Computational Physics Lab

Introduction to Numerical Integration

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Integration

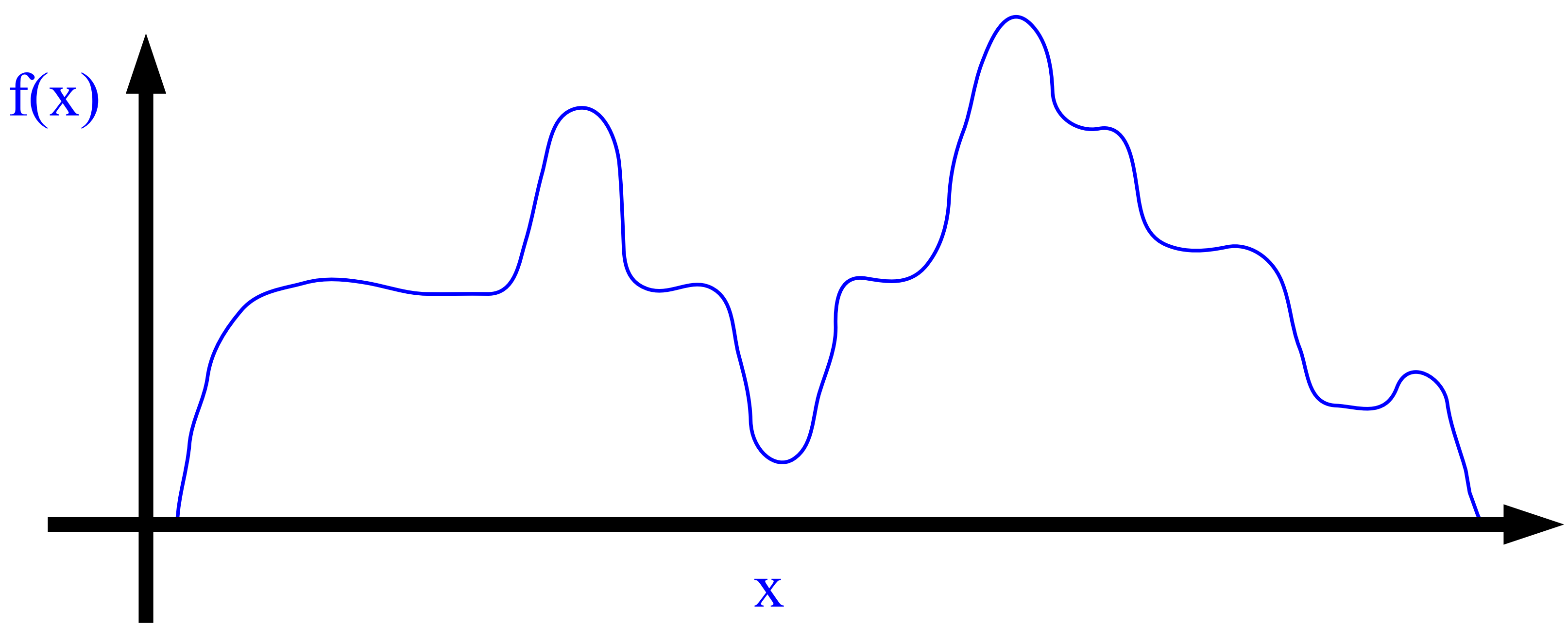
READ the discussion in

Chapters 5

Sections: 1 - 3

Numerical Integration

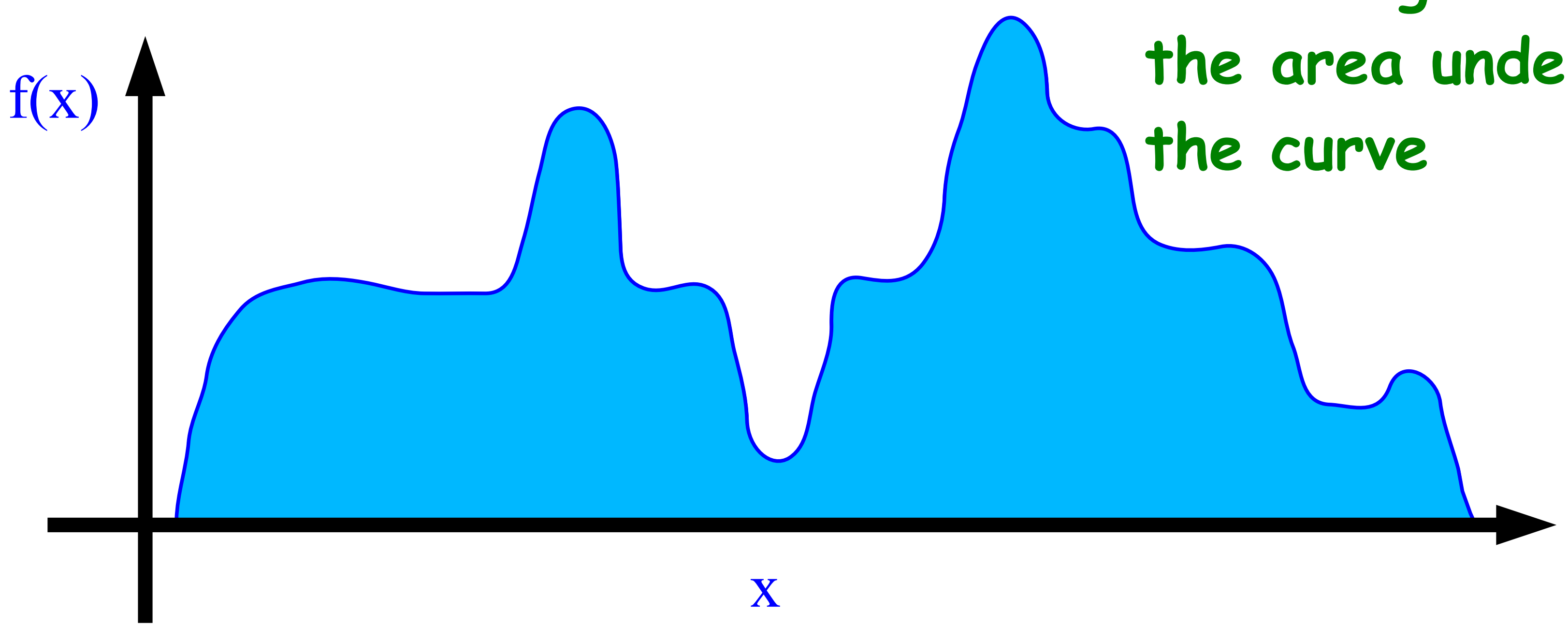
For a given function f(x) the solution can exist in an exact analytical form but frequently an analytical