Numerical differentiation and integration

NUMERICAL DIFFERENTIATION

The derivative of $f(x)$ at x_0 is:

$$f'(x_0) = \underset{h \to 0}{Limit} \frac{f(x_0 + h) - f(x_0)}{h}$$

An approximation to this is:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of h.

Forward Difference Formula

Let $f(x) = \ln x$ and $x_0 = 1.8$

Find an approximate value for $f'(1.8)$

h	$f(1.8)$	$f(1.8+h)$	$\dfrac{f(1.8+h) - f(1.8)}{h}$
0.1	0.5877867	0.6418539	0.5406720
0.01	0.5877867	0.5933268	0.5540100
0.001	0.5877867	0.5883421	0.5554000

The exact value of $f'(1.8) = 0.55\overline{5}$

Assume that a function goes through three points:

$$\left(x_0, f\left(x_0\right)\right), \left(x_1, f\left(x_1\right)\right) \text{ and } \left(x_2, f\left(x_2\right)\right).$$

$$f(x) \approx P(x)$$

$$P\left(x\right) = L_0\left(x\right) f\left(x_0\right) + L_1\left(x\right) f\left(x_1\right) + L_2\left(x\right) f\left(x_2\right)$$

Lagrange Interpolating Polynomial

$$P(x) = L_0(x) f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2)$$

$$P(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0)$$

$$+ \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1)$$

$$+ \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$f'(x) \approx P'(x)$$

$$P'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

If the points are equally spaced, i.e.,

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

$$P'(x_0) = \frac{2x_0 - (x_0 + h) - (x_0 + 2h)}{\{x_0 - (x_0 + h)\}\{x_0 - (x_0 + 2h)\}} f(x_0)$$

$$+ \frac{2x_0 - x_0 - (x_0 + 2h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 + 2h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 + 2h) - x_0\}\{(x_0 + 2h) - (x_0 + h)\}} f(x_2)$$

$$P'(x_0) = \frac{-3h}{2h^2} f(x_0) + \frac{-2h}{-h^2} f(x_1) + \frac{-h}{2h^2} f(x_2)$$

$$P'(x_0) = \frac{1}{2h}\{-3f(x_0) + 4f(x_1) - f(x_2)\}$$

Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\}$$

If the points are equally spaced with x_0 in the middle:

$$x_1 = x_0 - h \text{ and } x_2 = x_0 + h$$

$$P'(x_0) = \frac{2x_0 - (x_0 - h) - (x_0 + h)}{\{x_0 - (x_0 - h)\}\{(x_0 - (x_0 + h)\}} f(x_0)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 - h) - x_0\}\{(x_0 - h) - (x_0 + h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 - h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 - h)\}} f(x_2)$$

$$P'(x_0) = \frac{0}{-h^2} f(x_0) + \frac{-h}{2h^2} f(x_1) + \frac{h}{2h^2} f(x_2)$$

Another Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}$$

Alternate approach (Error estimate)

Take Taylor series expansion of $f(x+h)$ about x:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

$$f(x+h) - f(x) = hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

$$\frac{f(x+h) - f(x)}{h} = f'(x) + \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \cdots$$

.... (1)

$$\frac{f(x+h)-f(x)}{h} = f'(x)+O(h)$$

$$f'(x)=\frac{f(x+h)-f(x)}{h}-O(h)$$

$$f'(x)\approx\frac{f(x+h)-f(x)}{h}$$

Forward Difference Formula

$$O(h)=\frac{h}{2}f^{(2)}(x)+\frac{h^2}{3!}f^{(3)}(x)+\cdots$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2} f^{(2)}(x) + \frac{8h^3}{3!} f^{(3)}(x) + \cdots$$

$$f(x+2h) - f(x) = 2hf'(x) + \frac{4h^2}{2} f^{(2)}(x) + \frac{8h^3}{3!} f^{(3)}(x) + \cdots$$

$$\frac{f(x+2h) - f(x)}{2h} = f'(x) + \frac{2h}{2} f^{(2)}(x) + \frac{4h^2}{3!} f^{(3)}(x) + \cdots$$

.... (2)

$$\frac{f(x+h)-f(x)}{h} = f'(x) + \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \cdots$$

.... (1)

$$\frac{f(x+2h)-f(x)}{2h} = f'(x) + \frac{2h}{2} f^{(2)}(x) + \frac{4h^2}{3!} f^{(3)}(x) + \cdots$$

.... (2)

2 × Eqn. (1) – Eqn. (2)

$$2\frac{f(x+h)-f(x)}{h}-\frac{f(x+2h)-f(x)}{2h}$$

$$=f'(x)-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\cdots$$

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

$$=f'(x)-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\cdots$$

$$=f'(x)+O(h^2)$$

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}=f'(x)+O(h^2)$$

$$f'(x)=\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}-O(h^2)$$

$$f'(x)\approx\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

Three-point Formula

$$O(h^2)=-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\cdots$$

The Second Three-point Formula

Take Taylor series expansion of *f*(*x*+*h*) about *x*:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

Take Taylor series expansion of *f*(*x*-*h*) about *x*:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f^{(2)}(x) - \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

Subtract one expression from another

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!} f^{(3)}(x) + \frac{2h^6}{6!} f^{(6)}(x) + \cdots$$

$$f(x+h)-f(x-h)=2hf'(x)+\frac{2h^3}{3!}f^{(3)}(x)+\frac{2h^6}{6!}f^{(6)}(x)+\cdots$$

$$\frac{f(x+h)-f(x-h)}{2h}=f'(x)+\frac{h^2}{3!}f^{(3)}(x)+\frac{h^5}{6!}f^{(6)}(x)+\cdots$$

$$f'(x)=\frac{f(x+h)-f(x-h)}{2h}-\frac{h^2}{3!}f^{(3)}(x)-\frac{h^5}{6!}f^{(6)}(x)-\cdots$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

$$O(h^2) = -\frac{h^2}{3!} f^{(3)}(x) - \frac{h^5}{6!} f^{(6)}(x) - \cdots$$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Second Three-point Formula

