# Numerical Integration

**CH EN 2450**
**Numerical Methods**
**Fall 2019**

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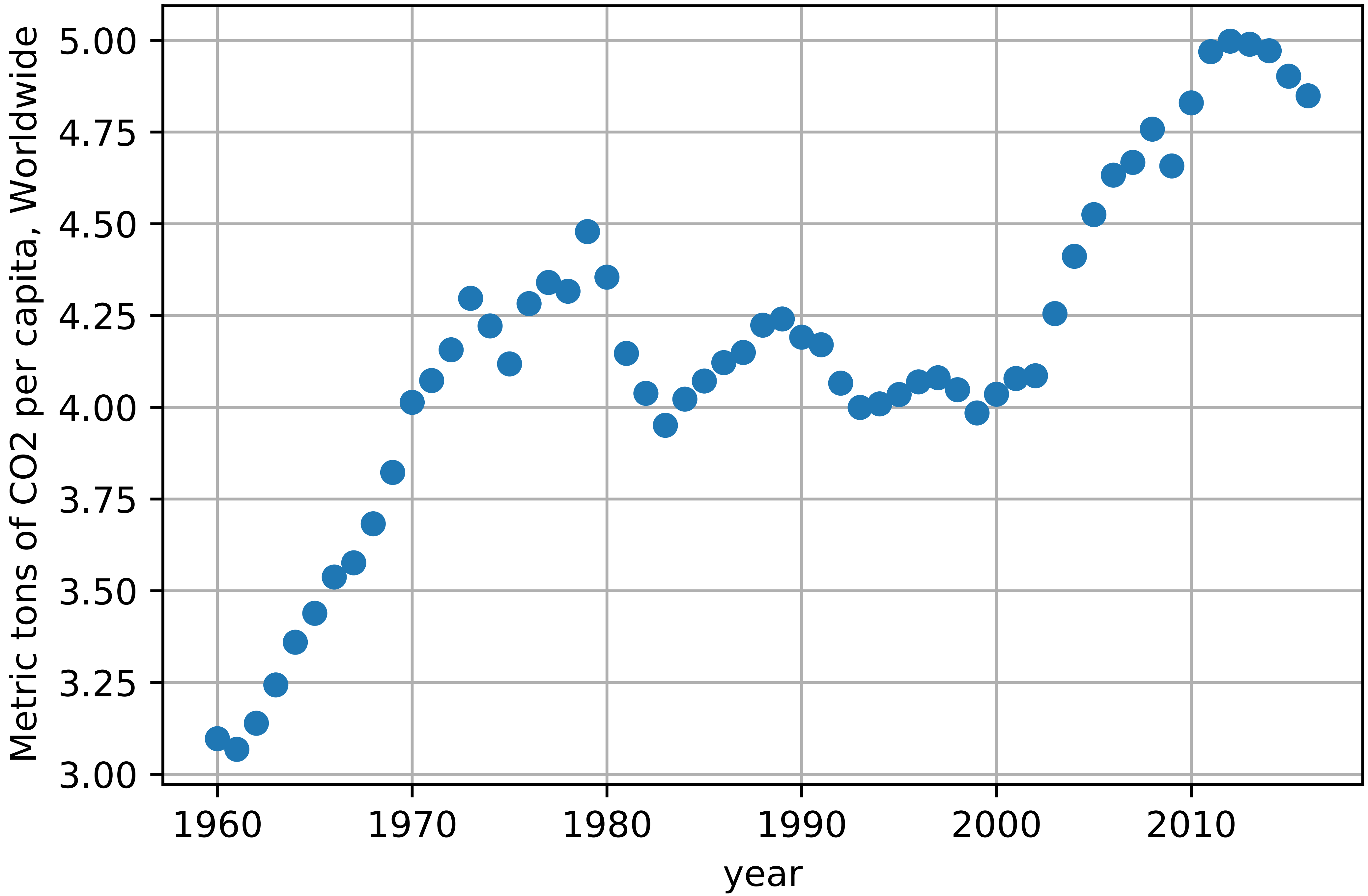
*University of Utah*




**Activity:**

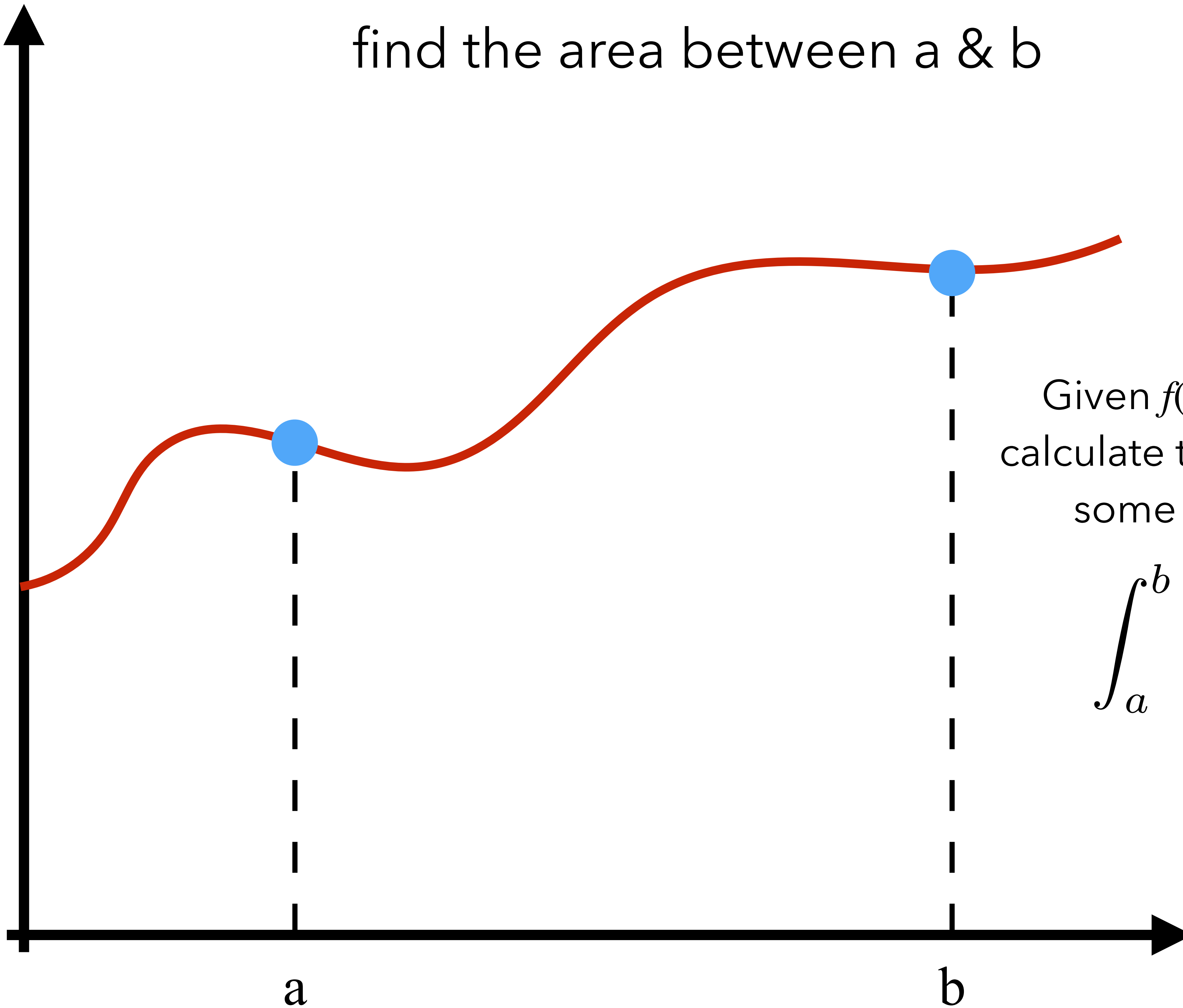
Calculate the total $CO_2$ emissions

# Learning Objectives

At the end of this chapter, you should be able to:

- Define what quadrature and numerical integration means
- Calculate the area under an analytical function using Newton-Cotes formulas
- Calculate the area under a discrete set of data point using Newton-Cotes formulas
- Use the left-point, right-point, midpoint, trapezoidal, and Simpson's 1/3 and 3/8th rules to calculate the integral of a function
- Determine which of the above integration formulas apply to equally-spaced and unequally-spaced data
- Estimate the error bounds for the midpoint, trapezoidal, and Simpson's 1/3 rules

# find the area between a & b




Given $f(x)$, we want to calculate the integral over some region $[a,b]$.

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

# Newton-Cotes Integration

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Concept:

Approximate $f(x)$ locally as a polynomial.

# Left/Right/Mid-point Rules

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Concept: Approximate $f(x)$ as a ***constant*** on the interval $[a,b]$.

$$f(x) \approx C$$

$$\int_a^b f(x)\mathrm{d}x \approx \int_a^b C\,\mathrm{d}x = Cx\big]_a^b = (b-a)C$$

We can chose C in a number of ways:

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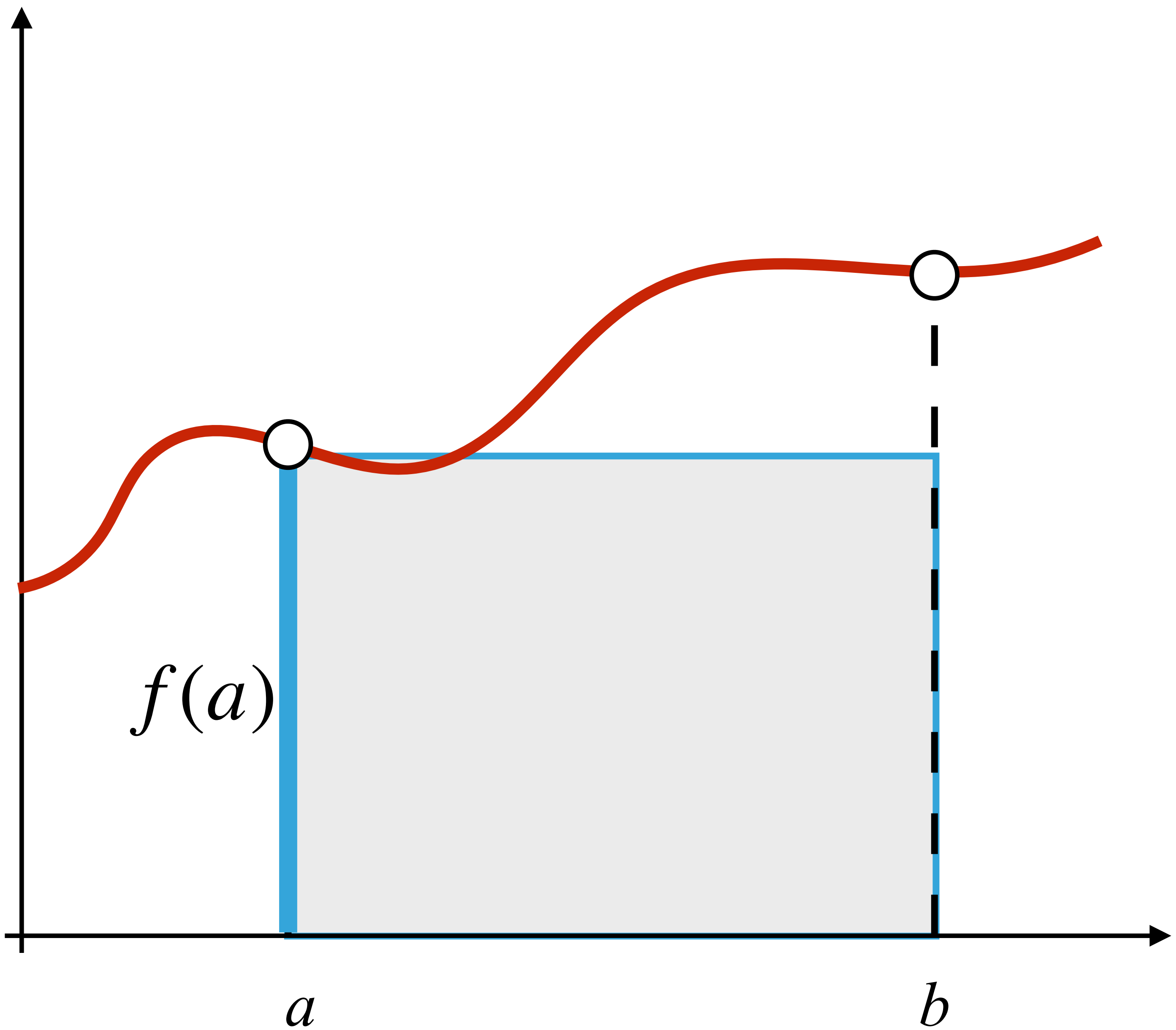


$$C = f(a)$$

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f(a)$$

(leftpoint rule)

Concept: Approximate $f(x)$ as a ***constant*** on the interval $[a,b]$.

