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Lecture 10

Numerical Differention

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Numerical Differentiation

Forward, backward, and central difference formulas for the first derivative

The forward, backward, and central finite difference formulas are the simplest finite difference approximations of the derivative. In these approximations, illustrated in Fig. 8-5, the derivative at point (x_i) is calculated from the values of two points. The derivative is estimated as the value of the slope of the line that connects the two points.

Forward difference is the slope of the line that connects points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$:

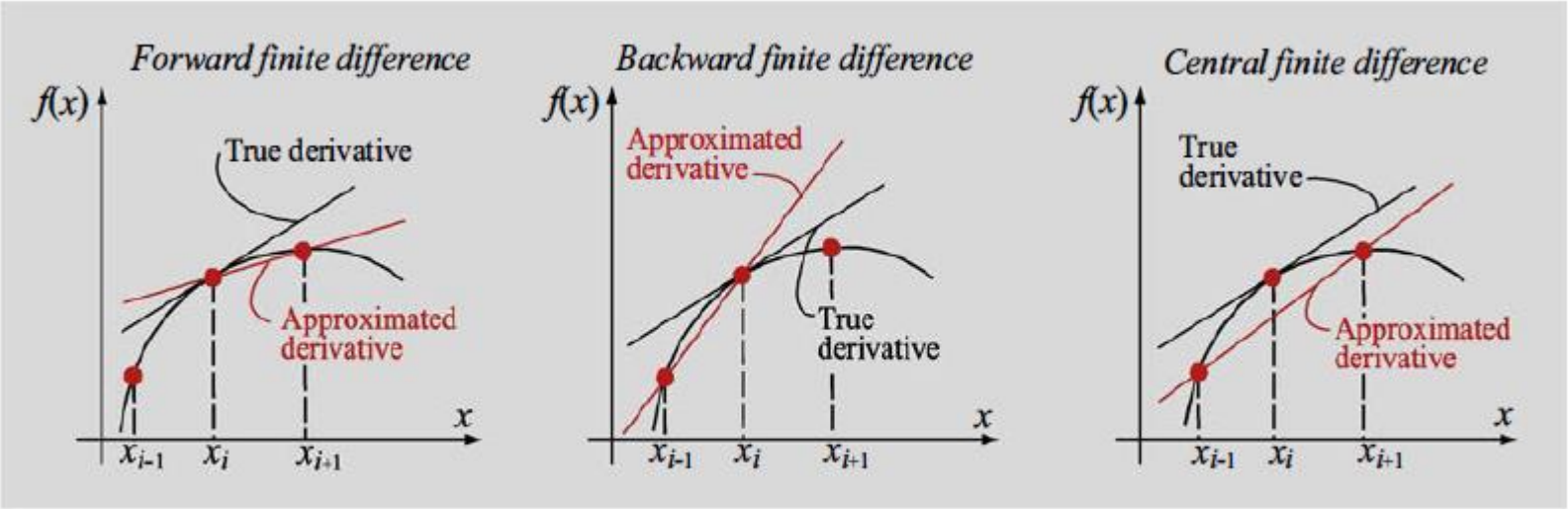
$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

Backward difference is the slope of the line that connects points $(x_{i-1}, f(x_{i-1}))$ and $(x_i, f(x_i))$:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

Central difference is the slope of the line that connects points $(x_{i-1}, f(x_{i-1}))$ and $(x_{i+1}, f(x_{i+1}))$:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$



Finite difference approximation of derivative.

Example

Consider the function $f(x) = x^3$. Calculate its first derivative at point $x = 3$ numerically with the forward, backward, and central finite difference formulas and using:

(*a*) Points $x = 2$, $x = 3$, and $x = 4$.

(*b*) Points $x = 2.75$, $x = 3$, and $x = 3.25$.

Compare the results with the exact (analytical) derivative.

SOLUTION

***Analytical differentiation*:** The derivative of the function is $f'(x) = 3x^2$, and the value of the derivative at $x = 3$ is $f'(3) = 3 \cdot 3^2 = 27$.

