Numerical integration

Recall that Lagrange interpolation of f by

$$f(x) = \underbrace{\sum_{i=0}^{n} f(x_i) L_{n,i}(x)}_{\text{Lagrange polynomial } P_n(x)} + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

So we can take integral on both sides:

$$\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x &= \int_a^b \sum_{i=0}^{n} f(x_i)\, L_{n,i}(x)\,\mathrm{d}x + \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)\,\mathrm{d}x \\
&= \sum_{i=0}^{n} a_i f(x_i) + E(f)
\end{aligned}$$

where for $i = 0, \dots, n$,

$$a_i = \int_a^b L_{n,i}(x)\,\mathrm{d}x \text{ and } E(f) = \frac{1}{(n+1)!} \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)\,\mathrm{d}x$$

Trapezoidal rule

Suppose we know f at $x_0 = a$ and $x_1 = b$, then

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)$$

Then taking integral of f yields

$$\int_a^b f(x)\,\mathrm{d}x = \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] \mathrm{d}x$$
$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))\,(x - x_0)\,(x - x_1)\,\mathrm{d}x$$

Trapezoidal rule

Integral of the first term on the right is straightforward.

Note that the second term on the right is

$$\begin{aligned}
&\int_{x_0}^{x_1} f''(\xi(x))\,(x-x_0)\,(x-x_1)\,\mathrm{d}x \\
&= f''(\xi)\int_{x_0}^{x_1} (x-x_0)\,(x-x_1)\,\mathrm{d}x \\
&= f''(\xi)\left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2}x^2 + x_0x_1x\right]_{x_0}^{x_1} \\
&= -\frac{h^3}{6}f''(\xi)
\end{aligned}$$

where $\xi \in (x_0, x_1)$ by MVT for integrals and

Trapezoidal rule

Therefore, we obtain

$$\int_a^b f(x)dx = \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1)\right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\xi)$$

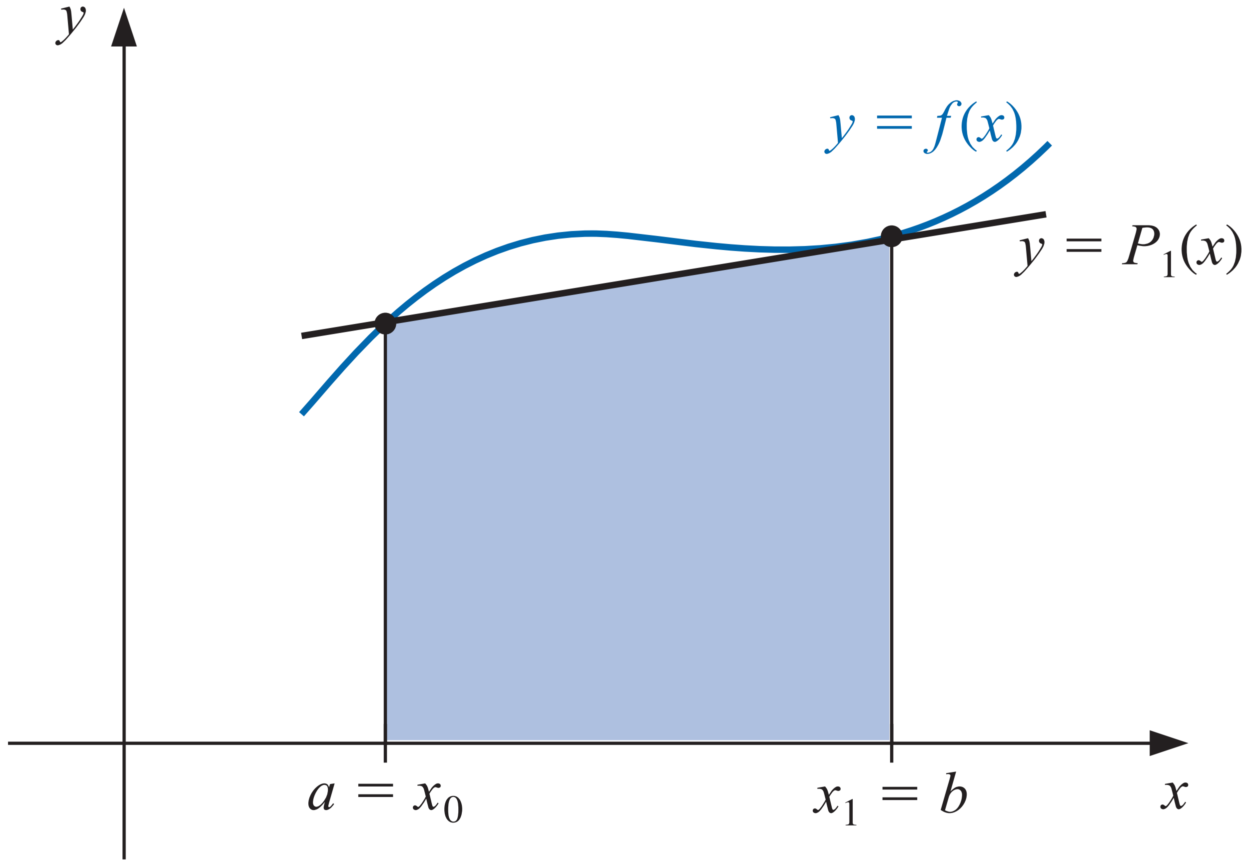
$$= \frac{(x_1-x_0)}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi)$$

Trapezoidal rule:

$$\int_a^b f(x)\,\mathrm{d}x = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi)$$

Trapezoidal rule

Illustration of Trapezoidal rule:



Simpson's rule

If we have values of f at $x_0 = a$, $x_1 = \frac{a+b}{2}$, and $x_2 = b$. Then

$$\int_a^b f(x)\,\mathrm{d}x = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right.$$