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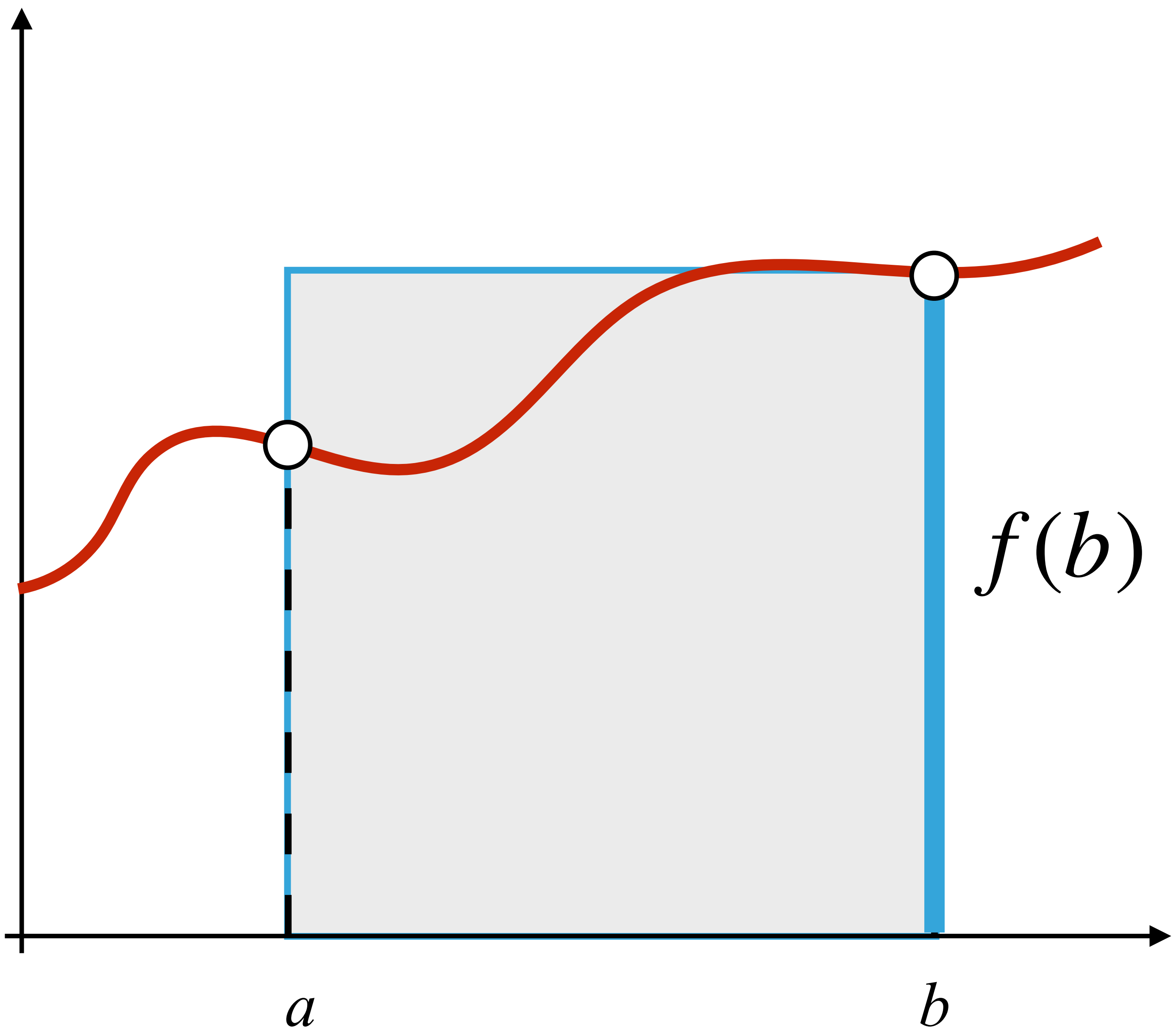



$$C = f(b)$$

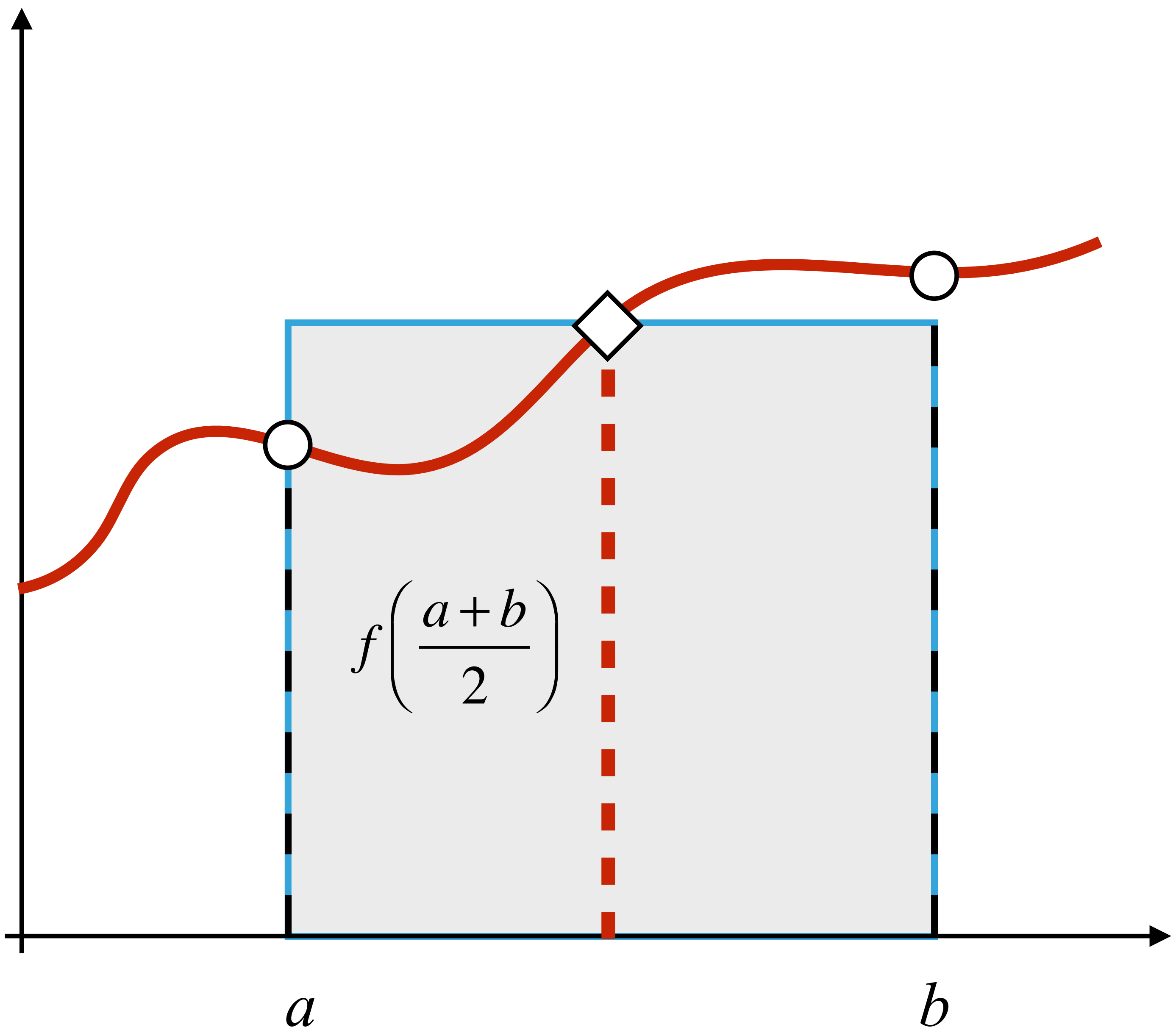
$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f(b)$$

(right-point rule)

Concept: Approximate $f(x)$ as a ***constant*** on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \int_a^b C\,\mathrm{d}x = Cx\Big]_a^b = (b-a)C$$

We can chose C in a number of ways:




$$C = f\left(\frac{a+b}{2}\right)$$

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f\left(\frac{a+b}{2}\right)$$

(midpoint rule)

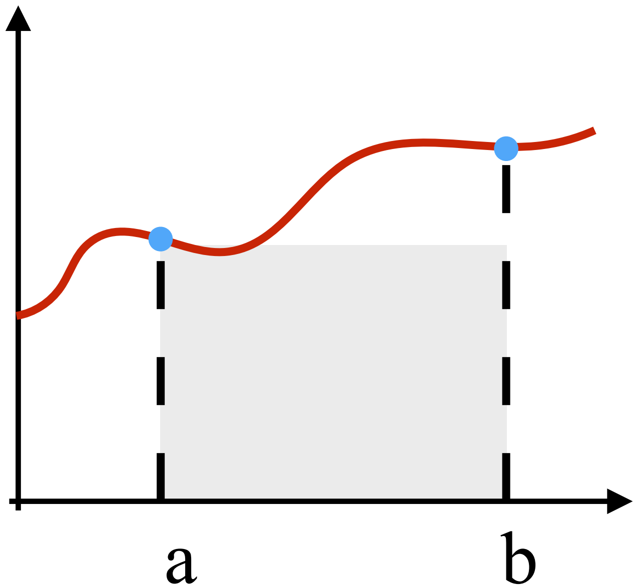
**Requires function value at the midpoint (can be a problem for tabular/discrete data).**

# Built-In Python Routines

## For Continuous Functions

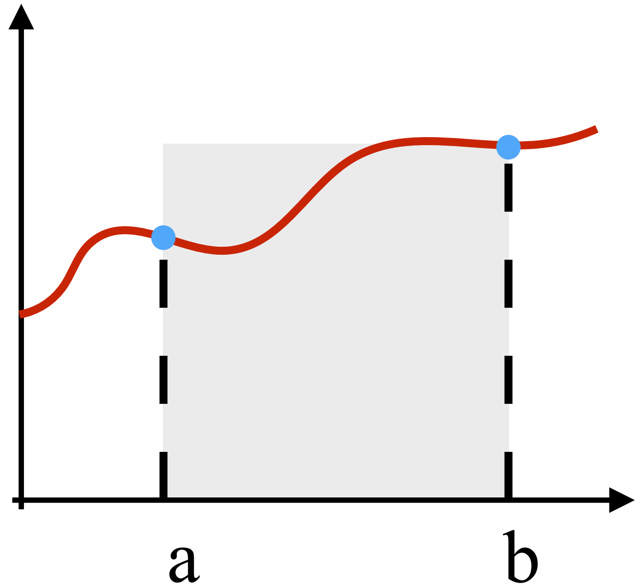
```
from scipy import integrate
result = integrate.quad(function_name,a,b)
```

