Section 4

Numerical Differentiation and Integration

Numerical differentiation

Recall the definition of derivative is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

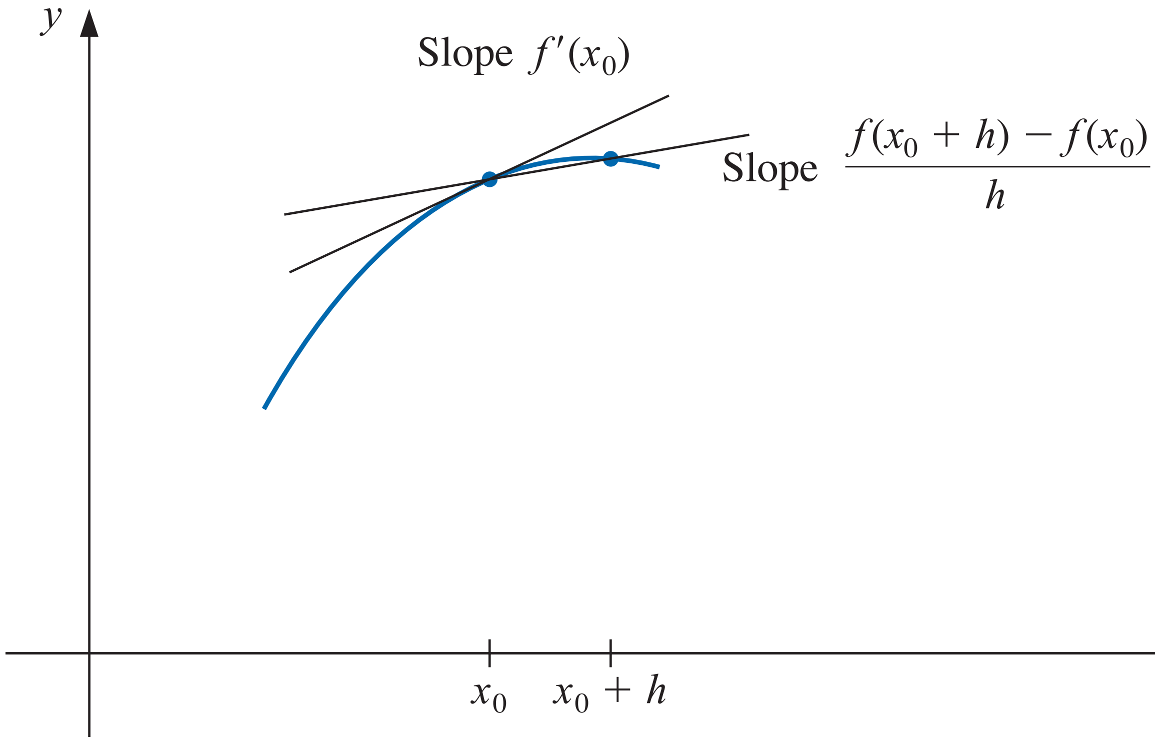
We can approximate $f'(x_0)$ by

$$\frac{f(x_0 + h) - f(x_0)}{h}, \quad \text{for some small } h$$

Numerical differentiation

Approximate $f'(x_0)$ by

$$\frac{f(x_0+h)-f(x_0)}{h}, \quad \text{for some small } h$$



How to quantify the error of this approximation?

Numerical differentiation

If $f \in C^2$, then Taylor's theorem says $\exists\, \xi \in (x_0, x_0 + h)$ s.t.

$$\begin{aligned} f(x_0 + h) &= f(x_0) + f'(x_0)h + \frac{1}{2} f''(\xi) h^2 \\ \iff \quad f'(x_0) &= \frac{f(x_0 + h) - f(x_0)}{h} - \frac{1}{2} f''(\xi) h \end{aligned}$$

If $\exists\, M > 0$ s.t. $|f''(x)| \leq M$ for all x near x_0, then

$$\text{Error} = \left| f'(x_0) - \frac{f(x_0 + h) - f(x_0)}{h} \right| = \left| \frac{1}{2} f''(\xi) h \right| \leq \frac{Mh}{2}$$

So the error is of order "$O(h)$".

