§7.1 Initial Value Problems

- Solve $\vec{y}' = \vec{F}(x, \vec{y}), \vec{y}(a) = \vec{\alpha}$.
- We call $y' = f(x, y)$ a <u>first-order</u> differential equation, where $y' = \dfrac{dy}{dx}$ and $f(x, y)$ are given.
- The solution contains an integration constant, so to find this constant we need to know a point on the solution curve: $y(a) = \alpha$.

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ODEs

- Ordinary differential equation (ODE) of order *n*:

$$y^{(n)} = f(x, y, y', y'', \ldots, y^{(n-1)})$$

- Can be transformed into *n* first-order equations:

$$\text{Let} \quad \begin{aligned} y_0 &= y \\ y_1 &= y' \\ y_2 &= y'' \\ &\vdots \\ y_{n-1} &= y^{(n-1)} \end{aligned} \qquad \text{Then,} \quad \begin{aligned} y_0' &= y_1 \\ y_1' &= y_2 \\ y_2' &= y_3 \\ &\vdots \\ y_{n-1}' &= f(x, y_0, y_1, y_2, \ldots, y_{n-1}) \end{aligned}$$

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IVPs

- For an initial value problem (IVP) we also have:

$$\left.\begin{aligned} y_0(a) &= \alpha_0 \\ y_1(a) &= \alpha_1 \\ y_2(a) &= \alpha_2 \\ &\vdots \\ y_{n-1}(a) &= \alpha_{n-1} \end{aligned}\right\} \text{All given at same value, x= } \alpha$$

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BVPs

- For a boundary value problem (BVP), the y_i are specified at different values of x:

IVP	BVP
$y'' = -y$	$y'' = -y$
$y(0) = 1$	$y(0) = 1$
$y'(0) = 0$	$y(\pi) = 0$

Notation

- A set of n first-order ODE's: $\vec{y}' = \vec{F}'(x, \vec{y}),\ \vec{y}(a) = \vec{\alpha}$,

$$\vec{F}'(x, \vec{y}) = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ f(x, \vec{y}) \end{bmatrix}.$$

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§7.2 Taylor Series Method

- Simple with fairly good accuracy.
- Consider Taylor Series (TS) for $\vec{y}$ about x:

$$\vec{y}(x+h) \approx \vec{y}(x) + \vec{y}'(x)h +$$

$$\frac{1}{2!}\vec{y}''(x)h^2 + \frac{1}{3!}\vec{y}'''(x)h^3 + \cdots + \frac{1}{m!}\vec{y}^{(m)}(x)h^m$$

Truncation Error: $E = \frac{1}{(m+1)!}\vec{y}^{(m+1)}(\xi)h^{m+1}, x < \xi < x+h$.

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Taylor Series Method

- Taylor Series (TS) for $\vec{y}$ about x yields a prediction for $\vec{y}$ at x+h given $\vec{y}(x)$ and its derivatives at x.
- Using FDA we have $\vec{y}^{(m+1)}(\xi) \approx \dfrac{\vec{y}^{(m)}(x+h) - \vec{y}^{(m)}(x)}{h}$, so truncation error becomes

$$E = \frac{h^m}{(m+1)!}\left[\vec{y}^{(m)}(x+h) - \vec{y}^{(m)}(x)\right].$$

A way to monitor error at each integration step.

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Taylor Series Example

- Example 7.1 (pp. 250-251) $y' + 4y = x^2, y(0) = 1$
  Determine y(0.1) with the 4th-order TS method using a single integration step. Estimate the error and compare with the actual error.

