System of ODEs

- If we have several dependent variables, y_i, i from 1 to m
- Derivatives could be functions of time and one or more y^s
- Initial conditions on all y^s should be given
- The system may be expressed as

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

$$\frac{dy_2}{dt} = f_2(t, y_1, y_2, ..., y_m) \qquad y_1\big|_{(t=0)} = y_{1,0};\, y_2\big|_{(t=0)} = y_{2,0};...;\, y_m\big|_{(t=0)} = y_{m,0}$$

$$...$$

$$\frac{dy_m}{dt} = f_m(t, y_1, y_2, ..., y_m)$$

Higher order ODEs

- If we have a higher order ODE, it could be converted into a system of ODEs
- For example, $$c_2 \frac{d^2 y}{dt^2} + c_1 \frac{dy}{dt} + c_0 y = f(t)$$
- Could be expressed as (using y_1=y and y_2=dy/dt):

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

$$\frac{dy_2}{dt} = f_2(t, y_1, y_2) = \frac{f(t) - c_0 y_1 - c_1 y_2}{c_2}$$

Higher order ODEs

- The only problem is with the boundary conditions
- There are two boundary conditions on y
- If both are specified at $t=t_0$ (e.g., y_0 and dy/dt_0): Initial Value Problem (IVP)
- If these are specified at different points (e.g., y_0 and y_T): Boundary Value Problem (BVP)
- Problems discussed till now were IVPs

Higher order ODEs

- The higher order IVP is readily convertible into a system of IVPs
- The BVPs require different technique and will be discussed later
- For now, we will look at only a system of IVPs, and will not consider higher-order IVPs separately, since these are equivalent!

System of ODEs

- All the methods described earlier for a single ODE, are applicable for a system
- Explicit methods pose no problem
- Implicit methods require the solution of a nonlinear system of algebraic equations
- Vector notation is used to write

$$\frac{d\{y\}}{dt} = \{f\} \text{ with } \{y\}_{t=0} = \{y_0\}$$

- where,

$$\{y\} = \{y_1, y_2, \ldots, y_m\}^{\mathrm{T}}; \{f\} = \{f_1, f_2, \ldots, f_m\}^{\mathrm{T}}; \{y_0\} = \{y_{1,0}, y_{2,0}, \ldots, y_{m,0}\}^{\mathrm{T}}$$

System of ODEs: Euler Forward

- Euler Forward method gives:

$$\{y\}_{n+1} = \{y\}_n + h\{f\}_n$$

- Or, in expanded form:

$$y_{1,n+1} = y_{1,n} + hf_1(t_n, y_{1,n}, y_{2,n}, \ldots, y_{m,n})$$
$$y_{2,n+1} = y_{2,n} + hf_2(t_n, y_{1,n}, y_{2,n}, \ldots, y_{m,n})$$
$$\ldots$$
$$y_{m,n+1} = y_{m,n} + hf_m(t_n, y_{1,n}, y_{2,n}, \ldots, y_{m,n})$$

- Similarly, for other explicit methods

System of ODEs: 4th order R-K

- For the 4th order R-K method:

$$\{y\}_{n+1} = \{y\}_n + \frac{h}{6}\left(\{k_1\}_n + 2\{k_2\}_n + 2\{k_3\}_n + \{k_4\}_n\right)$$

- The slopes are given by:

$$\{k_1\}_n = \{f\}_{(t_n, \{y\}_n)}$$

$$\{k_2\}_n = \{f\}_{(t_n + h/2, \{y\}_n + \{k_1\}_n h/2)}$$

$$\{k_3\}_n = \{f\}_{(t_n + h/2, \{y\}_n + \{k_2\}_n h/2)}$$

$$\{k_4\}_n = \{f\}_{(t_n + h, \{y\}_n + \{k_3\}_n h)}$$

System of ODEs: Euler Backward

- Euler Backward method results in:

$$\{y\}_{n+1} = \{y\}_n + h\{f\}_{n+1}$$

- Or, in expanded form:

$$y_{1,n+1} = y_{1,n} + f_1(t_{n+1}, y_{1,n+1}, y_{2,n+1}, \ldots, y_{m,n+1})$$

$$y_{2,n+1} = y_{2,n} + f_2(t_{n+1}, y_{1,n+1}, y_{2,n+1}, \ldots, y_{m,n+1})$$

$$\ldots$$

$$y_{m,n+1} = y_{m,n} + f_m(t_{n+1}, y_{1,n+1}, y_{2,n+1}, \ldots, y_{m,n+1})$$

- If the *f*s are linear in y, a set of linear algebraic equations:

$\{y\}_{n+1} = \{y\}_n + h([A]\{y\}_{n+1} + \{b\}_{n+1}) \Rightarrow [I - hA]\{y\}_{n+1} = \{y\}_n + h\{b\}_{n+1}$

System of ODEs: Euler Backward

- LU decomposition will work well, since the coefficient matrix is time-independent (if the time step is constant)
- Generally, a set of nonlinear equations
- Fixed-point or Newton methods could be used to solve

Stability of a System of IVPs

- As for a single ODE, we consider

$$\frac{d\{y\}}{dt} = [A]\{y\}$$

- Use Euler Forward:

$$\{y\}_{n+1} = \{y\}_n + h[A]\{y\}_n = [I + hA]\{y\}_n$$

- The amplification factor is defined as

$$\sigma = \frac{\left|\{y\}_{n+1}\right|}{\left|\{y\}_n\right|} \le \left\|I + hA\right\|$$

