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BSCS-V- Numerical Computing

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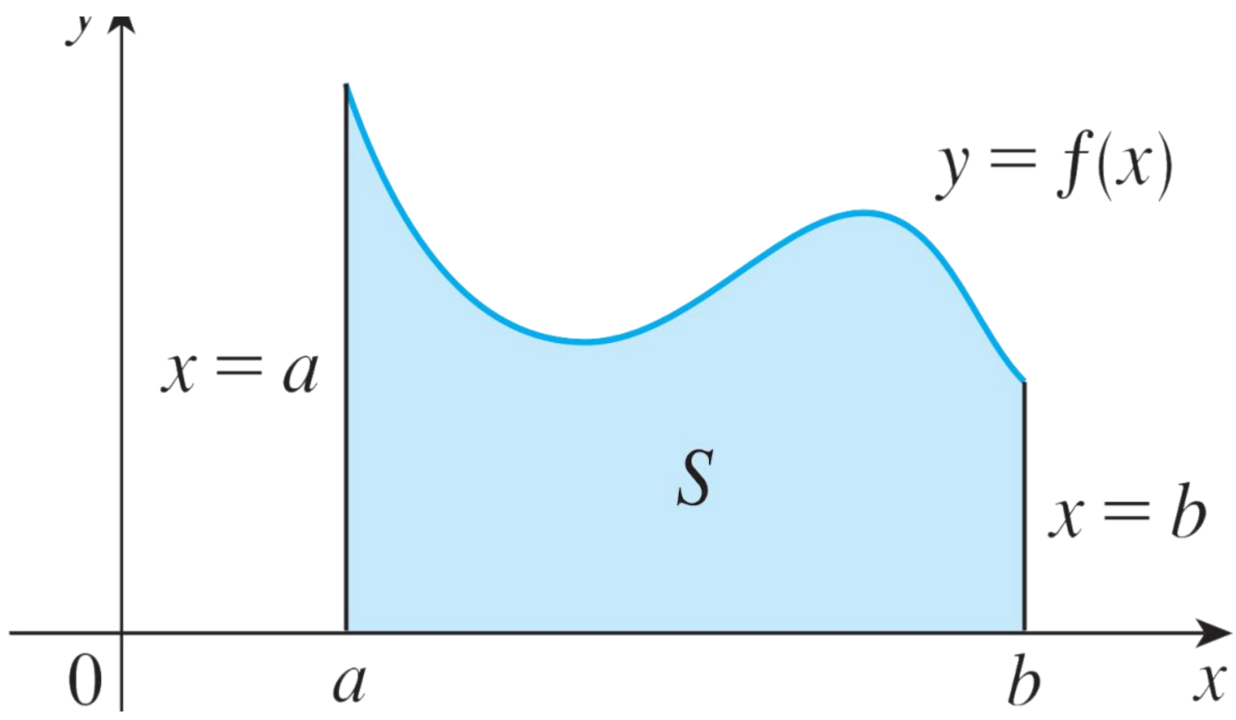
Numerical Integration

The use of numerical integration becomes necessary when a given function $f(x)$ cannot be integrated analytically, that is, $f(x)$ is not known explicitly.

A definite integral $\int_a^b f(x)\,dx$ can be interpreted or defined as "the area under the curve $y = f(x)$, bounded by the x-axis and the lines $x = a$ and $x = b$". This is shown graphically in the following diagram, in which S represents the area under the curve $y = f(x)$.



The general problem of numerical integration can be stated as follows.
Suppose that we are given a function $y = f(x)$, where usually $f(x)$ is not known explicitly, and a set of data points $(x_0, f(x_0)) = (a, f(a))$ and $(x_1, f(x_1)) = (b, f(b))$. It is required to compute the value of the definite integral

$$I = \int_{x_0}^{x_1} f(x)\, dx = \int_a^b y\, dx \text{——— Equation (1).}$$

Similar to numerical differentiation, we replace $f(x)$ by the Lagrange interpolation polynomial and, after integration, we obtain an approximate value of the definite integral. We have different integration rules that can be obtained depending upon the type of the interpolation formula used. That is, we use linear, quadratic or cubic Lagrange interpolation formula to obtain Trapezoidal, Simpson's 1/3 and Simpson's 3/8 rules respectively (see the previous lecture on interpolation for more details). We define