  Analytical solution of the ODE is:

$$y(x) = \frac{31}{32}e^{-4x} + \frac{1}{4}x^2 - \frac{1}{8}x + \frac{1}{32}.$$

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Taylor Series Example

- 4th-order TS method:

$$y(h) = y(0) + y'(0)h + \frac{1}{2!}y''(0)h^2 + \frac{1}{3!}y'''(0)h^3 + \frac{1}{4!}y^{(4)}(0)h^4$$

Using the original ODE we have…

$$y' = -4y + x^2$$

$$y'' = -4y' + 2x = -4(-4y + x^2) + 2x = 16y - 4x^2 + 2x$$

$$y''' = 16y' - 8x + 2 = -64y + 16x^2 - 8x + 2$$

$$y^{(4)} = -64y' + 32x - 8 = 256y - 64x^2 + 32x - 8$$

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Taylor Series Example

- At x=0, we have…

$$y'(0) = -4y(0) + (0)^2 = -4(1) = -4$$

$$y''(0) = 16y(0) - 4(0)^2 + 2(0) = 16$$

$$y'''(0) = -64y(0) + 16(0)^2 - 8(0) + 2 = -62$$

$$y^{(4)}(0) = 256y(0) - 64(0)^2 + 32(0) - 8 = 248$$

So, $$y(0.1) = 1 + (-4)(0.1) + \frac{1}{2!}(16)(0.1)^2 + \frac{1}{3!}(-62)(0.1)^3 + \frac{1}{4!}(248)(0.1)^4$$

$$= 0.6707$$

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Taylor Series Example

- For the error, we have $E = \frac{h^4}{5!}\left[\vec{y}^{(4)}(0.1) - \vec{y}^{(4)}(0)\right]$,
  where
  $$y^{(4)}(0) = 248,$$
  $$y^{(4)}(0.1) = 256(0.6707) - 64(0.1)^2 + 32(0.1) - 8$$
  $$= 166.259$$

So, $E = \frac{(0.1)^4}{5!}(166.259 - 248) = -6.8 \times 10^{-5}$

Using analytical solution, y(0.1)=0.670623 so actual error is

$$0.670623 - 0.670700 = -7.7 \times 10^{-5}$$

§7.3 Runge-Kutta Methods

- Taylor Series (TS) requires repeated differentiation (error-prone and tedious).
- RK methods are designed to eliminate the need for repeated differentiation.
- First-order RK method is equivalent to first-order Taylor Series integration: $\vec{y}(x+h)=\vec{y}(x)+\vec{y}'(x)h$

$$\vec{y}(x+h)=\vec{y}(x)+\vec{F}(x,\vec{y})h$$

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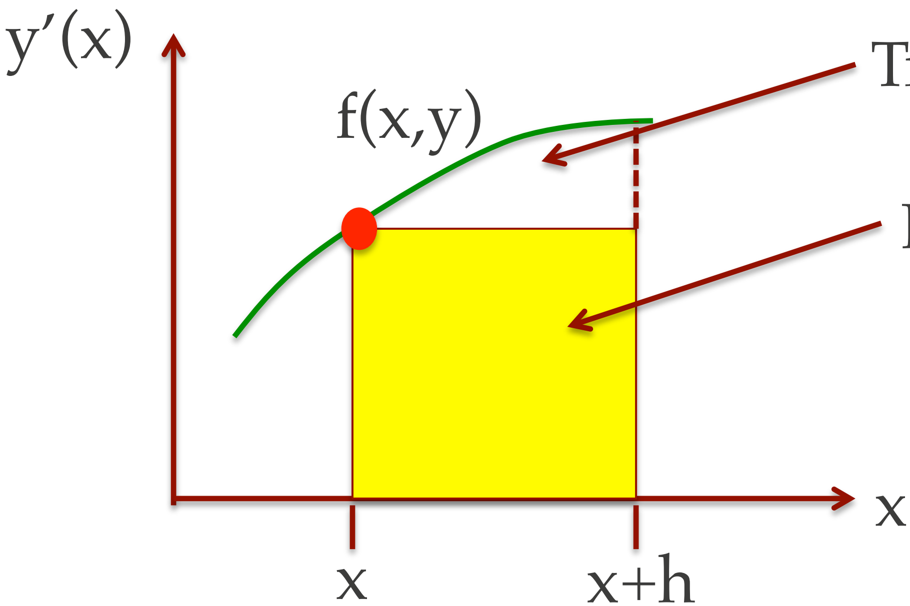
Euler's Method

- Graphical representation:



TE is proportional to the slope of the curve (i.e., y′′(x)).

$$y(x+h) - y(x) = \int_{x}^{x+h} y'\,dx = \int_{x}^{x+h} f(x,y)\,dx$$

Euler's Method Example

- Example 7.2 (pp. 251-252)

  Solve $y'' = -0.1y' - x, y(0) = 0, y'(0) = 1$

  from x=0 to x=2 using Euler's Method with h=0.05.

