

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	$f(1.8)$	$f(1.8+h)$	$\frac{f(1.8+h) - f(1.8)}{h}$
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 $f'(1.8) = 0.55\bar{5}$

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 1st 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 2nd 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	23.708450	1.541282
1st Three-point	22.032310	0.134858
2nd Three-point	22.228790	0.061622

Second-order Derivative

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

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

Add these two equations.

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

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

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

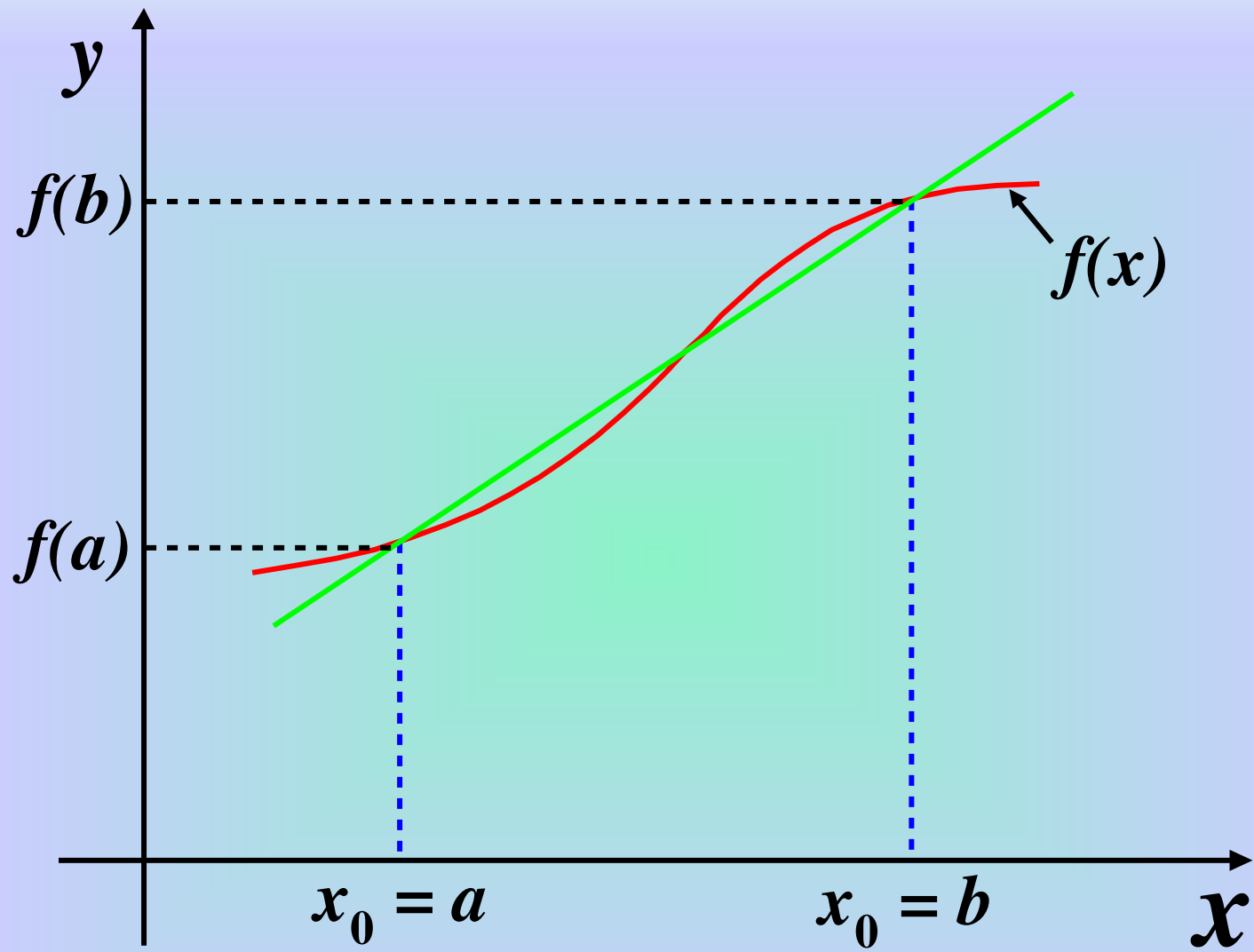
$$f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{2h^2}{4!} f^{(4)}(x) + \dots$$

