Chapter 6   Numerical Differentiation and Integration

6.1 Numerical Differentiation

When a function is given as a simple mathematical expression, the derivative can be determined analytically. When analytical differentiation of the expression is difficult or impossible, numerical differentiation has to be used. When the function is specified as a set of discrete data points, differentiation is done by a numerical method.

For a function given in terms of a set of data points, there are two approaches to calculate the numerical approximation of the derivative at one of the points:
1) Finite difference approximation
2) Derivative from curve fitting

6.1.1 Finite Difference Approximation

Finite difference approximation: the derivative at one point is approximated by the slope of the line that connects the two points at both sides of the point.

The derivative $f'(x)$ of a function $f(x)$ at point x=a is defined as

According to the two points used, the formula can be written into three types:
1) **Forward difference**:

2) **Backward difference**:

3) **Central difference**:

Example 6.1   Consider function $f(x)$=sin(x), using the data list below to calculate the first derivative at x=0.5 numerically with forward, backward and central difference formulas, compare them with true value.

xi	sin(xi)
0.45	0.43497
0.50	0.47943
0.55	0.522687

6.1.2 Differentiation Formulas Using Taylor Series

6.1.2.1 First-order Derivative Approximation

These differentiation formulas can be derived by Taylor series expansion. Taylor series can approximate the value of a function at x_{i+1} in terms of the value of the function and its derivatives at x_i as

Where $h = x_{i+1} - x_i$
Dropping the power higher than 2 gives,

This is forward difference formula, and the truncation error is

the error is of the order of h.

Similarly, backward difference can be shown from approximate $f(x_{i-1})$ in terms of $f(x_i)$ and its derivatives,

Where $h= x_i -x_{i-1}$. Dropping the power higher than 2 gives,

For central difference, from forward and back difference derivations, we can write

$$f(x_{i+1})= \tag{6.1}$$
$$f(x_{i-1})= \tag{6.2}$$

Where $h= x_{i+1} -x_i =x_i -x_{i-1}$. Dropping the power higher than 3 and substracting (6.2) from (6.1) give,

It is easily seen that the central difference formula gives more accurate approximation of the derivative and its truncation error is of the order of h^2. Central difference formula is useful only for interior points not for end points.

The formulas derived above are based on two-point values, we can also approximate the 1st-order derivative by three-point forward and backward difference.

Three-point forward difference: formula calculates the derivative at point x_i from the value at that point and the next two points x_{i+1} and x_{i+2}, and keep $h= x_{i+2} -x_{i+1} =x_{i+1} -x_i$.

$$f(x_{i+1})= \tag{6.3}$$
$$f(x_{i+2})= \tag{6.4}$$
(6.3)*4-(6.4) gives

Then

The truncation error is of order of h^2.

Example 6.2 Repeat Example 6.1 by three-point forward difference formula.

xi	sin(xi)
0.45	0.43497
0.50	0.47943
0.55	0.522687

6.1.2.2 Second-order Derivative Approximation

Similar to 1st-order derivative approximation, we can use Taylor series expansion to approximate higher order derivatives.

Note: for nth-order derivative approximation, it needs $(n+1)$-point values.

Three-point central difference formula:
For 2nd -order derivative approximation, it needs 3-point values.

$$f(x_{i+1})= \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (6.5)$$
$$f(x_{i-1})= \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (6.6)$$

(6.5)+(6.6) gives

The same way can be applied to develop higher order. For example, 4th-order derivative needs 5-point (x_{i+2} , x_{i+1}, x_i, x_{i-1}, x_{i-2}). You can find

Three-point forward difference formula:

Three-point backward difference formula:

6.1.3 Differentiation Formulas Using Lagrange Polynomials

The differentiation formulas can be derived by Lagrange polynomials. Given three points (x_i, y_i), (x_{i+1}, y_{i+1}), (x_{i+2}, y_{i+2}), the Lagrange polynomial that passes through the points is

$$f(x)=$$

$f'(x)=$ (6.7)

From (6.7), you can find the 1st-order derivative at any one point of the three given points (x_i, x_{i+1}, x_{i+2}) by replacing x with its corresponding value.

