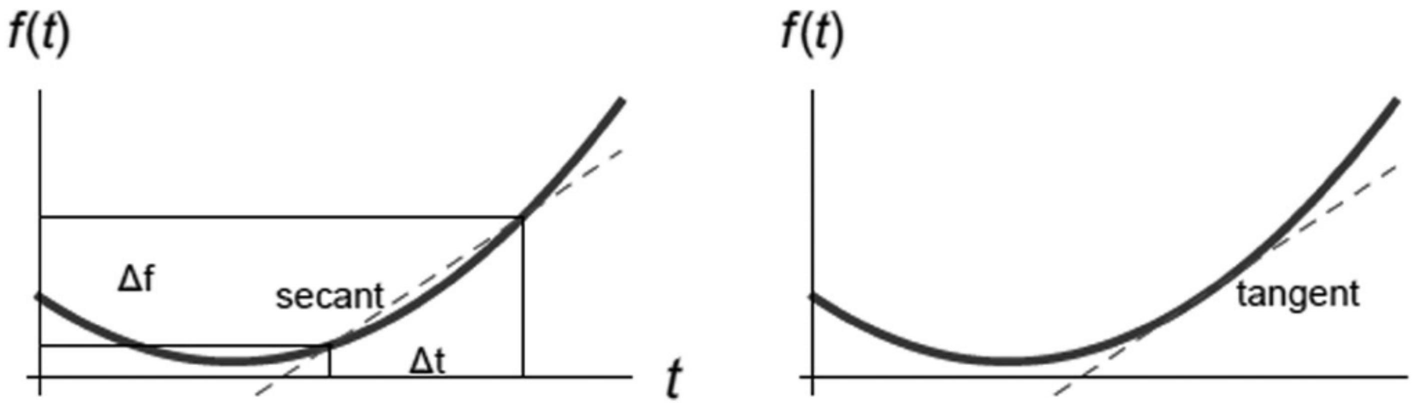
# 4 Calculus

Given the function $f(x)$, compute $d^n f/dx^n$ at given $x$

Compute $\int_a^b f(x)\,dx$, where $f(x)$ is a given function

## 4.1 Derivatives

- In mathematics, the rate of change of a function is referred to as the ***derivative***.
- For a function of a single variable, the derivative at a given point is the ***slope of the tangent***




**Centered difference form**

$$\frac{df}{dt} = \lim_{\Delta t \to 0}\left(\frac{f\left(t + \Delta t/2\right) - f\left(t - \Delta t/2\right)}{\Delta t}\right)$$

$$\frac{df}{dt} = \text{derivative of } f(t) \text{ with respect to } t = \lim_{\Delta t \to 0}\left(\frac{f\left(t + \Delta t\right) - f\left(t\right)}{\Delta t}\right)$$

**Forward difference form**

$$= \lim_{\Delta t \to 0}\left(\frac{f\left(t\right) - f\left(t - \Delta t\right)}{\Delta t}\right)$$

**Backward difference form**

# 4.1 Derivatives

$$v = \frac{dx}{dt} = \lim_{\Delta t \to 0}\left(\frac{x(t+\Delta t) - x(t)}{\Delta t}\right)$$

where

$v$ is velocity
$x$ is position
$t$ is time

**Velocity from Displacement**

$$\frac{d}{dt}\left(f\left(z\left(t\right)\right)\right) = \frac{df}{dz}\cdot\frac{dz}{dt}$$

**Chain rule**

$$\frac{d(f \cdot g)}{dt} = f\frac{dg}{dt} + g\frac{df}{dt}$$

**Product rule**

$$\frac{d\left(t^n\right)}{dt} = n \cdot t^{n-1}$$

**Derivative of $t^n$**

**Partial Derivatives**

$$z = f(x, y)$$

$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0}\left(\frac{f(x+\Delta x, y) - f(x, y)}{\Delta x}\right)$$

$$\frac{\partial f}{\partial y} = \lim_{\Delta y \to 0}\left(\frac{f(x, y+\Delta y) - f(x, y)}{\Delta y}\right)$$

## 4.2 Numerical Differentiation

- The derivation of the finite difference approximations for the derivatives of $f(x)$ are based on forward and backward Taylor series expansions of $f(x)$ about $x$, such as

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

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

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

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

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{12}f^{(4)}(x) + \cdots \qquad \text{(e)}$$

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \ldots \qquad \text{(f)}$$

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

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

- Equations (a)–(h) can be viewed as simultaneous equations that can be solved for various derivatives of $f(x)$.