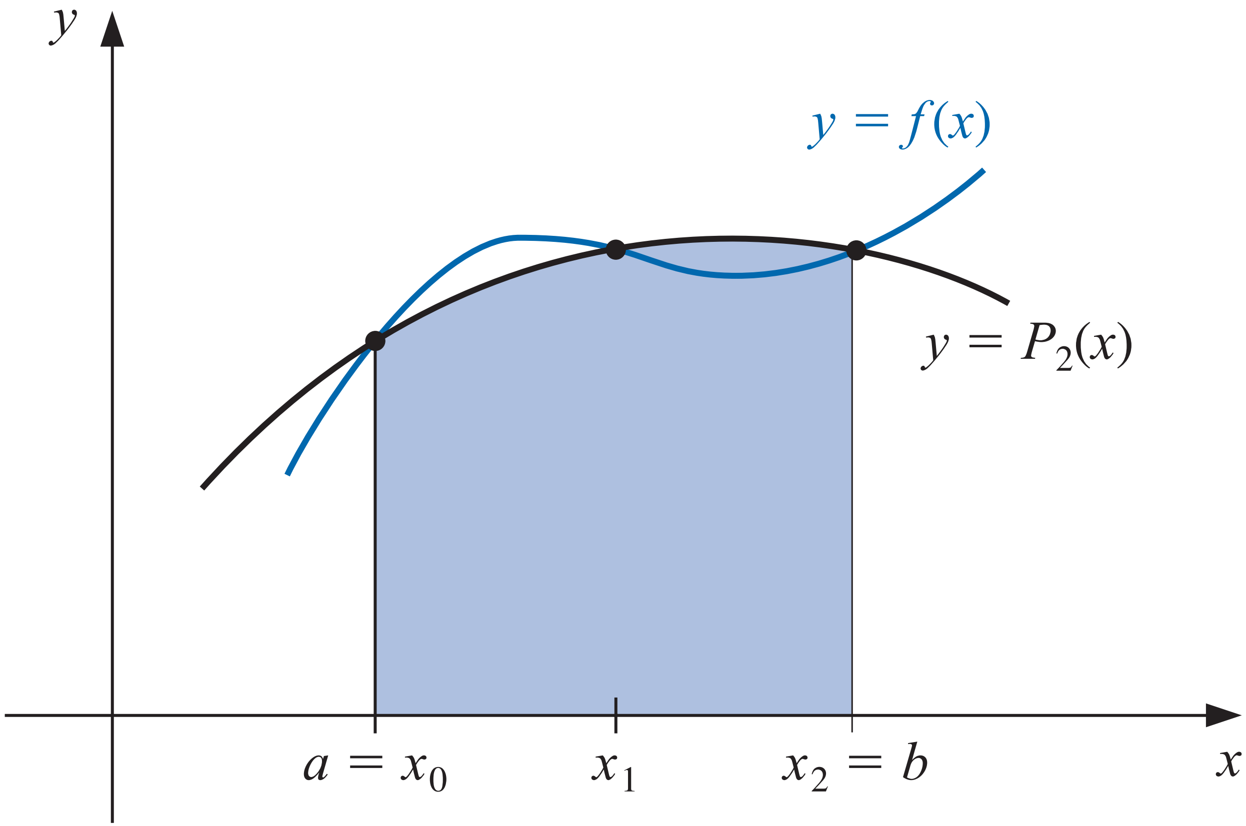
$$\left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] \mathrm{d}x$$

$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,\mathrm{d}x$$

Simpson's rule

With similar idea, we can derive the **Simpson's rule**:

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] - \frac{h^5}{90} f^{(4)}(\xi)$$



Example

Example (Trapezoidal and Simpson's rules for integration)

Compare Trapezoidal and Simpson's rules on $\int_0^2 f(x)\,\mathrm{d}x$ where f is

(a) x^2 (b) x^4 (c) $(x+1)^{-1}$
(d) $\sqrt{1+x^2}$ (e) $\sin x$ (f) e^x

Solution. Apply the the formulas respectively to get:

Problem	(a)	(b)	(c)	(d)	(e)	(f)
$f(x)$	x^2	x^4	$(x+1)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

Newton-Cotes formula

We can follow the same idea to get higher-order approximations, called the **Netwon-Cotes** formulas.

For $n = 3$ where $\xi \in (x_0, x_3)$:

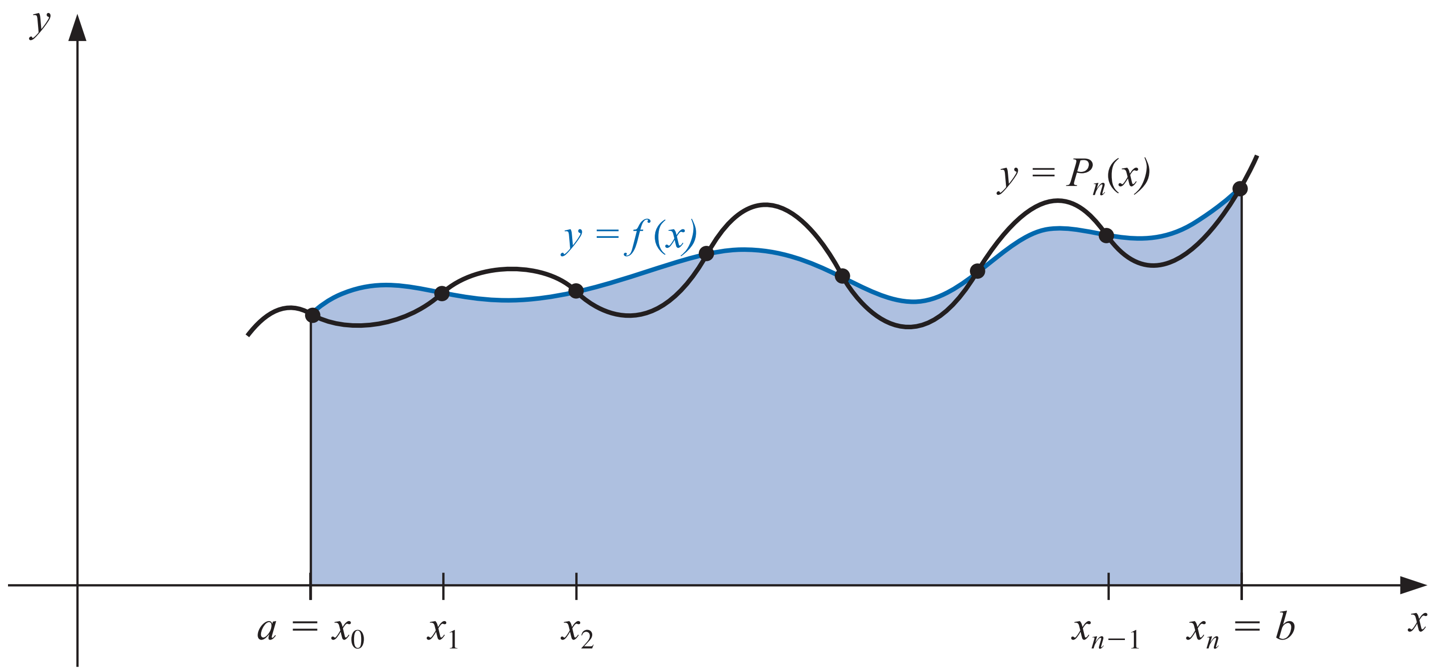
$$\int_{x_0}^{x_3} f(x)\,\mathrm{d}x = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] - \frac{3h^5}{80} f^{(4)}(\xi)$$

For $n = 4$ where $\xi \in (x_0, x_4)$:

$$\int_{x_0}^{x_4} f(x)\,\mathrm{d}x = \frac{2h}{45}\left[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\right] - \frac{8h^7}{945} f^{(6)}(\xi)$$

Composite numerical integration

Problem with Newton-Cotes rule for high degree is oscillations.

