1 Let $f(x) = e^x$. *Numerically* apply the forward-difference formula to approximate $f'(0)$, with $h = 10^{-k}$, $k = 2, 4, 6, 8, 10, 12$. What can you find? Explain it.

Solution The forward-difference formula is given by

$$f'(x) \approx \frac{f(x_0+h) + f(x_0)}{h}.$$

This gives us the following result:

h	Forward-difference approximation of $f'(0)$	Absolute error
10^{-2}	1.00501671	0.005016708416794913
10^{-4}	1.00005000	$5.0001667140975314 \times 10^{-5}$
10^{-6}	1.00000050	$4.999621836532242 \times 10^{-7}$
10^{-8}	0.99999999	$6.07747097092215 \times 10^{-9}$
10^{-10}	1.00000008	$8.274037099909037 \times 10^{-8}$
10^{-12}	1.00008890	$8.890058234101161 \times 10^{-5}$

The error started to increase after $h = 10^{-8}$. This is because for very small h, $f(x) - h$ is very close to $f(x)$, by continuity. As a result, we subtract two numbers that are almost the same, which introduces rounding errors.

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2 Suppose $f(x)$ is smooth, and $f'''(x)$ is bounded. Given the values of $f(x_0 - h)$, $f(x_0)$, and $f(x_0 + 2h)$, derive an approximation of $f'(x_0)$ such that the error can be bounded by

$$Ch^2 \max_{x\in\mathbb{R}} |f'''(x)|.$$

Solution By Taylor expansion, we get

$$\begin{aligned}
f(x_0 - h) &= f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(\xi_0)h^3 \\
f(x_0) &= f(x_0) \\
f(x_0 + 2h) &= f(x_0) + 2f'(x_0)h + 2f''(x_0)h^2 + \frac{4}{3}f'''(\xi_1)h^3.
\end{aligned}$$

We wish to find A, B, C so that $(Af(x_0 - h) + Bf(x_0) + Cf(x_0 + 2h))/h = f'(x_0) + \mathcal{O}(h^3)$. This gives us the system

$$\begin{cases} A + B + C = 0 \\ -A + 2C = 1 \\ \frac{1}{2}A + 2C = 0. \end{cases}$$

By inspection, we get $A = -2/3$, $B = 1/2$, $C = 1/6$, so

$$f'(x_0) = \frac{-\frac{2}{3}f(x_0 - h) + \frac{1}{2}f(x_0) + \frac{1}{6}f(x_0 + 2h)}{h},$$

and the error is then given by

$$\left| -\frac{1}{9}f'''(\xi_0)h^2 + \frac{2}{9}f'''(\xi_1)h^2 \right| \leq \frac{1}{9}|f'''(\xi_0)|h^2 + \frac{2}{9}|f'''(\xi_1)|h^2 \leq \frac{1}{3}h^2 \max_{x\in\mathbb{R}} |f''(x)|,$$

as desired.

3 Suppose f is smooth on $[a,b]$. A simple numerical quadrature rule, which is called the midpoint rule, uses the value of f at the midpoint of the interval to approximate f on the whole interval. It writes as follows:

$$\int_a^b f(x)\,\mathrm{d}x \approx (b-a) f\left(\frac{a+b}{2}\right).$$

Prove that

$$\int_a^b f(x)\,\mathrm{d}x - (b-a) f\left(\frac{a+b}{2}\right) = \frac{(b-a)^3}{24} f''(\xi),$$

for some $\xi \in [a,b]$.

Solution Notice that

$$\int_a^b f(x)\,\mathrm{d}x - (b-a) f\left(\frac{a+b}{2}\right) = \int_a^b f(x) - f\left(\frac{a+b}{2}\right) \mathrm{d}x.$$

By Taylor expansion at $(a+b)/2$, we get

$$f(x) - f\left(\frac{a+b}{2}\right) = f'\left(\frac{a+b}{2}\right)\left(x - \frac{a+b}{2}\right) + \frac{1}{2} f''(\xi_x)\left(x - \frac{a+b}{2}\right)^2.$$

