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MATEMÁTICA APLICADA I

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Source:
Chapra, Numerical Methods for Engineers, 2008

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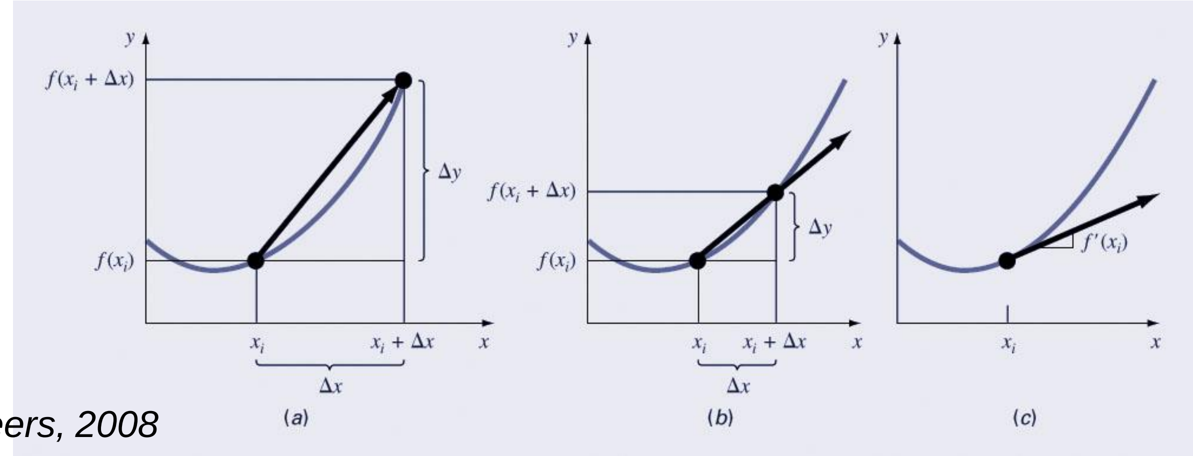
Differentiation

The mathematical definition of a derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

and as Δx is allowed to approach zero, the difference becomes a derivative:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



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High-Accuracy Differentiation Formulas

Taylor series expansion can be used to generate high-accuracy formulas for derivatives by using linear algebra to combine the expansion around several points.

Three categories for the formula include *forward finite-difference*, *backward finite-difference*, and *centered finite-difference*.