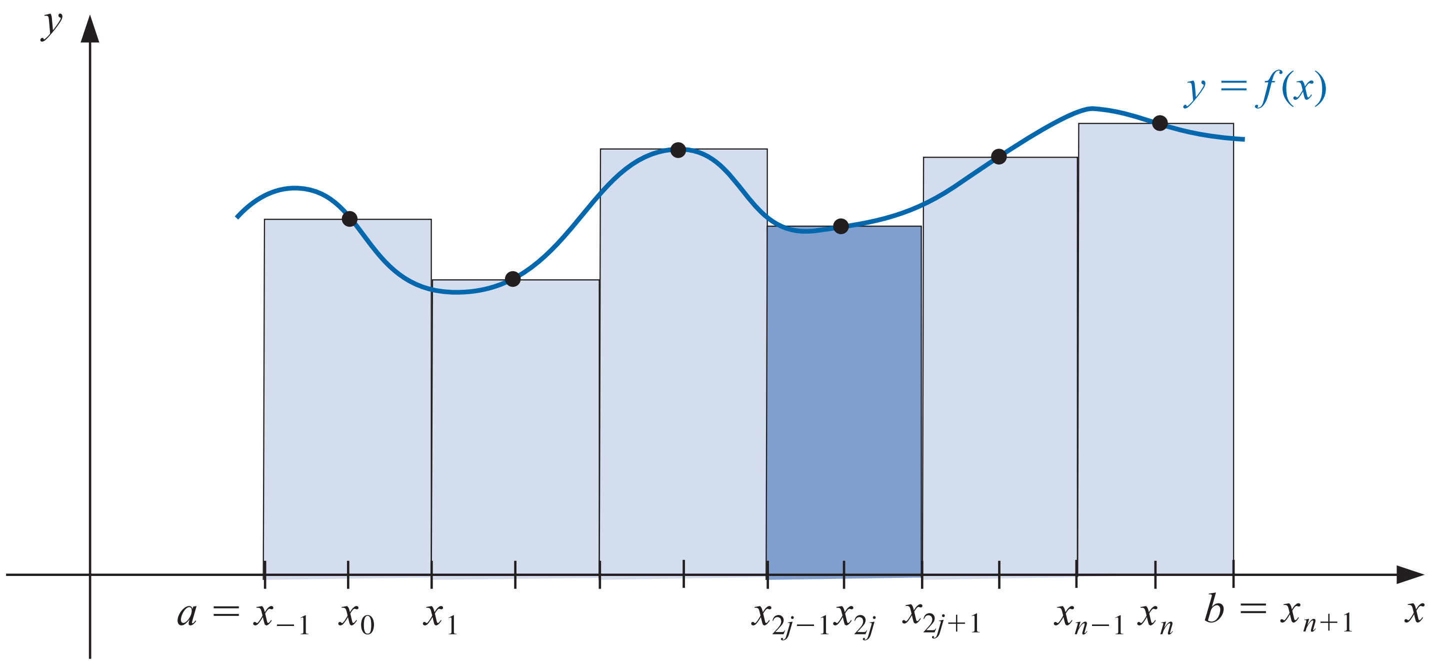


Instead, we can approximate the integral "piecewisely".

Composite midpoint rule

Let $x_{-1} = a, x_0, x_1, \ldots, x_n, x_{n+1} = b$ be a uniform partition of $[a, b]$ with $h = \frac{b-a}{n+2}$. Then we obtain the **composite midpoint rule**:

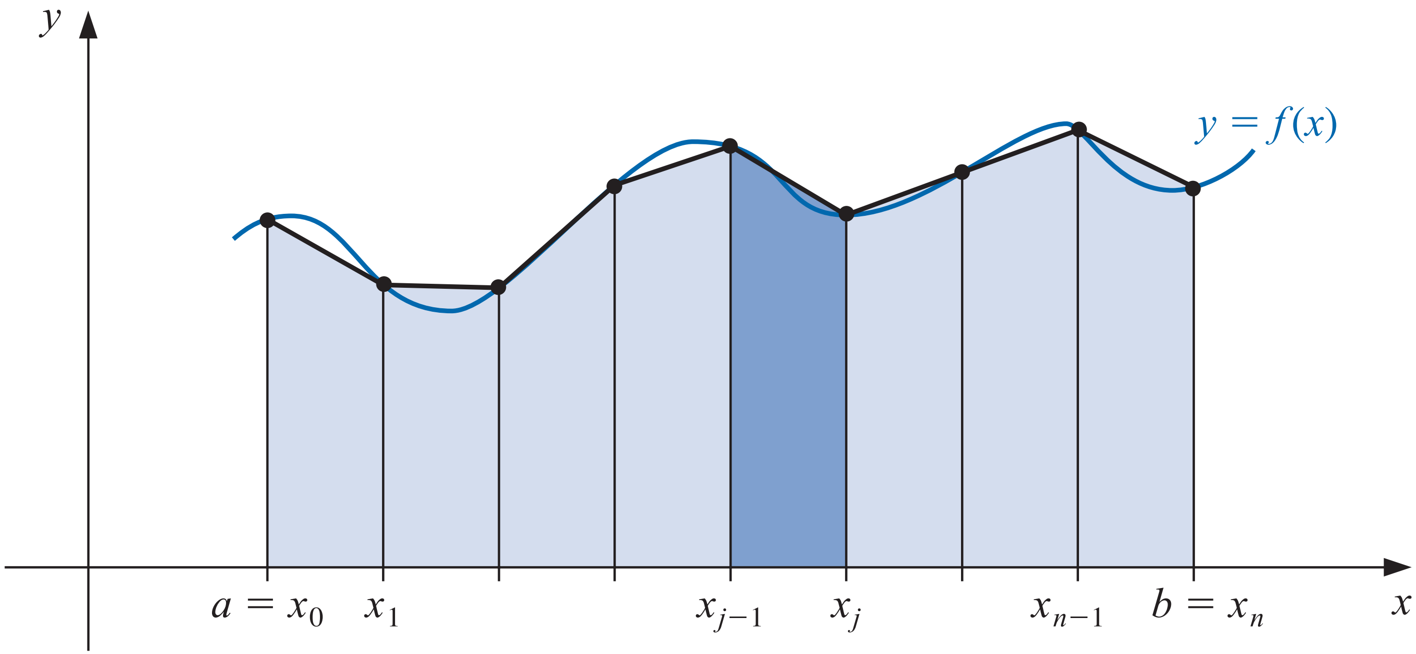
$$\int_a^b f(x)\,\mathrm{d}x = 2h \sum_{j=0}^{n/2} f\left(x_{2j}\right) + \frac{b-a}{6} h^2 f''(\mu)$$



