

Chapter1: Numerical Differentiation

1.1 Finite Difference Approximation of the Derivative

In finite difference approximations of the derivative, values of the function at different points in the neighborhood of the point $x=a$ are used for estimating the slope. It should be remembered that the function that is being differentiated is prescribed by a set of discrete points. Various finite difference approximation formulas exist. Three such formulas, where the derivative is calculated from the values of two points, are presented in this section.

1.1.1 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. 1-1, 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.

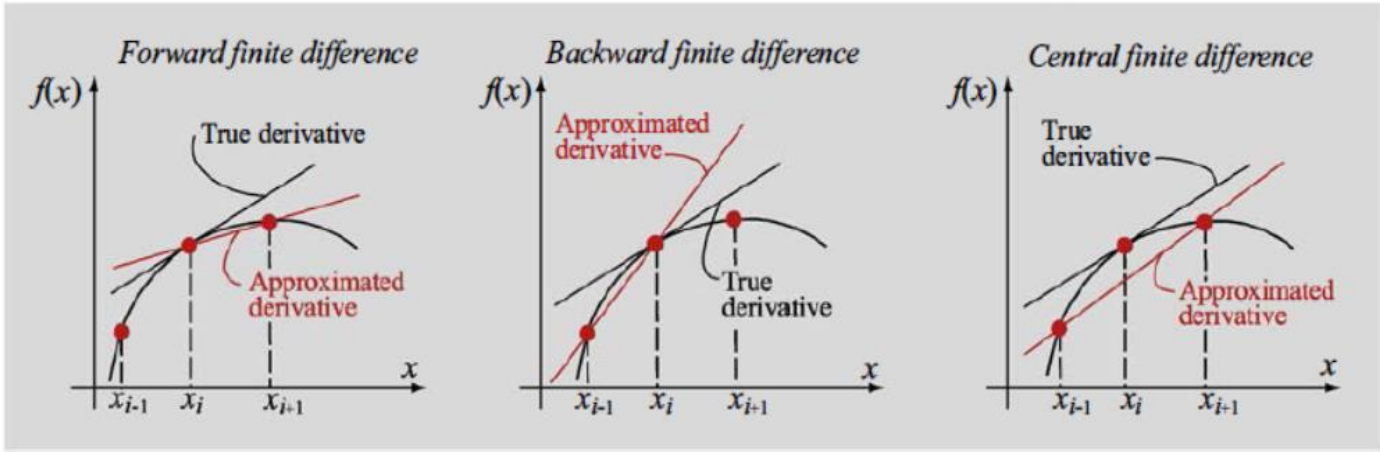


Figure 1-1: Finite difference approximation of derivative.

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

$$\left. \frac{df}{dx} \right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \quad (1.1)$$

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

$$\left. \frac{df}{dx} \right|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \quad (1.2)$$

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

$$\left. \frac{df}{dx} \right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} \quad (1.3)$$

Example 1-1: Comparing numerical and analytical differentiation.

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 $f'(3) = 3(3^2) = 27$.

Numerical differentiation:

(a) The points used for numerical differentiation are:

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

Using Eqs. (1.1) through (1.3), the derivatives using the forward, backward, and central finite difference formulas are:

Forward finite difference:

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

Backward finite difference:

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

Central finite difference:

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

(b) The points used for numerical differentiation are:

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

Using Eqs. (1.1) through (1.3), the derivatives using the forward, backward, and central finite difference formulas are:

Forward finite difference:

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

Backward finite difference:

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

Central finite difference:

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

The results show that the central finite difference formula gives a more accurate approximation. This will be discussed further in the next section. In addition, smaller separation between the points gives a significantly more accurate approximation.

1.2 Finite Difference Formulas Using Taylor Series Expansion

The forward, backward, and central difference formulas, as well as many other finite difference formulas for approximating derivatives, can be derived by using Taylor series expansion. The formulas give an estimate of the derivative at a point from the values of points in its neighborhood. The number of points used in the calculation varies with the formula, and the points can be ahead, behind, or on both sides of the point at which the derivative is calculated. One advantage of using Taylor series expansion for deriving the formulas is that it also provides an estimate for the truncation error in the approximation.

1.2.1 Finite Difference Formulas of First Derivative

Several formulas for approximating the first derivative at point x_i based on the values of the points near x_i are derived by using the Taylor series expansion. All the formulas derived in this section are for the case where the points are equally spaced.

