DTS104TC NUMERICAL METHODS

LECTURE 8

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CONTENTS

ORDINARY DIFFERENTIAL EQUATIONS (ODEs)

- 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.

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

v = dependent variable
t = independent variable

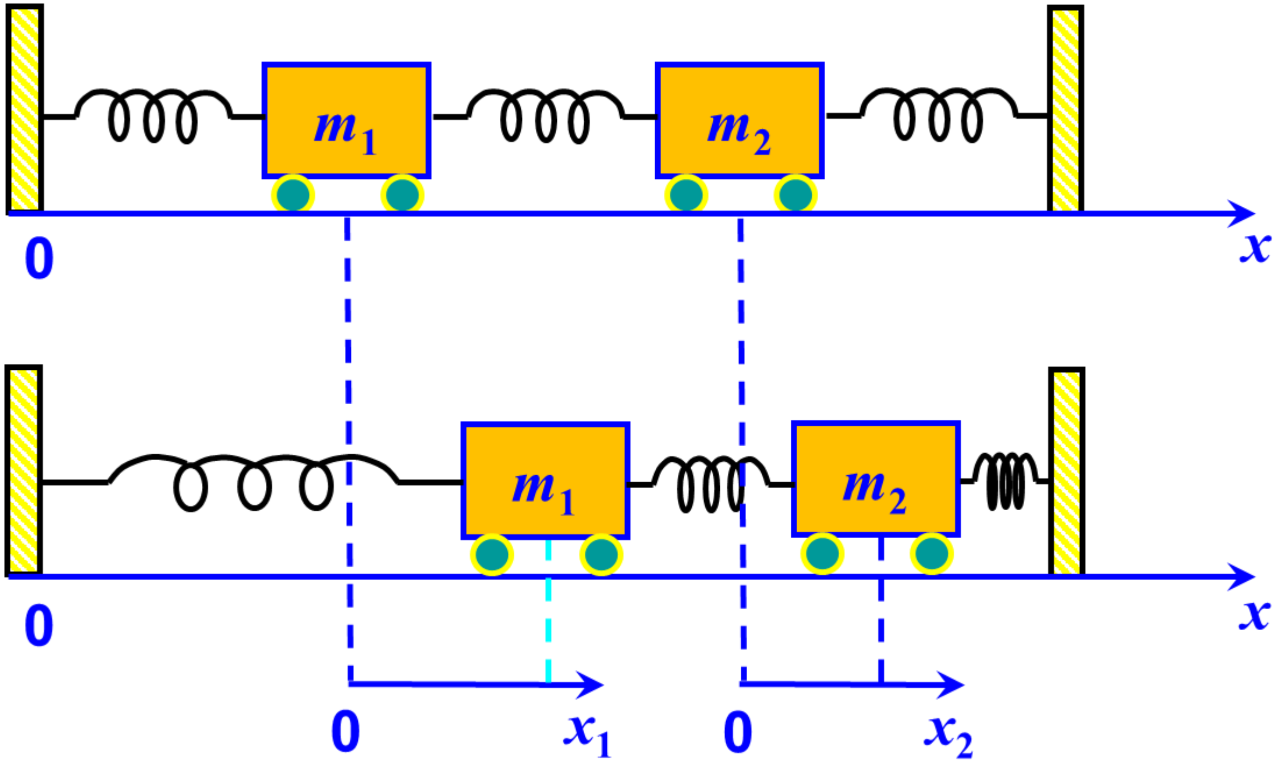
MATHEMATICAL BACKGROUND

When a function involves one independent 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.

EXAMPLE: MASS-SPRING SYSTEM



CONVERTING HIGHER ORDER ODEs INTO SYSTEM OF FIRST-ORDER ODEs

$$m_1 \frac{d^2 x_1}{dt^2} = -k\, x_1 + k(\boldsymbol{x}_2 - \boldsymbol{x}_1)$$

$$m_2 \frac{d^2 x_2}{dt^2} = -k(\boldsymbol{x}_2 - \boldsymbol{x}_1) - k\, x_2$$

Define:

$$\frac{dx_1}{dt} = v_1 \qquad \frac{dx_2}{dt} = v_2$$

$$\frac{d^2 x_1}{dt^2} = \frac{dv_1}{dt} \qquad \frac{d^2 x_2}{dt^2} = \frac{dv_2}{dt}$$

CONVERTING HIGHER ORDER ODEs INTO SYSTEM OF FIRST-ORDER ODEs

$$m_1 \frac{d^2 x_1}{dt^2} = -k\, x_1 + k(\boldsymbol{x}_2 - \boldsymbol{x}_1)$$

$$m_2 \frac{d^2 x_2}{dt^2} = -k(\boldsymbol{x}_2 - \boldsymbol{x}_1) - k\, x_2$$

$$\Rightarrow$$

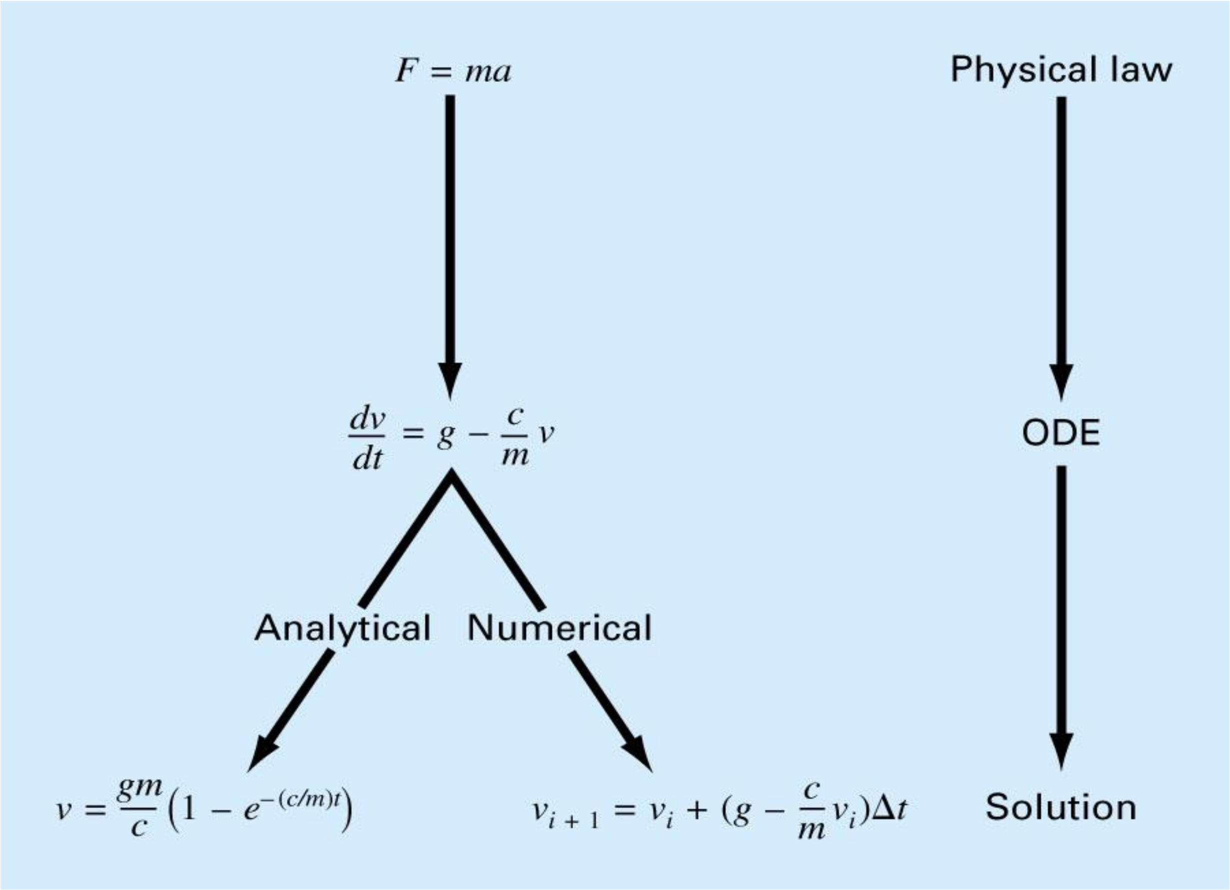
$$\frac{dx_1}{dt} = v_1$$

$$\frac{dx_2}{dt} = v_2$$

$$\frac{dv_1}{dt} = \frac{-k\, x_1 + k(\boldsymbol{x}_2 - \boldsymbol{x}_1)}{m_1}$$

$$\frac{dv_2}{dt} = \frac{-k(\boldsymbol{x}_2 - \boldsymbol{x}_1) - k\, x_2}{m_2}$$