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Forward Finite-Difference

First Derivative	Error
$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

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Backward Finite-Difference

	Error
First Derivative	
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

Source: Chapra, Numerical Methods for Engineers, 2008

Centered Finite-Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

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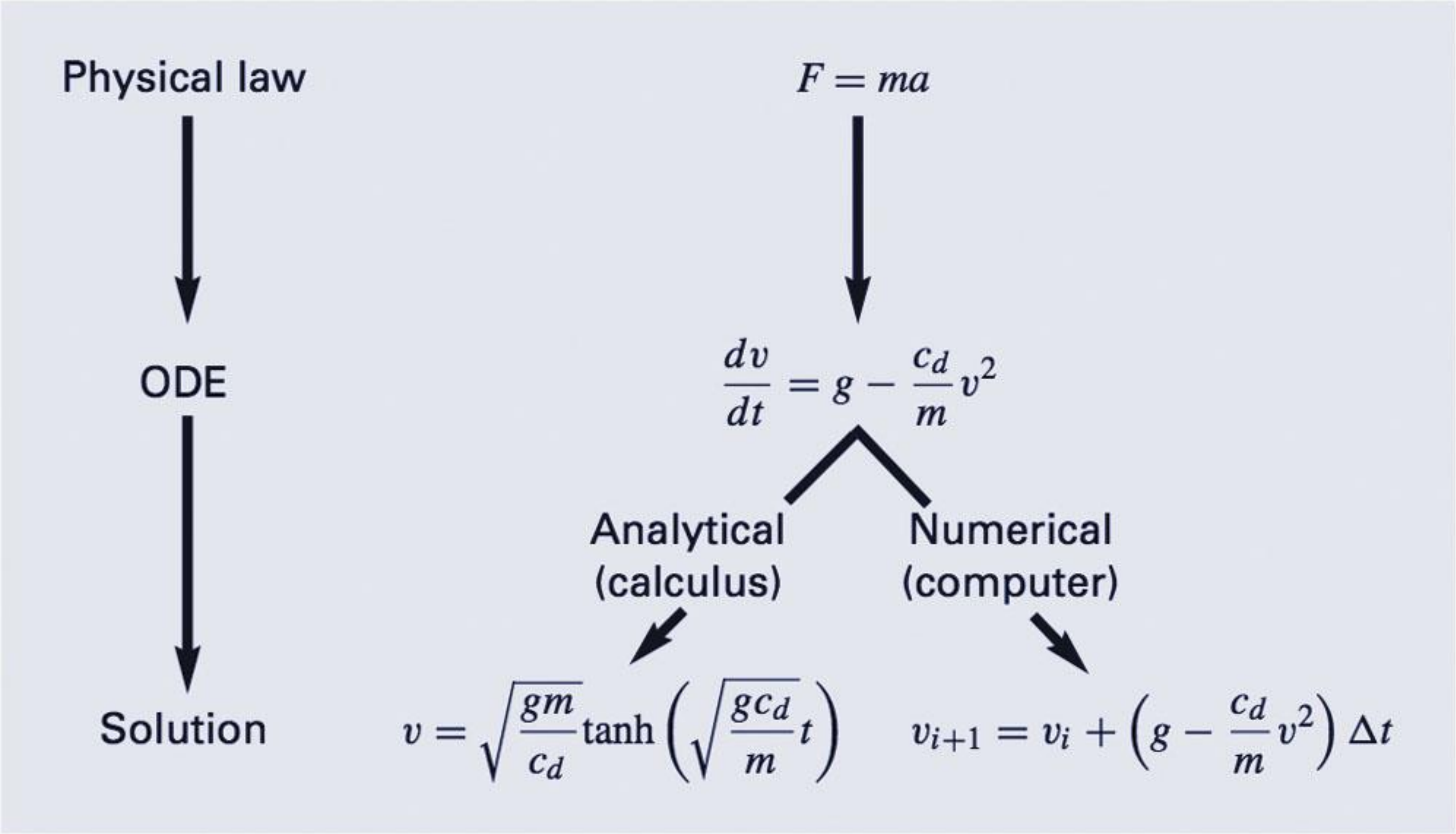


Ordinary Differential Equations

- Methods described here are for solving differential equations of the form:

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

- The methods in this chapter are all *one-step* methods and have the general format:

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

where ϕ is called an *increment function*, and is used to extrapolate from an old value y_i to a new value y_{i+1}.

Euler's Method

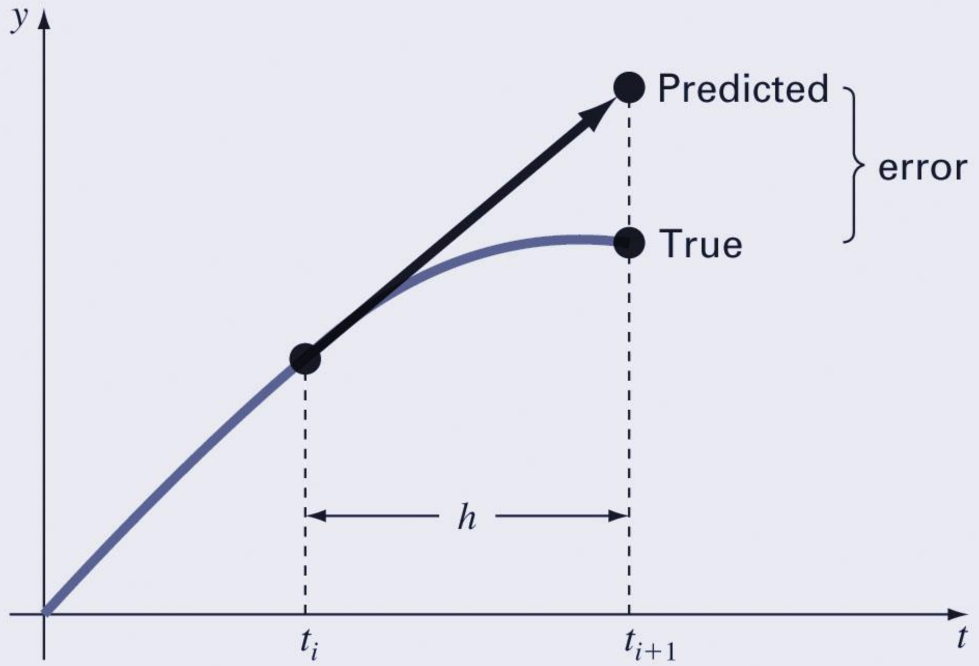
- The first derivative provides a direct estimate of the slope at t_i:

$$\left.\frac{dy}{dt}\right|_{t_i} = f(t_i, y_i)$$

and the Euler method uses that estimate as the increment function:

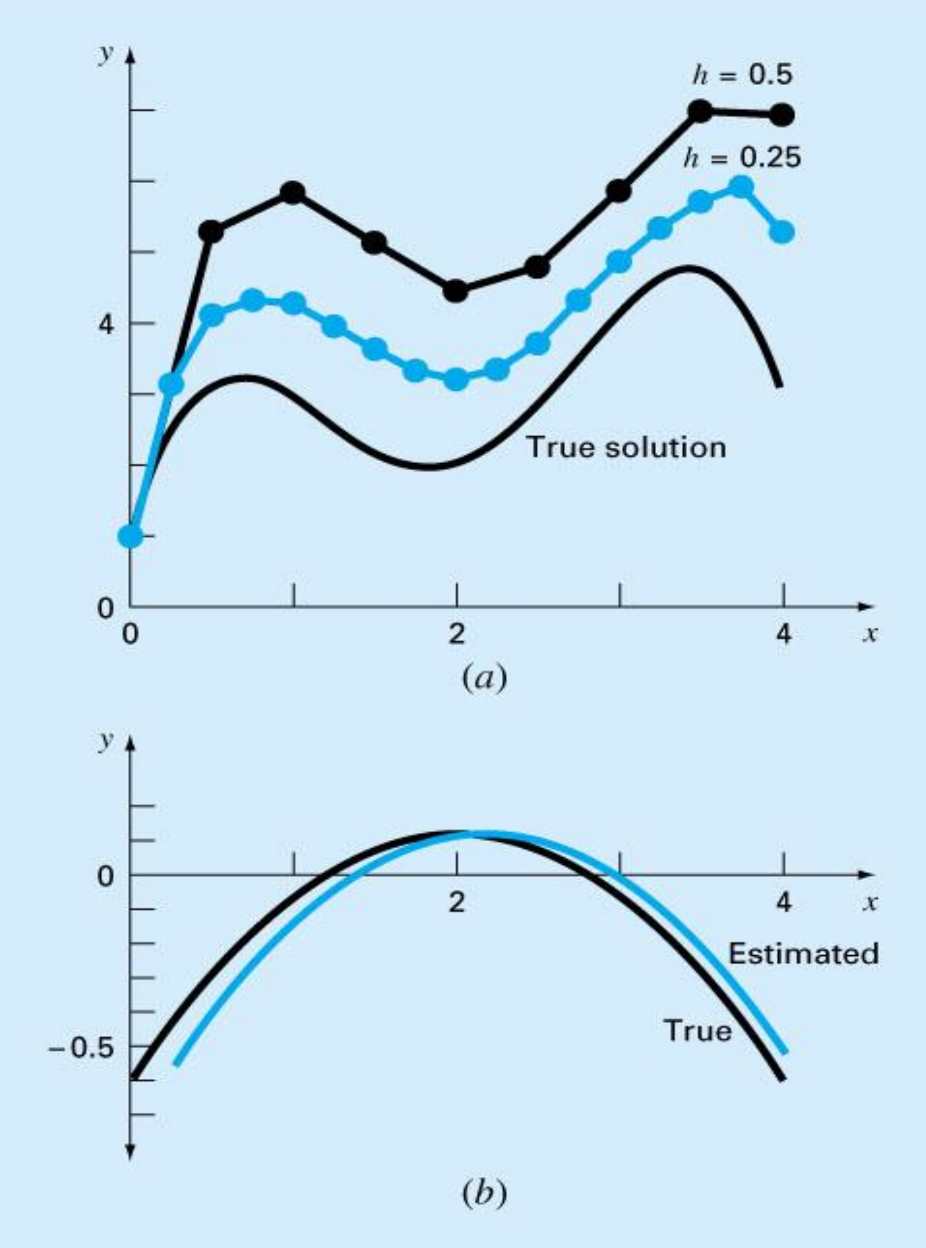
$$\phi = f(t_i, y_i)$$

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




y
60
40
20
0
True solution
Euler solution
0
1
2
3
4
t

Figure 25.4



Error Analysis for Euler's Method

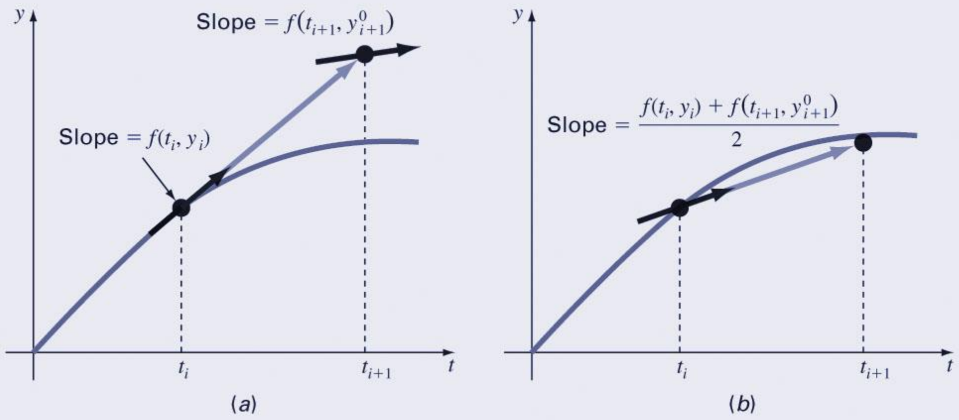
- The numerical solution of ODEs involves two types of error:
  - *Truncation errors*, caused by the nature of the techniques employed
  - *Roundoff errors*, caused by the limited numbers of significant digits that can be retained
- The total, or *global* truncation error can be further split into:
  - *local truncation error* that results from an application method in question over a single step, and
  - *propagated truncation error* that results from the approximations produced during previous steps.