solution does not exist and it is therefor necessary to solve the integral numerically



Numerical Integration

For a given function f(x) the solution can exist in an exact analytical form but frequently an analytical solution does not exist and it is therefor necessary to solve the integral numerically

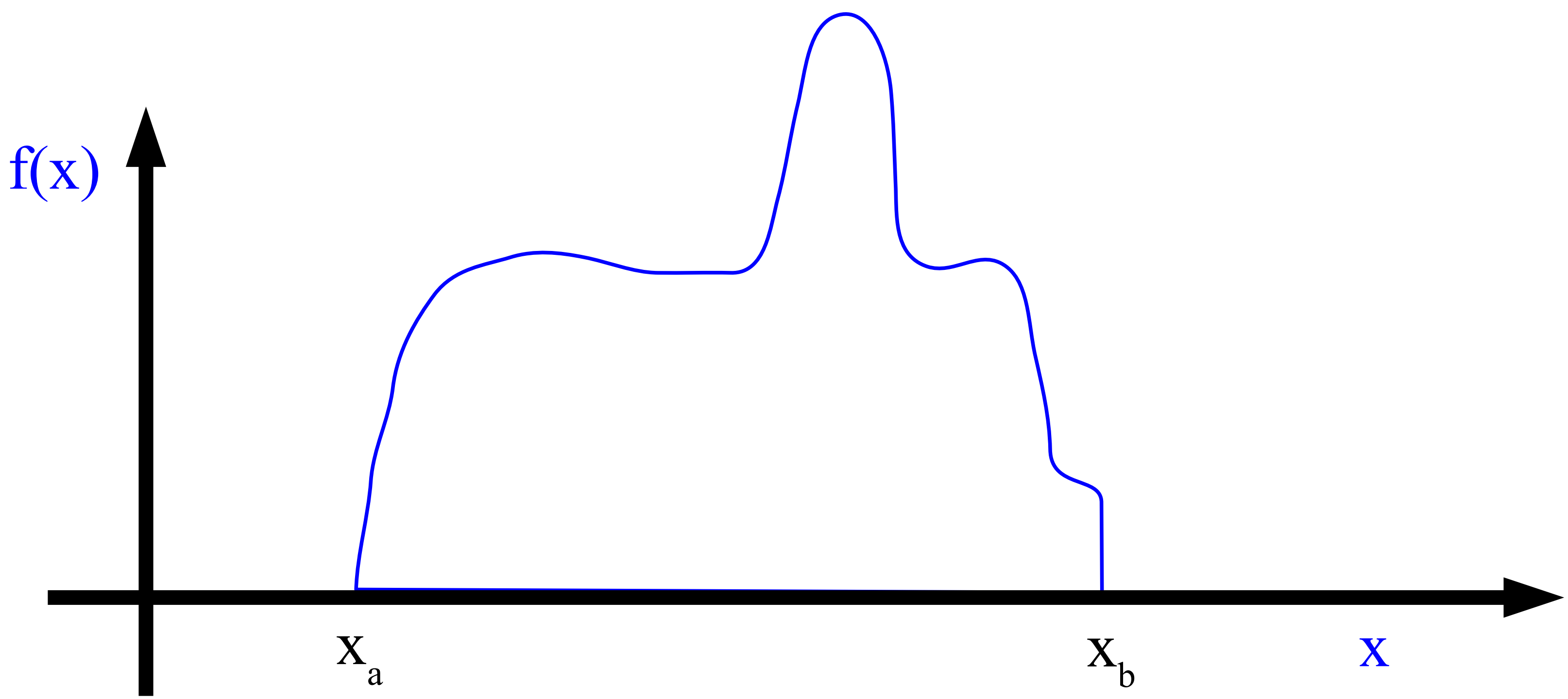
The integral is just the area under the curve



