Finite Difference Method

Motivation

For a given smooth function $f(x)$, we want to calculate the derivative $f'(x)$ at a given value of x.

Suppose we don't know how to compute the analytical expression for $f'(x)$, or it is computationally very expensive. However you do know how to evaluate the function value:

```python
def f(x):
    # do stuff here
    feval = ...
    return feval
```

We know that:

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

Can we just use $f'(x) \approx \frac{f(x+h)-f(x)}{h}$ as an approximation? How do we choose h? Can we get estimate the error of our approximation?

Finite difference method

For a differentiable function $f\colon \mathcal{R} \to \mathcal{R}$, the derivative is defined as:

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

Taylor Series centered at x, where $\bar{x} = x + h$

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

$$f(x+h) = f(x) + f'(x)\,h + O(h^2)$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

We define the **Forward Finite Difference** as:

$$df(x) = \frac{f(x+h) - f(x)}{h} \to \; f'(x) = df(x) + O(h)$$

Therefore, the **truncation error** of the forward finite difference approximation is bounded by:

$$|\; f'(x) - df(x)| \leq Mh$$

In a similar way, we can write:

$$f(x-h) = f(x) - f'(x)\,h + O(h^2) \rightarrow \; f'(x) = \frac{f(x) - f(x-h)}{h} + O(h^2)$$

And define the **Backward Finite Difference** as:

$$df(x) = \frac{f(x) - f(x-h)}{h} \rightarrow \; f'(x) = df(x) + O(h)$$

And subtracting the two Taylor approximations

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

$$f(x-h) = f(x) - f'(x)\,h + f''(x)\frac{h^2}{2} - f'''(x)\frac{h^3}{6} + \cdots$$

$$f(x+h) - f(x-h) = 2f'(x)\,h + f'''(x)\frac{h^3}{6} + O(h^5)$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

And define the **Central Finite Difference** as:

$$df(x) = \frac{f(x+h) - f(x-h)}{2h} \rightarrow \; f'(x) = df(x) + O(h^2)$$

How accurate is the finite difference approximation? How many function evaluations (in additional to $f(x)$)?

Forward Finite Difference:

$$df(x) = \frac{f(x+h)-f(x)}{h} \;\rightarrow\; f'(x) = df(x) + O(h)$$

Truncation error: $O(h)$
Cost: 1 function evaluation

Backward Finite Difference:

$$df(x) = \frac{f(x)-f(x-h)}{h} \;\rightarrow\; f'(x) = df(x) + O(h)$$

Truncation error: $O(h)$
Cost: 1 function evaluation

Central Finite Difference:

$$df(x) = \frac{f(x+h)-f(x-h)}{2h} \;\rightarrow\; f'(x) = df(x) + O(h^2)$$

Truncation error: $O(h^2)$
Cost: 2 function evaluation2

Our typical trade-off issue! We can get **better accuracy** with Central Finite Difference with the (possible) **increased computational** cost.

How small should the value of *h*?