Two-point forward difference formula for first derivative

The value of a function at point x_{i+1} can be approximated by a Taylor series in terms of the value of the function and its derivatives at point x_i :

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \dots \quad (1.4)$$

where $h = x_{i+1} - x_i$; is the spacing between the points. By using two terms Taylor series expansion with a remainder can be rewritten as:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \quad (1.5)$$

where ξ is a value of x between x_i and x_{i+1} . Solving Eq. (1.5) for $f'(x_i)$ yields:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(\xi)}{2!}h \quad (1.6)$$

An approximate value of the derivative $f'(x_i)$ can now be calculated if the second term on the right-hand side of Eq. (1.6) is ignored. Ignoring this second term introduces a truncation (discretization) error. Since this term is proportional to h , the truncation error is said to be on the order of h (written as $O(h)$):

$$\text{truncation error} = -\frac{f''(\xi)}{2!}h = O(h) \quad (1.7)$$

Using the notation of Eq. (1.7), the approximated value of the first derivative is:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - O(h) \quad (1.8)$$

The approximation in Eq. (1.8) is the same as the forward difference formula in Eq. (1.1).

Two-point backward difference formula for first derivative

The backward difference formula can also be derived by application of Taylor series expansion. The value of the function at point x_{i-1} is approximated by a Taylor series in terms of the value of the function and its derivatives at point x_i :

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 - \dots \quad (1.9)$$

where $h = x_i - x_{i-1}$; is the spacing between the points. By using two terms Taylor series expansion with a remainder can be rewritten as:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \quad (1.10)$$

where ξ is a value of x between x_i and x_{i+1} . Solving Eq. (1.10) for $f'(x_i)$ yields:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1}))}{h} + \frac{f''(\xi)}{2!} h \quad (1.11)$$

An approximate value of the derivative $f'(x_i)$ can now be calculated if the second term on the right-hand side of Eq. (1.11) is ignored. This yields:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1}))}{h} + O(h) \quad (1.12)$$

The approximation in Eq. (1.12) is the same as the forward difference formula in Eq. (1.2).

Two-point central difference formula for first derivative

The central difference formula can be derived by using three terms in the Taylor series expansion and a remainder. The value of the function at point x_{i+1} in terms of the value of the function and its derivatives at point x_i is given by:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!} h^2 + \frac{f'''(\zeta_1)}{3!} h^3 \quad (1.13)$$

where ζ_1 is a value of x between x_i and x_{i+1} . The value of the function at point x_{i-1} in terms of the value of the function and its derivatives at point x_i is given by:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!} h^2 - \frac{f'''(\zeta_2)}{3!} h^3 \quad (1.14)$$

where ζ_2 is a value of x between x_{i-1} and x_i . In the last two equations, the spacing of the intervals is taken to be equal so that $h = x_{i+1} - x_i = x_i - x_{i-1}$. Subtracting Eq. (1.14) from Eq. (1.13) gives:

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\zeta_1)}{3!} h^3 + \frac{f'''(\zeta_2)}{3!} h^3 \quad (1.15)$$

An estimate for the first derivative is obtained by solving Eq. (1.15) for $f'(x_i)$ while neglecting the remainder terms, which introduces a truncation error, which is of the order of h^2 :

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h} + O(h^2) \quad (1.16)$$

The approximation in Eq. (1.16) is the same as the central difference formula Eq. (1.3) for equally spaced intervals.

1.2.2 Finite Difference Formulas for the Second Derivative

The same approach used in Section 1.2.1 to develop finite difference formulas for the first derivative can be used to develop expressions for higher-order derivatives. In this section, expressions based on central differences, one-sided forward differences, and one-sided backward differences are presented for approximating the second derivative at a point x_i .

