Catastrophic Error Cancellation

- Single calculation can accumulate big error
- Examples:
  - c = a + b, with a >> b
  - c = a – b, with a ~ b

Catastrophic Error Cancellation

- To see how this creeps in “c = a – b”, consider
  - a = x.xxx xxxx xxxx1ssssss, where “x”, “s”, and “t” in [0-9]
  - b = x.xxx xxxx xxxx0tttttt

$$
\begin{array}{rl}
 & \overbrace{\mathrm{x.xxx\;xxxx\;xxxx}\,1}^{\text{available precision}} \\
- & \mathrm{x.xxx\;xxxx\;xxxx}\,0 \\
\hline
= & 0.000\;0000\;0000\,1\;\;\underbrace{\mathrm{uuuu\;uuuu\;uuuu}}_{\text{unassigned digits}} \\
= & 1.\mathrm{uuuu\;uuuu\;uuuu} \times 10^{-12}
\end{array}
$$

- In general ssssss-tttttt is not equal to uuuuuu

Quadratic Formula

- The equation

$$ax^2 + bx + c = 0$$

- has the roots

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

- Consider the equation

$$x^2 - 54.32x + 0.1 = 0$$

- The exact roots (to 11 decimal places) are
  - x1 = 54.318158995, and x2 = 0.0018410049576

4 digit floats

- Assume that we could only use 4 significant digits

$$\begin{aligned}\sqrt{b^2 - 4ac} &= \sqrt{(-54.32)^2 - 0.40000} \\ &= \sqrt{2951 - 0.4000} \\ &= \sqrt{2951} \\ &= 54.32\end{aligned}$$

- This leads to
  - $x1_4$ = 54.30 and $x2_4$=0 (which is completely wrong)

If we rationalize the formulae

- Consider

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \left(\frac{-b - \sqrt{b^2 - 4ac}}{-b - \sqrt{b^2 - 4ac}} \right)$$

$$x_1 = \frac{2c}{-b - \sqrt{b^2 - 4ac}}$$

- Similarly

$$x_2 = \frac{2c}{-b + \sqrt{b^2 - 4ac}}$$

4 digit floats

- For the same old example with these new formulae,

$$x_{2,4} = \frac{0.2000}{54.32 + 54.32} = \frac{0.2000}{108.6} = 0.001842$$

- But x1 goes to infinity!!!

Algorithmic Solution

- Evaluate

$$q = -\frac{1}{2}\left[b + \underline{\mathrm{sign}(b)}\sqrt{b^2 - 4ac}\right]$$

+1 or -1

- Roots to the quadratic

$$x_1 = \frac{q}{a}, \qquad x_2 = \frac{c}{q}$$

Truncation Error

- When we approximate an infinite series by chopping it
- Taylor series expansion of f(x) around x=a

