

Numerical Integration

Motivation. We have learned how to calculate some integrals analytically; such as

$$\int_0^1 x^2 dx = \left[\frac{1}{3}x^3 \right]_0^1 = \frac{1}{3}$$

But most integrals, e.g. $\int_1^4 e^{-x^2} dx$, cannot be calculated analytically. In this chapter we introduce several methods for approximating integrals.

A numerical integration formula is called a **quadrature**.

We employ three procedures to find quadratures:

$$\left\{ \begin{array}{l} \text{geometric arguments} \\ \text{interpolation} \\ \text{setting degree of exactness} \end{array} \right.$$

A quadrature for $\int_a^b f(x)dx$ uses some points of the interval $[a, b]$ to approximate this integral.

For example:

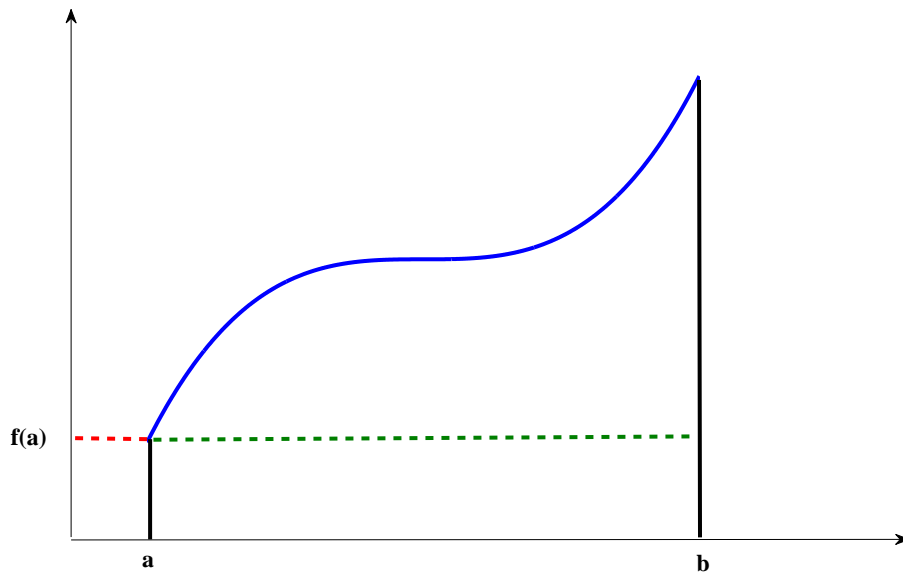
$$\text{midpoint method} \quad f\left(\frac{a+b}{2}\right)(b-a)$$

$$\text{Simpson method} \quad \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

The midpoint method uses the point $\frac{a+b}{2}$ and the Simpson method uses the points $\{a, \frac{a+b}{2}, b\}$ to approximate the true integral. The Simpson method uses the endpoints a and b ; therefore it is called a closed method. On the other hand, the midpoint rule is called an open method because it does not use the endpoints a and b .

1 **Rectangle and Midpoint methods** (some one-point methods) (from section 9.2)

In this method, the area under a curve $y = f(x)$ is approximated by the rectangle with one side being the interval $[a, b]$ and the other side being $f(a)$, as shown in the following figure.



So, in this method we approximate:

$$\int_a^b f(x)dx \approx (b - a)f(a)$$

Usually a better approximation is found if we divide the interval $[a, b]$ into a few subintervals of equal length, n subintervals each with length $h = \frac{b-a}{n}$:

$$a = x_1 < x_2 < \dots < x_n < x_{n+1} \quad x_{i+1} - x_i = \frac{b-a}{n}, \quad i = 1, \dots, n$$

we may denote this common length by h :

$$h = \frac{b-a}{n}$$

and then apply the rectangle rule to each subinterval :

$$\int_{x_1}^{x_2} f(x)dx \approx (x_2 - x_1)f(x_1) = h f(x_1)$$

Similarly :

$$\int_{x_2}^{x_3} f(x)dx \approx (x_3 - x_2)f(x_2) = h f(x_2)$$

and so on , and on the last subinterval we will have:

$$\int_{x_n}^{x_{n+1}} f(x)dx \approx (x_{n+1} - x_n)f(x_n) = h f(x_n)$$

Adding up these values gives:

$$\int_{x_1}^{x_2} f(x)dx + \int_{x_2}^{x_3} f(x)dx + \cdots + \int_{x_n}^{x_{n+1}} f(x)dx \approx h f(x_1) + h f(x_2) + \cdots + h f(x_n)$$

equivalently:

$$\int_a^b f(x)dx \approx h \{ f(x_1) + \cdots + f(x_n) \}$$

This quadrature is called the **composite rectangle method**

Example (from exercise 1 of the textbook). The following values of a function f are given:

x	0	0.3	0.6	0.9	1.2	1.5	1.8
f(x)	0.5	0.6	0.8	1.3	2	3.2	4.8

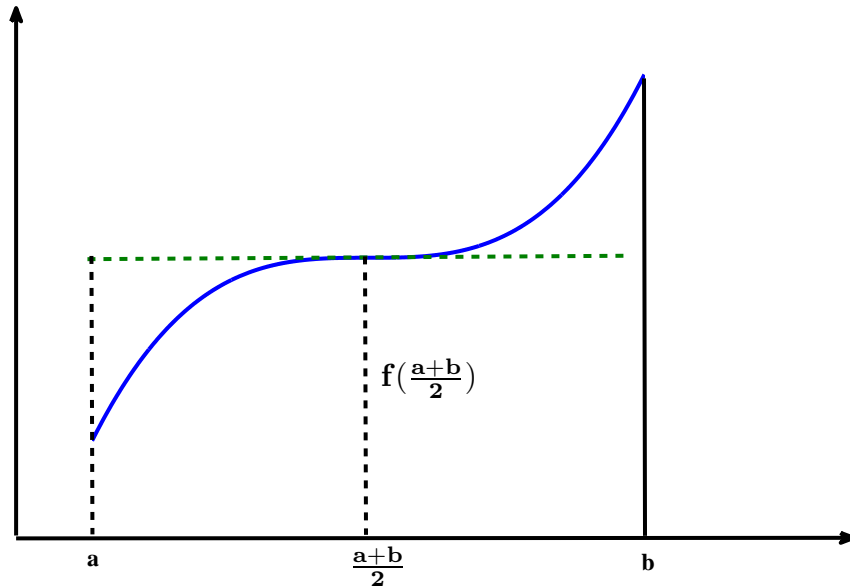
Use the composite rectangle method to approximate the integral $\int_0^{1.8} f(x)dx$

Solution.

