5.1 Numerical Differentiation

We develop $\boxed{\text{finite difference}}$ formulas for approximating derivatives.

5.1.1 Finite Difference Formulas

Recall from Calculus, $$\boxed{f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}}$$

Using Taylor's Theorem (w/ "center": x) we have:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi)$$

for some $\xi \in (x, x+h)$. This equation implies the following:

Two-point forward-difference formula

$$\boxed{f'(x) = \frac{f(x+h)-f(x)}{h} - \underbrace{\frac{h}{2} f''(\xi)}_{\text{"error"}}}$$ where $\xi \in (x, x+h)$.

(*) Note that for small h this gives us a <u>small error</u> quantity. We call the two-point forward-difference formula a <u>first order</u> method for approximating $f'(x)$.

In general, we say a method is $\boxed{\text{"order } n\text{"}}$ if the error is $\boxed{\mathcal{O}(h^n)}$, for an <u>approximation</u>.

The idea here is that for <u>first order</u> approximation, the <u>error</u> is <u>proportional</u> to h as $h \to 0$.

Ex. Use the Two-point forward-diff'ce formula with $h = 0.1$ to approximate $f'(x)$, where $f(x) = \frac{1}{x}$ @ $x = 2$.

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} = \underbrace{\frac{\frac{1}{2.1} - \frac{1}{2}}{0.1}}_{\text{slope of secant line}} \approx \boxed{-.2381}$$

True value: $f'(x) = -\frac{1}{x^2}$ @ $x = 2$ → error: $-.2381 - (-.2500) = \boxed{.0119}$

Compare the error to the predicted error given by: $\frac{h f''(c)}{2}$ for $c \in (2, 2.1)$

$f''(x) = \frac{2}{x^3}$ → error is b/w $(0.1)\cdot 2^{-3} \approx \underline{.0125}$ & $(0.1)(2.1)^{-3} \approx \underline{.0108}$,

which is consistent with our result.

· Next we consider a means to develop a second-order formula.

By Taylor's Theorem:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(c_1)$$

$$\ominus \quad f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(c_2)$$

where: $c_1 \in (x, x+h)$, $c_2 \in (x-h, x)$

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{6}\left[f'''(c_1) - f'''(c_2)\right]$$

→ Solving for $f'(x)$:

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \underbrace{\frac{h^2}{12}\left[f'''(c_1) - f'''(c_2)\right]}_{\text{"error"}}}$$

Before issuing a "nice", clean answer, we would like to first consolidate the error terms above. To do so, we use an extension of the IMVT from calculus.

Theorem Generalized Intermediate Value Theorem.

Let f be a continuous function on $[a,b]$. Let $x_1,\dots,x_n$ be points in $[a,b]$ & $a_1,\dots,a_n > 0$. Then there exists a number $\underline{c}$ in (a,b) such that: $\boxed{(a_1 + \dots + a_n)\, f(c) = a_1 f(x_1) + \dots + a_n f(x_n)}$

Proof Let $f(x_i)$ be the minimum & $f(x_j)$ the maximum of the n function values. Then:

$$a_1 f(x_i) + \dots + a_n f(x_i) \le a_1 f(x_1) + \dots + a_n f(x_n) \le a_1 f(x_j) + \dots + a_n f(x_j)$$

which implies that:

$$f(x_i) \le \frac{a_1 f(x_1) + \dots + a_n f(x_n)}{a_1 + \dots + a_n} \le f(x_j)$$

By the $\boxed{\text{IMVT}}$, there exists a number $c \in (x_i, x_j)$ such that

$$\boxed{f(c) = \frac{a_1 f(x_1) + \dots + a_n f(x_n)}{a_1 + \dots + a_n}}. \quad \square$$

Observe that the Generalized IMVT (above) indicates that we may consolidate the error terms from before, whereupon:

Three-point centered difference formula

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(c)} \qquad x-h < c < x+h$$

"Order Two" approximation!

Ex. Use the Three-point central difference formula w/ $h=0.1$

To approximate $f'(x)$ with $f(x)=\frac{1}{x}$, $x=2$.

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h} = \frac{\frac{1}{2.1}-\frac{1}{1.9}}{0.2} \approx \boxed{-.2506}$$

The error here is $\boxed{.0006}$, a significant improvement on the two-point forward difference used previously.

Q: How do we numerically approximate higher derivatives?

A: Simple: use Taylor series, as usual, & algebraically eliminate $f'(x)$ terms, & solve for $f''(x)$.

Recall:

$$f(x+h) = f(x) + h\cancel{f'(x)} + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_1)$$

$$\oplus\quad f(x-h) = f(x) - h\cancel{f'(x)} + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_2)$$

$$\downarrow$$

$$f(x+h)+f(x-h) - 2f(x) = h^2 f''(x) + \frac{h^4}{24}\left[f^{(4)}(c_1)+f^{(4)}(c_2)\right]$$

Once again we need the Generalized IMVT ...