Numerical differentiation

(*a*) The points used for numerical differentiation are:

x:	2	3	4
$f(x)$:	8	27	64

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(3)}{4-3} = \frac{64-27}{1} = 37 \qquad error = \left|\frac{37-27}{27}\cdot 100\right| = 37.04\,\%$$

Backward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2)}{3-2} = \frac{27-8}{1} = 19 \qquad error = \left|\frac{19-27}{27}\cdot 100\right| = 29.63\,\%$$

Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(2)}{4-2} = \frac{64-8}{2} = 28 \qquad error = \left|\frac{28-27}{27}\cdot 100\right| = 3.704\ \%$$

(*b*) The points used for numerical differentiation are:

x:	2.75	3	3.25
$f(x)$:	2.75^3	3^3	3.25^3

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(3)}{3.25-3} = \frac{3.25^3-27}{0.25} = 29.3125 \qquad error = \left|\frac{29.3125-27}{27}\right|\cdot 100 = 8.565\ \%$$

Backward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2.75)}{3-2.75} = \frac{27-2.75^3}{0.25} = 24.8125 \qquad error = \left|\frac{24.8125-27}{27}\right|\cdot 100 = 8.102\ \%$$

Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(2.75)}{3.25-2.75} = \frac{3.25^3-2.75^3}{0.5} = 27.0625 \qquad error = \left|\frac{27.0625-27}{27}\right|\cdot 100 = 0.2315\ \%$$

Finite Difference Formulas

define h as given below

$$h = x_{i+1} - x_i$$

Two-point forward difference formula for first derivative

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

Two-point backward difference formula for first derivative

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

Two-point central difference formula for first derivative

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

Three-point forward difference formulas for the first derivative

$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h} + O(h^2)$$

Three-point backward difference formulas for the first derivative

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2)$$

Example

Consider the function $f(x) = x^3$. Calculate the first derivative at point $x = 3$ numerically with the three-point forward difference formula, using:

(*a*) Points $x = 3$, $x = 4$, and $x = 5$.

(*b*) Points $x = 3$, $x = 3.25$, and $x = 3.5$.

Compare the results with the exact value of the derivative, obtained analytically.

SOLUTION

***Analytical differentiation*:** The derivative of the function is $f'(x) = 3x^2$, and the value of the derivative at $x = 3$ is $f'(3) = 3 \cdot 3^2 = 27$.

Numerical differentiation

(*a*) The points used for numerical differentiation are:

x:	3	4	5
$f(x)$:	27	64	125

Using Eq. (8.24), the derivative using the three-point forward difference formula is:

$$f'(3) = \frac{-3f(3)+4f(4)-f(5)}{2 \cdot 1} = \frac{-3 \cdot 27+4 \cdot 64-125}{2} = 25 \qquad error = \left|\frac{25-27}{27}\right| \cdot 100 = 7.41 \ \%$$

(*b*) The points used for numerical differentiation are:

x:	3	3.25	3.5
$f(x)$:	27	3.25^3	3.5^3

Using Eq. (8.24), the derivative using the three points forward finite difference formula is:

$$f'(3) = \frac{-3f(3)+4f(3.25)-f(3.5)}{2 \cdot 0.25} = \frac{-3 \cdot 27+4 \cdot 3.25^3-3.5^3}{0.5} = 26.875$$

$$error = \left|\frac{26.875-27}{27}\right| \cdot 100 = 0.46 \ \%$$

The results show that the three-point forward difference formula gives a much more accurate value for the first derivative than the two-point forward finite difference formula in Example 8-1. For $h = 1$ the error reduces from 37.04% to 7.4%, and for $h = 0.25$ the error reduces from 8.57% to 0.46%.

Finite Difference Formulas

First Derivative		
Method	**Formula**	**Truncation Error**
Two-point forward difference	$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Three-point forward difference	$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
Two-point backward difference	$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Three-point backward difference	$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$
Two-point central difference	$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
Four-point central difference	$f'(x_i) = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$	$O(h^4)$

Second Derivative		
Method	**Formula**	**Truncation Error**
Three-point forward difference	$f''(x_i) = \frac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2}$	$O(h)$
Four-point forward difference	$f''(x_i) = \frac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
Three-point backward difference	$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2}$	$O(h)$
Four-point backward difference	$f''(x_i) = \frac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Three-point central difference	$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$
Five-point central difference	$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2}$	$O(h^4)$

Example

Consider the function $f(x)=\frac{2^x}{x}$. Calculate the second derivative at $x=2$ numerically with the three-point central difference formula using:

(*a*) Points $x=1.8$, $x=2$, and $x=2.2$.