Composite trapezoidal rule

Let $x_0 = a, x_1, \ldots, x_n = b$ be a uniform partition of $[a, b]$ with $h = \frac{b-a}{n}$. Then we obtain the **composite Trapezoidal rule**:

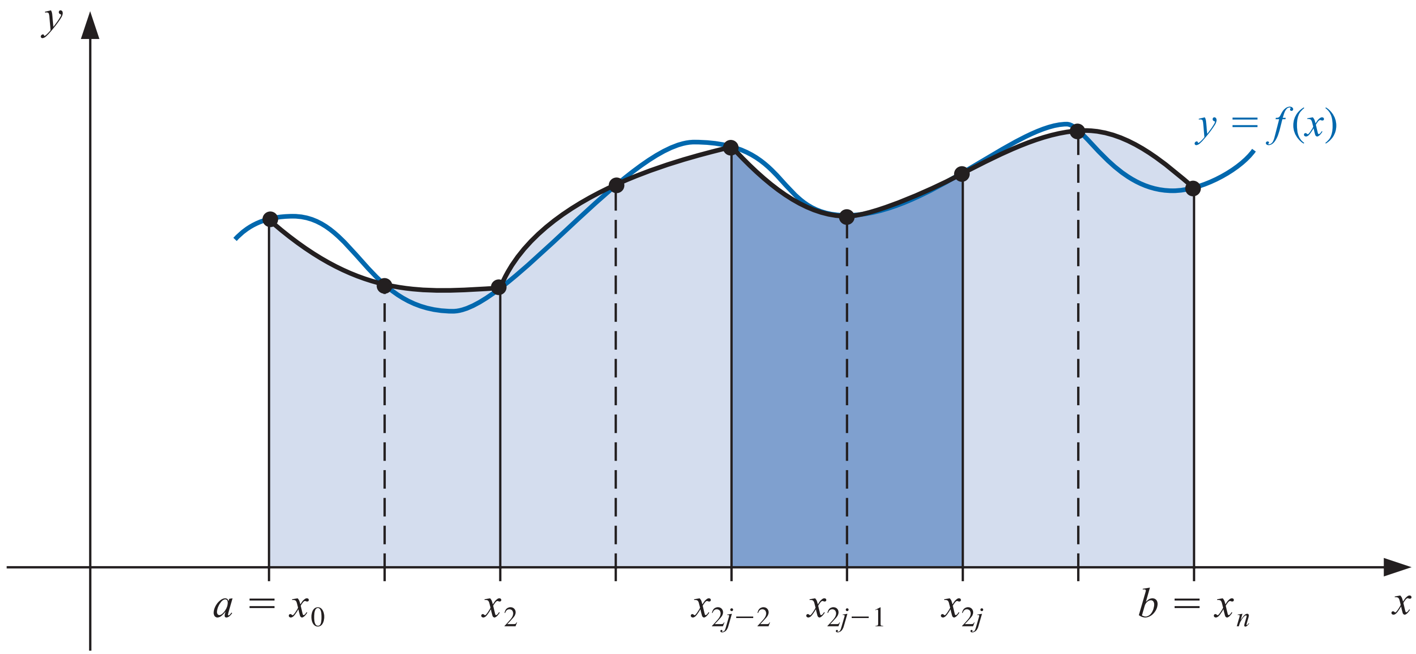
$$\int_a^b f(x)\,\mathrm{d}x = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f\left(x_j\right) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu)$$