  The analytical solution is

  $$y = 100x - 5x^2 + 990(e^{-0.1x} - 1)$$

  EM: $\vec{y}(x+h) \approx \vec{y}(x) + \vec{y}'(x)h$

  (See `euler.py` on pp. 248-249.)

Euler's Method Example

- Write ODE as a set of first-order equations using the substitutions y_0=y and y_1=y′:

$$\vec{y}' = \begin{bmatrix} y_0' \\ y_1' \end{bmatrix} = \begin{bmatrix} y_1 \\ -0.1y_1 - x \end{bmatrix}, \vec{y}(0) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

<u>Solution</u>: y(2)=0.543446

See `example7_2.py` for code (pp. 251-252).

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Second-Order RK Method

- General Form:

$$(\diamondsuit)\quad \vec{y}(x+h) = \vec{y}(x) + c_0\vec{F}(x,\vec{y})h + c_1\vec{F}[x+ph, \vec{y}+qh\vec{F}(x,\vec{y})]h$$

Determine c_o, c_1, p, and q by matching with Taylor Series.

Recall $$\vec{y}(x+h) = \vec{y}(x) + \vec{y}'(x)h + \frac{1}{2!}\vec{y}''(x)h^2 + O(h^3)$$

$$= \vec{y}(x) + \vec{F}(x,\vec{y})h + \frac{1}{2!}\vec{F}'(x,\vec{y})h^2 + O(h^3)$$

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Second-Order RK Method

- But $\vec{F}'(x,\vec{y}) = \dfrac{\partial \vec{F}}{\partial x} + \sum_{i=0}^{n-1} \dfrac{\partial \vec{F}}{\partial y_i} y_i' = \dfrac{\partial \vec{F}}{\partial x} + \sum_{i=0}^{n-1} \dfrac{\partial \vec{F}}{\partial y_i} F_i(x,\vec{y})$

  Hence,

  $$(✪)\quad \vec{y}(x+h) = \vec{y}(x) + \vec{F}(x,\vec{y})h + \frac{h^2}{2}\left(\frac{\partial \vec{F}}{\partial x} + \sum_{i=0}^{n-1} \frac{\partial \vec{F}}{\partial y_i} F_i(x,\vec{y})\right) + O(h^3)$$

  Returning to (❖),

$$\vec{F}[x+ph, \vec{y}+qh\vec{F}(x,\vec{y})] = \vec{F}(x,\vec{y}) + \frac{\partial \vec{F}}{\partial x} ph + qh \sum_{i=0}^{n-1} \frac{\partial \vec{F}}{\partial y_i} F_i(x,\vec{y}) + O(h^2)$$

(…via Taylor Series in several variables)

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Second-Order RK Method

- So, we can rewrite (❖) as

$$\vec{y}(x+h)=\vec{y}(x)+(c_0+c_1)\vec{F}(x,\vec{y})h+c_1\left[\frac{\partial\vec{F}}{\partial x}ph+qh\sum_{i=0}^{n-1}\frac{\partial\vec{F}}{\partial y_i}F_i(x,\vec{y})\right]h$$

Matching this form of (❖) with (✪) implies that we must have $c_0+c_1=1$, $c_1p=c_1q=½$.

<u>Popular Choices</u>:

c_0	c_1	p	q	
0	1	½	½	(Modified Euler's Method)
½	½	1	1	(Heun's Method)