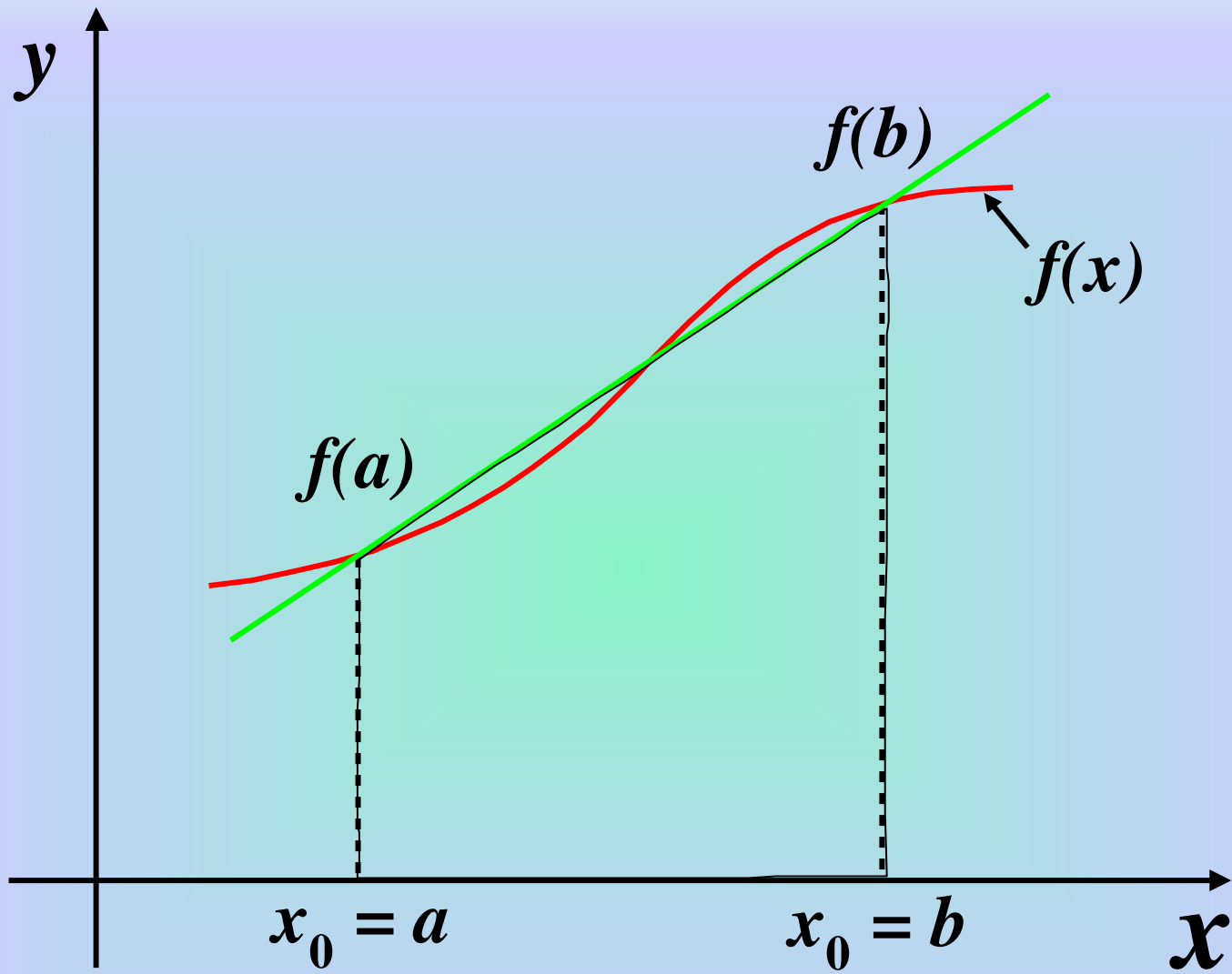
$$f^{(2)}(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

