Algoritmos Numéricos por Computadora

COM - 14105

"Actually, a person does not really understand something until he can teach it to a computer"
Donald Knuth, 1974

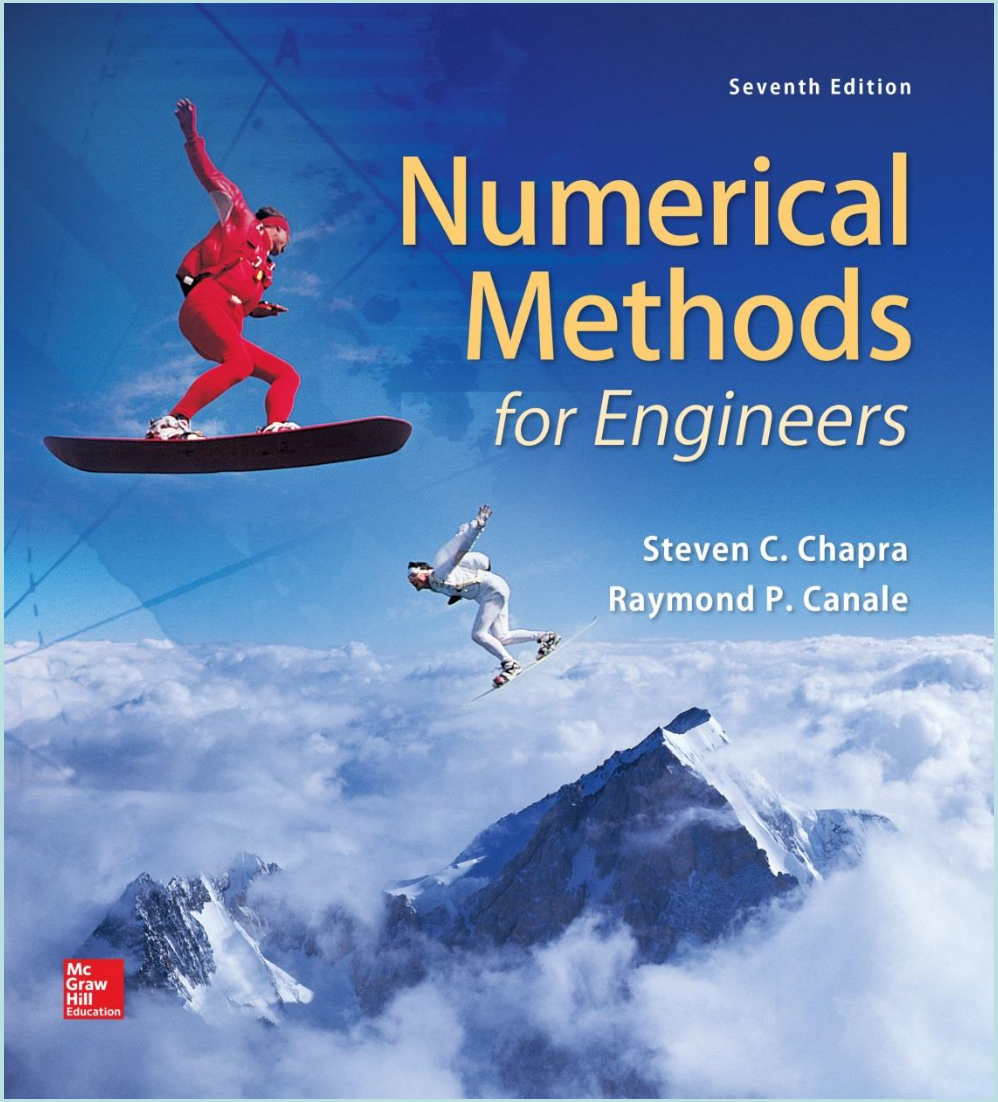
Objetivos

- Solucionar sistemas de ecuaciones lineales y ecuaciones diferenciales de forma numérica
- Entender el funcionamiento de diversos métodos numéricos
- Entender los errores numéricos de las soluciones computacionales
- Familiarizarse con el modelado matemático de sistemas físicos
- Usar un lenguaje de programación matricial de manera eficiente

Temario

1. Introducción
    1. Modelado de sistemas dinámicos
    2. Redondeo y truncamiento
    3. Raíces de funciones y optimización
    4. Números complejos
2. Sistemas lineales
    1. Valores y vectores propios
    2. Eliminación de Gauss
    3. Factorizaciones
    4. Métodos iterativos
    5. Sistemas no lineales
3. Ecuaciones diferenciales ordinarias
    1. Interpolación e integración
    2. Soluciones analíticas sencillas
    3. Problemas con valor inicial
    4. Sistemas de ecuaciones lineales de primer orden
    5. ODE de orden superior
    6. Métodos de paso variable, implícitos y multipasos
    7. Problemas con valores en la frontera
4. Ecuaciones diferenciales parciales (lineales de segundo orden)

Ecuaciones Diferenciales



Ordinary Differential Equations

Equations which are composed of an unknown function and its derivatives are called *differential equations*.

Differential equations play a fundamental role in engineering because many physical phenomena are best formulated mathematically in terms of their rate of change.

$$\frac{dv}{dt} = g - \frac{c_d}{m} v^2$$

v- dependent variable

t- independent variable

When a function involves one dependent variable, the equation is called an *ordinary differential equation (or ODE)*. A *partial differential equation (or PDE)* involves two or more independent variables.

Differential equations are also classified as to their order.

– *A first order equation* includes a first derivative as its highest derivative.
– *A second order equation* includes a second derivative.

Higher order equations can be reduced to a system of first order equations, by redefining a variable.

Physical law

$$F = ma$$

ODE

$$\frac{dv}{dt} = g - \frac{c_d}{m} v^2 \qquad \frac{dx}{dt} = v$$

Analytical (calculus)

Numerical (computer)

Solution

$$v = \sqrt{\frac{gm}{c_d}} \tanh\left(\sqrt{\frac{g c_d}{m}}\, t\right)$$

$$v_{i+1} = v_i + \left(g - \frac{c_d}{m} v^2\right) \Delta t$$

Initial Value Problems

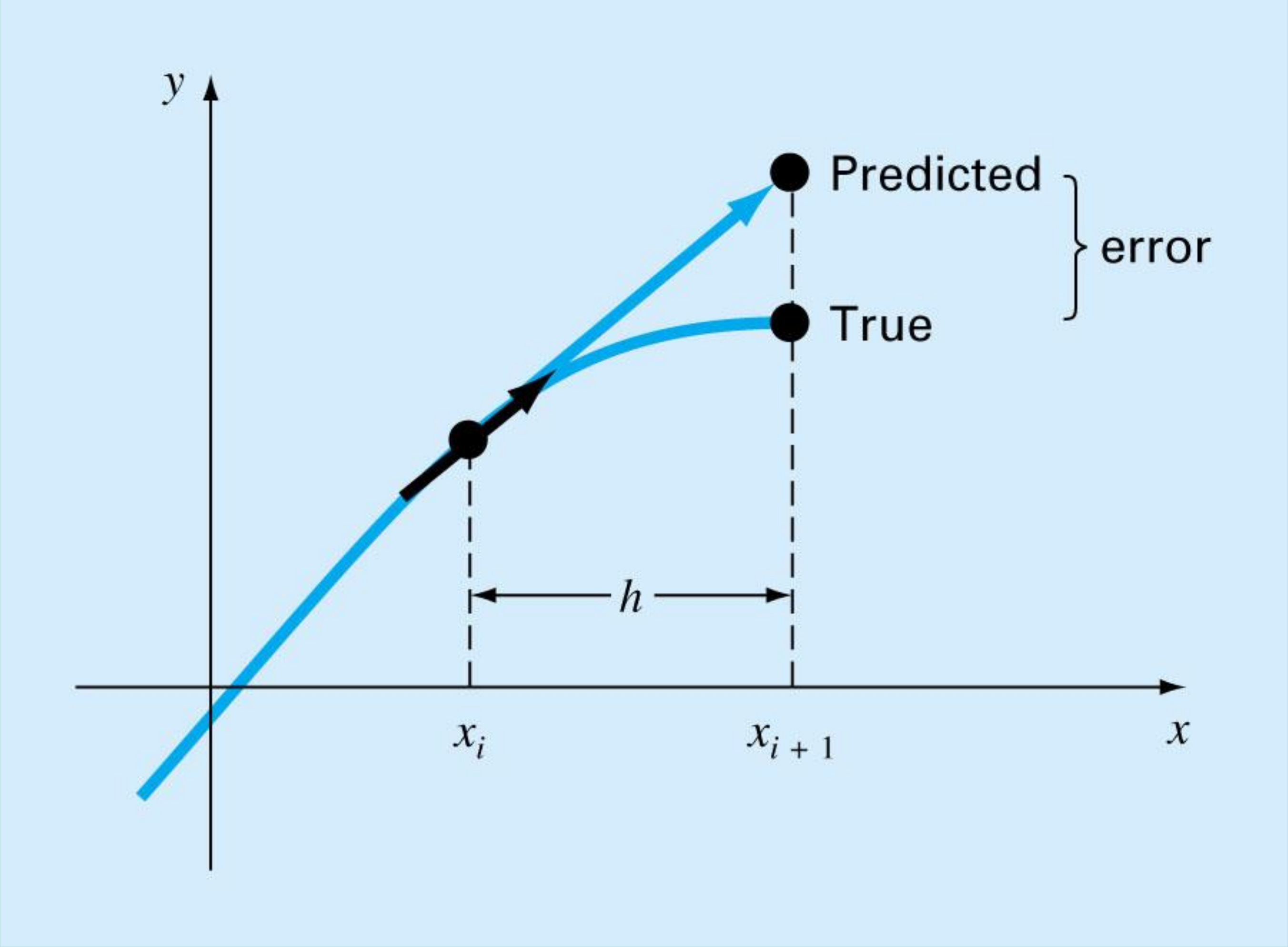
Solving ordinary differential equations of the form