- Numerically evaluate the function on the interval [a,b]
- Uses an integrator based on *adaptive* Simpson's quadrature



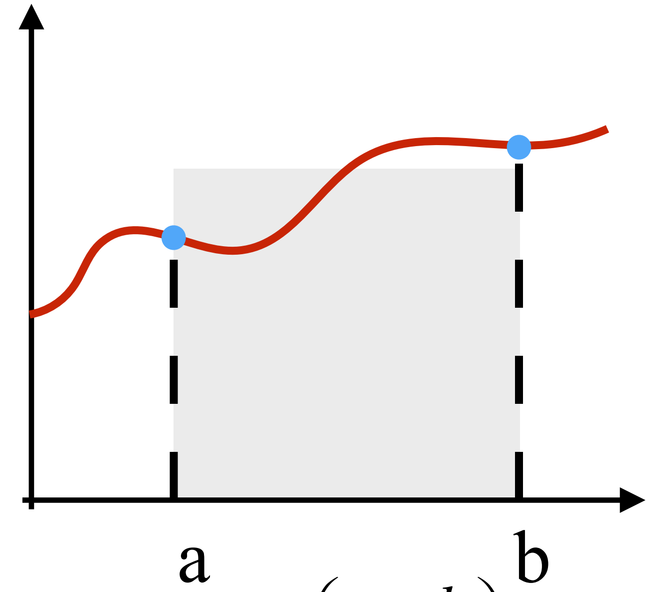

$$C = f(a)$$

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f(a)$$




$$C = f(b)$$

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f(b)$$




$$C = f\left(\frac{a+b}{2}\right)$$

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f\left(\frac{a+b}{2}\right)$$

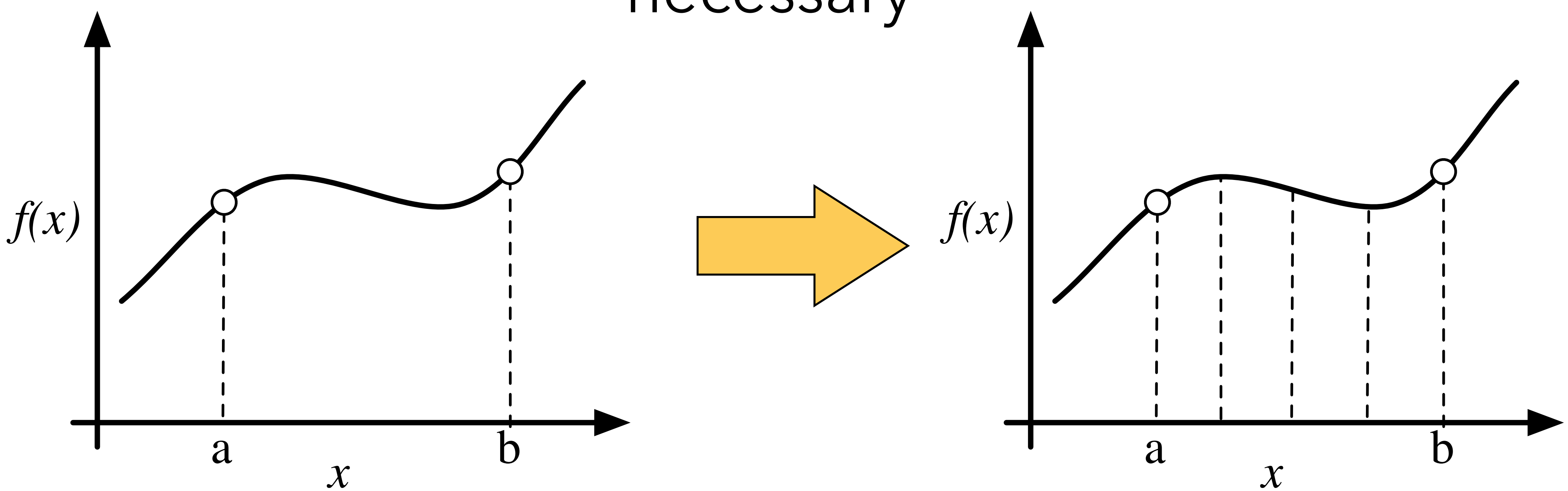
**<u>Coding Activity 1:</u>**

Develop three Python routines that implement the left-point, right-point, and mid-point formulas. The routine arguments must include: (1) a function, and (2) the interval (a,b) on which the function is to be evaluated.

Then apply these functions to calculate $\int_0^1 [1 + 0.5\sin^2(1.75\pi x)]\mathrm{d}x$ .

**Download the notebook: Quadrature (with gaps).ipynb from canvas**

To increase accuracy, these formulas can be applied to as many subintervals/segments as necessary




$$\int_a^b f(x)\mathrm{d}x \approx (x_2 - x_1) f\left(\frac{x_1 + x_2}{2}\right) + (x_3 - x_2) f\left(\frac{x_3 + x_2}{2}\right) + \ldots$$

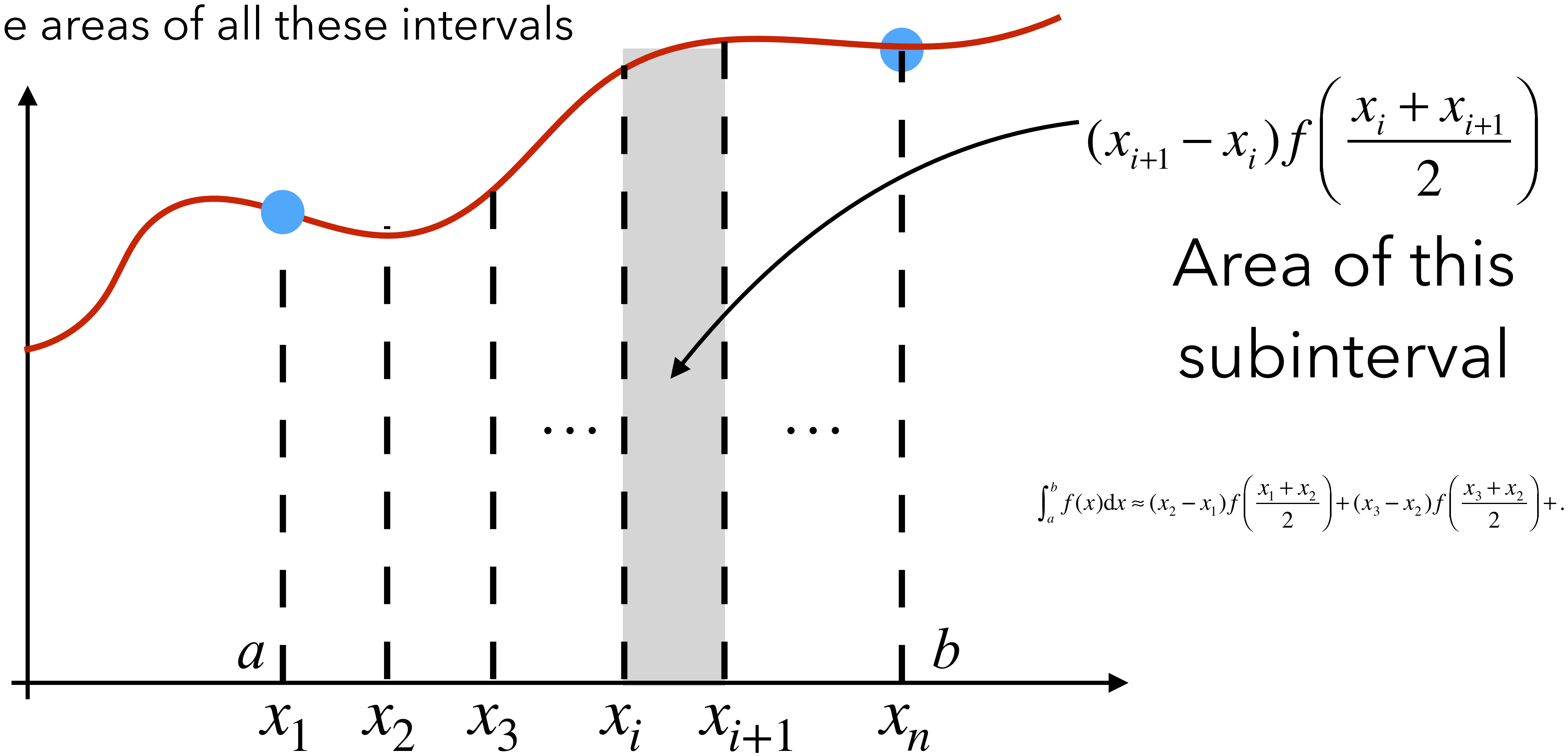
This procedure of dividing the area under a curve into smaller areas is called quadrature. Numerical integration is, from here onwards, equivalent to quadrature.

## Coding Activity 2:

Develop a Python code that computes the integral of an analytical function with arbitrary number of segments $n$. Use the left-point, right-point, and midpoint rules. Then apply these routines to calculate $\int_0^1 [1 + 0.5\sin^2(1.75\pi x)]\mathrm{d}x$ .

Hints:

- Create a **`linspace`** for the intervals
- Loop over each interval and apply the integration rule to that interval
- Add up the areas of all these intervals



```python
def midpoint(f, a, b, npts):
    '''
    f: Any Python function
    a: Lower integral bound
    b: Upper integral bound
    npts: Number of quadrature points

    Returns the integral of f(x) based on the midpoint rule
    '''
    x = np.linspace(a,b,npts)
    sum = 0.0
    for i in range(0,len(x)-1):
        a = x[i]
        b = x[i+1]
        sum += (b-a)*(f( (a+b)/2 ) )
    return sum
```