EXAMPLE: THE FALLING PARACHUTIST PROBLEM



RUNGA-KUTTA METHODS

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

$$\frac{dv}{dt} = f(t, v, g, c_d, m)$$

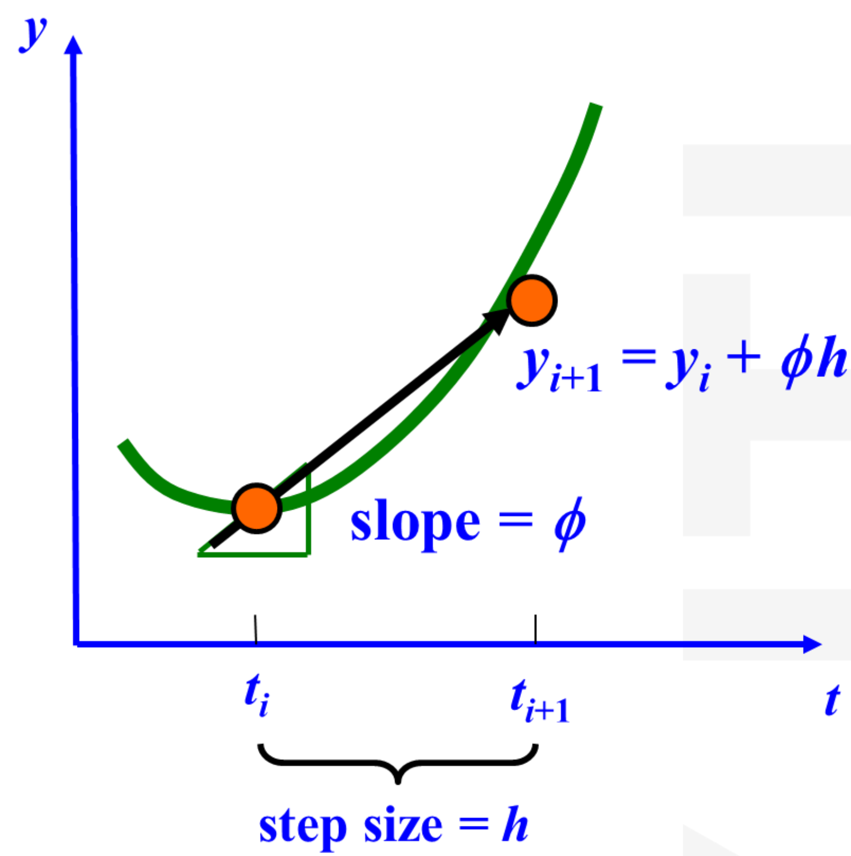
$$\frac{dv}{dt} = f(t, v)$$

R K (RUNGE-KUTTA) METHODS

$$\frac{dy}{dt} = f(t, y)$$

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

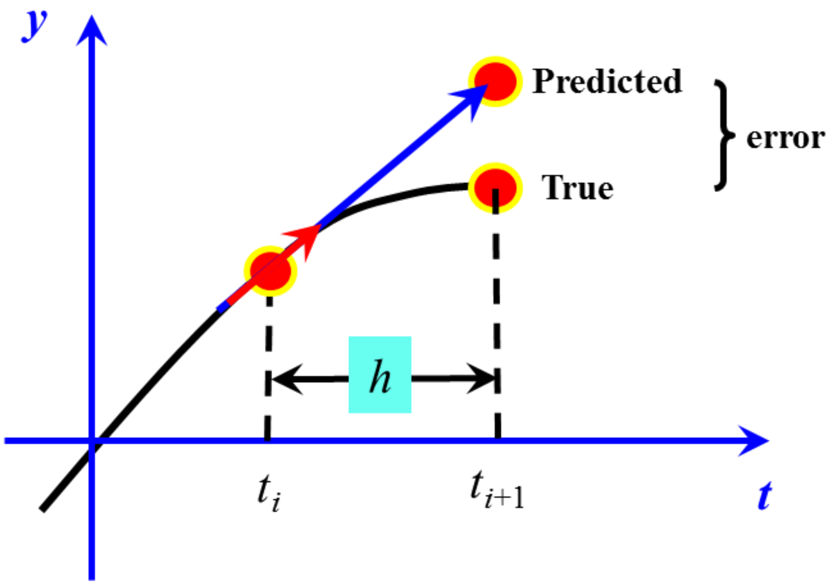
INCREMENT FUNCTION



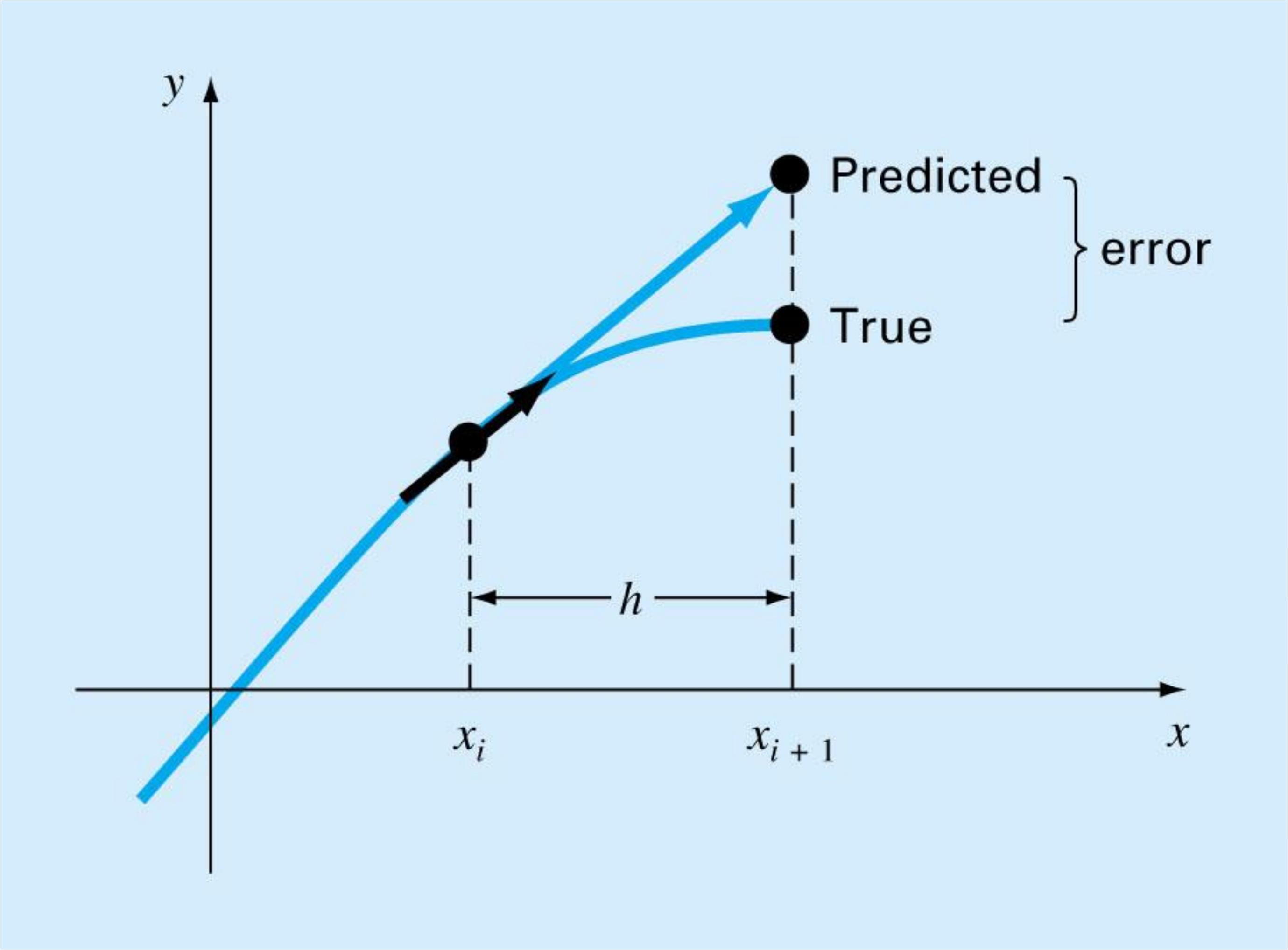
EULER'S METHOD

For Euler's method, the differential equation provides a direct estimate of the slope at x_i