Function = Polynomial + Error,

$$f(x) = P(x) + E \text{ ——— Equation (2).}$$

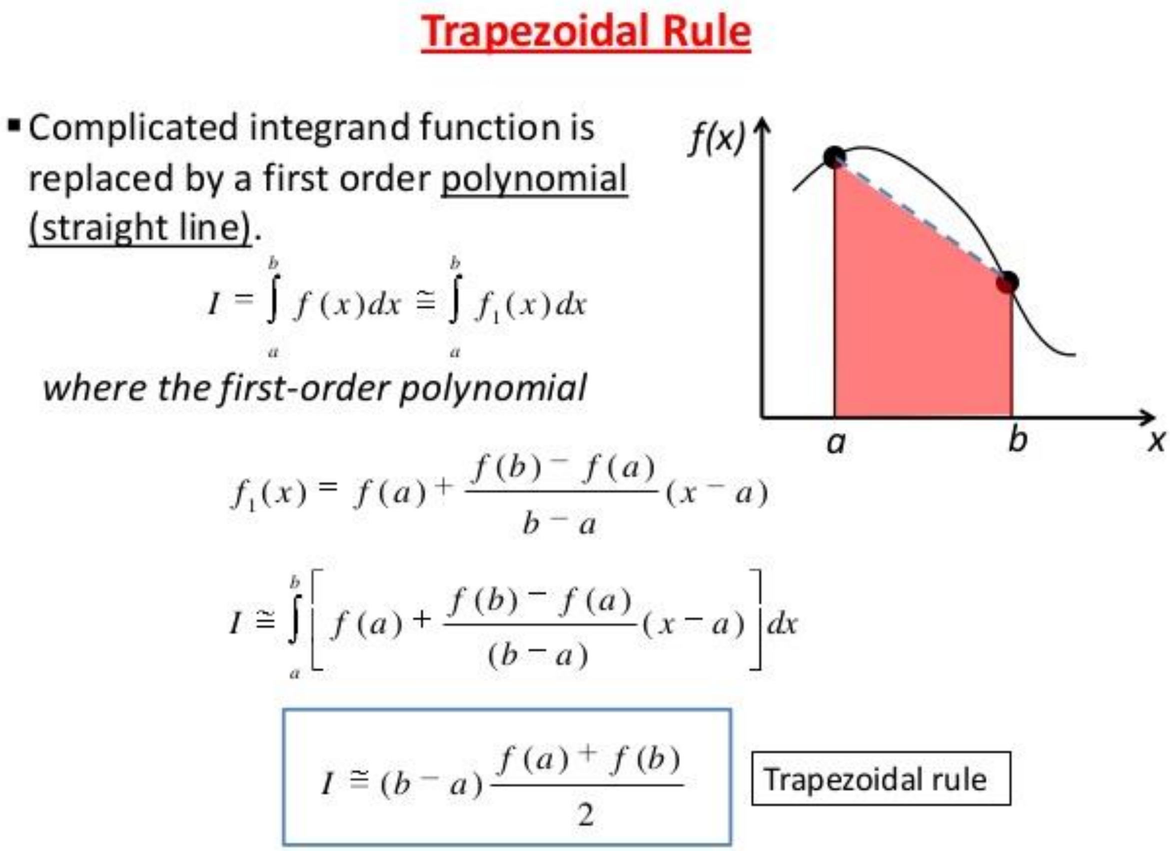
1. Trapezium or Trapezoidal Rule:

The very first method or rule that we shall study here is the trapezium or trapezoidal rule. The geometry or the graph of this rule has great resemblance with the shape of a trapezium and that's the reason that it's known as trapezium rule!

We use the Lagrange linear interpolation, using two points $\left(x_0, f(x_0)\right)$ and $\left(x_1, f(x_1)\right)$, to solve equation (1) numerically. That is, we approximate the curve $y = f(x)$ by a straight line $y = f_1(x) = P_1(x)$ passing through two points $\left(x_0, f(x_0)\right) = \left(a, f(a)\right)$ and $\left(x_1, f(x_1)\right) = \left(b, f(b)\right)$, and then we compute the area under the straight line $y = f_1(x) = P_1(x)$.

In the diagram below, $y = f(x)$ is represented by the black curve that is passing through two points $(a, f(a))$ and $(b, f(b))$, and $y = P_1(x)$ is represented by the dashed blue line that is joining these two points.

We let $x_0 = a,\ x_1 = b$ and $h = b - a$. Here h is defined as the width of the interval $[a, b]$.