- For convergence, the spectral norm of I+hA should be ≤ 1
- λ_{max} of [A] , $|1+h\,\lambda_{max}| \le 1$; $h \le 2/|\lambda_{max}|$

Stability of a System of IVPs

- Let us consider
$$\frac{d\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}}{dt} = \begin{bmatrix} 5.6 & -26.4 \\ 26.4 & -106.6 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}$$

  $y_1 = y_2 = 1$ at $t = 0$

- Solve by Euler Explicit

$$\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n+1} = \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_n + h\begin{bmatrix} 5.6 & -26.4 \\ 26.4 & -106.6 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_n$$
$$= \begin{Bmatrix} (1+5.6h)y_1 - 26.4hy_2 \\ 26.4hy_1 + (1-106.6h)y_2 \end{Bmatrix}_n$$

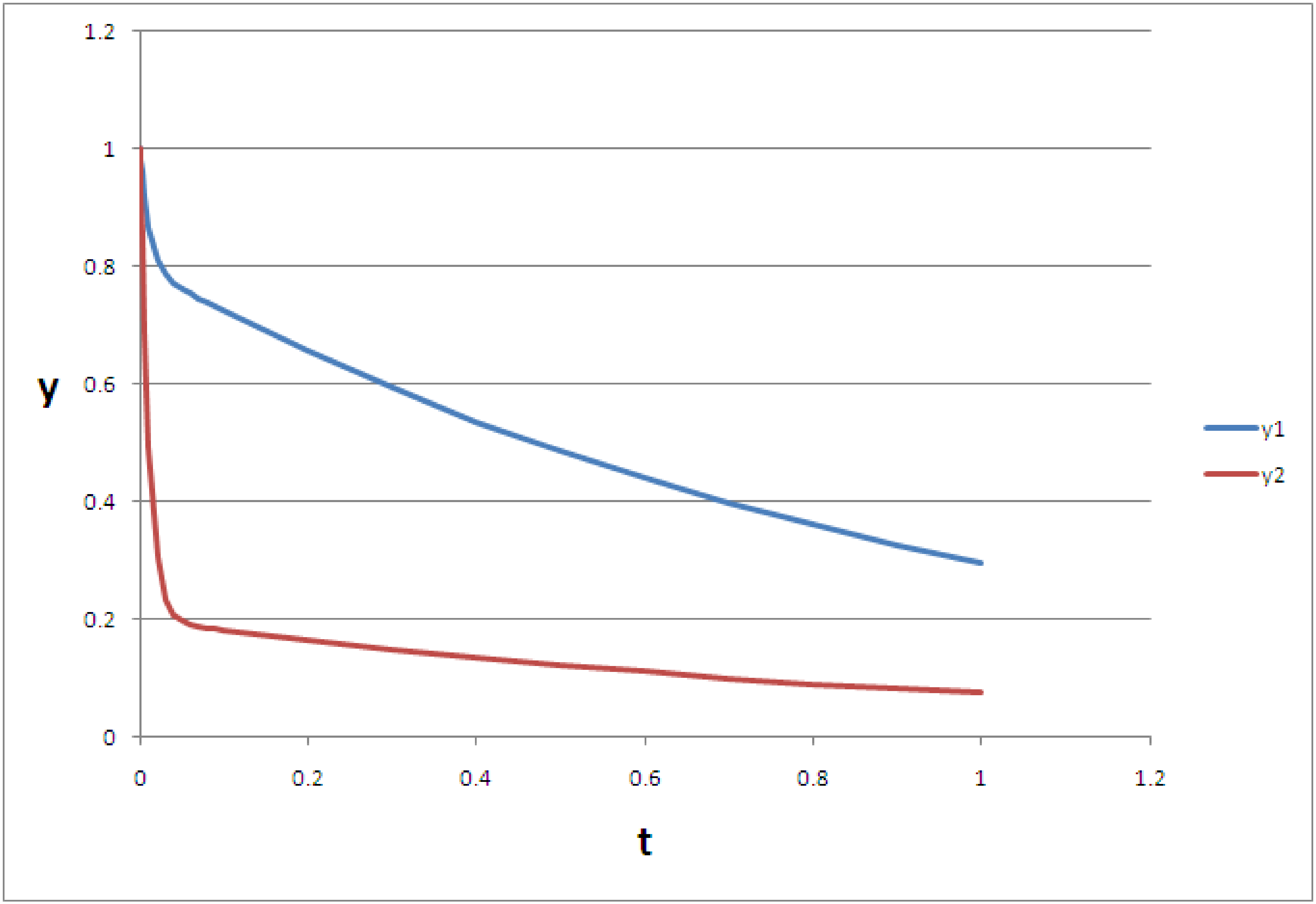
Stability of a System of IVPs

- Analytical solution is

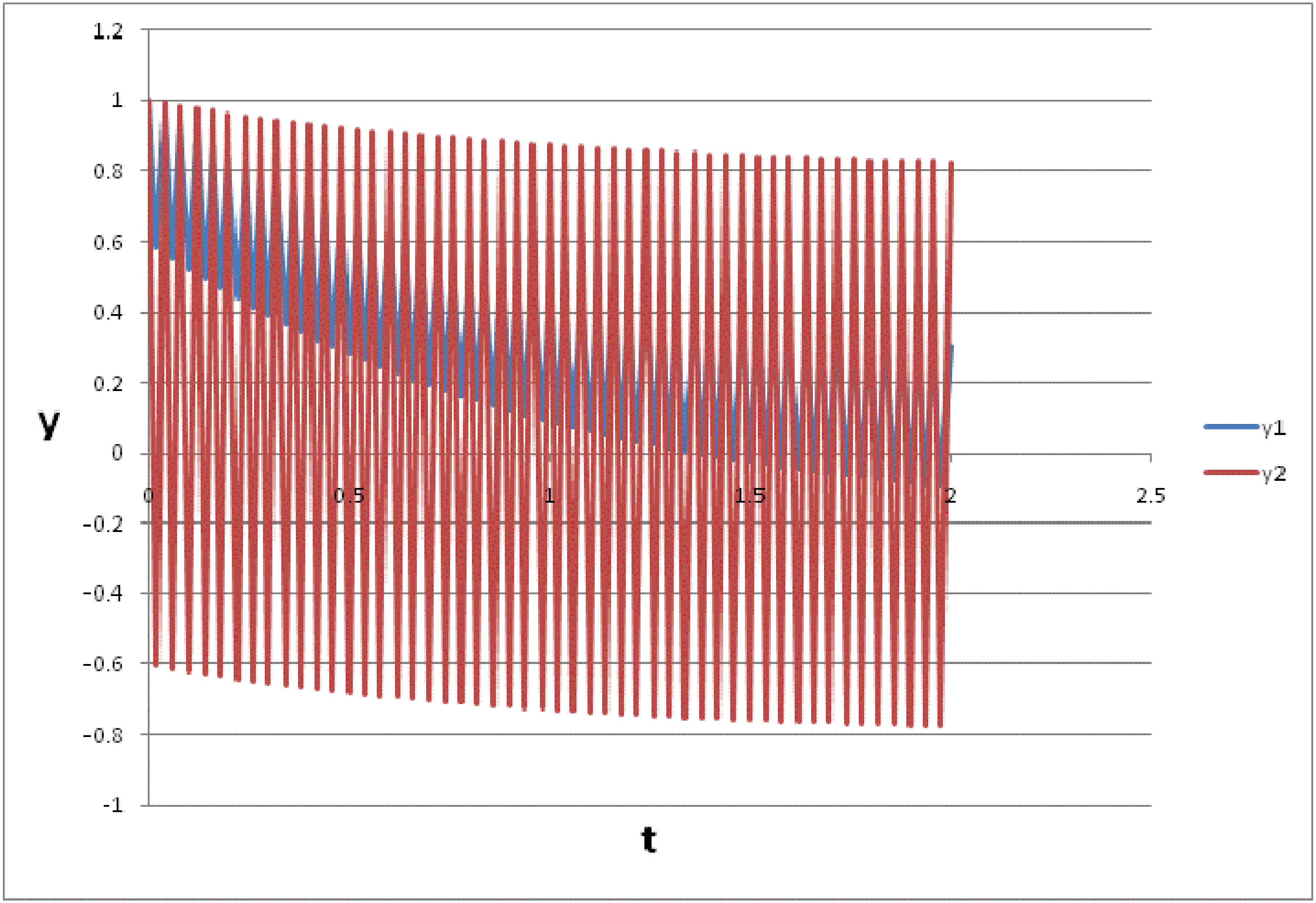
$$y_1 = 0.8e^{-t} + 0.2e^{-100t}$$
$$y_2 = 0.2e^{-t} + 0.8e^{-100t}$$

- Eigenvalues of [A] are -1, and -100

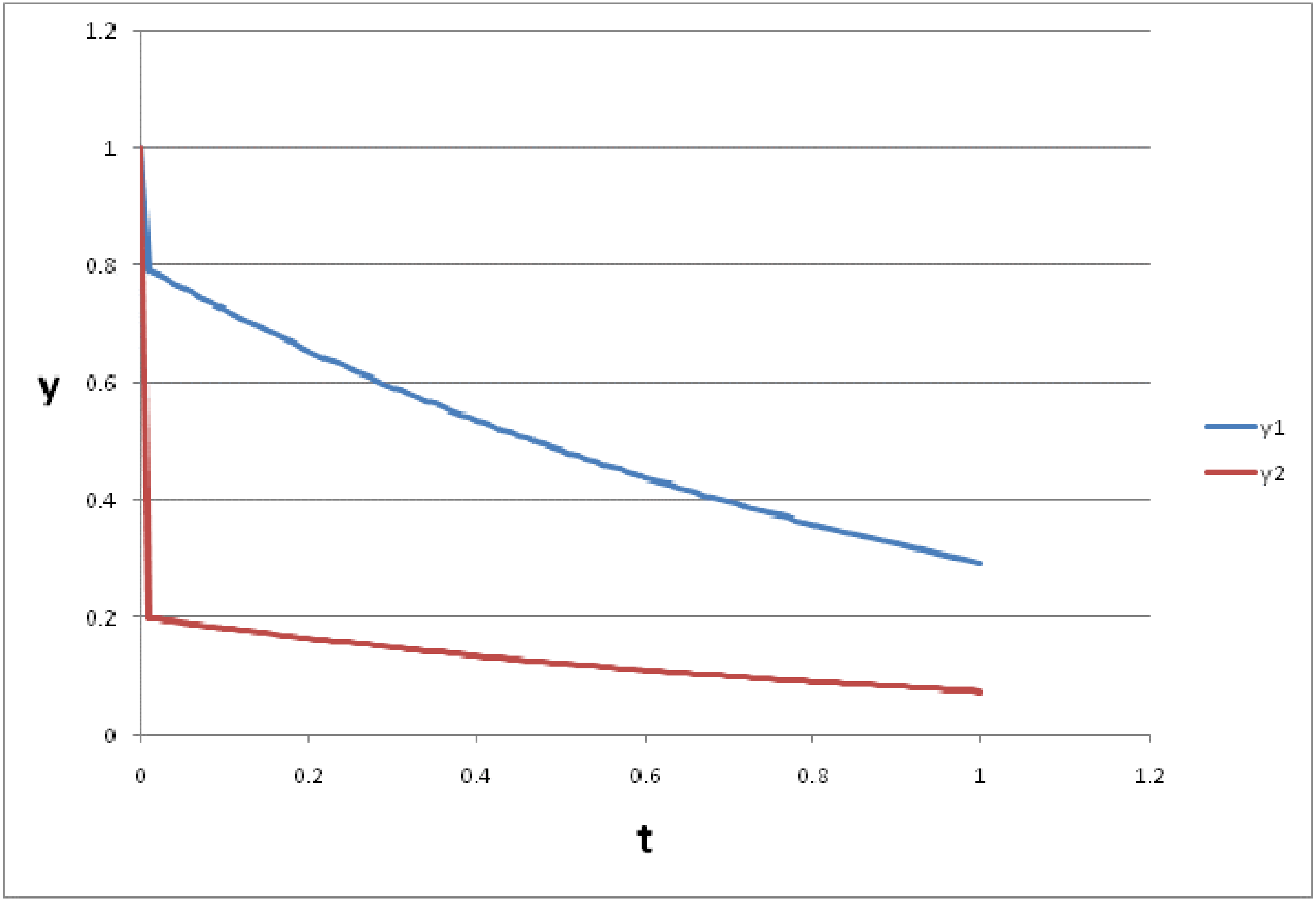
- The maximum time step for stability is given by $|1-100\,h| = 1 \Rightarrow h=0.02$