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



EULER'S METHOD



EULER'S METHOD

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

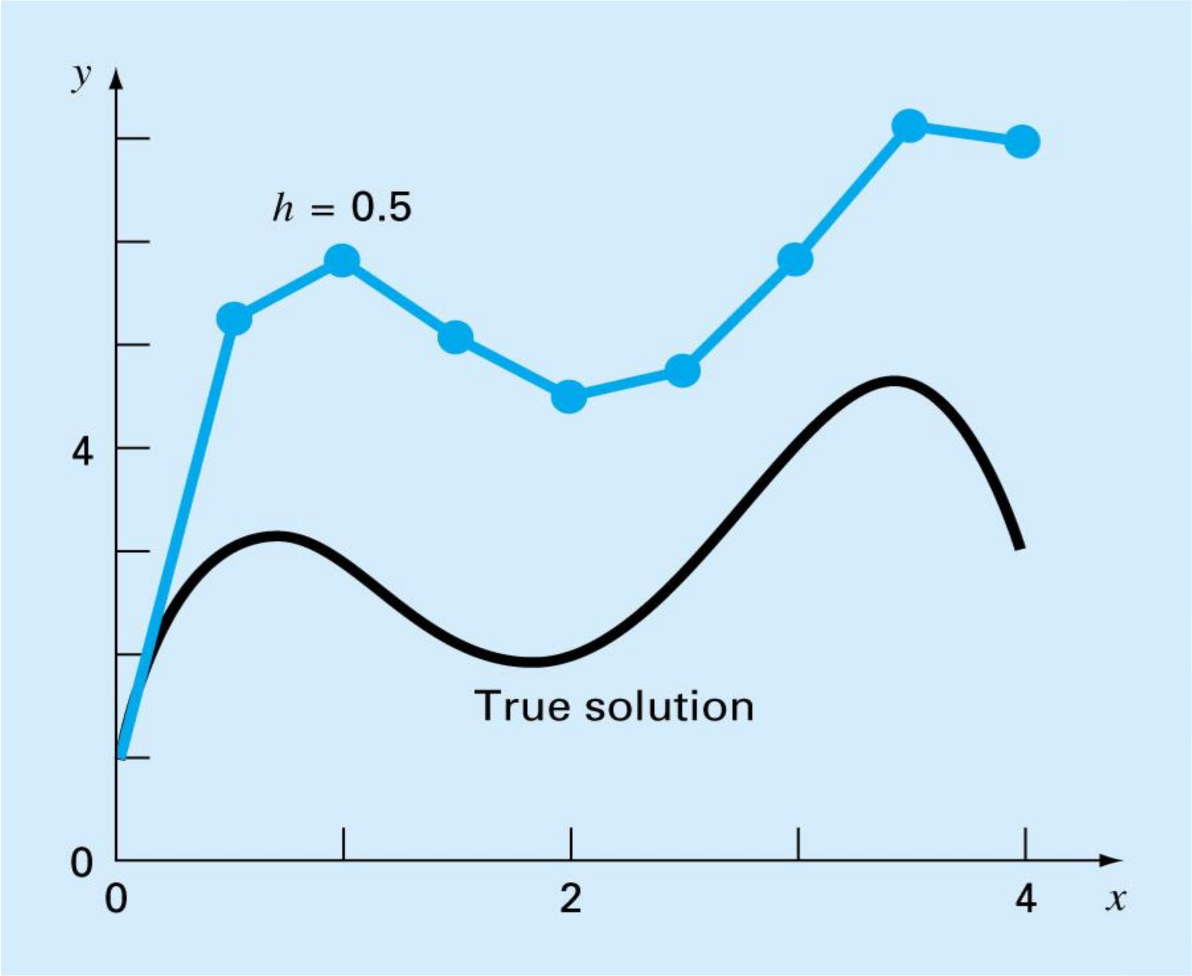
$$\varphi = f\left(x_i, y_i\right)$$

- 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:

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

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

EULER'S METHOD



Comparison of the true solution with a numerical solution using Euler's method for the integral of $y' = -2x^3 + 12x^2 - 20x + 8.5$ from $x = 0$ to $x = 4$ with a step size of 0.5. The initial condition at $x = 0$ is $y = 1$.

ERROR ANALYSIS FOR EULER'S METHOD

Numerical solutions of ODEs involves two types of error:

- ***Truncation*** errors.
  - ***Local truncation error***. *The error incurred on an each step.*

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

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

  - ***Propagated truncation error.*** Errors carried over from step to step.
    - The sum of the two is the ***total*** or **global truncation error.**
- ***Round-off*** errors.

ERROR ANALYSIS FOR EULER'S METHOD

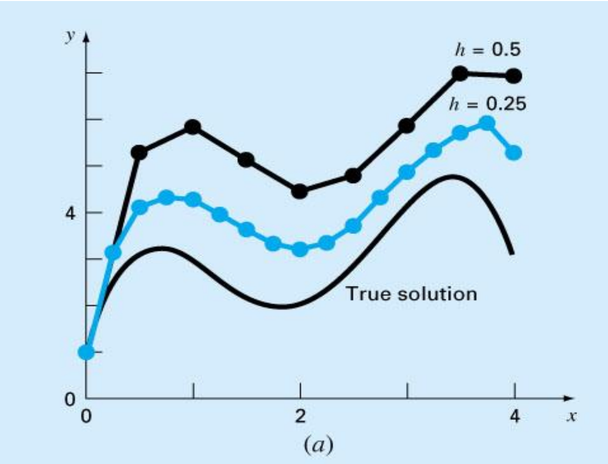
The Taylor series provides a means of quantifying the error in Euler's method. However;

- 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.

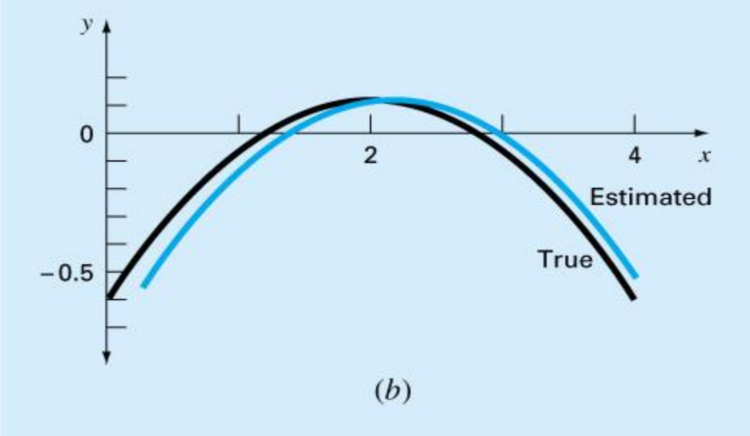
- In conclusion,
  - The error can be reduced by reducing the step size
  - If the solution to the differential equation is linear, the method will provide error free predictions as for a straight line the 2nd derivative would be zero.

ERROR ANALYSIS FOR EULER'S METHOD

(a) Comparison of two numerical solutions with Euler's method using step sizes of 0.5 and 0.25.



(b) Comparison of true and estimated local truncation error for the case where the step size is 0.5. Note that the "estimated" error is based on Equation



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 (or Improved Polygon) Method.

HEUN'S METHOD

One 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.

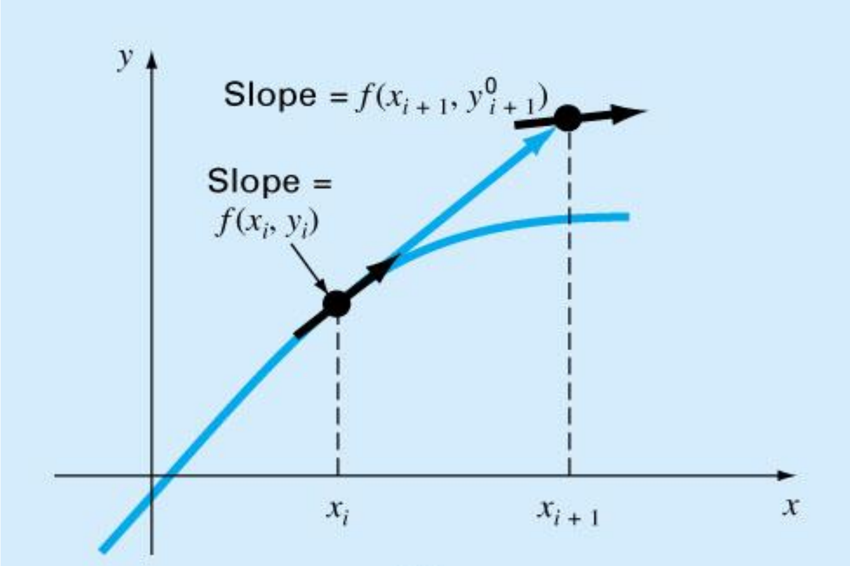
- The two derivatives are then averaged to obtain an improved estimate of the slope for the entire interval.