Example

$$f(x) = e^x - 2$$

$$f'(x) = e^x$$

We want to obtain an approximation for $f'(1)$

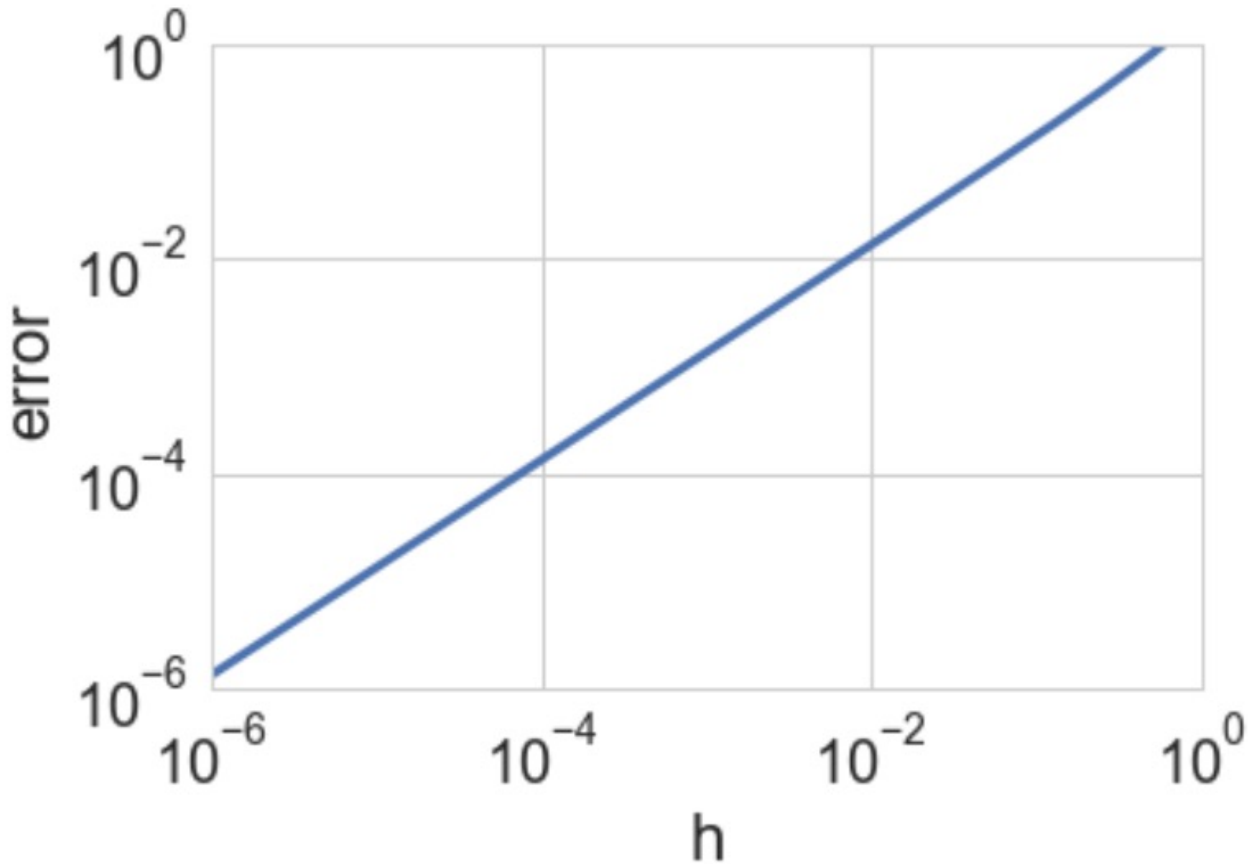
$$dfapprox = \frac{(e^{x+h}-2) - (e^x-2)}{h}$$