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots$$

- Applied to sine near x=0

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \ldots$$

- Consider truncating after 1 term

Truncation Error

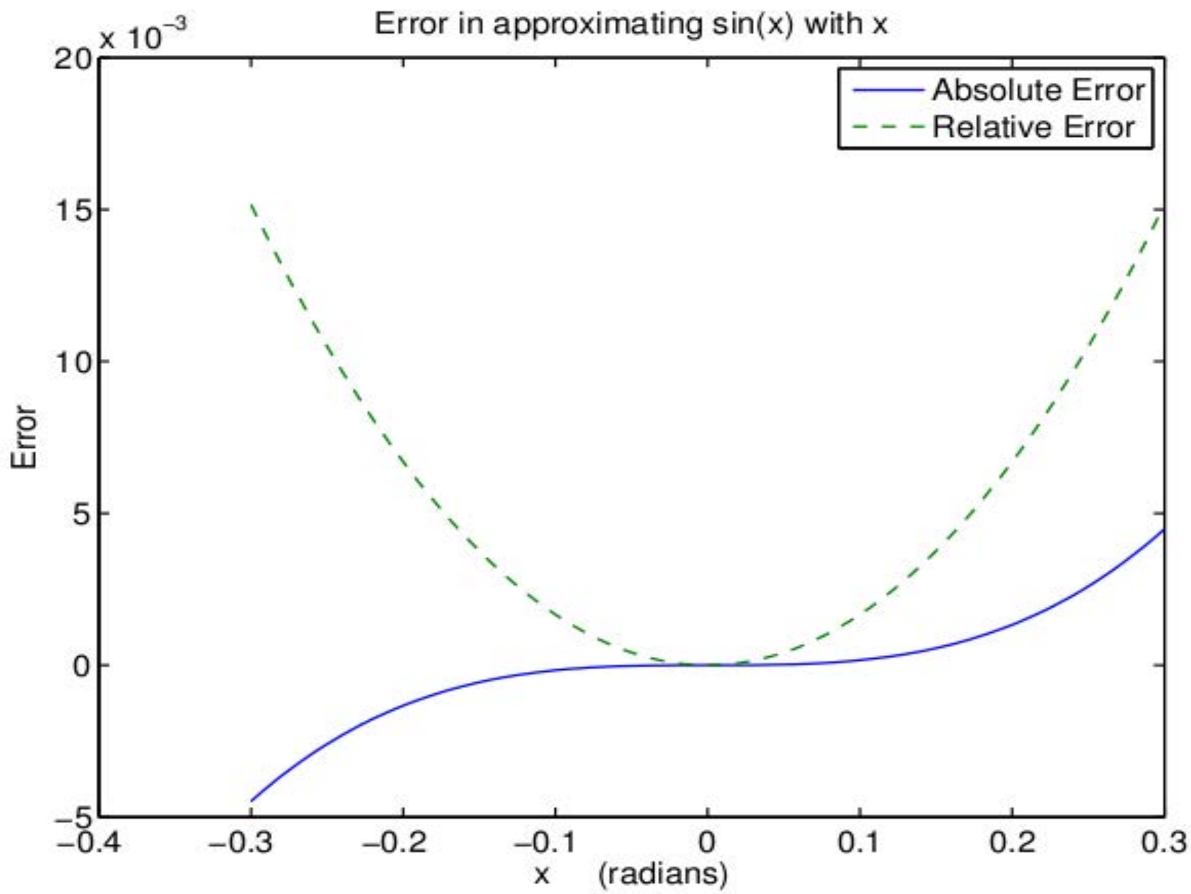
- Absolute Error

$$E_{abs} = x - \sin(x) = \frac{x^3}{3!} - \frac{x^5}{5!} + \cdots$$

- Relative Error

$$E_{rel} = \frac{x - \sin(x)}{\sin(x)} = \frac{x}{\sin(x)} - 1$$

Truncation Error



Truncation Error

- Depends on the number of terms included

h

$$f(x) = P_n(x) + O\left(\frac{(x-a)^{n+1}}{n+1!}\right)$$

- As h increases, truncation error increases

Round-off and Truncation Errors

- In many cases, round-off and truncation errors interact
- Consider finite differencing

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

- More accurate

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

Let's look at an example

- So lets look at an example where f(x) is the CDF of the normal distribution,

$$f(x) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{x}{\sqrt{2}}\right)\right]$$

