

**Problem Set # 8**  
**(No need to submit)**

1. Consider the following second-order homogeneous equation

$$y'' + 501y' + 500y = 2, \quad y(0) = 1, \quad y'(0) = -1$$

(i) Convert the above equation to the first-order problem

$$\frac{dz}{dx} = Az \quad ; \quad z(0) = z_0$$

(ii) Find the eigenvalues and eigenvectors of **A**.

(iii) Find the analytical solution of  $y(x)$ .

(iv) Why it is difficult to compute numerical solution of this system?

(v) What is the maximum step size that could be used in numerical computation with explicit Euler method in order to compute a stable solution.

(vi) What is the optimum step size one should use to guarantee accuracy of the solution to within  $1 \times 10^{-5}$  when forward Euler method is used?

2. Consider the following system of equations

$$x' = 1195x - 1995y, \quad x(0) = 2$$

$$y' = 1197x - 1997y, \quad y(0) = -2$$

(a) Find the analytical solution using eigenvalue-eigenvector method.

(b) State all steady-states and classify their stability.

(c) Calculate the solution after one step with step size  $h = 0.1$  using the Explicit Euler method.

(d) Calculate the solution after one step with step size  $h = 0.1$  using the Implicit Euler method.

(e) Compare results of part (c) and part (d) with exact solution.

(f) What is the maximum step size that could be used in numerical integration with the Explicit Euler method in order to compute a stable solution?

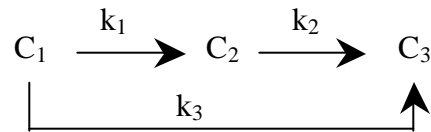
(g) What is the step size that should be used in numerical integration with the Explicit Euler method in order to compute a solution of maximum precision?

- (h) Why is the numerical integration of this dynamical system problematic, and in what sense is it problematic?
- (i) What would be the advantage of using the Implicit Euler method over the explicit Euler or 4<sup>th</sup>- order Runge-Kutta methods for this problem?
- (j) If your computer requires  $1 \times 10^{-6}$  sec of CPU time to do the computation in part (c), how much CPU time would it require if the 4<sup>th</sup>-order Runge-Kutta method was used instead?

3. Consider the following dynamical system:

$$\begin{aligned}x' &= 1.2x - 0.6xy, & x(0) &= 2 \\y' &= -0.8y + 0.2xy, & y(0) &= 1\end{aligned}$$

- (a) Calculate all steady states and determine whether the steady states are linearly stable.
- (b) State with reasons whether the stability of the above problem is time dependent.
- (c) How would you decide on the step size,  $h$ , to be used in the explicit and implicit methods for solutions to be numerically stable and accurate?
4. Catalytic cracking to convert crude oil fractions into gasoline is one of the largest volume man-made chemical processes in practice today. The key features of the process can be represented in a 3-component model developed by Weekman et. al of Mobil Oil Company:



where  $C_1$  represents the gas oil fraction of a crude feedstock,  $C_2$  represents the desired gasoline cut (i.e., molecules with 5 or more carbon atoms, up to a boiling point limit of 410 F). The process is accomplished in a fluid catalytic cracking (FCC) unit. This unit is essentially a vertical tubular reactor in which gas phase reactant (in this case gas oil) is introduced at the bottom of the reactor and products exit at the top. The catalyst is introduced as fine particles at the bottom of the reactor, and is carried along the vapour until they too are removed at the top of the reactor for recycle.

The equations that describe this process can be written:

$$\frac{dy_1}{dx} = -\frac{[k_1+k_3]}{S} \mathbf{j} y_1^2$$

$$\frac{dy_2}{dx} = y_1^2 - \frac{k_2}{S} \mathbf{j} y_2$$

where

$x = L/L_0 =$  dimensionless position.

$y_1 =$  mass fraction of the gas oil (= 1 at the reactor inlet).

$y_2 =$  mass fraction of gasoline fraction (= 0 at the inlet).

$S =$  liquid hourly space velocity of gas oil charge through the reactor

$=$  (mass of charge/hr) / (density of charge) / (volume of reactor)

$\phi =$  a catalyst deactivation factor =  $\exp(-\alpha x)$ .