# 4.2 Numerical Differentiation

## Coefficients of central finite difference approximations of $O(h^2)$

| | $f(x-2h)$ | $f(x-h)$ | $f(x)$ | $f(x+h)$ | $f(x+2h)$ |
|---|---|---|---|---|---|
| $2hf'(x)$ | | $-1$ | $0$ | $1$ | |
| $h^2f''(x)$ | | $1$ | $-2$ | $1$ | |
| $2h^3f'''(x)$ | $-1$ | $2$ | $0$ | $-2$ | $1$ |
| $h^4f^{(4)}(x)$ | $1$ | $-4$ | $6$ | $-4$ | $1$ |

## Coefficients of forward finite difference approximations of $O(h)$

| | $f(x)$ | $f(x+h)$ | $f(x+2h)$ | $f(x+3h)$ | $f(x+4h)$ |
|---|---|---|---|---|---|
| $hf'(x)$ | $-1$ | $1$ | | | |
| $h^2f''(x)$ | $1$ | $-2$ | $1$ | | |
| $h^3f'''(x)$ | $-1$ | $3$ | $-3$ | $1$ | |
| $h^4f^{(4)}(x)$ | $1$ | $-4$ | $6$ | $-4$ | $1$ |

## Coefficients of backward finite difference approximations of $O(h)$

| | $f(x-4h)$ | $f(x-3h)$ | $f(x-2h)$ | $f(x-h)$ | $f(x)$ |
|---|---|---|---|---|---|
| $hf'(x)$ | | | | $-1$ | $1$ |
| $h^2f''(x)$ | | | $1$ | $-2$ | $1$ |
| $h^3f'''(x)$ | | $-1$ | $3$ | $-3$ | $1$ |
| $h^4f^{(4)}(x)$ | $1$ | $-4$ | $6$ | $-4$ | $1$ |

Truncation error is now $O(h)$, which is not as good as the $O(h^2)$ error in central difference approximations.

# 4.2 Numerical Differentiation

## Coefficients of central finite difference approximations of $O(h^2)$

| | $f(x-2h)$ | $f(x-h)$ | $f(x)$ | $f(x+h)$ | $f(x+2h)$ |
|---|---|---|---|---|---|
| $2hf'(x)$ | | $-1$ | $0$ | $1$ | |
| $h^2 f''(x)$ | | $1$ | $-2$ | $1$ | |
| $2h^3 f'''(x)$ | $-1$ | $2$ | $0$ | $-2$ | $1$ |
| $h^4 f^{(4)}(x)$ | $1$ | $-4$ | $6$ | $-4$ | $1$ |

## Coefficients of forward finite difference approximations of $O(h^2)$

| | $f(x)$ | $f(x+h)$ | $f(x+2h)$ | $f(x+3h)$ | $f(x+4h)$ | $f(x+5h)$ |
|---|---|---|---|---|---|---|
| $2hf'(x)$ | $-3$ | $4$ | $-1$ | | | |
| $h^2 f''(x)$ | $2$ | $-5$ | $4$ | $-1$ | | |
| $2h^3 f'''(x)$ | $-5$ | $18$ | $-24$ | $14$ | $-3$ | |
| $h^4 f^{(4)}(x)$ | $3$ | $-14$ | $26$ | $-24$ | $11$ | $-2$ |

## Coefficients of backward finite difference approximations of $O(h^2)$

| | $f(x-5h)$ | $f(x-4h)$ | $f(x-3h)$ | $f(x-2h)$ | $f(x-h)$ | $f(x)$ |
|---|---|---|---|---|---|---|
| $2hf'(x)$ | | | | $1$ | $-4$ | $3$ |
| $h^2 f''(x)$ | | | $-1$ | $4$ | $-5$ | $2$ |
| $2h^3 f'''(x)$ | | $3$ | $-14$ | $24$ | $-18$ | $5$ |
| $h^4 f^{(4)}(x)$ | $-2$ | $11$ | $-24$ | $26$ | $-14$ | $3$ |

**Noncentral Finite Difference Approximations result in** $O(h^2)$ error.

## 4.2 Numerical Differentiation: Example

|  | $f(x-2h)$ | $f(x-h)$ | $f(x)$ | $f(x+h)$ | $f(x+2h)$ |
|---|---|---|---|---|---|
| $2hf'(x)$ |  | $-1$ | $0$ | $1$ |  |
| $h^2 f''(x)$ |  | $1$ | $-2$ | $1$ |  |
| $2h^3 f'''(x)$ | $-1$ | $2$ | $0$ | $-2$ | $1$ |
| $h^4 f^{(4)}(x)$ | $1$ | $-4$ | $6$ | $-4$ | $1$ |

Given the evenly spaced data points

| $x$ | 0 | 0.1 | 0.2 | 0.3 | 0.4 |
|---|---|---|---|---|---|
| $f(x)$ | 0.0000 | 0.0819 | 0.1341 | 0.1646 | 0.1797 |

compute $f'(x)$ and $f''(x)$ at $x = 0$ and 0.2 using finite difference approximations of $\mathcal{O}(h^2)$.

|  | $f(x)$ | $f(x+h)$ | $f(x+2h)$ | $f(x+3h)$ | $f(x+4h)$ | $f(x+5h)$ |
|---|---|---|---|---|---|---|
| $2hf'(x)$ | $-3$ | $4$ | $-1$ |  |  |  |
| $h^2 f''(x)$ | $2$ | $-5$ | $4$ | $-1$ |  |  |
| $2h^3 f'''(x)$ | $-5$ | $18$ | $-24$ | $14$ | $-3$ |  |
| $h^4 f^{(4)}(x)$ | $3$ | $-14$ | $26$ | $-24$ | $11$ | $-2$ |