# What about discrete data?

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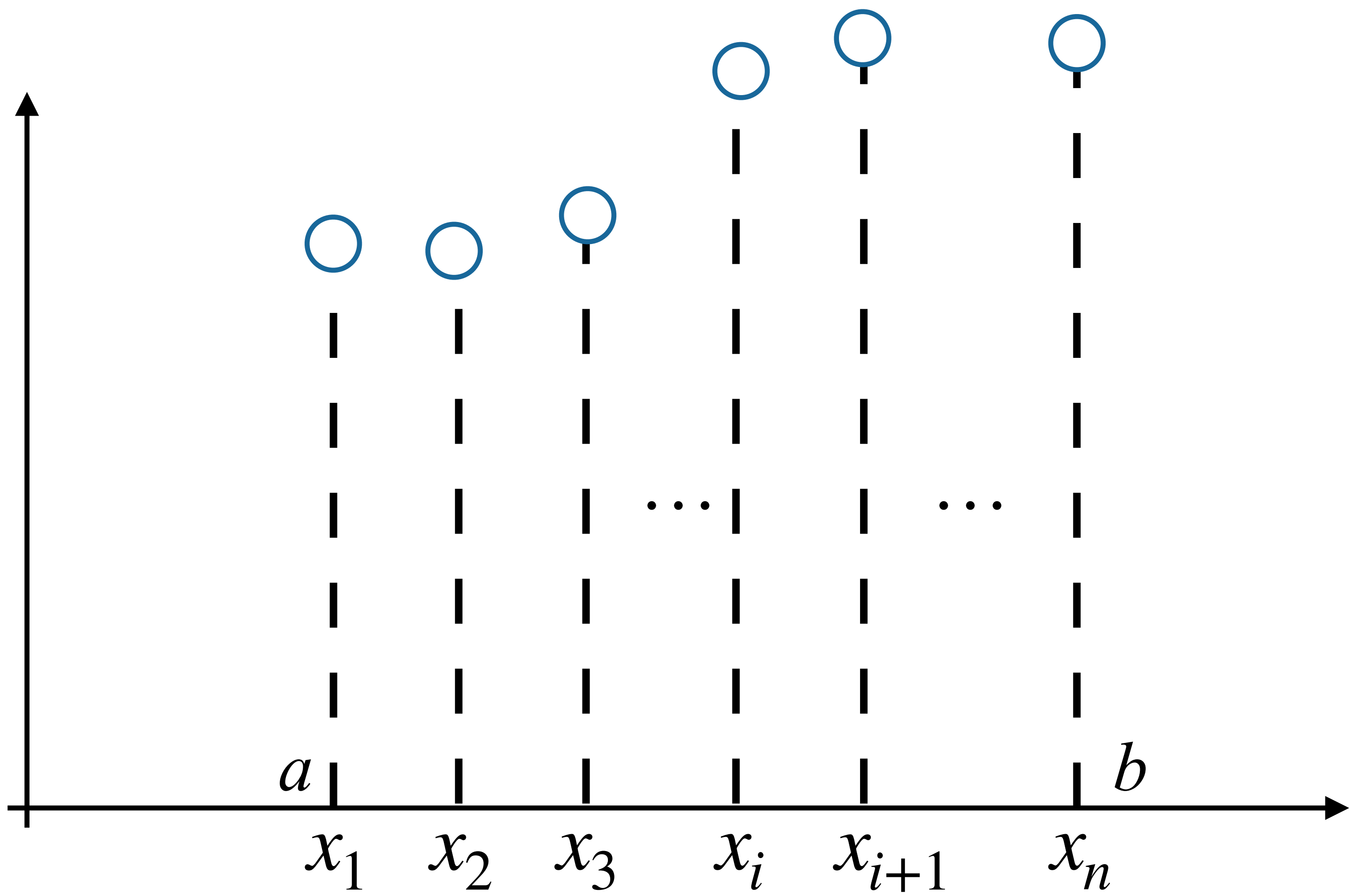
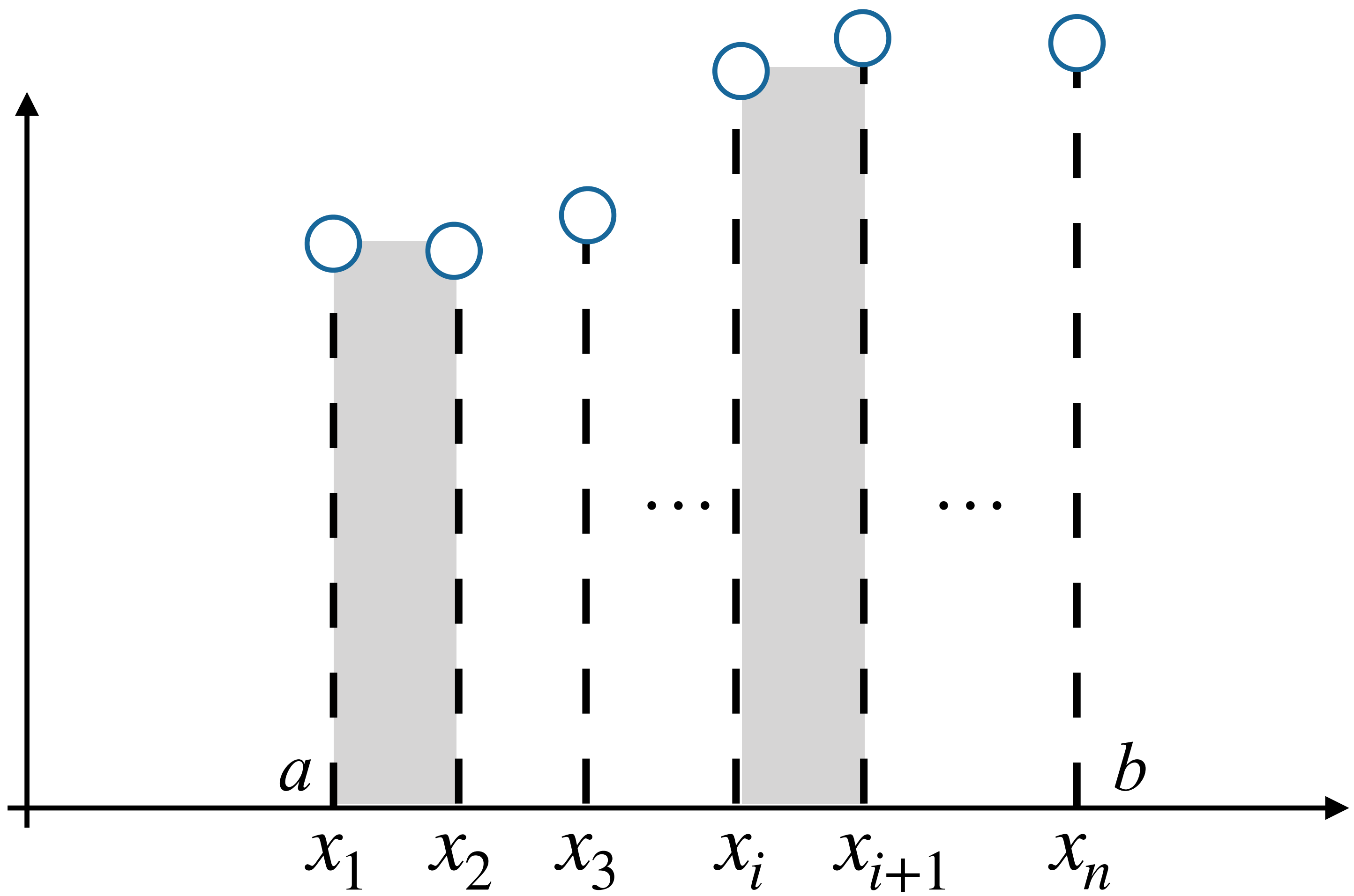


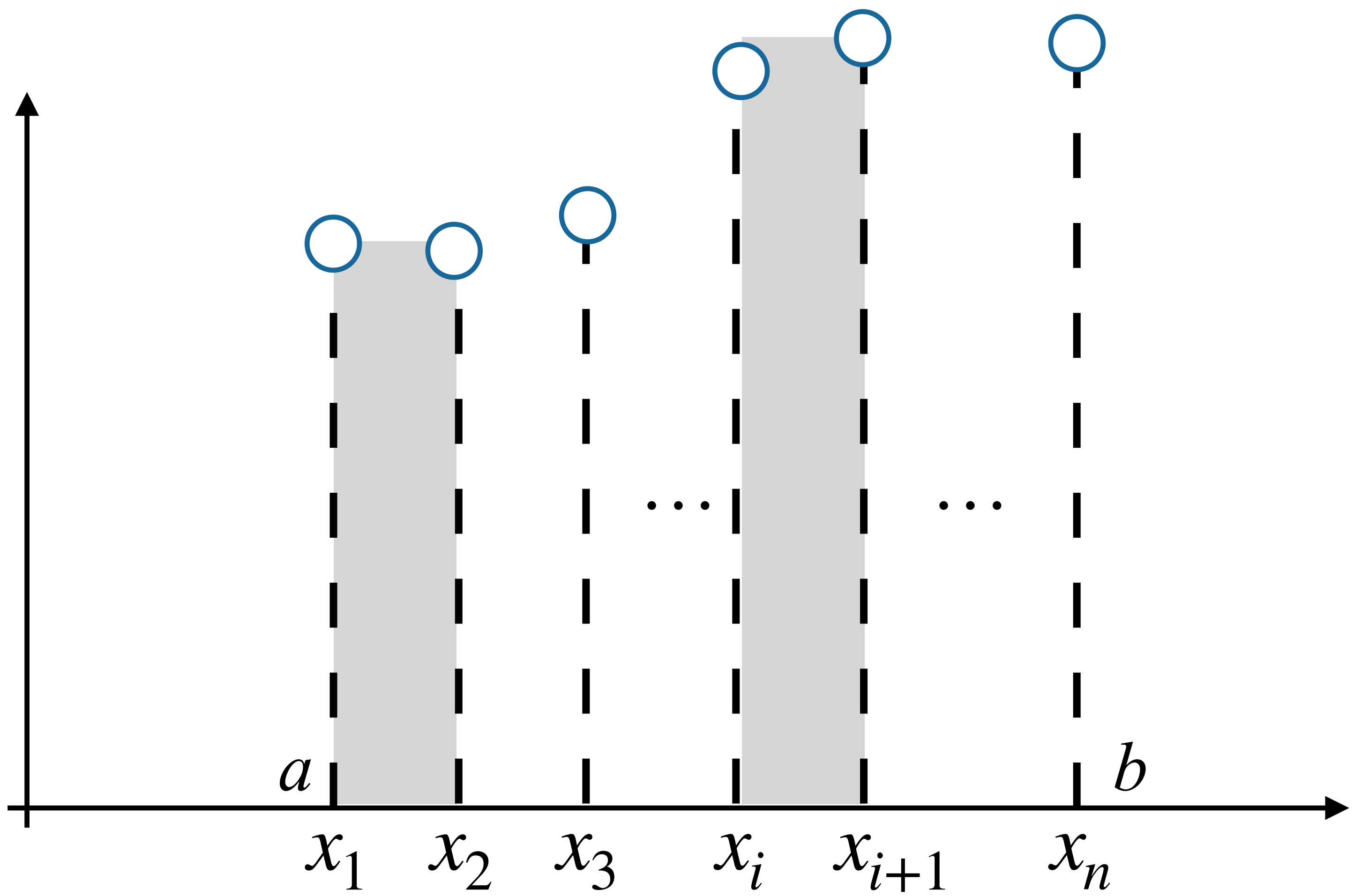
# What about discrete data?