Three-point central difference formula for the second derivative

Central difference formulas for the second derivative can be developed using any number of points on either side of the point x_i , where the second derivative is to be evaluated. The formulas are derived by writing the Taylor series expansion with a remainder at points on either side of x_i in terms of the value of the function and its derivatives at point x_i . Then, the equations are combined in such a way that the terms containing the first derivatives are eliminated. For example, for points x_{i+1} , and x_{i-1} the four-term Taylor series expansion with a remainder is:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\zeta_1)}{4!}h^4 \quad (1.17)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\zeta_2)}{4!}h^4 \quad (1.18)$$

where ζ_1 is a value of x between x_i and x_{i+1} . and ζ_2 is a value of x between x_{i-1} and x_i . Adding Eq. (1.17) and Eq. (1.18) gives:

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + 2\frac{f''(x_i)}{2!}h^2 + \frac{f^{(4)}(\zeta_1)}{4!}h^4 + \frac{f^{(4)}(\zeta_2)}{4!}h^4 \quad (1.19)$$

An estimate for the second derivative can be obtained by solving Eq.(1.19) for $f''(x_i)$ while neglecting the remainder terms. This introduces a truncation error of the order of h^2 .

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{h^2} + O(h^2) \quad (1.20)$$

Example 1-2: Comparing numerical and analytical differentiation.

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:

$$\begin{aligned} f'(x) &= \frac{2^x - x(\ln 2)2^x}{x^2} = \frac{2^x}{x^2} - \ln 2 \frac{2^x}{x} \\ f''(x) &= \frac{2^x(2x) - x^2(\ln 2)2^x}{x^4} - \ln 2 \left(\frac{2^x}{x^2} - \ln 2 \frac{2^x}{x} \right) \\ \Rightarrow f''(x) &= (\ln 2)^2 \frac{2^x}{x} - 2(\ln 2) \frac{2^x}{x^2} + 2 \frac{2^x}{x^3} \end{aligned}$$

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

Numerical differentiation

(a) The numerical differentiation is done by substituting the values of the points $x = 1.8$, $x = 2$, and $x = 2.2$ in Eq. (1.20). The operations are done with MATLAB, in the Command Window:

```
>> xa = [1.8 2 2.2];
>> ya = 2.^xa./xa;
>> df = (ya(1) - 2*ya(2) + ya(3))/0.2^2
df =
    0.57748177389232
```

(b) The numerical differentiation is done by substituting the values of the points $x = 1.9$, $x = 2$, and $x = 2.1$ in Eq. (1.20). The operations are done with MATLAB, in the Command Window:

```
>> xb = [1.9 2 2.1];
>> yb = 2.^xb./xb;
>> dfb = (yb(1) - 2*yb(2) + yb(3))/0.1^2
dfb =
    0.57532441566441
```

Error in part (a): $error = \frac{0.577482 - 0.574617}{0.574617} \cdot 100 = 0.4986 \%$

Error in part (b): $error = \frac{0.575324 - 0.574617}{0.574617} \cdot 100 = 0.1230 \%$

The results show that the three-point central difference formula gives a quite accurate approximation for the value of the second derivative.

1.3 Summary of Finite Difference Formulas for Numerical Differentiation

Table 3-1 lists difference formulas, of various accuracy, that can be used for numerical evaluation of first, second, third, and fourth derivatives. The formulas can be used when the function that is being differentiated is specified as a set of discrete points with the independent variable equally spaced.

Table 1-1: 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	$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2}))}{12h^2}$	$o(h^4)$

1.4 DIFFERENTIATION FORMULAS USING LAGRANGE POLYNOMIALS

The differentiation formulas can also be derived by using Lagrange polynomials. For the first derivative, the two-point central, three-point forward, and three-point backward difference formulas are obtained by considering three points (x_i, y_i) , (x_{i+1}, y_{i+1}) , and (x_{i+2}, y_{i+2}) . The polynomial, in Lagrange form, that passes through the points is given by:

$$f(x) = y_i \frac{(x-x_{i+1})(x-x_{i+2})}{(x_i-x_{i+1})(x_i-x_{i+2})} + y_{i+1} \frac{(x-x_i)(x-x_{i+2})}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} + y_{i+2} \frac{(x-x_i)(x-x_{i+1})}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} \quad (1.21)$$

Differentiating Eq.(1.21) gives:

$$f'(x) = y_i \frac{2x-x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})} + y_{i+1} \frac{2x-x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} + y_{i+2} \frac{2x-x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} \quad (1.22)$$

The first derivative at either one of the three points is calculated by substituting the corresponding value of x (x_i , x_{i+1} or x_{i+2}) in Eq. (1.22). This gives the following three formulas for the first derivative at the three points.

$$f'(x_i) = y_i \frac{2x_i-x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})} + y_{i+1} \frac{2x_i-x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} + y_{i+2} \frac{2x_i-x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} \quad (1.23)$$

