

# Numerical differentiation and integration

# NUMERICAL DIFFERENTIATION

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

$$f'(x_0) = \lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

An approximation to this is:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h} \quad \text{for small values of } h.$$

**Forward Difference  
Formula**

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

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

$h$	$f(1.8)$	$f(1.8+h)$	$\frac{f(1.8+h) - f(1.8)}{h}$
<b>0.1</b>	<b>0.5877867</b>	<b>0.6418539</b>	<b>0.5406720</b>
<b>0.01</b>	<b>0.5877867</b>	<b>0.5933268</b>	<b>0.5540100</b>
<b>0.001</b>	<b>0.5877867</b>	<b>0.5883421</b>	<b>0.5554000</b>

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

**Assume that a function goes through three points:**

**$(x_0, f(x_0)), (x_1, f(x_1))$  and  $(x_2, f(x_2))$ .**

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

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

**Lagrange Interpolating Polynomial**

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

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

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

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

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

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

$$\begin{aligned} P'(x_0) = & \frac{2x_0 - (x_0 + h) - (x_0 + 2h)}{\{x_0 - (x_0 + h)\}\{x_0 - (x_0 + 2h)\}} f(x_0) \\ & + \frac{2x_0 - x_0 - (x_0 + 2h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 + 2h)\}} f(x_1) \\ & + \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 + 2h) - x_0\}\{(x_0 + 2h) - (x_0 + h)\}} f(x_2) \end{aligned}$$

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

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

**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:

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

$$\begin{aligned} P'(x_0) = & \frac{2x_0 - (x_0 - h) - (x_0 + h)}{\{x_0 - (x_0 - h)\}\{(x_0 - (x_0 + h))\}} f(x_0) \\ & + \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 - h) - x_0\}\{(x_0 - h) - (x_0 + h)\}} f(x_1) \\ & + \frac{2x_0 - x_0 - (x_0 - h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 - h)\}} f(x_2) \end{aligned}$$

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

**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  $x$ :

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

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

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

..... (1)

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

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

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{Forward Difference Formula}$$

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

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

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

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

..... (2)

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

..... (1)

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

..... (2)

**2 × Eqn. (1) – Eqn. (2)**

$$\begin{aligned}
& 2 \frac{f(x+h) - f(x)}{h} - \frac{f(x+2h) - f(x)}{2h} \\
&= f'(x) - \frac{2h^2}{3!} f^{(3)}(x) - \frac{6h^3}{4!} f^{(4)}(x) - \dots \\
&\quad - \frac{f(x+2h) + 4f(x+h) - 3f(x)}{2h} \\
&= f'(x) - \frac{2h^2}{3!} f^{(3)}(x) - \frac{6h^3}{4!} f^{(4)}(x) - \dots \\
&= f'(x) + O(h^2)
\end{aligned}$$

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

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

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

**Three-point Formula**

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



# The Second Three-point Formula

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

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

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

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

Subtract one expression from another

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

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

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

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

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

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

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

**Second Three-point Formula**

## Summary of Errors

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{Forward Difference Formula}$$

**Error term**  $O(h) = \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \dots$

## Summary of Errors continued

### First Three-point Formula

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

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

## Summary of Errors continued

### Second Three-point Formula

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

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

**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 1<sup>st</sup> Three-point formula:

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

$$\begin{aligned} f'(2) &\approx \frac{1}{2 \times 0.1} [-3f(2) + 4f(2.1) - f(2.2)] \\ &= \frac{1}{0.2} [-3 \times 14.778112 + 4 \times 17.148957 \\ &\quad - 19.855030] \\ &= 22.032310 \end{aligned}$$

Using the 2<sup>nd</sup> Three-point formula:

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

$$\begin{aligned} f'(2) &\approx \frac{1}{2 \times 0.1} [f(2.1) - f(1.9)] \\ &= \frac{1}{0.2} [17.148957 - 12.703199] \\ &= 22.228790 \end{aligned}$$

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	<b>23.708450</b>	<b>1.541282</b>
1st Three-point	<b>22.032310</b>	<b>0.134858</b>
2nd Three-point	<b>22.228790</b>	<b>0.061622</b>