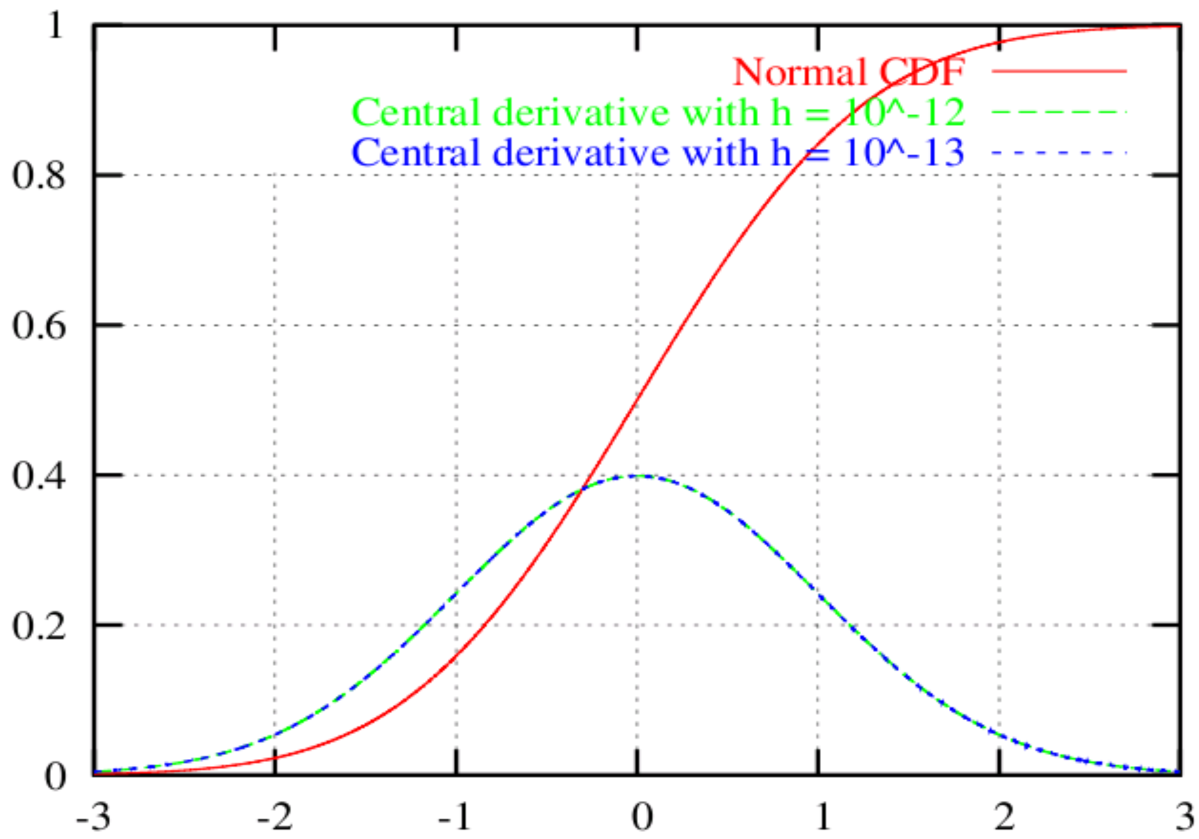
- consider centered difference formula,

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