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 $b-a$

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

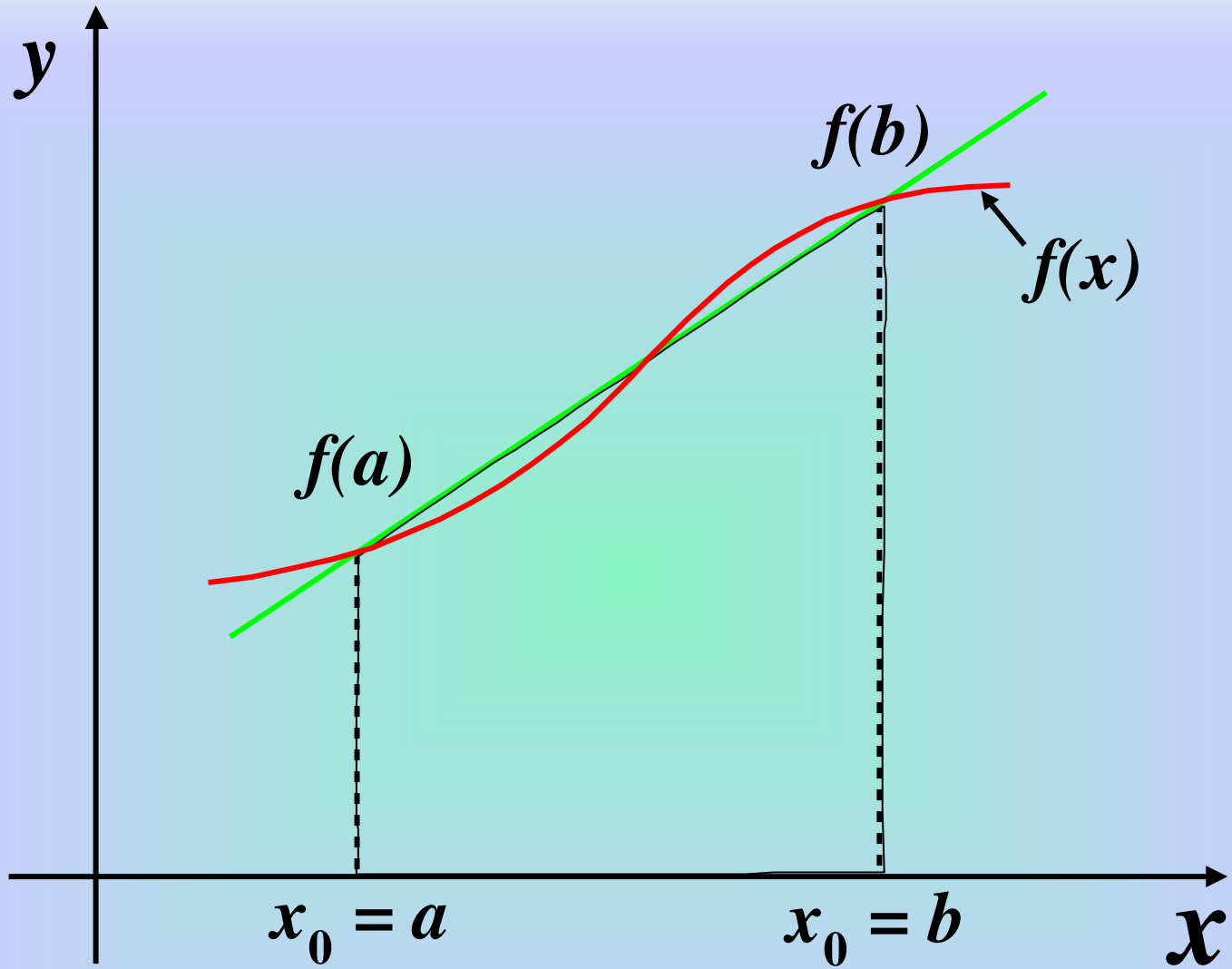
Simpson's Rule:

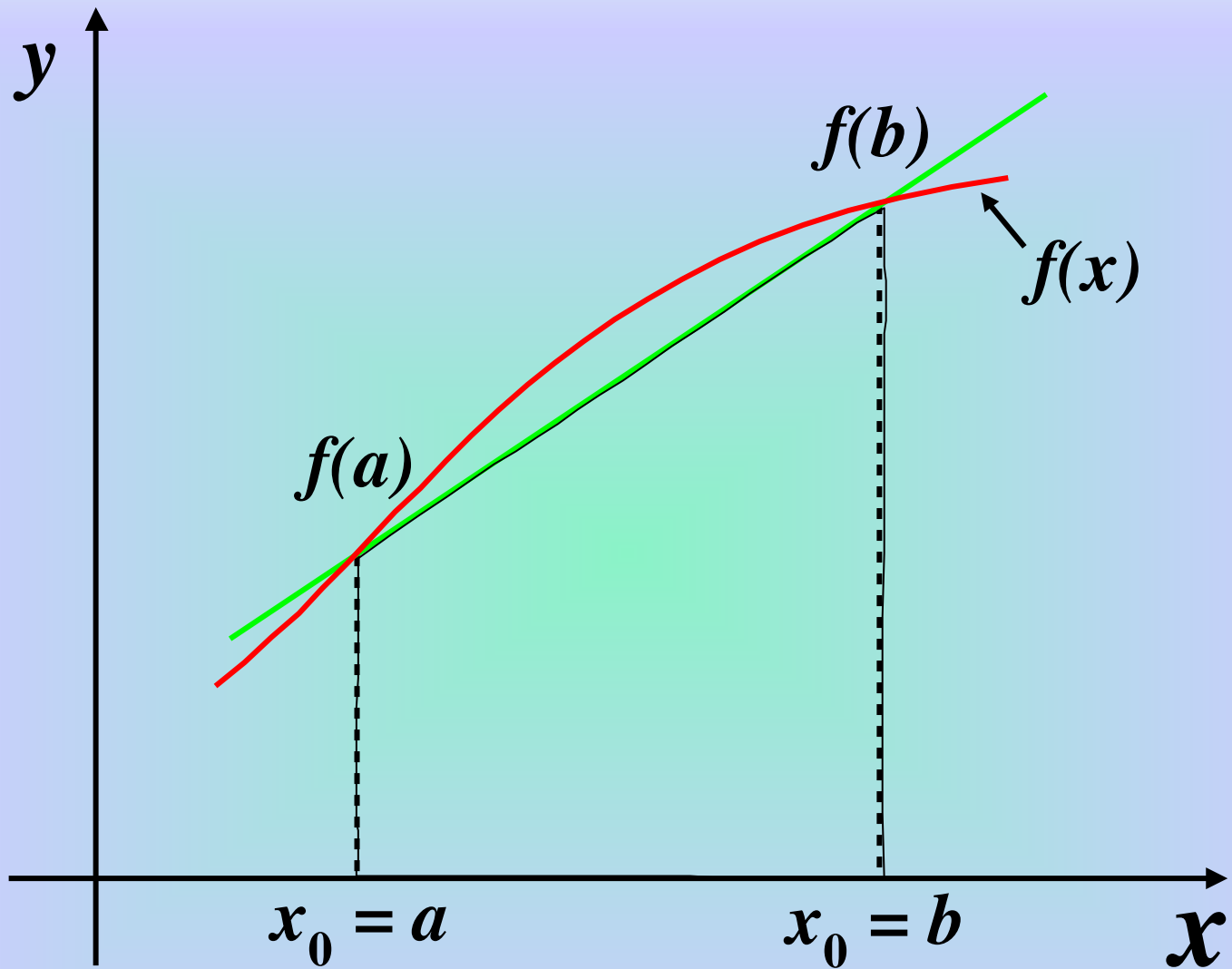
$$\int_{x_0}^{x_2} f(x) dx \approx \int_{x_0}^{x_2} P(x) dx$$