The step size $h = 0.3$.

$$\begin{aligned} \int_0^{1.8} f(x)dx &\approx h \{ f(0) + f(0.3) + f(0.6) + f(0.9) + f(1.2) + f(1.5) \} \\ &= (0.3) \{ 0.5 + 0.6 + 0.8 + 1.3 + 2 + 3.2 \} = 2.52 \end{aligned}$$

The next method in this section is the **midpoint method**. In this method we approximate the under-the-curve area with the area of the triangle with the length of one side being $b - a$ and the length of the other side being $f(\frac{a+b}{2})$.



$$\int_a^b f(x)dx \approx (b - a)f(a)$$

Usually a better approximation is found if we divide the interval $[a, b]$ into a few subintervals of equal length, n subintervals each with length $h = \frac{b-a}{n}$:

$$a = x_1 < x_2 < \dots < x_n < x_{n+1} \quad x_{i+1} - x_i = \frac{b-a}{n} \quad i = 1, \dots, n$$

we may denote this common length by h :

$$h = \frac{b-a}{n}$$

and then apply the midpoint rule to each subinterval :

$$\int_{x_1}^{x_2} f(x)dx \approx (x_2 - x_1)f\left(\frac{x_1 + x_2}{2}\right) = hf\left(\frac{x_1 + x_2}{2}\right)$$

Similarly :

$$\int_{x_2}^{x_3} f(x)dx \approx (x_3 - x_2)f\left(\frac{x_2 + x_3}{2}\right) = h f\left(\frac{x_2 + x_3}{2}\right)$$

and so on , and on the last subinterval we will have:

$$\int_{x_n}^{x_{n+1}} f(x)dx \approx (x_{n+1} - x_n)f\left(\frac{x_{n-1} + x_n}{2}\right) = h f\left(\frac{x_{n-1} + x_n}{2}\right)$$

Adding up these values gives:

$$\int_{x_1}^{x_2} f(x)dx + \int_{x_2}^{x_3} f(x)dx + \dots + \int_{x_n}^{x_{n+1}} f(x)dx \approx h f\left(\frac{x_1 + x_2}{2}\right) + h f\left(\frac{x_2 + x_3}{2}\right) + \dots + h f\left(\frac{x_{n-1} + x_n}{2}\right)$$

equivalently:

$$\int_a^b f(x)dx \approx h \left\{ f\left(\frac{x_1 + x_2}{2}\right) + \dots + f\left(\frac{x_{n-1} + x_n}{2}\right) \right\} \quad h = \frac{b-a}{n} \quad \text{step size}$$

This quadrature is called the **composite midpoint method**. This is an example of an open method.

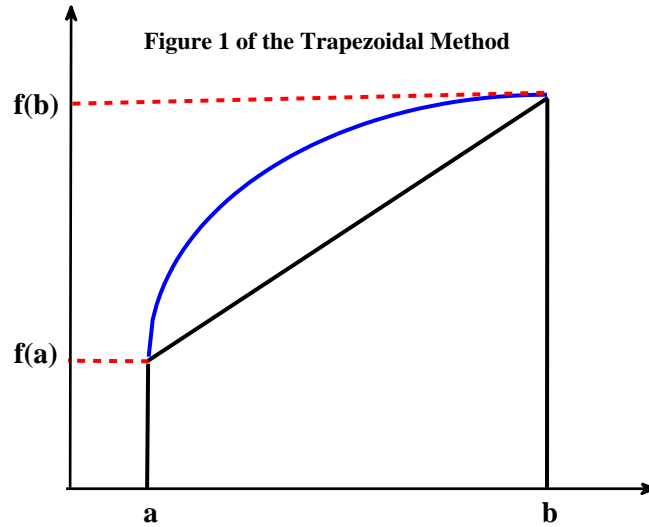
Example . Approximate the integral $\int_0^1 e^{x^2} dx$ using the composite midpoint rule with step size $h = \frac{b-a}{10} = \frac{1}{10} = 0.1$

Solution.

Set $f(x) = \exp(x^2)$. The nodes corresponding to $h = 0.1$ are

$$0, 0.1, 0.2, \dots, 0.9, 1$$

$$\begin{aligned} \int_0^1 f(x)dx &\approx h \left\{ f(0.05) + \dots + f(0.15) + \dots + f(0.95) \right\} \\ &= (0.1) \left\{ \exp(0.05^2) + \exp(0.15^2) + \exp(0.85^2) + \exp(0.95^2) \right\} \\ &= 1.4604 \end{aligned}$$



The next method we learn is the **trapezoidal method**. In this method we approximate the under-the-curve area with the area of the trapezoid as shown in the figure 1 below.

The trapezoid has the bases of lengths $f(a)$ and $f(b)$ and has height $b - a$, therefore its area is $\frac{1}{2}(b - a)[f(a) + f(b)]$. This is the value we use to approximate the area under the curve. So we approximate:

$$\int_a^b f(x)dx \approx \frac{b - a}{2} [f(a) + f(b)]$$

Question: What is the trapezoidal method on $[0, 1]$?

Answer:

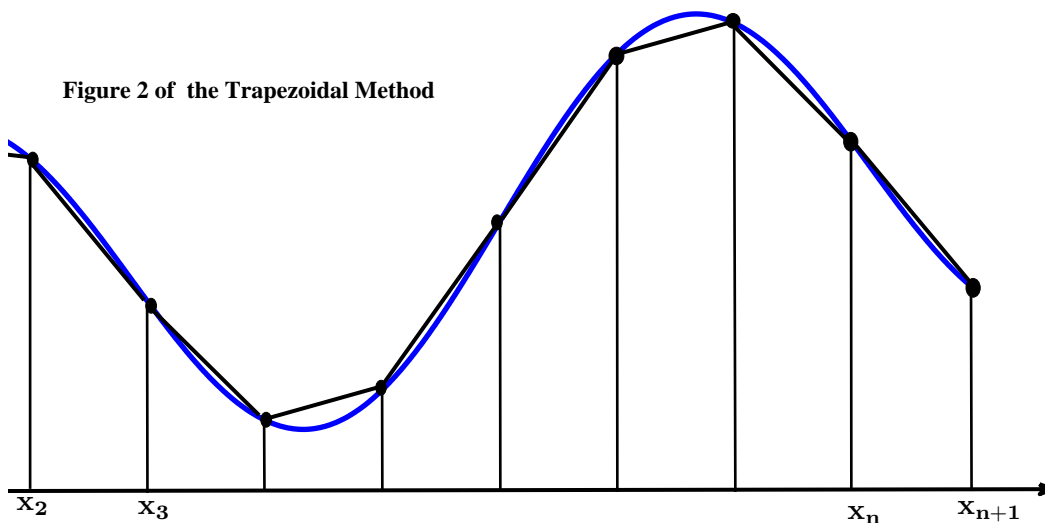
$$\int_0^1 f(x)dx \approx \frac{1}{2} [f(0) + f(1)] = \frac{1}{2}f(0) + \frac{1}{2}f(1)$$

Usually a better approximation is found if we divide the interval $[a, b]$ into a few subintervals and then apply the trapezoidal method to each subinterval.