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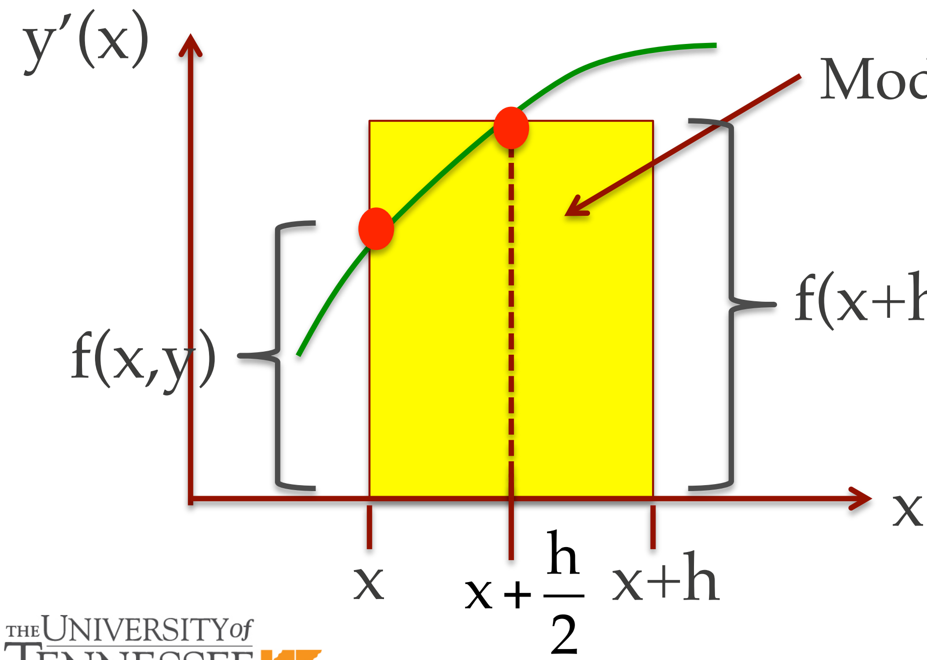
Modified Euler's Method

- Graphical rep. in 1D:

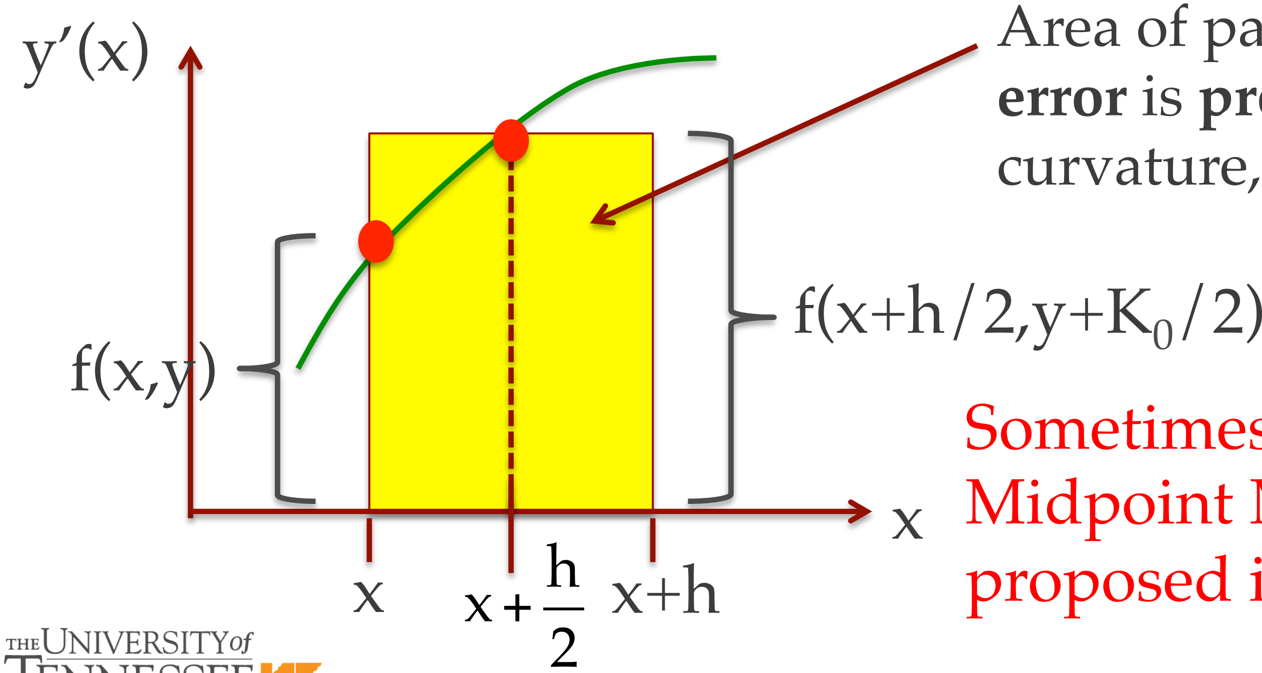
$$y\left(x+\frac{h}{2}\right)=y(x)+f(x,y)\cdot\frac{h}{2}=y(x)+\frac{K_0}{2}$$