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

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

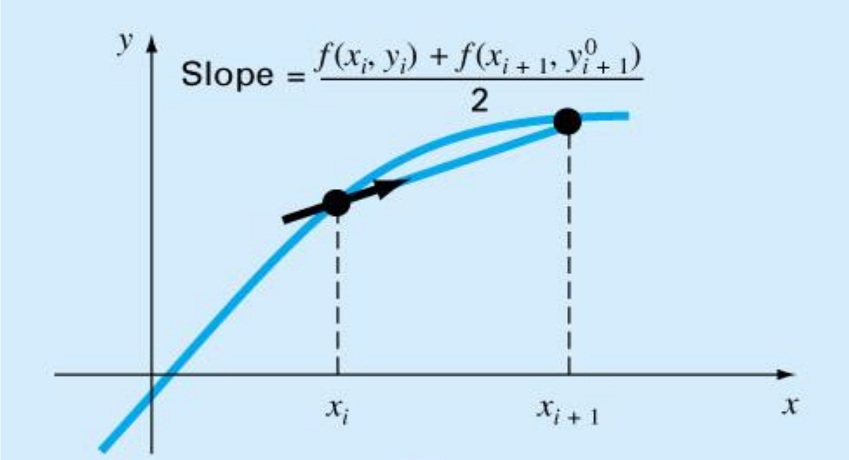
HEUN'S METHOD

Predictor



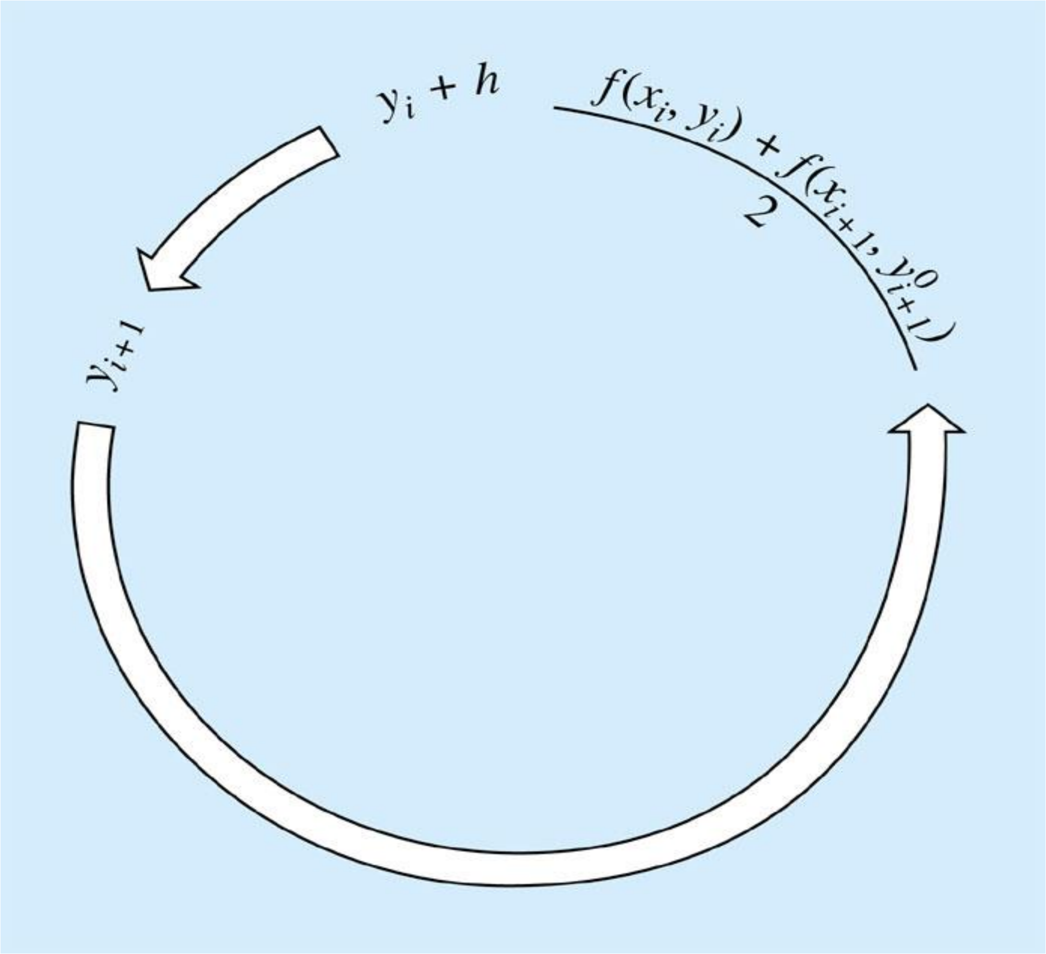
(*a*)

Corrector



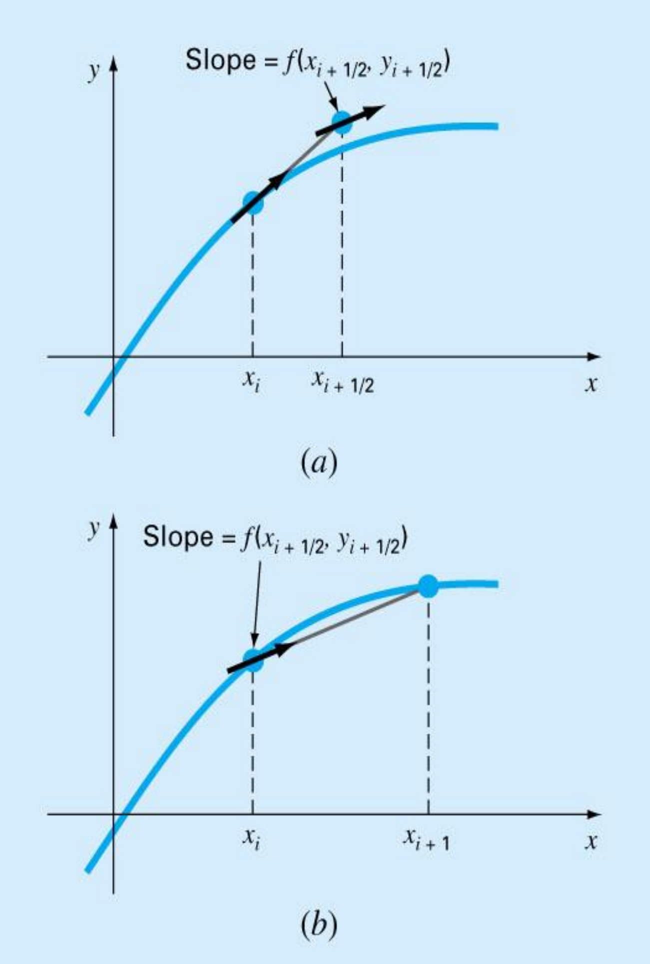
(*b*)

HEUN'S METHOD ITERATION



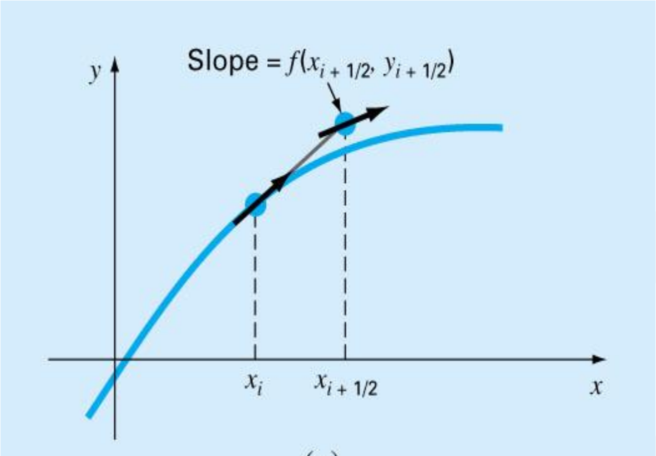
THE MIDPOINT (OR IMPROVED POLYGON) METHOD

- Uses Euler's method to predict a value of *y* at the midpoint of the interval.
- This value is substituted into the ODE to generate an improved slope which is then used to project from the beginning to the end of the interval.



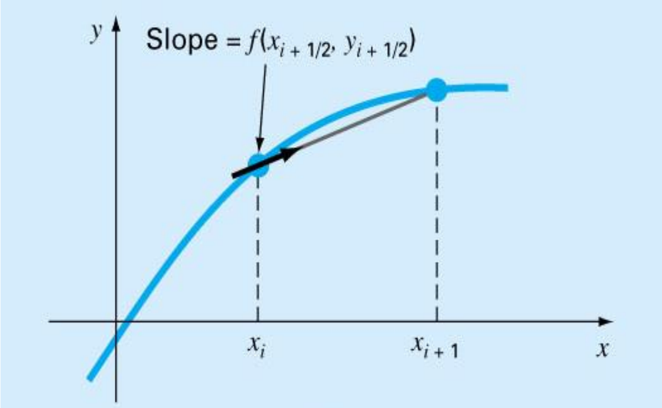
THE MIDPOINT (OR IMPROVED POLYGON) METHOD

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



(a)

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



(b)

RUNGE-KUTTA METHODS (R K)

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

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

  - Increment function

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

  - where *a's* = constants

$$\begin{aligned}
k_1 &= f(x_i, y_i) \\
k_2 &= f(x_i + p_1 h, y_i + q_{11} k_1 h) \\
k_3 &= f(x_i + p_3 h, y_i + q_{21} k_1 h + q_{22} k_2 h) \\
&\vdots \\
k_n &= f(x_i + p_{n-1} h, y_i + q_{n-1} k_1 h \\
&\qquad + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h)
\end{aligned}$$

RUNGE-KUTTA METHODS (R K)

- *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.

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h$$

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

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

DERIVATION OF A SECOND-ORDER R K METHOD

- Values of a_1, a_2, p_1, and q_{11} are evaluated by setting the second-order equation to a second-order Taylor series expansion. Comparing like terms leads to the following 3 equations to evaluate the 4 unknowns constants.

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

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

DERIVATION OF A SECOND-ORDER R K METHOD

Because we can choose an infinite number of values for a_2, there are an infinite number of second-order RK methods.