Error Analysis for Euler's Method

- The local truncation error for Euler's method is $O(h^2)$ and proportional to the derivative of $f(t,y)$ while the global truncation error is $O(h)$.
- This means:
  - The global error can be reduced by decreasing the step size, and
  - Euler's method will provide error-free predictions if the underlying function is linear.
- Euler's method is *conditionally stable*, depending on the size of h.

Heun’s Method

- One method to improve Euler’s method is to determine derivatives at the beginning and predicted ending of the interval and average them:

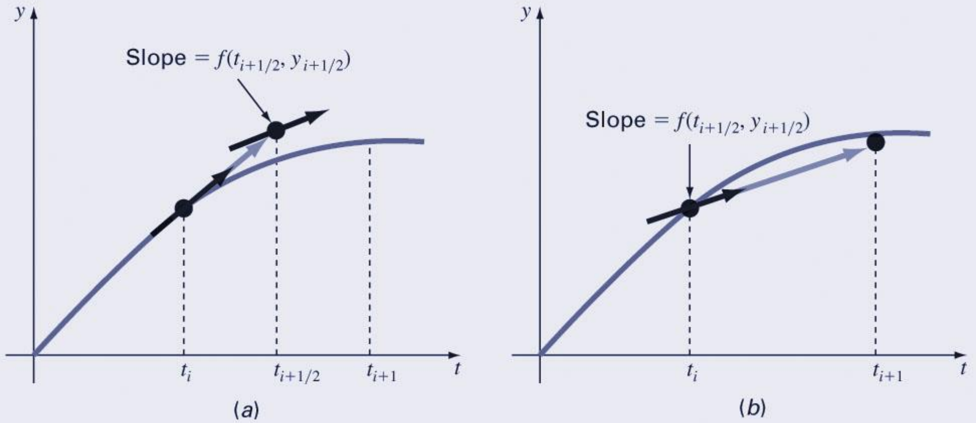


- This process relies on making a prediction of the new value of *y*, then correcting it based on the slope calculated at that new value.
- This predictor-corrector approach can be iterated to convergence:

$$y^j_{i+1} \longleftarrow y^m_i + \frac{f(t_i, y^m_i) + f(t_{i+1}, y^{j-1}_{i+1})}{2} h$$