Composite Simpson's rule

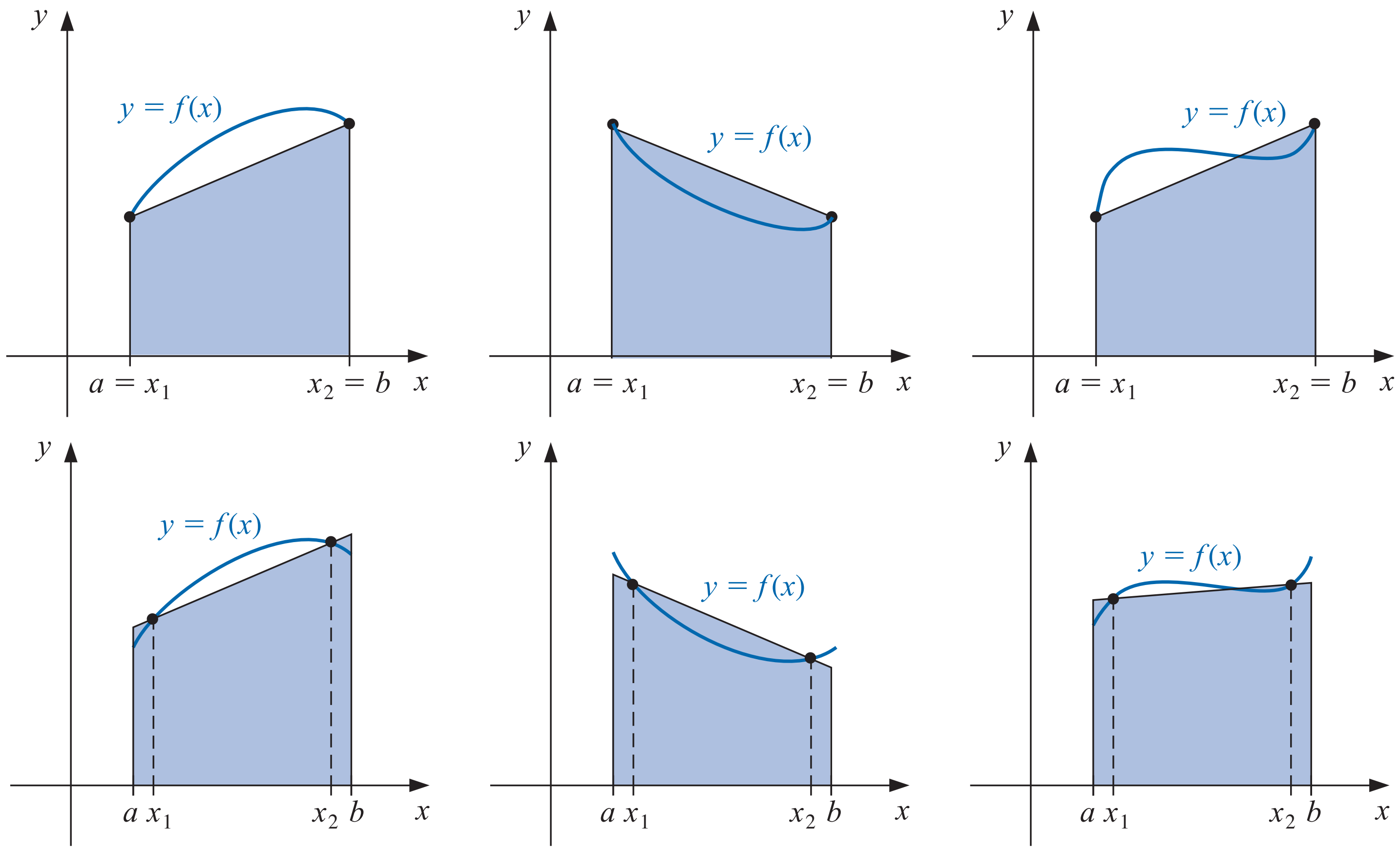
Let $x_0, x_1, \ldots, x_n$ (n even) be a uniform partition of $[a, b]$. Then apply Simpson's rule on $[x_0, x_2], [x_2, x_4], \ldots,$ a total of n such intervals. Then we obtain the **composite Simpson's rule**:

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\mu)$$



Gauss quadrature

Previously we chose points (nodes) with fixed gaps. What if we are allowed to to choose points $x_0, \ldots, x_n$ and evaluate f there?



Gauss quadrature

Gauss quadrature tries to determine $x_1, \dots, x_n$ and $c_1, \dots, c_n$ s.t.

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{i=1}^n c_i f(x_i)$$

Conceptually, since we have $2n$ parameters, i.e., c_i, x_i for $i = 1, \dots, n$, we expect to get "$=$" if $f(x)$ is a polynomial of degree $\leq 2n - 1$.

Gauss quadrature

Let's first try the case with interval $[-1, 1]$ and two points $x_1, x_2 \in [-1, 1]$. Then we need to find x_1, x_2, c_1, c_2 such that

$$\int_{-1}^{1} f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

and "$=$" holds for all polynomials of degree ≤ 3.

Gauss quadrature

We first note

$$\int \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right) \mathrm{d}x = a_0 \int 1 \, \mathrm{d}x + a_1 \int x \, \mathrm{d}x + a_2 \int x^2 \, \mathrm{d}x + a_3 \int x^3 \, \mathrm{d}x$$

Then we need x_1, x_2, c_1, c_2 s.t. $\int_{-1}^{1} f(x) \, \mathrm{d}x = c_1 f(x_1) + c_2 f(x_2)$ for $f(x) = 1, x, x^2$, and x^3:

$$\begin{aligned}
c_1 \cdot 1 + c_2 \cdot 1 &= \int_{-1}^{1} 1 \, \mathrm{d}x = 2, \\
c_1 \cdot x_1 + c_2 \cdot x_2 &= \int_{-1}^{1} x \, \mathrm{d}x = 0 \\
c_1 \cdot x_1^2 + c_2 \cdot x_2^2 &= \int_{-1}^{1} x^2 \, \mathrm{d}x = \frac{2}{3}, \\
c_1 \cdot x_1^3 + c_2 \cdot x_2^3 &= \int_{-1}^{1} x^3 \, \mathrm{d}x = 0
\end{aligned}$$

Gauss quadrature

Solve the system of four equations to obtain x_1, x_2, c_1, c_2:

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3}, \quad \text{and} \quad x_2 = \frac{\sqrt{3}}{3}$$

So the approximation is

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx f\left(\frac{-\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

which is exact for all polynomials of degree ≤ 3.

This point and weight selection is called **Gauss quadrature**.

Legendre polynomials

To obtain Gauss quadrature for larger n, we need **Legendre polynomials** $\{P_n : n = 0, 1, \dots\}$:

1. All P_n are monic (leading coefficient $=1$)
2. $$\int_{-1}^{1} P(x)P_n(x)\,\mathrm{d}x = 0$$

   for all polynomial P of degree less than n.

Legendre polynomials

The first five Legendre polynomials:

$$
\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= x^2 - \frac{1}{3} \\
P_3(x) &= x^3 - \frac{3}{5}x \\
P_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35}
\end{aligned}
$$

Gauss quadrature and Legendre polynomial

Theorem (Obtain Gauss quadrature by Legendre poly.)

Suppose $x_1, \ldots, x_n$ are the roots of the nth Legendre polynomial $P_n(x)$, and define

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \, \mathrm{d}x$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x) dx = \sum_{i=1}^{n} c_i P\left(x_i\right)$$

Gauss quadrature

n	**Roots** $r_{n,i}$	**Coefficients** $c_{n,i}$
2	0.5773502692	1.0000000000
	-0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	-0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	-0.3399810436	0.6521451549
	-0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	-0.5384693101	0.4786286705
	-0.9061798459	0.2369268850

Example

Example (Gauss quadrature)

Approximate $\int_{-1}^{1} e^x \cos x \, dx$ using Gauss quadrature with $n = 3$.

Solution. We need to use the roots of Legendre polynomial and coefficient values for $n = 3$:

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	-0.7745966692	0.5555555556

$$\begin{aligned}\int_{-1}^{1} e^x \cos x \, dx \approx & 0.\bar{5} e^{0.77459692} \cos(0.774596692) + 0.\bar{8} \cos(0) \\ & + 0.\bar{5} e^{-0.77459692} \cos(-0.774596692) \\ = & 1.9333904\end{aligned}$$

True value is $\int_{-1}^{1} e^x \cos x \, dx = 1.9334214$. Our error is 3.2×10^{-5}.