Calculate Area to Calculate Integral

Newton-Cotes Method of Order Zero [Rectangle Midpoint Rule]

- approximate f(x) as a constant
  - $f(x) \approx f(x = x_{midpoint})$
- area = $f(x_{mid}) * w$



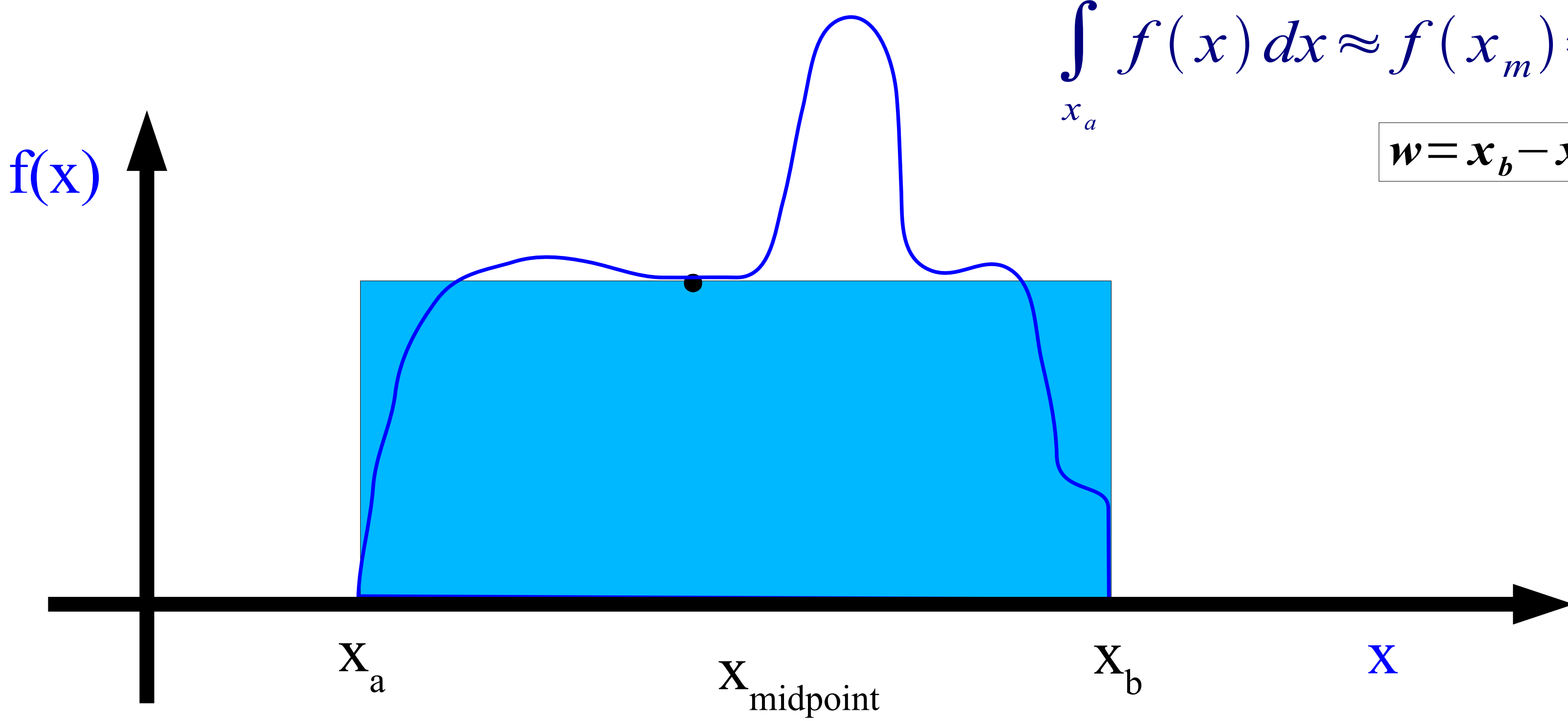
Calculate Area to Calculate Integral

Newton-Cotes Method of Order Zero [Rectangle Midpoint Rule]