Note that since a and b are equidistance from $(a+b)/2$,

$$\int_a^b x - \frac{a+b}{2}\,\mathrm{d}x = \frac{1}{2}\left(x - \frac{a+b}{2}\right)^2\Bigg|_a^b = \frac{1}{2}\left(b - \frac{a+b}{2}\right)^2 - \frac{1}{2}\left(a - \frac{a+b}{2}\right)^2 = 0.$$

Moreover, since $(x-(a+b)/2)^2 \geq 0$, if we write $m = \min_{x\in[a,b]} f''(x)$ and $M = \max_{x\in[a,b]} f''(x)$, we have

$$\int_a^b \frac{1}{2} m\left(x - \frac{a+b}{2}\right)^2 \mathrm{d}x \leq \int_a^b \frac{1}{2} f''(\xi_x)\left(x - \frac{a+b}{2}\right)^2 \mathrm{d}x \leq \int_a^b \frac{1}{2} M\left(x - \frac{a+b}{2}\right)^2 \mathrm{d}x.$$

Since

$$\int_a^b \frac{1}{2} f''(t)\left(x - \frac{a+b}{2}\right)^2 \mathrm{d}x$$

is continuous as a function of t, by the intermediate value theorem, there exists $\xi \in [a,b]$ such that

$$\int_a^b \frac{1}{2} f''(\xi_x)\left(x - \frac{a+b}{2}\right)^2 \mathrm{d}x = \int_a^b \frac{1}{2} f''(\xi)\left(x - \frac{a+b}{2}\right)^2 \mathrm{d}x = \frac{1}{6} f''(\xi)\left(x - \frac{a+b}{2}\right)^3\Bigg|_a^b = \frac{(b-a)^3}{24} f''(\xi).$$

Thus,

$$\int_a^b f(x)\,\mathrm{d}x - (b-a) f\left(\frac{a+b}{2}\right) = \frac{(b-a)^3}{24} f''(\xi).$$

4 Let $[a, b] = [0, 3h]$ $(h > 0)$, and let f be smooth on $[0, 3h]$.

a. Derive the Newton-Cotes formula for

$$\int_0^{3h} f(x)\,\mathrm{d}x$$

using the data points $(0, f(0))$, $(h, f(h))$, and $(3h, f(3h))$.

b. Derive an error estimate of your quadrature rule in terms of

$$\max_{y\in[0,3h]} |f'''(y)|.$$

c. What is the degree of precision of this quadrature rule? Justify your answer.

Solution a. The Lagrange polynomials are given as follows:

$$\begin{aligned} L_0(x) &= \frac{(x-h)(x-3h)}{3h^2} \\ L_h(x) &= \frac{x(x-3h)}{-2h^2} \\ L_{3h}(x) &= \frac{x(x-h)}{6h^2}. \end{aligned}$$

Thus, the coefficients are given by

$$\begin{aligned} \int_0^{3h} L_0(x)\,\mathrm{d}x &= 0 \\ \int_0^{3h} L_h(x)\,\mathrm{d}x &= \frac{9h}{4} \\ \int_0^{3h} L_{3h}(x)\,\mathrm{d}x &= \frac{3h}{4}. \end{aligned}$$

The error term is given by

$$\frac{f'''(\xi_x)}{3!}x(x-h)(x-3h),$$

so the formula is

$$\int_0^{3h} f(x)\,\mathrm{d}x = \frac{9h}{4}f(h) + \frac{3h}{4}f(3h) + \int_0^{3h} \frac{f'''(\xi_x)}{3!}x(x-h)(x-3h)\,\mathrm{d}x.$$

b. We just need to bound the error term.

$$\left|\int_0^{3h} \frac{f'''(\xi_x)}{3!}x(x-h)(x-3h)\,\mathrm{d}x\right| \le \int_0^{3h} \max_{y\in[0,3h]}|f'''(y)| \cdot 3h \cdot 2h \cdot 3h\,\mathrm{d}x = 54h^4 \max_{y\in[0,3h]}|f'''(y)|.$$

c. The error is 0 whenever $f'''(x) \equiv 0$, so the degree is 2, since second degree polynomials have vanishing third derivatives.