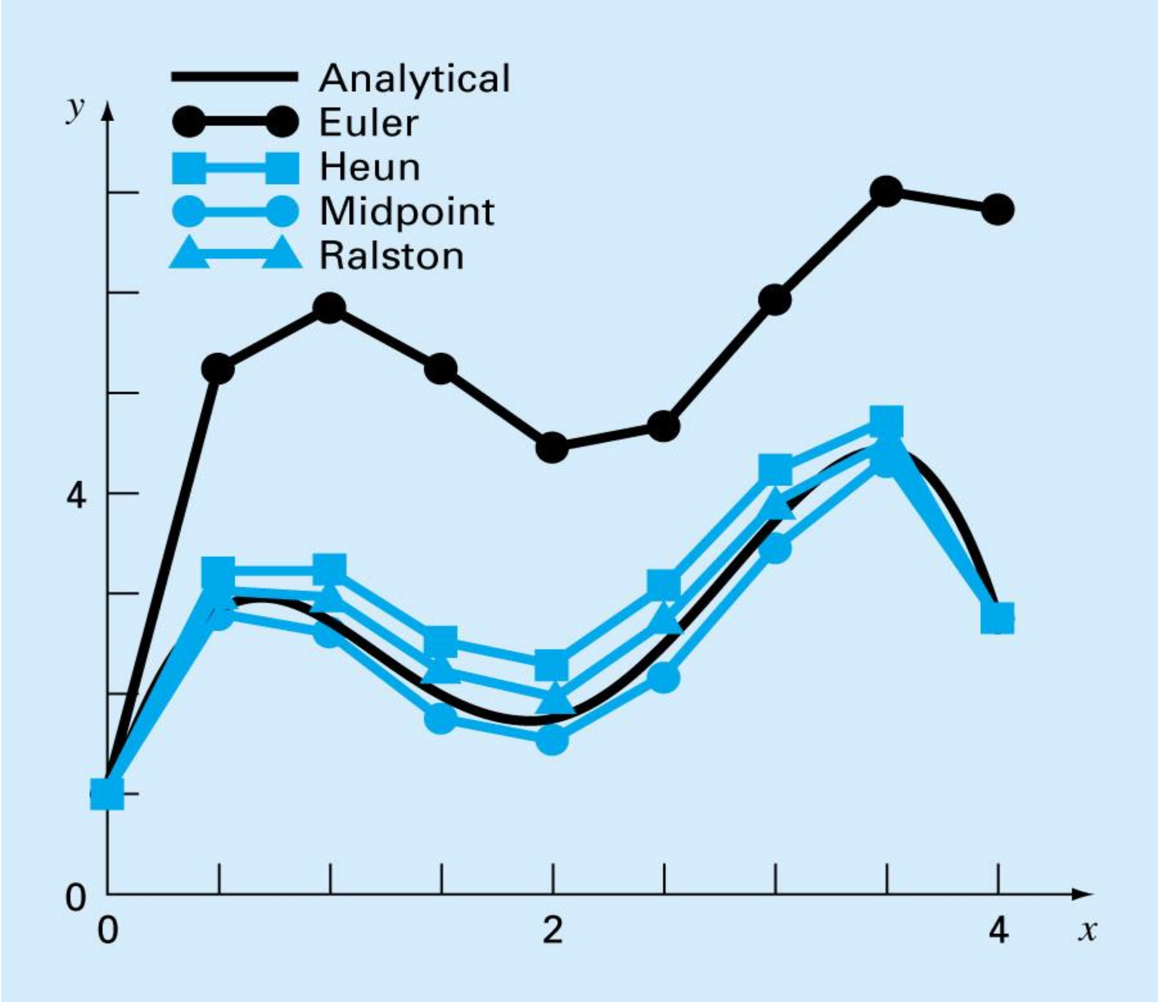
Every version would yield exactly the same results if the solution to ODE were quadratic, linear, or a constant.

However, they yield different results if the solution is more complicated (typically the case).

Three of the most commonly used methods are:

- Heun Method with a Single Corrector (a_2=1/2).
- The Midpoint Method (a_2=1).
- Ralston's Method (a_2=2/3).

DERIVATION OF A SECOND-ORDER R K METHOD



FOURTH-ORDER R K METHOD

Most popular RK method

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

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

$$k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$$

$$k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h)$$

$$k_4 = f(x_i + h, y_i + k_3 h)$$

SYSTEMS OF EQUATIONS

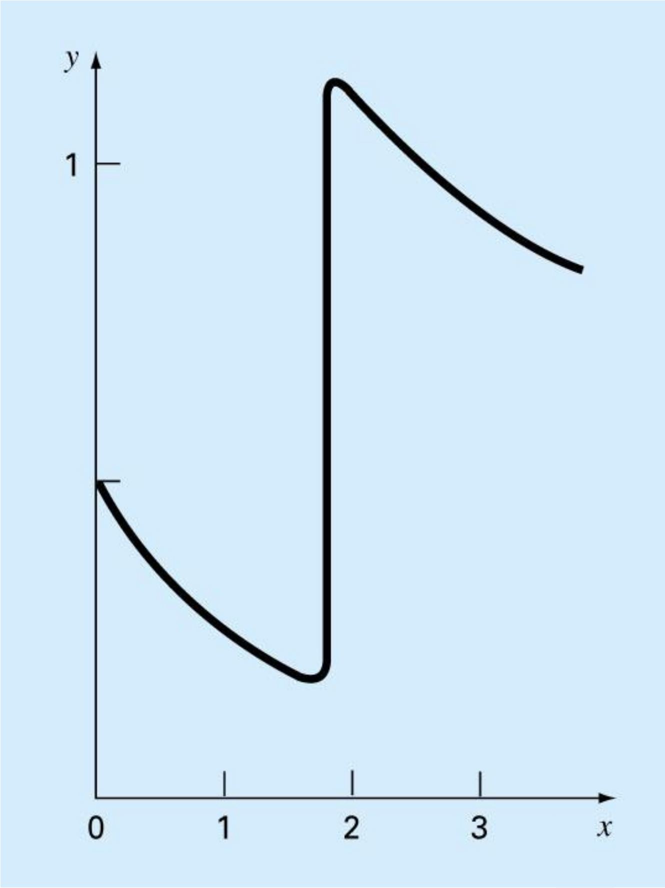
- Many practical problems in engineering and science require the solution of a system of simultaneous ordinary differential equations rather than a single equation:

$$\frac{dy_1}{dx} = f_1(x, y_1, y_2, \ldots, y_n)$$
$$\frac{dy_2}{dx} = f_2(x, y_1, y_2, \ldots, y_n)$$
$$\vdots$$
$$\frac{dy_n}{dx} = f_n(x, y_1, y_2, \ldots, y_n)$$

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

ADAPTIVE RUNGE-KUTTA METHODS

For an ODE with an abrupt changing solution, a constant step size can represent a serious limitation.



STEP-SIZE CONTROL OF RUNGE-KUTTA METHODS

- The strategy is to increase the step size if the error is too small and decrease it if the error is too large. Press et al. (1992) have suggested the following criterion to accomplish this:

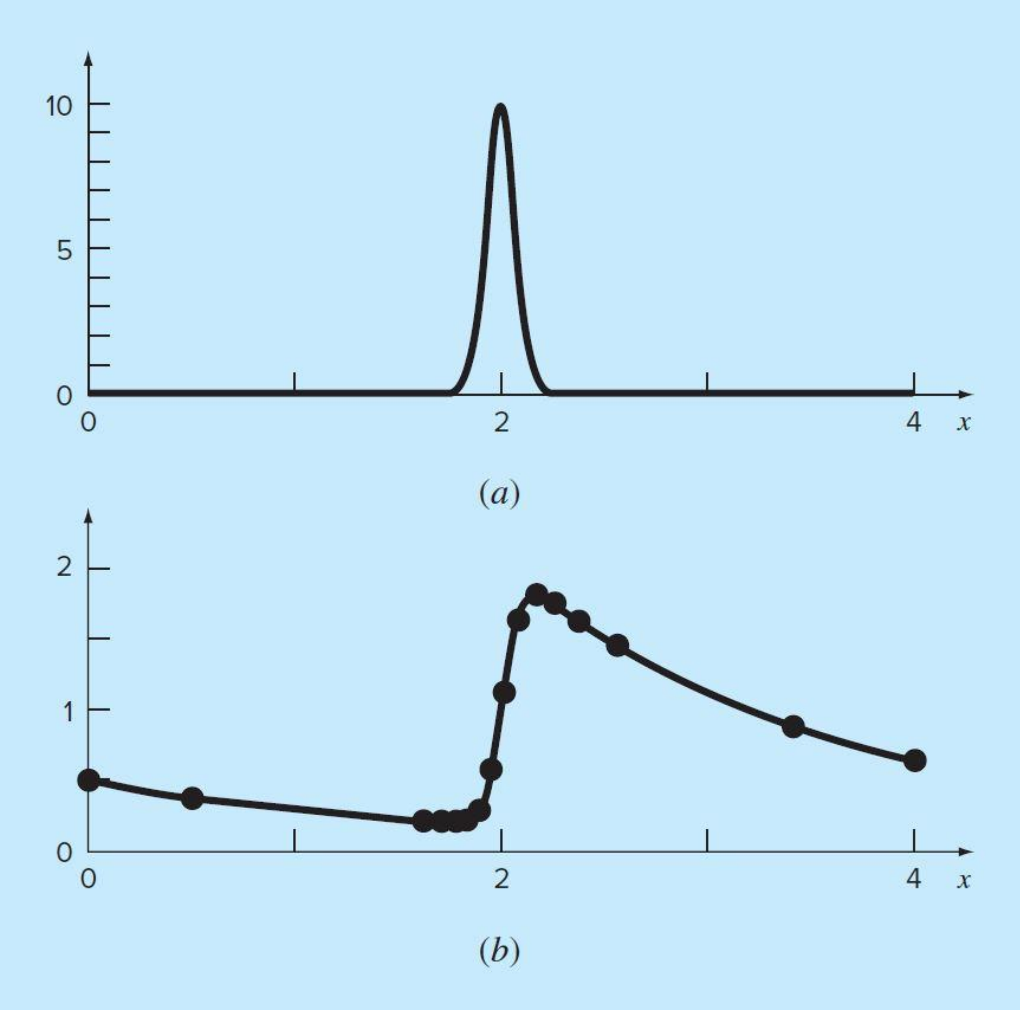
$$h_{\text{new}} = h_{\text{present}} \left| \frac{\Delta_{\text{new}}}{\Delta_{\text{present}}} \right|^{\alpha}$$

- $\Delta_{present}$ = computed present accuracy
- Δ_{new} = desired accuracy
- α = a constant power that is equal to 0.2 when step size increased and 0.25 when step size is decreased

STEP-SIZE CONTROL OF RUNGE-KUTTA METHODS

- Implementation of adaptive methods requires an estimate of the local truncation error at each step.
- The error estimate can then serve as a basis for either lengthening or decreasing step size.