We actually divide the interval $[a, b]$ into n subintervals each with length $\frac{b-a}{n}$:

$$a = x_1 < x_2 < \cdots < x_n < x_{n+1} \quad x_{i+1} - x_i = \frac{b - a}{n}, \quad i = 1, \dots, n$$

Figure 2 of the Trapezoidal Method



we may denote this common length by h and we call it the step size:

$$h = \frac{b - a}{n}$$

Then on the subintervals we have the following approximations; see Figure 2 below:

$$\int_{x_1}^{x_2} f(x)dx \approx \frac{x_2 - x_1}{2} [f(x_1) + f(x_2)] = \frac{h}{2} [f(x_1) + f(x_2)]$$

and

$$\int_{x_2}^{x_3} f(x)dx \approx \frac{x_3 - x_2}{2} [f(x_2) + f(x_3)] = \frac{h}{2} [f(x_2) + f(x_3)]$$

and so on , and on the last subinterval we will have:

$$\int_{x_n}^{x_{n+1}} f(x)dx \approx \frac{x_{n+1} - x_n}{2} [f(x_n) + f(x_{n+1})] = \frac{h}{2} [f(x_n) + f(x_{n+1})]$$

Adding up these values gives:

$$\begin{aligned} \int_{x_1}^{x_2} f(x)dx + \int_{x_2}^{x_3} f(x)dx + \cdots + \int_{x_n}^{x_{n+1}} f(x)dx &\approx \frac{h}{2} [f(x_1) + 2f(x_2) + \cdots + 2f(x_n) + f(x_{n+1})] \\ &= \frac{h}{2} [f(a) + 2f(x_2) + \cdots + 2f(x_n) + f(b)] \end{aligned}$$

so

$$\int_a^b f(x)dx \approx \frac{h}{2} [f(a) + 2f(x_1) + \cdots + 2f(x_n) + f(b)]$$

or equivalently, as written in the textbook:

$$\int_a^b f(x)dx \approx \frac{h}{2} [f(a) + f(b)] + h \{f(x_1) + \cdots + f(x_n)\}$$

This quadrature is called the **Composite Trapezoidal Method**

Example (from exercise 1 of the textbook). The following values of a function f are given:

x	0	0.3	0.6	0.9	1.2	1.5	1.8
f(x)	0.5	0.6	0.8	1.3	2	3.2	4.8

Use the composite rectangle method to approximate the integral $\int_0^{1.8} f(x)dx$

Solution.

The step size $h = 0.3$.

$$\begin{aligned} \int_0^{1.8} f(x)dx &\approx \frac{h}{2} \{f(0) + 2f(0.3) + 2f(0.6) + 2f(0.9) + 2f(1.2) + 2f(1.5) + f(1.8)\} \\ &= (0.15) \{(0.5) + 2(0.6) + 2(0.8) + 2(1.3) + 2(2) + 2(3.2) + (4.8)\} \\ &= 3.1650 \end{aligned}$$

compare this value with the approximate value we found from the composite rectangle method.

2 Numerical Integration Using Interpolating Polynomials

One method of approximating integrals is by use of interpolating polynomials. Indeed, if $p(x)$ is the interpolating polynomial of a function $f(x)$ at some distinct nodes $\{x_1, \dots, x_n\}$ from the interval $[a, b]$, then we may approximate the integral $\int_a^b f(x)dx$ by $\int_a^b p(x)dx$ which is easily calculated as $p(x)$ is a polynomial.

Example. The following data of a function f is given:

x	2	4	5	7
f(x)	5	-5	-40	10

By finding the interpolation polynomial, estimate the integral $\int_2^7 f(x)dx$.

cm

Solution.

x_k	$f[] = f()$	$f[,]$	$f[, ,]$	$f[, , ,]$
2	5			
		$\frac{-5-5}{4-2} = -5$		
4	-5		$\frac{-35-(-5)}{5-2} = -10$	
		$\frac{-40-(-5)}{5-4} = -35$		$\frac{20-(-10)}{7-2} = 6$
5	-40		$\frac{25-(-35)}{7-4} = 20$	
		$\frac{10-(-40)}{7-5} = 25$		
7	10			

and then

$$p(x) = 5 - 5(x - 2) - 10(x - 2)(x - 4) + 6(x - 2)(x - 4)(x - 5)$$

Collecting terms gives:

$$p(x) = 6x^3 - 76x^2 + 283x - 305$$

Then:

$$\begin{aligned} \int_2^7 f(x)dx &\approx \int_2^7 p(x)dx = \int_2^7 (6x^3 - 76x^2 + 283x - 305)dx \\ &= \left[\frac{6}{4}x^4 - \frac{76}{3}x^3 + \frac{283}{2}x^2 - 305x \right]_{x=2}^{x=7} = -\frac{200}{3} \end{aligned}$$

We saw in the preceding sections how to create some numerical quadratures base some logic.

For example, the trapezoidal method on the interval $[0, 1]$ is

$$\int_0^1 f(x)dx = \frac{1}{2}f(0) + \frac{1}{2}f(1)$$

Example. Find the quadrature $Af(a) + Bf(b)$ using two nodes $\{a, b\}$ for approximating the integral $\int_a^b f(x)dx$.

Solution.

$\mathbf{x_k}$	$\mathbf{f[] = f()}$	$\mathbf{f[,]}$
a	f(a)	$\frac{f(b)-f(a)}{b-a}$
b	f(b)	

The interpolating polynomial:

$$p(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

Now use this polynomial to approximate the integral of the function f :

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b p(x)dx = \int_a^b f(a)dx + \frac{f(b)-f(a)}{b-a} \int_a^b (x-a)dx \\
&= f(a)(b-a) + \frac{f(b)-f(a)}{b-a} \left[\frac{1}{2}(x-a)^2 \right]_{x=a}^{x=b} \\
&= f(a)(b-a) + \frac{f(b)-f(a)}{b-a} \frac{1}{2}(b-a)^2 \\
&= f(a)(b-a) + \frac{1}{2}[f(b) - f(a)](b-a) \\
&= \frac{b-a}{2}[f(a) + f(b)]
\end{aligned}$$

But this is the trapezoidal method for the nodes $\{a, b\}$!. This discussion in here substitutes the discussion that appears in the textbook from the beginning of section 9.3 up to the beginning of section 9.3.1.

Example. Find the quadrature using the nodes $\{a, \frac{a+b}{2}, b\}$ for approximating the integral $\int_a^b f(x)dx$.

