Given a univariate function

$$f: \mathbb{R} \to \mathbb{R}$$
,

compute

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

Only consider finite differences.

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Only consider finite differences.

- Solving differential equations
- Numerical optimization

Gradient of $f:\mathbb{R}^n \to \mathbb{R}$

$$\mathbf{g}_k = \frac{\partial f}{\partial x_k}$$

Hessian of $f: \mathbb{R}^n \to \mathbb{R}$

$$\mathbf{H}_{jk} = \frac{\partial^2 f}{\partial x_j \partial x_k}$$

Jacobian of $\mathbf{f}: \mathbb{R}^n \to \mathbb{R}^m$

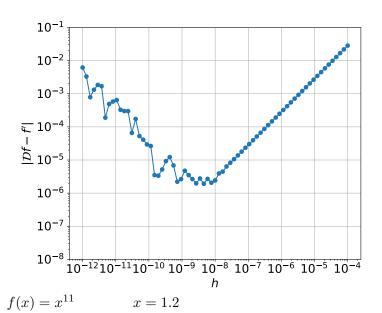
$$\mathbf{J}_{jk} = \frac{\partial f_j}{\partial x_k}$$

- ▶ Can compute f(x), a black box.
- Need to construct an approximation $\mathcal{D}f(x)$ for f'(x), balancing
 - Accuracy of the estimate (here: $|\mathcal{D}f f'| \to \min$)
 - Computational complexity (here: the number of evaluations of f)

The two-point forward difference scheme

$$\mathcal{D}f \equiv \frac{f(x+h) - f(x)}{h} \approx f'(x)$$

And the only thing left is to choose h?



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Numerical derivatives: truncation error

Assuming that f(x) is sufficiently smooth in the neighborhood of x, expand it into the Taylor series around x:

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

$$\mathcal{D}f \equiv \frac{f(x+h) - f(x)}{h} = f'(x) + \frac{f''(x)}{2}h + \cdots$$

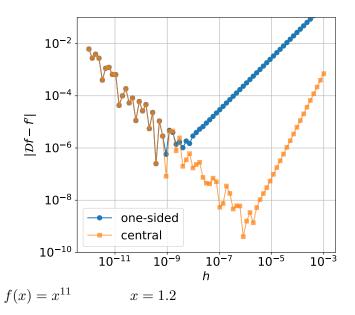
Numerical derivatives: two-point central scheme

Consider a central finite difference scheme

$$\mathcal{D}_c f \equiv \frac{f(x+h) - f(x-h)}{2h}$$

Expand $f(x \pm h)$ into the Taylor series around x,

$$\mathcal{D}_c f = f'(x) + \frac{f'''(x)}{6}h^2 + \cdots$$



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What is the step of the finite difference scheme?

With exact arithmetics,

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

With floating-point arithmetics, (x+h) is truncated to the nearest exactly representable number

```
>>> x = 1.0

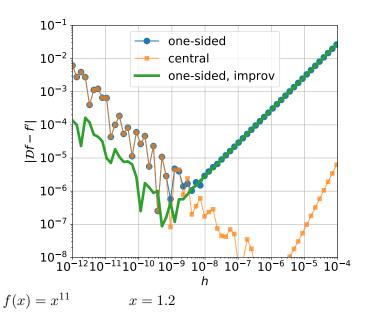
>>> h = np.array([1e-15, 1e-14, 1e-10])

>>> ((x + h) - x)/h - 1.0

array([ 1.1e-01, -8.0e-04, 8.3e-08])
```

What is the step of the finite difference scheme?

To keep the numerator and denominator of $\mathcal{D}f$ consistent, make sure that x+h and x differ by an exactly representable number:



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Numerical derivatives: roundoff errors

Consider a one-sided two-point scheme

$$\mathcal{D}f = \frac{f(x+h) - f(x)}{h} \approx f'(x)$$

and assume that the values of f(x) are computed to the relative accuracy ϵ_f .

Then the roundoff error of $\mathcal{D}f$ is

$$\epsilon_r \sim \epsilon_f \left| \frac{f(x)}{h} \right|$$

Numerical derivatives: roundoff errors

The total error is the combination of roundoff and linearization errors:

$$\epsilon_r + \epsilon_t \sim \epsilon_f \frac{f}{h} + f''h$$
.

This way, the total error has a minimum at

$$h_{\rm opt} \sim \epsilon_f^{1/2} \sqrt{f/f''}$$
.

and the minimum value of the total error is

$$\epsilon_{\min} \propto \epsilon_f^{1/2}$$

Numerical derivatives: roundoff errors

For a central finite difference scheme,

$$\mathcal{D}_c f \equiv \frac{f(x+h) - f(x-h)}{2h}$$
,

truncation error scales $\propto h^2$, thus

$$h_{
m opt} \propto \epsilon_f^{1/3}$$
 $\epsilon_{
m min} \propto \epsilon_f^{2/3}$

- The step and the denominator must be consistent
- lacktriangle For a scheme with the truncation error of $O(h^d)$, the optimal step of the finite difference

$$h_{\text{opt}} = \epsilon_f^{1/(d+1)} x_c$$

The simplest heuristics for x_c is $x_c = \max(1, x)$.

► The best total error scales as

$$\epsilon_{\rm min} \propto \epsilon_f^{d/(d+1)}$$

Finite differences: higher order schemes

Higher order finite differences

The main idea: form linear combinations of $f(x \pm h)$, $f(x \pm 2h)$ etc.

Example: construct a one-sided scheme of the order $\mathcal{O}(h^2)$ for the first derivative.

$$f(x+h) = f + f'h + \frac{1}{2}f''h^2 + \frac{1}{6}f'''h^3 + O(h^4)$$

Need three terms to cancel f(x) and f''(x).

Higher order finite differences

Use the method of indeterminate coefficients: write

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

and adjust A, B and C.

$$A f(x) + B f(x+h) + C f(x+2h) =$$

$$A f$$

$$+B \left(f + f' h + \frac{1}{2} f'' h^2 + \frac{1}{6} f''' h^3 + O(h^4) \right)$$

$$+C \left(f + f' 2h + \frac{1}{2} f'' 4h^2 + \frac{1}{6} f''' 8h^3 + O(h^4) \right)$$

Higher order finite differences

Solving the linear system for the coefficients in front of f(x), f'(x) and f''(x), we find

$$f'(x) = \frac{-\frac{3}{2}f(x) + 2f(x+h) - \frac{1}{2}f(x+2h)}{h} + O(h^2) .$$

Likewise,

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

For a better algorithm of generating such schemes see: B. Fornberg, *Generation of finite difference formulas on arbitrary spaced grids*, Mathematics of Computation **51**, 669 (1988).