Example

Example (Error of numerical differentiations)

Let $f(x) = \ln(x)$ at $x_0 = 1.8$. Use $h = 0.1, 0.05, 0.01$ to approximate $f'(x_0)$. Determine the approxiamtion errors.

Solution. We compute for $h = 0.1, 0.05, 0.01$ that

$$\frac{f(1.8+h) - f(1.8)}{h} = \frac{\ln(1.8+h) - \ln(1.8)}{h}$$

Then $|f''(x)| = |-\frac{1}{x^2}| \le \frac{1}{1.8^2} =: M$ for all $x > 1.8$. Error is bounded by $\frac{Mh}{2}$.

Numerical differentiation

Example (Error of numerical differentiations)

Let $f(x) = \ln(x)$ at $x_0 = 1.8$. Use $h = 0.1, 0.05, 0.01$ to approximate $f'(x_0)$. Determine the approxiamtion errors.

Solution (cont.)

h	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{Mh}{2}$
0.10	0.5406722	0.0154321
0.05	0.5479795	0.0077160
0.01	0.5540180	0.0015432

The exact value is $f'(1.8) = \frac{1}{1.8} = 0.55\bar{5}$.

Three-point endpoint formula

Recall the Lagrange interpolating polynomial for $x_0, \ldots, x_n$ is

$$f(x) = \sum_{k=0}^{n} f(x_k) L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

Suppose we have $x_0, x_1 \triangleq x_0 + h, x_2 \triangleq x_0 + 2h$, then

$$f(x) = \sum_{k=0}^{2} f(x_k) L_k(x) + \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))$$

where $\xi(x) \in (x_0, x_0 + 2h)$.

Three-point endpoint formula

Take derivative w.r.t. x of

$$f(x) = \sum_{k=0}^{2} f(x_k) L_k(x) + \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))$$

and set $x = x_0$ yields[4] the **Three-point endpoint formula**:

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

where $\xi(x_0) \in (x_0, x_0+2h)$.

[4] Note that $\frac{(x-x_0)(x-x_1)(x-x_2)}{6} \frac{\mathrm{d} f^{(3)}(\xi(x))}{\mathrm{d}x}\big|_{x=x_0} = 0$.

Three-point midpoint formula

Suppose we have $x_{-1} = x_0 - h, x_0, x_1 \triangleq x_0 + h$, then

$$f(x) = \sum_{k=-1}^{1} f(x_k) L_k(x) + \frac{(x - x_{-1})(x - x_0)(x - x_1)}{6} f^{(3)}(\xi_1)$$