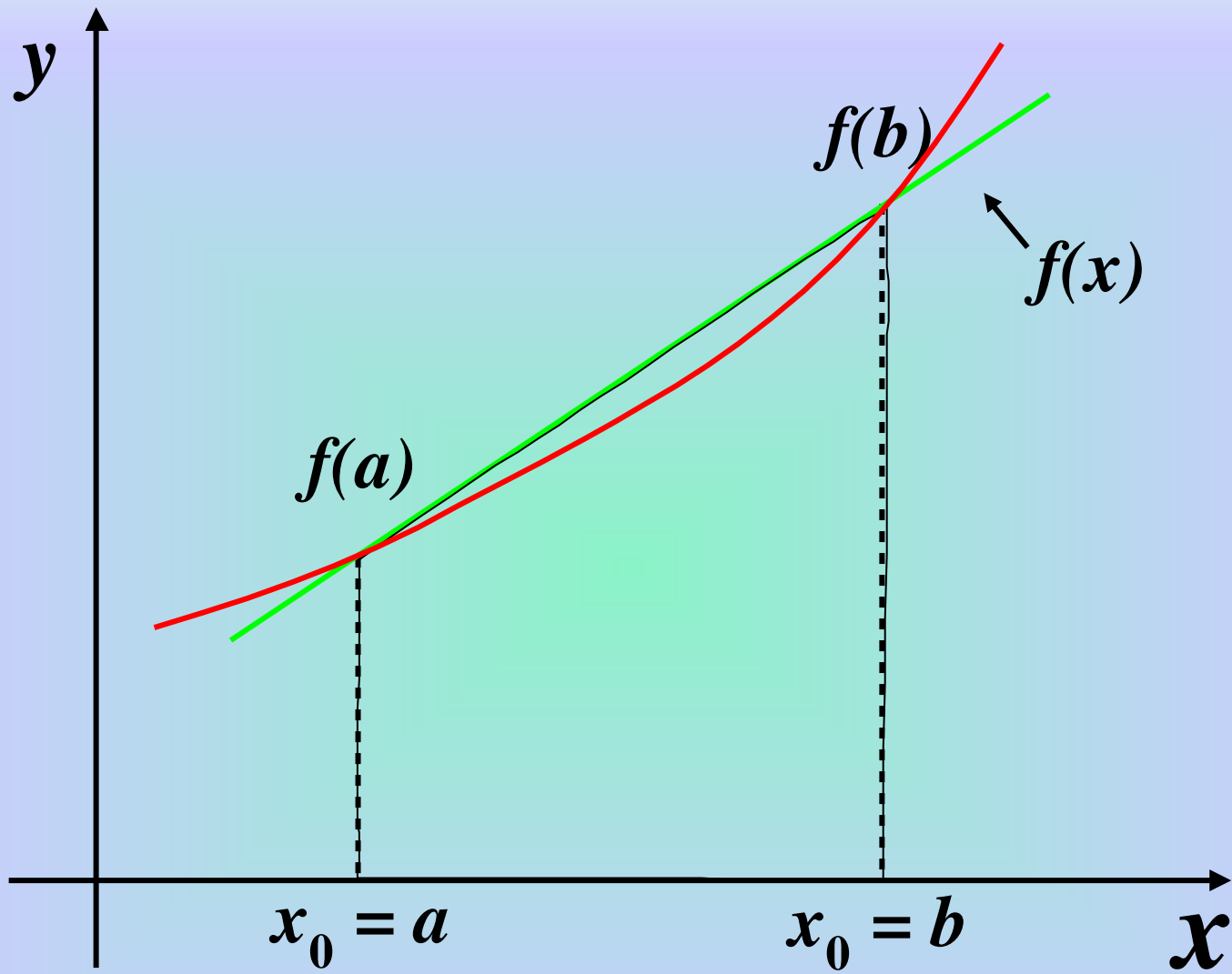
$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