THE RESULTS OF ADAPTIVE STEP-SIZE CONTROL



STIFFNESS

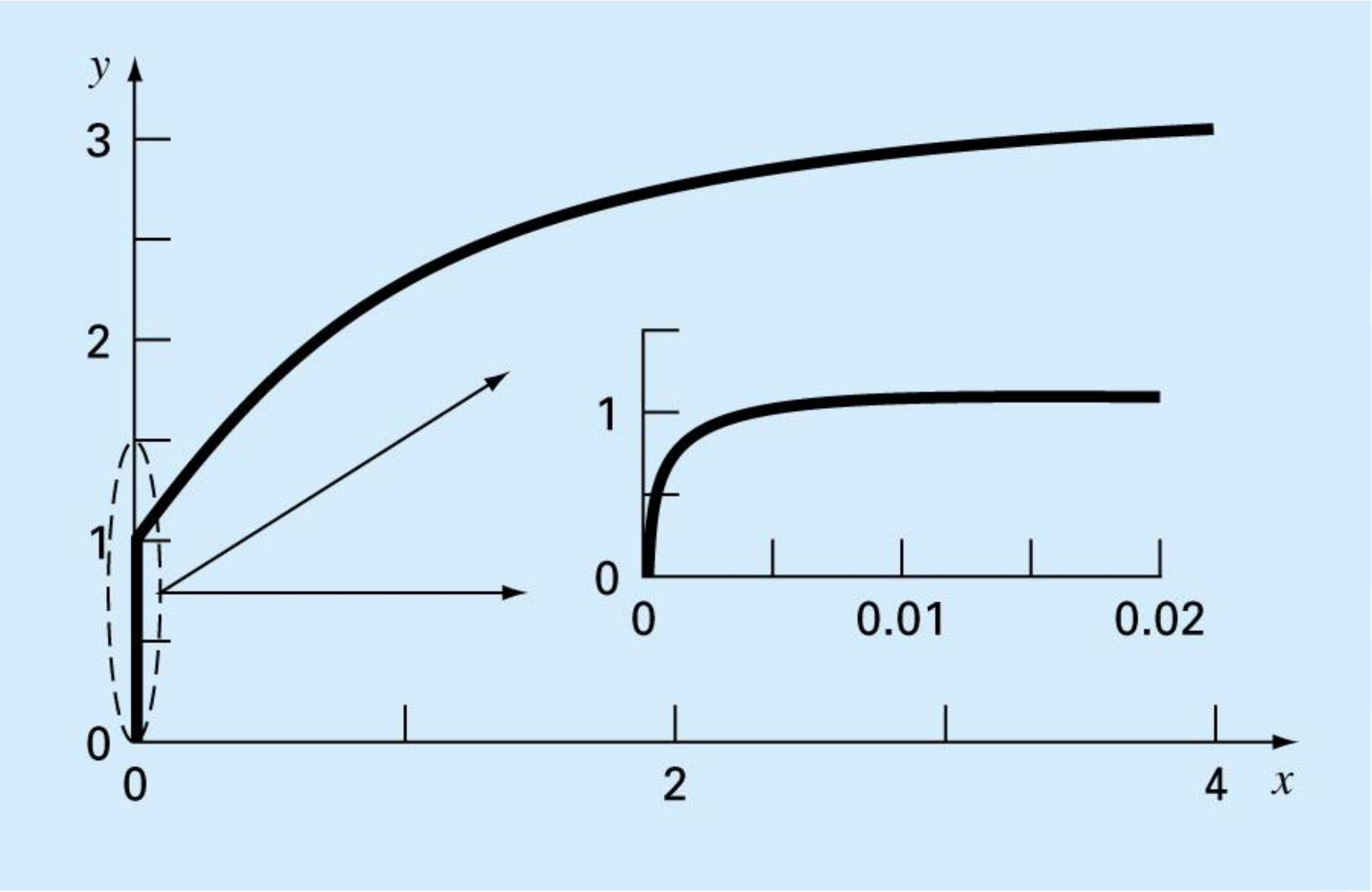
- A *stiff system* is the one involving rapidly changing components together with slowly changing ones.
- Both individual and systems of ODEs can be stiff:

$$\frac{dy}{dt} = -1000y + 3000 - 2000e^{-t}$$

- If $y(0) = 0$, the analytical solution is developed as:

$$y = 3 - 0.998e^{-1000t} - 2.002^{e-t}$$

STIFF SOLUTION OF AN ODE



ANALYSIS OF STABILITIES

- Insight into the step size required for stability of such a solution can be gained by examining the homogeneous part of the ODE:

$$\frac{dy}{dt} = -ay$$

- Given initial condition, $y = y_0$ at $t = 0$, the solution is

$$y = y_0 e^{-at}$$

- The solution starts at $y(0)=y_0$ and asymptotically approaches zero.

ANALYSIS OF STABILITY OF EXPLICIT EULER

- If the explicit form of Euler's method is used to solve the problem numerically:

$$y_{i+1} = y_i + \frac{dy_i}{dt} h$$

$$y_{i+1} = y_i - a y_i h \qquad \text{or} \qquad y_{i+1} = y_i (1 - ah)$$

- The stability of this formula depends on the step size *h*:

$$|1 - ah| < 1$$

$$h > 2/a \quad \Rightarrow \quad |y_i| \to \infty \quad \text{as} \quad i \to \infty$$

ANALYSIS OF STABILITY OF EXPLICIT EULER

- Thus, for transient part of the equation, the step size must be < 2/1000 = 0.002 to maintain stability.
- While this criterion maintains stability, an even smaller step size would be required to obtain an accurate solution.
- Rather than using explicit approaches, *implicit* methods offer an alternative remedy.
- An implicit form of Euler’s method can be developed by evaluating the derivative at a future time.

ANALYSIS OF STABILITY OF IMPLICIT EULER

- *Backward* or *implicit Euler's* method.