Truncation error

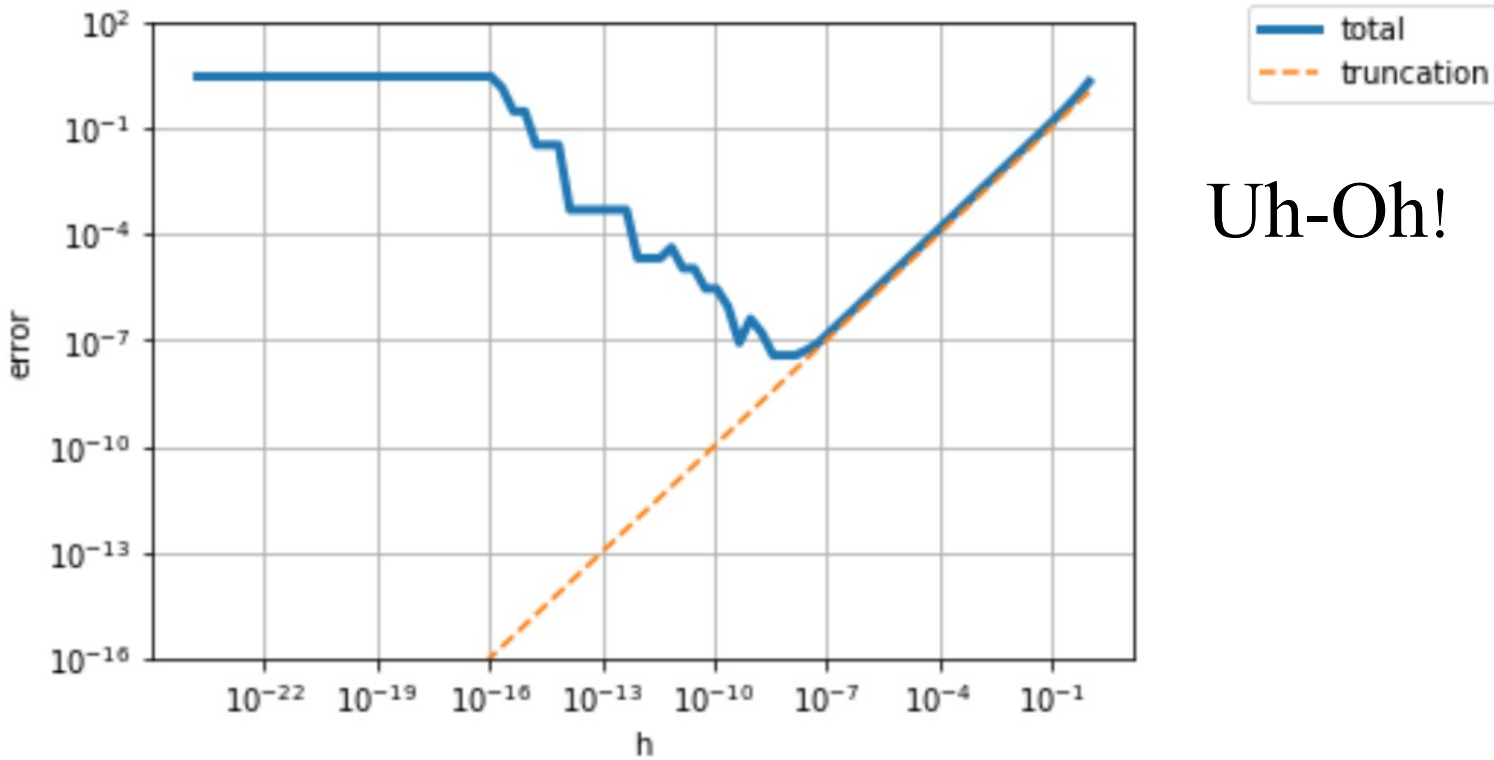
$$error(h) = abs(f'(x) - dfapprox)$$

h	$error$
1.000000E+00	1.952492E+00
5.000000E-01	8.085327E-01
2.500000E-01	3.699627E-01
1.250000E-01	1.771983E-01
6.250000E-02	8.674402E-02
3.125000E-02	4.291906E-02
1.562500E-02	2.134762E-02
7.812500E-03	1.064599E-02
3.906250E-03	5.316064E-03
1.953125E-03	2.656301E-03
9.765625E-04	1.327718E-03
4.882812E-04	6.637511E-04
2.441406E-04	3.318485E-04
1.220703E-04	1.659175E-04
6.103516E-05	8.295707E-05
3.051758E-05	4.147811E-05
1.525879E-05	2.073897E-05
7.629395E-06	1.036945E-05
3.814697E-06	5.184779E-06
1.907349E-06	2.592443E-06

Example



Should we just keep decreasing the perturbation h, in order to approach the limit $h \to 0$ and obtain a better approximation for the derivative?



Uh-Oh!