$$\frac{dy}{dx} = f(x, y) \qquad y(x_0) = y_0$$

$$y_{i+1} = y_i + \emptyset h$$

One-step methods
Constant step size

Euler's Method



First-order RK method

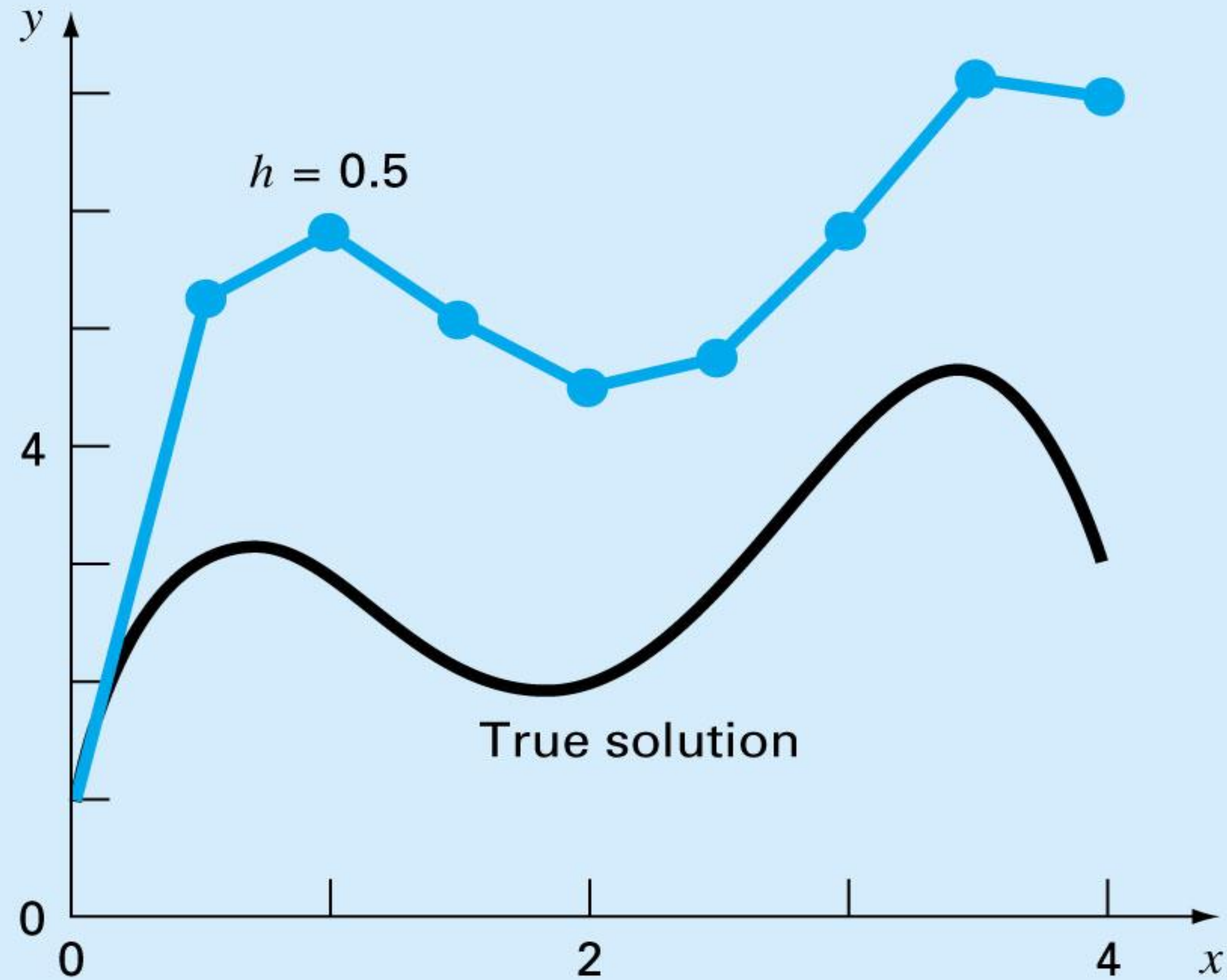
The first derivative provides a direct estimate of the slope at x_i

$$\phi = f(x_i, y_i)$$

where $f(x_i,y_i)$ is the differential equation evaluated at x_i and y_i. This estimate can be substituted into the equation:

$$y_{i+1} = y_i + f(x_i, y_i)h$$

A new value of y is predicted using the slope to extrapolate linearly over the step size h.


y
h = 0.5
4
True solution
0
0
2
4
x

Error Analysis for Euler's Method

- Numerical solutions of ODEs involves two types of error:

  - *Truncation* error
    - *Local truncation error*

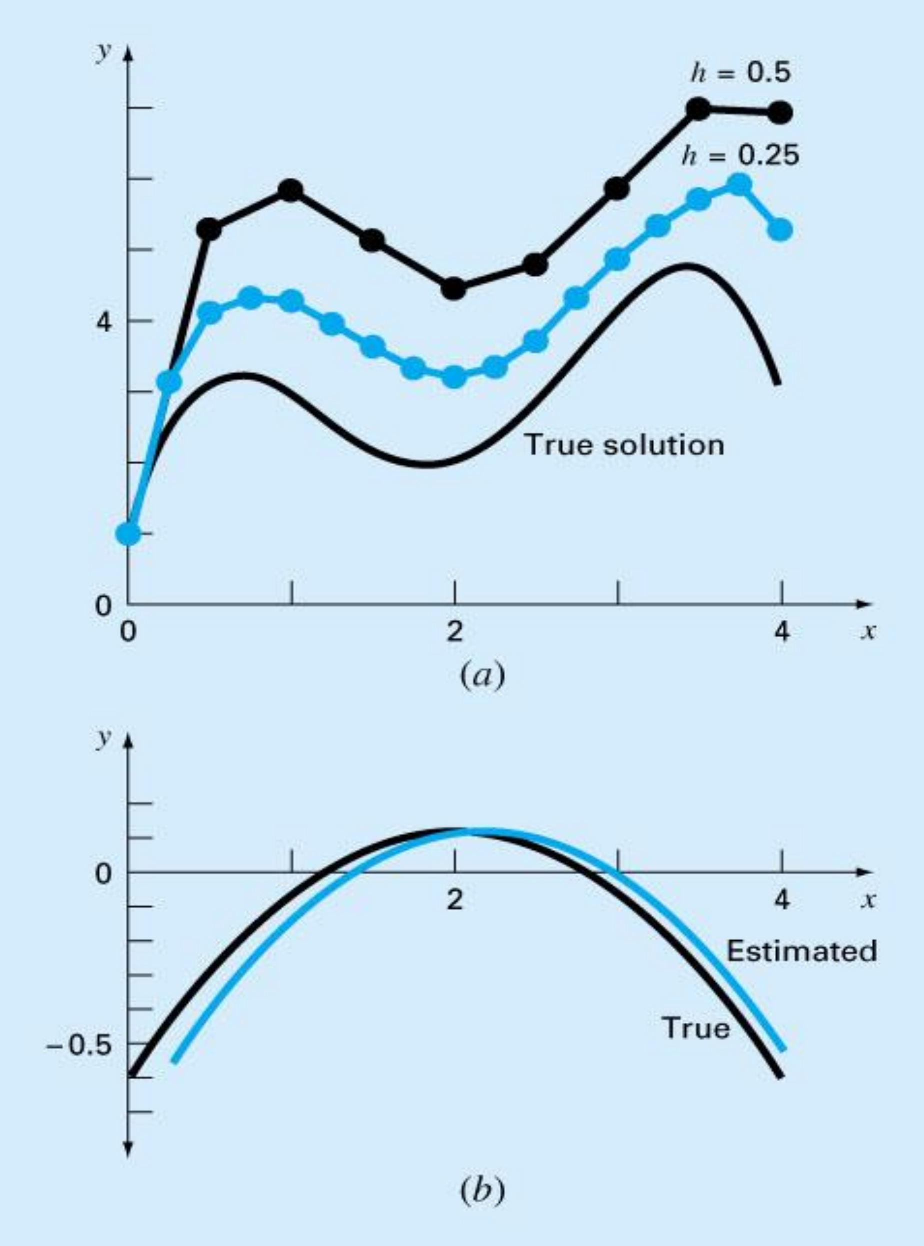
$$E_a = \frac{f'(x_i, y_i)}{2!} h^2$$

$$E_a = O(h^2)$$

    - *Propagated truncation error*   *O(h)*

  - *Round-off* errors

- The Taylor series provides a means of quantifying the error in Euler's method. However;
  - The Taylor series provides only an estimate of the local truncation error-that is, the error created during a single step of the method.
  - In actual problems, the functions are more complicated than simple polynomials. Consequently, the derivatives needed to evaluate the Taylor series expansion would not always be easy to obtain.
- In conclusion,
  - the error can be reduced by reducing the step size
  - If the solution to the differential equation is linear, the method will provide error free predictions as for a straight line the 2nd derivative would be zero.


y
h = 0.5
h = 0.25
4
True solution
0
0
2
4
x
(a)
y
0
2
4
x
Estimated
True
−0.5
(b)

Improvements of Euler's method

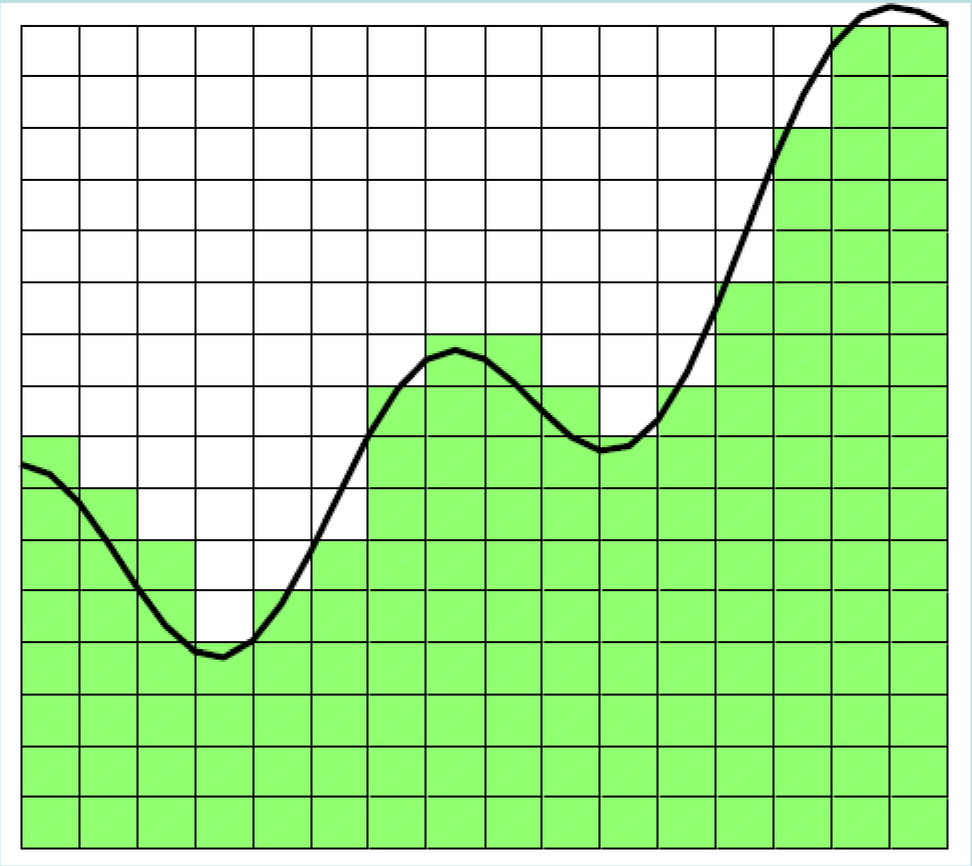
- A fundamental source of error in Euler's method is that the derivative at the beginning of the interval is assumed to apply across the entire interval.
- Two simple modifications are available to circumvent this shortcoming:
  - Heun's Method
  - The Midpoint Method