- and look at what happens as h is varied

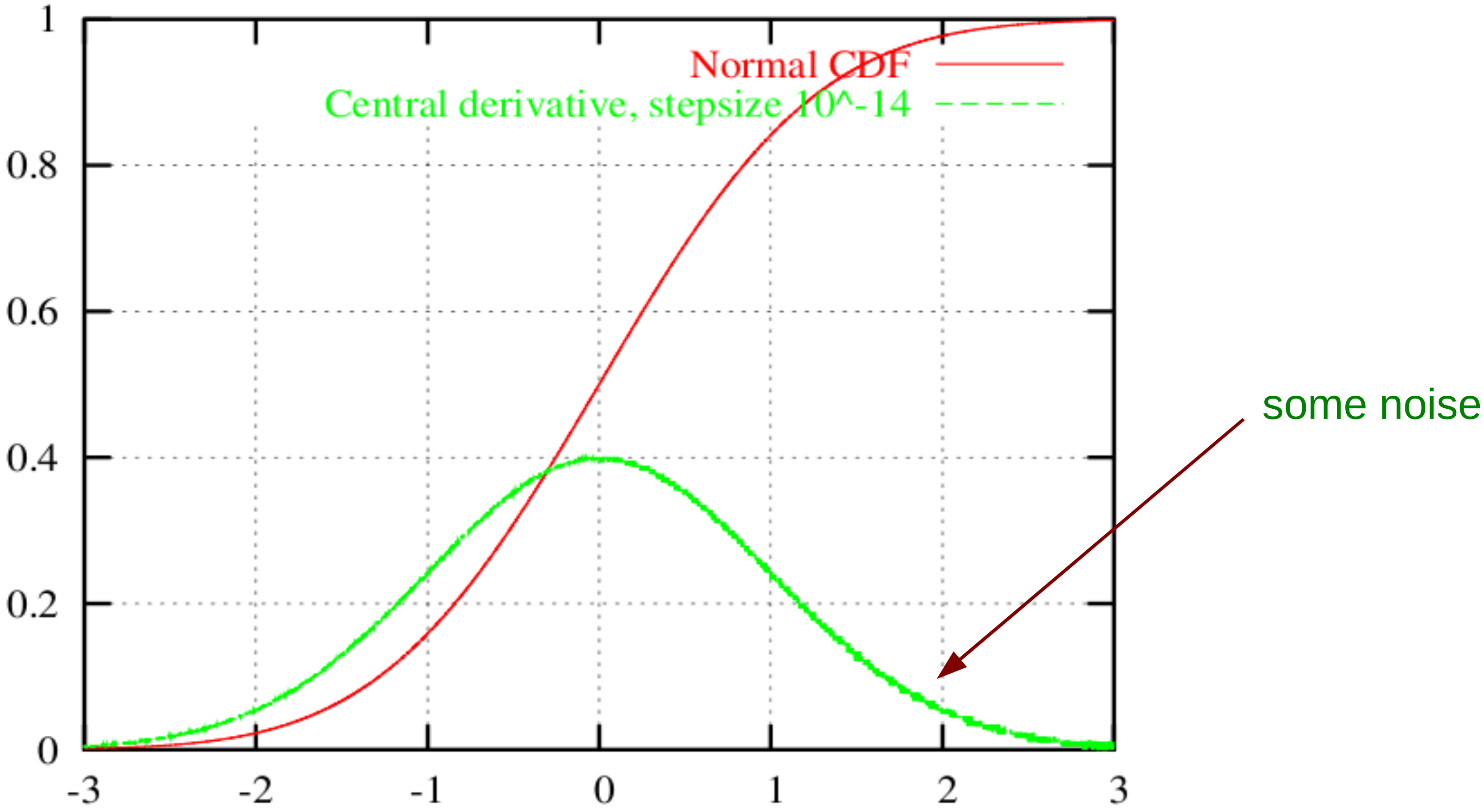
Example

- h = 10^{-12}, 10^{-13}



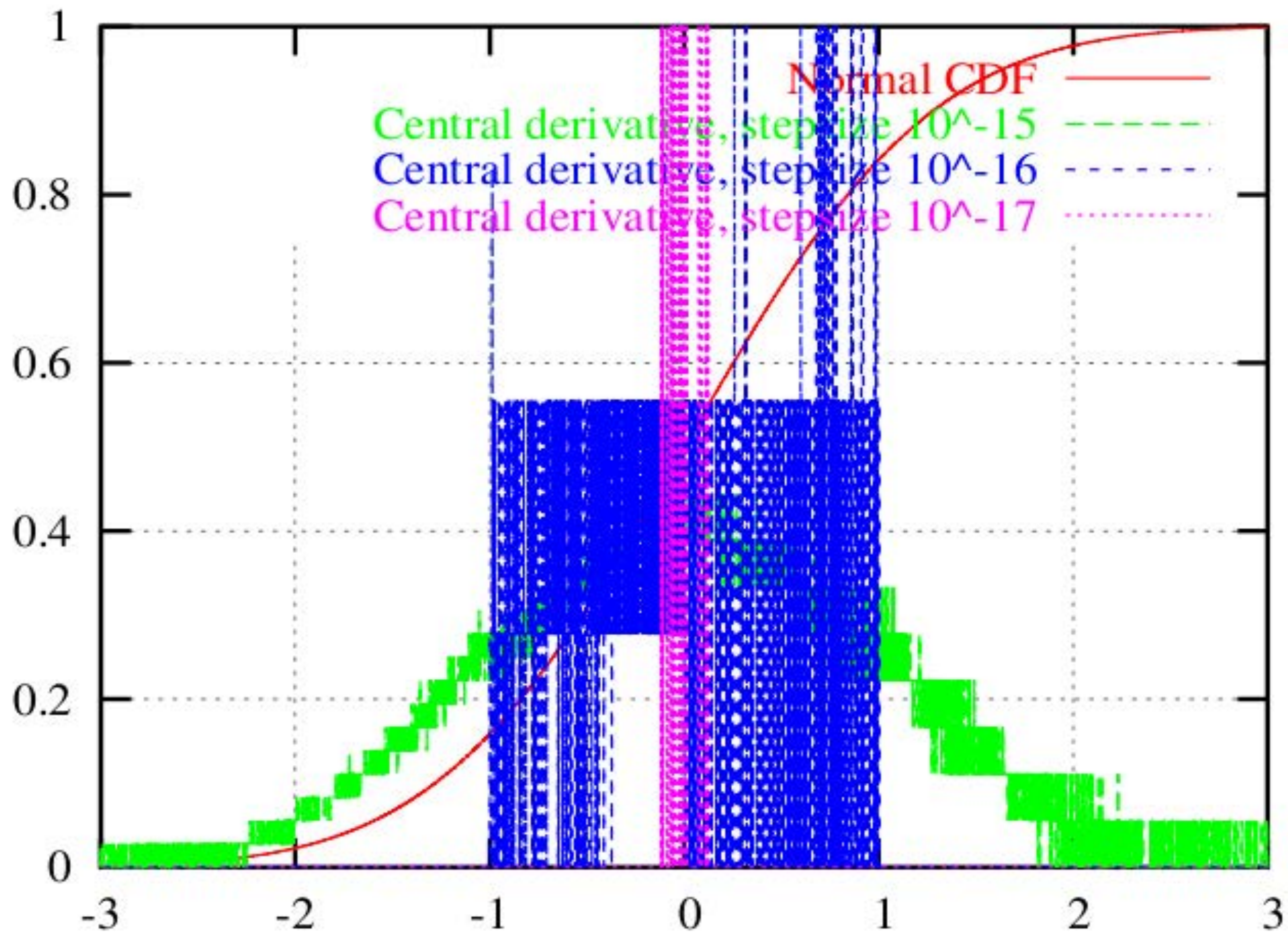