Solution. The discussion involving two nodes we just had seems to be more complicated if we have three nodes. Therefore we break the solution into two steps:

Step 1. We first solve the problem for simple case of three notes $\{-1, 0, 1\}$ and the integral $\int_{-1}^1 f(x) dx$. Then we deal with the general case.

x_k	$f[\] = f(\)$	$f[\ , \]$	$f[\ , \ , \]$
-1	$f(-1)$		
		$\frac{f(0)-f(-1)}{0-(-1)}$	
0	$f(0)$???
		$\frac{f(1)-f(0)}{1-0}$	
1	$f(1)$		

Simplify and continue:

x_k	$f[] = f()$	$f[,]$	$f[, ,]$
-1	$f(-1)$		
		$f(0) - f(-1)$	
0	$f(0)$		$\frac{(f(1)-f(0)) - (f(0)-f(-1))}{1-(-1)}$
		$f(1) - f(0)$	
1	$f(1)$		

Simplify:

x_k	$f[] = f()$	$f[,]$	$f[, ,]$
-1	$f(-1)$		
		$B = f(0) - f(-1)$	
0	$f(0)$		$C = \frac{1}{2}\{f(1) - 2f(0) + f(-1)\}$
		$f(1) - f(0)$	
1	$f(1)$		

The interpolating polynomial:

$$\begin{aligned}
 p(x) &= f(-1) + B(x+1) + C(x+1)(x-0) \\
 &= f(-1) + B(x+1) + C(x+1)x \\
 &= \{f(-1) + B\} + (B+C)x + Cx^2 \\
 &= f(0) + (B+C)x + Cx^2
 \end{aligned}$$

Approximate:

$$\int_{-1}^1 f(x) dx \approx \int_{-1}^1 p(x) dx = \left[f(0)x + \frac{B+C}{2}x^2 + \frac{C}{3}x^3 \right]_{-1}^1 = 2f(0) + 2\frac{C}{3}$$

$$= 2f(0) + \frac{1}{3}\{f(1) - 2f(0) + f(-1)\} = \frac{1}{3}\{f(1) + 4f(0) + f(-1)\}$$

So we have got the approximation:

$$\int_{-1}^1 f(x) dx \approx \frac{1}{3}\{f(1) + 4f(0) + f(-1)\}$$

Step 2 (the general case). Now we deal with the general case of approximating $\int_a^b f(x) dx$ by using a formula that would involve the nodes $\{a, \frac{a+b}{2}, b\}$. We first do a transformation and define a function g on $[-1, 1]$ through:

$$g(t) = f\left(\frac{a+b}{2} + t\frac{b-a}{2}\right)$$

By putting $x = \frac{a+b}{2} + t\frac{b-a}{2}$ we have $dx = \frac{b-a}{2} dt$ equivalently $dt = \frac{2}{b-a} dx$, and so through change of variable in integration we can write:

$$\int_{-1}^1 g(t) dt = \frac{2}{b-a} \int_a^b f(x) dx \quad \Rightarrow \quad \int_a^b f(x) dx = \frac{b-a}{2} \int_{-1}^1 g(t) dt$$

Then from the approximating formula we found for the functions on interval $[-1, 1]$ we can write:

$$\begin{aligned} \int_a^b f(x) dx &= \frac{b-a}{2} \int_{-1}^1 g(t) dt \approx \frac{b-a}{2} \left\{ \frac{1}{3} \{g(1) + 4g(0) + g(-1)\} \right\} \\ &= \frac{b-a}{6} \{g(1) + 4g(0) + g(-1)\} = \frac{b-a}{6} \left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right\} \end{aligned}$$

So:

$$\boxed{\int_a^b f(x) dx \approx \frac{b-a}{6} \left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right\}}$$

3 Finding Quadratures By Means of Setting Degree of Exactness

Example. Find a , b , and c such that the approximation

$$\int_0^2 f(x)dx \approx af(0) + bf(1) + cf(2)$$

is exact for polynomials of degree less than or equal to 2.

Solution. We force the above approximation to be exact for the polynomials 1 , x , x^2 :

$$af(0) + bf(1) + cf(2) = \int_0^2 f(x) dx \quad \text{for } f(x) = 1, f(x) = x, f(x) = x^2$$

$$\left\{ \begin{array}{l} f(x) = 1 \Rightarrow a + b + c = \int_0^2 (1)dx = 2 \quad (1) \\ f(x) = x \Rightarrow 0 + b + 2c = \int_0^2 (x)dx = \left[\frac{1}{2}x^2\right]_0^2 = 2 \quad (2) \\ f(x) = x^2 \Rightarrow 0 + b + 4c = \int_0^2 (x^2)dx = \left[\frac{1}{3}x^3\right]_0^2 = \frac{8}{3} \quad (3) \end{array} \right.$$

From (2) we have:

$$b = 2 - 2c$$

We put this value of b into equality (3) to get:

$$(2 - 2c) + 4c = \frac{8}{3} \Rightarrow 2 + 2c = \frac{8}{3} \Rightarrow \boxed{c = \frac{1}{3}}$$

$$\Rightarrow b = 2 - 2c = 2 - \frac{2}{3} = \frac{4}{3} \Rightarrow \boxed{b = \frac{4}{3}}$$

By putting these values of b and c into equality (1) we get:

$$a = 2 - b - c = 2 - \frac{4}{3} - \frac{1}{3} = \frac{1}{3} \quad \Rightarrow \quad \boxed{a = \frac{1}{3}}$$

So:

$$\int_0^2 f(x) dx \approx \frac{1}{3}f(0) + \frac{4}{3}f(1) + \frac{1}{3}f(2) \quad \checkmark$$

Example. Find A , B , such that the approximation

$$\int_{-1}^1 f(x) dx \approx A f(-1) + B f(0) + C f'(1)$$

is exact for polynomials of degree less than or equal to 2.

Solution. We force the above approximation to be exact for the polynomials 1 , x , x^2 :

$$A f(-1) + B f(0) + C f'(1) = \int_{-1}^1 f(x) dx \quad \text{for } f(x) = 1, f(x) = x, f(x) = x^2$$

$$\left\{ \begin{array}{l} f(x) = 1 \Rightarrow A + B + 0 = \int_{-1}^1 (1) dx = 2 \\ f(x) = x \Rightarrow -A + 0 + C = \int_{-1}^1 (x) dx = \left[\frac{1}{2}x^2 \right]_{-1}^1 = 0 \\ f(x) = x^2 \Rightarrow A + 0 + 2C = \int_{-1}^1 (x^2) dx = \left[\frac{1}{3}x^3 \right]_{-1}^1 = \frac{2}{3} \end{array} \right.$$

$$\begin{cases} A + B = 2 & (1) \\ -A + C = 0 & (2) \\ A + 2C = \frac{2}{3} & (3) \end{cases}$$

Solving this system, one gets:

$$A = \frac{2}{9} \quad B = \frac{16}{9} \quad C = \frac{2}{9}$$

4 The Simpson's Methods

(section 9.4)

The quadrature

$$\int_a^b f(x) dx \approx \frac{b-a}{6} \left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right\}$$

is called the **Simpson's $\frac{1}{3}$ -Method**. The name " $\frac{1}{3}$ -Method" comes from this: In this discussion, the nodes are $\{a, \frac{a+b}{2}, b\}$, so each step is worth $h = \frac{b-a}{2}$, and by putting h for $\frac{b-a}{2}$ in the recently found formula, we get

$$\int_a^b f(x) dx \approx \frac{h}{3} \left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right\}, \quad h = \frac{b-a}{2}$$