Second-order RK methods

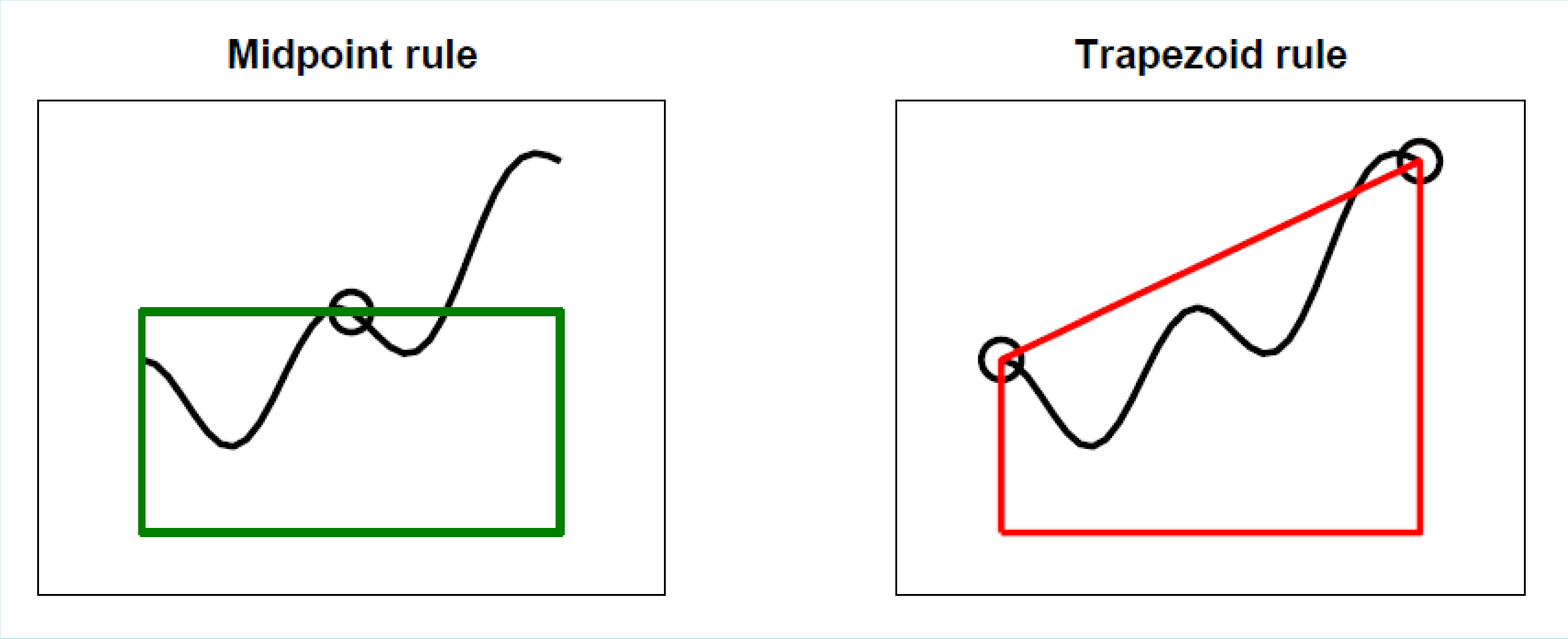
Numerical Integration

$$\frac{dy}{dx} = f(x, y)$$

$$y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} f(x, y)dx$$



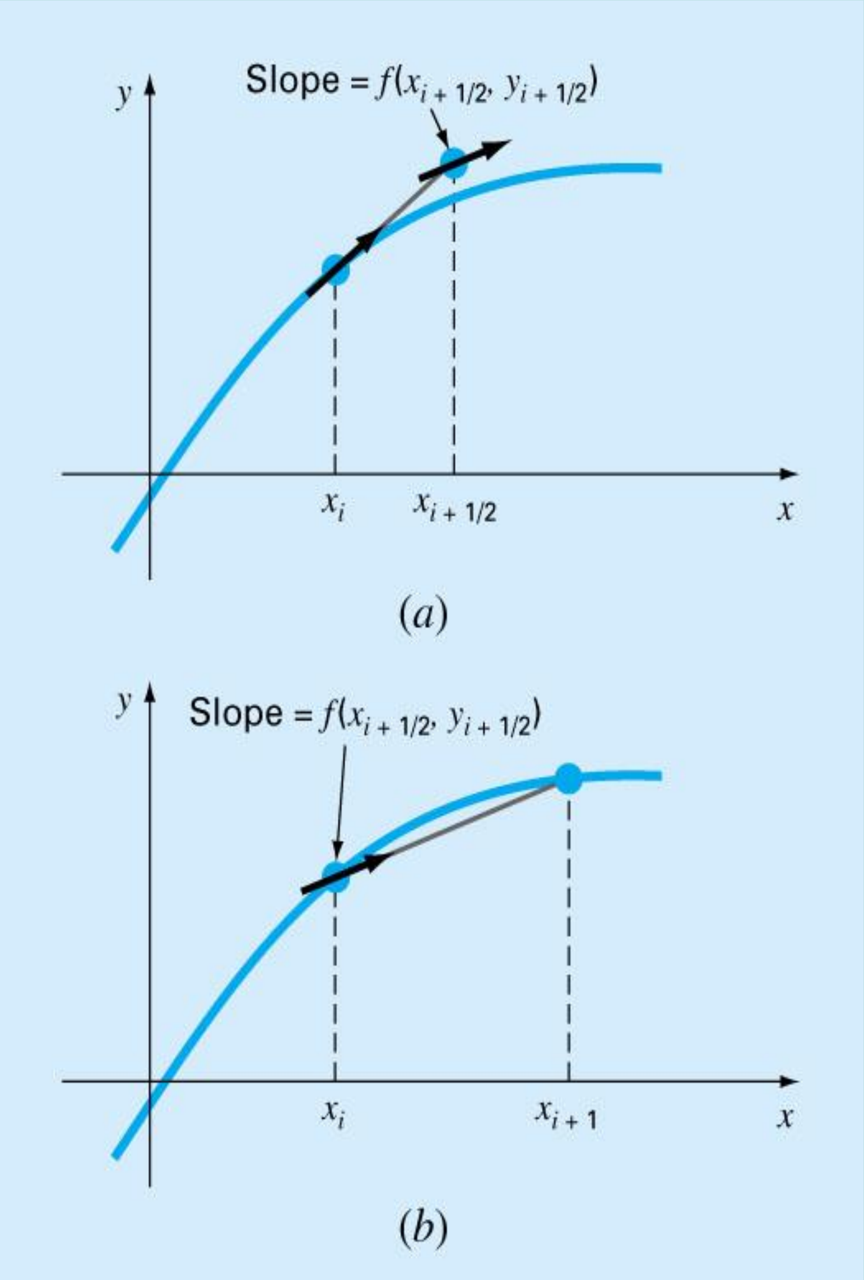
Numerical Integration



The Midpoint Method

- Uses Euler's method to predict a value of y at the midpoint of the interval $y_{i+1/2}$
- This derivative is then used as an improved estimate of the slope for the entire interval.

$$y_{i+1} = y_i + f(x_{i+1/2}, y_{i+1/2})h$$

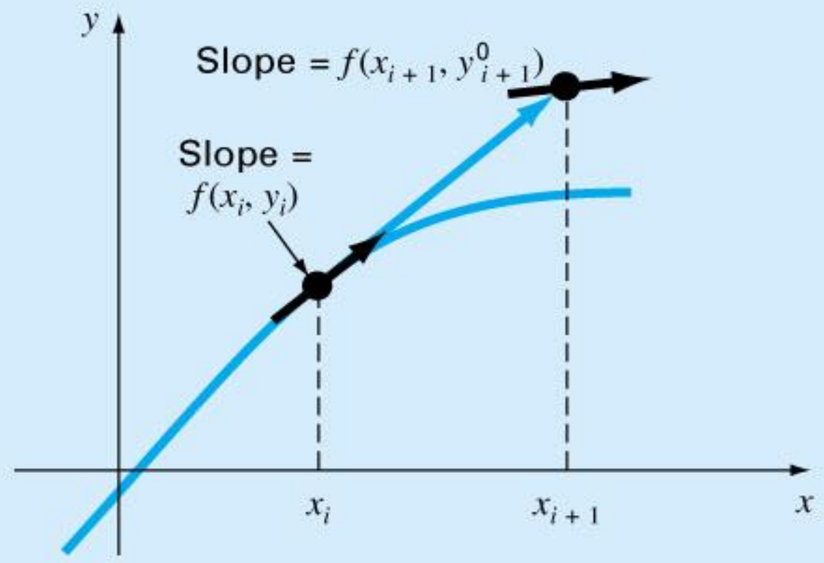

Slope = $f(x_{i+1/2}, y_{i+1/2})$
y
x_i
$x_{i+1/2}$
x
(a)
Slope = $f(x_{i+1/2}, y_{i+1/2})$
y
x_i
x_{i+1}
x
(b)

Heun's Method

- Another method to improve the estimate of the slope involves the determination of two derivatives for the interval:
  - At the initial point
  - At the end point
- The two derivatives are then averaged to obtain an improved estimate of the slope for the entire interval.

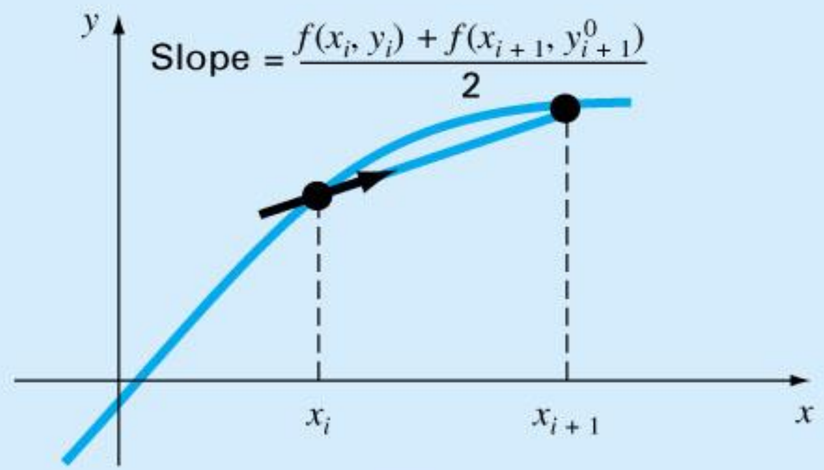
$$\text{Predictor:}\quad y_{i+1}^{0} = y_i + f(x_i, y_i)h$$

$$\text{Corrector:}\quad y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^{0})}{2}h$$