**Left-Point Rule** applies readily

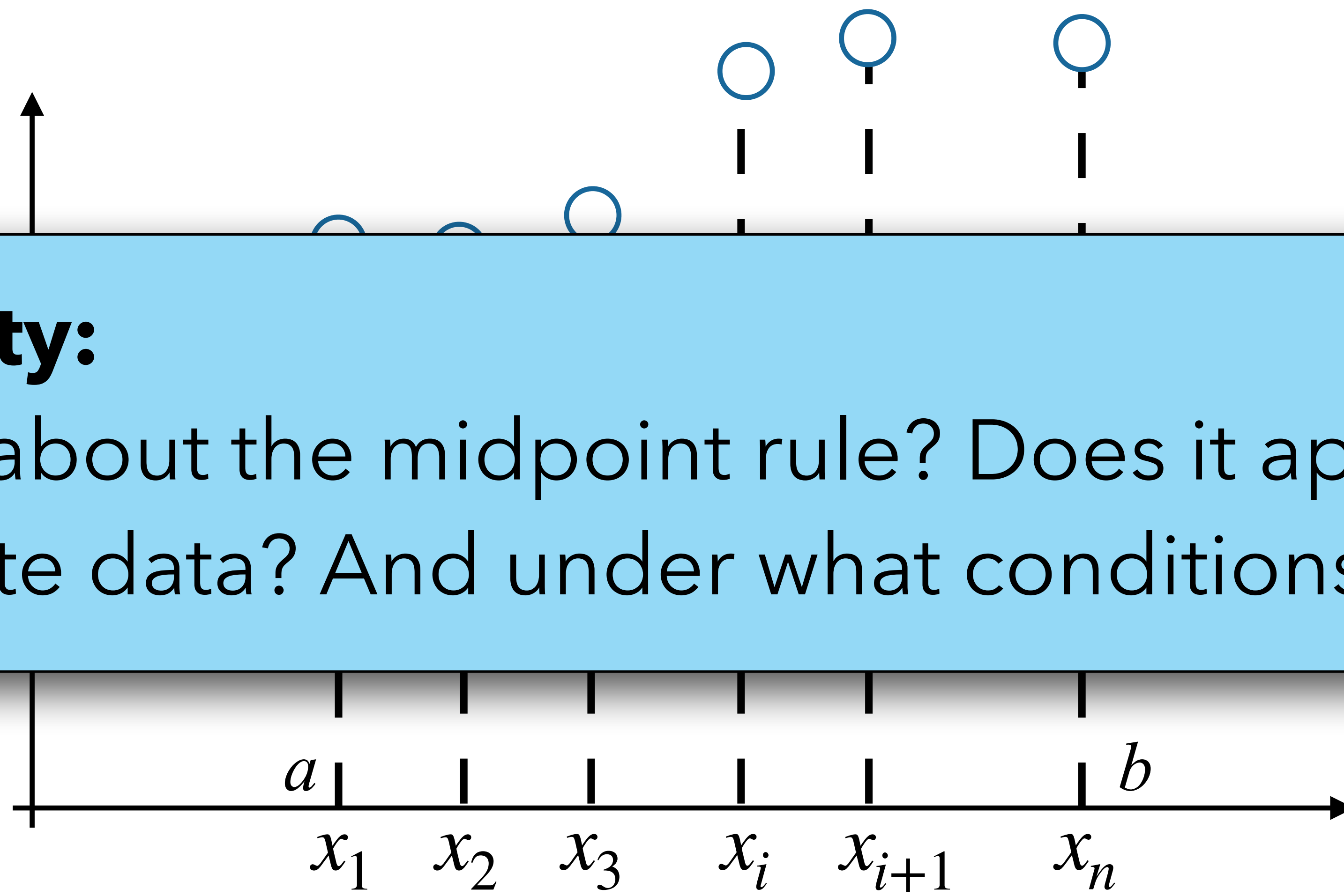


# What about discrete data?

**Right-Point Rule** applies readily



# What about discrete data?




**Activity:**

What about the midpoint rule? Does it apply to discrete data? And under what conditions?

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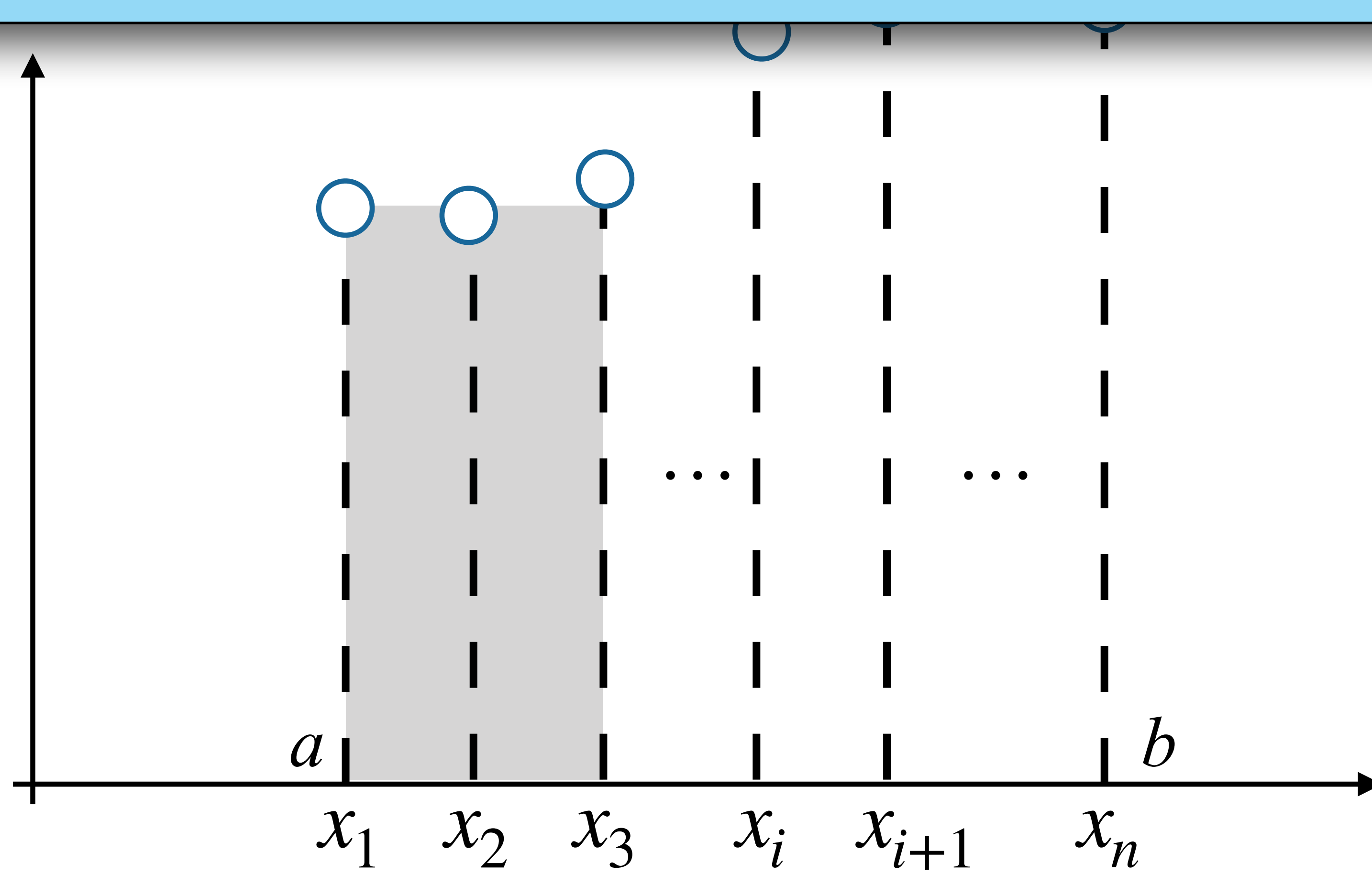
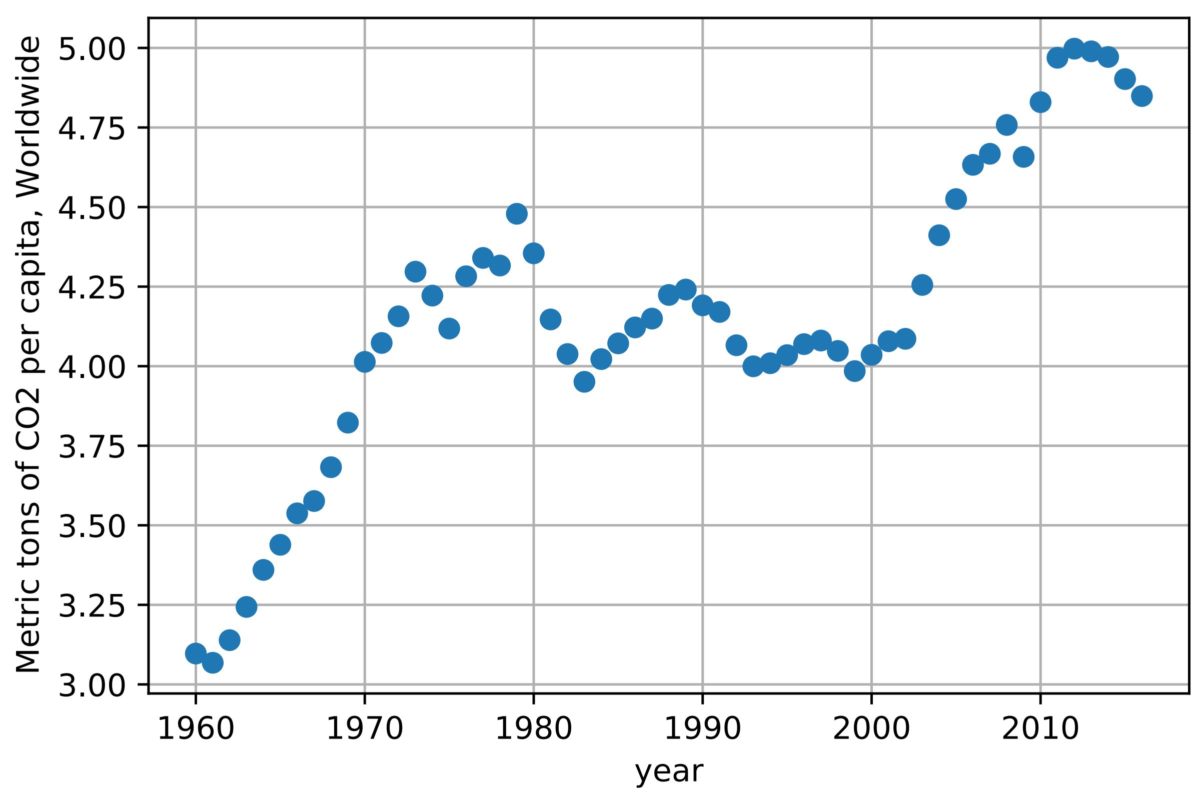
What about the midpoint rule? Does it apply to discrete data? And under what conditions?




The midpoint rule can be applied to equally-spaced discrete data, but you must take every two intervals at a time so that a midpoint can be defined.
***If the data is not equally spaced, the midpoint rule cannot be applied.***

**<u>Coding Activity 3:</u>**
Using the left-point and right-point rule, develop a Python code that integrates discrete data. Apply it to calculate the world emissions of CO2 per capita.