In order to derive the formula of the trapezoidal rule, we use the Lagrange linear interpolation formula

$$P_1(x) = L_0(x)f(x_0) \ + \ L_1(x)f(x_1).$$

We next integrate the both sides and use the definitions of $L_0(x)$ and $L_1(x)$ to write

$$\int_{x_0}^{x_1} P_1(x)\, dx = \int_{x_0}^{x_1} \left[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)\right] dx$$

$$= \frac{h}{2}[f(x_0) \ + \ f(x_1)] \text{——— Equation (3).}$$

This is similar to the area of a trapezium or trapezoid, which is

$$\text{Area} = \frac{height}{2}[base\ 1 + \ base\ 2].$$

Using $\boldsymbol{f(x) - P(x) = E}$, from equation (2), the error of the trapezoidal rule is

$$\boldsymbol{\int_{x_0}^{x_1} f(x)\,dx - \int_{x_0}^{x_1} P_1(x)\,dx = -\frac{h^3}{12} f''.}$$

This can be derived by expanding $y = f(x)$ in a Taylor's series and using equation (3).

Therefore, the trapezoidal rule with the error term is

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f'' \text{——— Equation (4).}$$

Remark 1: Note that the trapezoidal rule is exact if the given function $f(x)$ is linear, since in this case, the second derivate f'' is zero and so we do not have any error.

Example 1. Use the trapezoidal rule to evaluate

$$I = \int_0^1 (x + 1)\,dx.$$

Solution: We note that $f(x) = x + 1$ is linear and so we expect to get an exact solution using the trapezoidal rule (see Remark 1 for details).

The exact solution is

$$I = \int_0^1 (x + 1)dx = 3/2.$$

Given that $f(x) = x + 1$ and $h = x_1 - x_0 = 1 - 0 = 1$. Using the trapezoidal rule, we write

$$I = \int_0^1 (x + 1)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] = \frac{1}{2}[1 + 2] = 3/2.$$

Therefore, the trapezoidal rule gives the exact solution when $f(x)$ is linear.

Example 2. Use the trapezoidal rule to evaluate

$$I = \int_0^1 3x^2\, dx$$

and also calculate the absolute error.

Solution: The exact solution is

$$I = \int_0^1 3x^2 dx = 1.$$

Given that $f(x) = 3x^2$ and $h = x_1 - x_0 = 1 - 0 = 1.$

Using the trapezoidal rule, we write

$$I = \int_0^1 3x^2\, dx = \frac{h}{2}[f(x_0) + f(x_1)] = \frac{1}{2}[0 + 3] = 1.5.$$

Absolute Error = |Exact solution – Approximate solution|

= |1 – 1.5| = 0.5.

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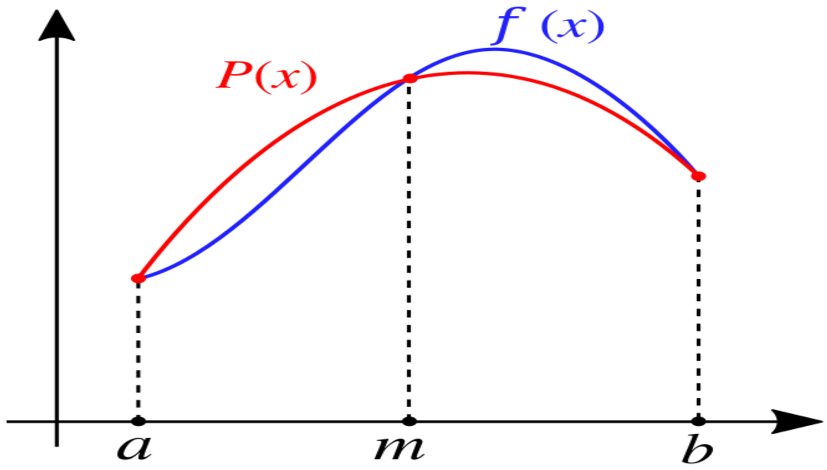
2 (a). Simpson's 1/3 Rule: In this rule, we use the Lagrange quadratic interpolation, using three points $(x_0, f(x_0))$, $(x_1, f(x_1))$ and $(x_2, f(x_2))$, to solve equation (1) numerically. That is, we approximate a given curve $y = f(x)$ by a parabola $y = P_2(x)$ passing through three points $(x_0, f(x_0))$, $(x_1, f(x_1))$ and $(x_2, f(x_2))$, and then we compute the area under the parabola $y = P_2(x)$.

We let $x_0 = a,\ x_1 = x_0 + h,\ \ x_2 = x_1 + h = b$ and $2h = b - a$.