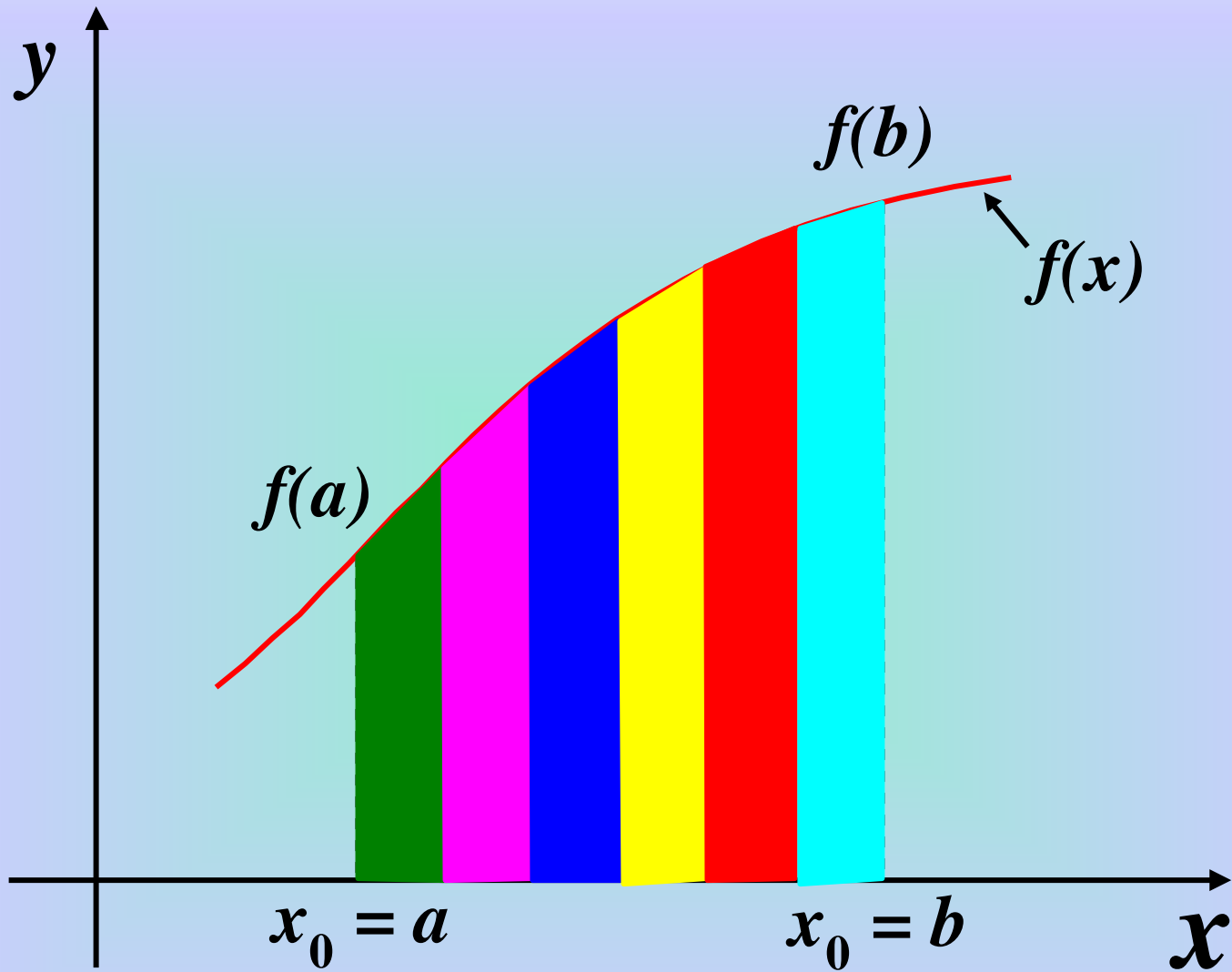
$$\begin{aligned}\int_{x_0}^{x_2} P(x) dx &= \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) dx \\ &+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) dx \\ &+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) dx\end{aligned}$$