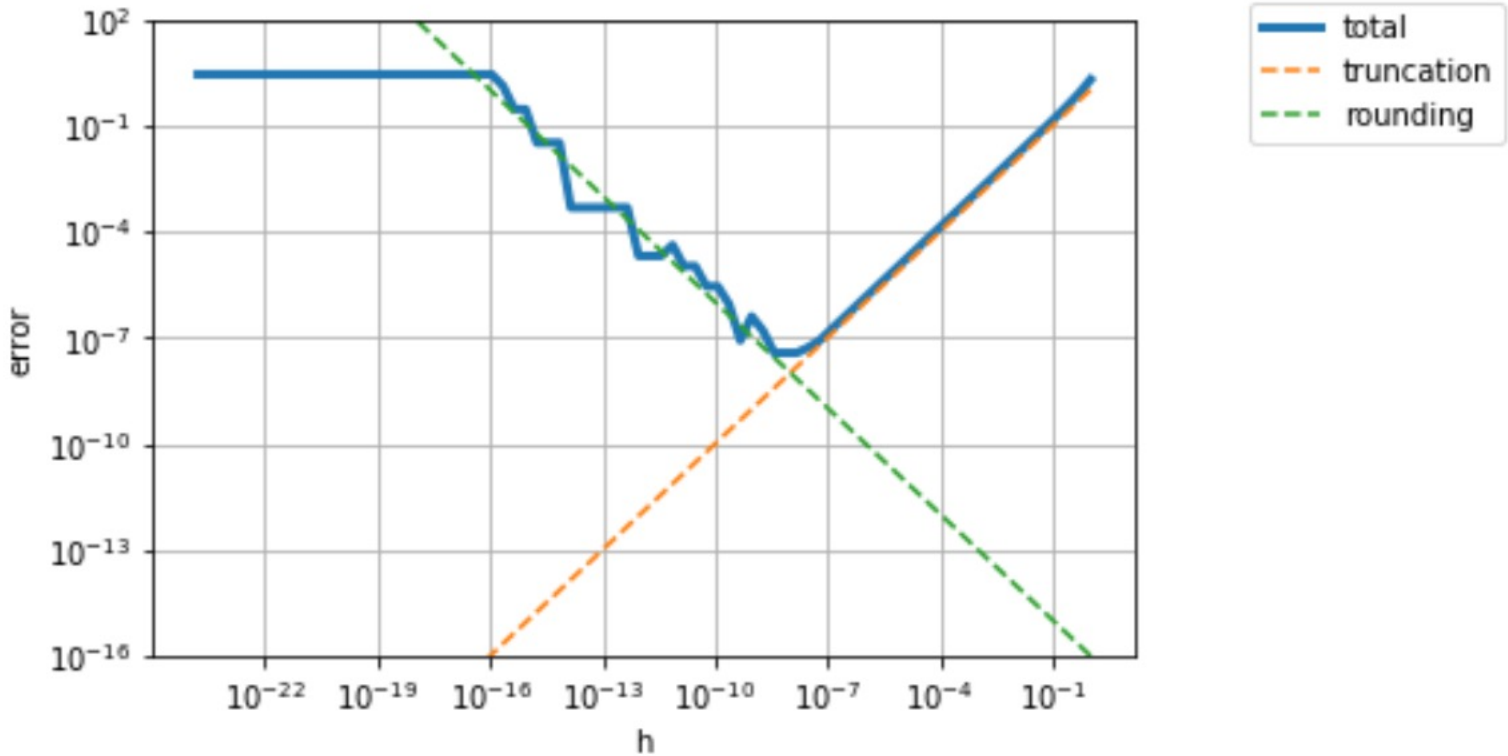
What happened here?

