CHAPTER 9

Numerical Differentiation

Numerical Differentiation

- Numerical differentiation requires us to find estimates for the derivative or slope of a function by using the function values at only a set of discrete points.
- Numerical differentiation is used because some functions are unknown or difficult (or impossible) to differentiate exactly.
- One must be very careful when using numerical techniques to estimate the rate of change of measured data, since small errors are exaggerated by differentiation.

Taylor Polynomials

- There are several formulas for approximating a first and second derivatives and these formulas can be found with the use of Taylor polynomials.

- Taylor polynomials, $f(x)$ at x_0 is,

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2$$

$$+ \frac{f'''(x_0)}{3!}(x - x_0)^3 + \ldots\ldots$$

- Let,

$$x = x_0 + h$$

$$h = x - x_0$$

$$f(x_0 + h) \approx f(x_0) + f'(x_0)h + f''(x_0)\frac{h^2}{2!} + f'''(x_0)\frac{h^3}{3!} + \ldots\ldots$$

First Derivatives

- 2 point formulas
  - Forward difference formula
  - Backward difference formula
- 3 point formulas
  - Forward difference formula
  - Backward difference formula
  - Central difference formula
- 5 point formulas
  - Forward difference formula
  - Central difference formula

Two-point formulas

- **2-points Forward** difference formula

$$f(x_i + h) = f(x_i) + f'(x_i)h + f''(x_i)\frac{h^2}{2!} + f'''(x_i)\frac{h^3}{3!} + \ldots\ldots$$

$$f(x_i + h) \approx f(x_i) + f'(x_i)h$$

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

- **2-points Backward** difference formula

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

$$f(x_i - h) \approx f(x_i) - f'(x_i)h$$

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

Example

- Given the following data:

x	1.00	1.05	1.10	1.15	1.20
$f(x)$	1.00000	1.02470	1.04881	1.07238	1.09545

- Use forward and backward two-point formulas to estimate f′(1.05).

Solution

- 2-points Forward difference formula:

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

$$f'(1.05) \approx \frac{f(1.05 + 0.05) - f(1.05)}{0.05}$$

$$f'(1.05) \approx \frac{f(1.10) - f(1.05)}{0.05}$$

$$f'(1.05) \approx \frac{1.04881 - 1.02470}{0.05} = 0.4822$$

Solution (cont.)

- Backward difference formula

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

$$f'(1.05) \approx \frac{f(1.05) - f(1.05 - 0.05)}{0.05}$$

$$f'(1.05) \approx \frac{f(1.05) - f(1.00)}{0.05}$$

$$f'(1.05) \approx \frac{1.02470 - 1.00000}{0.05} = 0.494$$

Three-point formulas

- **3-points Forward** difference formula

$$f(x_i+h) = f(x_i) + hf'(x_i) + \frac{h^2}{2!} f''(x_i) + \ldots\ldots$$

$$f(x_i+2h) = f(x_i) + 2hf'(x_i) + \frac{(2h)^2}{2!} f''(x_i) + \ldots\ldots$$

$$\begin{aligned} 4f(x_i+h) - f(x_i+2h) &= 3f(x_i) + 2hf'(x_i) - \ldots\ldots \\ &\approx 3f(x_i) + 2hf'(x_i) \end{aligned}$$

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

- **3-points Backward** difference formula

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

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

$$\begin{aligned} 4f(x_i - h) - f(x_i - 2h) &= 3f(x_i) - 2hf'(x_i) + \ldots\ldots \\ &\approx 3f(x_i) - 2hf'(x_i) \end{aligned}$$

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

- **3-points Central** difference formula

$$f(x_i + h) = f(x_i) + f'(x_i)h + f''(x_i)\frac{h^2}{2!} + f'''(x_i)\frac{h^3}{3!} + \ldots\ldots$$

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

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

$$f(x_i + h) - f(x_i - h) \approx 2hf'(x_i)$$

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i - h)}{2h}$$

Example

- Given the following data:

x	1.00	1.05	1.10	1.15	1.20
$f(x)$	1.00000	1.02470	1.04881	1.07238	1.09545

- Use forward, backward and central three-point formulas to estimate $f'(1.10)$.

Solution

- 3-points Forward difference formula

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

$$f'(1.10) \approx \frac{1}{2(0.05)}[-3f(1.10) + 4f(1.10+0.05) - f(1.10+2(0.05))]$$

$$\begin{aligned} f'(1.10) \quad &\approx \frac{1}{0.1}[-3f(1.10) + 4f(1.15) - f(1.20)] \\ &\approx \frac{1}{0.1}[-3(1.04881) + 4(1.07238) - 1.09545] \\ &\approx 0.4764 \end{aligned}$$

Solution (cont.)

- 3-points Backward difference formula

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

$$f'(1.10) \approx \frac{1}{2(0.05)}[f(1.10 - 2(0.05)) - 4f(1.10 - 0.05) + 3f(1.10)]$$

$$f'(1.10) \approx \frac{1}{0.1}[f(1.00) - 4f(1.05) + 3f(1.10)]$$

$$\approx \frac{1}{0.1}[1.00000 - 4(1.02470) + 3(1.04881)]$$

$$\approx 0.4763$$

Solution (cont.)

