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 \textit{continuous} quantities, which cannot be represented on a computer \(\rightarrow\) 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 \( O(h) \).
Similarly, we derive **backward differences**

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

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

We can also derive **central differences**

\[
f'(x) \approx \frac{f(x + h) - f(x - h)}{2h},
\]

which are second order \[\left| \frac{f(x + h) - f(x - h)}{2h} - f'(x) \right| \leq Mh^2.\]

Here \( M \) depends on \( f''' \).
Finite differences cont’d

Higher-order approximations:

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

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 $f(x) = x^2 + \sin(x)$

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

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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:

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

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

or the other way around

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

\[ = \frac{f(x + h) - 2f(x) + f(x - h)}{h^2} \]
Second order derivatives cont’d

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

\[ f''(x) \stackrel{ctr.}{\Rightarrow} \frac{f'(x + h/2) - f'(x - h/2)}{h} \stackrel{ctr.}{\Rightarrow} \frac{f(x+h) - f(x) - f(x)-f(x-h)}{h} \]

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

Higher-order approximation:

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