When the points are equally spaced, Eq. (1.23) reduces to the **three point forward difference formula**:

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

$$f'(x_{i+1}) = y_i \frac{2x_{i+1}-x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})} + y_{i+1} \frac{2x_{i+1}-x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} + y_{i+2} \frac{2x_{i+1}-x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} \quad (1.24)$$

When the points are equally spaced, Eq. (1.24) reduces to the **two point central difference formula**:

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

Which is:

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

$$f'(x_{i+2}) = y_i \frac{2x_{i+2}-x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})} + y_{i+1} \frac{2x_{i+2}-x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} + y_{i+2} \frac{2x_{i+2}-x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} \quad (1.25)$$

When the points are equally spaced, Eq. (1.24) reduces to the **three point backward difference formula**:

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

(1.4) First Derivatives From Interpolating Polynomials:

We begin with a Newton-Gregory forward polynomial:

$$f(x_t) = f_0 + t\Delta f_0 + \frac{t(t-1)}{2!}\Delta^2 f_0 + \frac{t(t-1)(t-2)}{3!}\Delta^3 f_0 + \dots + \frac{t(t-1)\dots(t-n+1)}{n!}\Delta^n f_0 + \dots \quad (1.26)$$

Differentiating Eq.(1.26) , remembering that f_0 and all the Δ -terms are constants (after all, they are just the numbers from the difference table), we have:

$$\begin{aligned} f'(x_t) &= \frac{d}{dx} [f(x_t)] = \frac{d}{dt} [f(x_t)] \frac{1}{h} \\ &= \frac{1}{h} \left[\Delta f_0 + \frac{(2t-1)}{2!}\Delta^2 f_0 + \frac{3t^2-6t+2}{3!}\Delta^3 f_0 + \dots \right] \end{aligned} \quad (1.27)$$

If we let $t=0$, giving us the derivative corresponding to x_0 , we have:

$$f'(x_0) = \frac{1}{h} \left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \frac{1}{4}\Delta^4 f_0 \dots \right] \quad (1.28)$$

1.5 Use of MATLAB Built-In Functions for Numerical Differentiation

In general, it is recommended that the techniques described in this chapter be used to develop script files that perform the desired differentiation. MATLAB does not have built-in functions that perform numerical differentiation of an arbitrary function or discrete data. There is, however, a built-in function called **diff**, which can be used to perform numerical differentiation, and another built-in function called **polyder**, which determines the derivative of polynomial.

1.5.1 The diff command

The built-in function **diff** calculates the derivative of the functions:

```
>> syms x
>> diff(x^3+2*x^2-1)
ans =
3*x^2 + 4*x
>> diff(x^3+2*x^2-1,2)
ans =
6*x + 4
>> diff(x^3+2*x^2-1,3)
ans =
6
```

1.5.2 The polyder command

The built-in function **polyder** can calculate the derivative of a polynomial (it can also calculate the derivative of a product and quotient of two polynomials).

```
>> p=[4 0 2 5]
p =
    4    0    2    5
>> polyder(p)
ans =
   12    0    2
```

1.6 PROBLEMS

- Given the following data:

x	1	1.2	1.3	1.4	1.5
f(x)	0.6133	0.7882	0.9716	1.1814	1.4117

Find the first derivative $f'(x)$ at the point $x = 1.3$.

- Use the three-point forward difference formula.
- Use the three-point backward difference formula.
- Use the two-point central difference formula.

- The following data is given for the stopping distance of a car on a wet road versus the speed at which it begins braking.

v(mi/h)	12.5	25	37.5	50	62.5	75
d(ft)	20	59	118	197	299	420

Calculate the rate of change of the stopping distance at a speed of 62.5 mph using:

- the two-point backward difference formula, and
 - the three-point backward difference formula.
- Use Lagrange interpolation polynomials to find the finite difference formula for the second derivative at the point $x = x_i$ using the unequally spaced points $x = x_{i+1}$, and $x = x_{i+2}$. What is the second derivative at $x = x_{i+1}$ and at $x = x_{i+2}$?
- Find the first derivative from backward polynomial approximated to the forth difference.
 - Find the second derivative from forward polynomial to the forth difference.
 - Use the data below to estimate the derivative of y at x=1.7:

x	1.3	1.5	1.7	1.9	2.1	2.3	2.5
f(x)	3.669	4.482	5.474	6.686	8.166	9.974	12.182