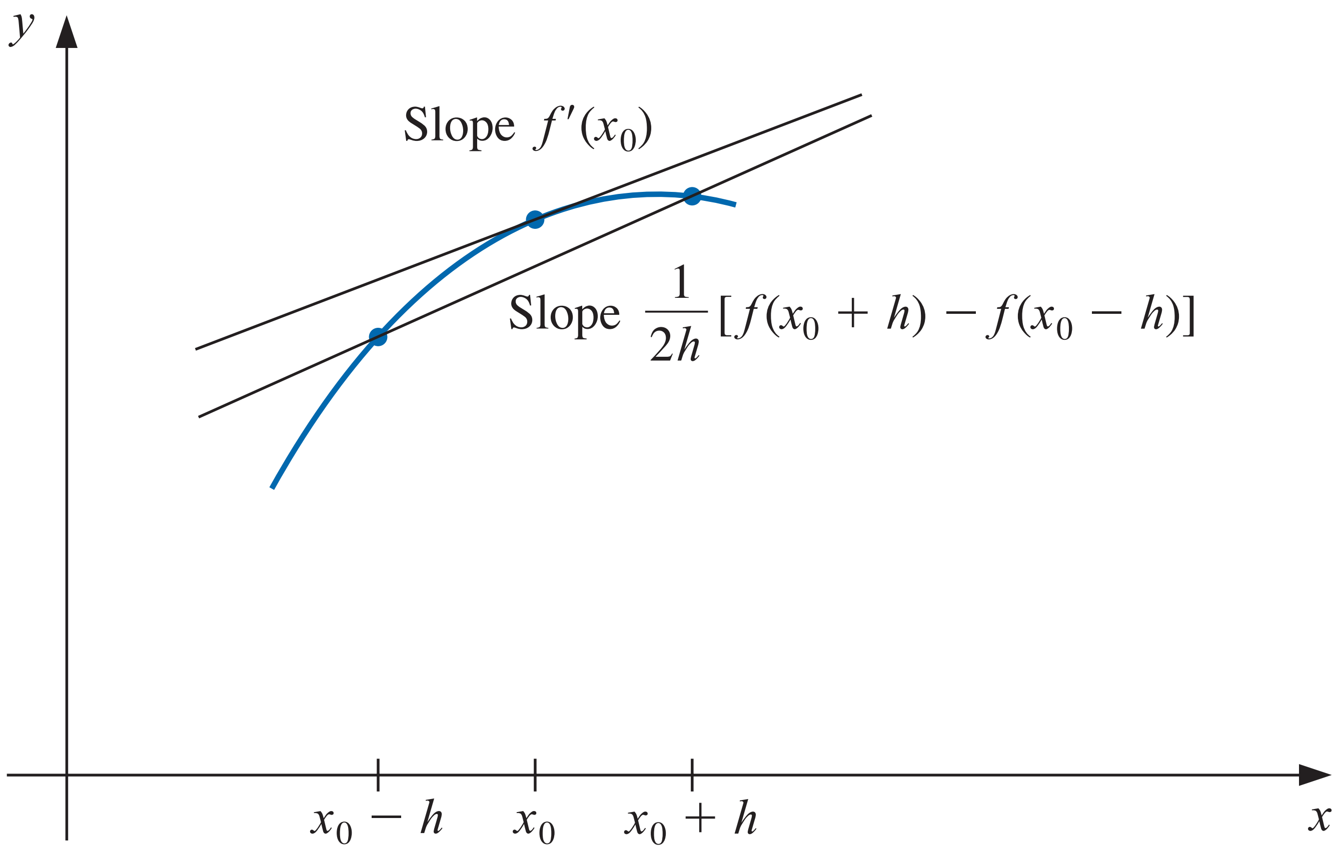
where $\xi_1 \in (x_0 - h, x_0 + h)$.

Take derivative w.r.t. x, and set $x = x_0$ yields **Three-point midpoint formula**:

$$f'(x_0) = \frac{1}{2h}\left[f(x_0 + h) - f(x_0 - h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Three-point midpoint formula

Illustration of **Three-point midpoint formula**:



Five-point midpoint formula

We can also consider $x_k = x_0 + kh$ for $k = -2, -1, 0, 1, 2$, then

$$f(x) = \sum_{k=-2}^{2} f(x_k) L_k(x) + \frac{\prod_{k=-2}^{2}(x - x_k)}{5!} f^{(5)}(\xi_0)$$

where $\xi_0 \in (x_0 - 2h, x_0 + 2h)$.

Show that you can get the **Five-point midpoint formula**:

$$f'(x_0) = \frac{1}{12h}\left[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^4}{30} f^{(5)}(\xi_0)$$

Five-point endpoint formula

We can also consider $x_k = x_0 + kh$ for $k = 0, 1, \ldots, 4$, then

$$f(x) = \sum_{k=0}^{4} f(x_k) L_k(x) + \frac{\prod_{k=0}^{4}(x - x_k)}{5!} f^{(5)}(\xi_0)$$

where $\xi_0 \in (x_0, x_0 + 4h)$.

Show that you can get the **Five-point endpoint formula**:

$$f'(x_0) = \frac{1}{12h}\Big[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h) \Big] + \frac{h^4}{5} f^{(5)}(\xi_0)$$

Example

Example (3-point and 5-point formulas)

Use the values in the table to find $f'(2.0)$:

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Compare your result with the true value $f'(2) = 22.167168$.