Summary of Errors

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Forward Difference Formula

Error term

$$O(h) = \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \cdots$$

Summary of Errors continued

First Three-point Formula

$$f'(x) \approx \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h}$$

Error term $O(h^2) = -\frac{2h^2}{3!} f^{(3)}(x) - \frac{6h^3}{4!} f^{(4)}(x) - \cdots$

Summary of Errors continued

Second Three-point Formula

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Error term $O(h^2) = -\frac{h^2}{3!} f^{(3)}(x) - \frac{h^5}{6!} f^{(6)}(x) - \cdots$

Example:

$$f(x) = xe^{x}$$

Find the approximate value of $f'(2)$ **with** $h = 0.1$

x	$f(x)$
1.9	**12.703199**
2.0	**14.778112**
2.1	**17.148957**
2.2	**19.855030**

Using the Forward Difference formula:

$$f'(x_0) \approx \frac{1}{h}\{f(x_0+h) - f(x_0)\}$$

$$f'(2) \approx \frac{1}{0.1}\{f(2.1) - f(2)\}$$

$$= \frac{1}{0.1}\{17.148957 - 14.778112\}$$

$$= 23.708450$$

Using the 1st Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{-3f(x_0)+4f(x_0+h)-f(x_0+2h)\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}[-3f(2)+4f(2.1)-f(2.2)]$$

$$= \frac{1}{0.2}[-3\times 14.778112+4\times 17.148957 - 19.855030]$$

$$= 22.032310$$

Using the 2nd Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}[f(2.1) - f(1.9)]$$

$$= \frac{1}{0.2}[17.148957 - 12.703199]$$

$$= 22.228790$$

The exact value of $f'(2)$ is: 22.167168

Comparison of the results with $h = 0.1$

The exact value of $f'(2)$ is 22.167168

Formula	$f'(2)$	Error
Forward Difference	23.708450	1.541282
1st Three-point	22.032310	0.134858
2nd Three-point	22.228790	0.061622

Second-order Derivative

$$f(x+h)=f(x)+hf'(x)+\frac{h^2}{2}f^{(2)}(x)+\frac{h^3}{3!}f^{(3)}(x)+\cdots$$

$$f(x-h)=f(x)-hf'(x)+\frac{h^2}{2}f^{(2)}(x)-\frac{h^3}{3!}f^{(3)}(x)+\cdots$$

Add these two equations.

$$f(x+h)+f(x-h)=2f(x)+\frac{2h^2}{2}f^{(2)}(x)+\frac{2h^4}{4!}f^{(4)}(x)+\cdots$$

$$f(x+h)-2f(x)+f(x-h)=\frac{2h^2}{2}f^{(2)}(x)+\frac{2h^4}{4!}f^{(4)}(x)+\cdots$$

$$\frac{f(x+h)-2f(x)+f(x-h)}{h^2}=f^{(2)}(x)+\frac{2h^2}{4!}f^{(4)}(x)+\cdots$$

$$f^{(2)}(x)=\frac{f(x+h)-2f(x)+f(x-h)}{h^2}-\frac{2h^2}{4!}f^{(4)}(x)+\cdots$$

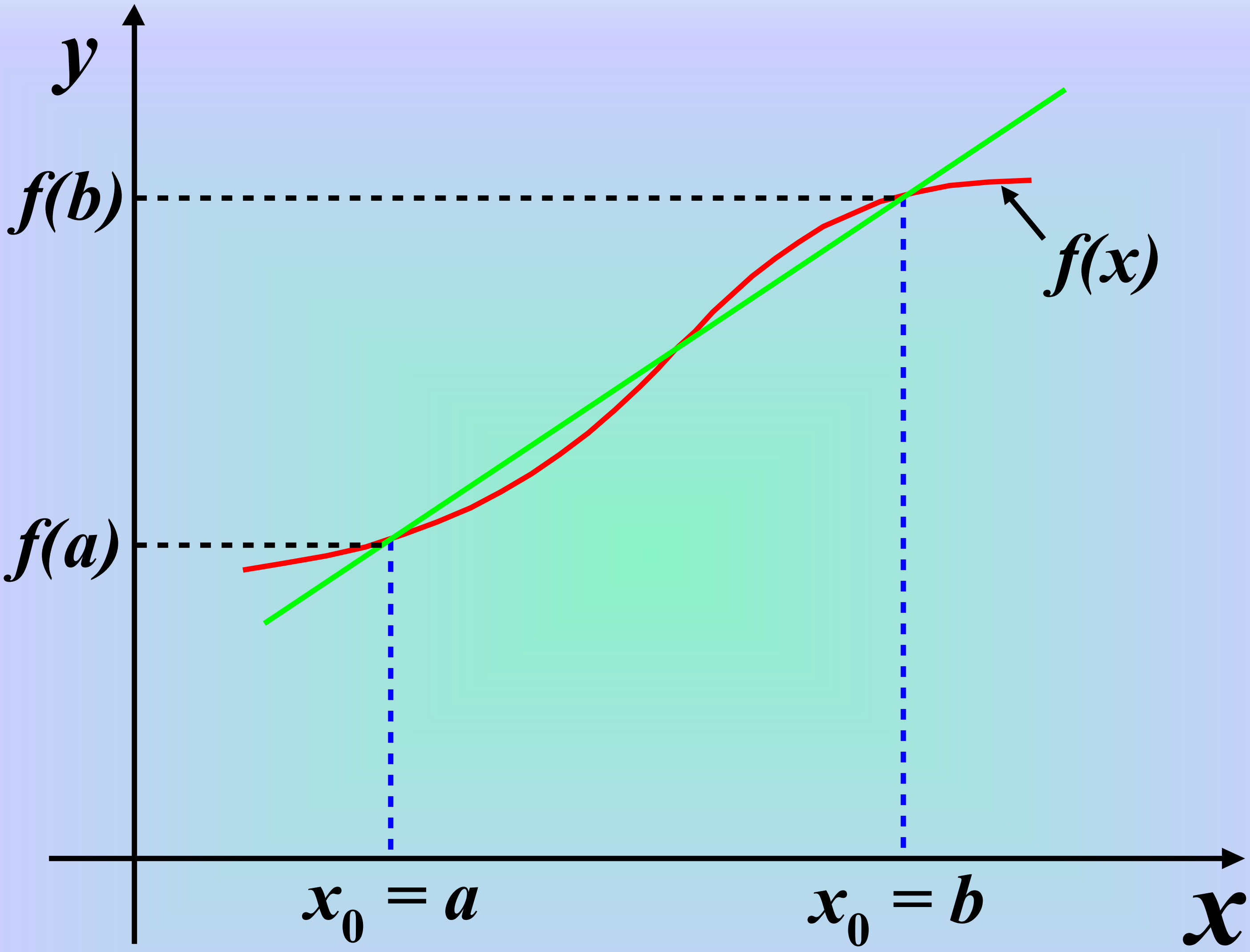
$$f^{(2)}(x)\approx\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