**Solution** From the forward difference formulas in Table 5.3a, we get

$$f'(0) = \frac{-3f(0) + 4f(0.1) - f(0.2)}{2(0.1)} = \frac{-3(0) + 4(0.0819) - 0.1341}{0.2} = 0.967$$

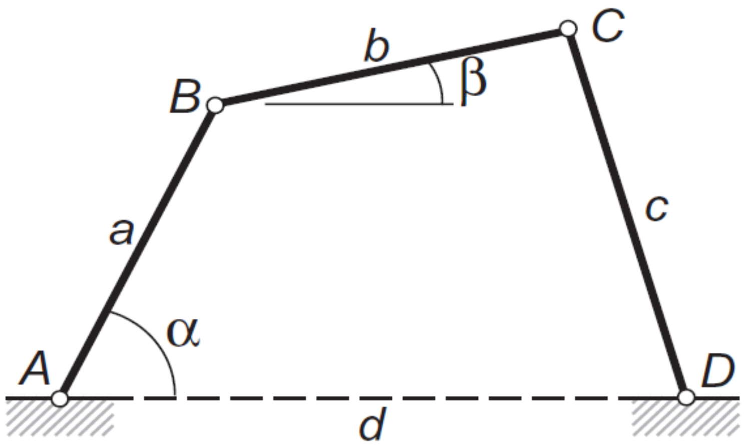
$$f''(0) = \frac{2f(0) - 5f(0.1) + 4f(0.2) - f(0.3)}{(0.1)^2}$$
$$= \frac{2(0) - 5(0.0819) + 4(0.1341) - 0.1646}{(0.1)^2} = -3.77$$

The central difference approximations in Table 5.1 yield

$$f'(0.2) = \frac{-f(0.1) + f(0.3)}{2(0.1)} = \frac{-0.0819 + 0.1646}{0.2} = 0.4135$$

$$f''(0.2) = \frac{f(0.1) - 2f(0.2) + f(0.3)}{(0.1)^2} = \frac{0.0819 - 2(0.1341) + 0.1646}{(0.1)^2} = -2.17$$

# 4.2 Numerical Differentiation: Example




The linkage shown has the dimensions $a = 100$ mm, $b = 120$ mm, $c = 150$ mm, and $d = 180$ mm. It can be shown by geometry that the relationship between the angles $\alpha$ and $\beta$ is

$$(d - a\cos\alpha - b\cos\beta)^2 + (a\sin\alpha + b\sin\beta)^2 - c^2 = 0$$

For a given value of $\alpha$, we can solve this transcendental equation for $\beta$ by one of the root-finding methods

| $\alpha$ (deg) | 0 | 5 | 10 | 15 | 20 | 25 | 30 |
|---|---|---|---|---|---|---|---|
| $\beta$ (rad) | 1.6595 | 1.5434 | 1.4186 | 1.2925 | 1.1712 | 1.0585 | 0.9561 |

If link $AB$ rotates with the constant angular velocity of 25 rad/s, use finite difference approximations of $\mathcal{O}(h^2)$ to tabulate the angular velocity $d\beta/dt$ of link $BC$ against $\alpha$.

## 4.2 Numerical Differentiation: Example

| | $f(x-2h)$ | $f(x-h)$ | $f(x)$ | $f(x+h)$ | $f(x+2h)$ |
|---|---|---|---|---|---|
| $2hf'(x)$ | | $-1$ | 0 | 1 | |
| $h^2 f''(x)$ | | 1 | $-2$ | 1 | |
| $2h^3 f'''(x)$ | $-1$ | 2 | 0 | $-2$ | 1 |
| $h^4 f^{(4)}(x)$ | 1 | $-4$ | 6 | $-4$ | 1 |

**Solution** The angular speed of $BC$ is

$$\frac{d\beta}{dt} = \frac{d\beta}{d\alpha}\frac{d\alpha}{dt} = 25\frac{d\beta}{d\alpha}\ \text{rad/s}$$

where $d\beta/d\alpha$ is computed from finite difference approximations using the data in the table. Forward and backward differences of $\mathcal{O}(h^2)$ are used at the endpoints, central differences elsewhere. Note that the increment of $\alpha$ is

| | $f(x)$ | $f(x+h)$ | $f(x+2h)$ | $f(x+3h)$ | $f(x+4h)$ | $f(x+5h)$ |
|---|---|---|---|---|---|---|
| $2hf'(x)$ | $-3$ | 4 | $-1$ | | | |
| $h^2 f''(x)$ | 2 | $-5$ | 4 | $-1$ | | |
| $2h^3 f'''(x)$ | $-5$ | 18 | $-24$ | 14 | $-3$ | |
| $h^4 f^{(4)}(x)$ | 3 | $-14$ | 26 | $-24$ | 11 | $-2$ |

$$h = (5\ \text{deg})\left(\frac{\pi}{180}\text{rad / deg}\right) = 0.087266\ \text{rad}$$