Three-Point Centered-Difference Formula for Second Derivative

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

where $c \in (x-h, x+h)$.

A caveat for numerical differentiation (*)

Each of the previous methods in §5.1 relies, fundamentally, on <u>subtracting/dividing nearly equal quantities</u>. Unfortunately, when using floating point arithmetic (i.e. performing computations on a computer with a finite $\boxed{\varepsilon_{mach}}$) such computations can lead to significant deterioration in the quality of approximations due to <u>loss of significance</u>. We illustrate this phenomenon with an example.

$\boxed{\text{Ex.}}$ Approximate $f'(x)$ when $f(x) = e^x$ @ $x=0$.

<u>Two-point formula:</u>

$$f'(x) \approx \frac{e^{x+h} - e^x}{h}$$

<u>Three point:</u>

$$f'(x) \approx \frac{e^{x+h} - e^{x-h}}{2h} \quad (\text{set } x=0)$$

h	error for 2-point	error for 3-point
10^{-1}	$-.0517\ldots$	$-.001667$
10^{-2}	$-.00501$	$-.00001666$
$\vdots$	$\vdots$	$\vdots$
10^{-9}	$-.00000827$	$-.0000002722$

error increased

error increased

Why does this happen? Consider 3-point error:

$$f'(x) - \hat{f}'(x) = f'(x) - \frac{f(x+h) + \epsilon_1 - (f(x-h) + \epsilon_2)}{2h} = \cdots$$

$$= \underbrace{f'(x) - \frac{f(x+h) - f(x-h)}{2h}}_{\text{correct formula}} + \underbrace{\frac{\epsilon_2 - \epsilon_1}{2h}}_{\text{rounding error}}$$

<u>Moral</u>: when <u>h becomes too small</u> error can actually increase!

Extrapolation

Assume that we have an $\boxed{\text{order } n}$ formula $F(h)$ for approximating the quantity Q. This tells us that:

$$\boxed{Q \approx F(h) + \underbrace{Kh^n}_{\text{error}}}$$

, where K is roughly constant over the range of h. $(*)$

As before, we would like to algebraically manipulate this formula of order n so as to produce a higher order approximation. The key insight here is that we use $\boxed{\frac{h}{2}}$ instead of h, as this should reduce the error from a constant times h^n to a constant times $\left(\frac{h}{2}\right)^n$, i.e. we reduce the error by a factor of 2^n.

That is to say, we expect:

$$Q - F\left(\frac{h}{2}\right) \approx \frac{1}{2^n}\left[Q - F(h)\right]$$

Solving for Q...

Extrapolation for order n formula ("Richardson Extrapolation")

$$\boxed{Q \approx \frac{2^n F(h/2) - F(h)}{2^n - 1}}$$

— This formula typically renders a higher-order approximation of Q.

why?

$$Q = \underbrace{F_n(h)}_{n\text{-order formula}} + Kh^n + \mathcal{O}\left(h^{n+1}\right)$$

Now we cut h in half.

$$Q = F_n\left(\tfrac{h}{2}\right) + K\left(\frac{h^n}{2^n}\right) + \mathcal{O}(h^{n+1})$$

& The extrapolated version which we call $F_{n+1}(h)$ satisfies:

$$\underbrace{F_{n+1}(h)}_{\text{"Q"}} = \frac{2^n F_n(h/2) - F_n(h)}{2^n - 1}$$

$$= \frac{2^n\left(Q - Kh^n/2^n - \mathcal{O}(h^{n+1})\right) - \left(Q - Kh^n - \mathcal{O}(h^{n+1})\right)}{2^n - 1}$$

$$= Q + \frac{-Kh^n + Kh^n + \mathcal{O}(h^{n+1})}{2^n - 1} = \underline{Q + \mathcal{O}(h^{n+1})}. \square$$

This shows that $F_{n+1}(h)$ is at least an order $n+1$ formula for approximating the quantity Q.

$\boxed{\text{Ex.}}$ Apply the extrapolation formula for second-order centered-diff. $F_2(h)$ for $f'(x)$

$$F_4(x) = \frac{2^2 F_2(h/2) - F_2(h)}{2^2 - 1} = \left[4 \cdot \frac{f(x+h/2) - 2f(x) + f(x-h/2)}{h^2/4} - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}\right] \Big/ 3$$

$$= \boxed{\frac{-f(x-h) - 8f(x-h/2) + 8f(x+h/2) - f(x+h)}{6h}}$$

→ A five-point centered differ formula!
(This is an order 4 formula)