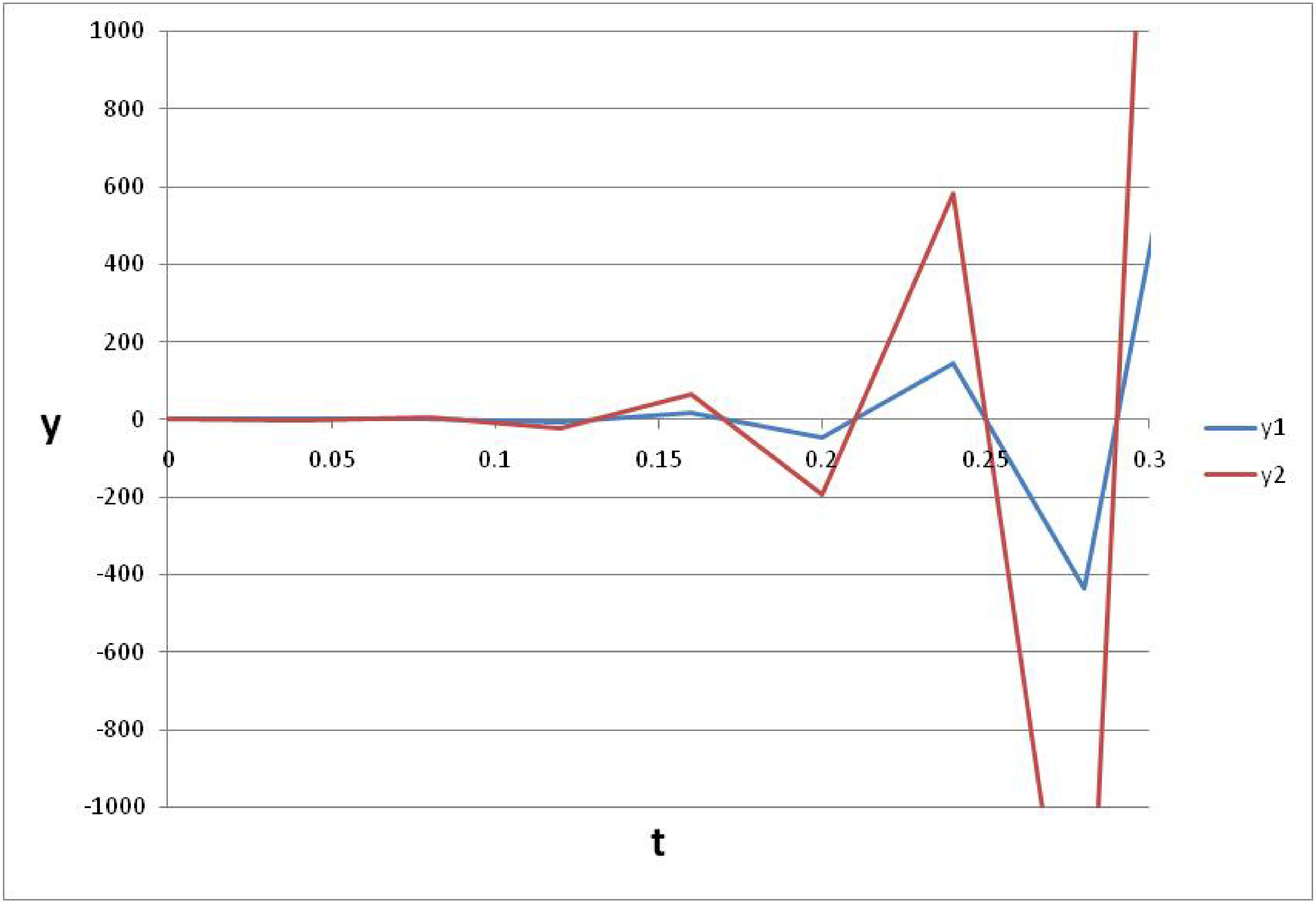
1.2
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
1.2
t
y1
y2



h=0.02



h=0.01


1000
800
600
400
200
0
-200
-400
-600
-800
-1000
0
0.05
0.1
0.15
0.2
0.25
0.3
y
t
y1
y2