Now we seek a composite form of this method. In the composite method we first divide the interval $[a, b]$ into an even number $2n$ of subintervals all of equal length $h = \frac{b-a}{2n}$ (**step size**); the endpoints of the intervals are:

$$a = x_1, x_2, x_3, x_4, x_5, \dots, x_{2n-1}, x_{2n}, x_{2n+1}$$

Then on each pair of subintervals we approximate:

$$\int_{x_1}^{x_3} f(x) dx \approx \frac{h}{3} [f(x_1) + 4f(x_2) + f(x_3)]$$

$$\int_{x_3}^{x_5} f(x) dx \approx \frac{h}{3} [f(x_3) + 4f(x_4) + f(x_5)]$$

⋮

$$\int_{x_{2n-1}}^{x_{2n+1}} f(x) dx \approx \frac{h}{3} [f(x_{2n-1}) + 4f(x_{2n}) + f(x_{2n+1})]$$

$$\int_{x_{2n-1}}^{x_{2n+1}} f(x) dx \approx \frac{h}{3} [f(x_{2n-1}) + 4f(x_{2n}) + f(x_{2n+1})]$$

Adding up these values, one gets an approximation for $\int_a^b f(x) dx$ by the following expression:

$$\frac{h}{3} \left[f(x_1) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_5) + \cdots + 2f(x_{2n-1}) + 4f(x_{2n}) + f(x_{2n+1}) \right]$$

But as $x_1 = a$ and $x_{2n+1} = b$, we equivalently get the approximation:

$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(a) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_5) + \cdots + 2f(x_{2n-1}) + 4f(x_{2n}) + f(b) \right]$$

This method for approximating integrals is called the **Composite Simpson's $\frac{1}{3}$ -Method**. In this formula, and every method we have seen so far, h is the step size and is equal to the common length of the subintervals.

Example . The following values of a function f are given:

x	-18	-12	-6	0	6	12	18
f(x)	0	2.6	3.2	4.8	5.6	6	6.2

Use the composite rectangle method to approximate the integral $\int_{-18}^{18} f(x) dx$

Solution. Since the number of nodes is even and the subintervals are of equal length, we can apply the composite Simpson's $\frac{1}{3}$ -Method. We have $h = 6$. Then

$$\begin{aligned} \int_{-18}^{18} f(x) dx &\approx \frac{h}{3} \left[f(x_1) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_5) + 4f(x_6) + f(x_7) \right] \\ &= \frac{6}{3} \left[(0) + 4(2.6) + 2(3.2) + 4(4.8) + 2(5.6) + 4(6) + (6.2) \right] = 154.8 \end{aligned}$$

Example . Find a quadrature

$$\int_0^3 f(x) dx \approx A f(0) + B f(1) + C f(2) + D f(3)$$

that is exact for polynomials of degree less than or equal to 3.

Solution . We force the above approximation to be exact for the polynomials 1 , x , x^2 , and x^3 :

$$A f(0) + B f(1) + C f(2) + D f(3) = \int_0^3 f(x) dx \quad \text{for } f(x) = 1, f(x) = x, f(x) = x^2, f(x) = x^3$$

$$\left\{ \begin{array}{l} f(x) = 1 \Rightarrow A + B + C + D = \int_0^3 (1) dx = 3 \\ f(x) = x \Rightarrow 0 + B + 2C + 3D = \int_0^3 (x) dx = \left[\frac{1}{2} x^2 \right]_0^3 = \frac{9}{2} \\ f(x) = x^2 \Rightarrow 0 + B + 4C + 9D = \int_0^3 (x^2) dx = \left[\frac{1}{3} x^3 \right]_0^3 = 9 \\ f(x) = x^3 \Rightarrow 0 + B + 8C + 27D = \int_0^3 (x^3) dx = \left[\frac{1}{4} x^4 \right]_0^3 = \frac{81}{4} \end{array} \right.$$

In summary, we get the following system:

$$\left\{ \begin{array}{l} A + B + C + D = 3 \quad (1) \\ B + 2C + 3D = \frac{9}{2} \quad (2) \\ B + 4C + 9D = 9 \quad (3) \\ B + 8C + 27D = \frac{81}{4} \quad (4) \end{array} \right.$$

Note. If one takes a quadrature

$$\int_0^3 f(x) dx \approx A f(0) + B f(1) + C f(2) + D f(3)$$

and imposes the condition that the formula be exact for the polynomials with degree less than or equal to 3, then one gets these values:

$$A = \frac{3}{8} \quad B = \frac{9}{8} \quad C = \frac{9}{8} \quad D = \frac{3}{8}$$

$$\text{Solve for } A, B, C, \text{ and } D \Rightarrow A = \frac{3}{8}, B = \frac{9}{8}, C = \frac{9}{8}, D = \frac{3}{8}$$

so the quadrature becomes

$$\int_0^3 f(x) dx \approx \frac{3}{8}f(0) + \frac{9}{8}f(1) + \frac{9}{8}f(2) + \frac{3}{8}f(3) = \frac{3}{8} [f(0) + 3f(1) + 3f(2) + f(3)]$$

By use of transformation, we can find a formula on any interval $[a, b]$. In fact, one must divide this interval into 3 subintervals each of length h , and then a transformation will change the above formula to this formula over $[a, b]$:

$$\int_a^b f(x) dx \approx \frac{3}{8} h [f(a) + 3f(x_2) + 3f(x_3) + f(b)]$$

Now let's transform this quadrature to a quadrature on an arbitrary interval $\int_a^b f(x)dx$.

Correspondingly we divide the interval $[a, b]$ into three subintervals of equal length. For this we need the nodes:

$$a \quad , \quad x_1 = \frac{2a + b}{3} \quad , \quad x_2 = \frac{a + 2b}{3} \quad , \quad b$$

The step size is $h = \frac{b-a}{3}$. Now to transform this "old" interval to the "new" interval $[0, 3]$ we do the transformation

$$t = \frac{(x - a) \times (\text{length of new interval})}{\text{length of old interval}} \quad \Rightarrow \quad \begin{cases} t = \frac{3(x-a)}{b-a} \\ dt = \frac{3dx}{b-a} \end{cases}$$

Then, corresponding to the function f on $[a, b]$ we define a function g on $[0, 3]$ via

$$g(t) = f(x)$$

$$\int_a^b f(x) dx = \int_0^3 g(t) \left(\frac{b-a}{3} \right) dt = \frac{b-a}{3} \int_0^3 g(t) dt = h \int_0^3 g(t) dt \approx$$

$$\approx h \left(\frac{3}{8} \right) [g(0) + 3g(1) + 3g(2) + g(3)] = \frac{3}{8} h [f(a) + 3f(x_1) + 3f(x_2) + f(b)]$$

So:

$$\int_a^b \mathbf{f}(\mathbf{x}) d\mathbf{x} \approx \frac{3}{8} \mathbf{h} [\mathbf{f}(\mathbf{a}) + 3\mathbf{f}(\mathbf{x}_1) + 3\mathbf{f}(\mathbf{x}_2) + \mathbf{f}(\mathbf{b})]$$

This method for approximating integrals is called the **Simpson's $\frac{3}{8}$ -Method**. In this formula, and every method we have seen so far, h is the step size and is equal to the common length of the subintervals.