Two advantages:
1).

2).

6.1.4 Differentiation Using Curve Fitting

The differentiation can also be found by curve fitting method. For a set of given points, find a differentiable analytical function by curve fitting those data points, then calculate its derivative at the point of interest.

6.1.5 MATLAB Built-in Function for Differentiation

Two built-in functions that are important in calculating numerical difference are:
1). D= diff(X)
    diff(X) calculates the difference between adjacent elements of a vector.
    where vector X=[x_1, x_2, …, x_{n-1}, x_n], difference vector D=[(x_2-x_1), (x_3-x_2), …, (x_n-x_{n-1})].

To calculate the finite forward difference for Y=[y_1, y_2, …, y_{n-1}, y_n], use

>>Y$_{der}$=
The result is a difference vector

For equal spacing points, $h=$
It can be simplified as

2). DP=polyder(P)
    polyder(P) calculates the derivative of the polynomial whose coefficients are given by the vector P.

Example 6.3 Find the derivative of $f(x)=5x^3+4x^2+7$ by MATLAB function polyder().

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6.2 Numerical Integration

Integration has been widely used in engineering and science. The general form of a definite integral is

where *f(x)* is the integrand. The integral result is a number when the upper and lower limits *a* and *b* are numbers.

If *f(x)* is a very complex function of x or its analytical form is not available (i.e. only discrete data points by measurement), the anti-derivative is impossible to found, then the integral needs to be determined by numerical integration methods.

The numerical integration methods include:
(1). Rectangle and midpoint methods
(2). Trapezoidal method
(3). Simpson's method
(4). Gauss quadrature method
The idea of all the methods is based on Newton-Cotes integration formulas.

6.2.1 Newton-Cotes Integration Formula

Newton-Cotes Integration Formula: Replace a complicated integrand function with a polynomial that is easy to integrate

Where $F_n(x)=$, and it can be found by interpolation or curve fitting.

6.2.2 Rectangle and Midpoint Methods

6.2.2.1 Composite Rectangle Method

Composite Rectangle Method: divides the integration domain [a, b] into N subintervals. The integral in each subinterval is calculated as area of a rectangle, and the whole integral is obtained by adding the values of the integrals in all the subintervals.

If the height of each rectangle in the subinterval is assumed as the value of the integrand at the left end-point of the subinterval, then

I(*f*)=

However, this method may cause overestimation or underestimation for the result when the integrand function is monotonically increasing or decreasing.

When the subintervals have the same width *h*, the equation above can be simplified as

I(*f*)=

6.2.2.2 Composite Midpoint Method

Composite Midpoint Method: is basically the same as composite rectangle method, but it improves the accuracy by using the value of the integrand at the middle of the subinterval as the rectangle height.

I(*f*)=

When the subintervals have the same width *h*, the equation above can be simplified as

I(*f*)=

6.2.3 Trapezoidal Method

Composite Trapezoidal Method: approximates the integrand in each subinterval by a line function (1st-order polynomial) that passes through both end points of the subinterval. The integral in each subinterval is calculated as area of a trapezoid, and the whole integral is obtained by adding the values of the integrals in all the subintervals.

I(*f*)=

When the subintervals have the same width *h*, the equation above can be simplified as

I(*f*)=

Example 6.4 Use composite trapezoidal method to integrate
$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ between [0, 0.8].

MATLAB built-in Trapezoidal integration function:

I=trapz(X, Y)

Integral of Y with respect to X, where Y is vector of integrand values corresponding to vector X.

Example 6.4 cont. Repeat Example 6.4 using MATLAB function trapz().

n	I
2	1.0688
3	1.3639
4	1.4848
5	1.5399
6	1.5703

6.2.4 Simpson's Method

Simpson's Method: approximates the integrand in each subinterval by a higher order polynomial that passes through some points of the subinterval. The integral in each subinterval is calculated as area of a trapezoid, and the whole integral is obtained by adding the values of the integrals in all the subintervals.