Example

- h = 10^{-14}



Example

- h = 10^{-15}, 10^{-16}, 10^{-17}



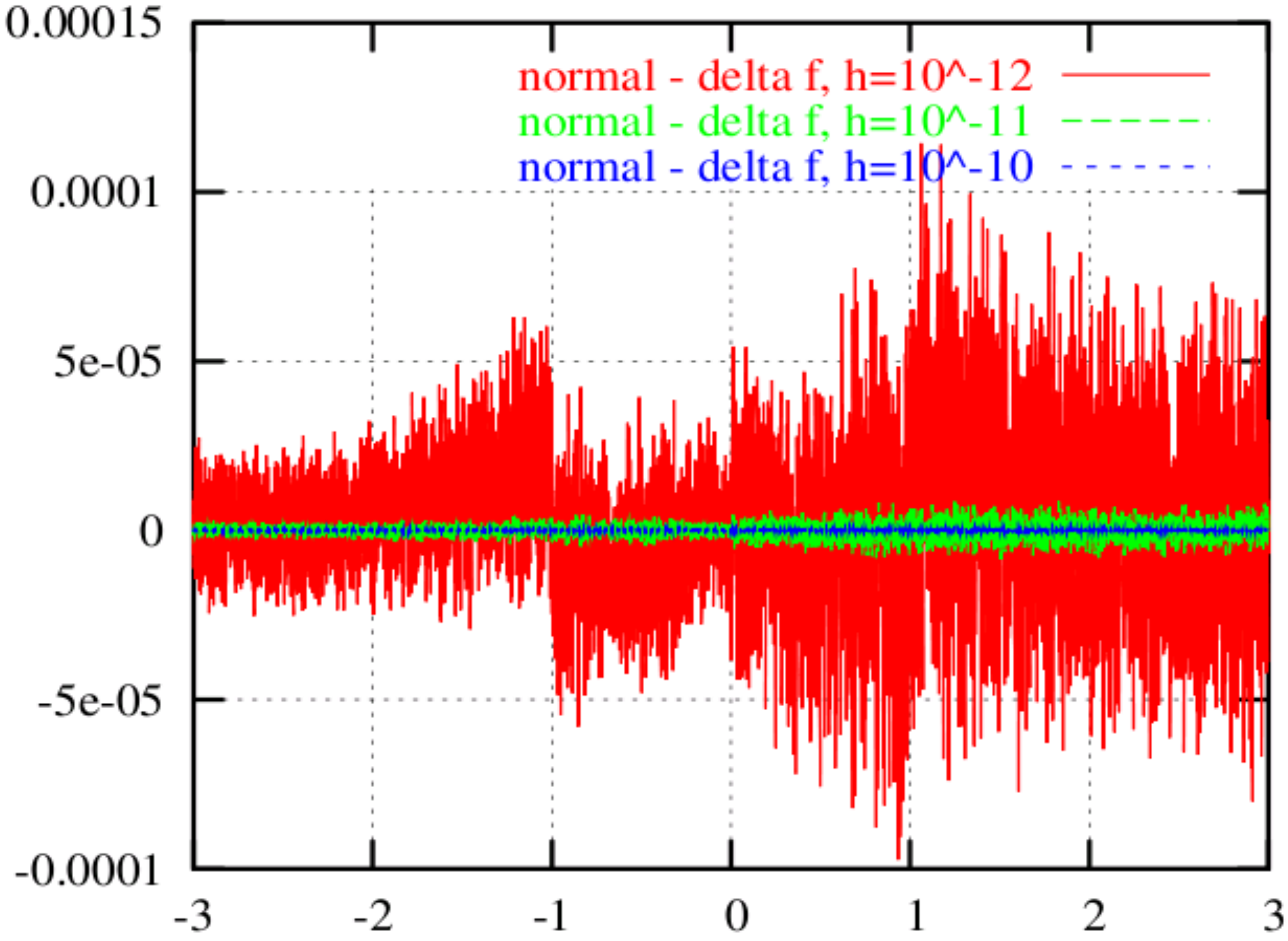
whoa!!!

What just happened?