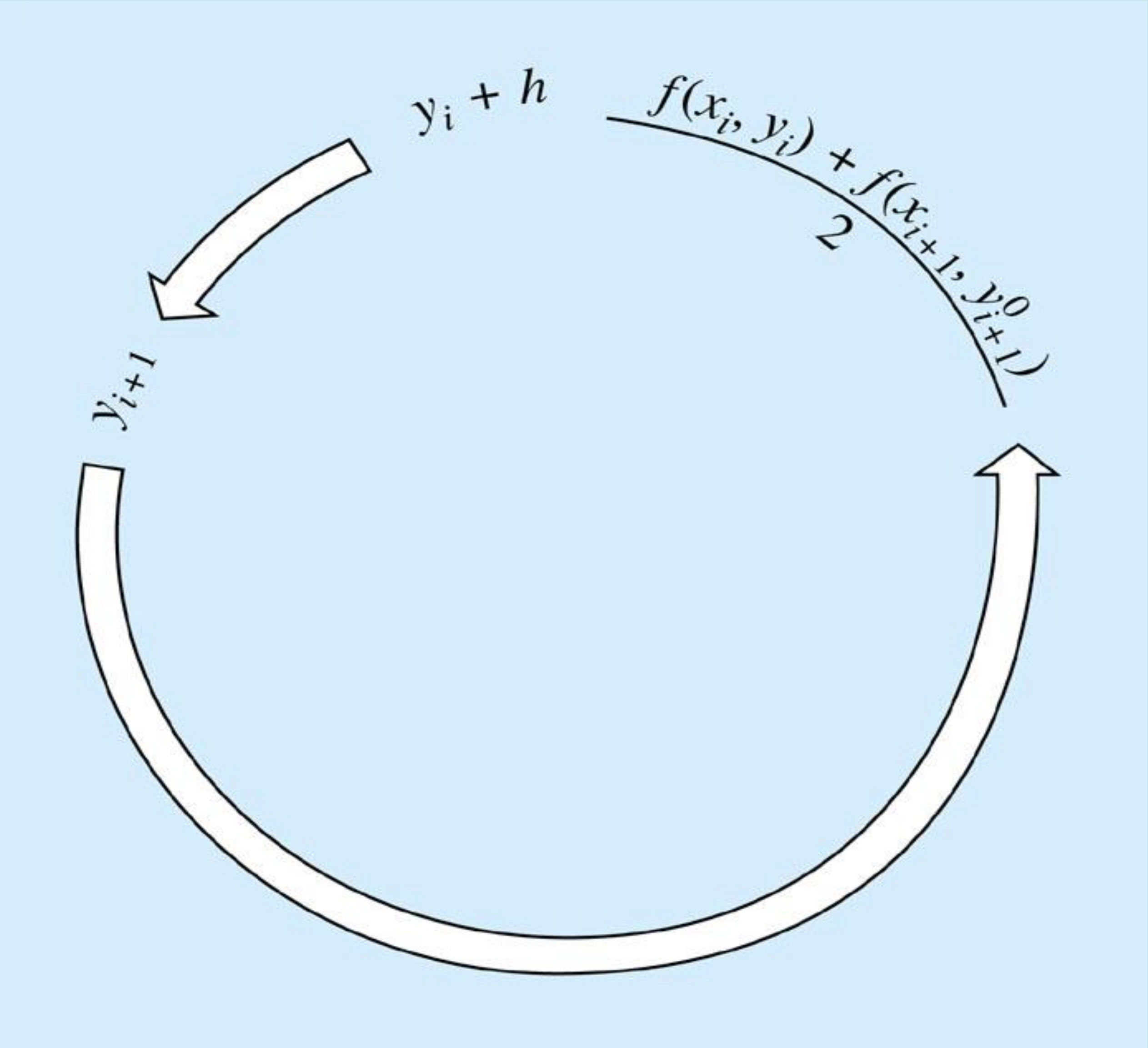
y
Slope = $f(x_{i+1}, y^0_{i+1})$
Slope = $f(x_i, y_i)$
x_i
x_{i+1}
x

(a)



y
Slope = $\dfrac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1})}{2}$
x_i
x_{i+1}
x

(b)


$y_i + h \dfrac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^0)}{2}$
y_{i+1}

Runge-Kutta Methods (RK)

- Runge-Kutta methods achieve the accuracy of a Taylor series approach without requiring the calculation of higher derivatives.

$$y_{i+1} = y_i + \phi(x_i, y_i, h)h$$

$$\phi = a_1 k_1 + a_2 k_2 + \cdots + a_n k_n$$ ***Increment function***

$$a's = \text{constants}$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$ ***p's and q's are constants***

$$k_3 = f(x_i + p_3 h, y_i + q_{21} k_1 h + q_{22} k_2 h)$$

$$\vdots$$

$$k_n = f(x_i + p_{n-1} h, y_i + q_{n-1} k_1 h + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h)$$

- k's are recurrence functions. Because each k is a functional evaluation, this recurrence makes RK methods efficient for computer calculations.
- Various types of RK methods can be devised by employing different number of terms in the increment function as specified by n.
- First order RK method with $n=1$ is in fact Euler's method.
- Once n is chosen, values of a's, p's, and q's are evaluated by setting general equation equal to terms in a Taylor series expansion.

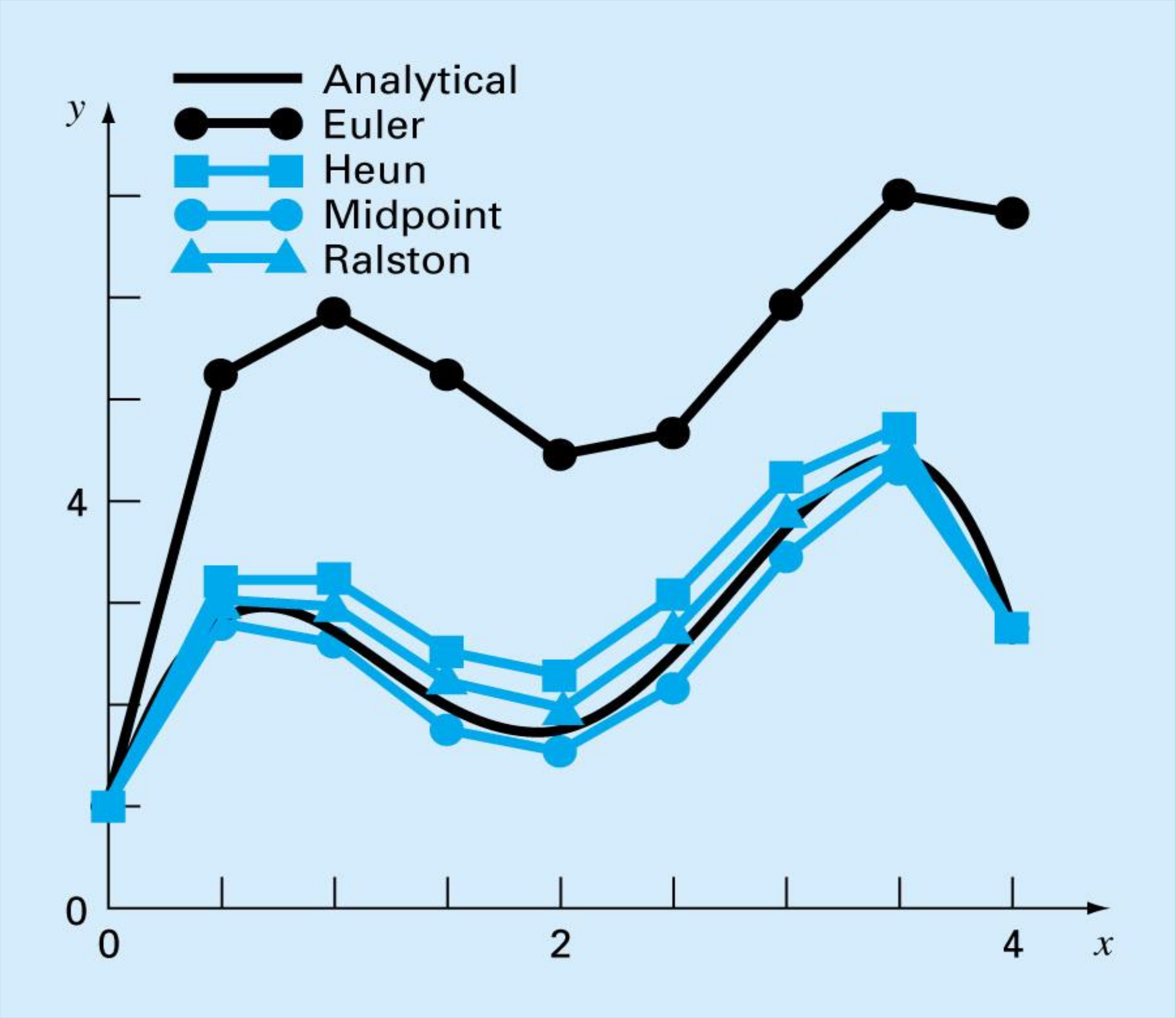
$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2) h$$
$$k_1 = f(x_i, y_i)$$
$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

- Values of a_1, a_2, p_1, and q_{11} are evaluated by setting the second order equation to Taylor series expansion to the second order term. Three equations to evaluate four unknowns constants are derived.

