# 5. Differentiation

# Derivatives

Numerical methods can be used to find the value of derivatives, if they can't be obtained analytically.
With *finite difference*, we use approximate formulas that are exact in the limit of a size parameter going to zero.

# Centered finite difference for the first derivative

Subtracting Taylor series,

$$
\begin{array}{rlll}
f(x+h) = f(x) & +hf'(x) + \frac{h^2}{2}f''(x) & +\frac{h^3}{6}f'''(\xi_+) \\
f(x-h) = f(x) & -hf'(x) + \frac{h^2}{2}f''(x) & -\frac{h^3}{6}f'''(\xi_-) \\
\hline
f(x+h) - f(x-h) = & 2hf'(x) & +\frac{h^3}{3}f'''(\xi)
\end{array}
$$

$$\text{so } f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

with absolute error $\frac{h^2}{6}|f'''(\xi)|$, or $|\frac{h^2}{6}f'''(x) + \frac{h^4}{120}f^{(5)}(x) + \frac{h^6}{5040}f^{(7)}(x) + \ldots|$. Since the error is $\mathcal{O}(h^2)$, this formula is said to be second-order accurate.

More accurate (higher order) centered finite difference formulas can be derived by adding, e.g., $f(x-2h)$ and $f(x+2h)$ to the formula, which enables canceling out more initial terms in the Taylor series.

# Centered finite difference for the second derivative

Adding Taylor series,

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) \quad + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_+) \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) \quad - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_-)
\end{aligned}
$$

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$$
f(x+h) + f(x-h) - 2f(x) = h^2 f''(x) \qquad + \frac{h^4}{12}f^{(4)}(\xi)
$$

$$
\text{so } f''(x) \approx \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}
$$

with absolute error $\frac{h^2}{12}|f^{(4)}(\xi)|$. Again, the error is $\mathcal{O}(h^2)$, so this formula is second-order accurate.

# Forward finite difference for the first derivative

$$
\begin{array}{rcll}
f(x+h) &=& f(x) & +hf'(x) + \frac{h^2}{2}f''(x) \quad +\frac{h^3}{6}f'''(\xi_1) \\
f(x+2h) &=& f(x) & +2hf'(x) + 2h^2 f''(x) \quad +\frac{4}{3}h^3 f'''(\xi_2) \\
\hline
4f(x+h) - f(x+2h) &=& 3f(x) & +2hf'(x) \qquad\qquad -\frac{2}{3}h^3 f'''(\xi)
\end{array}
$$

$$\text{so } f'(x) \approx \frac{4f(x+h) - f(x+2h) - 3f(x)}{2h}$$

This is a non-centered finite-difference formula that is second-order accurate – absolute error is $\frac{2}{3}h^2|f'''(\xi)|$. A backward finite-difference formula $f'(x) \approx \frac{-4f(x-h)+f(x-2h)+3f(x)}{2h}$ can similarly be derived, with the same level of accuracy.

# Example

Let $f(x) = \sqrt{x}$. We can estimate $f'(1)$ using the finite difference formulas with $h = 0.1$ as 0.50063 (centered), 0.49895 (forward), 0.49847 (backward). Similarly, we can estimate $f''(1)$ as $-0.25079$

Exercise: check these values and determine the fractional error of each compared to the analytic derivatives.

# Truncation and roundoff errors

Taking the $\mathcal{O}(h^2)$ centered finite difference first-derivative formula as an example,
Absolute truncation error $\sim \frac{h^2}{6}|f'''(x)|$, increasing with $h$
Absolute roundoff error $\sim \frac{\epsilon|f(x)|}{2h}$, decreasing with $h$
Total error $\sim$ truncation + roundoff $\sim \frac{h^2}{6}|f'''(x)| + \frac{\epsilon|f(x)|}{2h}$
We can take the derivative of the total error expression with respect to $h$ and set it to 0 to estimate where the total error is minimum. The result is $h_{\text{optim}} \sim \sqrt[3]{\frac{3}{2}\left|\frac{f(x)}{f'''(x)}\right|\epsilon}$, so if we take $h$ smaller than $\mathcal{O}(\epsilon^{1/3})$, roundoff error will likely result in the finite-difference formula giving inaccurate results.

# Combining different finite difference estimates to reduce truncation error

Consider the series form of the centered finite difference first-derivative formula truncation error:

$$\left|\frac{h^2}{6}f'''(x) + \frac{h^4}{120}f^{(5)}(x) + \frac{h^6}{5040}f^{(7)}(x) + \ldots\right|$$

If we calculate the formula results for two $h$ values, $h_1$ and $h_2 = \frac{h_1}{2}$, we can cancel out the first (lowest-order) error term by combining the two results as $r = \frac{4}{3}r_2 - \frac{1}{3}r_1$. The error series for $r$ is

$$\left|\frac{(\frac{4}{3}h_2^2 - \frac{1}{3}h_1^2)}{6}f'''(x) + \frac{(\frac{4}{3}h_2^4 - \frac{1}{3}h_1^4)}{120}f^{(5)}(x) + \frac{(\frac{4}{3}h_2^6 - \frac{1}{3}h_1^6)}{5040}f^{(7)}(x) + \ldots\right|$$
$$= \left|\frac{-\frac{1}{4}h_1^4}{120}f^{(5)}(x) + \frac{-\frac{5}{16}h_1^6}{5040}f^{(7)}(x) + \ldots\right|$$

We can repeat this process to then cancel out more terms ($h^4, h^6, \ldots$), improving the accuracy for small enough $h$.

# Richardson extrapolation

This is systematized in an algorithm as follows:
Given a function $f$, where $D_0^0$ is the derivative estimate using centered finite difference with step size $h_0$, i.e.
$D_0^0 = \frac{f(x+h_0)-f(x-h_0)}{2h_0}$
Estimates with smaller step size are obtained as
$D_i^0 = \frac{f(x+h_i)-f(x-h_i)}{2h_i}$, with $h_i = \frac{h_0}{2^i}, i = 1, 2, \ldots$
Combined estimates, which cancel out terms in the error series, are obtained as

$$D_i^j \equiv \frac{4^j}{4^j - 1} D_{i+1}^{j-1} - \frac{1}{4^j - 1} D_i^{j-1},$$

for $j = 1, 2, \ldots$

# Example

For $f(x) = \sqrt{x}$, we can estimate $f'(1)$ using Richardson extrapolation with $h_0 = 0.4$ via

$D_0^0 = \frac{\sqrt{1.4}-\sqrt{0.6}}{0.8} = 0.51077$
$D_1^0 = \frac{\sqrt{1.2}-\sqrt{0.8}}{0.4} = 0.50254$
$D_0^1 = \frac{4}{3}D_1^0 - \frac{1}{3}D_0^0 = 0.49980$
$D_2^0 = \frac{\sqrt{1.1}-\sqrt{0.9}}{0.2} = 0.50063$
$D_1^1 = \frac{4}{3}D_2^0 - \frac{1}{3}D_1^0 = 0.49999$
$D_0^2 = \frac{16}{15}D_1^1 - \frac{1}{15}D_0^1 = 0.500001$

If we reached a certain maximum $j \geq 1$, we can estimate the absolute error in our highest-order estimate $D_0^j$ using the difference between it and the second-best estimate: $|D_0^j - D_1^{j-1}|$