Differentiation

Given a function f, the derivative f' of f is defined as

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

A difference approximation of the derivative is

$$f'(x_0) \approx \underbrace{\frac{f(x_0+h) - f(x_0)}{h}}_{D_h(x_0)}.$$

Error analysis I

Write $f(x) = p_1(x) + R_1(x)$. We have

$$f(x) = f(x_0) + f(x_0)'(x - x_0) + R_1(x).$$

Hence

$$f(x_0 + h) = f(x_0) + f'(x_0)h + R_1(x_0 + h).$$

Rearranging, we get

$$f'(x_0) = \underbrace{\frac{f(x_0 + h) - f(x_0)}{h}}_{D_h(x_0)} - \frac{1}{h} R_1(x_0 + h).$$

Hence

$$\underbrace{\left| \frac{f(x_0 + h) - f(x_0)}{h} - f'(x_0) \right|}_{e_h(x)} \leq \frac{1}{h} |R_1(x_0 + h)|$$

Error analysis II

Using the error bound for Taylor polynomials, we have

$$|R_1(x_0+h)| \le B_1(x_0+h) = \frac{|x_0+h-x_0|^2}{2!} \max_{\zeta\in[x_0,x_0+h]} |f''(\zeta)|.$$

Let $C_2(x_0,\bar{h}) = \max_{\zeta\in[x_0,x_0+\bar{h}]} |f''(\zeta)|$. Then for any $\bar{h}>0$, we have

$$\begin{aligned}|R_1(x_0+h)| \le B_1(x_0+h) &= \frac{|x_0+h-x_0|^2}{2!} C_2(x_0,\bar{h}) \\ &= \frac{C_2(x_0,\bar{h})}{2} h^2 \quad \text{for all } h\in(0,\bar{h}).\end{aligned}$$

We see that $\boxed{e_h(x) = \frac{1}{h}|R_1(x_0+h)| = \mathcal{O}(h) \text{ as } h\downarrow 0}$.

Example

Let $f(x) = \frac{x^4}{4}$. We use the D_h to approximate the derivative of f at $x_0 = 2$.

We have $f(x_0) = 4$, $f'(x_0) = x_0^3 = 8$.

h	$D_h(x_0)$	$e_h(x_0)$
1	16.25	8.25
10^{-1}	8.6203	0.6203
10^{-2}	8.0602	0.0602
10^{-3}	8.0060	0.0060
$\vdots$		
10^{-8}	8.0000	4.020×10^{-8}
10^{-9}	8.0000	6.619×10^{-7}

The error decreases with order $\mathcal{O}(h)$ as $h \downarrow 0$ roughly until 10^{-8}.

Second-order approximation I

Observe that

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + R_2(x_0+h)$$
$$f(x_0+h) = f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2}h^2 + R_2(x_0-h),$$

and

$$f(x_0+h) - f(x_0-h) = 2hf'(x_0) + R_2(x_0+h) - R_2(x_0-h).$$

Therefore,

$$\underbrace{\frac{f(x_0+h) - f(x_0-h)}{2h}}_{\hat{D}_h(x_0)} = f'(x_0) + \frac{1}{2h}\left(R_2(x_0+h) - R_2(x_0-h)\right)$$

Second-order approximation II

The error in this case is

$$\underbrace{\left|\frac{f(x_0+h)-f(x_0-h)}{2h}-f'(x_0)\right|}_{\hat{e}_h(x_0)} = \frac{1}{2h}\left|R_2(x_0+h)-R_2(x_0-h)\right|.$$

Let $C_3(x_0,\bar{h}) = \max_{\zeta\in[x_0-\bar{h},x_0+\bar{h}]}|f'''(\zeta)|$. Following the same procedure as before, we have

$$|\hat{e}_h(x_0)| \le \frac{C_3(x_0,\bar{h})}{3!}h^2 \quad \text{for all } h\in(0,\bar{h}).$$

That is, $\boxed{\hat{e}_h(x_0)=\mathcal{O}(h^2)}$.