## Python Built-in for Discrete Data Integration

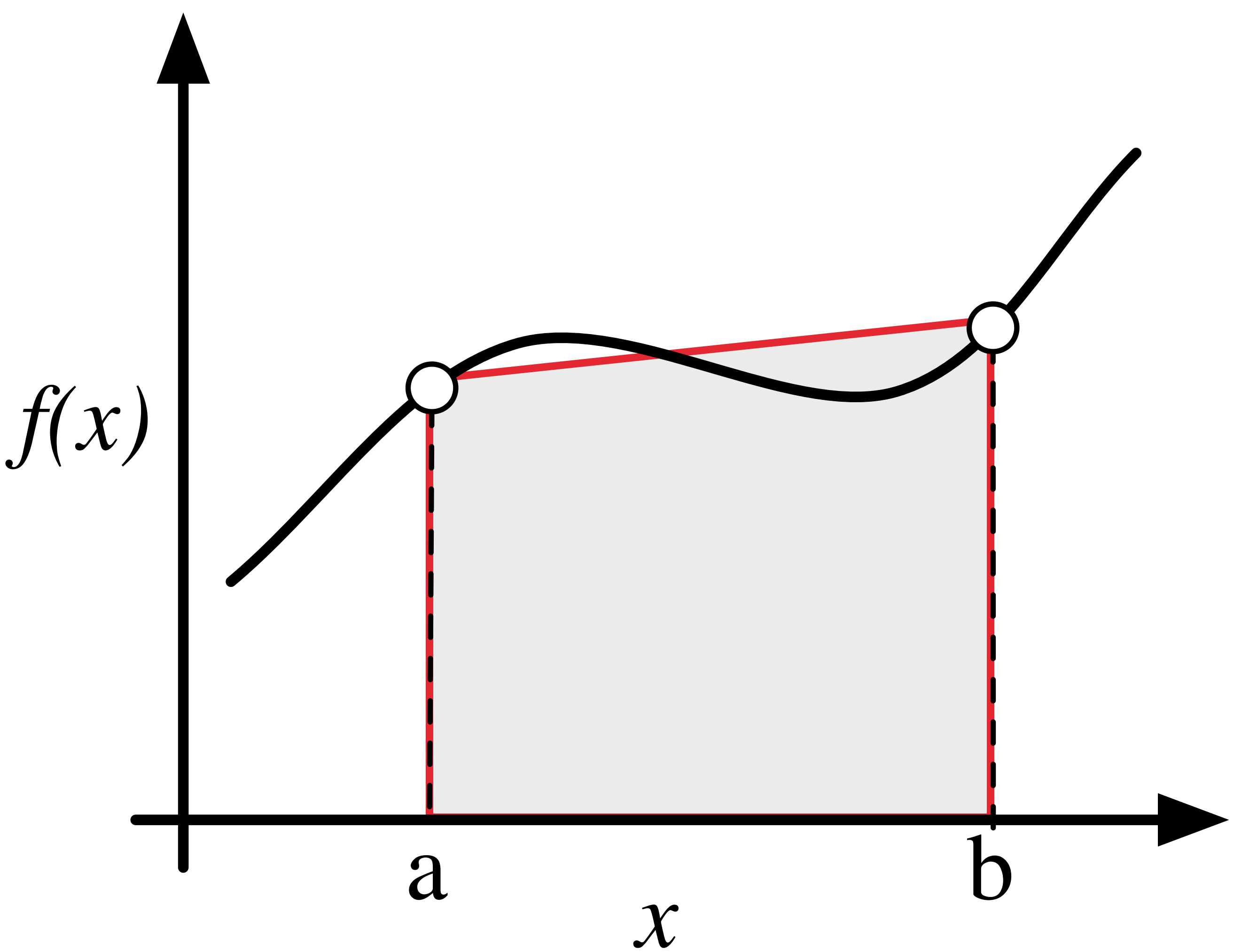
```
import numpy as np
result = np.trapz(y,x)
```

- Integrate discrete data numerically using the trapezoid method.

# More Accurate Methods

# Trapezoidal Rule

Concept: Approximate $f(x)$ as a ***linear*** function on the interval $[a,b]$.



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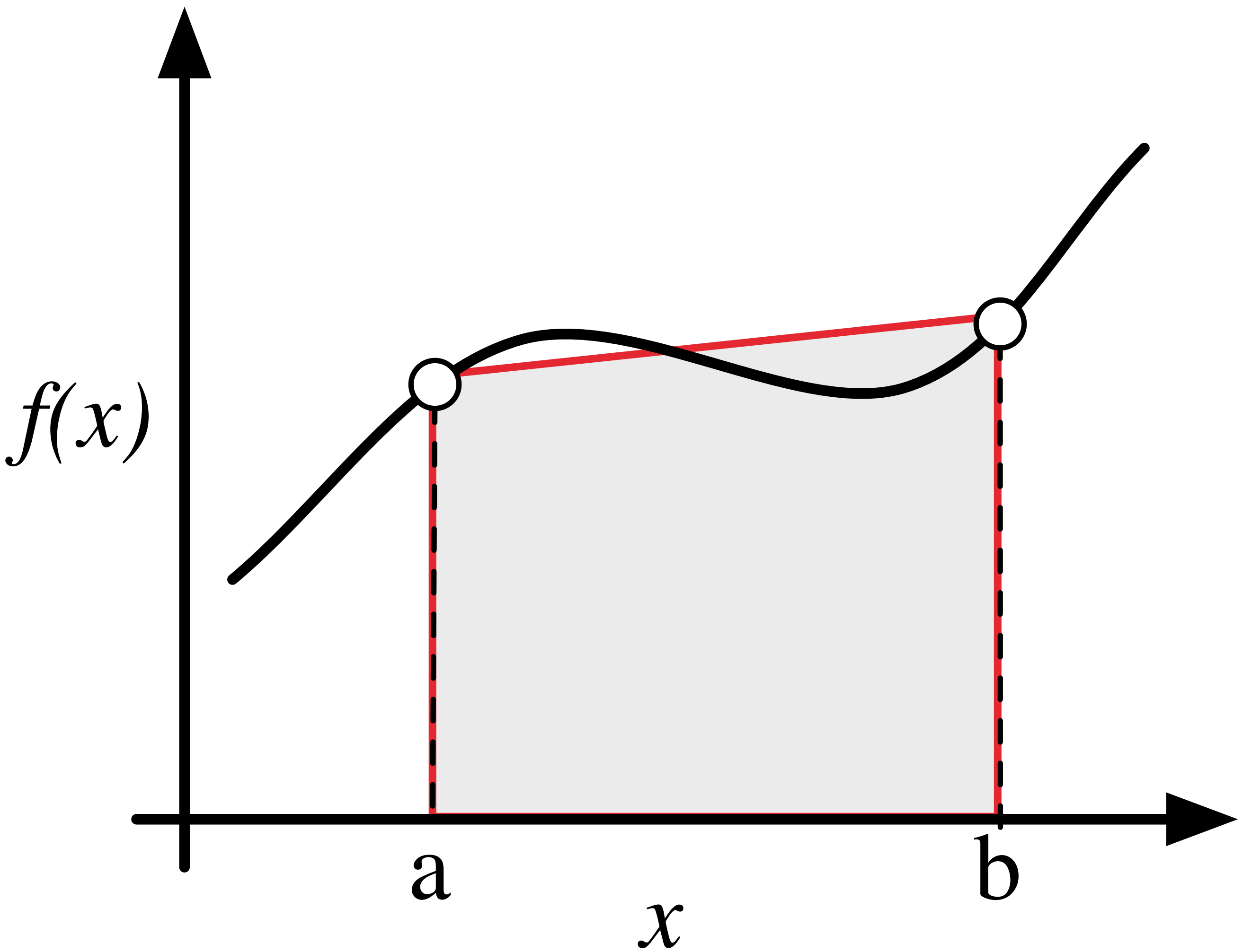
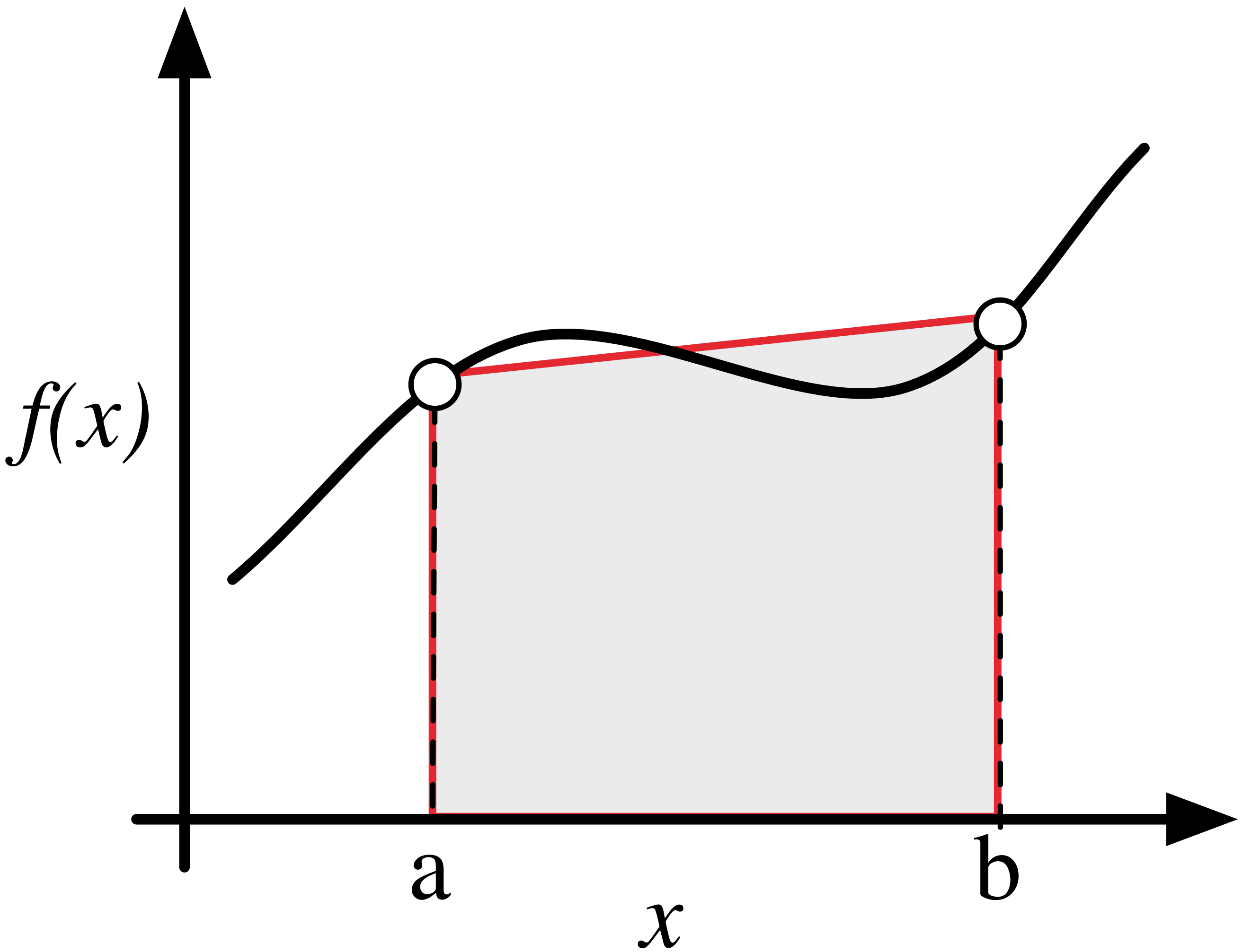



**Activity (2 min, Group):**
Calculate the area under this line between $a$ and $b$. HINT: Use geometry to compute the area.

Concept: Approximate $f(x)$ as a ***linear*** function on the interval $[a,b]$.