Example . Use the Simpson's $\frac{3}{8}$ -Method to approximate the integral $\int_{-1.2}^{2.3} (x^2 - 1)e^{-x^2} dx$

Solution .

Each step size is $\frac{2.3 - (-1.2)}{3} = 1.667$. So the nodes are:

$$-1.2 \quad , \quad -0.0333 \quad , \quad 1.1333 \quad , \quad 2.3$$

$$f(x) = (x^2 - 1)e^{-x^2} \quad \Rightarrow \quad \left\{ \begin{array}{l} f(-1.2) = 0.1042 \\ f(-0.0333) = -0.9978 \\ f(1.1333) = 0.0787 \\ f(2.3) = 0.0216 \end{array} \right.$$

Then:

$$\begin{aligned} \int_{-1.2}^{2.3} (x^2 - 1)e^{-x^2} dx &\approx \frac{3}{8} h [f(a) + 3f(x_1) + 3f(x_2) + f(b)] \\ &= \frac{3}{8} h [f(-1.2) + 3f(-0.0333) + 3f(1.1333) + f(2.3)] \\ &= \left(\frac{3}{8}\right)(1.667) [(0.1042) + 3(-0.9978) + 3(0.0787) + (0.0216)] = -1.6450 \end{aligned}$$

The **Composite Simpson's $\frac{3}{8}$ -Method** is this :

$$\int_a^b f(x) dx \approx \frac{3}{8} h \left[f(a) + 3 \sum_{i=2,5,8,\dots} [f(x_i) + f(x_{i+1})] + 2 \sum_{i=4,7,10,\dots} f(x_i) + f(b) \right]$$

Note . This formula is good if you want to write a Matlab code.

Example . Write the Composite Simpson's $\frac{3}{8}$ -Method for the interval $[0, 15]$ if we divide this

interval into 15 subintervals ((note that for the $\frac{3}{8}$ -method the number of subintervals must be a multiple of 3).

Solution . The step size is $h = \frac{b-a}{15} = \frac{15}{15} = 1$. So , the nodes are:

$$0 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15$$

These points are the points

$$x_1 , x_2 , \dots , x_{16}$$

So,

$$\begin{aligned} & \frac{3}{8}h\{f(0) + 3f(1) + 3f(2) + f(3)\} + \frac{3}{8}h\{f(3) + 3f(4) + 3f(5) + f(6)\} \\ & + \frac{3}{8}h\{f(6) + 3f(7) + 3f(8) + f(9)\} + \frac{3}{8}h\{f(9) + 3f(10) + 3f(11) + f(12)\} \\ & + \frac{3}{8}h\{f(12) + 3f(13) + 3f(14) + f(15)\} \end{aligned}$$

which due to $h = 1$, it simplifies to:

$$\begin{aligned} & \frac{3}{8}\{f(0) + 3f(1) + 3f(2) + 2f(3) + 3f(4) + 3f(5) + 2f(6) + 3f(7) \\ & + 3f(8) + 2f(9) + 3f(10) + 3f(11) + 2f(12) + 3f(13) + 3f(14) + f(15)\} \end{aligned}$$

5 Romberg Integration

(section 9.10)

Consider a composite model, e.g. the composite trapezoidal method or a composite Simpson method. You may want to know what step size h , which is the length of each subinterval, gives a better approximation. Do we get better approximation if h is small?. The following order of convergence can be verified for the composite methods but an exact analysis requires some advanced knowledge of Calculus, so we skip it.

Composite Method	Order of Convergence
composite midpoint method	$O(h^2)$
composite trapezoidal method	$O(h^2)$
composite Simpson's $\frac{1}{3}$ -method	$O(h^4)$
composite Simpson's $\frac{3}{8}$ -method	$O(h^4)$

Let us study the composite trapezoidal method :

$$\int_a^b f(x)dx = \underbrace{\frac{h}{2} [f(a) + f(b)] + h \{f(x_1) + \dots + f(x_n)\}}_{D(h)} + O(h^2)$$

$$\int_a^b f(x)dx = D(h) + O(h^2)$$

In more advanced courses of Numerical Analysis it is shown that there are some constants $\gamma_1, \gamma_2, \dots$, not depending on h such that

$$\int_a^b f(x)dx = D(h) + \gamma_1 h^2 + \gamma_2 h^4 + \gamma_3 h^6 + \dots$$

We can improve the composite trapezoidal method by applying the extrapolation technique:

$$\frac{1}{3} \left\{ 4D\left(\frac{h}{2}\right) - D(h) \right\}$$

This gets rid of the term h^2 and we will have

$$\int_a^b f(x)dx = \frac{1}{3} \left\{ 4D\left(\frac{h}{2}\right) - D(h) \right\} + \gamma'_2 h^4 + \gamma'_3 h^6 + \dots$$

with some new constants $\gamma'_2, \gamma'_3, \dots$

Now let us divide the interval $[a, b]$ in to $n, 2n, 4n, \dots$ number of subintervals, and calculate the composite trapezoidal approximation for each. Put the approximate values in the first column and call them $I_{1,1}, I_{2,1}, I_{3,1}, \dots$, as shown below:

# of subintervals	composite trapezoidal
n	$I_{1,1}$
2n	$I_{2,1}$
4n	$I_{3,1}$
8n	$I_{4,1}$

Note that $I_{1,1}$ is the composite trapezoidal approximation corresponding to some initial step size $h_0 = \frac{b-a}{n}$ while $I_{2,1}$ is the composite trapezoidal approximation corresponding to the step size $\frac{h_0}{2} = \frac{b-a}{2n}$; so if $I_{1,1}$ is denoted by $D(h)$, then $I_{2,1}$ is actually $D(\frac{h}{2})$. But we recall from the extrapolation method that in order to get an improved approximate value, we must take the combination $\frac{1}{3}\{4D(\frac{h}{2}) - D(h)\}$, which is $\frac{1}{3}\{4I_{2,1} - I_{1,1}\}$. Indeed, to improve the values $I_{i,1}$ of the first column, one should form the combinations $\frac{1}{3}\{4I_{i+1,1} - I_{i,1}\}$. We denote these combinations by $I_{i,2}$:

$$I_{i,2} = \frac{1}{3}\{4I_{i+1,1} - I_{i,1}\}$$

We put these values in the second column:

step size	composite trapezoidal
h_0	$I_{1,1}$
	$I_{1,2}$
$\frac{h_0}{2}$	$I_{2,1}$
	$I_{2,2}$
$\frac{h_0}{4}$	$I_{3,1}$
	$I_{3,2}$
$\frac{h_0}{8}$	$I_{4,1}$