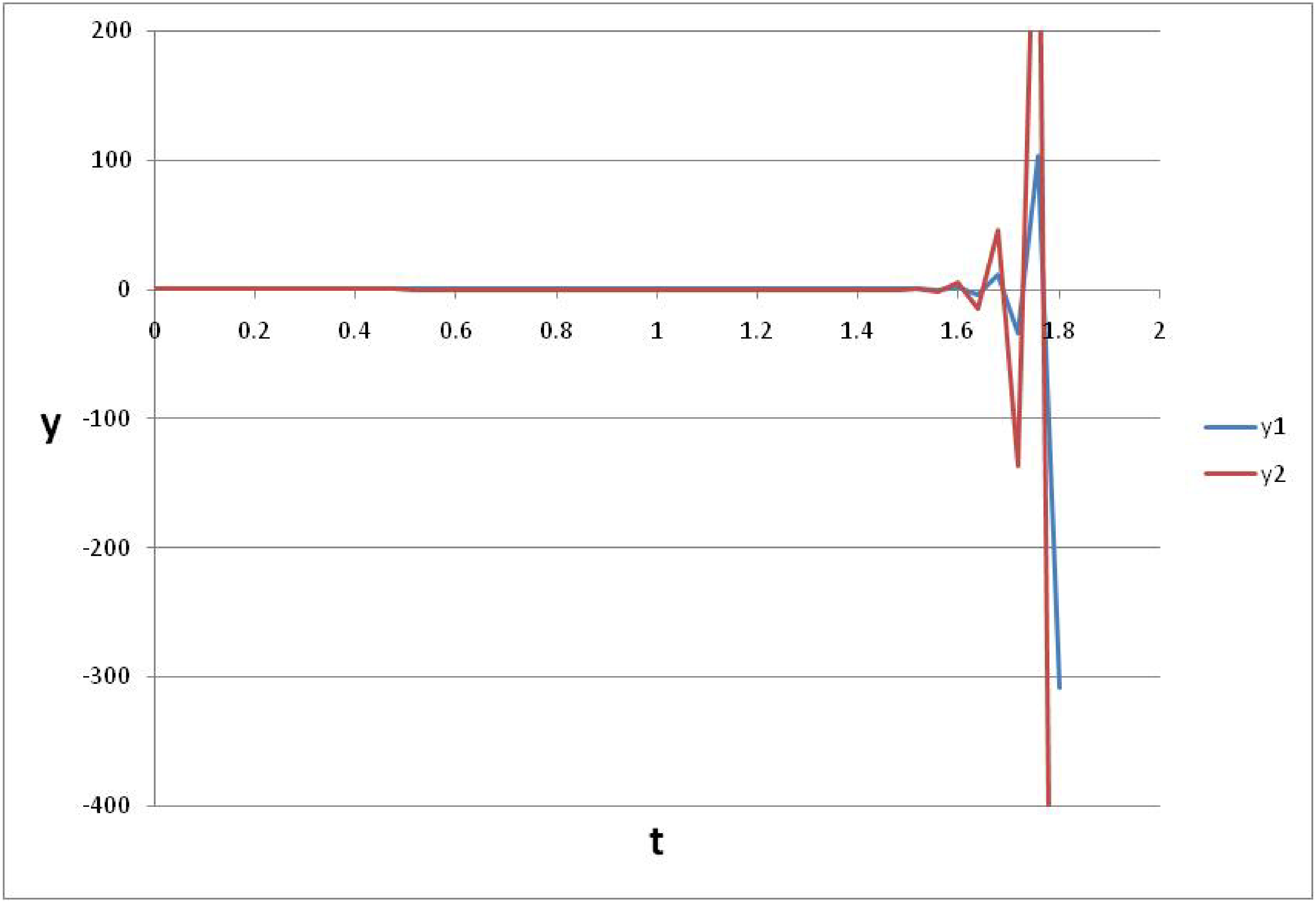
h=0.04

Stability of a System of IVPs

- For stability, the limit depends on λ_{max}
- For accuracy, h should be smaller than the stability limit of $2/|\lambda_{max}|$
- The analytical solution is of the form

$$\{y\} = \{c_1\}e^{\lambda_1 t} + \{c_2\}e^{\lambda_2 t}$$

- The part corresponding to the largest magnitude eigenvalue decays fast
- Physically, therefore, a larger time step could be used after the initial period



h=0.01 up to 0.1, then 0.02 up to 0.2, 0.04 after that

Stiff Systems

- If the ratio $|\lambda_{max}|/ |\lambda_{min}|$ is large (typically more than 100)
- The "early" time step should depend on λ_{max} and the subsequent time step could be increased substantially
- Does not work for Forward Euler
- Using Backward Euler, we need to solve a set of linear equations
- But we get a better stability