The most common Simpson's methods include:
1). Simpson's 1/3 Method
2). Simpson's 3/8 Method

Note: All the subintervals should have same width.

6.2.4.1 Composite Simpson's 1/3 Method

Composite Simpson's 1/3 Method: approximates the integrand in every 2 subintervals by a 2nd-order polynomial that passes through three points of 2 adjacent subintervals. The integral in each subinterval is calculated as area of a trapezoid, and the whole integral is obtained by adding the values of the integrals in all the subintervals.

It is easily to know that the number of subintervals must be an even number.

The 2nd-order polynomial can be written in Newton's form

$p(x)=$

since
$p(x_{i-1})=$
$p(x_i)=$
$p(x_{i+1})=$

We can find

then

$Ii(f)=$

Consider all the subintervals

I(f)=

By collecting similar terms, then

I(f)≈

Or I(f)≈

Example 6.5 Repeat Example 6.4 using composite Simpson's 1/3 method with N=4 subintervals.

6.2.4.2 Composite Simpson's 3/8 Method

Composite Simpson's 3/8 Method: approximates the integrand in every 3 subintervals by a 3rd-order polynomial that passes through four points of 3 adjacent subintervals. The integral in each subinterval is calculated as area of a trapezoid, and the whole integral is obtained by adding the values of the integrals in all the subintervals.

It is easily to know that the number of subintervals must be dividable by 3.

The 3rd-order polynomial can be written as

p(x)=

since
p(x_i)=
p(x_{i+1})=
p(x_{i+2})=
p(x_{i+3})=

We can determine the coefficients and find

Ii(f)=

Consider all the subintervals

I(f)≈

By collecting similar terms, then

I(f)≈

Or I(f)≈

Example 6.6 Repeat Example 6.4 using composite Simpson's 3/8 method with N=6 subintervals.

MATLAB built-in Simpson's integration function:
I=quad('**function**', a, b)
Calculates the integral of '**function**' between [a, b] with an absolute error less than 10^{-6}, where **function** can be a string, name of a function file, or the name of an inline function.

Example 6.7 Repeat Example 6.4 using MATLAB function quad().

6.2.5 Gauss Quadrature Method

All the integration methods introduced before are using polynomial functions passing through subinterval endpoints.

Gauss Quadrature Method: evaluates the integral by using weighted addition of values of integrand at Gaussian points that are not equally spaced and do not include the end points.

Gauss quadrature integration of $\boxed{\int_{-1}^{1} f(x)dx}$.

Write the integral in Gauss quadrature form as

$$\int_{-1}^{1} f(x)dx \approx$$

The coefficients C_i and the location of Gauss points x_i are determined by enforcing the above equation to be **exact** for the cases when $f(x) = 1, x, x^2, x^3, \cdots$ The number of cases needed depends on the value of n (number of Gauss points).

For example for n=2,

$$\int_{-1}^{1} f(x)dx \approx \tag{6.8}$$

There will be four unknowns C_1, C_2, x_1, x_2, thus the following 4 cases are required:
Case 1:

Case 2:

Case 3:

Case 4:

We can find

Then substituting these constants into equation (6.8) gives

$$(6.9)$$

You can check (6.9) works for $f(x) = 1, x, x^2, x^3$. However, when $f(x)$ is different from these, Gauss quadrature only approximates the value for the integral.

Example 6.8 Evaluate $\int_{-1}^{1} \cos(x)dx$ by Gauss quadrature method with n=2.

Note: The accuracy of Gauss quadrature can be increased by using a higher value for n (Gauss points). The Gauss points and coefficients for higher value of number are provided by Table 7.1 on P285.

Q: How to evaluate $\int_{a}^{b} f(x)dx$ by Gauss quadrature?

A: Transform $\int_{a}^{b} f(x)dx$ into the form $\int_{-1}^{1} f(t)dt$ by changing variable.

Let

Then

Example 6.9 Evaluate $\int_{0}^{3} e^{-x^2} dx$ by Gauss quadrature method with n=4.