The values of the first column, which are some composite trapezoidal values, are of order $O(h^2)$. The improved values, which are in the second column, are of order $O(h^4)$. To improve the values of the second column we must employ an extrapolation technique for improving $O(h^4)$ methods. Generally, as we have learned before, to improve a method $D(h)$ of order $O(h^m)$ we must take the combination $\frac{1}{4^m - 1} \left\{ 4^m D\left(\frac{h}{2}\right) - D(h) \right\}$. Therefore to improve the values of the second column, we take the combinations

$$\frac{1}{2^4 - 1} \left\{ 2^4 I_{i+1,2} - I_{i,2} \right\} = \frac{1}{4^2 - 1} \left\{ 4^2 I_{i+1,2} - I_{i,2} \right\}$$

We denote these values by $I_{i,3}$ and put them in the third column:

$$I_{i,3} = \frac{1}{4^2 - 1} \left\{ 4^2 I_{i+1,2} - I_{i,2} \right\}$$

step size	composite trapezoidal
h_0	$I_{1,1}$
	$I_{1,2}$
$\frac{h_0}{2}$	$I_{2,1}$
	$I_{2,2}$
$\frac{h_0}{4}$	$I_{3,1}$
	$I_{3,2}$
$\frac{h_0}{8}$	$I_{4,1}$

As you guess, the elements in the next column are form from:

$$I_{i,4} = \frac{1}{4^3 - 1} \{4^3 I_{i+1,3} - I_{i,3}\}$$

step size	composite			
	trapezoidal			
h_0	$I_{1,1}$			
		$I_{1,2}$		
$\frac{h_0}{2}$	$I_{2,1}$		$I_{1,3}$	
		$I_{2,2}$		$I_{1,4}$
$\frac{h_0}{4}$	$I_{3,1}$		$I_{2,3}$	
		$I_{3,2}$		
$\frac{h_0}{8}$	$I_{4,1}$			

and in general if we want to construct the elements of the j -th column , we use the formula:

$$I_{i,j} = \frac{1}{4^{j-1} - 1} \{4^{j-1} I_{i+1,j-1} - I_{i,j-1}\}$$

In Matlab, due to format of arrays, we put them in this order:

step size	composite			
	trapezoidal			
h_0	$I_{1,1}$	$I_{1,2}$	$I_{1,3}$	$I_{1,4}$
$\frac{h_0}{2}$	$I_{2,1}$	$I_{2,2}$	$I_{2,3}$	
$\frac{h_0}{4}$	$I_{3,1}$	$I_{3,2}$		
$\frac{h_0}{8}$	$I_{4,1}$			

Example. Here we approximate the integral $\int_0^\pi \sin x \, dx$ using the Romberg Integration technique. The true value of this integral is 2. We start with $h_0 = \pi$ as the initial step size.

h	$I_{i,1}$	$I_{i,2}$	$I_{i,3}$	$I_{i,4}$	$I_{i,5}$	$I_{i,6}$
$\pi=3.1416$	0.00000000	0.95221404	2.37929775	1.97462375	2.00040288	1.99999842
$\frac{\pi}{2}=1.5708$	0.71416053	A =2.29010502	C =1.98094678	2.00030218	1.99999882	
$\frac{\pi}{4}=0.7854$	1.89611890	B =2.00026917	1.99999975	2.00000000		
$\frac{\pi}{8}=0.3927$	1.97423160	2.00001659	2.00000000			
$\frac{\pi}{16}=0.1963$	1.99357034	2.00000103				
$\frac{\pi}{32}=0.0982$	1.99839336					

$$C = \frac{4^2 B - A}{4^2 - 1} = \frac{16B - A}{15}$$

6 Integrals With Singularities

(section 9.11.1)

Definition. A singularity for an integral $\int_a^b f(x)dx$ is a point in the interval at which the function f is undefined. For example, in the integral $\int_{-1}^1 \frac{1}{|x|}dx$ the integrand is not defined at $x = 0$, so the point $x = 0$ is considered as a singularity for the integral. The point $x = 1$ is a singularity for the integral $\int_1^3 \frac{1}{\sqrt{(x-1)^2}}$. Some of such integrals are convergent, meaning that the value of the integral exists, and some are divergent. For example, the integral $\int_1^3 \frac{1}{\sqrt{(x-1)^2}}$ is convergent and the integral $\int_{-1}^1 \frac{1}{|x|}dx$ is divergent. Numerical procedures can be applied to evaluate the values of the convergent integrals. To evaluate the value of the integrals such as $\int_{-1}^1 \frac{1}{\sqrt{|x|}}dx$ where the singularity is an interior point, one must split the integral into two parts such that the singularity appear at one endpoint; so we write

$$\int_{-1}^1 \frac{1}{\sqrt{|x|}}dx = \int_{-1}^0 \frac{1}{\sqrt{|x|}}dx + \int_0^1 \frac{1}{\sqrt{|x|}}dx$$

So we are always able to put a singularity at one of the endpoints. Let us now see how to deal with an integral such as $\int_1^3 \frac{1}{\sqrt{(x-1)^2}}$ in which the singularity is at one of the endpoints. For such integral we use an “Open Method” such as the composite midpoint method. For example we may split the interval $[1, 4]$ into 10 subintervals with step size $h = \frac{4-1}{10} = 0.3$ using these nodes :

$$1, 1.3, 1.6, 1.9, 2.2, 2.5, 2.8, 3.1, 3.4, 3.7, 4$$

Now on each subinterval take the midpoint; here are the midpoints:

$$1.15, 1.45, 1.75, 2.05, 2.35, 2.65, 2.95, 3.25, 3.55, 3.85$$

$$\int_1^3 \frac{1}{\sqrt{(x-1)^2}} \approx$$

$$h\{f(1.15)+f(1.45)+f(1.75)+f(2.05)+f(2.35)+f(2.65)+f(2.95)+f(3.25)+f(3.55)+f(3.85)\}$$

$$= 0.3 \left\{ (44.4444) + (4.9383) + (1.7778) + (0.9070) + (0.5487) + (0.3673) + (0.2630) + (0.1975) + (0.1538) + (0.1231) \right\} = 16.1163$$

7 Integrals With Unbounded Limits

(section 9.11.2)

Integrals of the forms $\int_{-\infty}^b f(x)dx$ and $I = \int_a^{\infty} f(x)dx$ and $\int_{-\infty}^{+\infty} f(x)dx$ can be evaluated either of the following method:

For example to evaluate the integral $\int_0^{\infty} e^{-x^2} dx$ we may first approximate it with an integral $\int_0^M e^{-x^2} dx$ where M is large, and then apply one the methods of this chapter to $\int_0^M e^{-x^2} dx$.