## Second-order Derivative

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

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

**Add these two equations.**

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

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

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

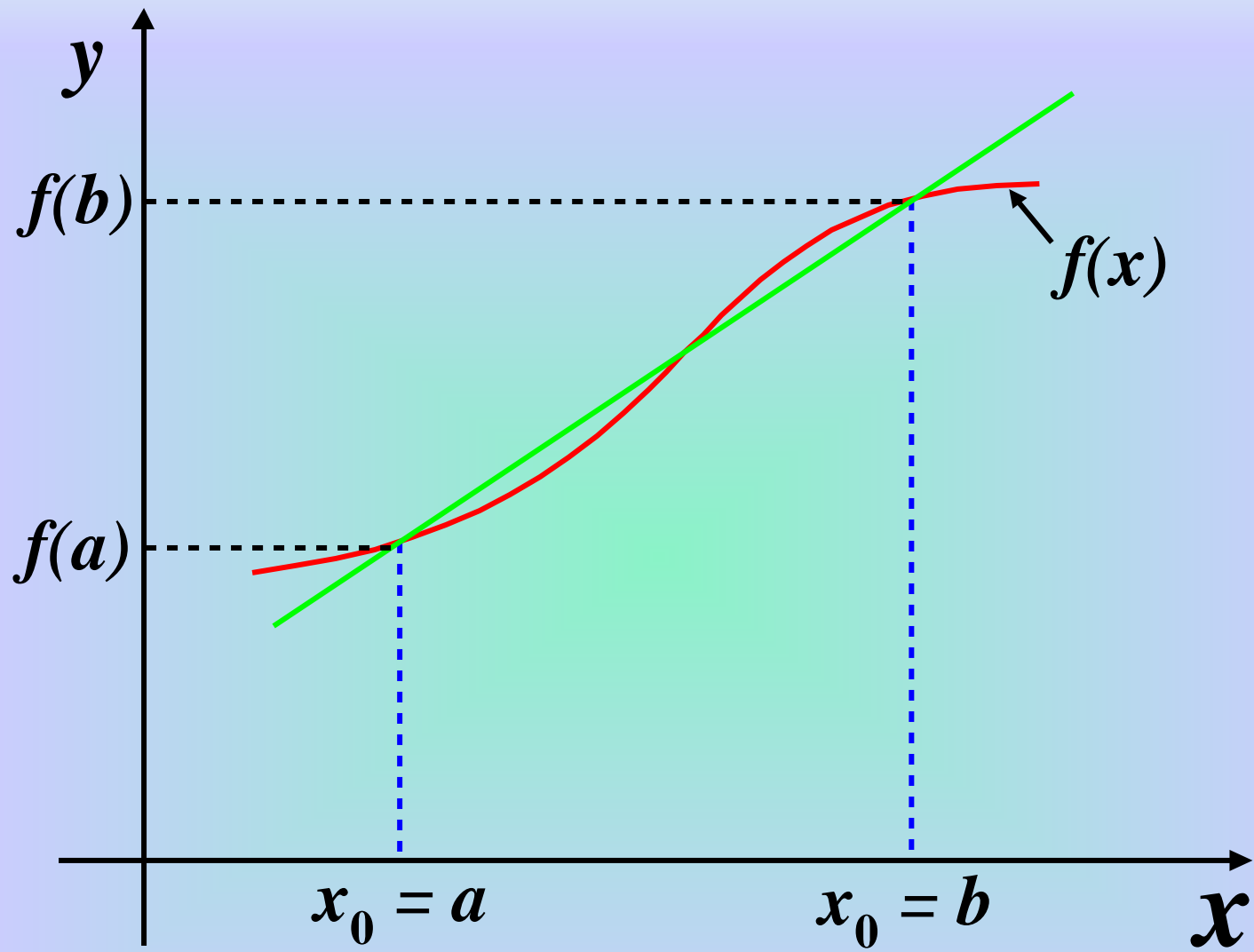
$$f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{2h^2}{4!} f^{(4)}(x) + \dots$$

