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Lecture Title: Numerical differentiation

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Numerical differentiation

Finite difference formulas:

By definition, the derivative of $f(x)$ at a value x is

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \qquad (1)$$

Using Taylor theorem then

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

Where (c) is between (x) and (x + h) Equation (2) implies the following formula:

Two – point forward difference formula

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

Where (c) is between(x)and (x + h)

The approximate formula:

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

Example

Use the two-point forward difference formula with h=0.1 to approximate the derivative of $f(x) = 1/x$ at x=2

The two-point forward

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} = \frac{\frac{1}{2.1} - \frac{1}{2}}{0.1} \approx -0.2381$$

The difference between this approximation and the correct derivative $f'(x) = -x^{-2}$ at x=2 is the error

-0.2381-(-0.2500)=0.0119

Compare this to the error predicted by the formula, which is $h\ f''(c)/2$ for some c between 2 and 2.1. Since $f''(x) = 2x^{-3}$, the error must be between

$(0.1)2^{-3} \approx 0.0125$ and $(0.1)(2.1)^{-3} \approx 0.0108$

Two - point centered- difference formula:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(c)$$

Where $x - h < c < x + h$

Example:

Use the two-point centered-difference formula with h=0.1 to approximate the derivative of $f(x) = 1/x$ at x=2

The two – point centered-difference formula evaluates to

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \approx \frac{\frac{1}{2.1} - \frac{1}{1.9}}{0.2} \approx -0.2506$$

The first differentiation:

Forward difference formulas:

- Two- points

$$f'(x_i) = \frac{1}{h}(f_{i+1} - f_i) + o(h)$$

Central difference formula:

- Two - point

$$f'(x_i) = \frac{1}{2h}(f_{i+1} - f_{i-1}) + o(h^2)$$

Backward difference formula:

- Two-point

$$f'(x_i) = \frac{1}{h}(f_i - f_{i-1}) + o(h)$$

Where:

$h \equiv$ The step

$x_i \equiv$ the point at which we want to determine the value of the differentiation

$f_i \equiv f(x_i)$

$f_{i+1} \equiv f(x_i + h)$

$f_{i-1} \equiv f(x_i - h)$

$o(h),\ o(h^2) \equiv$ The error in the formula and depends on the value of h. (but always these errors are neglected)

Example

If $f(x) = 4x^3 - 5x$. Calculate the value of $f'(2.0)$ using all formulas, take (h=0.01)

The solution:

x	F(x)
1.99	21.57240
2.00	22.00000

2.01	22.43240

1-Forward formula:

$$f'(x_i) = \frac{1}{h}(f_{i+1} - f_i)$$

$$f'(2.0) = \frac{1}{0.01}((22.43240) - (22.00000)) = 43.24000$$

2-Central formula:

$$f'(x_i) = \frac{1}{2h}(f_{i+1} - f_{i-1})$$

$$f'(2.0) = \frac{1}{2(0.01)}((22.43240) - (21.57240)) = 43.00000$$

3-Backward formula:

$$f'(x_i) = \frac{1}{h}(f_i - f_{i-1})$$

$$f'(2.0)=\frac{1}{0.01}((22.00000)-(21.57240))=42.76000$$

The exact of this differentiation

$$f'(x)=12x^2-5 \Rightarrow f'(2.0)=12(2)^2-5=43$$

So : the central formula is more accurate than the forward & backward

The second differentiation:

1-Forward difference formulas:

- Three - points

$$f''(x_i)=\frac{1}{h^2}(f_{i+2}-2f_{i+1}+f_i)+o(h)$$

2-Central difference formula:

- Three - point

$$f''(x_i) = \frac{1}{h^2}(f_{i+1} - 2f_i + f_{i-1}) + o(h^2)$$

3-Backward difference formula:

- Three - point

$$f''(x_i) = \frac{1}{h^2}(f_i - 2f_{i-1} + f_{i-2}) + o(h)$$

Where:

$h \equiv$ The step

$x_i \equiv$ The point at which we want to determine the value of the differentiation

$f_i \equiv f(x_i)$

$f_{i+1} \equiv f(x_i + h)$

$f_{i-1} \equiv f(x_i - h)$

$f_{i+2} \equiv f(x_i + 2h)$

$f_{i-2} \equiv f(x_i - 2h)$

$o(h), o(h^2) \equiv$ The error in the formula and depends on the value of h. (but always these errors are neglected)

Example

If $f(x) = x^3 + 5x^2 - 7x + 9$. Calculate the value of $f''(1.0)$ using all formulas, take

(h=0.005)

The solution:

x	F(x)
0.990	7.94080
0.995	7.97020
1.000	8.00000
1.005	8.03020
1.01	8.0608

0	0

1-Forward formula:

$$f''(x_i) = \frac{1}{h^2}(f_{i+2} - 2f_{i+1} + f_i)$$

$$f''(1.0) = \frac{1}{(0.005)^2}((8.06080) - 2(8.03020) + (8.00000)) = 16.00000$$

2-Central formula:

$$f''(x_i) = \frac{1}{h^2}(f_{i+1} - 2f_i + f_{i-1})$$

$$f''(1.0) = \frac{1}{(0.005)^2}((8.03020) - 2(8.00000) + (7.97020)) = 16.00000$$

3-Backward formula:

$$f''(x_i) = \frac{1}{h^2}(f_i - 2f_{i-1} + f_{i-2})$$

$$f''(1.0) = \frac{1}{(0.005)^2}((8.00000) - 2(7.97020) + (7.94080)) = 16.00000$$

The exact of this differentiation

$$f'(x) = 3x^2 + 10x - 7 \Rightarrow f''(x) = 6x + 10 \Rightarrow f''(1.0) = 16$$

Exercises

1-Use all formulas to approximate $f'(1)$ and find the approximation error, where $f(x) = \ln x$ for

$(i)\ h = 0.1, \quad (ii)\ h = 0.01 \quad (iii)\ h = 0.001$

2-Use all formulas to approximate $f''(1)$, where $f(x) = x^{-1}$ for $(i)\ h = 0.1,\ (ii)\ h = 0.01\ (iii)\ h = 0.001$ and find the approximation error