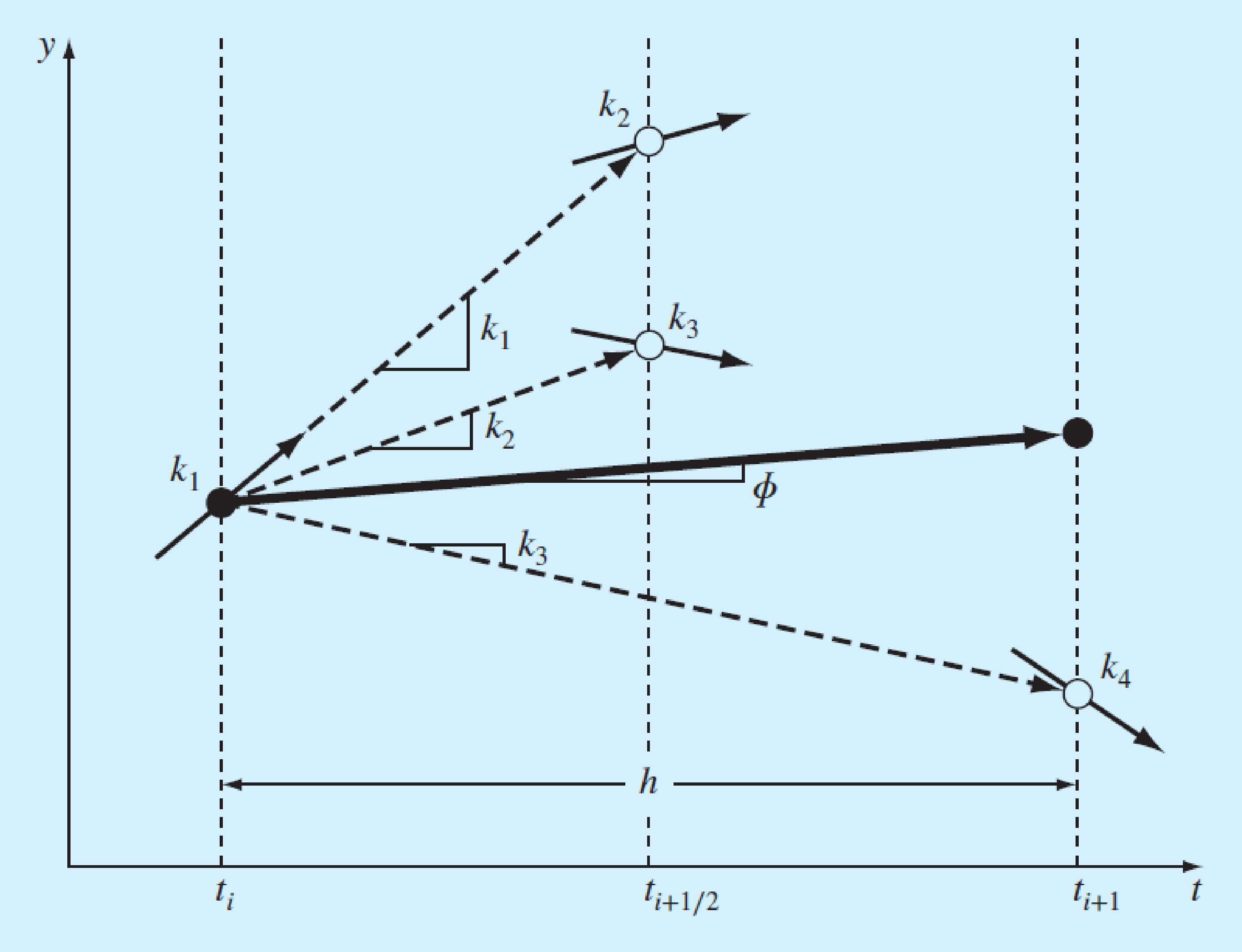
$$\left.\begin{aligned} a_1 + a_2 &= 1 \\ a_2 p_1 &= \frac{1}{2} \\ a_2 q_{11} &= \frac{1}{2} \end{aligned}\right\}$$

A value is assumed for one of the unknowns to solve for the other three.

- Because we can choose an infinite number of values for a_2, there are an infinite number of second-order RK methods.
- Every version would yield exactly the same results if the solution to ODE were quadratic, linear, or a constant.
- However, they yield different results if the solution is more complicated (typically the case).
- Three of the most commonly used methods are:
  - Huen Method with a Single Corrector ($a_2=1/2$)
  - The Midpoint Method ($a_2=1$)
  - Raltson's Method ($a_2=2/3$)


Analytical
Euler
Heun
Midpoint
Ralston
y
4
0
0
2
4
x

Classical RK-4



Systems of Equations

- Many practical problems in engineering and science require the solution of a system of simultaneous ordinary differential equations rather than a single equation:

$$\frac{dy_1}{dx} = f_1(x, y_1, y_2, \ldots, y_n)$$

$$\frac{dy_2}{dx} = f_2(x, y_1, y_2, \ldots, y_n)$$

$$\vdots$$

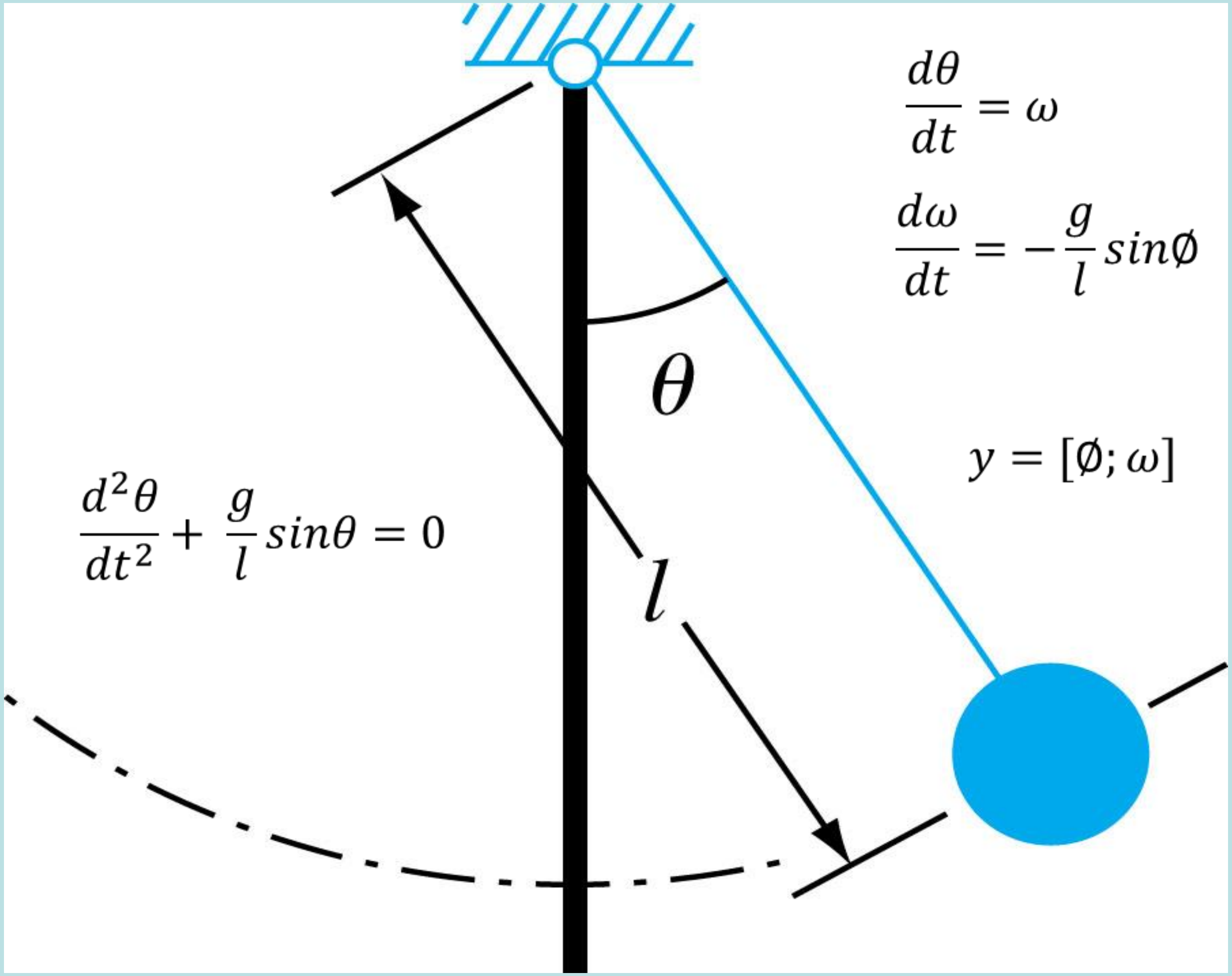
$$\frac{dy_n}{dx} = f_n(x, y_1, y_2, \ldots, y_n)$$