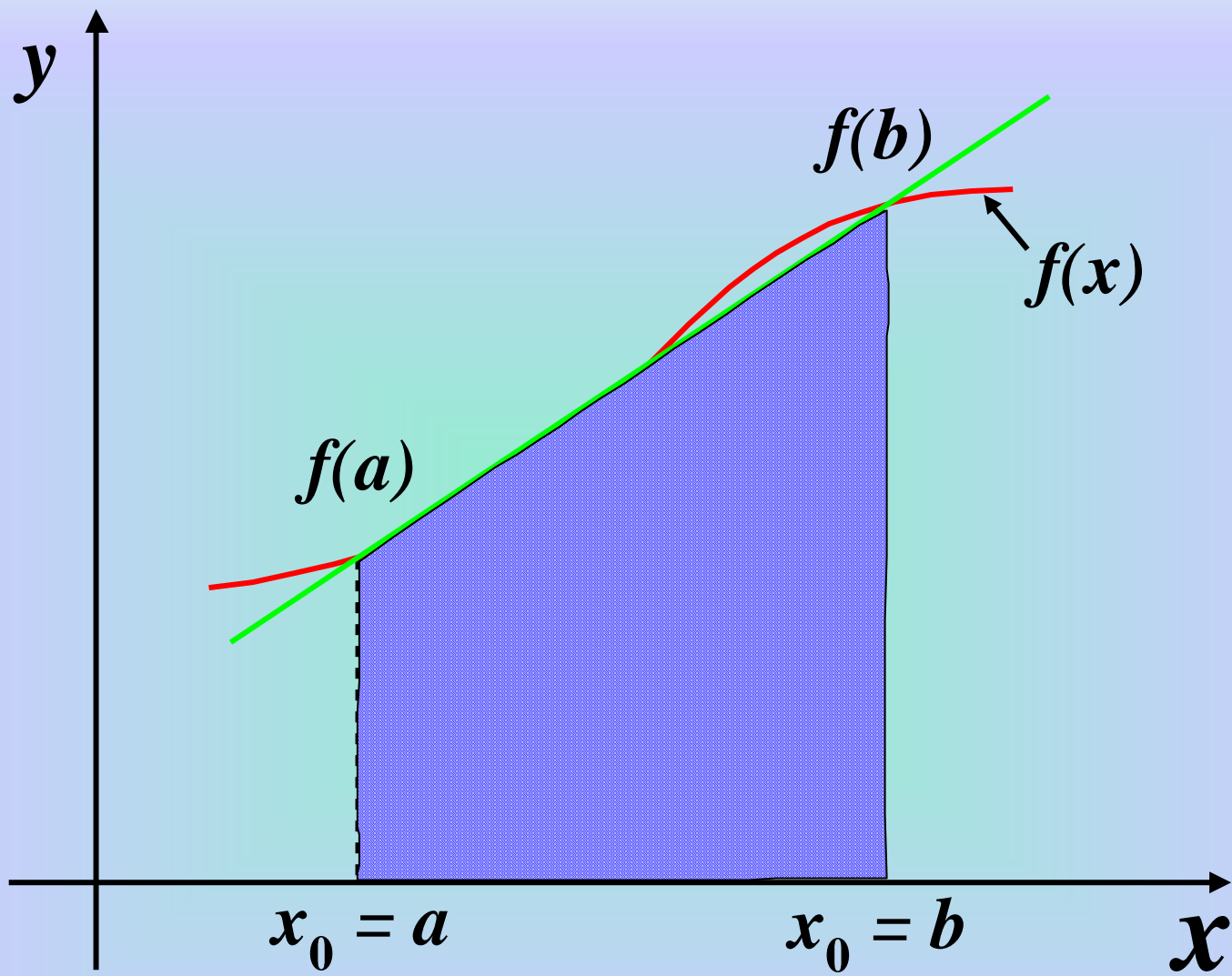
$$f^{(2)}(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

# NUMERICAL INTEGRATION

$$\int_a^b f(x)dx = \text{area under the curve } f(x) \text{ between } x = a \text{ to } x = b.$$

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.







## Area of the trapezoid

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

The height is  $b-a$

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

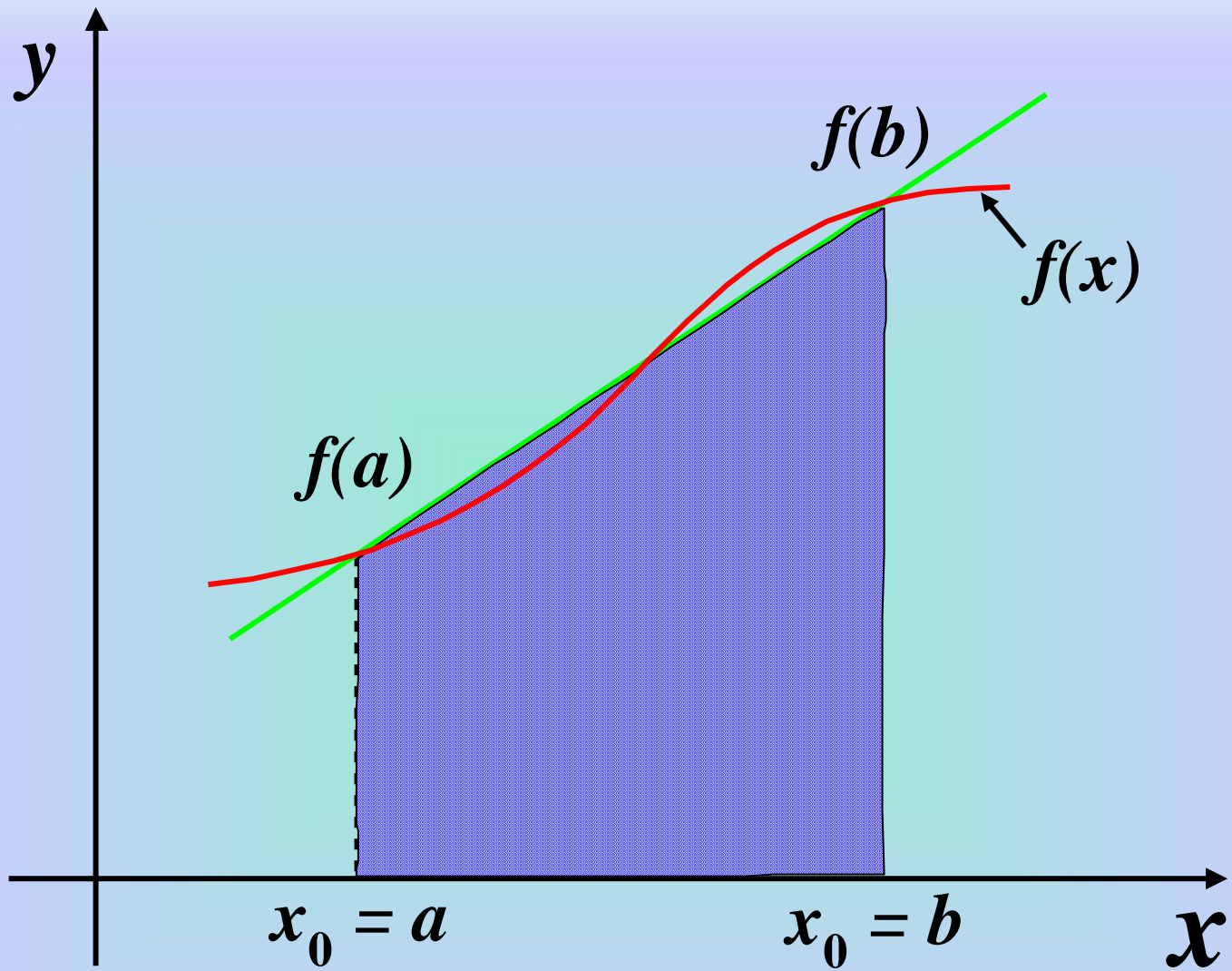
## Simpson's Rule:

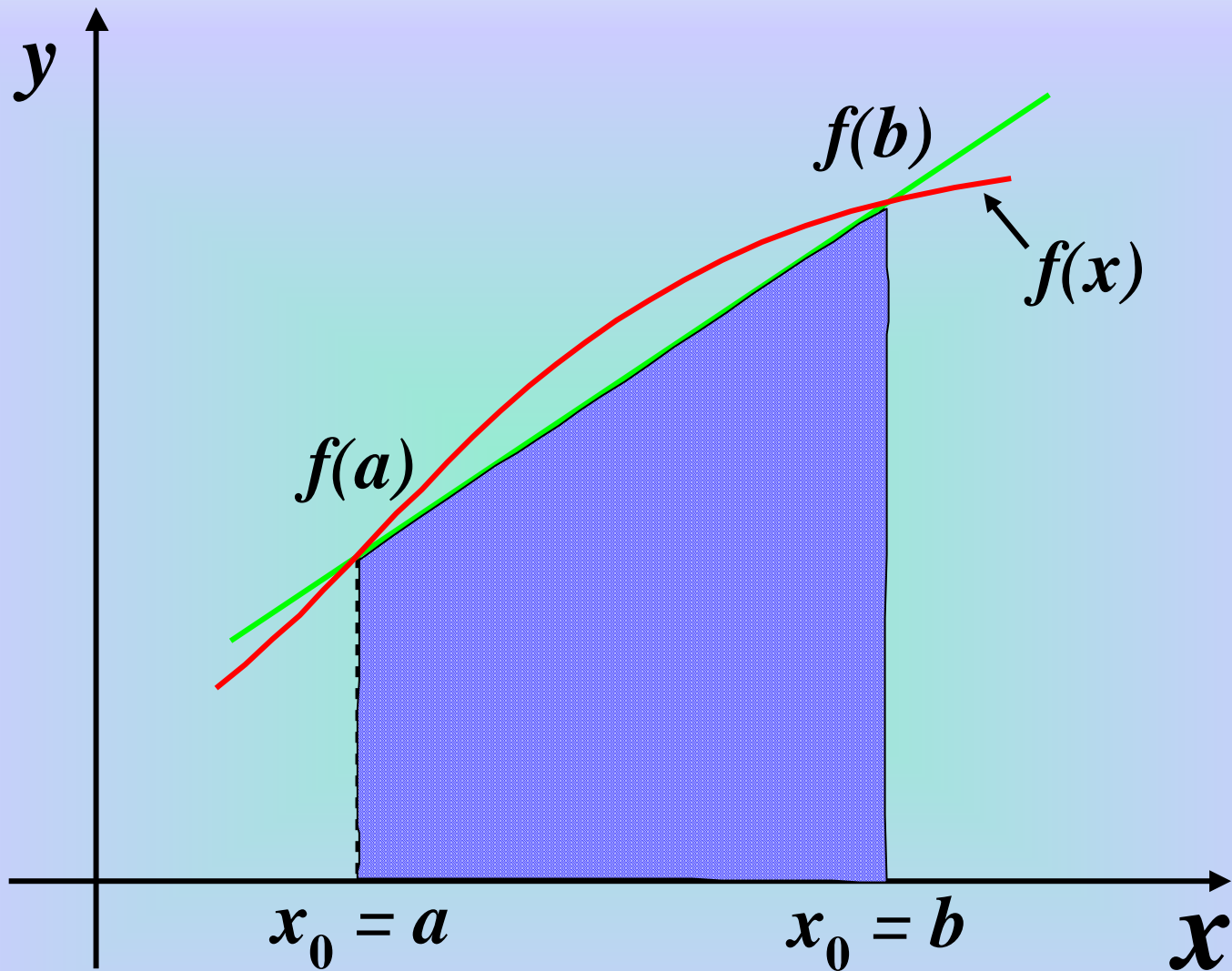
$$\int_{x_0}^{x_2} f(x) dx \approx \int_{x_0}^{x_2} P(x) dx$$

