NUMERICAL METHODS
BEKG2452
NUMERICAL DIFFERENTIATION
(Second Derivative)

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Learning Outcomes

At the end of this topic, student should be able to:

1. Find the second derivative of a function by using forward, backward and central difference approximation.

2. Find the second derivative of a function by using high accuracy differentiation formula.

Numerical Differentiation

(Estimating the derivative of a function at a specific point)

Forward, Backward, Central Difference Approximation of First Derivatives

Forward, Backward, Central Difference Approximation of Second Derivatives

Taylor Series Expansion / Interpolation

Forward D.A. Backward D.A.	Accuracy $O(h)$:
Centered D.A. High Accuracy F.D.A. High Accuracy B.D.A.	Accuracy $O(h^2)$:
High Accuracy C.D.A.	Accuracy $O(h^4)$:

Forward D.A. Backward D.A.	Accuracy $O(h)$:
Centered D.A. High Accuracy F.D.A. High Accuracy B.D.A.	Accuracy $O(h^2)$:
High Accuracy C.D.A.	Accuracy $O(h^4)$:

5.4 Finite Divided Difference Approximations

- Taylor series expansions can be used to derive finite-divided-difference approximations of derivatives.

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \dots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n + R_n$$

5.4 Finite Divided Difference Approximations

- The second derivative of a function/ a set of data can be obtained by using:

  - ❑ forward difference approximation
  - ❑ backward difference approximation
  - ❑ centered difference approximation
  - ❑ high-accuracy difference formulas

5.5 Finite difference approximates of second derivative

- Forward difference approximation, $O(h)$

$$f'' \approx \frac{1}{h^2}[f(x) - 2f(x+h) + f(x+2h)]$$

5.5 Finite difference approximates of second derivative

Example

Use forward difference approximation to estimate the second derivative of:

$$f(x) = 0.13x^5 - 0.75x^3 + 0.12x^2 - 0.5x + 1$$

at $x = 0.5$ and step size of $h = 0.25$.

Find the percentage of relative error if the solution f"(0.5) is -1.685.

5.5 Finite difference approximates of second derivative

Solution

x$= 0.5 \quad \longrightarrow \quad f(x) = 0.6903$

x$+h = 0.75 \quad \longrightarrow \quad f(x+h) = 0.4069$

x$+2h = 1 \quad \longrightarrow \quad f(x+2h) = 0$

- $f'' \approx \frac{1}{h^2}[f(x) - 2f(x+h) + f(x+2h)]$

$$f''(0.5) = \frac{1}{0.25^2}[0.6903 - 2(0.4069) + 0]$$

$$= -1.976$$

Percentage of relative error $= \frac{|-1.685-(-1.976)|}{|-1.685|} \times 100\% = 17.27\%$

5.5 Finite difference approximates of second derivative

- Backward difference approximation, $O(h)$

$$f''(x) \approx \frac{1}{h^2}[f(x-2h) - 2f(x-h) + f(x)]$$

5.5 Finite difference approximates of second derivative

Example

Use backward difference approximation to estimate the second derivative of:

$$f(x) = 0.13x^5 - 0.75x^3 + 0.12x^2 - 0.5x + 1$$

at $x = 0.5$ and step size of $h = 0.25$. Hence, calculate the percentage of relative error.

5.5 Finite difference approximates of second derivative

Solution

x= $0.5 \quad \longrightarrow \quad f(x) = 0.6903$

$x - h = 0.25 \quad \longrightarrow \quad f(x-h) = 0.8709$

$x - 2h = 0 \quad \longrightarrow \quad f(x-2h) = 1$

- $f''(x) \approx \frac{1}{h^2}[f(x-2h) - 2f(x-h) + f(x)]$

$$f''(0.5) = \frac{1}{0.25^2}[1 - 2(0.8709) + 0.6903]$$
$$= -0.824$$

Percentage of relative error $= \frac{|-1.685-(-0.824)|}{|-1.685|} \times 100\% = 51.1\%$

5.5 Finite difference approximates of second derivative

- Centered difference approximation, $O(h^2)$

$$f''(x) \approx \frac{1}{h^2}[f(x+h) - 2f(x) + f(x-h)]$$

5.5 Finite difference approximates of second derivative

Example

Use centered difference approximation to estimate the second derivative of:

$$f(x) = 0.13x^5 - 0.75x^3 + 0.12x^2 - 0.5x + 1$$

at $x = 0.5$ and step size of $h = 0.25$.

