Exercises: Numerical Calculus (Solutions)

1. (Derivation of the third-order forward difference formulan; solution by extrapolation)

   Let $V = f'(x)$ and $V_h = D_h^{[1f]}\{f\}(x)$, the first-order forward difference formula, for simplicity. Recall that

$$
\begin{aligned}
V_h &= V + \underbrace{\frac{f''(x)}{2}}_{b_1} h + \underbrace{\frac{f'''(x)}{6}}_{b_2} h^2 + \underbrace{\frac{f^{(4)}(x)}{24}}_{b_3} h^3 + O(h^4). \\
&= V + b_1 h + b_2 h^2 + b_3 h^3 + O(h^4).
\end{aligned}
$$

   To obtain a third-order method, the first two error terms $b_1 h$ and $b_2 h^2$ must be eliminated. To this end, we look for a linear combination of V_h, V_{2h}, and V_{3h} such that

$$
\alpha_1 V_h + \alpha_2 V_{2h} + \alpha_3 V_{3h} = V + O(h^3),
$$

   where α_j are to be determined. Writing the left-hand side out and collecting like-terms, we have

$$
\begin{aligned}
&\alpha_1 V_h + \alpha_2 V_{2h} + \alpha_3 V_{3h} \\
&\qquad = (\alpha_1 + \alpha_2 + \alpha_3) V + (\alpha_1 + 2\alpha_2 + 3\alpha_3) b_1 h + (\alpha_1 + 4\alpha_2 + 9\alpha_3) b_2 h^2 + O(h^3).
\end{aligned}
$$

   Matching coefficients, we obtain a linear system of three equations for the unknown weights α_j, for $j = 1, 2, 3$:

$$
\begin{array}{rcrcrcr}
\alpha_1 & + & \alpha_2 & + & \alpha_3 & = & 1 \\
\alpha_1 & + & 2\alpha_2 & + & 3\alpha_3 & = & 0 \\
\alpha_1 & + & 4\alpha_2 & + & 9\alpha_3 & = & 0
\end{array}
$$

   Solving the system (say by Gaussian elimination), we obtain

$$
\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -3 \\ 1 \end{bmatrix}.
$$

   Therefore, $3V_h - 3V_{2h} + V_{3h}$ is a new formula approximating V with third-order accuracy:

$$
\begin{aligned}
D_h^{[3f]}\{f\}(x) &= 3V_h - 3V_{2h} + V_{3h} \\
&= 3\frac{f(x+h) - f(x)}{h} - 3\frac{f(x+2h) - f(x)}{2h} + \frac{f(x+3h) - f(x)}{3h} \\
&= \frac{-11f(x) + 18f(x+h) - 9f(x+2h) + 2f(x+3h)}{6h}.
\end{aligned}
$$

2. (**LM** 14.1–12)

(a) Recall that

$$D_h^{[2c]}\{f\}(x) = f'(x) + c_2 h^2 + c_4 h^4 + O(h^6).$$

It follows that

$$D_{2h}^{[2c]}\{f\}(x) = f'(x) + 4c_2 h^2 + 16 c_4 h^4 + O(h^6),$$

and so

$$\frac{4D_h^{[2c]}\{f\}(x) - D_{2h}^{[2c]}\{f\}(x)}{3} = f'(x) - 4c_4 h^4 + O(h^6).$$

Therefore, the fourth-order centered difference formula is given by

$$\begin{aligned} D_h^{[4c]}\{f\}(x) &= \frac{4D_h^{[2c]}\{f\}(x) - D_{2h}^{[2c]}\{f\}(x)}{3} \\ &= \frac{4}{3}\frac{f(x+h) - f(x-h)}{2h} - \frac{1}{3}\frac{f(x+2h) - f(x-2h)}{4h} \\ &= \frac{f(x-2h) - 8f(x-h) + 8(x+h) - f(x+2h)}{12h}. \end{aligned}$$

(c) The second-order centered difference formula for $f''(x)$ is given by

$$D_h^2\{f\}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{1}{12}f''''(x)h^2 + O(h^4).$$

(See Lecture 33 or **LM** p.1766-7.) By a similar argument as above, we see that

$$\frac{4D_h^2\{f\}(x) - D_{2h}^2\{f\}(x)}{3} = f''(x) + O(h^4),$$

yields a fourth-order centered difference formula for $f''(x)$:

$$\begin{aligned} &(\text{4th-order CD for } f''(x)) \\ &= \frac{4D_h^2\{f\}(x) - D_{2h}^2\{f\}(x)}{3} \\ &= \frac{4}{3}\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{3}\frac{f(x+2h) - 2f(x) + f(x-2h)}{4h^2} \\ &= \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2}. \end{aligned}$$

3. (Approximating π again; **LM** 14.1–17) Applying the suggested change of variables $h = 1/n$ and Taylor-expanding about $h = 0$, we obtain

$$\begin{aligned} p_n &= \frac{\sin(\pi h)}{h} = \pi - \frac{\pi^3}{6}h^2 + \frac{\pi^5}{120}h^4 + \cdots = \pi + a_1 h^2 + a_2 h^4 + \cdots \\ P_n &= \frac{\tan(\pi h)}{h} = \pi + \frac{\pi^3}{3}h^2 + \frac{2\pi^5}{15}h^4 + \cdots = \pi + b_1 h^2 + b_2 h^4 + \cdots. \end{aligned}$$

Note that both are second-order accurate. The average of the two algorithms gives another second-order algorithm as h^2 term survives:

$$\mathfrak{B}_n = \pi + c_1 h^2 + c_2 h^4 + \cdots,$$

where

$$c_1 = \frac{a_1 + b_1}{2} = \frac{\pi^3}{12}, \quad c_2 = \frac{a_2 + b_2}{2} = \frac{17\pi^5}{240}.$$

One way to obtain a fourth-order algorithm is to extrapolate p_n and P_n. Calculation shows that

$$\mathfrak{R}_n \equiv \frac{2}{3}p_n + \frac{1}{3}P_n = \pi + \frac{\pi^5}{20}h^4 + \cdots .$$

The above is not the only way. One may, for instance, construct another fourth-order algorithm by extrapolating $\mathfrak{B}_\mathfrak{n}$ and $\mathfrak{B}_{\mathfrak{n}/2}$:

$$\mathfrak{S}_n \equiv \frac{4}{3}\mathfrak{B}_n - \frac{1}{3}\mathfrak{B}_{n/2} = \pi - \frac{17\pi^5}{60}h^4 + \cdots .$$