NUMERICAL INTEGRATION

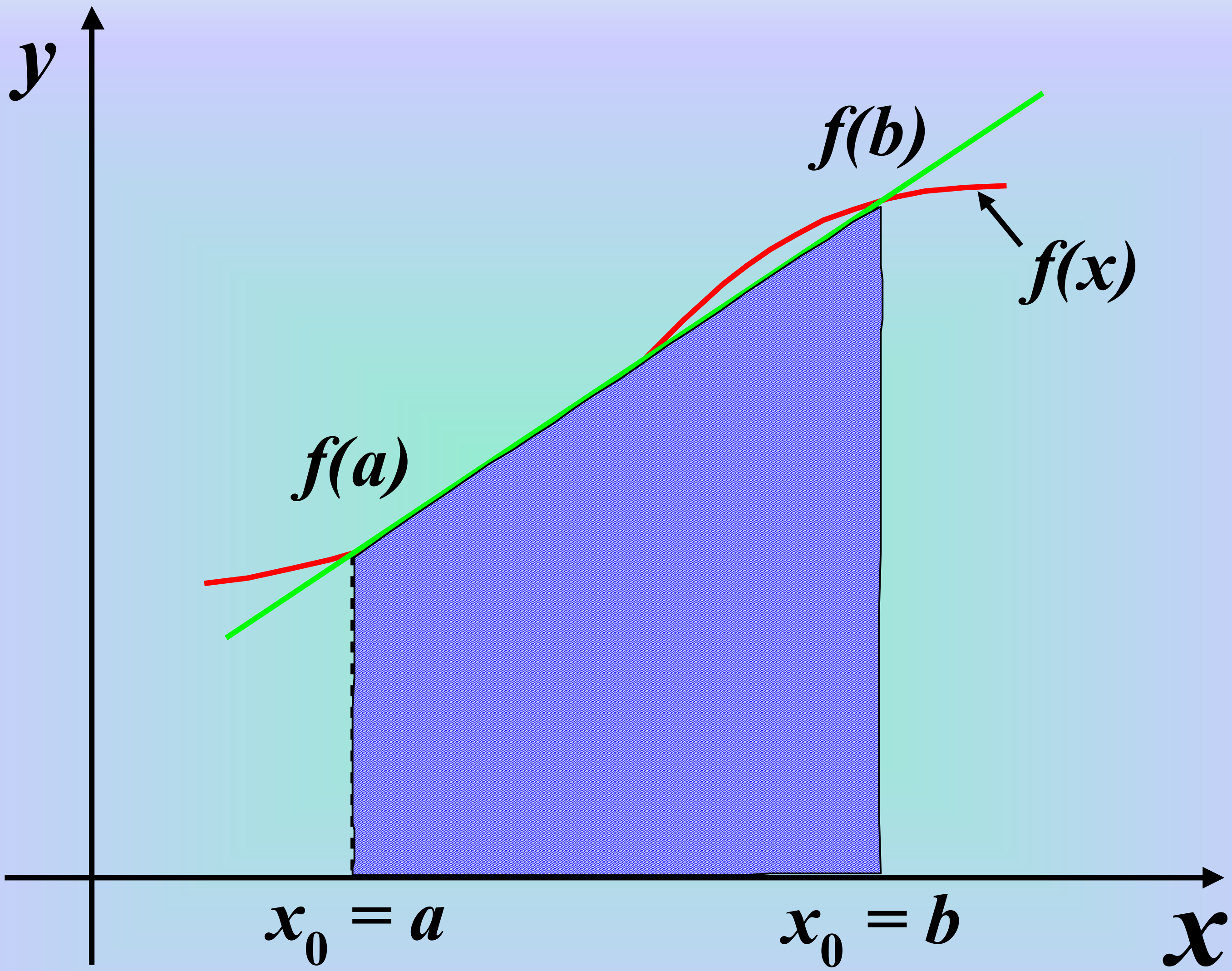
$$\int_a^b f(x)dx =$$ **area under the curve *f(x)* between**

$$x = a \text{ to } x = b.$$

In many cases a mathematical expression for *f(x)* is unknown and in some cases even if *f(x)* is known its complex form makes it difficult to perform the integration.