5.5 Finite difference approximates of second derivative

Solution

x= 0.5 $\quad \longrightarrow \quad f(x) = 0.6903$

$x + h = 0.75 \quad \longrightarrow \quad f(x+h) = 0.4069$

$x - h = 0.25 \quad \longrightarrow \quad f(x-h) = 0.8709$

- $f''(x) \approx \frac{1}{h^2}[f(x+h) - 2f(x) + f(x-h)]$

$$f''(0.5) = \frac{1}{0.25^2}[0.4069 - 2(0.6903) + 0.8709]$$

=-1.6448

Percentage of relative error $= \frac{|-1.685-(-1.6448)|}{|-1.685|} \times 100\% = 2.39\%$

5.5 Finite difference approximates of second derivative

Example

Given the following data

t	1	2	3	4	5	6	7
$f(t)$	-1.8	-3.8	4.2	34.2	103	232.2	448.2

Calculate $f''(4)$ with step size of 1 by using forward and backward difference approximation of $O(h)$ and centered difference approximation of $O(h^2)$.

5.5 Finite difference approximates of second derivative

Solution

$$t = 4 \quad \dashrightarrow \quad f(t) = 34.2$$
$$t + h = 5 \quad \dashrightarrow \quad f(t+h) = 103$$
$$t + 2h = 6 \quad \dashrightarrow \quad f(t+2h) = 232.2$$
$$t - h = 3 \quad \dashrightarrow \quad f(t-h) = 4.2$$
$$t - 2h = 2 \quad \dashrightarrow \quad f(t-2h) = -3.8$$

- Forward difference approximation, *O*(*h*)

$$f'' \approx \frac{1}{h^2}[f(t) - 2f(t+h) + f(t+2h)]$$
$$f''(4) = \frac{1}{1^2}[34.2 - 2(103) + 232.2] = 60.4$$

5.5 Finite difference approximates of second derivative

Solution (cont.)

- Backward difference approximation, $O(h)$

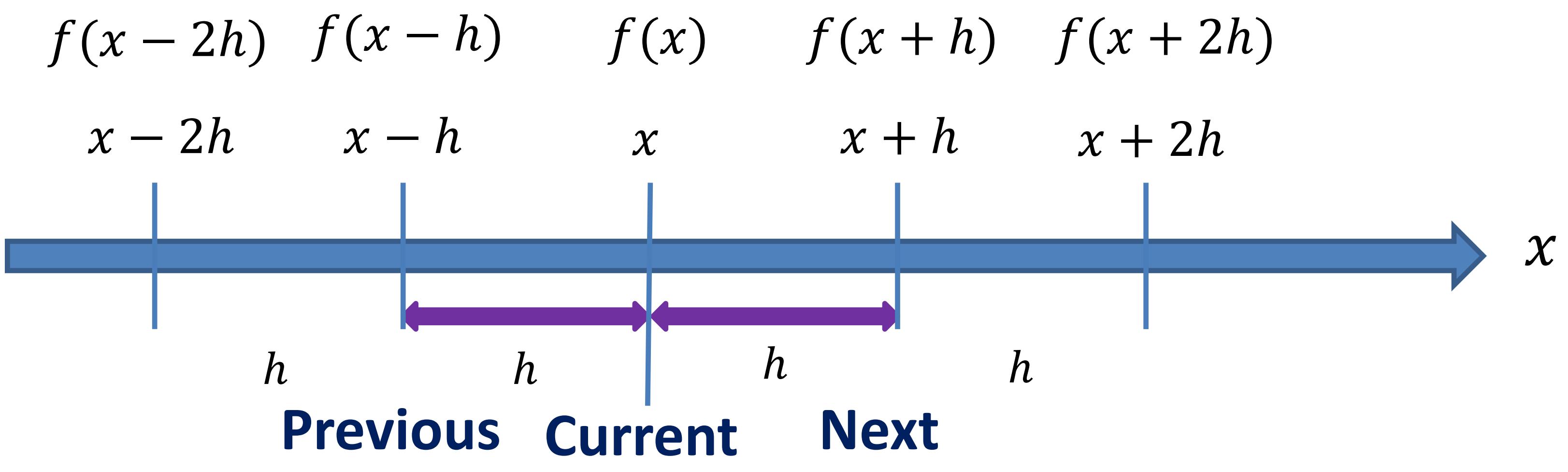
$$f''(t) \approx \frac{1}{h^2}[f(t-2h) - 2f(t-h) + f(t)]$$
$$f''(4) = \frac{1}{1^2}[-3.8 - 2(4.2) + 34.2] = 22$$