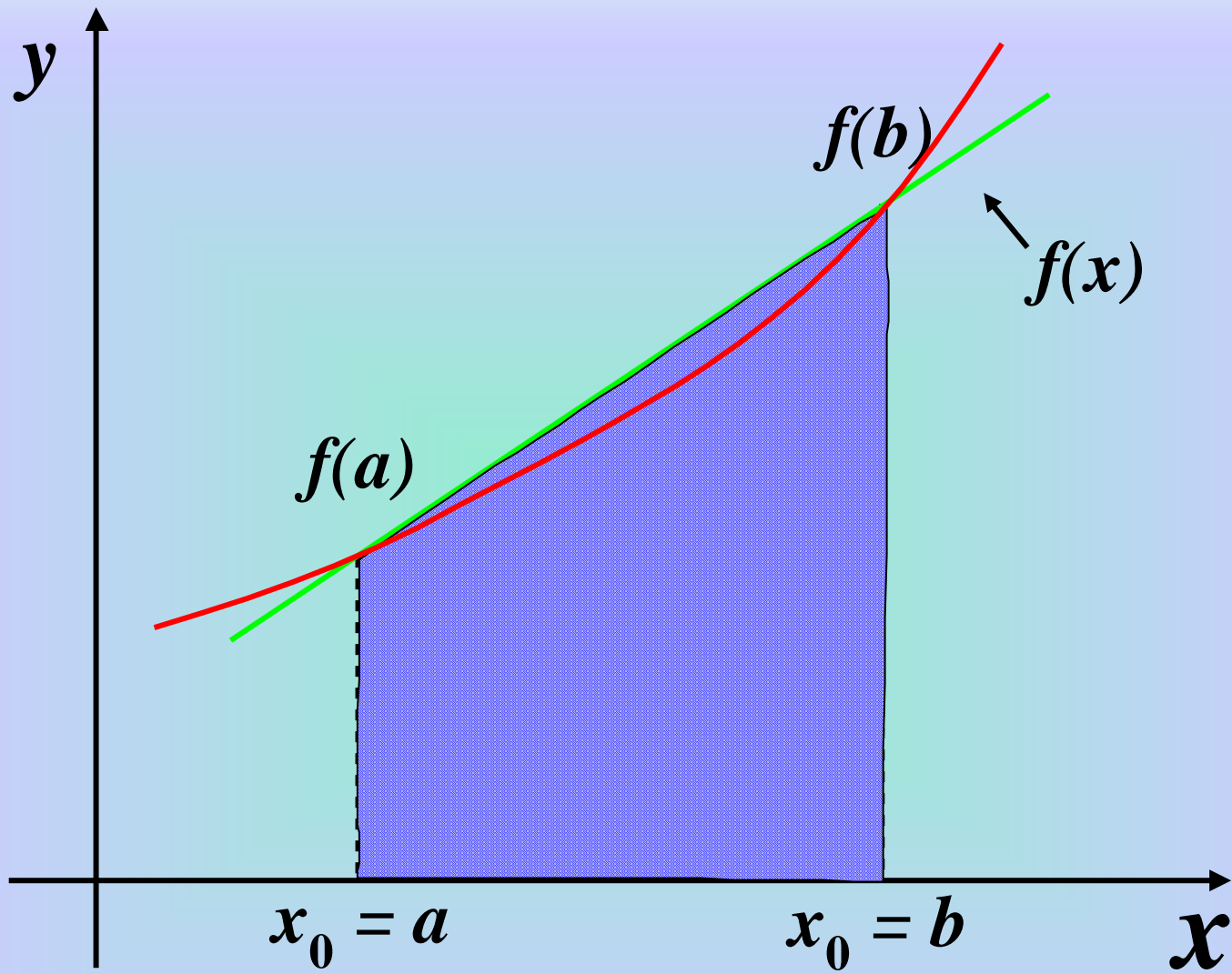
$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h$$