Gauss quadrature on arbitrary interval

So far the Gauss quadrature is only considered on $[-1,1]$.

To find Gauss quadrature on arbitrary $x \in [a,b]$, just do a change of variable:

$$t = \frac{2x-a-b}{b-a} \quad \Longleftrightarrow \quad x = \frac{1}{2}[(b-a)t+a+b]$$

Then $t \in [-1,1]$ and the integral is

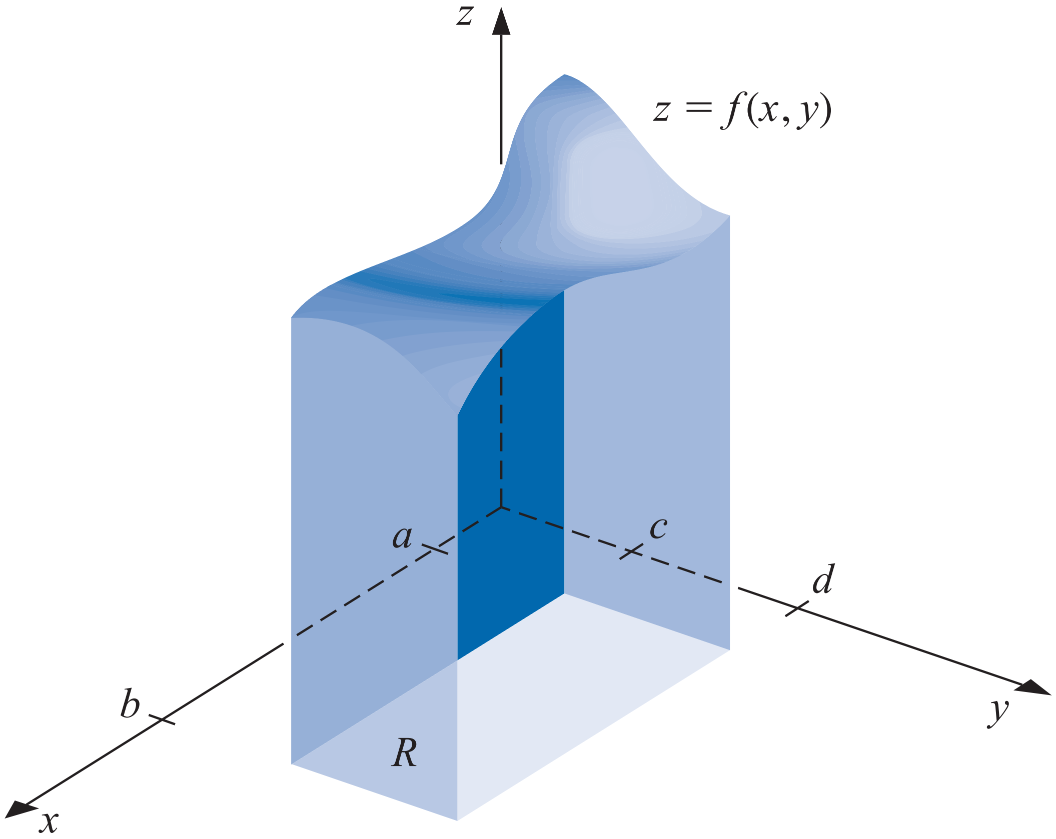
$$\int_a^b f(x)\,\mathrm{d}x = \int_{-1}^1 f\left(\frac{(b-a)t+(b+a)}{2}\right)\frac{(b-a)}{2}\,\mathrm{d}t$$

Then apply Gauss quadrature to the right side.

Multiple integrals

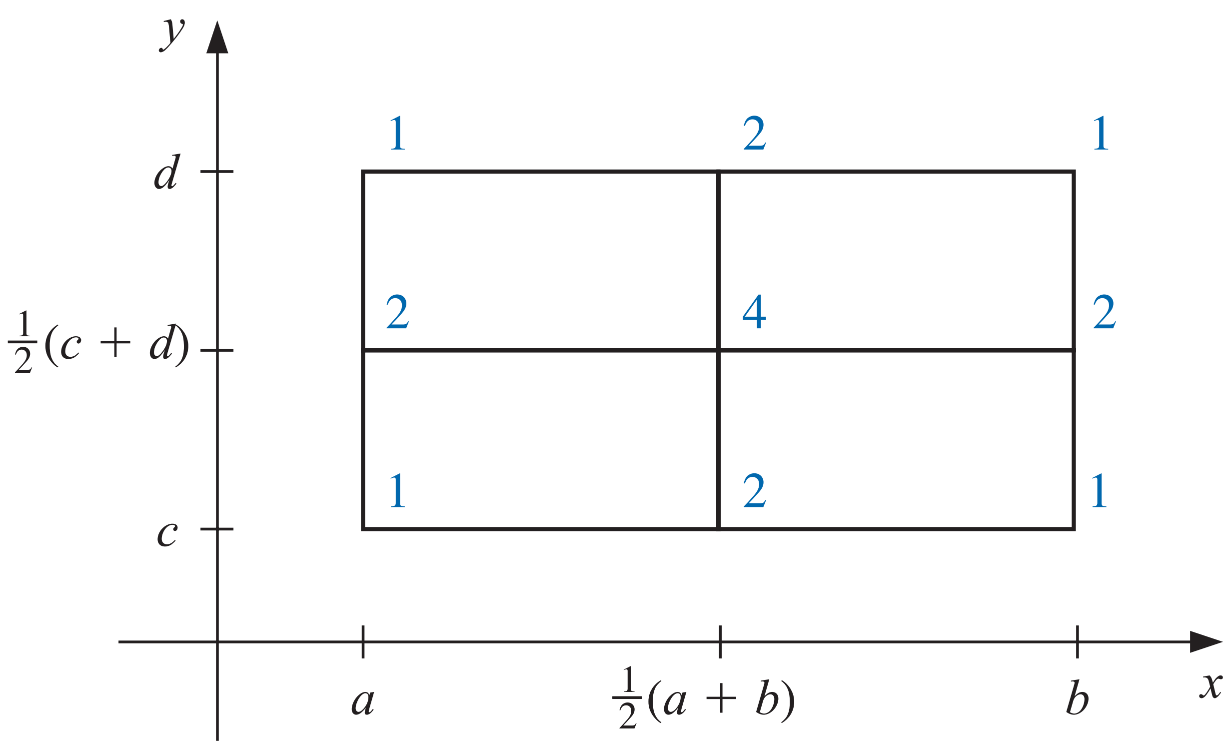
Now we consider multiple integral

$$\int_a^b \int_c^d f(x, y)\, \mathrm{d}y\, \mathrm{d}x$$



Multiple integrals

First consider a 2×2 grid on the domain $[a, b] \times [c, d]$:



Here $k = \frac{d-c}{2}$ and $h = \frac{b-a}{2}$.