$$f(x) = e^x - 2, \qquad f'(x) = e^x \rightarrow f'(1) \approx 2.7$$

Forward Finite Difference

$$df(1) = \frac{f(1+h) - f(1)}{h}$$

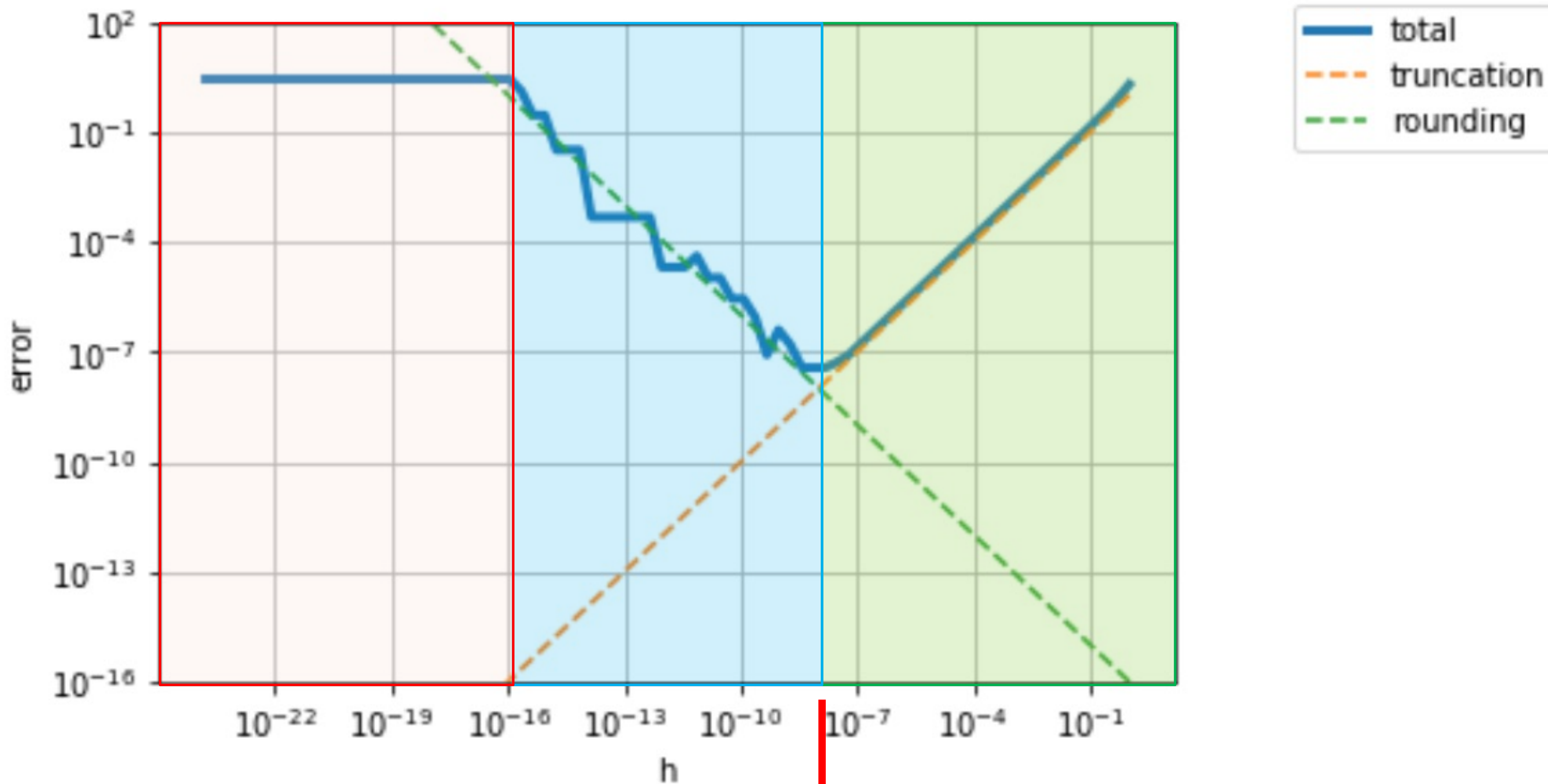
If h is very "small", we will have the issue of cancelation!



When computing the finite difference approximation, we have two competing source of errors: Truncation errors and **Rounding errors**

$$df(x) = \frac{f(x+h) - f(x)}{h} \leq \frac{\epsilon_m \, |f(x)|}{h}$$

Loss of accuracy
due to rounding



Optimal "h"

Minimize the total error

$$error \sim \frac{\epsilon_m |f(x)|}{h} + Mh$$

Gives

$$h = \sqrt{\epsilon_m |f(x)|/M}$$

Truncation error: $error \sim M\,h$

Rounding error: $error \sim \dfrac{\epsilon_m |f(x)|}{h}$