$$\vec{y}(x+h)=y(x)+\vec{F}(x,\vec{y})h+$$
$$\vec{F}\left[x+\frac{h}{2},\vec{y}+\frac{h}{2}\vec{F}(x,\vec{y})\right]h$$

Modified Euler's Method

- Graphical rep. in 1D:



Area of panel is such that the **error** is **proportional** to the curvature, i.e., $(y')'' = y'''$.

Sometimes called Runge's Midpoint Method – proposed in 1895.

Modified Euler's Method

- ME can be represented in three steps:

$$K_0 = h\vec{F}(x, \vec{y})$$

Get estimate of y at midpoint via EM

$$K_1 = h\vec{F}\left(x + \frac{h}{2}, \vec{y} + \frac{K_0}{2}\right)$$

$$\vec{y}(x+h) = \vec{y}(x) + K_1$$

Then, get area of panel so error is proportional to the curvature.

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Fourth-Order RK Method

- See `run_kut4.py` on pp. 255-256.

(determine stepsize *h* by trial and error)

$$\vec{K}_0 = h\vec{F}(x, \vec{y})$$

$$\vec{K}_1 = h\vec{F}\left(x + \frac{h}{2}, \vec{y} + \frac{\vec{K}_0}{2}\right)$$

$$\vec{K}_2 = h\vec{F}\left(x + \frac{h}{2}, \vec{y} + \frac{\vec{K}_1}{2}\right)$$

$$\vec{K}_3 = h\vec{F}\left(x + h, \vec{y} + \vec{K}_2\right)$$

$$\vec{y}(x + h) = \vec{y}(x) + \frac{1}{6}\left(K_0 + 2K_1 + 2K_2 + K_3\right)$$

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RK Examples

- Example 7.3 on pp. 256-257:
  Use 2nd order RK (i.e., ME) to integrate $y' = \sin y,\ y(0) = 1$ from x=0 to x=0.5 with stepsize h=0.1 (keep 4 decimal places).

Solution: $F(x,y) = \sin y$

$$K_0 = hF(x,y) = 0.1\sin y$$

$$K_1 = hF\left(x + \frac{h}{2}, y + \frac{K_0}{2}\right) = 0.1\sin\left(y + \frac{K_0}{2}\right)$$

$$y(x+h) = y(x) + K_1$$

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RK Examples

- Example 7.3 on pp. 256-257:

Given y(0)=1…

$$
\begin{aligned}
K_0 &= 0.1\sin(1.0000) = 0.0841 \\
K_1 &= 0.1\sin\left(1.0000 + \frac{0.0841}{2}\right) = 0.0863 \\
y(0.1) &= 1.0 + 0.0863 = 1.0863 \\
K_0 &= 0.1\sin(1.0863) = 0.0855 \\
K_1 &= 0.1\sin\left(1.0863 + \frac{0.0855}{2}\right) = 0.0905 \\
y(0.2) &= 1.0863 + 0.0905 = 1.1768
\end{aligned}
$$

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RK Examples

- Example 7.3 on pp. 256-257:
  Tabulated results…

Exact solution is x(y)=ln (csc y- cot y) + 0.604582

x(1.4664)=0.5

x	y	K_0	K_1
0.0	1.0000	0.0841	0.0863
0.1	1.0863	0.0885	0.0905
0.2	1.1768	0.0923	0.0940
0.3	1.2708	0.0955	0.0968
0.4	1.3676	0.0979	0.0988
0.5	1.4664		

RK Examples

- Example 7.4 on pp. 257-258:

Use 4th order RK to integrate $y'' = -0.1y' - x,\ y(0) = 0,\ y'(0) = 1$ from x=0 to x=2 with stepsize h=0.25.