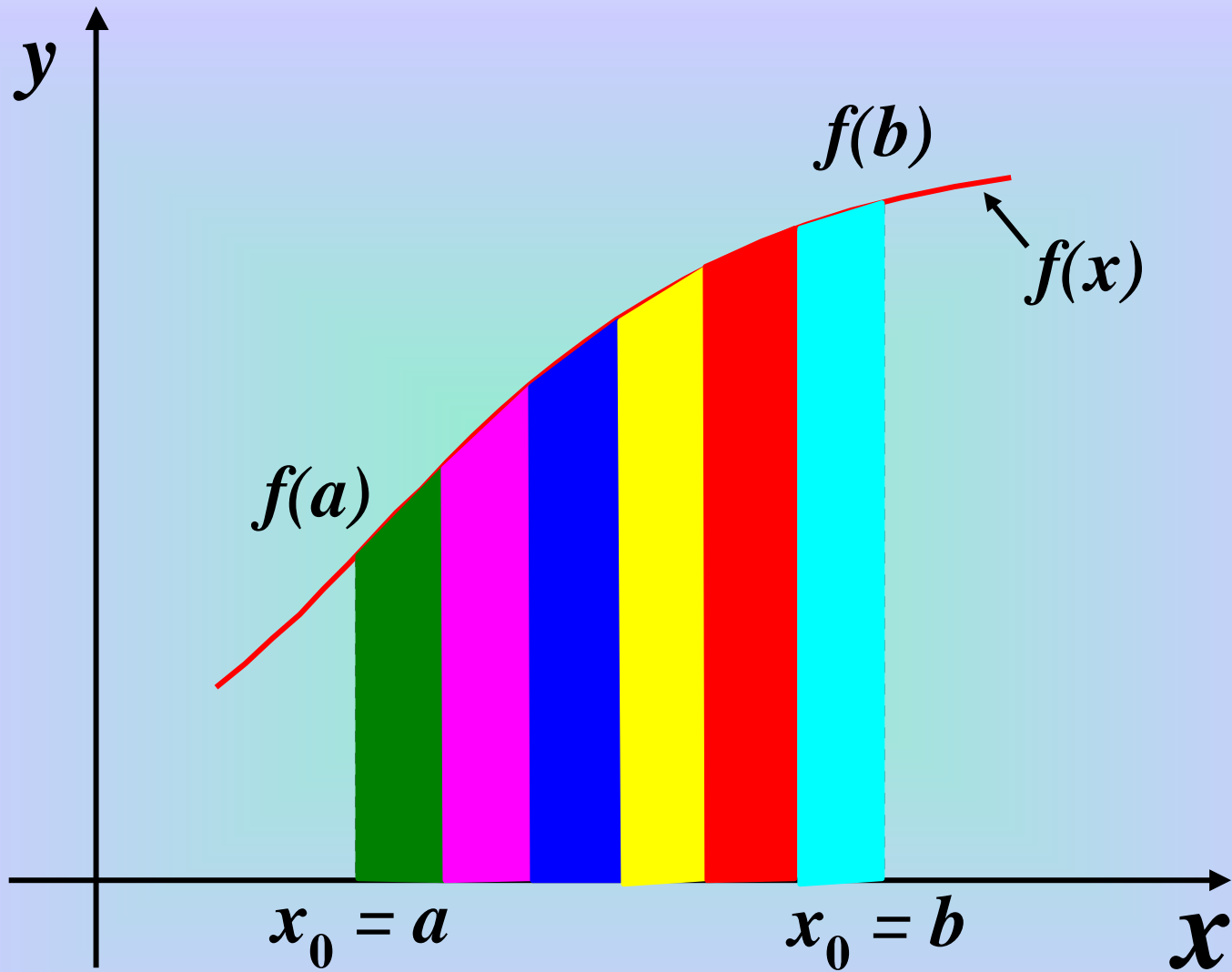
$$\begin{aligned}\int_{x_0}^{x_2} P(x) dx &= \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) dx \\ &+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) dx \\ &+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) dx\end{aligned}$$

$$\int_{x_0}^{x_2} f(x) dx \approx \int_{x_0}^{x_2} P(x) dx$$
$$= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$