- approximate f(x) as a constant
  - $f(x) \approx f(x = x_{midpoint})$
- area = $f(x_{mid}) * w$

$$\int_{x_a}^{x_b} f(x)\,dx \approx f(x_m) * w$$

$$w = x_b - x_a$$



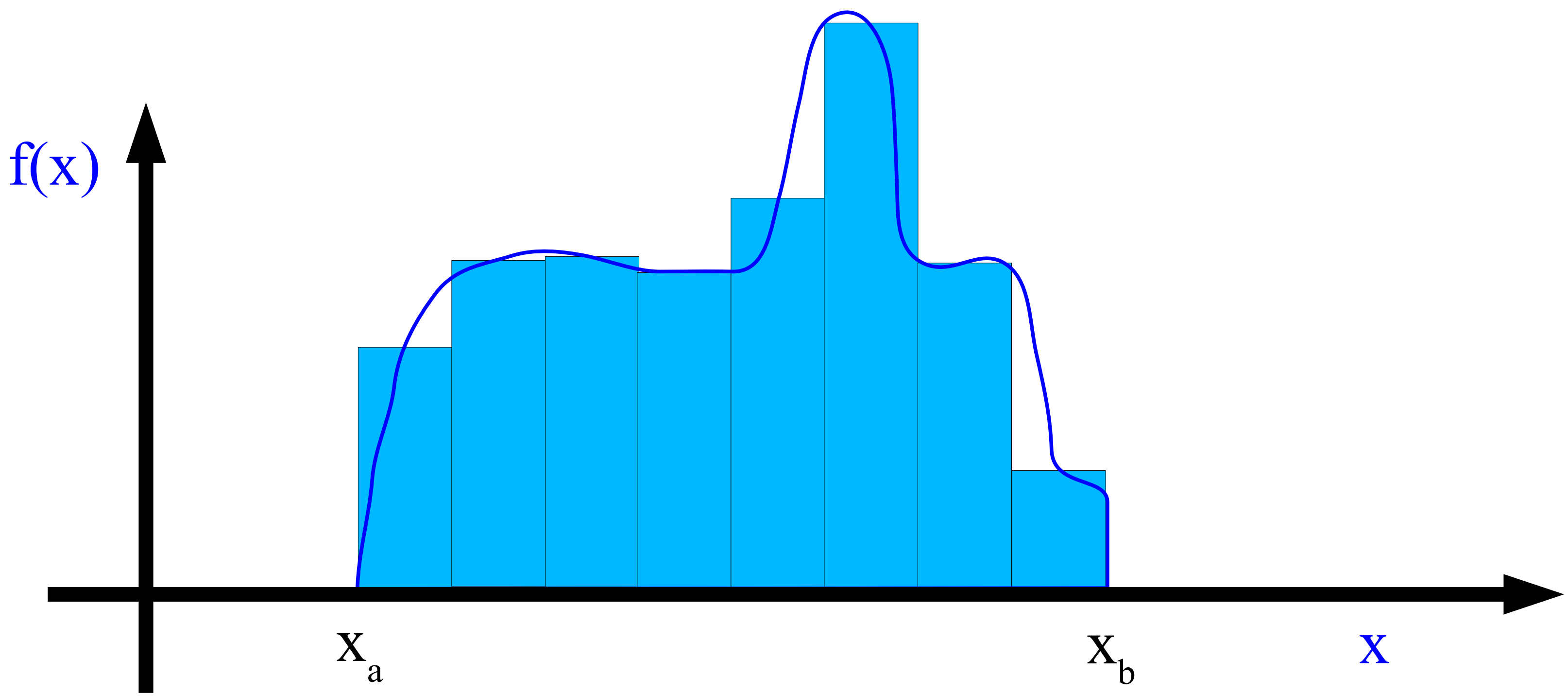
Composite Midpoint Method

- break up interval into small pieces
- approximate interval area via rectangle
  - area = $f(x_{mid}) * w$
- add up all of the areas