Hint: Use three-point midpoint formula with $h = 0.1, 0.2$, endpoint with $h = \pm 0.1$, and five-pint midpoint formula with $h = 0.1$.

Second derivative midpoint formula

Expand f in a third Taylor polynomial about a point x_0 and evaluate at $x_0 + h$ and $x_0 - h$:

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$
$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4$$

where $\xi_{\pm 1}$ is between x_0 and $x_0 \pm h$.

Adding the two and using IVT $f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$ (assuming $f \in C^4$) yield:

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0 - h) - 2f(x_0) + f(x_0 + h)\right] - \frac{h^2}{12}f^{(4)}(\xi)$$

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

Roundoff error instability

Recall we have three-point midpoint approximation

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

for $\xi_1 \in (x_0 - h, x_0 + h)$.

Will we get better accuracy as $h \to 0$? Not necessarily.

Round-off error instability

In numerical computations, round-off error is inevitable:

$$f(x_0 + h) = \tilde{f}(x_0 + h) + e(x_0 + h)$$
$$f(x_0 - h) = \tilde{f}(x_0 - h) + e(x_0 - h)$$

Hence we're approximating $f'(x_0)$ by $\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}$ with error:

$$f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} = \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Suppose $|e(x)| \leq \varepsilon$, $\forall x$, then the error bound is:

$$\left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

So the error does not go to 0 as $h \to 0$, due to the round-off error.

Richardson's extrapolation

Goal: generate high-accuracy results by *low-order* formula.

Suppose we have formula $N_1(h)$ to approximate M with [5]

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

with some unknown $K_1, K_2, K_3, \ldots$.

For h small enough, the error is dominated by $K_1 h$, then

$$M = N_1\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots$$

[5] E.g., $M = f'(x_0)$ and $N_1(h) = \frac{f(x_0+h)-f(x_0)}{h}$.

Richardson's extrapolation

Therefore

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots$$

Define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

then M can be approximated by $N_2(h)$ with order $O(h^2)$:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots$$

Example

Example (Richardson's extrapolation)

Let $f(x) = \ln(x)$. Approximate f at $x = 1.8$ with forward difference using $h = 0.1$ and $h = 0.05$. Then approximate using $N_2(0.1)$.

Solution. We know the forward difference is $O(h)$, and

$$N_1(h) = f(x_0) - \frac{f(x_0+h) - f(x_0)}{h} = \begin{cases} 0.5406722, & \text{for } h = 0.1 \\ 0.5479795, & \text{for } h = 0.05 \end{cases}$$

$$N_2(0.1) = N_1(0.05) + (N_1(0,05) - N_1(0.1)) = 0.555287.$$

Formula	$N_1(0.1)$	$N_1(0.05)$	$N_2(0.1)$
Error	1.5×10^{-2}	7.7×10^{-3}	2.7×10^{-4}

Richardson's extrapolation

Suppose $M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \dots$, then for $j = 2, 3, \dots$, we have $O(h^{2j})$ approximation:

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}$$

We can show the order of generating these $N_j(h)$ [6]:

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
1: $N_1(h)$			
2: $N_1(\frac{h}{2})$	3: $N_2(h)$		
4: $N_1(\frac{h}{4})$	5: $N_2(\frac{h}{2})$	6: $N_3(h)$	
7: $N_1(\frac{h}{8})$	8: $N_2(\frac{h}{4})$	9: $N_3(\frac{h}{2})$	10: $N_4(h)$

[6] Exercise: write a computer program for Richardson's extrapolation.

Example

Example (Richardson's extrapolation)

Consider approximation of $f'(x_0)$:

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots$$

Find the approximation errors of order $O(h^2), O(h^4), O(h^6)$ for $f'(2.0)$ when $f(x) = xe^x$ and $h = 0.2$.

Solution. We have $O(h^2)$ approximation

$$f'(x_0) = N_1(h) - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots$$

where $N_1(h) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right]$. Then compute $N_1(h), N_1(\frac{h}{2}), N_2(h), N_1(\frac{h}{4}), N_2(\frac{h}{2}), \ldots$ in order.