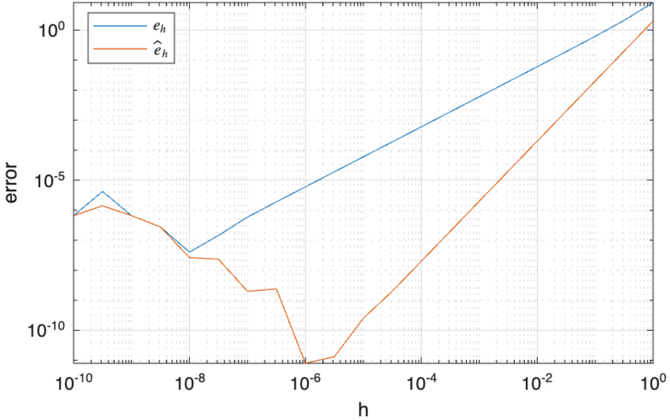
Example

h	$\hat{D}_h(x_0)$	$\hat{e}_h(x_0)$
1	10	2
10^{-1}	8.0200	0.0200
10^{-2}	8.0000	0.0002
10^{-3}	8.0000	2.0×10^{-6}
10^{-4}	8.0000	2.0×10^{-8}
10^{-5}	8.0000	2.5×10^{-10}
10^{-6}	8.0000	8.0×10^{-12}
10^{-7}	8.0000	2.0×10^{-9}

The error decreases with order $\mathcal{O}(h^2)$ as $h \downarrow 0$ roughly until 10^{-5}.

Plotting the results

Due to the polynomial order of the error in relation to h, e_h and $\hat{E}_h$ vs. h should be plotted in a log-log plot.



The slope of the linear portion in the log-log plot corresponds to the order of the derivative approximation.

Catastrophic subtraction I

Why the order estimate doesn't hold in for h too small

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

Suppose $h = 10^{-8}$. If $f(x_0) = 0.a_1a_2a_3a_4\cdots a_{16}$, $f'(x_0) = 0.b_1b_2b_3b_4\cdots b_{16}$ and $\frac{f''(x_0)}{2} = 0.c_1c_2c_3c_4\cdots c_{16}$, then on a 16-digit machine

$$
\begin{aligned}
&f(x) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 \\
&= 0.a_1a_2a_3a_4\cdots a_{16} + 0.00000000b_1b_2b_3b_4\cdots b_8 \\
&\qquad + 0.0000000000000000c_1\cdots c_{16} \\
&= 0.a_1a_2\cdots a_8[a_9+b_1][a_{10}+b_2]\cdots[a_{16}+b_8].
\end{aligned}
$$

Catastrophic subtraction II

Why the order estimate doesn't hold in for h too small

Therefore, the numerator in D_h is $0.00000000 b_1 b_2 b_3 b_4 \cdots b_8$, and the digits b_9 through b_{16} are lost with $h = 10^{-8}$.
D_h in this case is computed to be $0.b_1 b_2 \cdots b_8 xxxxxxxx$ where the last 8 digits are unreliable.

Fourth-order approximation

By combining $\hat{D}_{2h}(x_0)$ and $\hat{D}_h(x_0)$ to cancel out even higher order terms in the Taylor expansion, we get

$$\begin{aligned}\check{D}(x_0) &= \frac{4\hat{D}_h(x_0) - \hat{D}_{2h}(x_0)}{3} \\ &= \frac{8[f(x_0+h) - f(x_0-h)] - [f(x_0+2h) - f(x_0-2h)]]}{12h}.\end{aligned}$$

This is an $\mathcal{O}(h^4)$ approximation of the derivative.

When computing derivatives, it is useful to measure the computational cost using "FEs", i.e. the number of function evaluations.

D_h requires 2 FEs (or 1 if $f(x)$ is reused) and is $\mathcal{O}(h)$.
$\hat{D}_h$ requires 2 FEs and is $\mathcal{O}(h^2)$.
$\breve{D}_h$ requires 4 FEs and is $\mathcal{O}(h^4)$.