The computations yield

$$\dot\beta(0^\circ) = 25\frac{-3\beta(0^\circ) + 4\beta(5^\circ) - \beta(10^\circ)}{2h} = 25\frac{-3(1.6595) + 4(1.5434) - 1.4186}{2\,(0.087266)}$$

$$= -32.01\ \text{rad/s}$$

$$\dot\beta(5^\circ) = 25\frac{\beta(10^\circ) - \beta(0^\circ)}{2h} = 25\frac{1.4186 - 1.6595}{2(0.087266)} = -34.51\ \text{rad/s}$$

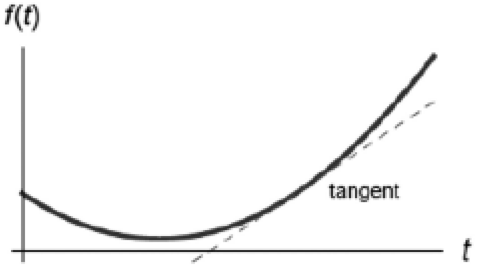
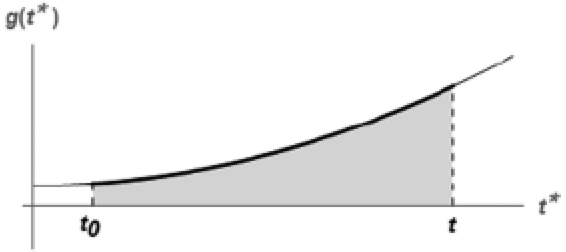
and so forth.

```
alpha=[0:5:30]'*pi/180
beta=[1.6595;1.5434;1.4186;1.2925;1.1712;1.0585;0.9561]
dbeta_dt=25*gradient(beta,alpha)
```

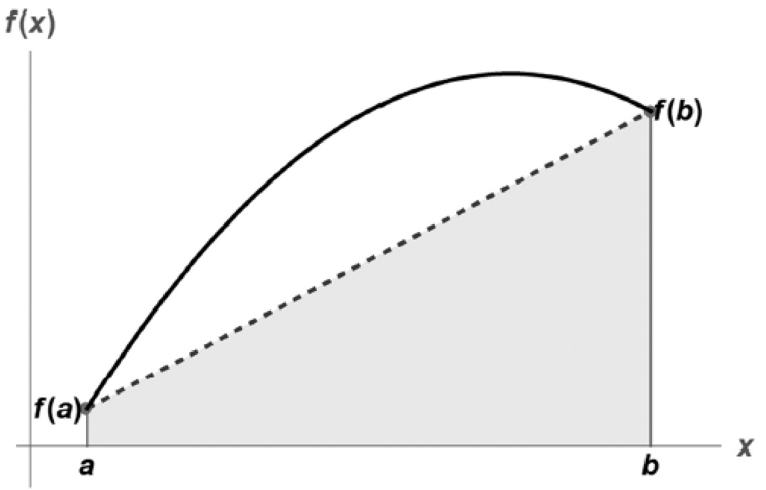
The complete set of results is

| $\alpha$ (deg) | 0 | 5 | 10 | 15 | 20 | 25 | 30 |
|---|---|---|---|---|---|---|---|
| $\dot\beta$ (rad/s) | $-32.01$ | $-34.51$ | $-35.94$ | $-35.44$ | $-33.52$ | $-30.81$ | $-27.86$ |

# 4.3 Integrals

| | Derivatives | Integrals |
|---|---|---|
| **Concept** | *Differentiation* is the process of finding $g(t)$ from $f(t)$. $$\overbrace{g(t)}^{?} = \frac{d\overbrace{f}^{\surd}}{dt}$$ | *Integration* is the process of finding the anti-derivative $f(t)$ from $g(t)$. $$\overbrace{g(t)}^{\surd} = \frac{d\overbrace{f}^{?}}{dt}$$ |
| **Numerical Approximation** | $$\frac{df}{dt} \cong \frac{f(t+\Delta t) - f(t)}{\Delta t}$$ | $$f(t) - f(t_1) \cong \sum_{i=1}^{n} g(t_i)\Delta t$$ $$t_i = t_1 + i\Delta t$$ |
| **Mathematical Definition** | $$g(t) = \frac{df}{dt}$$ $$= \lim_{\Delta t \to 0}\left(\frac{f(t+\Delta t) - f(t)}{\Delta t}\right)$$ | $$f(t) - f(t_0) = \int_{t^*=t_0}^{t} g(t^*)dt^*$$ $$= \lim_{\Delta t \to 0}\left(\sum_{i=1}^{n} g(t_i)\Delta t\right)$$ |
| **Geometric Interpretation** | $\frac{df}{dt}$ is the *slope* of the $f(t)$ curve.   | $\int_{t^*=t_0}^{t} g(t^*)dt^*$ is the *area* under the $g(t)$ curve.   |