$$y = [y_1; y_2; \ldots; y_n]$$

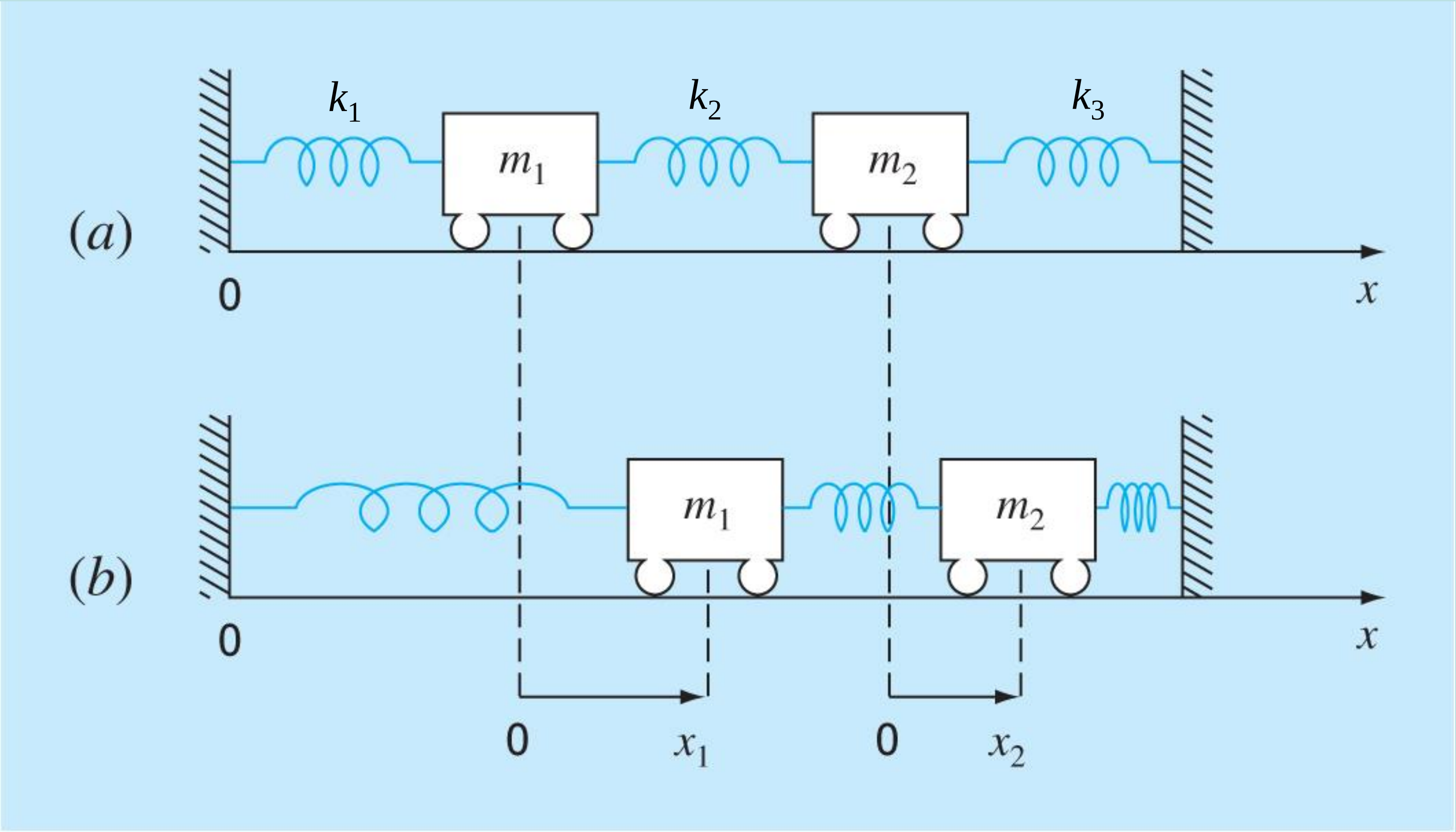
$$y' = [f_1; f_2; \ldots; f_n]$$

- Solution requires that n initial conditions be known at the starting value of x.

ODEs and Engineering Practice



ODEs and Engineering Practice



Eigenvalues and eigenvectors

Boundary-Value Problems

- An ODE is accompanied by auxiliary conditions. These conditions are used to evaluate the integral that result during the solution of the equation. An n^{th} order equation requires n conditions.

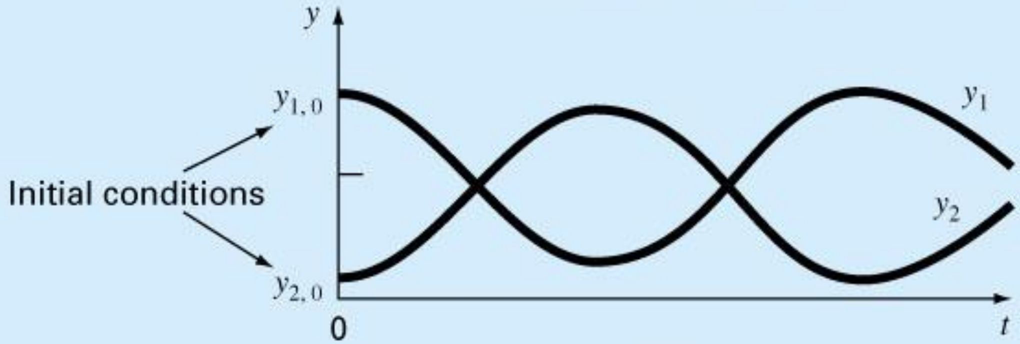
- If all conditions are specified at the same value of the independent variable, then we have an *initial-value problem*.

- If the conditions are specified at different values of the independent variable, usually at extreme points or boundaries of a system, then we have a *boundary-value problem*.

$$\frac{dy_1}{dt} = f_1(t, y_1, y_2)$$

$$\frac{dy_2}{dt} = f_2(t, y_1, y_2)$$

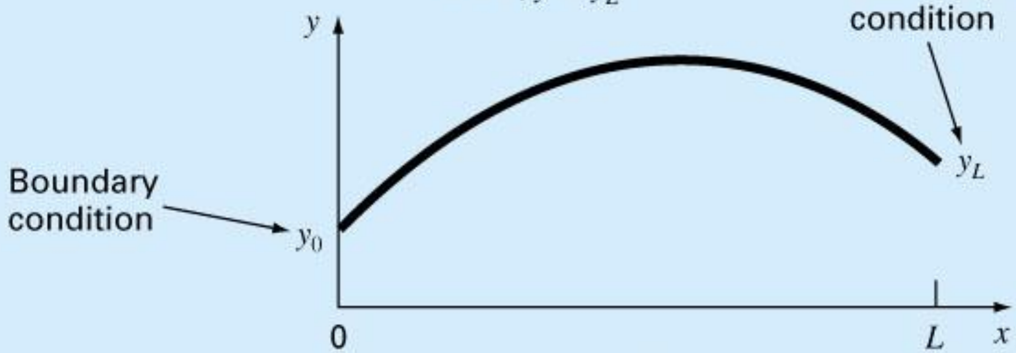
where at $t = 0$, $y_1 = y_{1,0}$ and $y_2 = y_{2,0}$



(a)