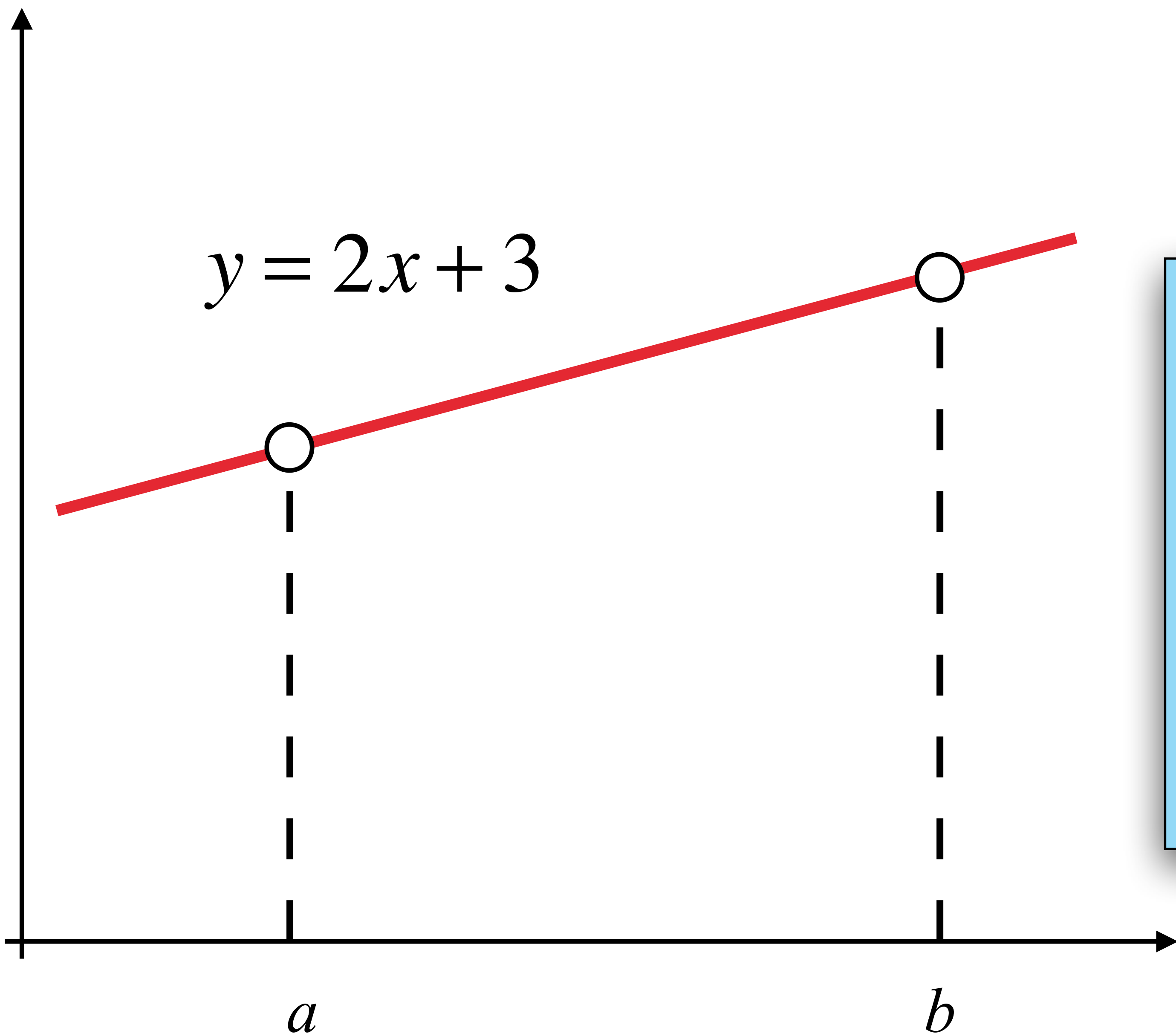



## Trapezoidal Rule

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

- Convenient form for tabular (discrete) data.
- Does not require equally spaced data.

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




**Activity (2 mins, Group):**
Calculate the true error in integrating $y = 2x + 3$ on the interval [0,2] using the Trapezoidal rule. The exact integral: $\int_0^2 (2x+3)\mathrm{d}x = 10$

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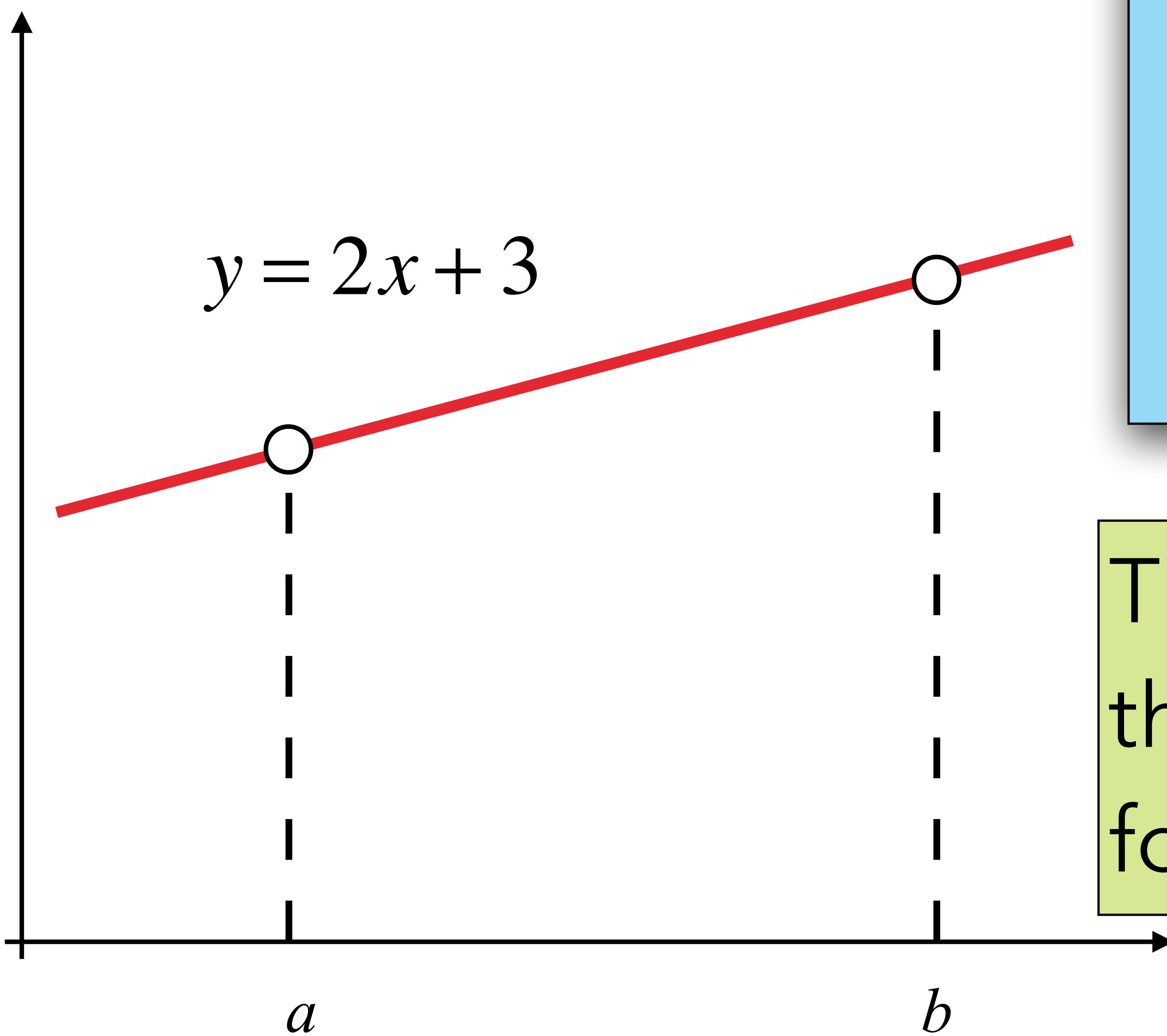



**Activity (2 mins, Group):**
Calculate the true error in integrating $y = 2x + 3$ on the interval [0,2] using the Trapezoidal rule. The exact integral: $\int_0^2 (2x+3)\mathrm{d}x = 10$

The error is zero because the trapezoidal rule is exact for a straight line.

**Activity (1 min, Group):**
What is the true error in integrating $y = \text{constant}$ on the interval [a, b] using the Trapezoidal rule.

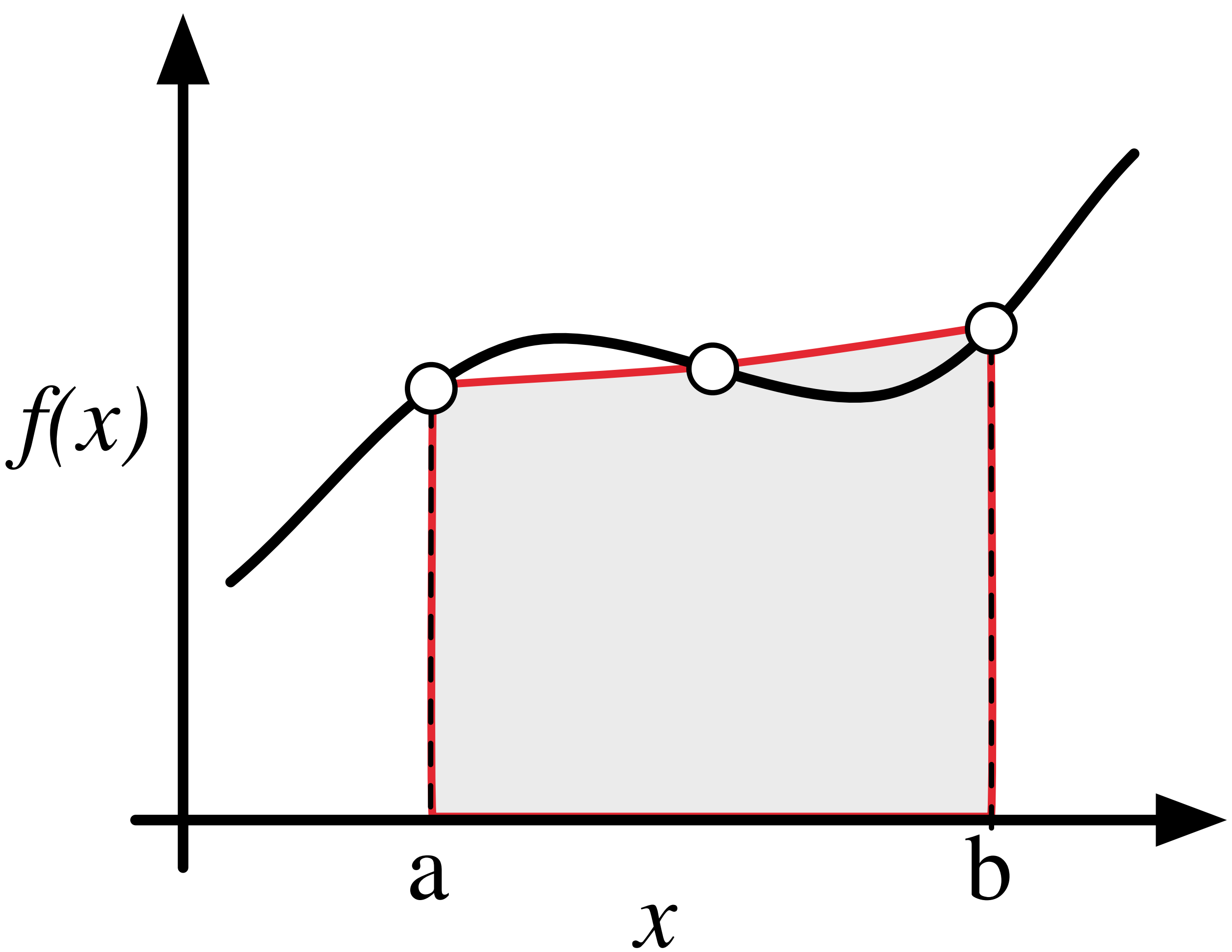
The error is zero because the trapezoidal rule is exact for a constant function. A constant function is simply a straight line with zero slope.

# Simpson's 1/3 Rule

<u>Concept</u>: Approximate $f(x)$ as a ***quadratic*** on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \frac{\Delta x}{3}\left[f(a) + 4f\left(\tfrac{a+b}{2}\right) + f(b)\right]$$

$$\Delta x = \frac{b-a}{2}$$




Requires **three** equally spaced points on interval $[a,b]$.