# 4.6 Numerical Integration: Trapezoidal Rule



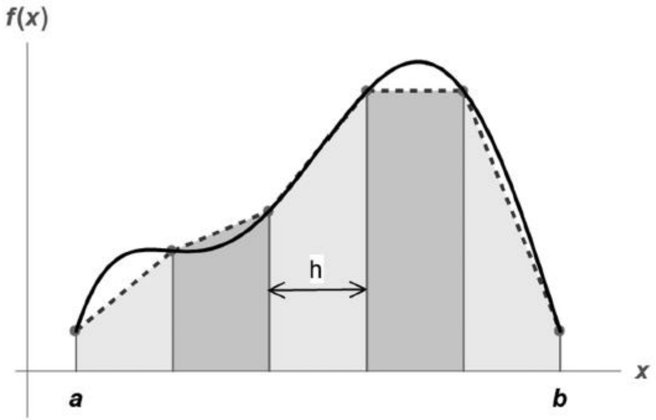

$$I = \int_{x=a}^{b} f(x)\,dx$$

- The *trapezoid rule* uses a linear interpolation to approximate *f*(*x*). An integral using the trapezoid rule approximation is shown in Figure

$$I = \int_a^b f(x)\,dx \cong \int_a^b \left( f(a) + \frac{f(b)-f(a)}{b-a}(x-a) \right) dx$$

$$I \cong (b-a)\left( \frac{f(a)+f(b)}{2} \right)$$

# 4.6 Numerical Integration: Trapezoidal Rule




$$I = \int_{x=a}^{b} f(x)\,dx$$

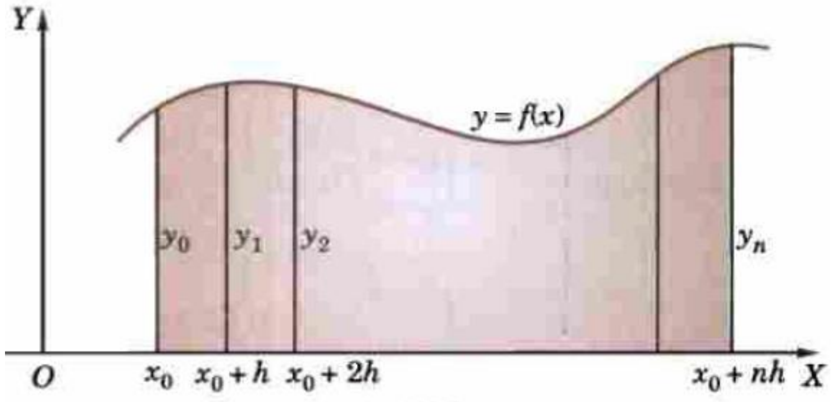
$$I = \int_{x=a}^{b} f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx$$

$$\cong h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2}$$

$$I \cong \frac{h}{2}\left(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right)$$

$$I = \underbrace{(b-a)}_{\text{width}} \underbrace{\frac{1}{2n}\left(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right)}_{\text{average height}}$$

$$E = -\frac{1}{12}(b-a)h^2\overline{f''}$$




$$\int_{x_0}^{x_0+nh} f(x)\,dx = \frac{h}{2}[(y_0 + y_n) + 2(y_1 + y_2 + \dots + y_{n-1})]$$