Composite Midpoint Method

$$\int_{x_a}^{x_b} f(x)\,dx \approx \sum_{i=0}^{n-1} f(x_a+(i+1/2)w)*w$$

$$w=(x_b-x_a)/n$$

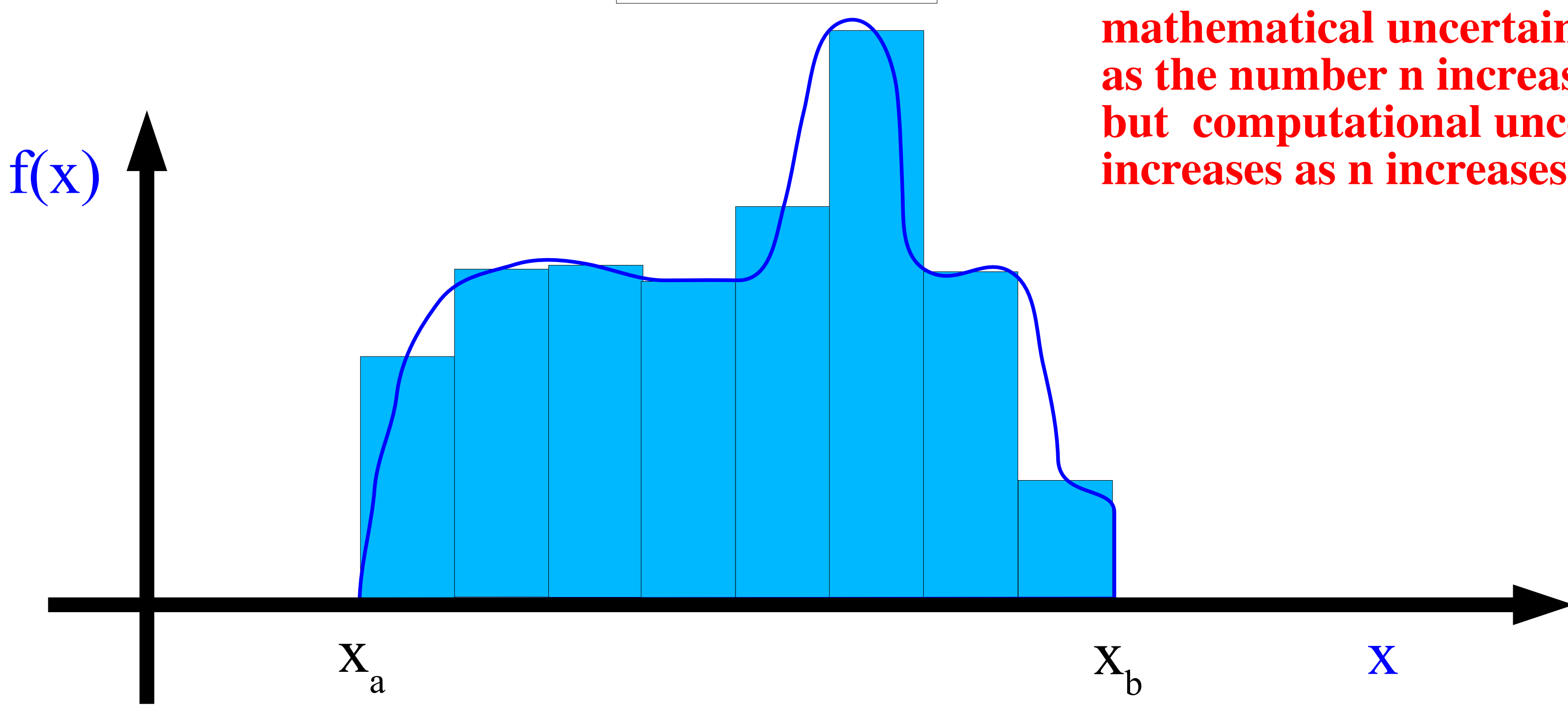


Composite Midpoint Method

$$\int_{x_a}^{x_b} f(x)\,dx \approx \sum_{i=0}^{n-1} f(x_a+(i+1/2)w) * w$$

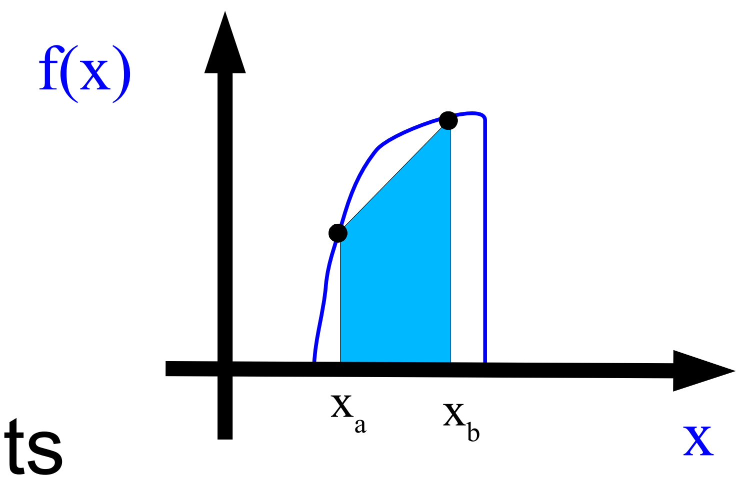
$$\boldsymbol{w=(x_b-x_a)/n}$$