- Short answer
  - We hit machine precision
- Long answer
  - IEEE “double” standard (64 bit) has 52 bit mantissa (+1 for sign)
  - can represent upto $2^{-52} \sim 10^{-16}$ or only 16 decimal digits
  - as we approach $h = 10^{-16}$, we hit this limit relentlessly
- So small is not necessarily good
- In fact, there is more bizarre stuff!
  - we know the derivative of this function analytically
  - we can look for the absolute error

Example continued

- Compare absolute error (y-axis)

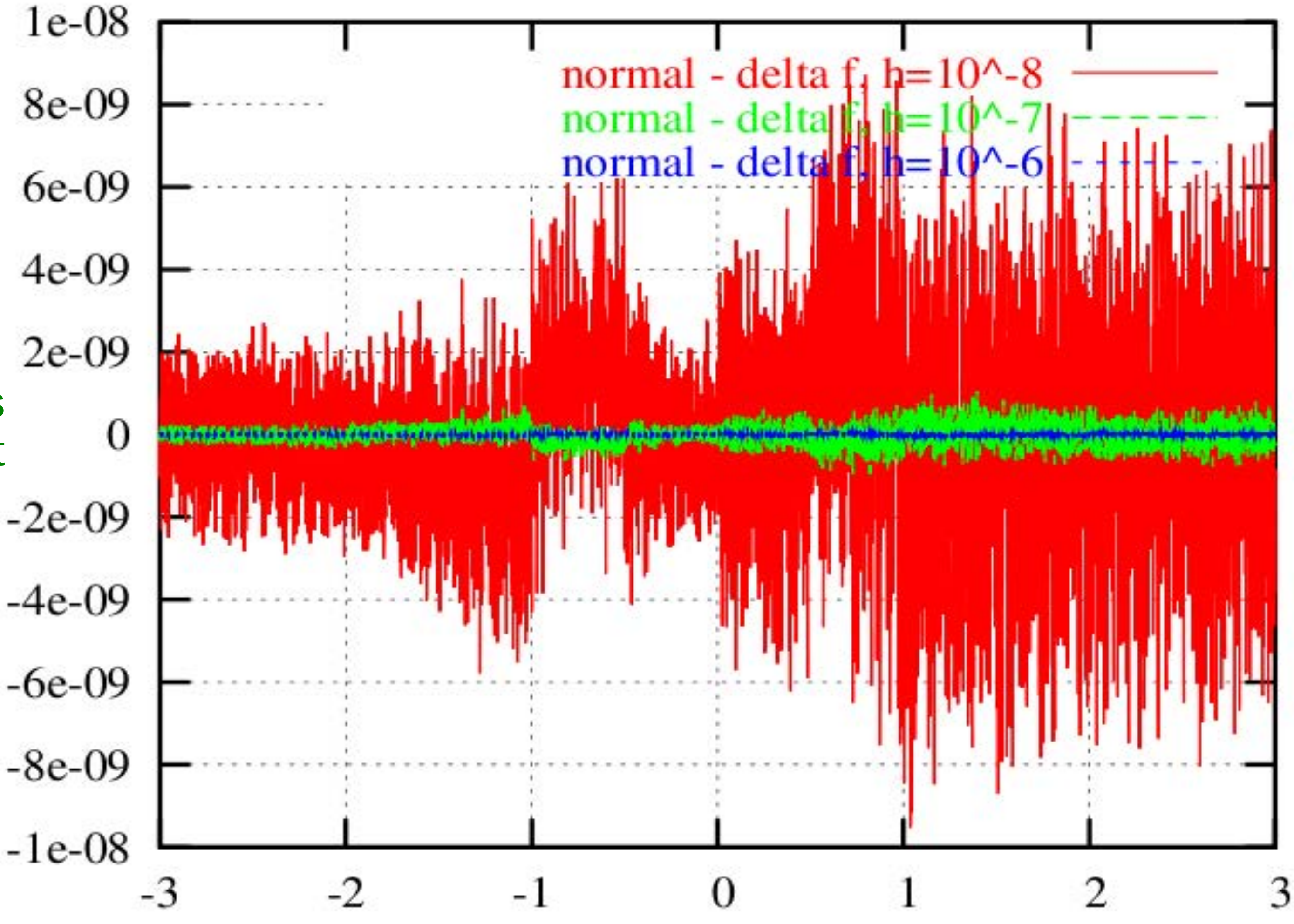


it actually seems to get better as h is ***increased***!