# 4.6 Numerical Integration: Trapezoidal Rule (Example)

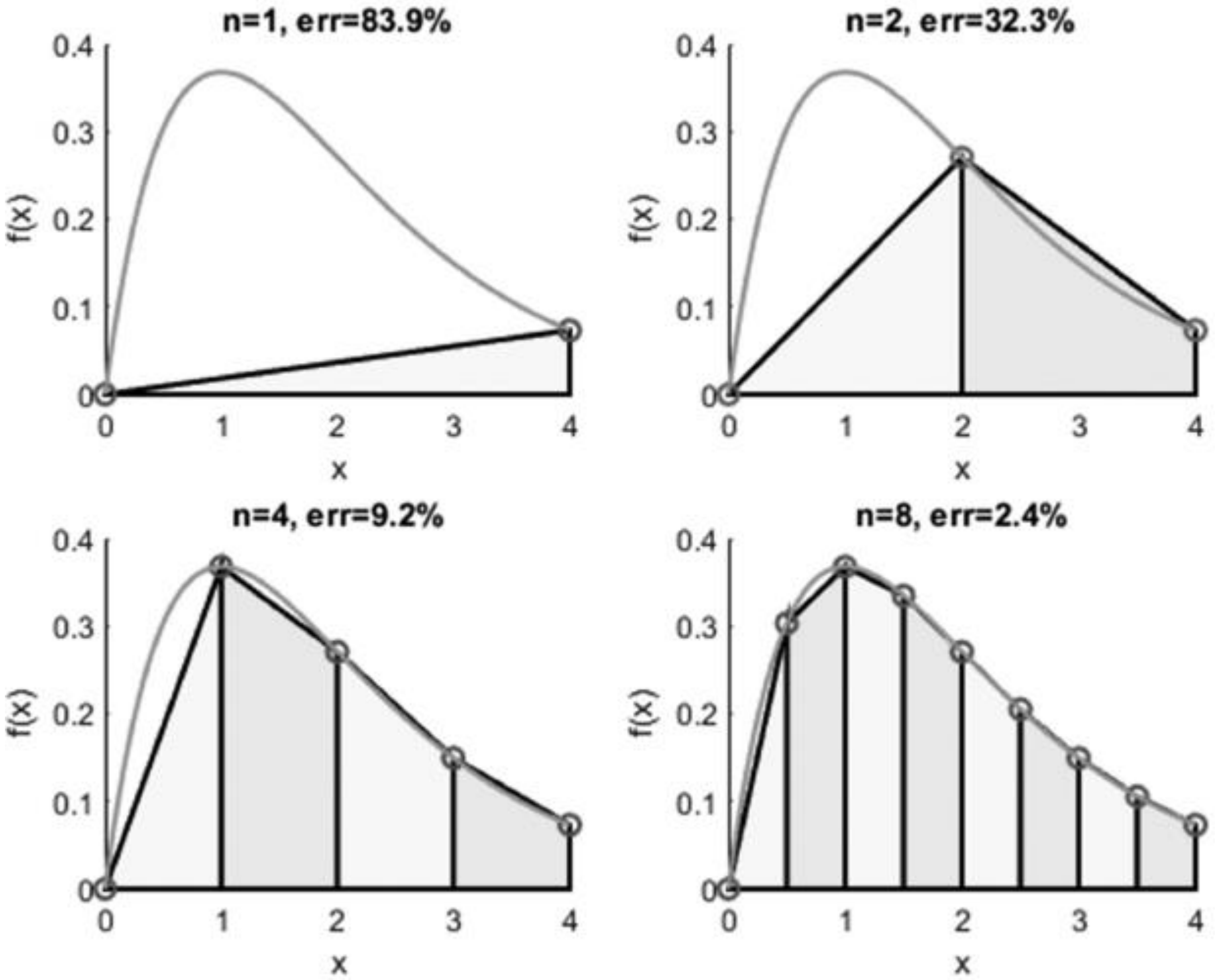
As an example, consider the integral

$$I = \int_{x=a}^{b} f(x)\,dx = \int_{x=a}^{b} xe^{-x}\,dx$$

In this case, the exact integral can be determined as

$$I_{\text{exact}} = \left(-xe^{-x} - e^{-x}\right)_{x=a}^{x=b} = \left(-be^{-b} - e^{-b}\right) - \left(-ae^{-a} - e^{-a}\right)$$

Choosing $a=0$ and $b=4$ gives $I_{\text{exact}}=0.9084$.



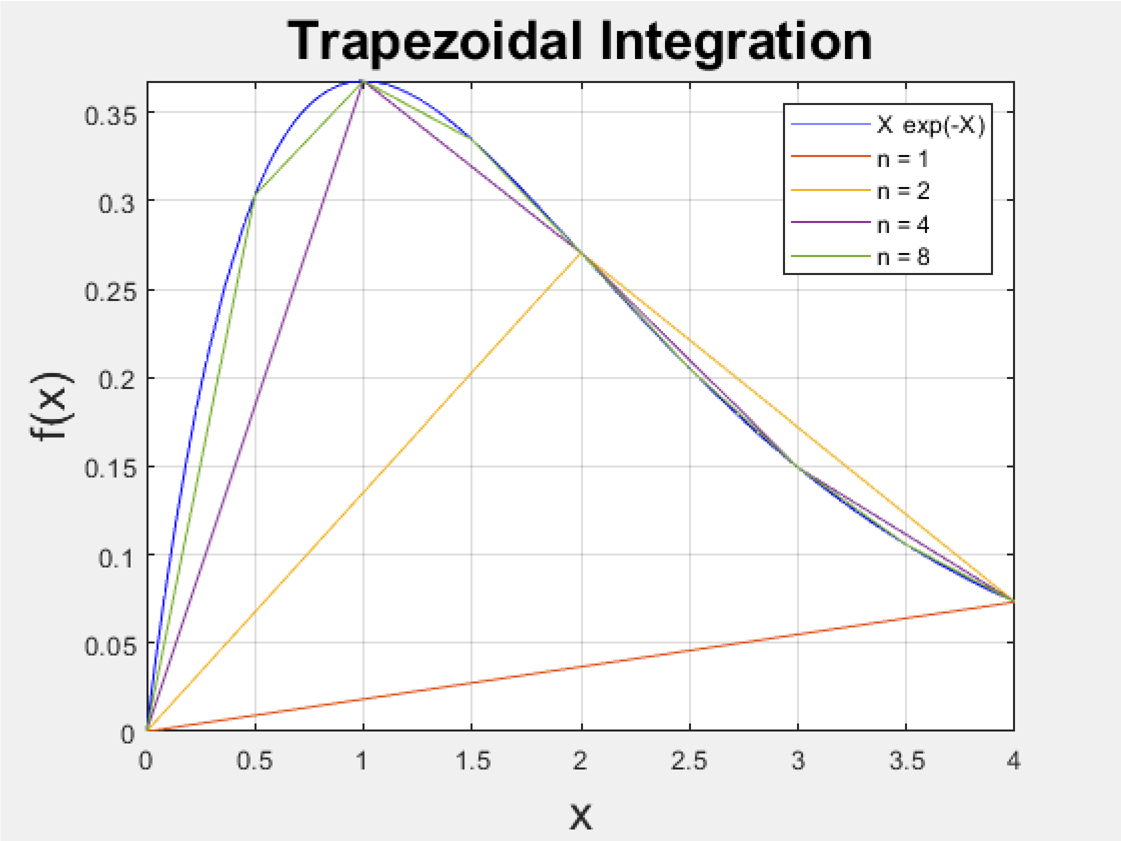
# 4.6 Numerical Integration: Trapezoidal Rule (Example)