(*b*) Points $x=1.9$, $x=2$, and $x=2.1$.

Compare the results with the exact (analytical) derivative.

SOLUTION

***Analytical differentiation*:** The second derivative of the function $f(x)=\frac{2^x}{x}$ is:

$$f''(x)=\frac{2^x[\ln(2)]^2}{x}-\frac{2\cdot 2^x\ln(2)}{x^2}+\frac{2\cdot 2^x}{x^3}$$

and the value of the derivative at $x=2$ is $f''(2)=0.574617$.

(*a*) The numerical differentiation is done by substituting the values of the points $x=1.8$, $x=2$, and $x=2.2$ in equation given below

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

The operations are done with MATLAB, in the Command Window:

```
>> x=[1.8  2  2.2  ];
>>  f=(2.^x)./(x)
f =
    1.9346    2.0000    2.0885

>> h=0.2;
>>
>> df=(f(1)-2*f(2)+f(3))./h.^2

df =
    0.5775
```

(*b*) The numerical differentiation is done by substituting the values of the points $x = 1.9$, $x = 2$, and $x = 2.1$ The operations are done with MATLAB, in the Command Window:

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

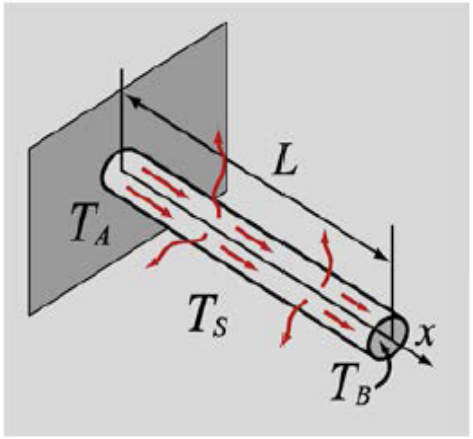
```
>> x=[1.9  2  2.1];
>>  f=(2.^x)./(x)
f =
    1.9643    2.0000    2.0415
>> h=0.1;
>>
>> df=(f(1)-2*f(2)+f(3))./h.^2
df =
    0.5753
```

Example

A fin is an extended surface used to transfer heat from a base material (at $x = 0$) to an ambient. Heat flows from the base material through the base of the fin, through its outer surface, and through the tip. Measurement of the temperature distribution along a pin fin gives the following data:

x (cm)	0	1	2	3	4	5	6	7	8	9	10
T (K)	473	446.3	422.6	401.2	382	364.3	348.0	332.7	318.1	304.0	290.1

The fin has a length $L = 10$ cm, constant cross-sectional area of 1.6×10^{-5} m^2, and thermal conductivity $k = 240$ W/m/K. The heat flux (W/m^2) is given by $q_x = -k\frac{dT}{dx}$



(*a*) Determine the heat flux at $x = 0$. Use the three-point forward difference formula for calculating the derivative.

(*b*) Determine the heat flux at $x = L$. Use the three-point backward difference formula for calculating the derivative.

(*c*) Determine the amount of heat (in W) lost between $x = 0$ and $x = L$. (The heat flow per unit time in Watts is the heat flux multiplied by the cross-sectional area of the fin.)

Solution

(*a*) The three point forward difference formula for the derivative is:

$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$$

In the present problem $h = 0.01\text{m}$. Applying the formula at $x = 0$ yields:

$$\left.\frac{dT}{dx}\right|_{x=0} = \frac{-3T(0) + 4T(1) - T(2)}{2(0.01)} = \frac{-3(473) + 4(446.3) - 422.6}{0.02} = -2820 \text{ K/m}$$

Therefore, the heat flux at $x = 0$ is: $q_x|_{x=0} = -k\left.\frac{dT}{dx}\right|_{x=0} = -(240)(-2820) = 676.8 \text{ kW/m}^2$

(*b*) The three point backward difference formula for the derivative is:

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$$

Applying the formula at $x = 0.1\text{ m}$ yields:

$$\left.\frac{dT}{dx}\right|_{x=10} = \frac{T(8) - 4T(9) + 3T(10)}{2(0.01)} = \frac{318.1 - 4(304) + 3(290.1)}{0.02} = -1380 \text{ K/cm}$$