Stiff Systems

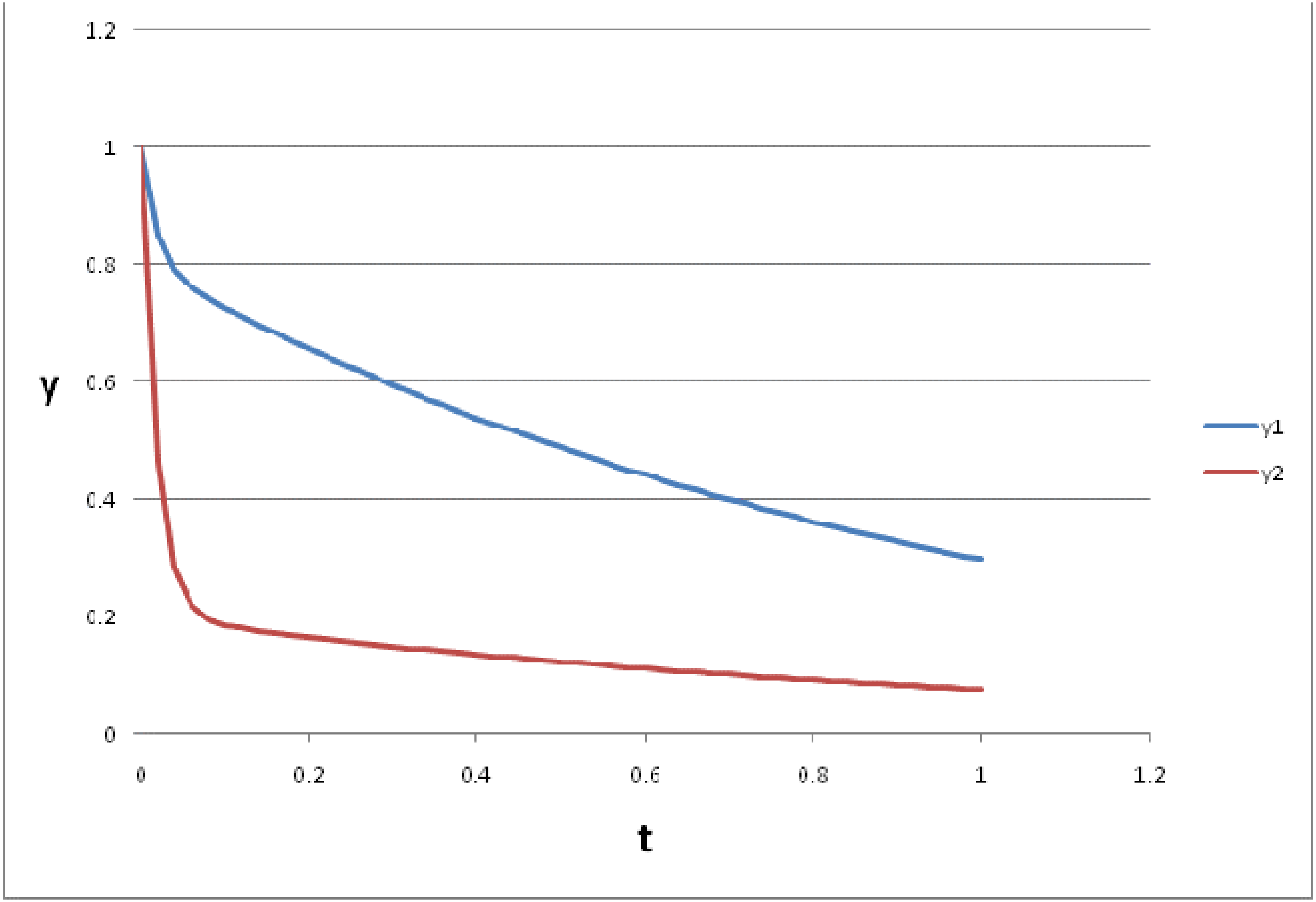
- Backward Euler:

$$\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n+1} = \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n} + h\begin{bmatrix} 5.6 & -26.4 \\ 26.4 & -106.6 \end{bmatrix}\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n+1}$$