$$y_{i+1} = y_i + \frac{dy_{i+1}}{dt} h$$

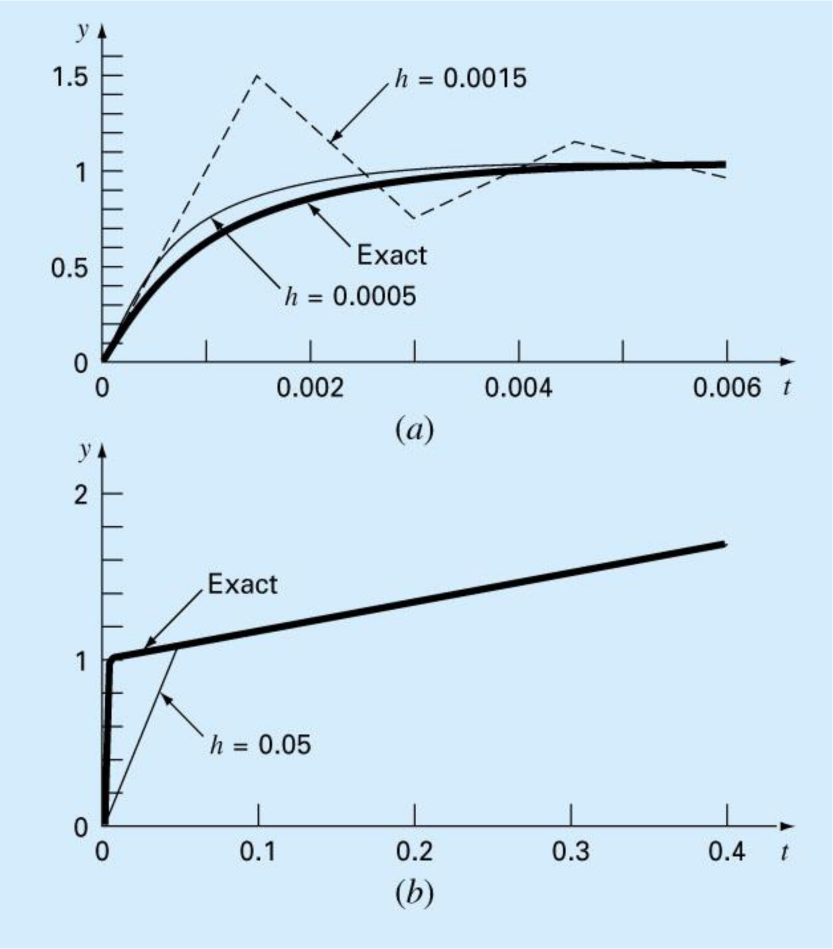
$$y_{i+1} = y_i - a y_{i+1} h$$

$$y_{i+1} = \frac{y_i}{1 + ah}$$

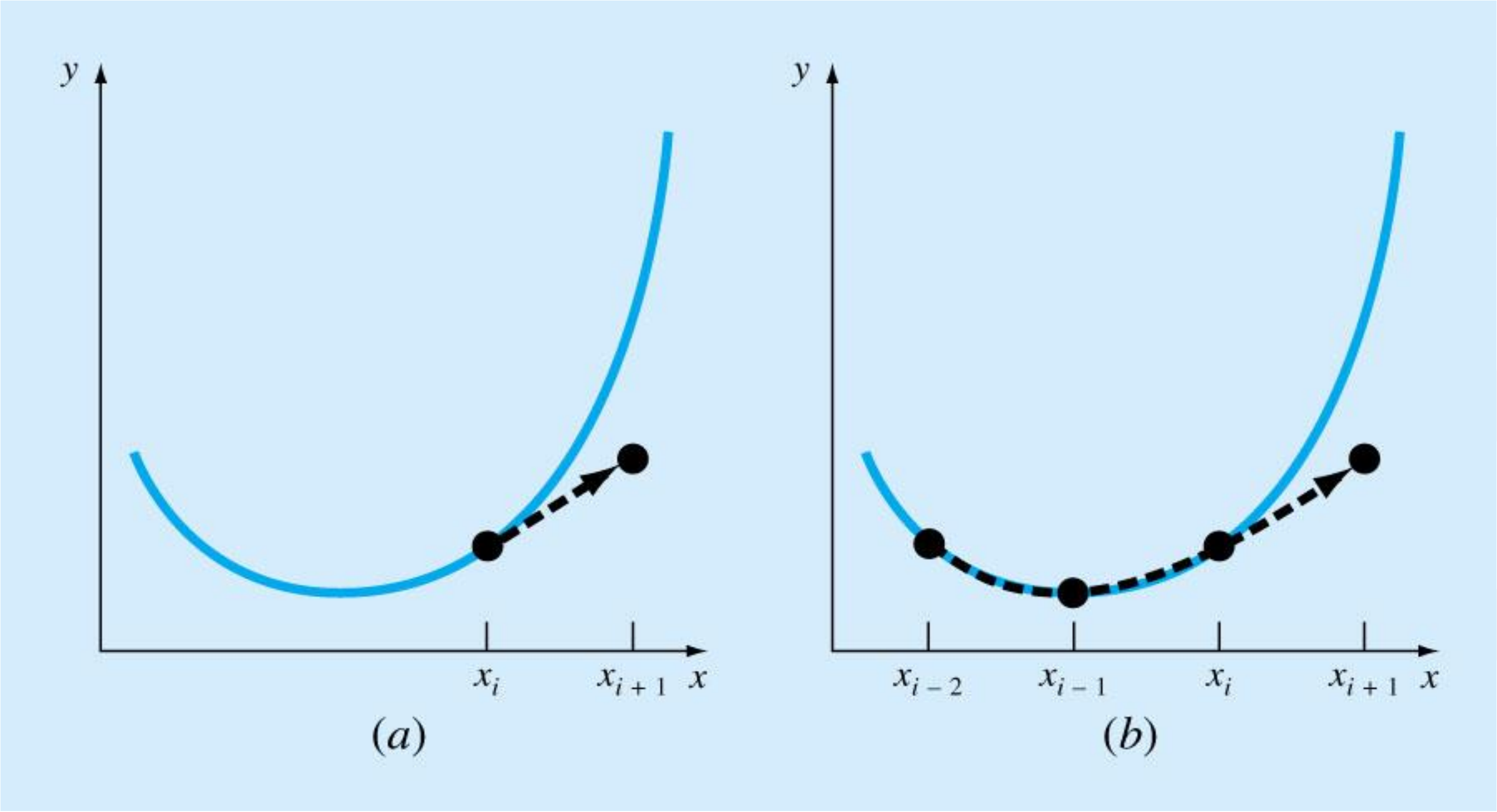
- The approach is called *unconditionally stable*. Regardless of the step size:

$$|y_i| \to 0 \quad as \quad i \to \infty$$

COMPARISON OF (A) EXPLICIT AND (B) IMPLICIT EULER SOLUTIONS



(A)ONE-STEP VERSUS
(B) MULTISTEP METHODS FOR SOLVING ODEs

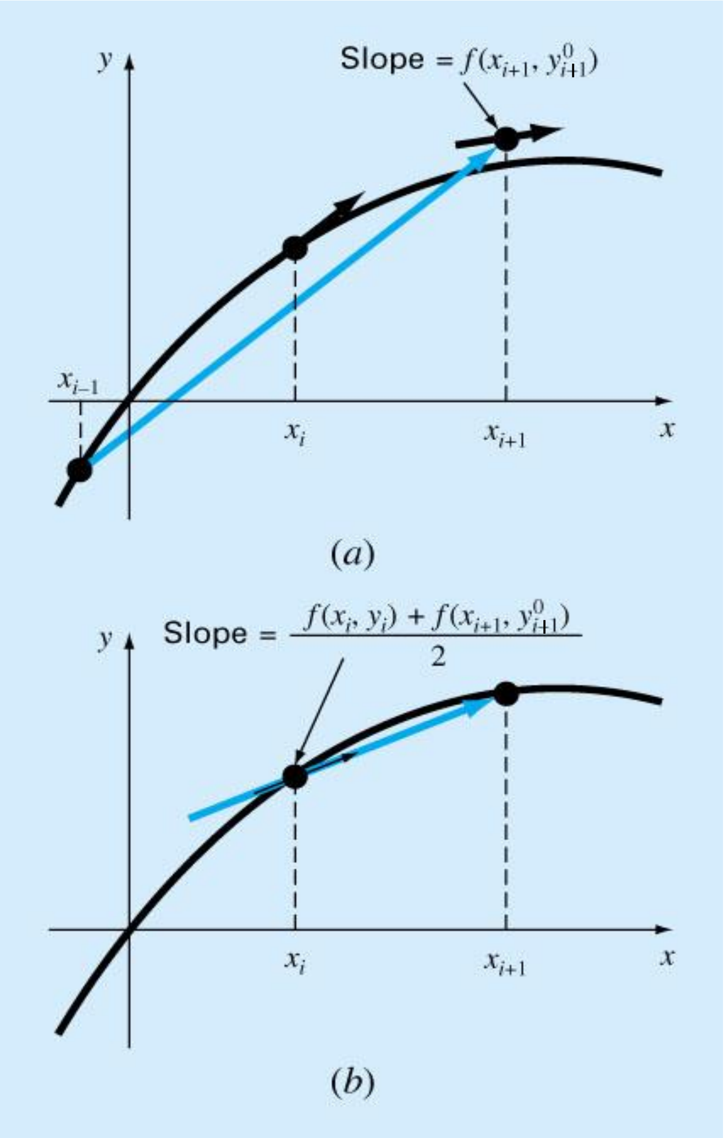


THE NON-SELF-STARTING HEUN METHOD

- Heun method uses *Euler's method* as a *predictor* and *trapezoidal rule* as a *corrector*.
- Predictor is the weak link in the method because it has the greatest error, $O(h^2)$.
- One way to improve Heun's method is to develop a predictor that has a local error of $O(h^3)$.

$$y_{i+1}^{0} = y_{i-1} + f(x_i, y_i)2h$$

THE NON-SELF-STARTING HEUN METHOD



STEP-SIZE CONTROL OF NON-SELF-STARTING HEUN METHOD

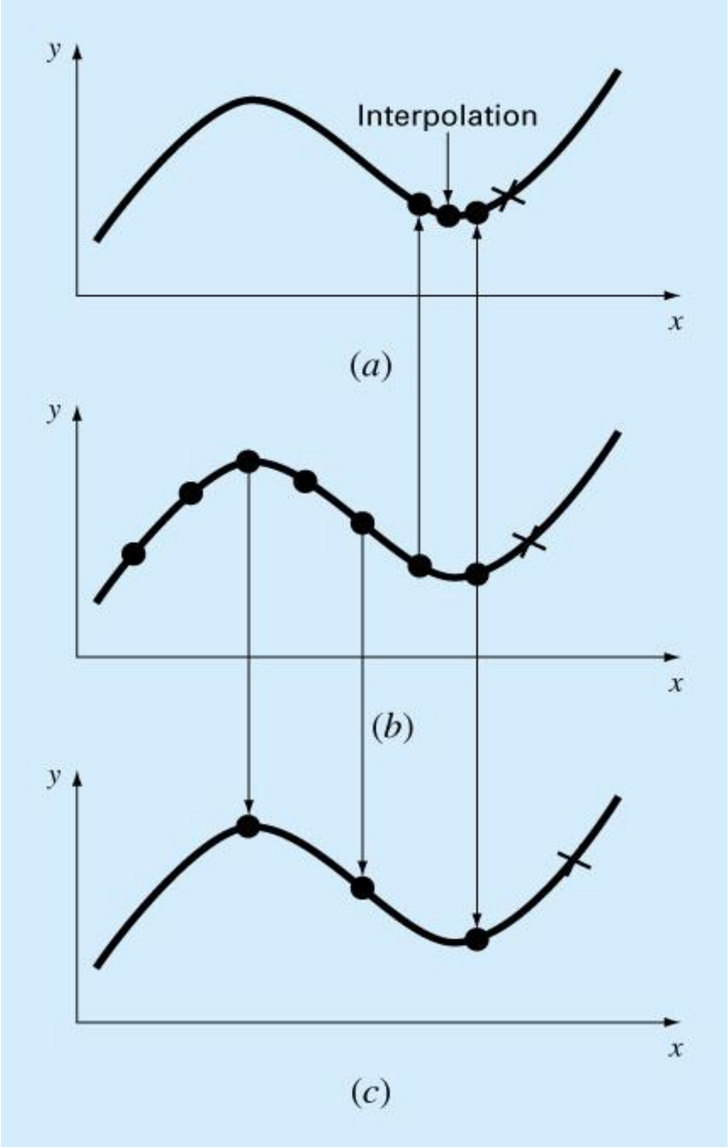
Constant Step Size.

- A value for h must be chosen prior to computation.
- It must be small enough to yield a sufficiently small truncation error.
- It should also be as large as possible to minimize run time cost and round-off error.

