Numerical differentiation

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1. Introduction

Why do we need to approximate derivatives at all?

Several reasons

There could be several situations where we would be needing numerical evaluations of derivatives:

- Let us say that we have a set of sampled data points. This may have an underlying function satisfying the data points which we do not know.
- Let us say that the sampled/discrete data points do not have any underlying function satisfying the data
- There are situations where the given function is too complicated to calculate the functional derivative.
- We will see later while solving ordinary differential equations that solutions are discrete approximations defined on grids. Hence, to find a derivative, we need numerical methods.

Introduction to Numerical Differentiation

Approximating a Derivative

- Derivative of a function $f(x)$ at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

- As an approximation, we can just write

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h}$$

  and this is applicable for very small values of h.

- But we will start the discussion with this.

Introduction to Numerical Differentiation

Taylor expansion of $f(x+h)$

We can start with Taylor expansion of $f(x+h)$ about x as

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

Looking at above we can write

$$\boxed{\boxed{f'(x) = \frac{f(x+h)-f(x)}{h}} - \frac{1}{2}hf''(x)} \tag{1}$$

Eq. 1 shows that approximation of derivative by $\dfrac{f(x+h)-f(x)}{h}$ induces an error (called truncation error) which is of the order of h (written as $O(h)$).

Introduction to Numerical Differentiation

Forward-difference formula

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

Eqs. 1 and 2 are known as the forward-difference formula if $h > 0$ and the backward-difference formula if $h < 0$.

To note: If the second derivative is close to zero, this simple two point formula can be used to approximate the derivative.

Numerical Differentiation

Example

Use the forward-difference formula to approximate the derivative of $f(x) = ln\ x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.

h	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{h}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

The exact answer at 1.8 is 0.555. And we see that as h decreases answer gets better, and the error bound become smaller.

Numerical Differentiation

Consider the following two Taylor series expansions of $f(x+h)$

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

By subtraction, we obtain

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2}{3!}h^3 f'''(x) + \frac{2}{5!}f^{(5)}(x) + \ldots\ldots$$

The above can be rewritten

$$\boxed{f'(x) = \frac{1}{2h}[f(x+h) - f(x-h)]} - \frac{h^2}{3!}f'''(x) - \frac{h^4}{5!}f^{(5)}(x) - \ldots.. \quad (3)$$

Numerical Differentiation

Central difference formula, also called 3-point midpoint formula

$$f'(x) \equiv \frac{1}{2h}[f(x+h) - f(x-h)] \tag{4}$$

where the truncation error is $\frac{-1}{6}h^2 f'''(x)$ which makes it $O(h^2)$, smaller than the previous formula. This is the second-order approximation to the first derivative. We will use this while discussing the solution time-dependent Schrödinger's equation.

Numerical Differentiation

Three point Endpoint Formula or second-order forward difference formula

$$f'(x) = \frac{1}{2h}[-3f(x) + 4f(x+h) - f(x+2h)] + \frac{h^2}{3}f^{(3)}(x) \tag{5}$$

Similar to the 3-point formulas, 5-point formulas can also be derived.

Numerical Differentiation

Compute the first-derivative of $f(x) = exp(x)$ using

1. first-order forward difference
2. second-order Central-difference formula
3. second-order forward difference, Eq. 5

Use $h = 0.4$, 0.2 and 0.1. Make a table.

2nd derivatives

In a similar fashion like in the previous slides, formula for 2nd and 3rd degree derivatives can also be derived. Below we show the formula for 2nd derivatives.

2nd derivative: backward-difference

- 1^{st}-order formulae:
  $f''(x) = \frac{1}{h^2}(f(x) - 2f(x-h) + f(x-2h) + O(h))$
- 2^{nd}-order formulae:
  $f''(x) = \frac{1}{h^2}(2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h) + O(h^2))$

2nd derivative: forward-difference

- 1^{st}-order formulae:
  $f''(x) = \frac{1}{h^2}(f(x+2h) - 2f(x+h) + f(x) + O(h))$
- 2^{nd}-order formulae:
  $f''(x) = \frac{1}{h^2}(-f(x+3h) + 4f(x+2h) - 5f(x+h) + 2f(x) + O(h^2))$

2nd derivatives

2nd derivative: central-difference

- 2^{nd}-order formulae:
$f''(x) = \frac{1}{h^2}(f(x+h) - 2f(x) + f(x-h) + O(h^2))$
- 4^{th}-order formulae: $f''(x) = \frac{1}{12h^2}(-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)) + O(h^4)$

Assignment

Let $f(x) = cos(x)$.

- Calculate approximations for $f'(0.8)$ with $h =$ 0.1, 0.001 and 0.0001 using 2nd-order central-difference formula and the central-difference formula of 4th-order. Remember that we have not seen the 4th-order formula yet. Either derive it or look up online.
- Calculate approximations for $f''(0.8)$ with $h =$ 0.1, 0.001 using the 2nd-order central-difference formula.

END