In the diagram below, $P_2(x) = P(x)$ and $x_1 = m$.



In order to derive the formula of the Simpson's 1/3 rule, we use the Lagrange quadratic interpolation formula

$$P_2(x) = L_0(x)f(x_0) \ + \ L_1(x)f(x_1) \ + \ L_2(x)f(x_2).$$

Similar to the trapezoidal rule, we next integrate the both sides, use the definitions of $L_0(x)$, $L_1(x)$ and $L_2(x)$ and then, at the end of the day, we derive the formula of Simpson's 1/3 rule, which is

$$\int_{x_0}^{x_2} P_2(x)\, dx \ = \frac{h}{3}[f(x_0) \ + 4f(x_1) + \ f(x_2)] \text{——— Equation (5).}$$

Similar to the trapezoidal rule, the error of Simpson's 1/3 rule is

$$\boldsymbol{\int_{x_0}^{x_2} f(x)\, dx - \int_{x_0}^{x_2} P_2(x)\, dx = -\frac{h^5}{90} f'''' \ = -\frac{h^5}{90} f^{(4)}}.$$

Therefore, Simpson's 1/3 rule with the error term is

$$\int_{x_0}^{x_2} f(x)\, dx = \frac{h}{3}[f(x_0) \ + 4f(x_1) + \ f(x_2)] - \frac{h^5}{90} f^{(4)} \text{ - Equation (6).}$$

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2 (b). Simpson's 3/8 Rule: In this rule, we use the Lagrange cubic interpolation, using four points $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$ and $(x_3, f(x_3))$, to solve equation (1) numerically.

We let $x_0 = a,\ \ x_1 = x_0 + h,\ \ x_2 = x_1 + h,\ \ x_3 = x_2 + h\ = b$ and $3h = b - a$.

In order to derive the formula of the Simpson's 3/8 rule, we use the Lagrange cubic interpolation formula

$$P_3(x) = L_0(x)f(x_0)\ +\ L_1(x)f(x_1)\ +\ L_2(x)f(x_2)\ +\ L_3(x)f(x_3).$$

Similar to previous rules, we next integrate the both sides, use the definitions of $L_0(x)$, $L_1(x)$, $L_2(x)$ and $L_3(x)$ and then, at the end of the day, we derive the formula of Simpson's 3/8 rule

$\int_{x_0}^{x_3} P_3(x)\,dx\ = \frac{3h}{8}[f(x_0)\ + 3f(x_1) +\ 3f(x_2)\ +\ f(x_3)]$ - Eq. (7).

Similar to the previous rule, the error of Simpson's 3/8 rule is

$$\boldsymbol{\int_{x_0}^{x_3} f(x)\,dx - \int_{x_0}^{x_3} P_3(x)\,dx = -\frac{3h^5}{80} f''''\ = -\frac{3h^5}{80} f^{(4)}}.$$

Therefore, Simpson's 3/8 rule with the error term is

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

$-\frac{3h^5}{80} f^{(4)}$ ——— Equation (8).

<u>Remark 2</u>: From equations (6) and (8), we note that both Simpson's 1/3 and Simpson's 3/8 rules are exact if the given function $f(x)$ is linear, quadratic or cubic, since in this case, the fourth derivate $f^{(4)}$ is zero and so we do not have any error.

<u>Example 3</u>: Use the trapezoidal rule and Simpson's rules to estimate the integral $I\ = \int_1^3 (x^3 - \ 2x^2 +\ 7x - 5)\,dx$.

In addition, calculate the absolute error in each case.

<u>Solution</u>: We note that $f(x) = x^3 - \ 2x^2 +\ 7x - 5$ is cubic and so we expect to get an exact solution using Simpson's 1/3 and 3/8 rules (see Remark 2 for details).

The exact solution is

$$I = \int_1^3 (x^3 - 2x^2 + 7x - 5)\, dx = 62/3.$$

1. <u>Trapezoidal Rule</u>:

Given that

$f(x) = x^3 - 2x^2 + 7x - 5,\ x_0 = 1,\ x_1 = 3$ and $h = x_1 - x_0 = 3 - 1 = 2.$

Using the trapezoidal rule, we write

$I = \int_1^3 f(x)\, dx = \frac{h}{2}[f(x_0) + f(x_1)] = \frac{2}{2}[1 + 25] = 26.$

Absolute Error $=$|Exact solution – Approximate solution|

$= |(62/3) - 26| = 5.33333.$

2a. <u>Simpson's 1/3 Rule</u>:

Given that $f(x) = x^3 - 2x^2 + 7x - 5,$

$x_0 = 1,\ x_1 = x_0 + h,\ x_2 = 3$ and $h = (x_2 - x_0)/2 = (3 - 1)/2 = 1.$

Using Simpson's 1/3 rule, we write

$$\int_1^3 f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]$$
$$= \frac{1}{3}[1 + 4(9) + 25] = 62/3.$$

This is the same as the exact solution and hence there is no absolute error. That is, Absolute Error = 0.