- Centered difference approximation, $O(h^2)$

$$f''(t) \approx \frac{1}{h^2}[f(t+h) - 2f(t) + f(t-h)]$$
$$f''(4) \approx \frac{1}{1^2}[103 - 2(34.2) + 4.2] = 38.8$$

5.5 Finite difference approximates of second derivative

Time Line:



Step size: h

5.5 Finite difference approximates of second derivative

Exercise

Given a function

$$f(t) = 2e^{\cos 3t}.$$

Use forward and backward difference approximation of $O(h)$ and centered difference approximation of $O(h^2)$ to approximate $f''(0.7)$ with step size of 0.1.

ANSWER:

Forward= 10.3596; Backward= 16.6756; Centered= 13.5844

5.6 High accuracy second derivative formula

❖ Forward difference approximation, $O(h^2)$

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

❖ Backward difference approximation, $O(h^2)$

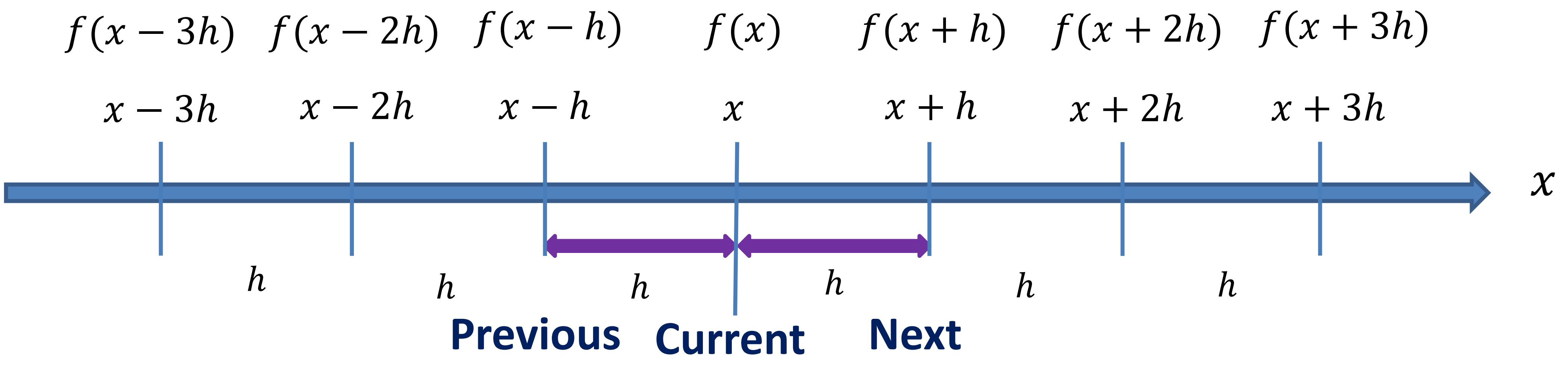
$$f''(x) \approx \frac{1}{h^2}[2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h)]$$

❖ Centered difference approximation, $O(h^4)$

$$f''(x) \approx \frac{1}{12h^2}[-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)]$$

5.6 High accuracy second derivative formula

Time Line:



Step size: h

5.6 High accuracy second derivative formula

Example

Use high accuracy difference approximation to estimate the second derivative of:

$$f(t) = 4e^{\sin 2t} - 1$$

at $x = 0.5$ and step size of $h = 0.1$.

5.6 High accuracy second derivative formula

Solution

- $f(t) = 4e^{\sin 2t} - 1$

t	0.2	0.3	0.4	0.5	0.6	0.7	0.8
f(t)	4.9045	6.0353	7.1960	8.2791	9.1587	9.7161	9.8685

- Forward difference, $O(h^2)$

$$f''(t) \approx \frac{1}{h^2}[-f(t+3h) + 4f(t+2h) - 5f(t+h) + 2f(t)]$$

$f''(0.5)$= -23.9665

5.6 High accuracy second derivative formula

Solution (cont.)