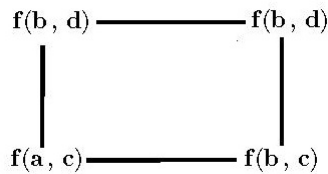
For example

$$\int_0^{\infty} e^{-x^2} dx \approx \int_0^{10} e^{-x^2} dx = \text{using the trapezoidal method with } h=0.5 = 0.8862$$

8 Solving Double Integrals Numerically

Consider a double integral $I = \int_a^b \int_c^d f(x, y) dx dy = \int_a^b \left[\int_c^d f(x, y) dy \right] dx$. We may, for example, apply the trapezoidal rule on the variable y first and then on the variable x to write:

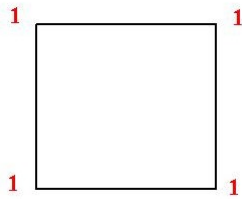
$$\begin{aligned}
 I &= \int_a^b \left[\int_c^d f(x, y) dy \right] dx \\
 &\approx \int_a^b \left\{ \frac{d-c}{2} [f(x, c) + f(x, d)] \right\} dx \\
 &= \frac{d-c}{2} \int_a^b [f(x, c) + f(x, d)] dx \\
 &= \frac{d-c}{2} \left\{ \int_a^b f(x, c) dx + \int_a^b f(x, d) dx \right\} \\
 &\approx \frac{d-c}{2} \left\{ \frac{b-a}{2} \{f(a, c) + f(b, c)\} + \frac{b-a}{2} \{f(a, d) + f(b, d)\} \right\} \\
 &= \frac{b-a}{2} \frac{d-c}{2} \{f(a, c) + f(b, c) + f(a, d) + f(b, d)\} \\
 &= \frac{hk}{4} \{f(a, c) + f(b, c) + f(a, d) + f(b, d)\} \quad h \text{ and } k \text{ are step sizes}
 \end{aligned}$$



If we denote the four values by $\begin{cases} f_{11} = f(a, c) \\ f_{1,2} = f(b, c) \\ f_{2,1} = f(b, d) \\ f_{2,2} = f(a, d) \end{cases}$, then we rewrite:

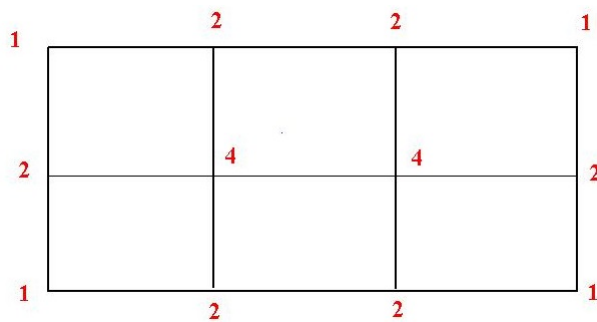
$$I \approx \frac{hk}{4} \{f_{1,1} + f_{1,2} + f_{2,1} + f_{2,2}\}$$

In the following figure you see the coefficients of these terms.



Now if you want to use a composite trapezoidal on both x and y , with step sizes $h = \frac{b-a}{3}$ and $k = \frac{d-c}{2}$ for example, then the coefficients are as follows:

$$\begin{aligned} & \frac{hk}{4} \left\{ \{f_{11} + 2f_{12} + 2f_{13} + f_{14}\} + 2\{f_{21} + 2f_{22} + 2f_{23} + f_{24}\} + \{f_{31} + 2f_{32} + 2f_{33} + f_{34}\} \right\} \\ &= \frac{hk}{4} \left\{ \{f_{11} + 2f_{12} + 2f_{13} + f_{14}\} + \{2f_{21} + 4f_{22} + 4f_{23} + 2f_{24}\} + \{f_{31} + 2f_{32} + 2f_{33} + f_{34}\} \right\} \end{aligned}$$



In general, the coefficients of a composite trapezoidal method are:

$$\begin{array}{ccccccc}
1 & 2 & 2 & 2 & \cdots & 2 & 2 & 1 \\
2 & 4 & 4 & 4 & \cdots & 4 & 4 & 2 \\
2 & 4 & 4 & 4 & \cdots & 4 & 4 & 2 \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\
2 & 4 & 4 & 4 & \cdots & 4 & 4 & 2 \\
2 & 4 & 4 & 4 & \cdots & 4 & 4 & 2 \\
1 & 2 & 2 & 2 & \cdots & 2 & 2 & 1
\end{array}$$

and for a composite Simpson they are:

$$\begin{array}{ccccccc}
1 & 4 & 2 & 4 & 2 & \cdots & 2 & 4 & 1 \\
4 & 16 & 8 & 16 & 8 & \cdots & 8 & 16 & 4 \\
2 & 8 & 4 & 8 & 4 & \cdots & 4 & 8 & 2 \\
4 & 16 & 8 & 16 & 8 & \cdots & 8 & 16 & 4 \\
2 & 8 & 4 & 8 & 4 & \cdots & 4 & 8 & 2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\
2 & 8 & 4 & 8 & 4 & \cdots & 4 & 8 & 2 \\
4 & 16 & 8 & 16 & 8 & \cdots & 8 & 16 & 4 \\
1 & 4 & 2 & 4 & 2 & \cdots & 2 & 4 & 1
\end{array}$$

Example . Approximate the integral $\int_0^\pi \int_0^\pi \cos(x+y) dx dy$ using the trapezoidal composite rule with step sizes $h = \frac{b-a}{3} = \frac{\pi}{3} = 1.0472$ and $k = \frac{c-d}{2} = \frac{\pi}{2} = 1.5708$.

Solution . The x -nodes are:

$$0, \frac{\pi}{3}, \frac{2\pi}{3}, \pi$$

and the y -nodes are:

$$0, \frac{\pi}{2}, \pi$$

The location of the double-nodes on the plane:

$(0, \pi)$	$(\frac{\pi}{3}, \pi)$	$(\frac{2\pi}{3}, \pi)$	(π, π)
$(0, \frac{\pi}{2})$	$(\frac{\pi}{3}, \frac{\pi}{2})$	$(\frac{2\pi}{3}, \frac{\pi}{2})$	$(\pi, \frac{\pi}{2})$
$(0, 0)$	$(\frac{\pi}{3}, 0)$	$(\frac{2\pi}{3}, 0)$	$(\pi, 0)$

Then the values of the function multiplies by the weights:

$$A =$$

$f(0, \pi)$	$2f(\frac{\pi}{3}, \pi)$	$2f(\frac{2\pi}{3}, \pi)$	$f(\pi, \pi)$
$2f(0, \frac{\pi}{2})$	$4f(\frac{\pi}{3}, \frac{\pi}{2})$	$4f(\frac{2\pi}{3}, \frac{\pi}{2})$	$2f(\pi, \frac{\pi}{2})$
$f(0, 0)$	$2f(\frac{\pi}{3}, 0)$	$2f(\frac{2\pi}{3}, 0)$	$f(\pi, 0)$

$$A =$$

-1.0000	1.0000	1.0000	1.0000
0.0000	-3.4641	-3.4641	-0.0000
1.0000	1.0000	-1.0000	-1.0000

Add up these values: -6.9282

Then multiply by $\frac{hk}{4} = \frac{(1.0472)(1.5708)}{4} = 0.4112$ to get the approximate value for the integral:

$$(-6.9282)(0.4112) = -2.8489$$