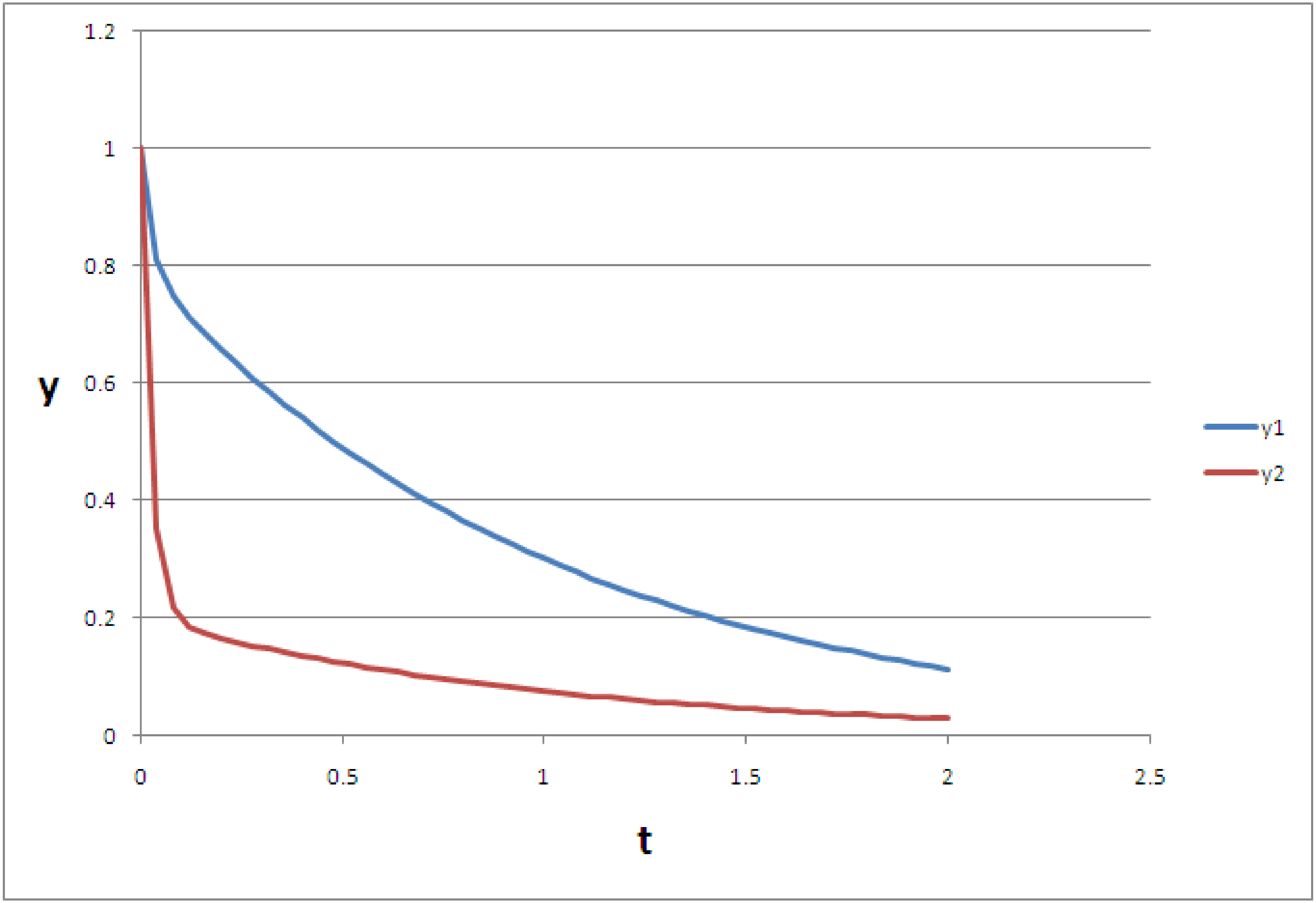
$$\begin{bmatrix} 1-5.6h & 26.4h \\ -26.4h & 1+106.6h \end{bmatrix}\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n+1} = \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n}$$

- For a small number of equation, inverse may be obtained:

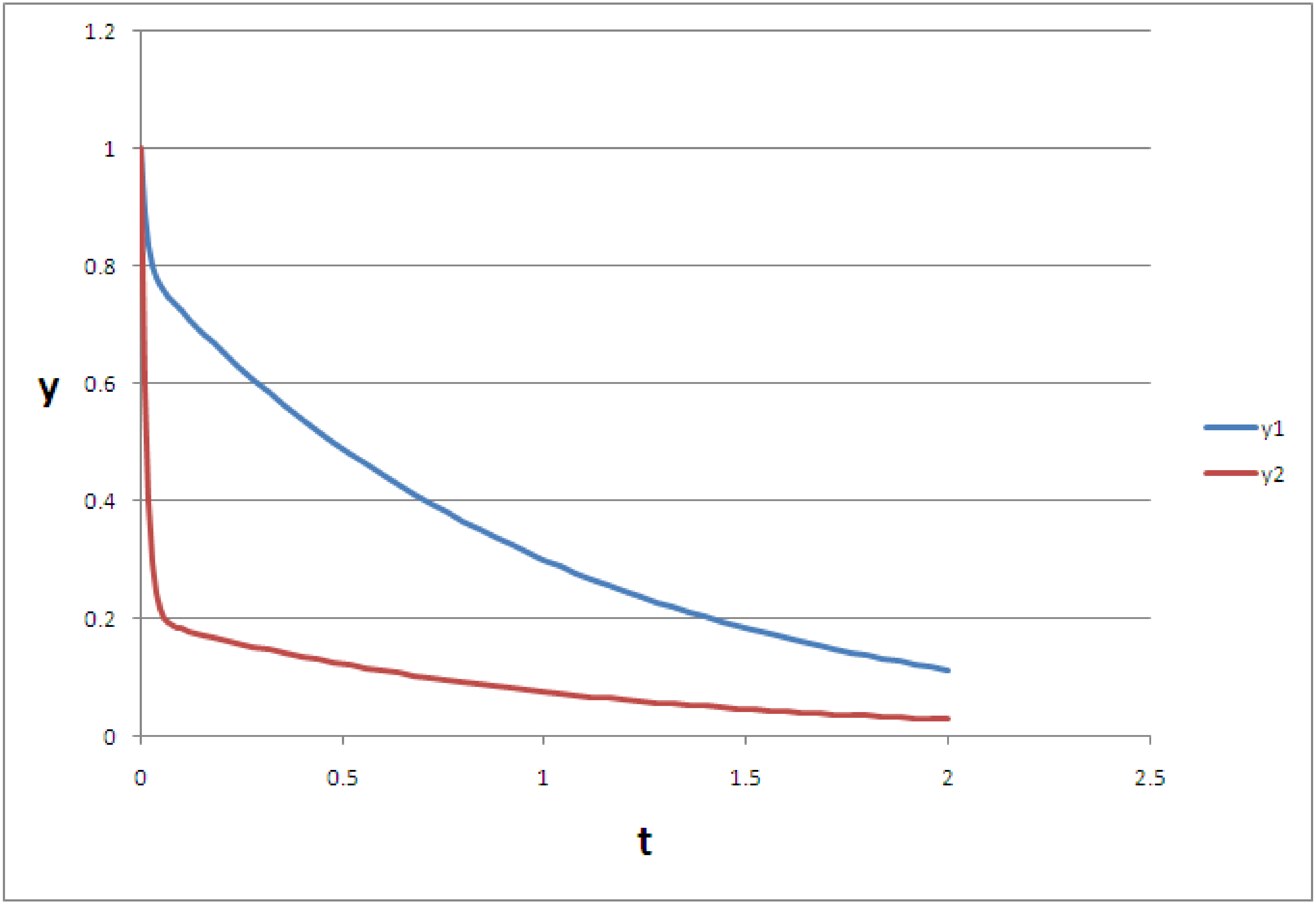
$$\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n+1} = \frac{1}{1+101h+100h^2}\begin{bmatrix} 1+106.6h & -26.4h \\ 26.4h & 1-5.6h \end{bmatrix}\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix}_{n}$$