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









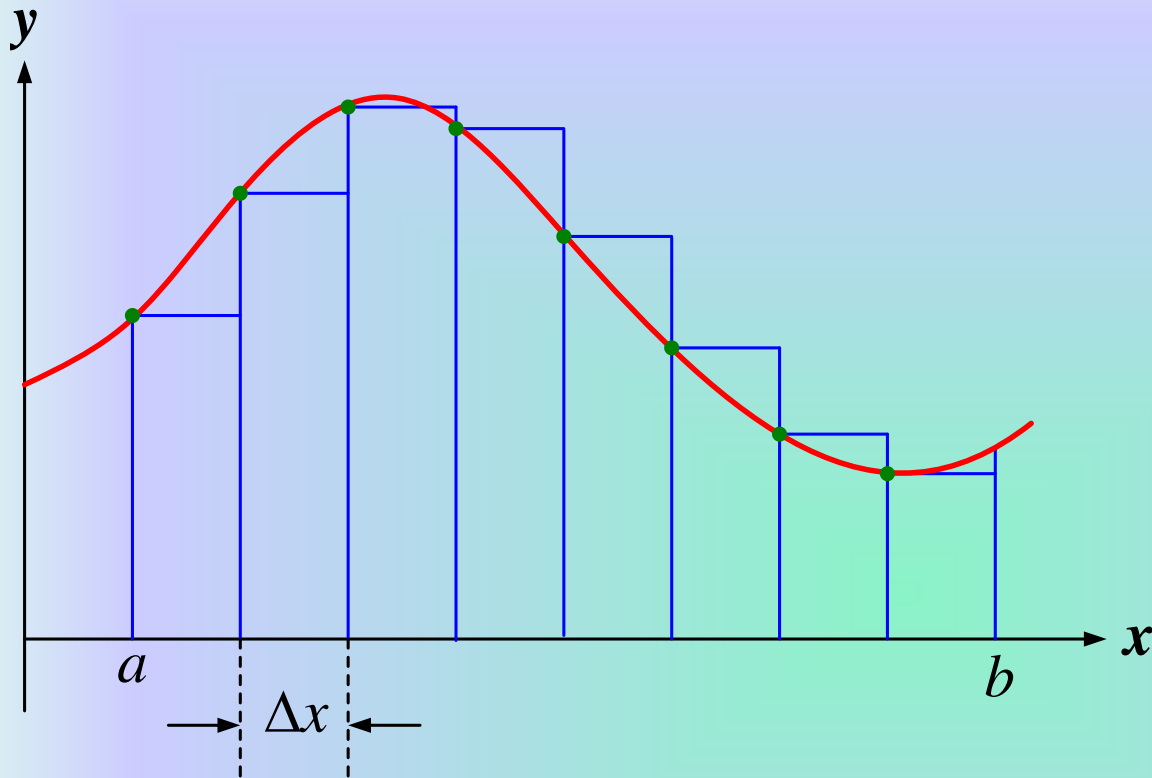
Composite Numerical Integration

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

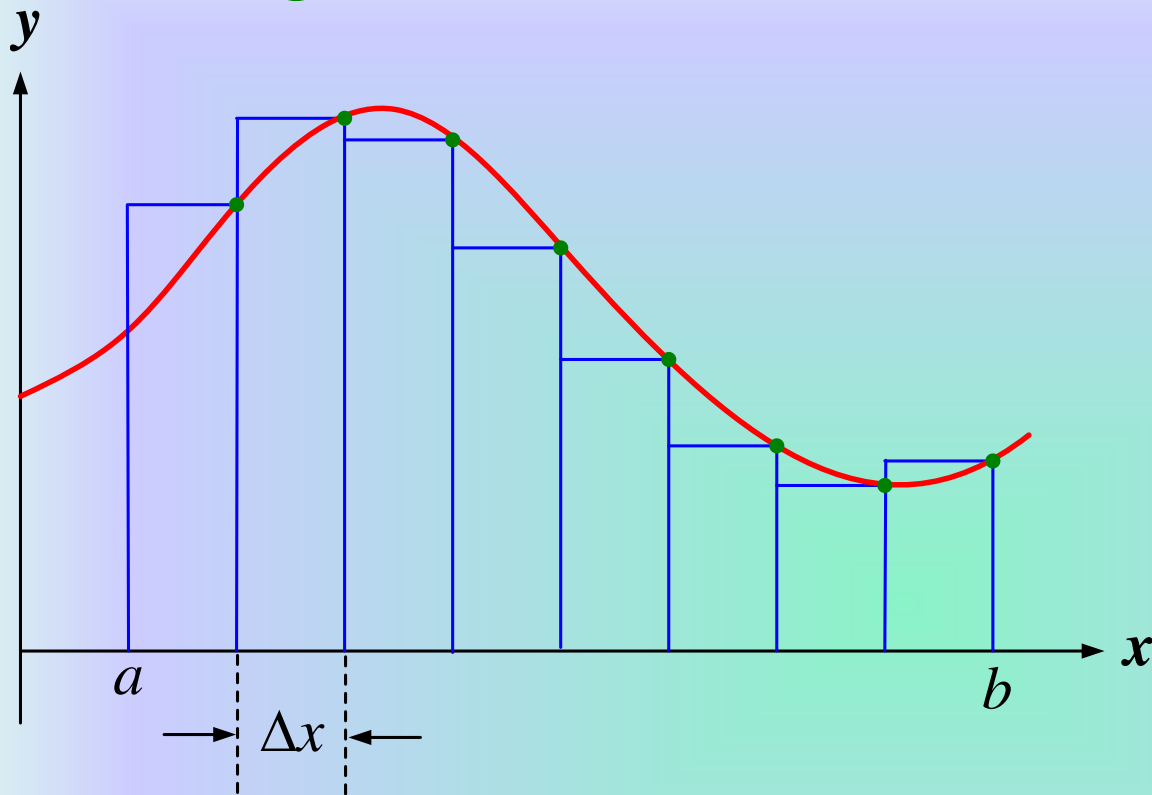
$x_2 = a + \Delta x$ is used as the height of the individual