mathematical uncertainty decreases as the number n increases, but computational uncertainty increases as n increases!



Trapezoidal Method

- **Trapezoidal Rule**
  - linear f(x) approximation
  - uses both a start & end points
  - area = $[(f(x_1)+f(x_2))/2\ ]*w$



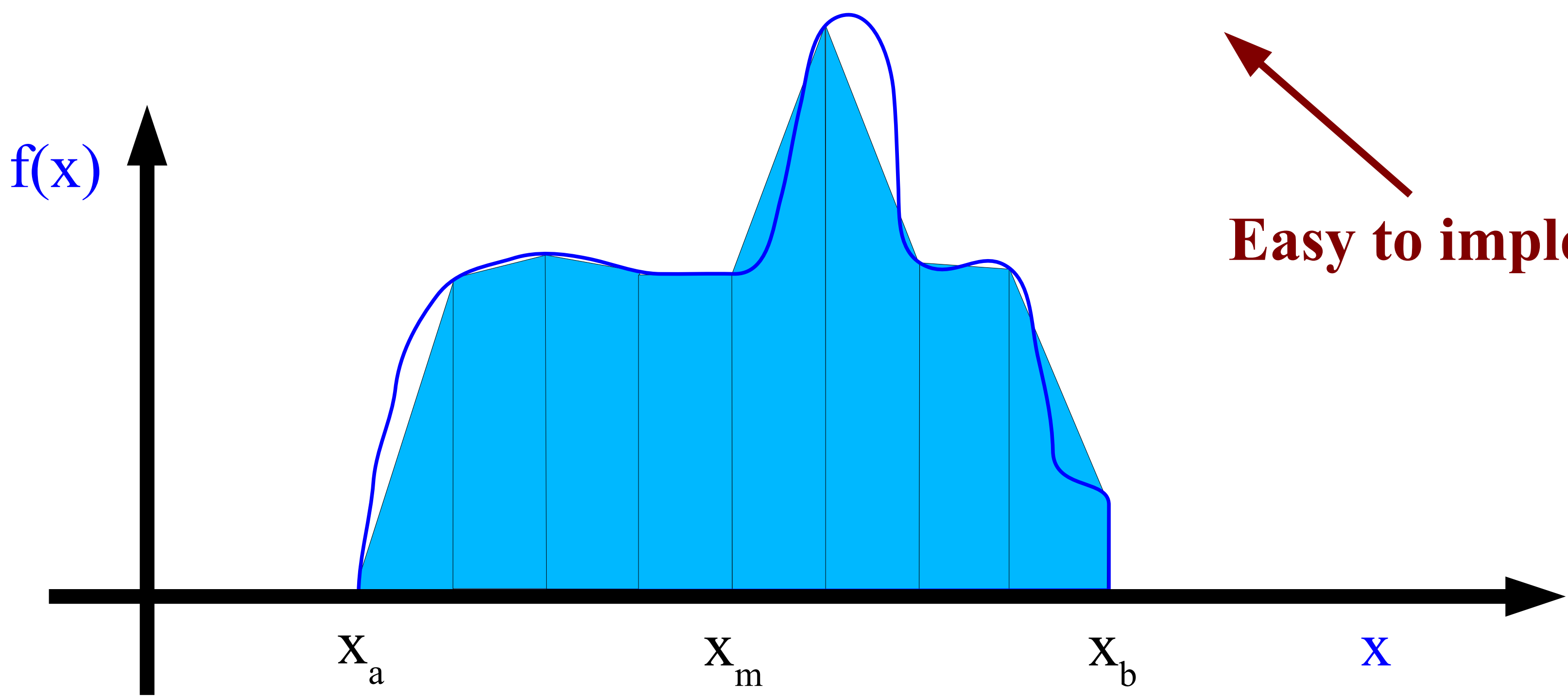
Composite Trapezoidal Method

$$\int_{x_a}^{x_b} f(x)\,dx = \frac{w}{2}\sum_{i=1}^{N}\left[f(x_a+(i-1)w)+f(x_a+iw)\right] + O(w^2)$$