2b. <u>Simpson's 3/8 Rule</u>:

Given that $f(x) = x^3 - 2x^2 + 7x - 5,$

$x_0 = 1,\ x_1 = x_0 + h, x_2 = x_1 + h, x_3 = 3$ and
$h = (x_3 - x_0)/3 = (3 - 1)/3 = 2/3.$

Using Simpson’s 3/8 rule, we write

$$\int_{x_0}^{x_3} f(x)dx \ = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

$$= (3/8)(2/3)[1 \ + 3(155/27) + \ 3(355/27) \ + \ 25] = 62/3.$$

This is also the same as the exact solution and hence there is no absolute error. That is, Absolute Error = 0.

Remark 3: Remember that h is defined as the width of the interval. The smaller the h, the more accurate the approximate solution. Therefore, h and the accuracy of the numerical solution are inversely proportional to each other. That is, when we have a small interval, we have a small value of h and so we have a more accurate numerical solution. Based on this analysis, we can see that among the trapezoidal, Simpson 1/3 and Simpson's 3/8 rules, the most accurate solution will be obtained when we use Simpson's 3/8 rule because this rule has the smallest value of h, when the given function is of the 4th or the higher order polynomial. This is demonstrated in the following exercise.

Exercise:

Apply the trapezoidal, Simpson 1/3 and Simpson's 3/8 rules to the following definite integral

$$I \ = \int_1^2 x^4 \, dx$$

and calculate the absolute error in each case.

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3. <u>Composite Numerical Integration (Composite Rules):</u>

Suppose that we want to find an approximate solution of

$$I = \int_0^4 e^x \, dx$$

using Simpson's 1/3 rule (for example), with $f(x) = e^x,\ x_0 = 0,\ x_1 = x_0 + h, x_2 = 4$ and $h = (x_2 - x_0)/2 = (4-0)/2 = 2$,

$$\int_0^4 f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] = 56.76958.$$

The exact solution is

$$I = \int_0^4 e^x \, dx = e^4 - e^0 = 53.59815.$$

Absolute Error = |Exact solution – Approximate solution| = 3.17. (a large error!)

The problem of having a large error is mainly because of a large interval. However, we can easily solve that problem by dividing the large interval into two, four or even eight small subintervals, apply Simpson' 1/3 rule on each of the subinterval and then we can add them up! In fact, the more we divide an interval into small subintervals, the more accurate our solution will be. That is, the smaller the h, the more accurate the approximate solution (see Remark 3 for more details). The value of h should remain the same in each of these subintervals. This process is called <u>composite numerical integration or composite rules</u>.

We divide the given interval into four subintervals, use Simpson's 1/3 rule on each of these subintervals and then we add these subintervals as follows.
(Note that $h = 1/2$ in all of these four subintervals.)

$$I = \int_0^4 e^x \, dx = \int_0^1 e^x \, dx + \int_1^2 e^x \, dx + \int_2^3 e^x \, dx + \int_3^4 e^x \, dx$$

$$= (1/6)\left[e^0 + 4e^{(1/2)} + e^1\right] + (1/6)\left[e^1 + 4e^{(3/2)} + e^2\right]$$

$$+(1/6)[e^2 + 4e^{(5/2)} + e^3] + (1/6)[e^3 + 4e^{(7/2)} + e^4] = 53.6162.$$

Absolute Error $=$|Exact solution – Approximate solution|

$=$0.018, which is a small error.

This was an example of composite Simpson's 1/3 rule.

Exercises:

1. Apply composite trapezoidal and composite Simpson's 3/8 rules to the same example

$$I = \int_0^4 e^x \, dx$$

by taking four subintervals and calculate the absolute error in each case.

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2. Apply composite trapezoidal, composite Simpson's 1/3 and 3/8 rules to

$$I = \int_1^2 x^5 \, dx$$

by taking four subintervals and calculate the absolute error in each case.

Last Modified: 9th May 2022.