y
f(b)
f(a)
f(x)
x0 = a
x0 = b
x


y
f(b)
f(x)
f(a)
$x_0 = a$
$x_0 = b$
x

Area of the trapezoid

The length of the two parallel sides of the trapezoid are: *f(a)* and *f(b)*

The height is *b-a*

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

$$=\frac{h}{2}\left[f(a)+f(b)\right]$$

Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} P(x)dx$$

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

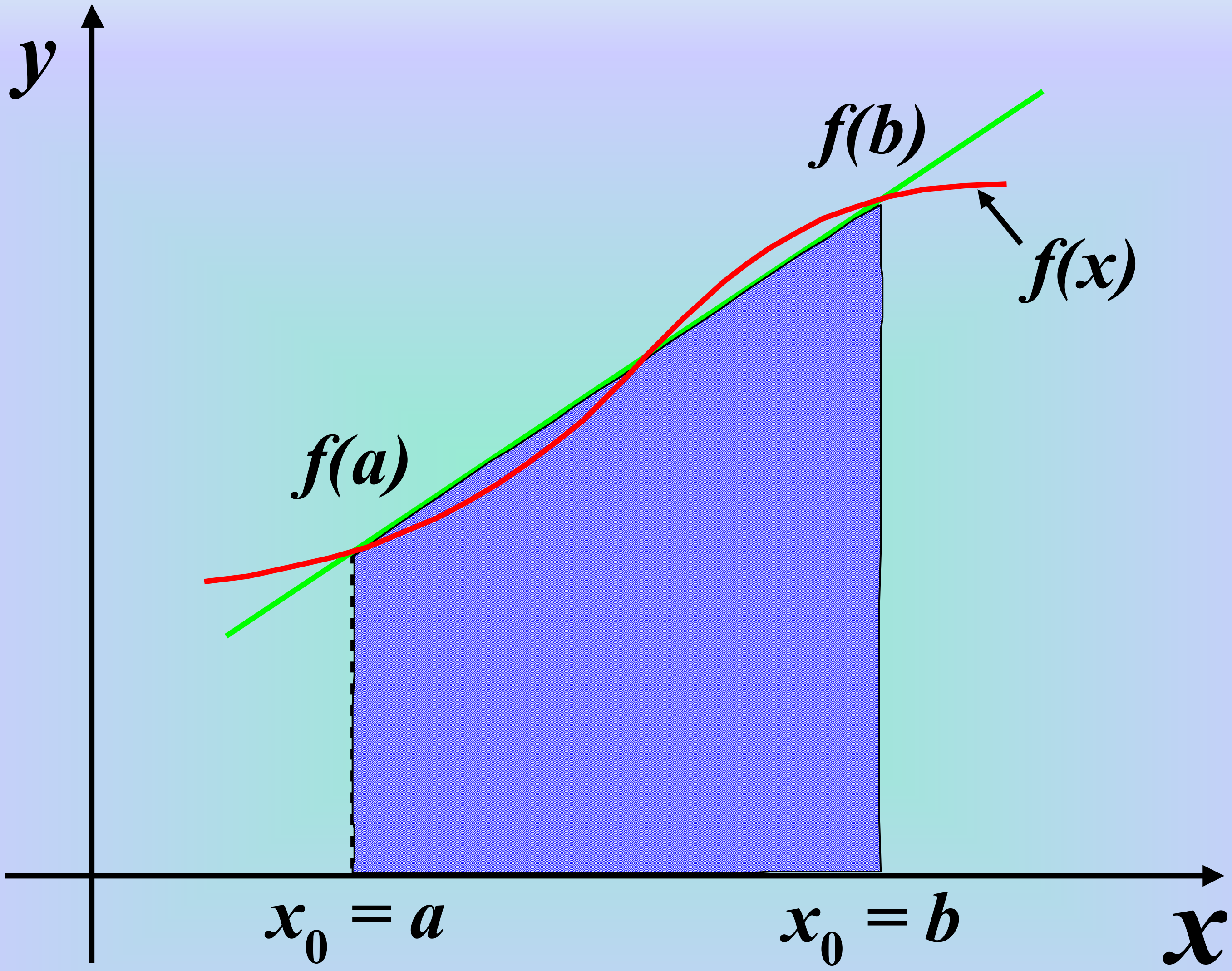
$$\int_{x_0}^{x_2} P(x)\,dx = \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0)\,dx$$