Variable Step Size.

- If the corrector error is greater than some specified error, the step size is decreased.
- A step size is chosen so that the convergence criterion of the corrector is satisfied in two iterations.
- Efficient strategy is to increase and decrease by doubling and halving the step size.

ADVANTAGE OF HALVING AND DOUBLING STEP SIZE



NEWTON-COTES FORMULAS

Open Formulas

$$y_{i+1} = y_{i-n} + \int_{x_{i-n}}^{x_{i+1}} f_n(x)\,dx$$

where $f_n(x)$ is an n^{th} order interpolating polynomial.

Closed Formulas

$$y_{i+1} = y_{i-n+1} + \int_{x_{i-n+1}}^{x_{i+1}} f_n(x)\,dx$$

ADAMS FORMULAS (ADAMS-BASHFORTH)

Open Formulas.

- The Adams formulas can be derived in a variety of ways. One way is to write a forward Taylor series expansion around x_i. A second order open Adams formula:

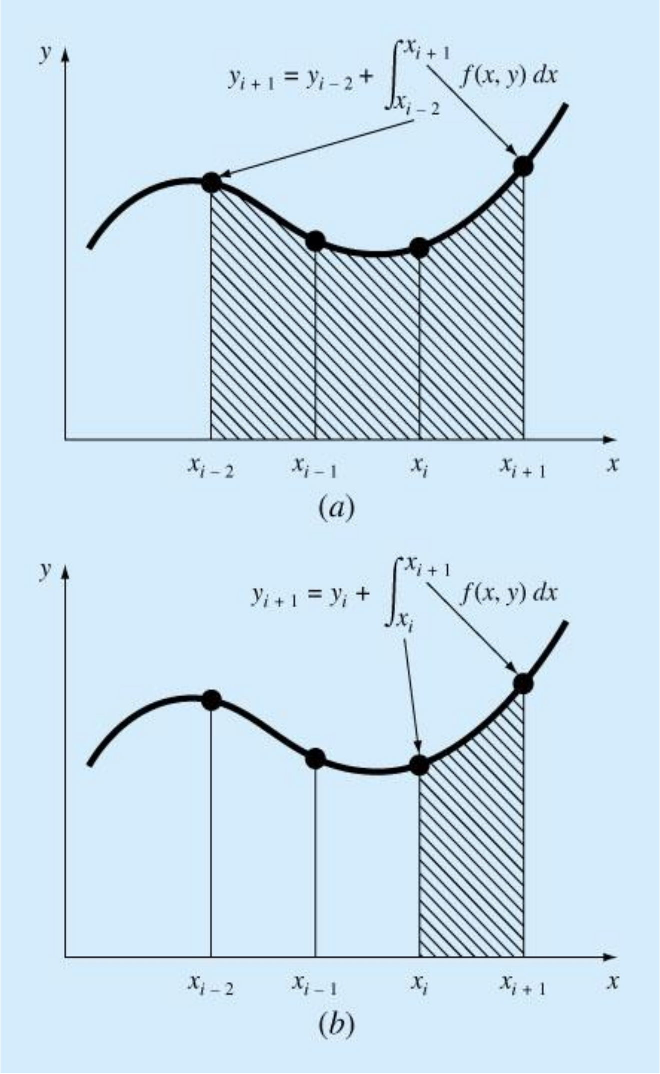
$$y_{i+1} = y_i + h\left(\frac{3}{2} f_i - \frac{1}{2} f_{i-1}\right) + \frac{5}{12} h^3 f_i'' + O(h^4)$$

- *Closed Formulas.*
- A backward Taylor series around x_{i+1} can be written:

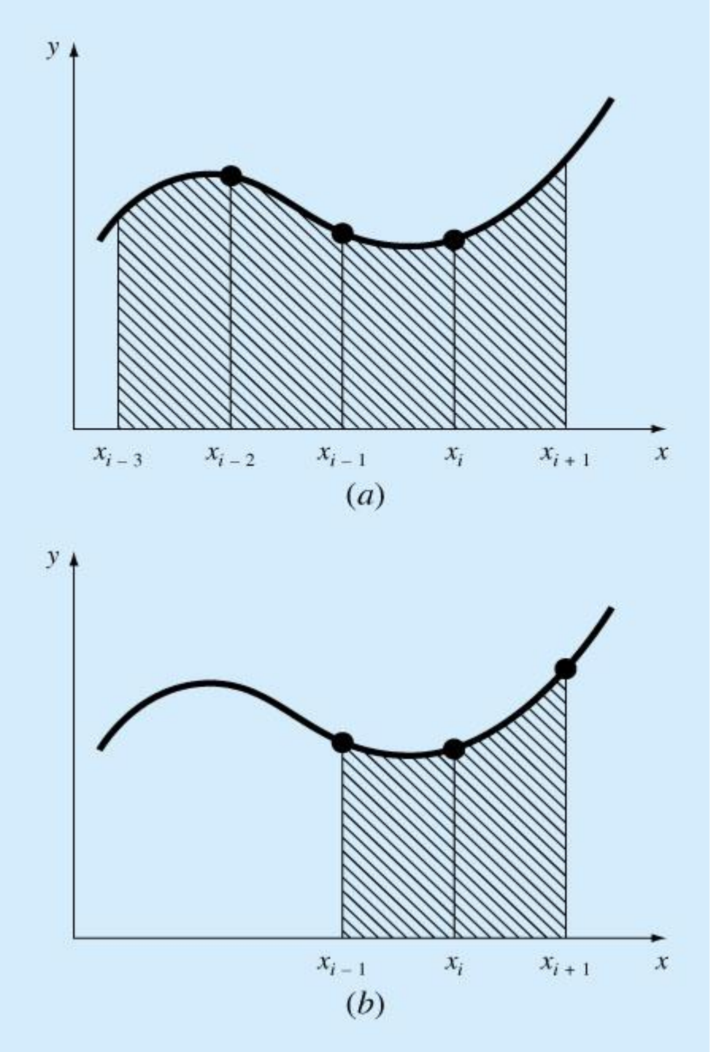
$$y_{i+1} = y_i + h\sum_{k=0}^{n-1} \beta_k f_{i+1-k} + O(h^{n+1})$$

Coefficients for Adams-Bashforth predictors

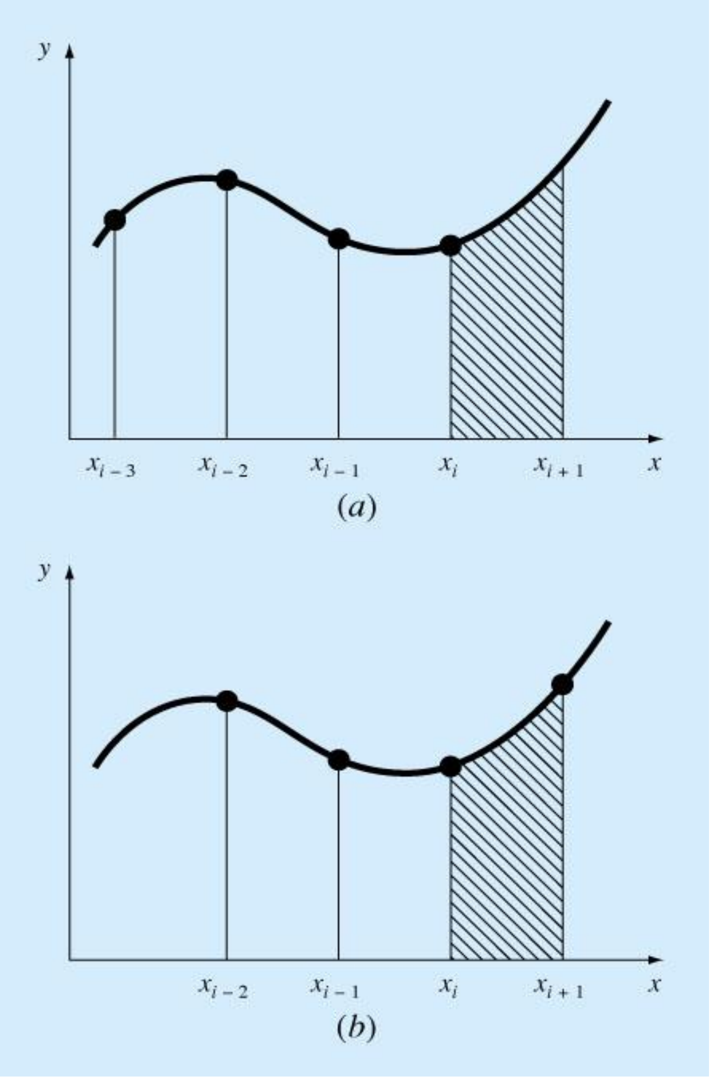
(A) NEWTON-COTES VERSUS
(B) ADAMS INTEGRATION FORMULAS



(A) OPEN & (B) CLOSED NEWTON-COTES INTEGRATION FORMULAS



(A) OPEN VERSUS (B) CLOSED ADAMS INTEGRATION FORMULAS



HIGHER-ORDER MULTISTEP METHODS

Milne's Method

- Uses the three point Newton-Cotes open formula as a predictor and three point Newton-Cotes closed formula as a corrector.

Fourth-Order Adams Method

- Based on the Adams integration formulas. Uses the fourth-order Adams-Bashforth formula as the predictor and fourth-order Adams-Moulton formula as the corrector.