Introduction to Finite Differences

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Ordinary and Partial Differential Equations

What is an ordinary differential equation (ODE)?

An equation relating a function to its derivatives of a single variable (in such a way that the function itself can be determined)

Convention regarding notation:

- time-derivatives are denoted by a dot $\dot{y}(t) = \frac{dy}{dt}(t)$
- other derivatives are denoted by a prime $y'(x) = \frac{dy}{dx}(x)$

Equations relating derivatives of more than one independent variables are called partial differential equations (PDEs)
Different notations:

$$\frac{\partial u}{\partial x} = \partial_x u = u_x$$

Motivation

In this course we will study simulation of differential equations:

- steady heat equation (elliptic): $\nabla^2 u = u_{xx} + u_{yy} = q$
- heat equation (parabolic): $u_t = \nabla^2 u,$
- wave equation (hyperbolic): $u_{tt} = \nabla^2 u,$
- transport equations: $u_t + \nabla f(u) = \varepsilon \nabla^2 u,$

Common for all: relates various derivatives of unknown functions

These are all *continous* quantities, which cannot be represented on a computer $\longrightarrow$ we need discrete quantities.

Computing Derivatives

Question:

How do we compute the derivative of a given function $f(x)$ on a computer?

Consider the definition of the derivative:

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

Idea: use a finite h to estimate $f'(x)$:

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

This is a forward finite difference. Clearly h must be small for this to be a good approximation

Finite differences

'Rigorous' derivation from MacLoren series:

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

for $x \leq \xi \leq x+h$. We can rearrange to

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

Thus, the error we make by using forward differences is

$$\left| \frac{f(x+h) - f(x)}{h} - f'(x) \right| \leq Mh,$$

where M depends on f''. We call the approximation first order since the error is $\mathcal{O}(h)$.

Finite differences cont'd

Similarly, we derive backward differences

$$f'(x) \approx \frac{f(x) - f(x-h)}{h},$$

which also are first order: $|\frac{f(x)-f(x-h)}{h} - f'(x)| \leq Mh$.

We can also derive central differences

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

which are second order $|\frac{f(x+h)-f(x-h)}{2h} - f'(x)| \leq Mh^2$.
Here M depends on f'''.

Finite differences cont'd

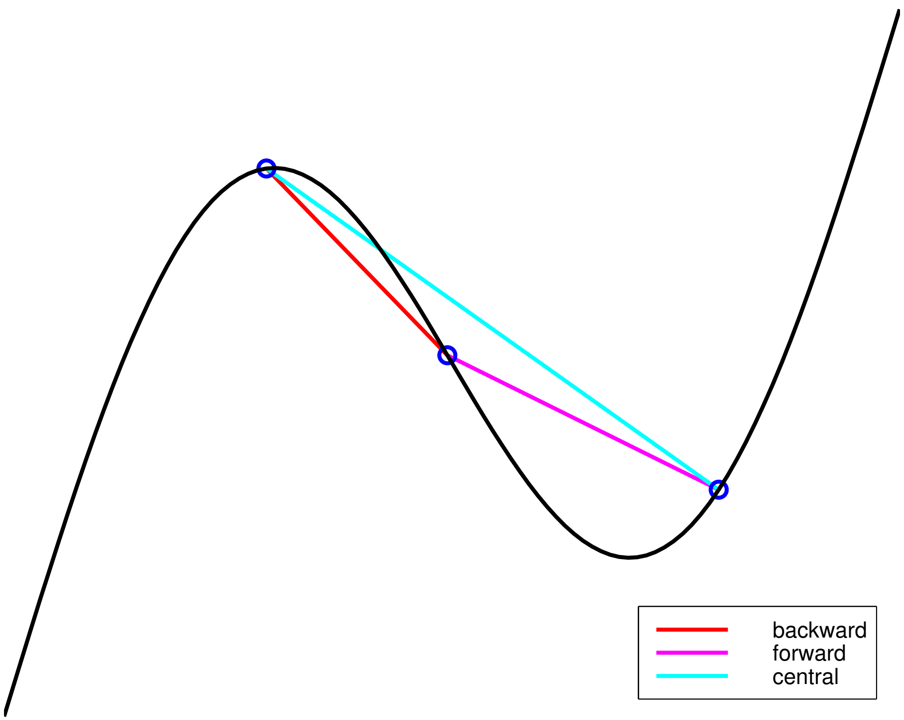
Higher-order approximations:

- second order: $f'(x) = \frac{-f(x+2h)+4f(x+h)-3f(x)}{3h} + \mathcal{O}(h^2)$
- third order: $f'(x) = \frac{2f(x+h)+3f(x)-6f(x-h)+f(x-2h)}{6h} + \mathcal{O}(h^3)$
- fourth order:
  $f'(x) = \frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h} + \mathcal{O}(h^4)$
- ....