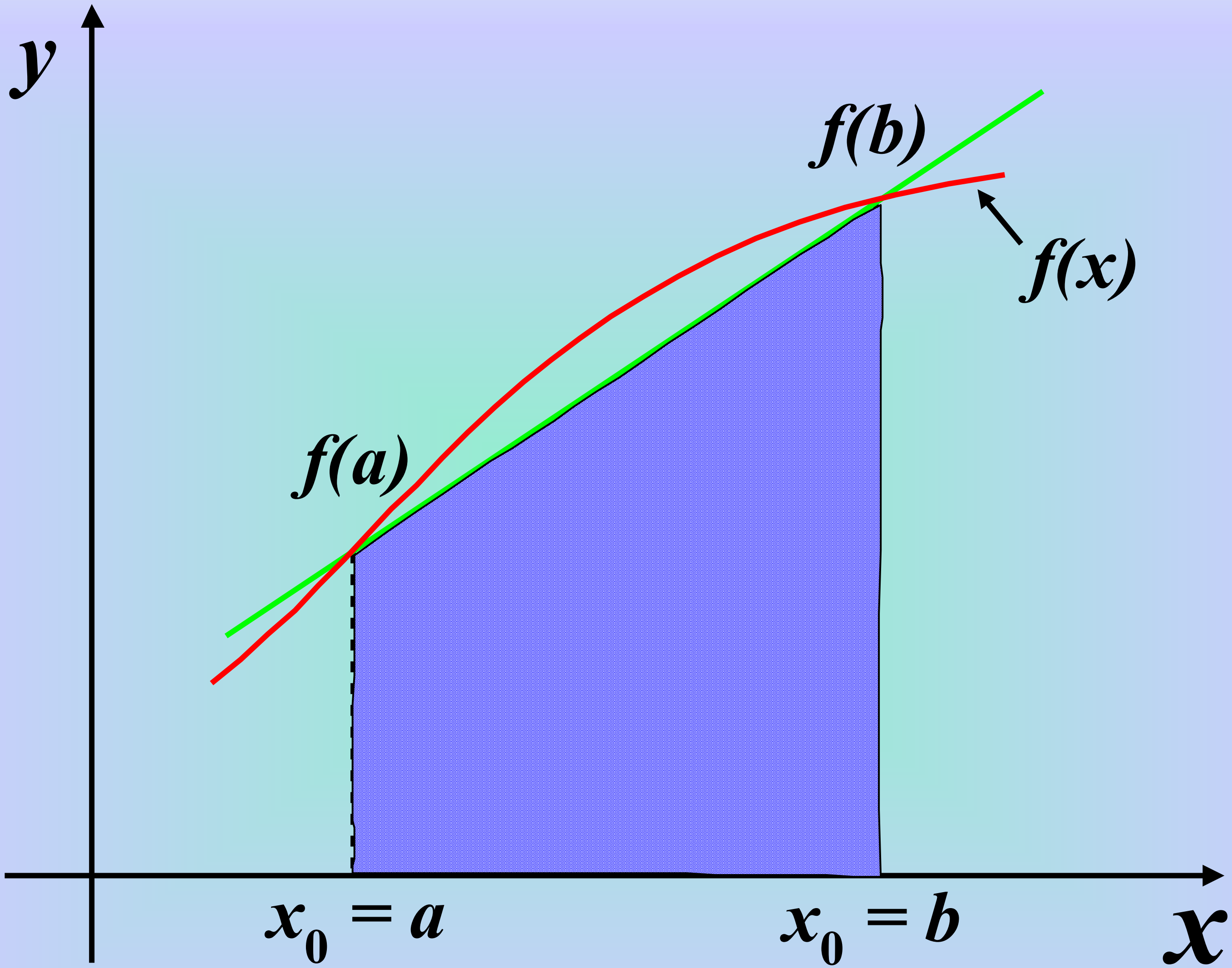
$$+\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1)\,dx$$

$$+\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)\,dx$$

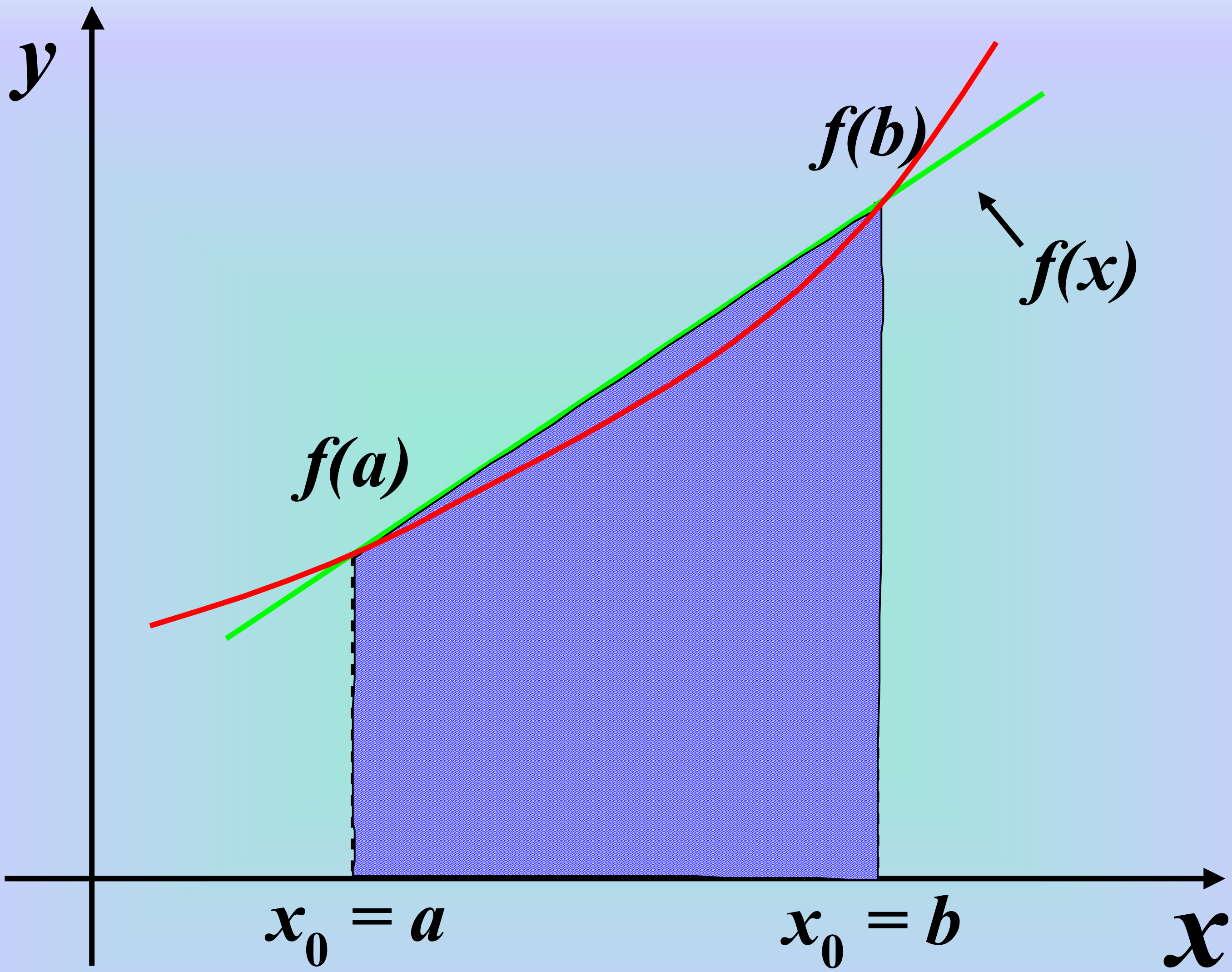
$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} P(x)dx$$