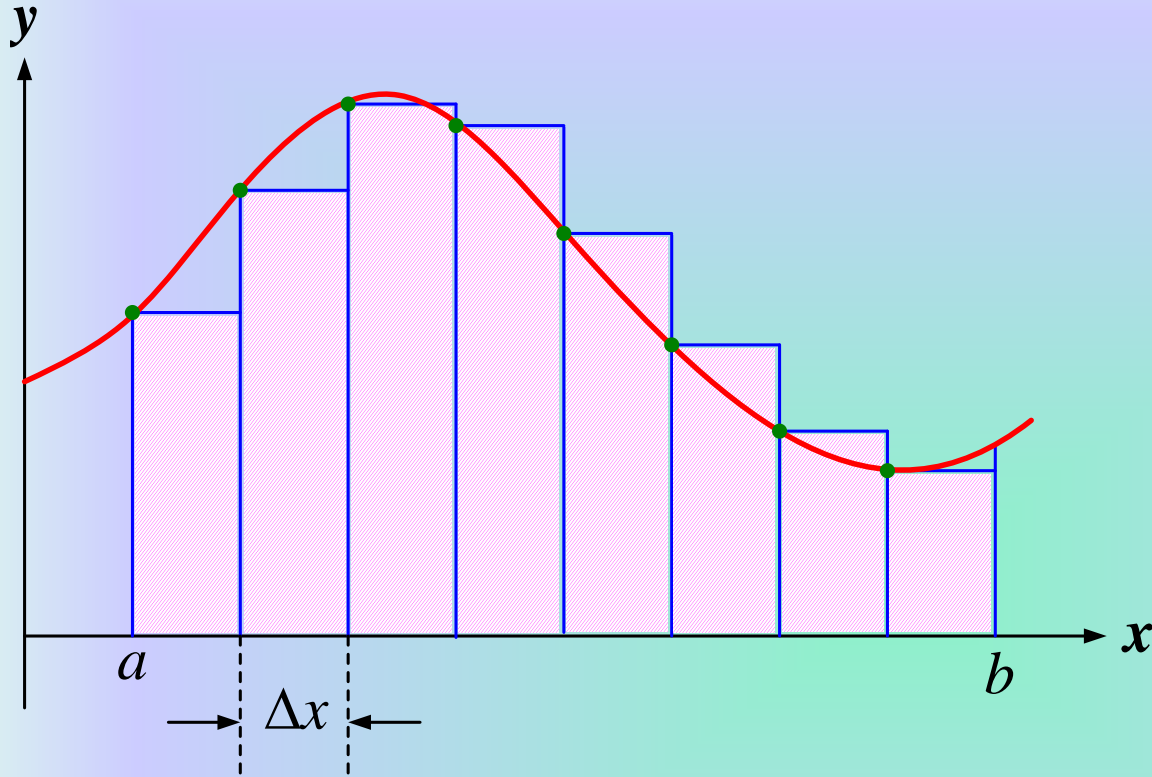
# Composite Numerical Integration

## **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

$x_1 = a$ , the left-side sample of the function is

$x_2 = a + \Delta x$  is used as the

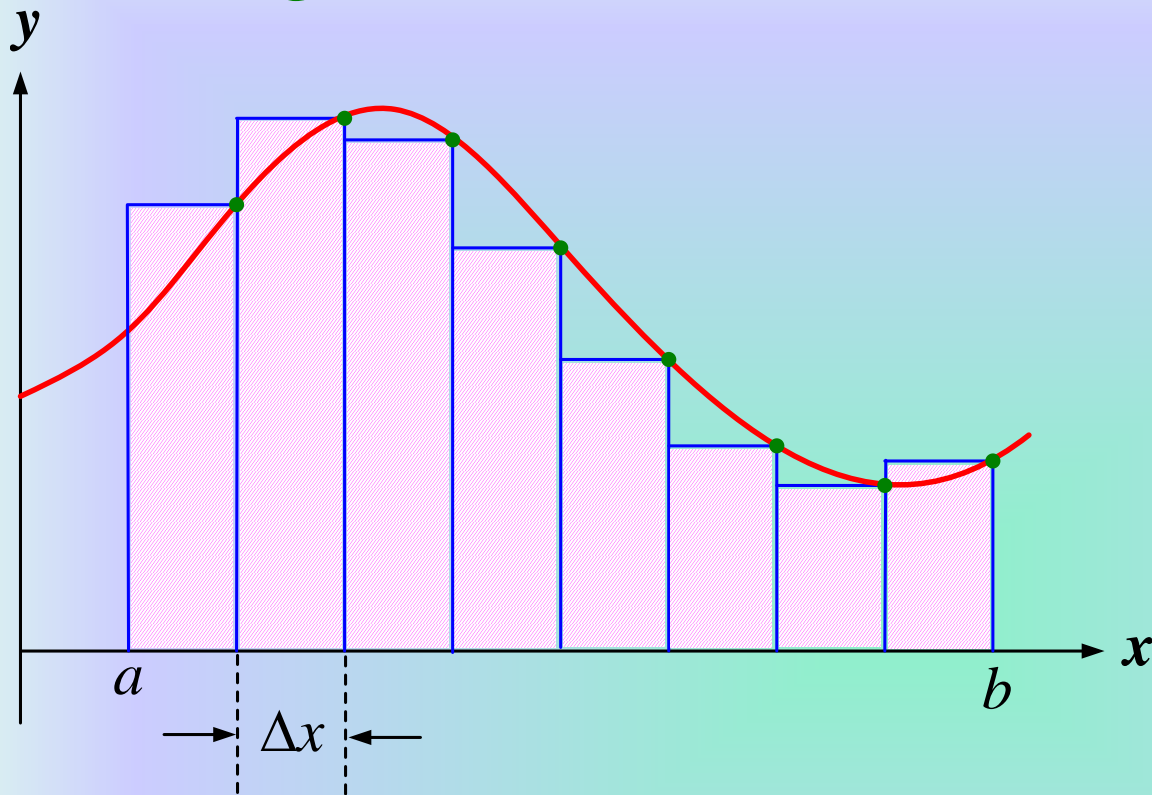
$x_3 = a + 2\Delta x$  height of the

individual rectangle.