Example continued

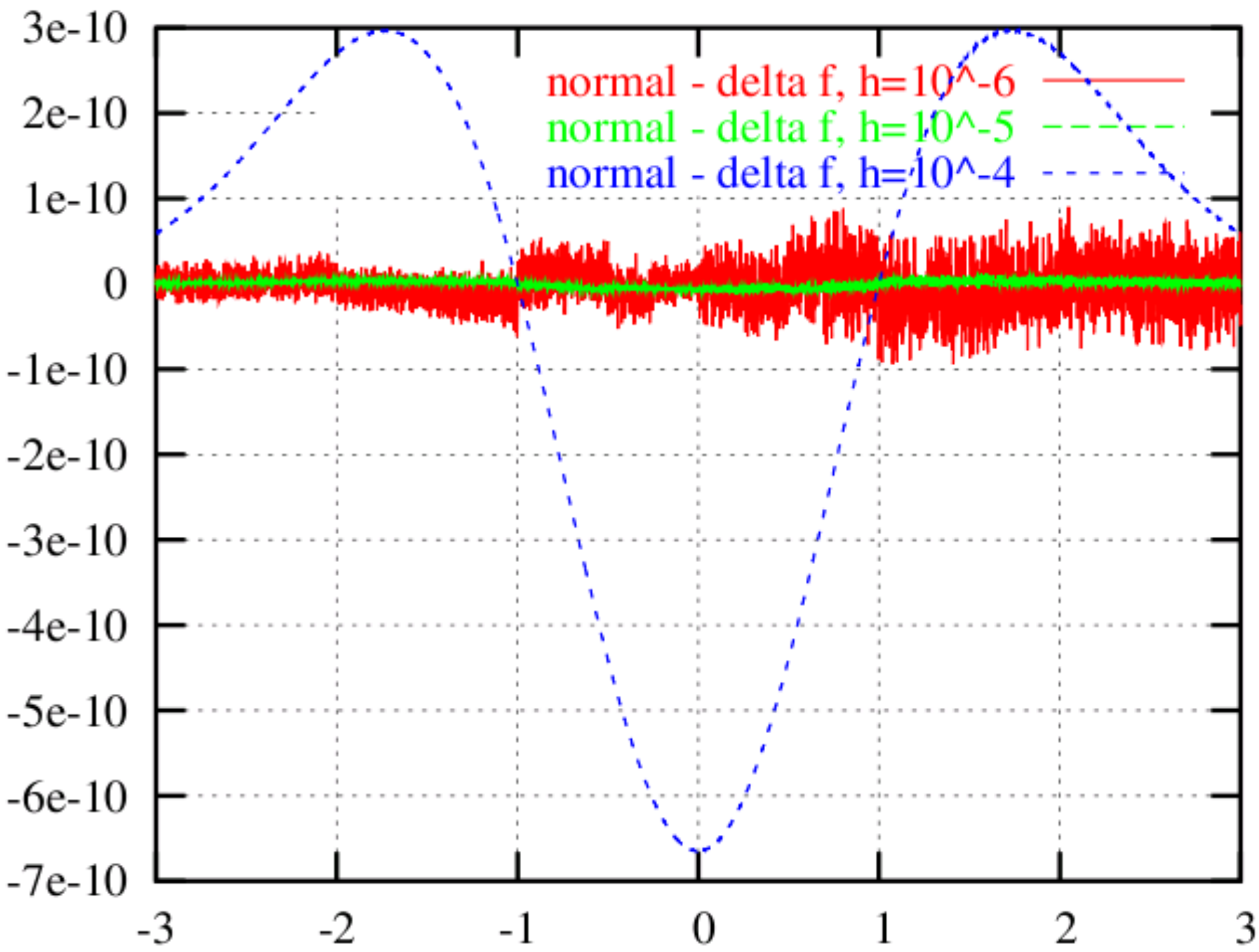
- The story continues

note y axis is
stretched out



Example continued

- Until finally, “commonsense” prevails



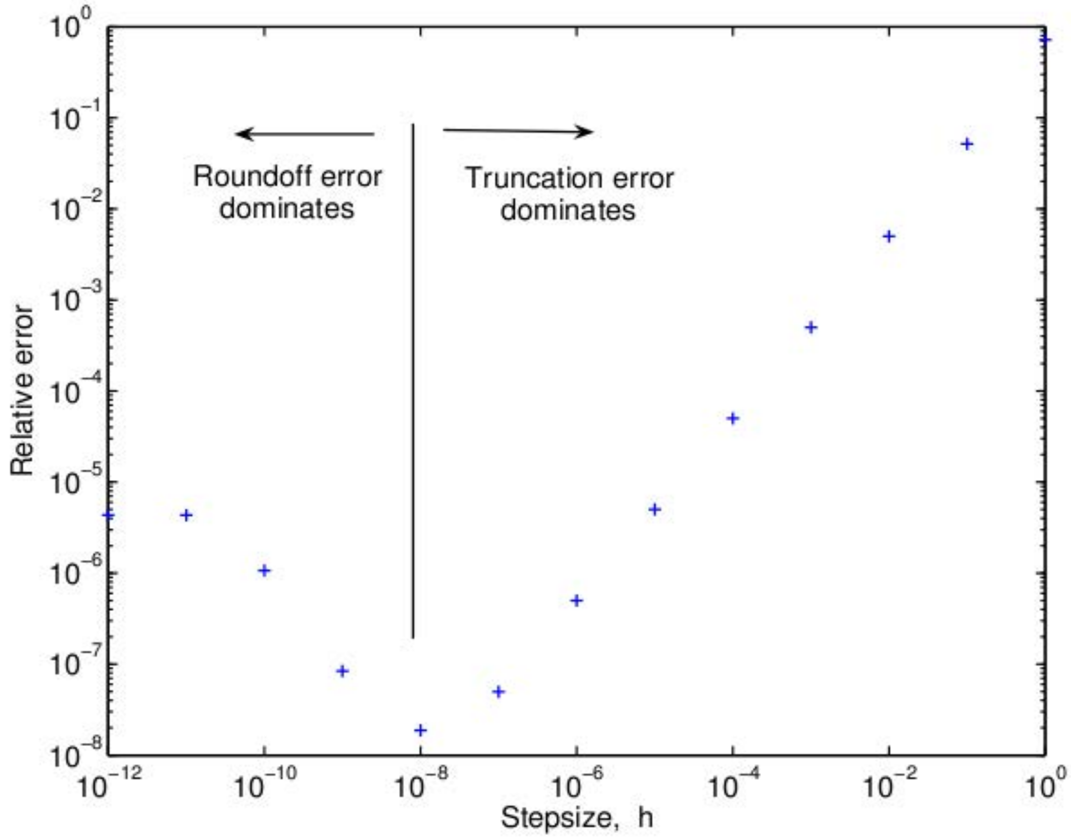
h = 10^{-5} is the best choice? who would have thought?

Summary

- At very low h we hit finite-precision/round-off issues
- But why does the story stay the same far away from that limit?
  - 10^{-5} and 10^{-16} are far apart!
- We looked at a particular f(x), but the story is the essentially the same for other functions
- Two important sources of error
  - Truncation error: (increases with increasing h)
  - Roundoff error: (increases with decreasing h)

Another example

- Forward difference formula (not centered)
- To get derivatives of f(x) = exp(x)



location of minima is different, but story is the same!

Cancellation Error

- Taylor series

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

$$f(x-h) = f(x) - hf'(x) + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \ldots$$

$$f(x+h) - f(x-h) = 2hf'(x) + 2\frac{f'''(x)}{3!}h^3 + \ldots$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \underline{\frac{f'''(x)}{3!}h^2 + \ldots}$$

gets larger as h increases

Cancellation Error