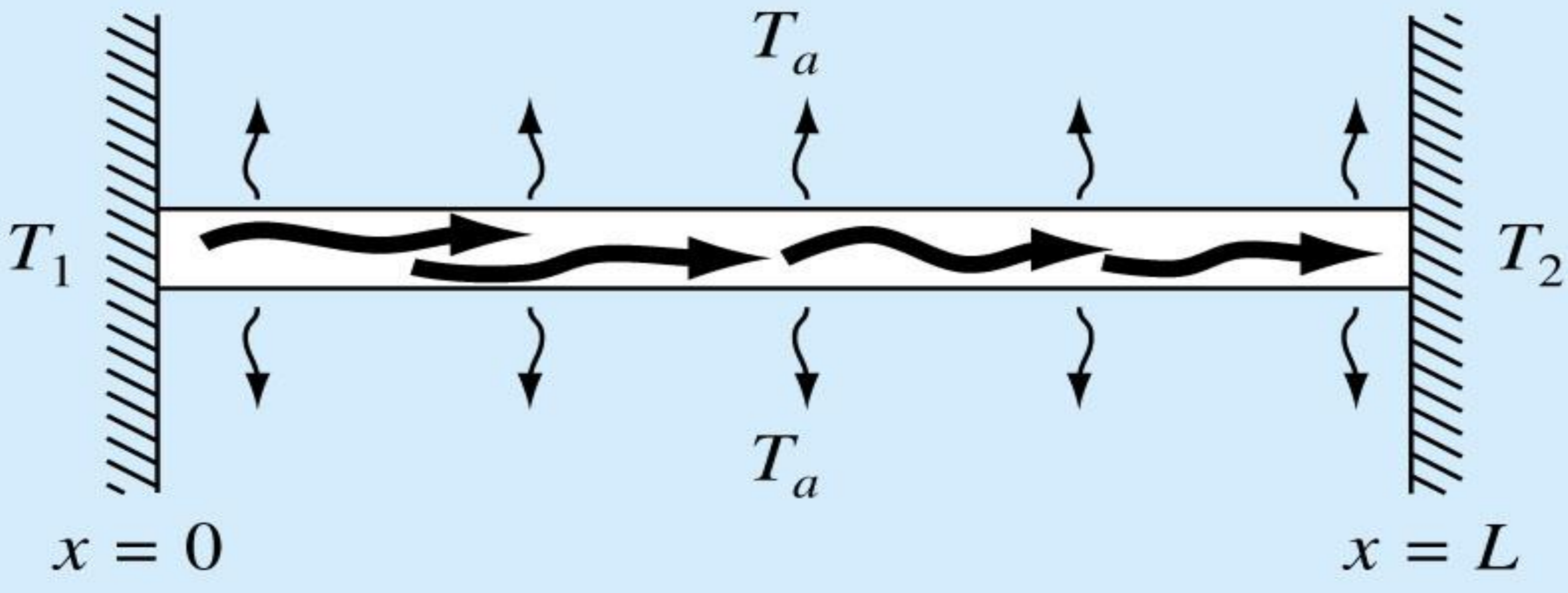
$$\frac{d^2y}{dx^2} = f(x, y)$$

where at $x = 0$, $y = y_0$
$x = L$, $y = y_L$



(b)

Heated Rod



$$\frac{d^2T}{dx^2} + h'(T_a - T) = 0$$

$$T_a = 20$$

$$L = 10\, m$$

$$h' = 0.01 m^{-2}$$

$$\left.\begin{aligned} T(0) &= T_1 = 40 \\ T(L) &= T_2 = 200 \end{aligned}\right\}$$ **Boundary Conditions**

Analytical Solution:

$$T = 73.4523e^{0.1x} - 53.4523e^{-0.1x} + 20$$

The Shooting Method

- Converts the boundary value problem to initial-value problem. A trial-and-error approach is then implemented to solve the initial value approach.
- For example, the 2nd order equation can be expressed as two first order ODEs:

$$\frac{dT}{dx} = z$$

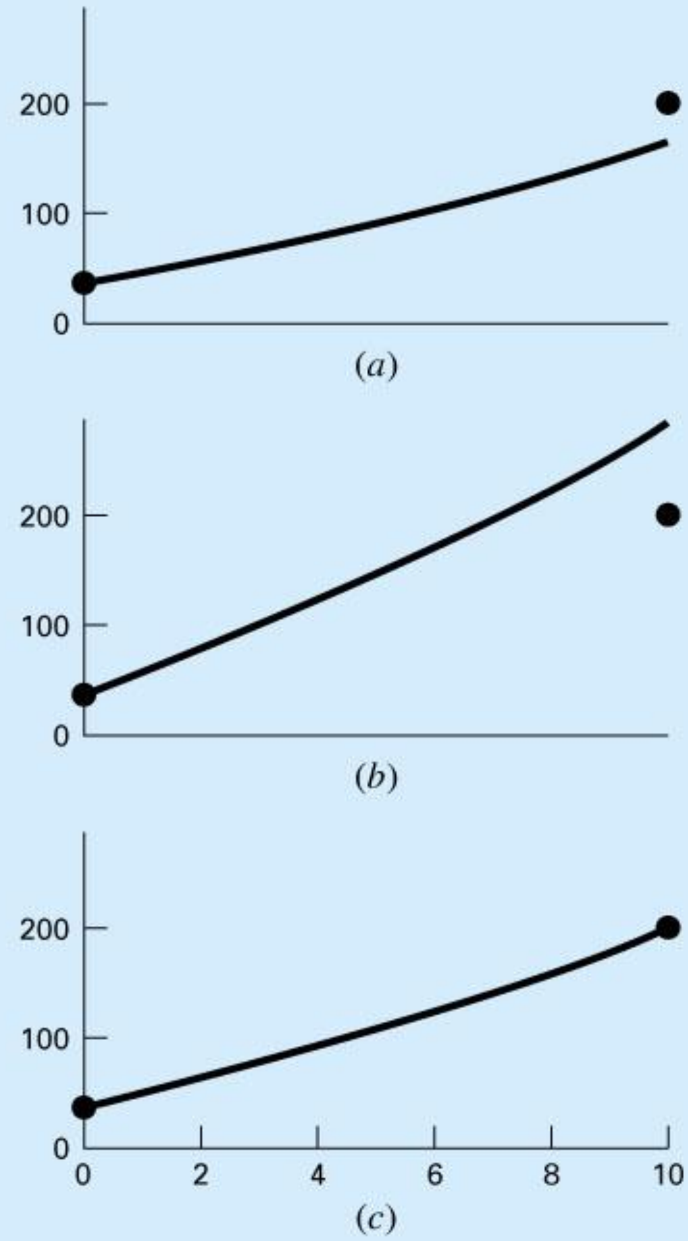
$$\frac{dz}{dx} = h'(T - T_a)$$

- An initial value is guessed, say *z(0)=10*.
- The solution is then obtained by integrating the two 1st order ODEs simultaneously.

- Using a 4^{th} order RK method with a step size of *2*:
  T(10)=168.3797.

- This differs from *T(10)=200*. Therefore a new guess is made, *z(0)=20* and the computation is performed again.
  z(0)=20   *T(10)=285.8980*

- Since the two sets of points, $(z, T)_1$ *and* $(z, T)_2$, are linearly related, a linear interpolation formula is used to compute the value of *z(0)* as *12.6907* to determine the correct solution.


200
100
0
(a)
200
100
0
(b)
200
100
0
0
2
4
6
8
10
(c)

- For a nonlinear problem a better approach involves recasting it as a roots problem.

$$T_{10} = f(z_0)$$
$$200 = f(z_0)$$
$$g(z_0) = f(z_0) - 200$$

- Driving this new function, *$g(z_0)$,* to zero provides the solution.

Finite Differences Methods.

- The most common alternatives to the shooting method.
- Finite differences are substituted for the derivatives in the original equation.

$$\frac{d^2T}{dx^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} - h'(T_i - T_a) = 0$$

$$-T_{i-1} + (2 + h'\Delta x^2)T_i - T_{i+1} = h'\Delta x^2 T_a$$

- Finite differences equation applies for each of the interior nodes. The first and last interior nodes, T_{i-1} and T_{i+1}, respectively, are specified by the boundary conditions.
- Thus, a linear equation transformed into a set of simultaneous algebraic equations can be solved efficiently.