Midpoint Method

- Another improvement to Euler's method is similar to Heun's method, but predicts the slope at the midpoint of an interval rather than at the end:



- This method has a local truncation error of $O(h^3)$ and global error of $O(h^2)$

Runge-Kutta Methods

- Runge-Kutta (RK) methods achieve the accuracy of a Taylor series approach without requiring the calculation of higher derivatives.
- For RK methods, the increment function ϕ can be generally written as:

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

where the *a*'s are constants and the *k*'s are

$$\begin{aligned}
k_1 &= f(t_i, y_i) \\
k_2 &= f(t_i + p_1 h, y_i + q_{11} k_1 h) \\
k_3 &= f(t_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h) \\
&\vdots \\
k_n &= f(t_i + p_{n-1} h, y_i + q_{n-1,1} k_1 h + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h)
\end{aligned}$$

where the *p*'s and *q*'s are constants.

Classical Fourth-Order Runge-Kutta Method

- The most popular RK methods are fourth-order, and the most commonly used form is:

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

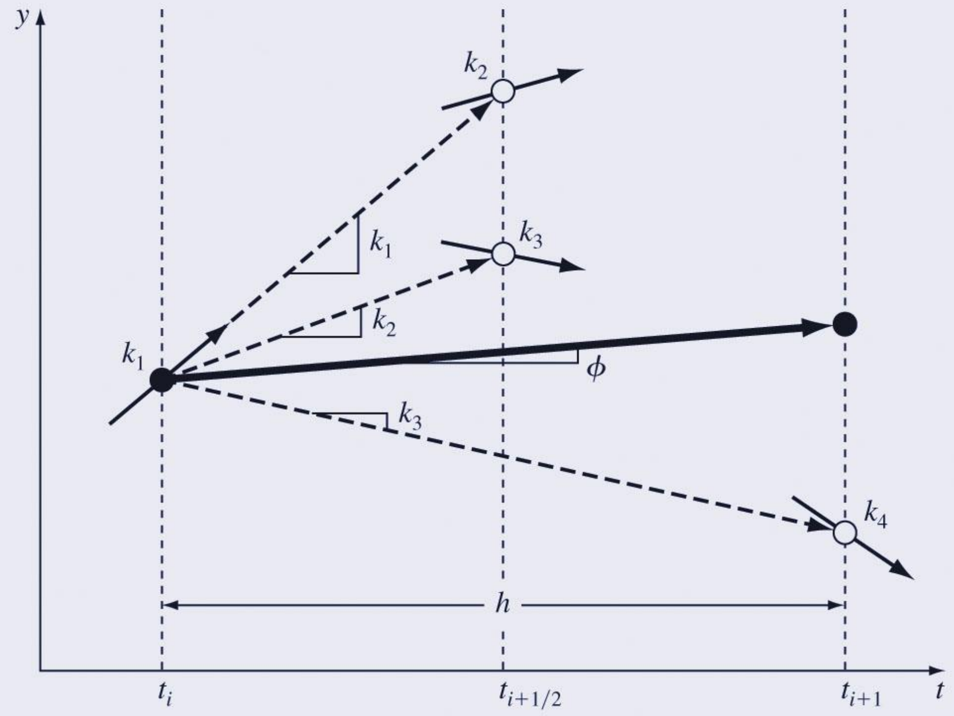
where:

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

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

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

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

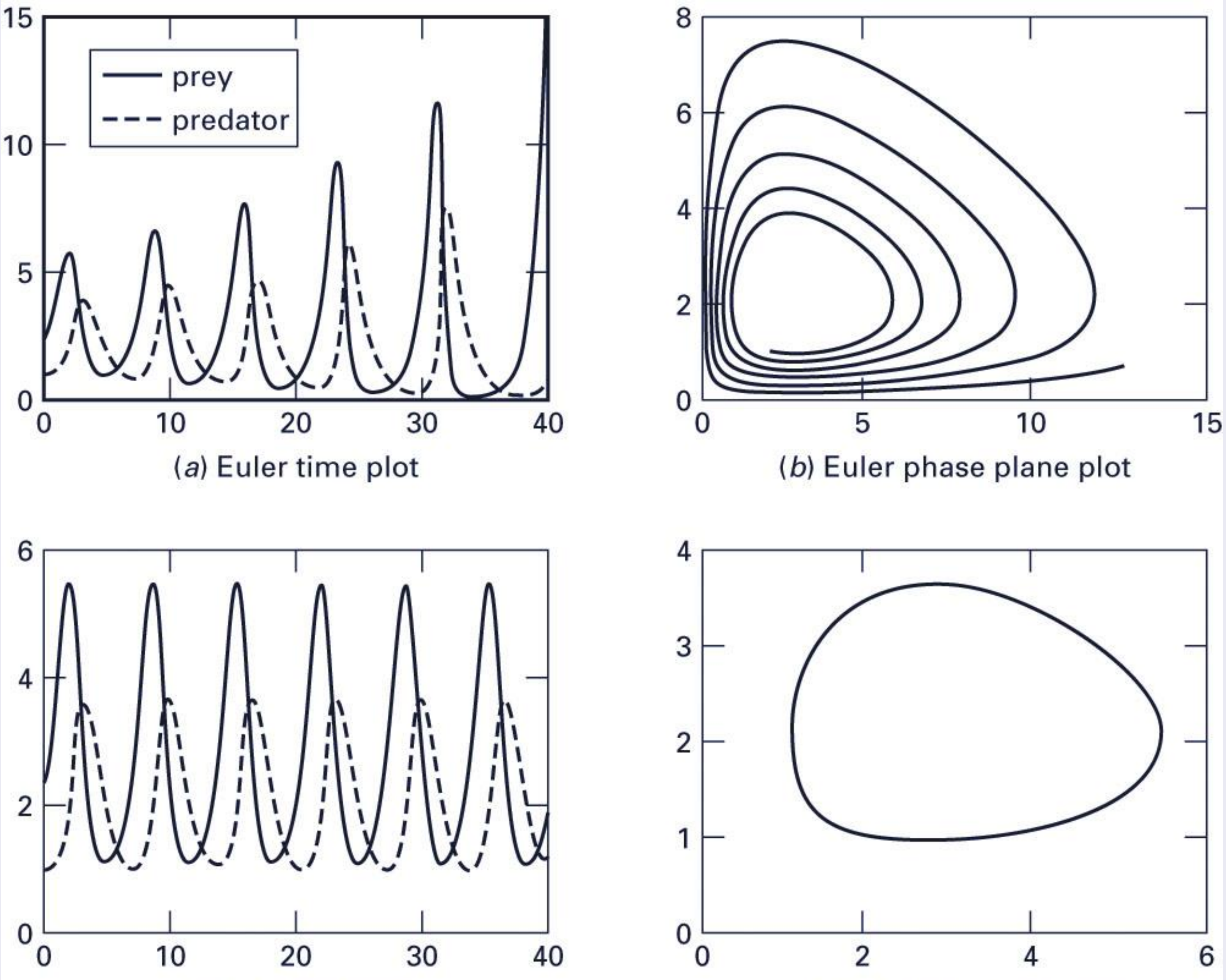


Systems of Equations

- Many practical problems require the solution of a *system* of equations:

$$\frac{dy_1}{dt} = f_1(t, y_1, y_2, \cdots, y_n)$$
$$\frac{dy_2}{dt} = f_2(t, y_1, y_2, \cdots, y_n)$$
$$\vdots$$
$$\frac{dy_n}{dt} = f_n(t, y_1, y_2, \cdots, y_n)$$

- The solution of such a system requires that *n* initial conditions be known at the starting value of *t*.