Solution: Let $y_0 = y$ and $y_1 = y'$

$$\vec{y}' = \vec{F}(x,\vec{y}) = \begin{bmatrix} y_0' \\ y_1' \end{bmatrix} = \begin{bmatrix} y_1 \\ -0.1y_1 - x \end{bmatrix}$$

```
def F(x,y):
    F=zeros((2),dtype=float64)
    F[0]=y[1]
    F[1]=-0.1*y[1]-x
    return F
```

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RK Examples

- Example 7.4 on pp. 257-258:

```
x=0.0
xStop=2.0
y=array([0.0,1.0])
h=0.25
freq=1
X,Y=integrate(F,x,y,xStop,h) # RK4 function
printSoln(X,Y,freq)          # Output table of results
Input("\nPress return to exit")
```

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RK Examples

- Example 7.4 on pp. 257-258:

x	y[0]	y[1]
0.0000e+000	0.0000e+000	1.0000e+000
2.5000e-001	2.4431e-001	9.4432e-001
…	…	…
1.0000e+000	7.8904e-001	4.2110e-001
…	…	…
2.0000e+000	5.4345e-001	-1.0543e+000

Would be same estimate from Taylor Series Method of Order 4

RK Examples

- Example 7.5 on p. 259:

  Use 4th order RK to integrate $y' = 3y - 4e^{-x},\ y(0) = 1$ from x=0 to x=10 with stepsize h=0.1; the analytical solution is $y=e^{-x}$.

```
def F(x,y):
  F=zeros((1),dtype=float64)
  F[0]=3.0*y[0]-4.0*exp(-x)
  return F
```

```
x=0.0
xStop=10.0
y=array([1.0])
h=0.1
freq=20
X,Y=integrate(F,x,y,xStop,h)
printSoln(X,Y,freq)
input("\nHit return to exit")
```

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RK Examples

- Example 7.5 on p. 259:

Output:

x	y[0]
0.0000e+000	1.0000e+000
2.0000e+000	1.3250e-001
4.0000e+000	-1.1237e+000
6.0000e+000	-4.6056e+002
8.0000e+000	-1.8575e+005
1.0000e+001	-7.4912e+007

What is happening?

Seeing numerical instability in y, but why? Recall that analytical solution is $y=e^{-x}$.

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RK Examples

- Example 7.5 on p. 259:
  Use 4th order RK to integrate $y' = 3y - 4e^{-x},\ y(0) = 1$

  The general solution to the ODE is $y=Ce^{3x}+e^{-x}$
  and suppose there is a small error (ε) in the initial condition, i.e., $y(0)=1+\varepsilon$. Then, the analytical (particular) solution becomes $y=\varepsilon e^{3x}+e^{-x}$.

  term dominants as x approaches ∞^{+}

  Sensitivity of IC is a source of *numerical instability* of the solution – nothing wrong with Python code.

§7.4 Stability and Stiffness

- Numerical integration is **stable** means that the effects of local errors **do not accumulate**, i.e., the global error stays bounded.
- Stability has nothing to do with accuracy–there are inaccurate methods that are stable.
- Stability is determined by: (1) ODE, (2), Method of solution, and (3) stepsize h.

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Stability and Stiffness

- Q: What is the stability of Euler's Method?

Consider $y' = -\lambda y$, $y(0) = \beta$ in which the analytical solution is $y(x) = \beta e^{-\lambda x}$.

Since EM is given by $y(x+h) = y(x) + hy'(x)$, then via substitution for our ODE we have

$$y(x+h) = y(x) + h[-\lambda y(x)] = (1-\lambda h)y(x).$$

So, if $|1-\lambda h| > 1$, the method will be **unstable**. Why?

EM is stable if $h \leq$ ____________.

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§7.4 Stability and Stiffness

- An IVP is **stiff**, if some terms in the solution vector y(x) vary more rapidly with x than with the other terms. For example, y''+1001y'+1000y=0 is a stiff ODE since it can be shown that EM would require $h \le 2/1000 = .002$ to be stable; RK methods would require very small h as well.
- RK methods are generally impractical for stiff ODE's– sometimes the remedy is to reduce the order of the method at the cost of increasing the truncation error.

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