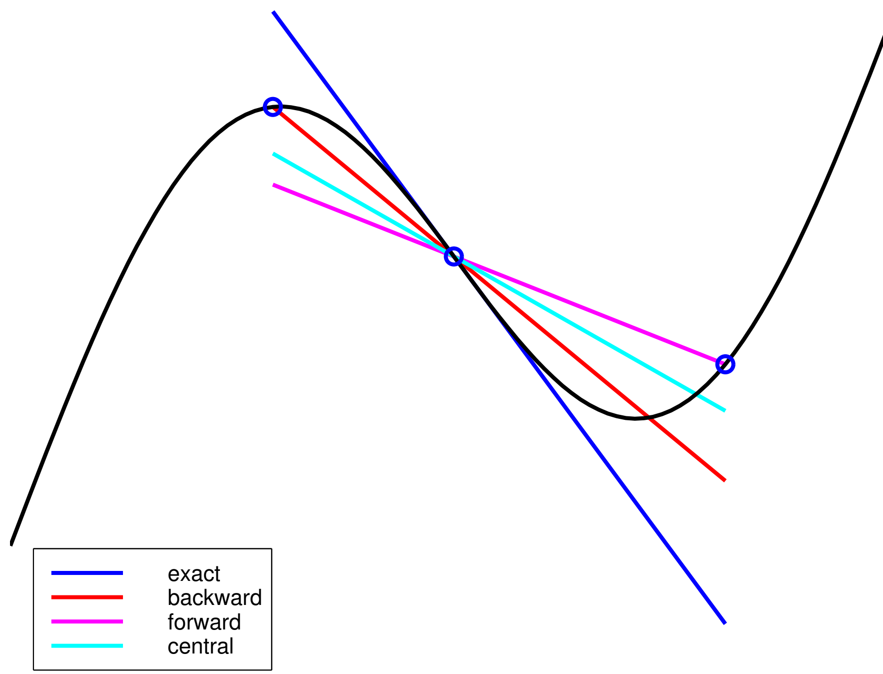
Playing with Taylor series, one can define a host of approximations....

Exercise: Verify some of the above formulas.

Graphical interpretation



discrete points



slopes

Example: $f'(1.0)$ for $f(x) = x^2 + \sin(x)$

$$F'_f(x) = \frac{f(x+h) - f(x)}{h}, \quad F'_b(x) = \frac{f(x+h) - f(x)}{h}, \quad F'_c(x) = \frac{f(x+h) - f(x-h)}{2h}$$

N	$f'(x)$	$F'_f(x)$	$F'_f - f'$	$F'_b(x)$	$F'_b - f'$	$F'_c(x)$	$F'_c - f'$
8	2.5403	2.6114	7.11e-02	2.4664	-7.39e-02	2.5389	-1.41e-03
16	2.5403	2.5762	3.59e-02	2.5037	-3.66e-02	2.5400	-3.52e-04
32	2.5403	2.5583	1.80e-02	2.5221	-1.82e-02	2.5402	-8.79e-05
64	2.5403	2.5493	9.03e-03	2.5312	-9.07e-03	2.5403	-2.20e-05
128	2.5403	2.5448	4.52e-03	2.5358	-4.53e-03	2.5403	-5.50e-06
256	2.5403	2.5426	2.26e-03	2.5380	-2.26e-03	2.5403	-1.37e-06

Second order derivatives

Consider once more the Taylor series

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

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f^{(3)}(x) + \frac{h^4}{24}f^{(4)}(\eta)$$

Adding and rearranging terms we obtain

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

where the error is bounded by $|e^h(x)| \leq \sup_x |f^{(4)}(x)|h^2/12$.

Second order derivatives cont'd

Alternatively, we can use forward and backward approximations:

$$f''(x) \xrightarrow{\text{fwd.}} \frac{f'(x+h) - f'(x)}{h} \xrightarrow{\text{bwd.}} \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h}$$

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

or the other way around

$$f''(x) \xrightarrow{\text{bwd.}} \frac{f'(x) - f'(x-h)}{h} \xrightarrow{\text{fwd.}} \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h}$$

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

Second order derivatives cont'd

And to make the confusion complete; we can apply central differences twice

$$f''(x) \xrightarrow{\text{ctr.}} \frac{f'(x+h/2) - f'(x-h/2)}{h} \xrightarrow{\text{ctr.}} \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h}$$
$$= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Higher-order approximation:

$$f''(x) = \frac{-f(x+2h) + 16f(x) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} + \mathcal{O}(h^4)$$