- Backward difference, $O(h^2)$

$$f''(t) \approx \frac{1}{h^2}[2f(t) - 5f(t-h) + 4f(t-2h) - f(t-3h)]$$

$f''(0.5)$= -18.5345

- Centered difference, $O(h^4)$

$$f''(t) \approx \frac{1}{12h^2}[-f(t+2h) + 16f(t+h) - 30f(t) + 16f(t-h) - f(t-2h)]$$

$f''(0.5)$= -20.4027

5.6 High accuracy second derivative formula

Example

Given the following data

t	1	2	3	4	5	6	7
f(t)	-1.8	-3.8	4.2	34.2	103	232.2	448.2

Use forward and backward difference approximation of $O(h^2)$ and centered difference approximation of $O(h^4)$ to find $f''(4)$ with h=1. Find the percentage of relative error for each approximations if the true value is 38.4.

5.6 High accuracy second derivative formula

Solution

t	1	2	3	4	5	6	7
f(t)	-1.8	-3.8	4.2	34.2	103	232.2	448.2

- Forward difference, $O(h^2)$

$$f''(t) \approx \frac{1}{h^2}[-f(t+3h) + 4f(t+2h) - 5f(t+h) + 2f(t)]$$

$$f''(4) \approx \frac{1}{1^2}[-f(7) + 4f(6) - 5f(5) + 2f(4)]$$

$f''(4) = 34$

Percent relative error $= \frac{|38.4 - 34|}{38.4} \times 100\% = 11.46\%$

5.6 High accuracy second derivative formula

Solution (cont.)

t	1	2	3	4	5	6	7
f(t)	-1.8	-3.8	4.2	34.2	103	232.2	448.2

- Backward, $O(h^2)$

$$f''(t) \approx \frac{1}{h^2}[2f(t) - 5f(t-h) + 4f(t-2h) - f(t-3h)]$$

$$f''(4) \approx \frac{1}{1^2}[2f(4) - 5f(3) + 4f(2) - f(1)]$$

$f''(4) = 34$

Percent relative error $= \frac{|38.4 - 34|}{38.4} \times 100\% = 11.46\%$

5.6 High accuracy second derivative formula

Solution (cont.)

t	1	2	3	4	5	6	7
f(t)	-1.8	-3.8	4.2	34.2	103	232.2	448.2

- Centered, $O(h^4)$

$$f''(t) \approx \frac{1}{12h^2}[-f(t+2h) + 16f(t+h) - 30f(t) + 16f(t-h) - f(t-2h)]$$

$$f''(4) \approx \frac{1}{12(1^2)}[-f(6) + 16f(5) - 30f(4) + 16f(3) - f(2)]$$

$$f''(4) = 38.4$$

$$\text{Percent relative error} = \frac{|38.4 - 38.4|}{38.4} \times 100\% = 0\%$$

5.6 High accuracy second derivative formula

Exercise 1

Given a function

$$f(t) = 2e^{\cos 3t}.$$

Use forward and backward difference approximation of $O(h)$ and centered difference approximation of $O(h^2)$ to approximate $f''(0.7)$ with step size of 0.1. Suppose the true value is 13.5807. Calculate the percent relative error for each method.

ANSWER:

Forward=12.6984, ε= 6.5%; Backward=15.9764, ε=17.64%;

Centered=13.5955, ε=0.11%

5.6 High accuracy second derivative formula

Exercise 2

Given that

x	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3
$f(x)$	24.5325	29.9641	36.5982	44.7012	54.5982	66.6863	81.4509	99.4843

Use the high accuracy forward and backward difference approximation of $O(h^2)$ and centered difference approximations of $O(h^2)$ and $O(h^4)$ of the second derivatives formula to estimate $f''(2.0)$ using $h = 0.1$.

ANSWER:

Forward=208.42; Backward=211.91; Centered=218.37

5.6 High accuracy second derivative formula

Exercise 3

Given a function

$$f(t) = t\cos t.$$

Use approximation of $O(h^2)$ and $O(h^4)$ to find $f''(2.0)$ with step size h= 0.2.