Multiple integrals

We first approximate the inner integral using composite Trapezoidal rule:

$$\begin{aligned}\int_c^d f(x,y)\,\mathrm{d}y &= \int_c^{c+k} f(x,y)\,\mathrm{d}y + \int_{c+k}^d f(x,y)\,\mathrm{d}y \\ &\approx \frac{k}{2}(f(x,c)+f(x,c+k)) + \frac{k}{2}(f(x,c+k)+f(x,d)) \\ &= \frac{k}{2}(f(x,c)+2f(x,c+k)+f(x,d)) =: g(x)\end{aligned}$$

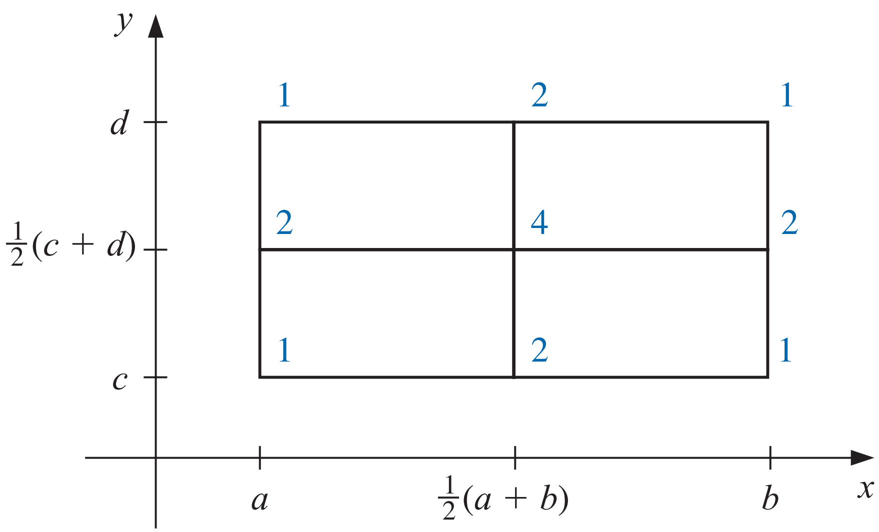
Then approximate the outer integral:

$$\int_a^b g(x)\,\mathrm{d}x = \frac{h}{2}(g(a)+2g(a+h)+g(b))$$

Multiple integrals

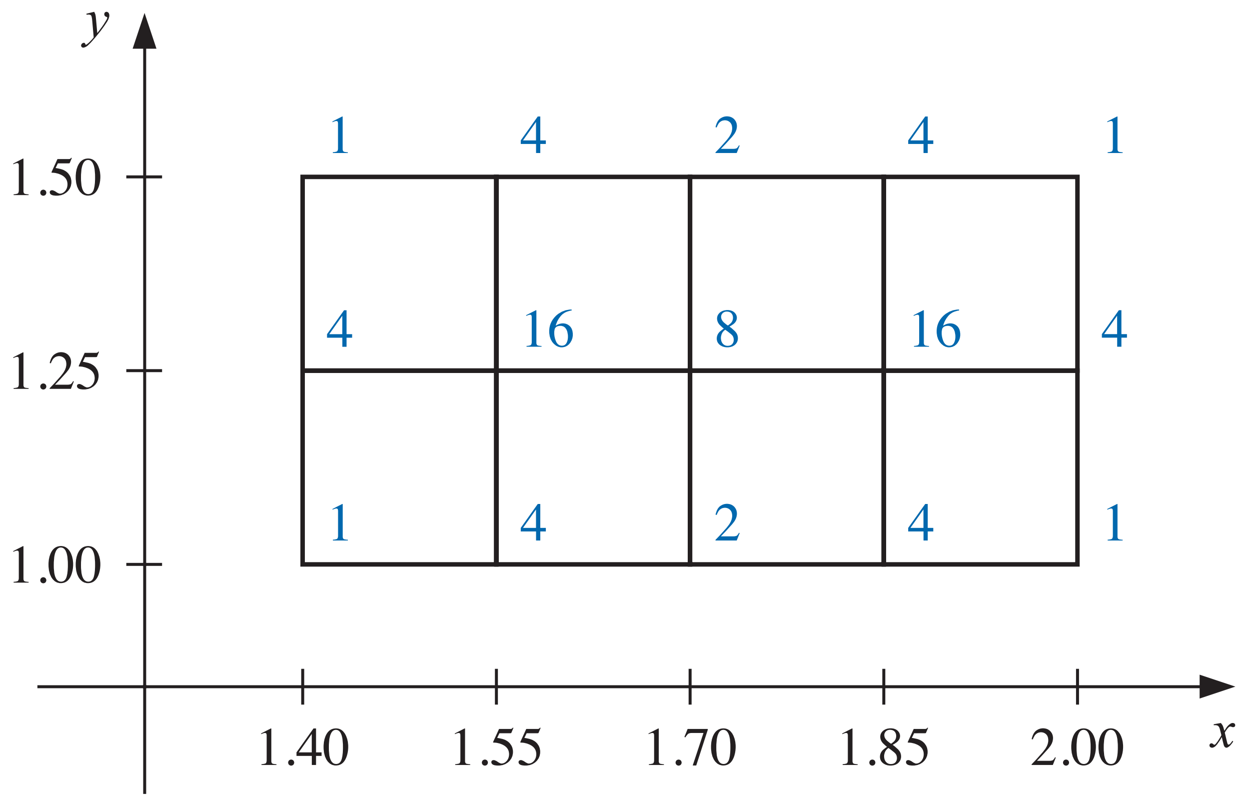
Combine the two to obtain:

$$\int_a^b \left(\int_c^d f(x,y)\,\mathrm{d}y \right) \mathrm{d}x = \frac{(b-a)(d-c)}{16} \Bigg\{ f(a,c) + f(a,d) + f(b,c) + f(b,d) + 2\left[f\left(\frac{a+b}{2}, c\right) + f\left(\frac{a+b}{2}, d\right) + f\left(a, \frac{c+d}{2}\right) + f\left(b, \frac{c+d}{2}\right) \right] + 4f\left(\frac{a+b}{2}, \frac{c+d}{2}\right) \Bigg\}$$