h=0.02



h=0.04



h=0.01 up to 0.1, then 0.02 up to 0.2, 0.04 after that

Stiff Systems

- Backward Euler is stable for large time steps
- Error becomes large as we move in time
- Why not use higher order methods as we increase the time step in later part?
- Most common technique for stiff systems is the Gear's method
- Use Backward difference formulae (BDF) of orders 1 - 6, with gradual increase in h

Backward Difference Formulae

$$hf_{n+1} = \sum_{i=0}^{k} \alpha_i y_{n+1-i}; \ \mathrm{k} = 0,1,2,\ldots,\mathrm{n}+1$$

- k=1 (Euler Implicit, BDF1): $hf_{n+1} = y_{n+1} - y_n$
- k=2: $hf_{n+1} = \frac{3}{2} y_{n+1} - 2y_n + \frac{1}{2} y_{n-1}$
- k=3: $hf_{n+1} = \frac{11}{6} y_{n+1} - 3y_n + \frac{3}{2} y_{n-1} - \frac{1}{3} y_{n-2}$
- k=6 (BDF6):

$$hf_{n+1} = \frac{49}{20} y_{n+1} - 6y_n + \frac{15}{2} y_{n-1} - \frac{20}{3} y_{n-2} + \frac{15}{4} y_{n-3} - \frac{6}{5} y_{n-4} + \frac{1}{6} y_{n-5}$$

Stiff Systems: Gear's Method

- Use BDF1 (Backward Euler) for "a few" time steps with step size h
- Then use BDF2 with a step size of 2h
- Since BDF2 requires y_{n-1} also, BDF1 has to be used for at least 2 steps of h
- Similarly, after at least 3 steps of BDF2 with step size 2h, we could switch to BDF3 with step size 4h; and so on

Gear's Method

- This allows us to use the "equal spaced" formulae derived for BDF
- We could also use unequal spacing of previous points, when changing the step size, but it requires re-derivation
- The recommended size of the initial time step is $1/|\lambda_{max}|$
- BDF7 is unstable. BDF6 is stable but not robust (stability region is small)
- Therefore, sometimes we stop at BDF5

Gear's Method: Example

- Same Problem:

$$\frac{d\{y\}}{dt} = \begin{bmatrix} 5.6 & -26.4 \\ 26.4 & -106.6 \end{bmatrix} \{y\}$$

- Start with h=0.01 (=1/| λ_{max} |)
- Euler Implicit for 2 steps, to get

$$\{y\}_{0.01} = \begin{Bmatrix} 0.892079 \\ 0.598020 \end{Bmatrix}; \{y\}_{0.02} = \begin{Bmatrix} 0.834237 \\ 0.396059 \end{Bmatrix}$$

- BDF2 at y=0.02, with h=0.02

Gear's Method: Example

- BDF2:

$$hf_{0.04} = \frac{3}{2} y_{0.04} - 2 y_{0.02} + \frac{1}{2} y_0$$

- The y^s at 0 and 0.02 are known

$$0.02 \begin{bmatrix} 5.6 & -26.4 \\ 26.4 & -106.6 \end{bmatrix} \{y\}_{0.04} = \frac{3}{2} \{y\}_{0.04} - 2 \begin{Bmatrix} 0.834237 \\ 0.396059 \end{Bmatrix} + \frac{1}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

- Solve to get

$$\{y\}_{0.04} = \begin{Bmatrix} 0.768733 \\ 0.192183 \end{Bmatrix}$$

- Repeat to get y at 0.06 and 0.08
- Use BDF3 with h=0.04 (use 0, .04 and .08)

Gear's Method: Example

- BDF3:

$$hf_{0.12} = \frac{11}{6} y_{0.12} - 3y_{0.08} + \frac{3}{2} y_{0.04} - \frac{1}{3} y_0$$

- The y^s at 0, 0.04, and 0.08 are known
- Solve to get y at 0.12
- Repeat to get y at 0.16, 0.20, 0.24
- Use BDF4 with h=0.08 (use the known values at 0, 0.08, 0.16 and 0.24)
- Get y at 0.32. Repeat to get 0.40, 0.48, 0.56, and 0.64)

Gear's Method: Example

- Use BDF5 with h=0.16 (use the known values at 0, 0.16, 0.32, 0.48 and 0.64)
- Solve to get y at 0.80
- Repeat to get y at 0.96, 1.12, 1.28,1.44
- Use BDF6 with h=0.32 (use the known values at 0, 0.32, 0.64,0.96,1.28 and 1.44)
- Get y at 1.76. Repeat to get 2.08 and beyond, till the desired time
- We could have used h=0.01 for more than 2 steps, say up to t=0.1!