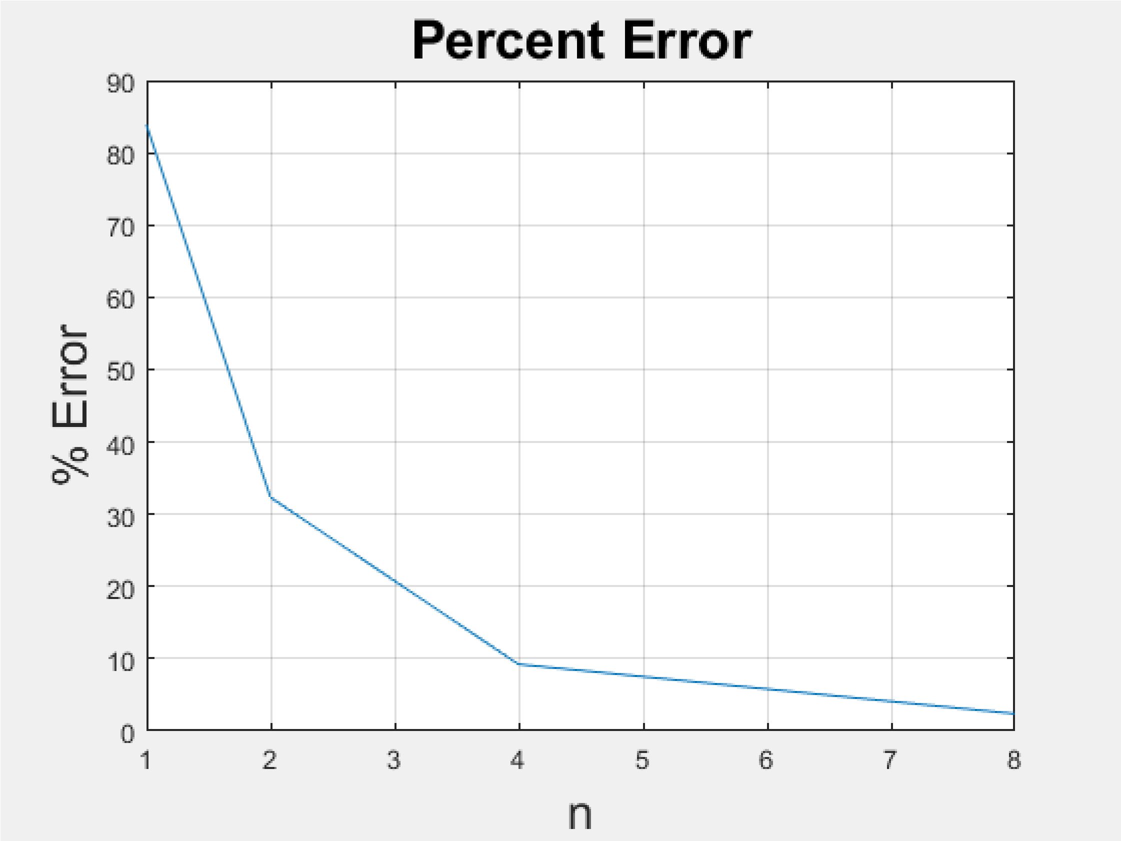
```
% House Keeping
clc
clear
clear all

% Exact Function
syms X
a=0
b=4
n=[1;2;4;8]
exact=vpa(int(X.*exp(-X),a,b))
figure(1)
fplot(@(X) X*exp(-X),[a b],'b')
title('Trapezoidal Integration','FontSize',20); % Title
xlabel('x','FontSize',18); % Labels the x-axis
ylabel('f(x)','FontSize',18); % Labels the y-axis
grid; %Includes grid lines in the plot
hold on
```

```
% Trapezoidal Rule
for i=1:max(size(n))
   x=[a:(b-a)/n(i):b]
   y=x.*exp(-x)
   txt = ['n = ',num2str(n(i))];
   plot(x,y,'DisplayName',txt)
   legend show
   I=trapz(x,y)
error(i)=100*(exact-I)/exact
end
figure(2)
plot(n,error)
title('Percent Error','FontSize',20); % Title
xlabel('n','FontSize',18); % Labels the x-axis
ylabel('% Error','FontSize',18); % Labels the y-axis
grid; %Includes grid lines in the plot
```