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

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

## Right Riemann Sum

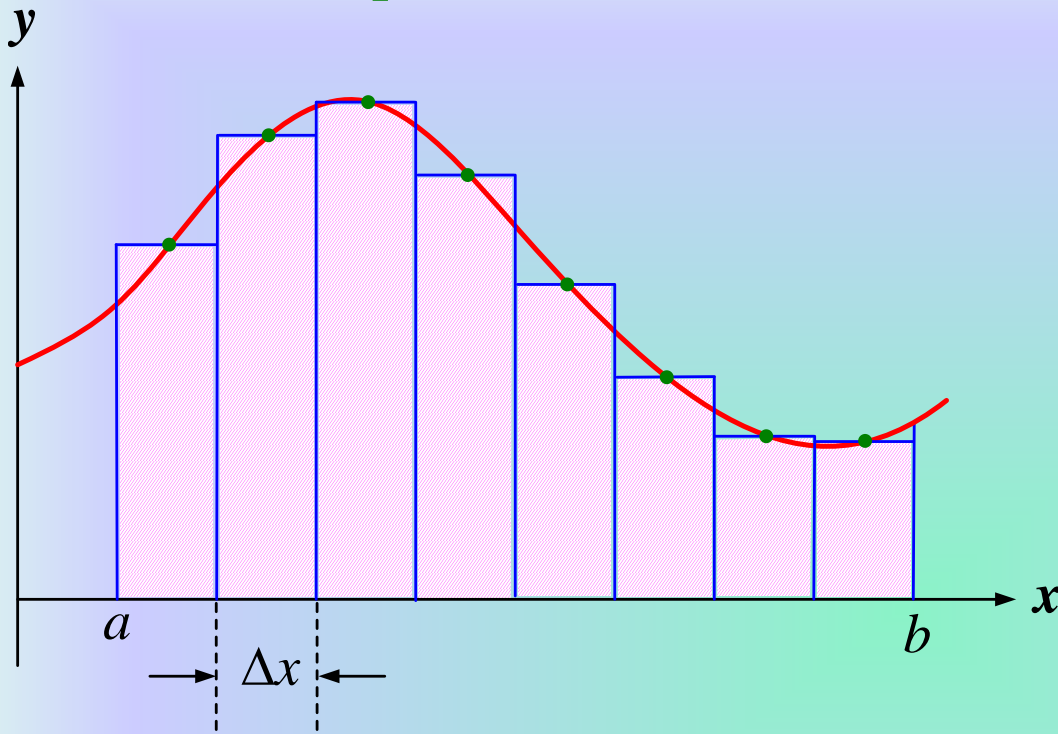


$\Delta x = (b - a) / n$   
In Right Riemann sum, the right-side sample of the function is used as the height of the individual rectangle.

$$\begin{aligned}x_1 &= a + \Delta x \\x_2 &= a + 2\Delta x \\x_3 &= a + 3\Delta x \\&\vdots \\x_i &= a + i\Delta x\end{aligned}$$

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

## Midpoint Rule



$\Delta x = (b - a) / n$   
In the Midpoint Rule, the sample at the middle of the subinterval is used as the height of the individual rectangle.  
 $\vdots$

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

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

## 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

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

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

**by dividing the interval into 20 subintervals.**

$$n = 20$$

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

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

$$\begin{aligned}\int_0^{\pi} \sin(x) dx &\approx \frac{h}{2} \left[ f(a) + 2 \sum_{k=1}^{n-1} f(x_k) + f(b) \right] \\ &= \frac{\pi}{40} \left[ \sin(0) + 2 \sum_{k=1}^{19} \sin\left(\frac{k\pi}{20}\right) + \sin(\pi) \right] \\ &= 1.995886\end{aligned}$$



## 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

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

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

by dividing the interval into 20 subintervals.

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

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

$$\begin{aligned}
\int_0^{\pi} \sin(x) dx &\approx \frac{\pi}{60} \left[ \sin(0) + 2 \sum_{k=1}^9 \sin\left(\frac{2k\pi}{20}\right) \right. \\
&\quad \left. + 4 \sum_{k=1}^{10} \sin\left(\frac{(2k-1)\pi}{20}\right) + \sin(\pi) \right] \\
&= 2.000006
\end{aligned}$$