- accurate to O(w)
- has error $O(w^2)$

$$\int_{x_a}^{x_b} f(x)\,dx \approx \frac{w}{2}*\left(f(x_a)+f(x_b)+2\sum_{i=1}^{N-1}\left[f(x_a+i\,w)\right]\right)$$

Easy to implement!



$$w=(x_b-x_a)/N$$

Error on Integration

$$\int_{x_a}^{x_b} f(x)\,dx = \frac{w}{2}\sum_{i=1}^{N}\left[f(x_a+(i-1)w)+f(x_a+iw)\right] + O(w^2)$$

$$\epsilon = \frac{1}{12}w^2\left[f'(x_a)-f'(x_b)\right]$$

Euler-Maclaurin formula for the error on the trapezoidal rule

Practical Estimation of Errors

$$\int_{x_a}^{x_b} f(x)\,dx = I = I_{N_1} + \epsilon_1$$

with $\epsilon_k = c\,w_k^2$

$$= I_{N_2} + c\,w_2^2$$

$$I_{N_2} - I_{N_1} = -3c\,w_2^2$$

increasing $N \to 2N, \quad w_1 = 2w_2$

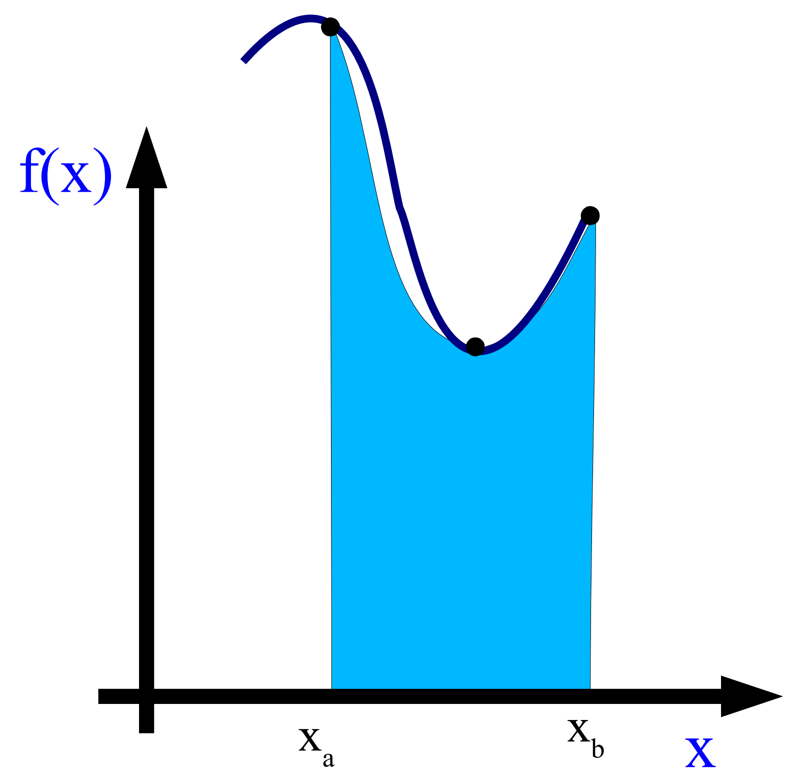
$$\epsilon_2 = \frac{1}{3}\left|I_{N_2} - I_{N_1}\right|$$

error on 2nd integration

3-Point Simpson Method

- **3-Point Simpson Rule**
  - quadratic f(x) approximation
  - uses both a start, mid & end points
  - area