- 3-points Central difference formula

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i - h)}{2h}$$

$$f'(1.10) \approx \frac{f(1.10 + 0.05) - f(1.10 - 0.05)}{2(0.05)}$$

$$\approx \frac{f(1.15) - f(1.05)}{0.1} = \frac{1.07238 - 1.02470}{0.1}$$

$$\approx 0.4768$$

Five-point Formulas

- **5-points Central** difference formula

$$f'(x) \approx \frac{1}{12h}\begin{bmatrix} f(x_i - 2h) - 8f(x_i - h) + \\ 8f(x_i + h) - f(x_i + 2h) \end{bmatrix}$$

- **5-points Forward** difference formula

$$f'(x_i) \approx \frac{1}{12h}[-25f(x_i) + 48f(x_i + h)$$
$$-36f(x_i + 2h) + 16f(x_i + 3h) - 3f(x_i + 4h)]$$

Example

- Given the following data:

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
$f(x)$	1.00000	1.02470	1.04881	1.07238	1.09545	1.11803	1.14018

- Use forward and central five-point formulas to estimate $f'(1.10)$.

Solution

- 5-points Central difference formula

$$f'(1.10) \approx \frac{1}{12(0.05)}[f(1.10-2(0.05))-8f(1.10-0.05)$$
$$+8f(1.10+0.05)-f(1.10+2(0.05))]$$

$$= \frac{1}{12(0.05)}[f(1.00)-8f(1.05)+8f(1.15)-f(1.20)]$$

$$= \frac{1}{0.6}[1.00000-8(1.02470)+8(1.07238)-1.09545]$$
$$= 0.47665$$

Solution (cont.)

- 5-points Forward difference formula

$$f'(1.10) \approx \frac{1}{12(0.05)}[-25f(1.10)+48f(1.15)-36f(1.20)$$
$$+16f(1.25)-3f(1.30)]$$

$$=\frac{1}{0.6}[-25(1.04881)+48(1.07238)-36(1.09545)$$
$$+16(1.11803)-3(1.14018)]$$

$$=0.4762$$

- In general, using more evaluation points with small values of *h* produces greater accuracy.

Second Derivatives

- 3 point formulas
  - Central difference formula

- 5 point formulas
  - Central difference formula

Three-point formulas

- Central difference formula

$$f(x_i+h)=f(x_i)+f'(x_i)h+f''(x_i)\frac{h^2}{2!}+f'''(x_i)\frac{h^3}{3!}+\ldots\ldots$$

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

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

$$f(x_i+h)+f(x_i-h)\approx 2f(x_i)+h^2f''(x_i)$$

- **3-points Central** difference formula (second derivative):

$$f''(x_i) \approx \frac{f(x_i - h) - 2f(x_i) + f(x_i + h)}{h^2}$$

Example

- Given the following data:

x	1.00	1.05	1.10	1.15	1.20
$f(x)$	1.00000	1.02470	1.04881	1.07238	1.09545

- Use central three-point formulas to estimate $f''(1.10)$ with h = 0.05

Solution

- Central three-point difference formula

$$f''(x_i) \approx \frac{f(x_i - h) - 2f(x_i) + f(x_i + h)}{h^2}$$

$$f''(1.10) \approx \frac{1.02470 - 2(1.04881) + (1.07238)}{0.05^2}$$

$$f''(1.10) \approx -0.212$$

Five-point Formulas

- **5-points Central** difference formula (second derivative):

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

Example

- Given the following data:

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
$f(x)$	1.00000	1.02470	1.04881	1.07238	1.09545	1.11803	1.14018

- Use central five-point formulas to estimate $f''(1.10)$.

Solution

- Central difference formula

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

$$f''(x_i) \approx \frac{1}{12(0.05)^2}[-f(1.10 - 2(0.05)) + 16f(1.10 - 0.05) - 30f(1.10) + 16f(1.10 + 0.05) - f(1.10 + 2(0.05))]$$

Solution (cont.)

$$f''(x_i) \approx \frac{1}{0.03}[-f(1.00)+16f(1.05)$$
$$-30f(1.10)+16f(1.15)-f(1.20))]$$
$$\approx \frac{1}{0.03}[-1.00000+16(1.02470)$$
$$-30(1.04881)+16(1.07238)-1.09545)]$$
$$\approx \text{-}0.21567$$

Exercise #1

i) Estimate $f'(1.2)$ using

a) Forward and backward two-point formulas

b) Forward, backward, and central three-point formulas

c) Forward and central five-point formulas

with h=0.1 and h=0.001.

ii) Find the exact value of $f'(1.2)$ and calculate the error for each estimation.

x	$f(x) = cos(x)$
1.000	0.54030
1.100	0.45360
1.198	0.36422
1.199	0.36329
1.200	0.36236
1.201	0.36143
1.202	0.36049
1.300	0.26750
1.400	0.16997

Exercise # 2

i) Estimate $f''(1.2)$ using

a) Central three-point formulas

b) Central five-point formulas

with h = 0.1 and h = 0.001.

ii) Find the exact value of $f''(1.2)$ and calculate the error for each estimation.

x	$f(x) = cos(x)$
1.000	0.54030
1.100	0.45360
1.198	0.36422
1.199	0.36329
1.200	0.36236
1.201	0.36143
1.202	0.36049
1.300	0.26750
1.400	0.16997