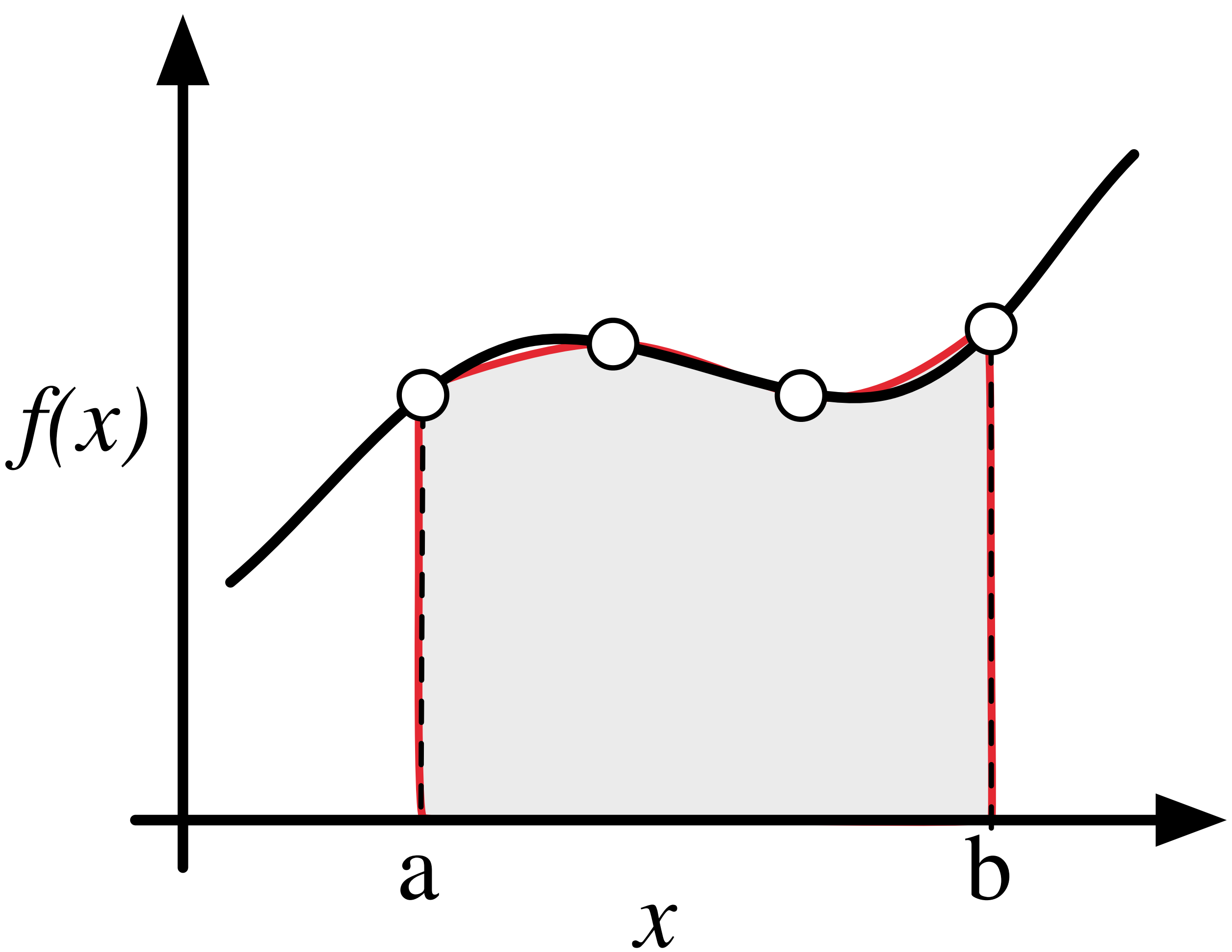
**Activity (1 min, Individual):**
What is the error in integrating $y = \alpha x^2 + \beta x + \gamma$ on the interval [a, b] using Simpson's 1/3 rule?

# Simpson's 3/8 Rule

Concept: Approximate $f(x)$ as a ***cubic*** on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \frac{3\Delta x}{8}\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right)$$

$$\Delta x = \frac{b-a}{3} \qquad x_i = a + i\Delta x$$



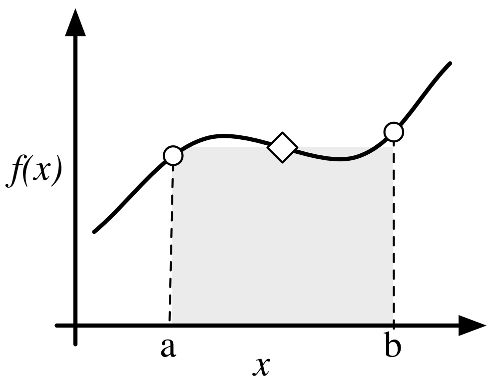

Requires **four** equally spaced points on interval $[a,b]$.

**Activity (1 min, Individual):**
What is the error in integrating $y = \alpha x^3 + \beta x^2 + \gamma x + \delta$ on the interval [a, b] using Simpson's 3/8 rule?

# Midpoint Rule

<u>Concept</u>: Approximate $f(x)$ as a *constant* on the interval $[a,b]$.

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

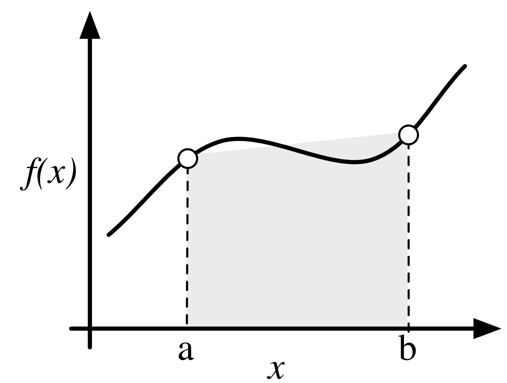



- Requires function value at the midpoint (can be a problem for tabular/discrete data).

# Trapezoid Rule

<u>Concept</u>: Approximate $f(x)$ as a *linear* function on the interval $[a,b]$.

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

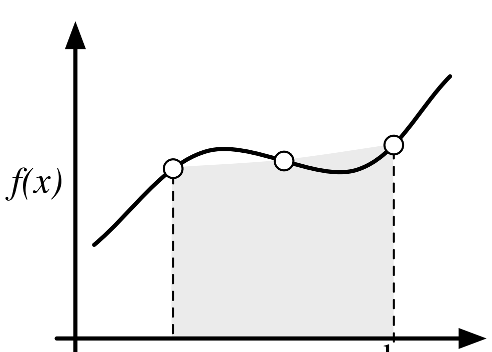



- Convenient form for tabular (discrete) data.
- Doesn't require equally spaced data.
- $\Delta x = b-a$

# Simpson's 1/3 Rule

<u>Concept</u>: Approximate $f(x)$ as a *quadratic* on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \frac{\Delta x}{3}\left[f(a) + 4f\left(\tfrac{a+b}{2}\right) + f(b)\right]$$

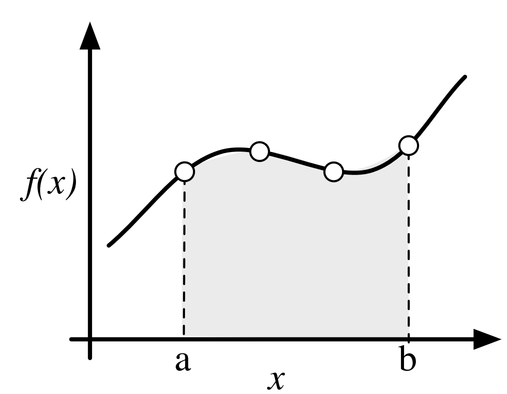



- Requires three equally spaced points on interval $[a,b]$.
- $\Delta x = (b-a)/2$

# Simpson's 3/8 Rule

<u>Concept</u>: Approximate $f(x)$ as a *cubic* on the interval $[a,b]$.

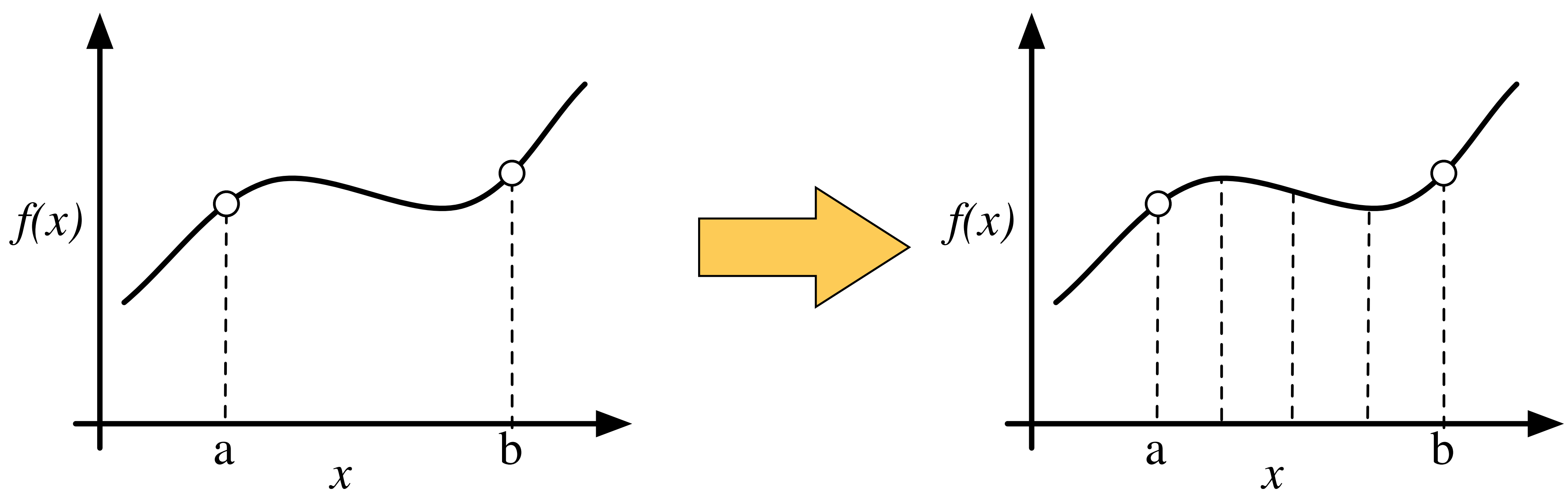
$$\int_a^b f(x)\mathrm{d}x \approx \frac{3\Delta x}{8}\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right)$$




- Requires four equally spaced points on interval $[a,b]$.
- $\Delta x = (b-a)/3$
- $x_i = a + i\Delta x$

We can apply these concepts to either tabulated data or complex functions

can be applied to as many subintervals as available/necessary



**Trapezoid Rule** $\int_a^b f(x)\mathrm{d}x \approx \frac{(b-a)}{2}[f(a)+f(b)]$

**Simpson's 1/3 Rule** $\int_a^b f(x)\mathrm{d}x \approx \frac{\Delta x}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$

**Simpson's 3/8 Rule** $\int_a^b f(x)\mathrm{d}x \approx \frac{3\Delta x}{8}\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right)$

**Activity (1 min, Individual):**
Which of the three Simpon's rules can be easily applied to discrete data?

## Trapezoidal Rule

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

**Coding Activity 4 (3 min, Group):**

Develop a Python routine that computes the integral of a function using the Trapezoidal rule for an arbitrary number of segments $n$, and use it to calculate $\int_0^1 [1 + 0.5\sin^2(1.75\pi x)]\mathrm{d}x$

Trapezoidal Rule

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

**<u>Coding Activity 5 (3 min, Group):</u>**
Using the Trapezoidal rule, develop a Python routine that computes the integral of discrete data $(x_i, y_i)$. Test your routine on the World Emissions of CO2.

# Error Bounds

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

n = Number of segments

$|f''(x)| \leq K \quad |f''''(x)| \leq M$ on [a,b]

| Midpoint | Trapezoid | Simpson's 1/3 |
|---|---|---|
| $E_M \leq K\dfrac{(b-a)^3}{24n^2}$ | $E_T \leq K\dfrac{(b-a)^3}{12n^2}$ | $E_S \leq M\dfrac{(b-a)^5}{18n^4}$ |

**Note, these are only UPPER bounds. The actual error may be much smaller depending on the function.**