$$A = \frac{w}{6}\left[f(x_a) + 4 f(x_{mid}) + f(x_b) \right]$$

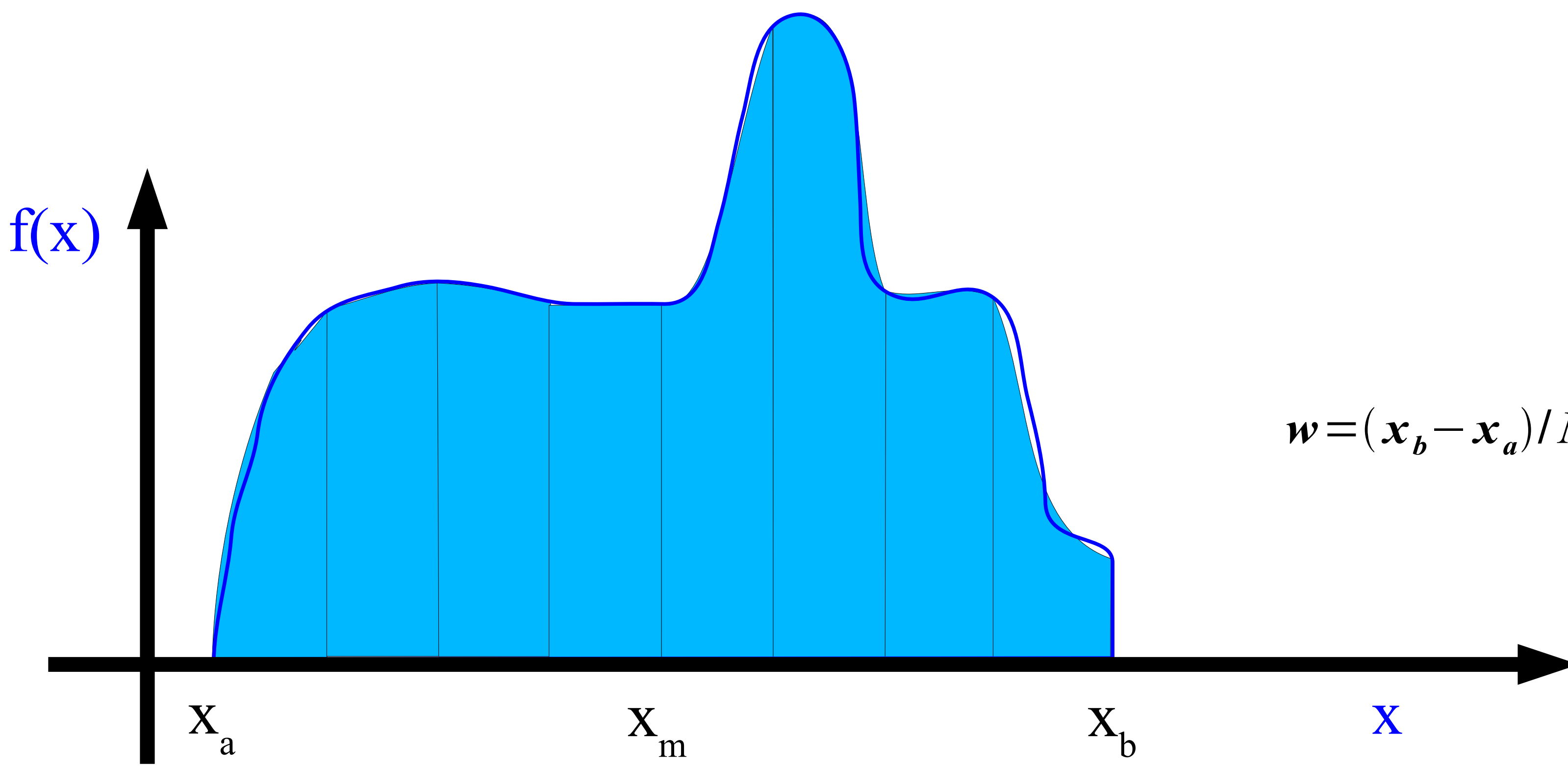


Composite 3-Point Simpson Method

$$\int_{x_a}^{x_b} f(x)\,dx = \frac{w}{6}\sum_{i=0}^{N-1}\left[f(x_a+iw)+4f(x_a+w(i+1/2))+f(x_a+(i+1)w)\right] + O(w^4)$$

- accurate to $O(w^3)$
- has error $O(w^4)$

$$I_N = \frac{w}{6}\left[f(x_a)+f(x_b)+2\sum_{i=1}^{N-1} f(x_a+iw)+4\sum_{i=0}^{N-1} f(x_a+w(i+1/2))\right]$$



$$\boldsymbol{w=(x_b-x_a)/N}$$

Error on Simpson's rule

$$\int_{x_a}^{x_b} f(x)\,dx = I = I_N + O(w^4)$$

$$\epsilon = \frac{1}{90} w^4 [f'''(x_a) - f'''(x_b)]$$

error on the Simpson's rule integration

Practical Estimation of Errors

$$\int_{x_a}^{x_b} f(x)\,dx = I = I_{N_1} + \epsilon_1$$

with $\epsilon_k = c\, w_k^4$

$$= I_{N_2} + c\, w_2^4$$

$$I_{N_2} - I_{N_1} = -15\, c\, w_2^4$$ *increasing* $N \to 2N$, $w_1 = 2 w_2$

$$\epsilon_2 = \frac{1}{15} |I_{N_2} - I_{N_1}|$$

error on 2nd integration

Let's get working on Exercise 5