$x_3 = a + 2\Delta x$ 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

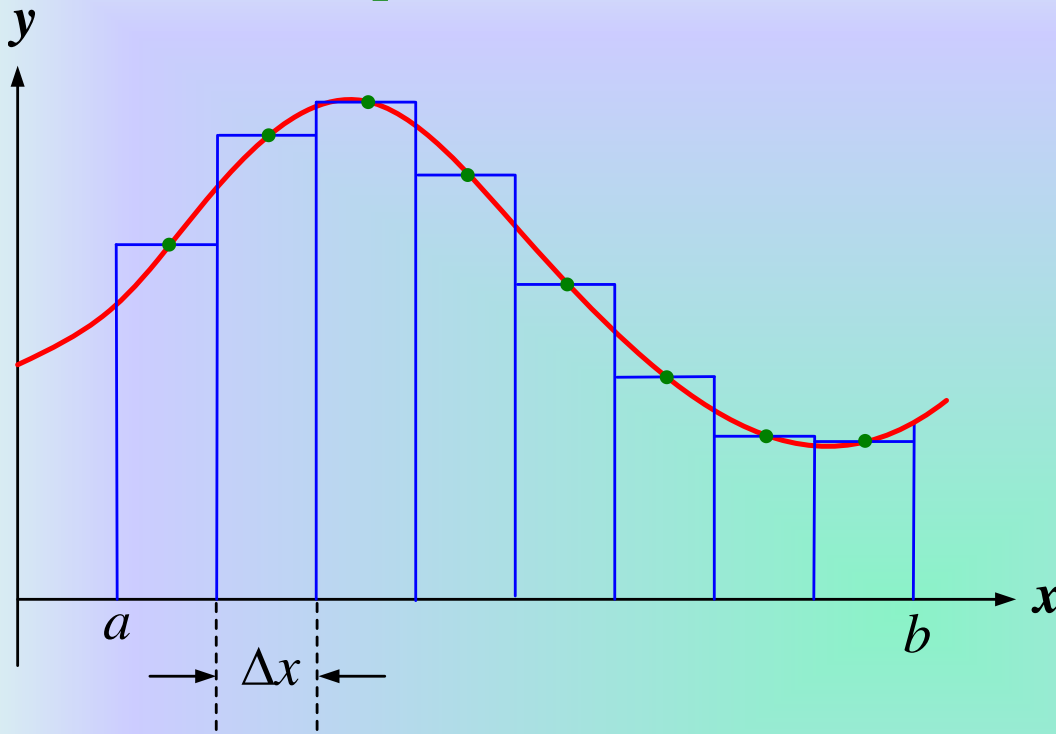


$\Delta x = (b - a) / n$
In Right Riemann sum, the right-side sample of the function is used as the height of the individual rectangle.

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

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

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.

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

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

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