} = -0.0625195 \end{aligned}$$

To compute the error bound for our approximation, we use the following error formula

$$E_C(f, h) = -\frac{h^2}{12} f^{(4)}(\eta(x_1)), \quad \text{for} \quad \eta(x_1) \in (1.9, 2.1)$$

or

$$|E_C(f, h)| = \left| -\frac{h^2}{12} \right| |f^{(4)}(\eta(x_1))|, \quad \text{for} \quad \eta(x_1) \in (1.9, 2.1)$$

The fourth derivative of the given function at $\eta(x_1)$ is

$$f^{(4)}(\eta(x_1)) = -6/(\eta(x_1) + 2)^4$$

and it cannot be computed exactly because $\eta(x_1)$ is not known. But one can bound the error by computing the largest possible value for $|f^{(4)}(\eta(x_1))|$. So bound $|f^{(4)}|$ on the interval $(1.9, 2.1)$ is

$$M = \max_{1.9 \leq x \leq 2.1} |-6/(x+2)^4| = 0.0259354$$

at $x = 1.9$, Thus, for $|f^{(4)}(\eta(x))| \leq M$, we have

$$|E_C(f, h)| \leq \frac{h^2}{12} M$$

Taking $M = 0.0259354$ and $h = 0.1$, we obtain

$$|E_C(f, h)| \leq \frac{0.01}{12}(0.0259354) = 0.0000216$$

which is the possible maximum error in our approximation.
The actual error is

$$Error = f''(2) + 0.0625195 = -0.0625000 + 0.0625195 = 0.0000195$$

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28. Use a suitable composite integration formula for the approximation of the integral $\int_1^2 \frac{dx}{3-x}$, with $n = 5$. Compute an upper bound for your approximation.

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29. Use the composite Trapezoidal rule for the approximation of the integral $\displaystyle\int_1^3 \frac{dx}{7-2x}$ with $h = 0.5$. Also, compute an error term.

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30. Find the step size h so that the absolute value of the error for the composite Trapezoidal rule is less than 5×10^{-4} when it is used to approximate the integral $\displaystyle\int_2^7 \frac{dx}{x}$.

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35. Evaluate $\int_0^1 e^{x^2} dx$ by the Simpson's rule choosing h small enough to guarantee five decimal accuracy. How large can h be ?