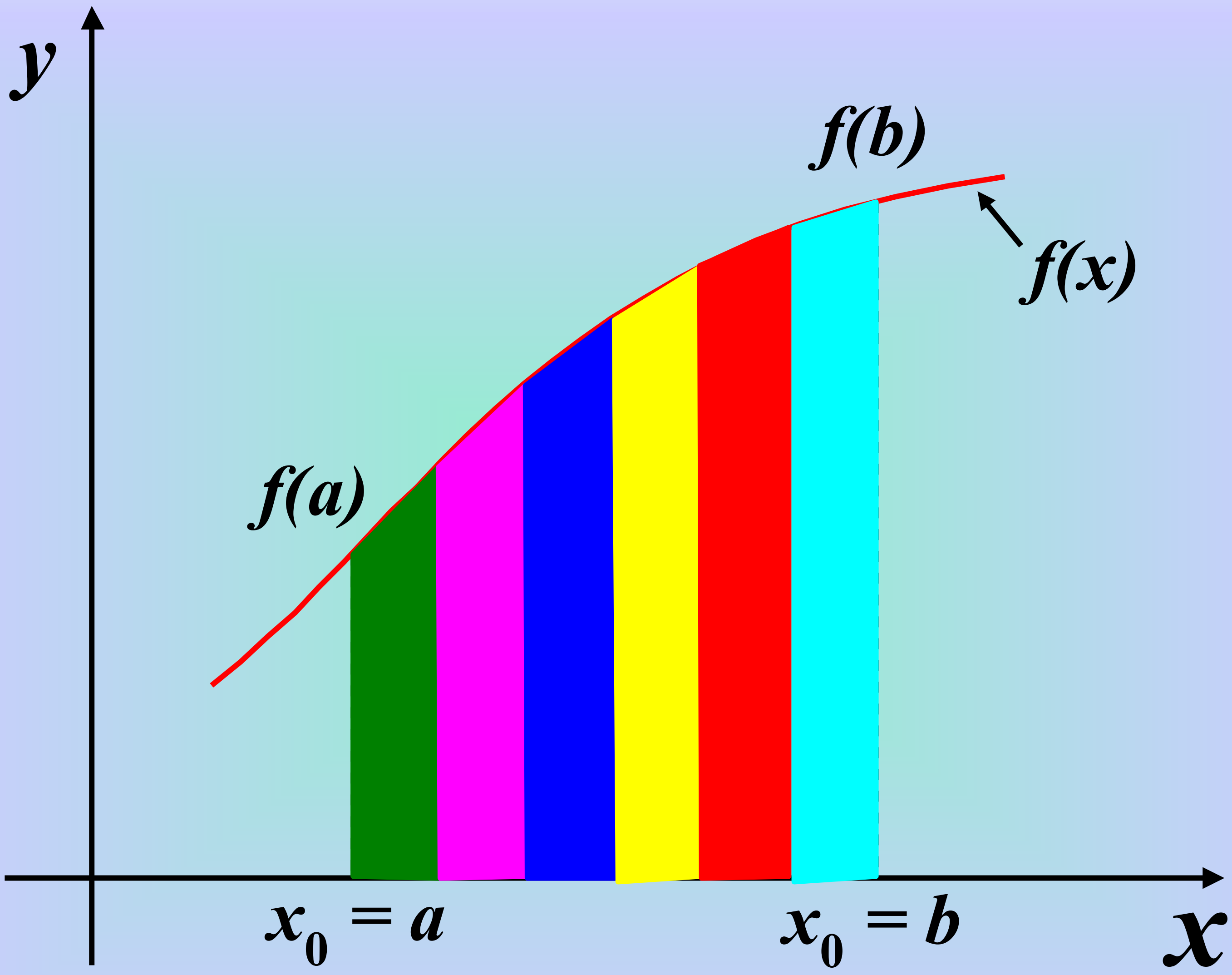
$$= \frac{h}{3}\left[f\left(x_0\right) + 4f(x_1) + f(x_2)\right]$$