- As h decreases $f(x+h) - f(x-h)$ gets small
  - catastophic cancellation error
- Consider a crude way of getting a handle on cancellation error
- Due to finite number of significant digits

$$\bar{f}(x) = f(x) + \alpha(x) f(x)$$

measured — $\bar{f}(x)$; actual — $f(x)$; $\alpha(x)$ — relative accuracy, "effect of discarded digits", random variable

  - If accuracy of the order of machine precision

$$|\alpha(x)| \sim 2^{-53}$$

  - If 5 significant decimal places

$$|\alpha(x)| \sim 10^{-5}$$

Cancellation Error

- Therefore,

$$\bar{f}(x+h) - \bar{f}(x-h) = f(x+h) - f(x-h) + \alpha(x+h)f(x+h) - \alpha(x-h)f(x-h)$$

- Crudely,

$$\bar{f}(x+h) - \bar{f}(x-h) \approx f(x+h) - f(x-h) + \alpha(x)f(x)$$

when h is small these differences are also small

- Thus, Δf is dominated by the relative error term
  - sets up the optimization problem

Optimal "h"

- Want to minimize truncation and cancellation error
- Start from

$$\frac{f(x+h)-f(x-h)}{2h} \approx f'(x) + \underline{\frac{f'''(x)}{3!}h^2 + \frac{\alpha(x)f(x)}{2h}}$$

want to minimize this with respect to h

- Setting

$$\frac{d}{dh}\left[\frac{f'''(x)}{3!}h^2 + \frac{\alpha(x)f(x)}{2h}\right] = 0$$

- Yields

$$h = \left(\frac{3\alpha f}{f'''}\right)^{1/3}$$