(*a*) Euler time plot

(*b*) Euler phase plane plot

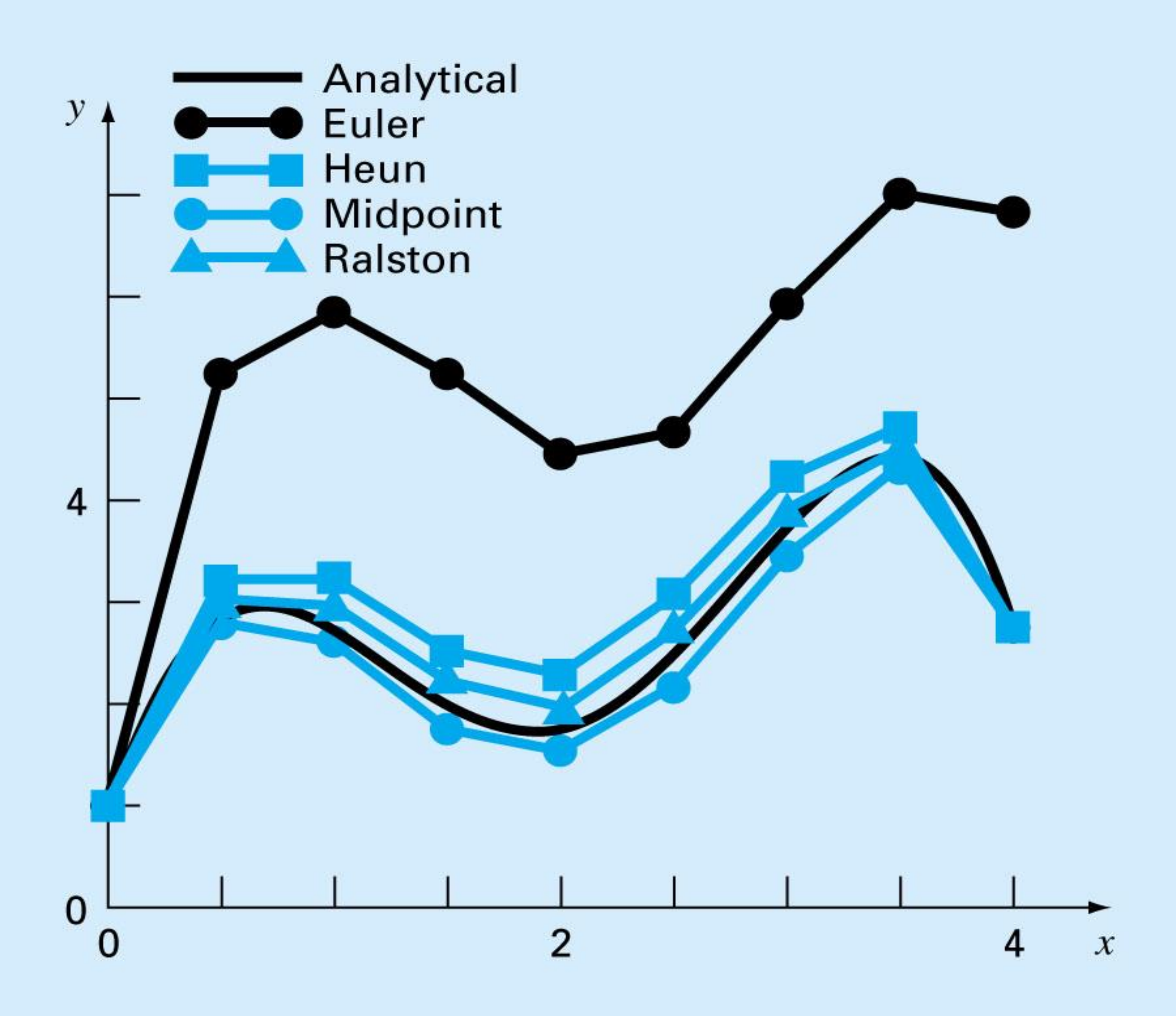
(*c*) RK4 time plot

(*d*) RK4 phase plane plot

Solution Methods

- Single-equation methods can be used to solve systems of ODE’s as well; for example, Euler’s method can be used on systems of equations - the one-step method is applied for every equation at each step before proceeding to the next step.
- Fourth-order Runge-Kutta methods can also be used, but care must be taken in calculating the *k*’s.

Figure 25.14



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