y
f(b)
f(x)
f(a)
x₀ = a
x₀ = b
x



y
f(b)
f(x)
f(a)
x0 = a
x0 = b
x


y
f(b)
f(x)
f(a)
x0 = a
x0 = b
x



y
f(b)
f(x)
f(a)
$x_0 = a$
$x_0 = b$
x

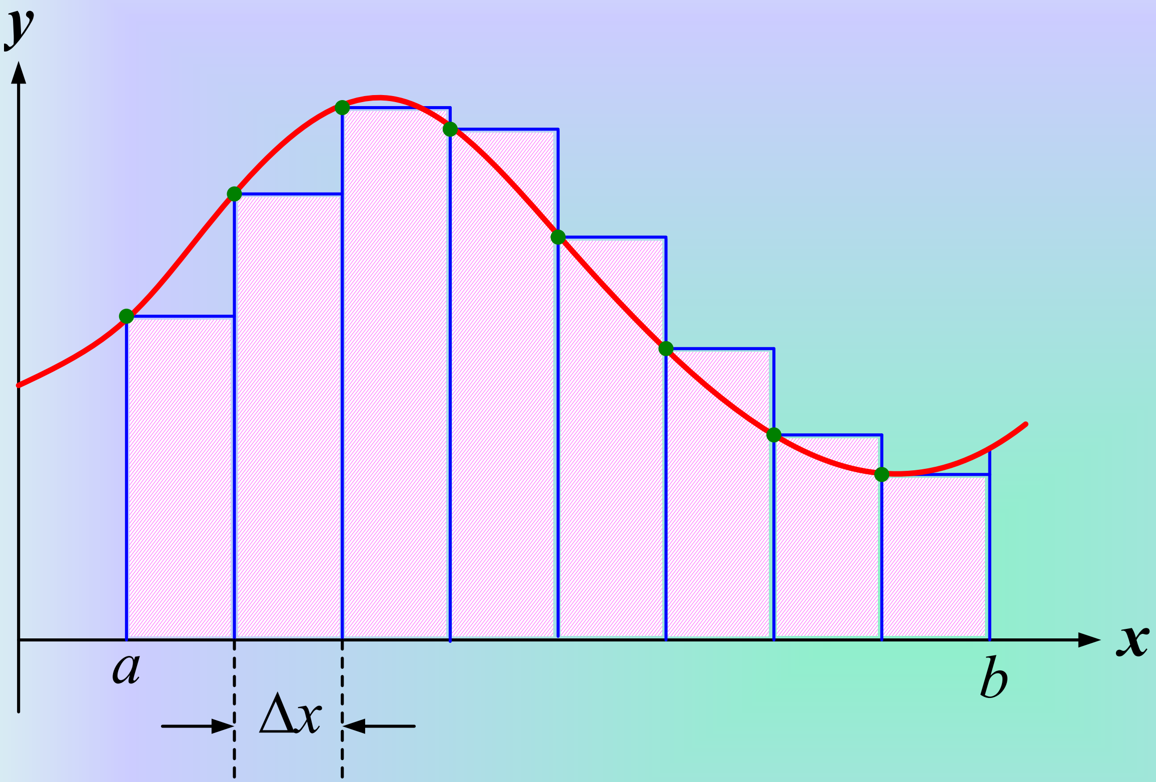
Composite Numerical Integration

Riemann Sum

The area under the curve is subdivided into n subintervals. Each subinterval is treated as a rectangle. The area of all subintervals are added to determine the area under the curve.

There are several variations of Riemann sum as applied to composite integration.

Left Riemann Sum



$$\Delta x = (b-a)/n$$

In Left Riemann sum, the left-side sample of the function is used as the height of the rectangle.

$$x_1 = a$$

$$x_2 = a + \Delta x$$

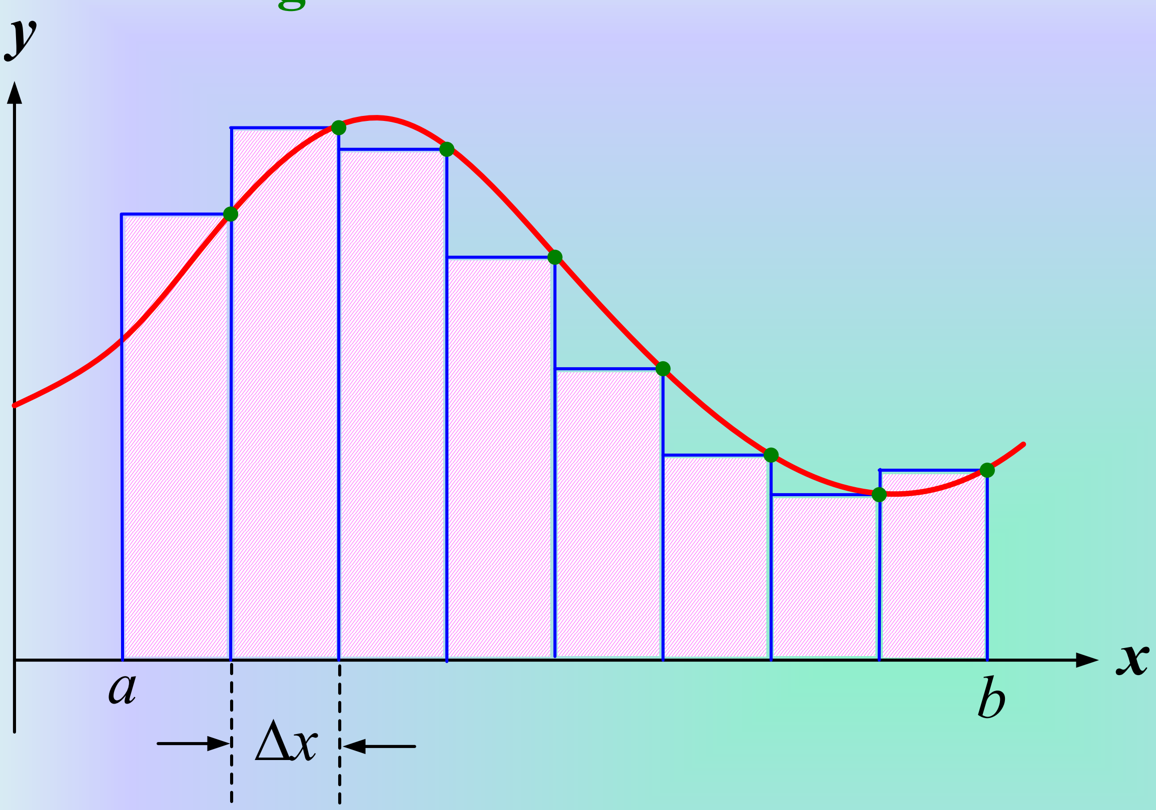
$$x_3 = a + 2\Delta x$$

$$\vdots$$

$$x_i = a + (i-1)\Delta x$$

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} f(x_i)\Delta x$$

Right Riemann Sum



In Right Riemann sum, the right-side sample of the function is used as the height of the individual rectangle.