Multiple integrals

We can also consider a 2×4 grid on the domain $[a, b] \times [c, d]$:

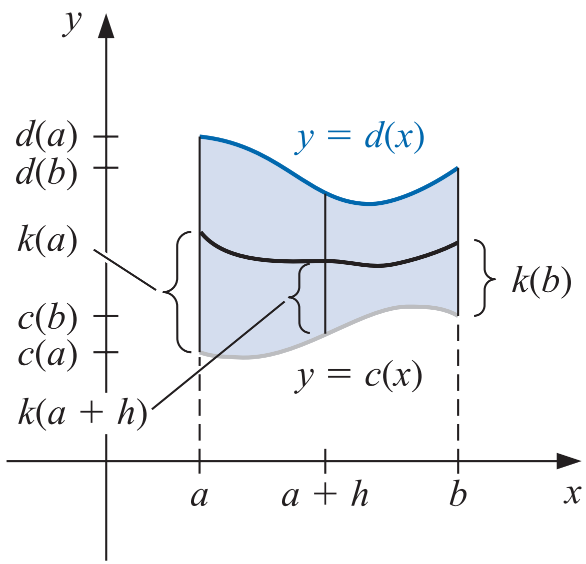


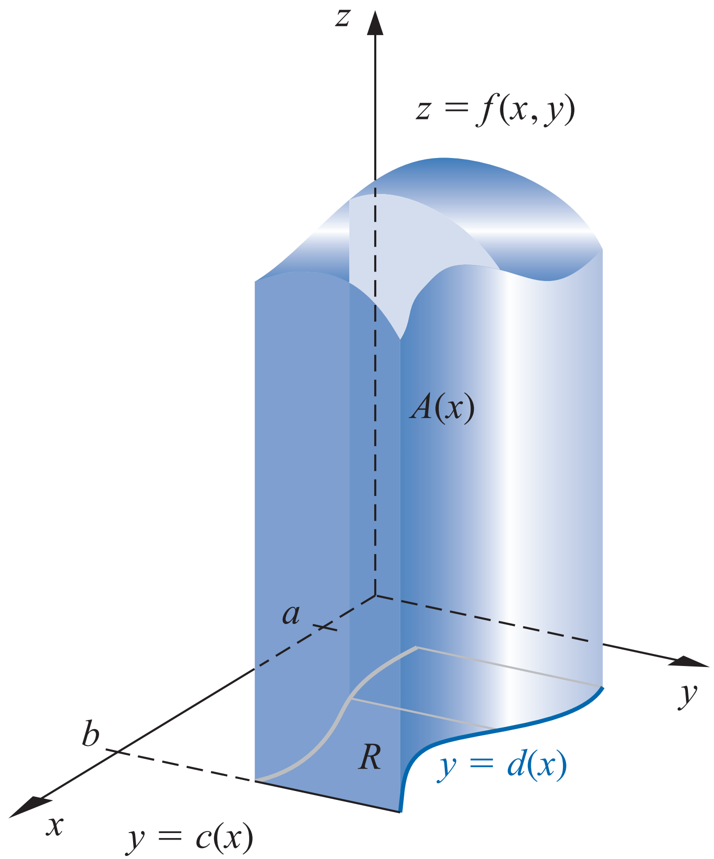
Here $k = \frac{d-c}{4}$ and $h = \frac{b-a}{2}$.

Gauss quadrature for non-rectangular region

We can also use Gauss quadrature for non-rectangular region:

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y)\,\mathrm{d}y\,\mathrm{d}x$$





Composite Simpson's rule on non-rectangular region

Now we consider multiple integrals on non-rectangular regions:

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,\mathrm{d}y\,\mathrm{d}x$$

For each integral set $k(x) = \frac{d(x)-c(x)}{2}$, then

$$\begin{aligned}
\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,\mathrm{d}y\,\mathrm{d}x \approx & \int_a^b \frac{k(x)}{3}[f(x,c(x)) + 4f(x,c(x)+k(x)) + f(x,d(x))]\,\mathrm{d}x \\
\approx & \frac{h}{3}\left\{ \frac{k(a)}{3}[f(a,c(a)) + 4f(a,c(a)+k(a)) + f(a,d(a))] \right. \\
& + \frac{4k(a+h)}{3}[f(a+h,c(a+h)) + 4f(a+h,c(a+h) \\
& + k(a+h)) + f(a+h,d(a+h))] \\
& \left. + \frac{k(b)}{3}\Big[f(b,c(b)) + 4f(b,c(b)+k(b)) + f(b,d(b))\Big] \right\}
\end{aligned}$$

Gauss quadrature for non-rectangular region

We can also use Gauss quadrature for non-rectangular region:

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y)\, \mathrm{d}y\, \mathrm{d}x$$

For each $x \in [a, b]$, transform $[c(x), d(x)]$ into variable t in $[-1, 1]$:

$$f(x, y) = f\left(x, \frac{(d(x) - c(x))t + d(x) + c(x)}{2}\right)$$

$$\mathrm{d}y = \frac{d(x) - c(x)}{2}\, \mathrm{d}t$$

Gauss quadrature for non-rectangular region

So the inner integral can be approximated by Gauss quadrature:

$$\begin{aligned}\int_{c(x)}^{d(x)} f(x,y)\,\mathrm{d}y &= \frac{d(x)-c(x)}{2}\int_{-1}^{1} f\left(x, \frac{(d(x)-c(x))t+d(x)+c(x)}{2}\right)\mathrm{d}t \\ &\approx \frac{d(x)-c(x)}{2}\sum_{j=1}^{n} c_{n,j} f\left(x, \frac{(d(x)-c(x))r_{n,j}+d(x)+c(x)}{2}\right) \\ &=: g(x)\end{aligned}$$

Then we apply Gauss quadrature to the outer integral:

$$\begin{aligned}\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,\mathrm{d}y\,\mathrm{d}x &\approx \int_a^b g(x)\,\mathrm{d}x \\ &= \int_{-1}^{1} g\left(\frac{(b-a)t+(b+a)}{2}\right)\frac{(b-a)}{2}\,\mathrm{d}t \\ &\approx \sum_{i=1}^{m} c_{m,i}\, g\left(\frac{(b-a)r_{m,i}+(b+a)}{2}\right)\frac{(b-a)}{2}\end{aligned}$$