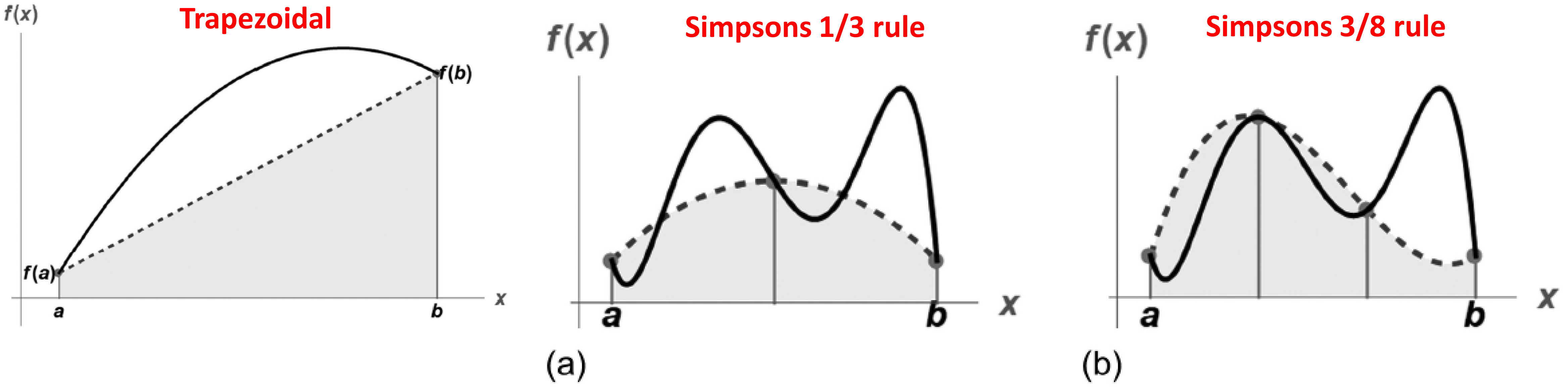
# 4.6 Numerical Integration: Trapezoidal Rule (Example)



# 4.6 Numerical Integration: Simpsons one-third rule

- Instead of a linear interpolation as used with the trapezoid rule, Simpson's rules use higher-order polynomials. The quadratic and cubic interpolating functions are shown in the following Figure




$$\int_{x_0}^{x_0+nh} f(x)\,dx = \frac{h}{3}[(y_0+y_n)+4(y_1+y_3)+\dots+y_{n-1})+2(y_2+y_4+\dots+y_{n-2})]$$

**Simpsons 1/3 rule**

$$I \cong \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right)$$

$$\int_{x_0}^{x_0+nh} f(x)\,dx = \frac{3h}{8}[(y_0+y_n)+3(y_1+y_2+y_4+y_5+\dots+y_{n-1})+2(y_3+y_6+\dots+y_{n-3}]$$

**Simpsons 3/8 rule**

$$I = \frac{3h}{8}\left(f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right)$$

# 4.6 Numerical Integration: Example

- Evaluate $\int_0^6 \frac{dx}{1+x^2}$ using a) Trapezoidal rule; b) Simpson's 1/3 rule; c) Simpson's 3/8 rule.

| x | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|---|
| f(x) | 1 | 1.5 | 0.2 | 0.1 | 0.05884 | 0.0385 | 0.027 |
| y | y0 | y1 | y2 | y3 | y4 | y5 | y6 |

By Trapezoidal rule,

$$\int_0^6 \frac{1}{1+x^2} = \frac{h}{2}[(y_0+y_6)+2(y_1+y_2+y_3+y_4+y_5)]$$

$$= \frac{1}{2}[(1+\ 0.027)+2(0.5+0.2+0.1+0.0588+0.0385)] = 1.4108.$$

By Simpson's 1/3 rule,

$$\int_0^6 \frac{1}{1+x^2} = \frac{h}{3}[(y_0+y_6)+4(y_1+y_3+y_5)+2(y_2+y_4)]$$

$$= \frac{1}{3}[(1+0.027)+4(0.5+0.1+0.0385)+2(0.2+0.0588)] = 1.3662.$$

By Simpson's 3/8 rule,

$$\int_0^6 \frac{1}{1+x^2} = \frac{3h}{8}[(y_0+y_6)+3(y_1+y_2+y_4+y_5)+2y_3]$$

$$= \frac{3}{8}[(1+0.027)+3(0.5+0.2+0.0588+0.0385)+2(0.1)] = 1.3571.$$

# 4.6 Numerical Integration: Example

- Evaluate $\int_0^6 \frac{dx}{1+x^2}$ using a) Trapezoidal rule; b) Simpson's 1/3 rule; c) Simpson's 3/8 rule.

```
% House Keeping
clc
clear
clear all

% Exact Function
syms X
a=0
b=6
n=6
exact=vpa(int(1/(1+X.^2),a,b))

% Data
x=[a:(b-a)/n:b]
y=1./(1+x.^2)

% Trapezoidal
I_trap=trapz(x,y)
error_I_3_8=100*(exact-I_trap)/exact

% Simpson's 1/3
I_1_3=simpson(x,y,[],'1/3')
error_I_1_3=100*(exact-I_1_3)/exact

% Simpson's 3/8
I_3_8=simpson(x,y,[],'3/8')
error_I_3_8=100*(exact-I_3_8)/exact
```

```
I_trap =

   1.4108


error_I_3_8 =

-0.36644546083921529896209780771262


I_1_3 =

   1.3662


error_I_1_3 =

2.8082596776963738498539098910662


I_3_8 =

   1.3571


error_I_3_8 =

3.4551199875076057272490144906671
```

# References


- *Applied Engineering Mathematics*, Brian Vick, CRC Press, 2020
- *Numerical Methods in Engineering with MATLAB*, Jaan Klusalaas, Cambridge University Press, 2012