$$\Delta x = (b-a)/n$$

$$x_1 = a + \Delta x$$

$$x_2 = a + 2\Delta x$$

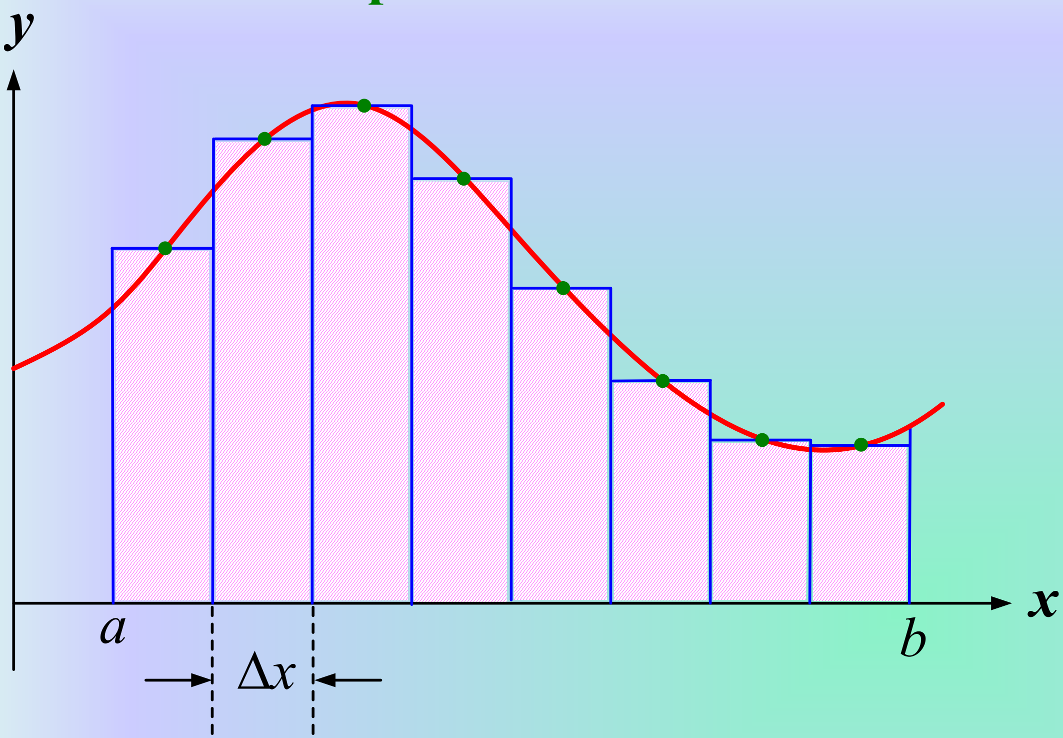
$$x_3 = a + 3\Delta x$$

$$\vdots$$

$$x_i = a + i\Delta x$$

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} f(x_i)\Delta x$$

Midpoint Rule



In the Midpoint Rule, the sample at the middle of the subinterval is used as the height of the individual
e.

$$\Delta x = (b-a)/n$$

$$x_1 = a + (2\times 1 - 1)(\Delta x / 2)$$

$$x_2 = a + (2\times 2 - 1)(\Delta x / 2)$$

$$x_3 = a + (2\times 3 - 1)(\Delta x / 2)$$

$$\vdots$$

$$x_i = a + (2\times i - 1)(\Delta x / 2)$$

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} f(x_i)\Delta x$$

Composite Trapezoidal Rule:

Divide the interval into n subintervals and apply Trapezoidal Rule in each subinterval.

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(a) + 2\sum_{k=1}^{n-1} f(x_k) + f(b) \right]$$

where

$$h = \frac{b-a}{n} \quad \text{and } x_k = a + kh \quad \text{for } k = 0, 1, 2, \ldots, n$$

Find $\int_{0}^{\pi} \sin(x)dx$

by dividing the interval into 20 subintervals.

$$n = 20$$

$$h = \frac{b-a}{n} = \frac{\pi}{20}$$

$$x_k = a + kh = \frac{k\pi}{20}, \quad k = 0, 1, 2, \ldots\ldots, 20$$

$$\int_0^{\pi} \sin(x)dx \approx \frac{h}{2}\left[f(a) + 2\sum_{k=1}^{n-1} f(x_k) + f(b) \right]$$

$$= \frac{\pi}{40}\left[\sin(0) + 2\sum_{k=1}^{19} \sin\left(\frac{k\pi}{20}\right) + \sin(\pi) \right]$$

$$= 1.995886$$

Composite Simpson's Rule:

Divide the interval into *n* subintervals and apply Simpson's Rule on each consecutive pair of subinterval. Note that *n* must be even.

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

where

$$h = \frac{b-a}{n} \text{ and } x_k = a + kh \quad \text{for } k = 0, 1, 2, \ldots, n$$

Find $\int_0^{\pi} \sin(x)\,dx$

by dividing the interval into 20 subintervals.

$$n = 20 \qquad h = \frac{b-a}{n} = \frac{\pi}{20}$$

$$x_k = a + kh = \frac{k\pi}{20}, \quad k = 0, 1, 2, \ldots\ldots, 20$$

$$\int_0^{\pi} \sin(x)\,dx \approx \frac{\pi}{60}\left[\sin(0) + 2\sum_{k=1}^{9}\sin\left(\frac{2k\pi}{20}\right) + 4\sum_{k=1}^{10}\sin\left(\frac{(2k-1)\pi}{20}\right) + \sin(\pi)\right]$$

$$= 2.000006$$