Reported values for the rate constants for a particular catalyst are:

$$k_1 = 18.1 \text{ hr}^{-1}, \quad k_2 = 1.7 \text{ hr}^{-1}, \quad k_3 = 4.8 \text{ hr}^{-1}.$$

Solve the problem using fourth-order Runge-Kutta method for values of  $S = 20, 50$  and  $100 \text{ hr}^{-1}$ , and  $\alpha = 0, 1$ , and  $2$ . Commercially, values of  $\alpha = 2$  are not uncommon, which is the reason that a fluidized bed design is used, i.e., to remove and regenerate the catalyst.

5. Consider the following plot of  $\log [E_t(y(t_f))]$  vs  $\log [h]$  obtained from integrating a dynamical system to the same final time,  $t_f$ , starting with the same initial condition. The values of  $h$  in the figure differ by a factor of 2. The straight lines are lines of slope 1, 2, 3 and 4.

- What methods were used for the integration of the data points shown in the figure as squares and circles?
- Why does data point A deviate from a straight line?
- Why does data point C deviate from a straight line?
- What approximately is  $[E_t(y(t_f))]$  in case D as compared to case E?

- (e) How much CPU time approximately was required to compute  $y_1(t_f)$  in case D as compared to case E? What you have assumed about the type of numerical method used?
- (f) How much CPU time approximately was required to compute  $y_1(t_f)$  in case B as compared to case C? What you have assumed about the type of numerical method used?

### **Problem Set #8**

*Q 1.*

$$y'' + 500y' + 500y = 2$$

$$y = z_1$$

$$y' = z_1' = z_2, \quad z_1(0) = 1$$

$$y'' = z_1'' = z_2' = -501z_2 - 500z_1 + 2, \quad z_2(0) = -1$$

(i)

$$\frac{d}{dx} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -500 & -501 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 2 \end{bmatrix}, \quad \begin{bmatrix} z_1(0) \\ z_2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\frac{dZ}{dx} = \mathbf{A}Z + \mathbf{b}, \quad Z(0) = Z_0$$

$$Z = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} 0 & 1 \\ -500 & -501 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$$

(ii) Eigenvalues of  $\mathbf{A}$

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ -500 & -501 \end{bmatrix}, \quad \mathbf{A} - I\mathbf{I} = \begin{bmatrix} 0 - I & 1 \\ -500 & -501 - I \end{bmatrix}$$

$$I^2 + 501I + 500 = 0$$

$$(I + 1)(I + 500) = 0$$

$$I_1 = -1, I_2 = -500$$

for  $I_1 = -1$

$$\text{adj}(\mathbf{A} - I_1\mathbf{I}) = \text{adj} \begin{bmatrix} 1 & 1 \\ -500 & -500 \end{bmatrix} = \begin{bmatrix} -500 & -1 \\ 500 & 1 \end{bmatrix} \Rightarrow \mathbf{v}_1 = \mathbf{a} \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

for  $I_1 = -500$

$$\text{adj}(\mathbf{A} - \mathbf{I}_2\mathbf{I}) = \text{adj} \begin{bmatrix} 500 & 1 \\ -500 & -1 \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ 500 & 500 \end{bmatrix} \Rightarrow \mathbf{v}_2 = \mathbf{a} \begin{bmatrix} -1 \\ 500 \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} -1 & -1 \\ 1 & 500 \end{bmatrix}, \quad \mathbf{U}^{-1} = \frac{1}{-499} \begin{bmatrix} 500 & 1 \\ -1 & -1 \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} -1 & 0 \\ 0 & -500 \end{bmatrix}$$

$$(iii) \mathbf{Z} = c_1 \mathbf{v}_1 e^{I_1 t} + c_2 \mathbf{v}_2 e^{I_2 t} - \mathbf{A}^{-1} \mathbf{b}$$

$$\mathbf{Z} = c_1 \begin{bmatrix} -1 \\ 1 \end{bmatrix} e^{-t} + c_2 \begin{bmatrix} -1 \\ 500 \end{bmatrix} e^{-500t} - \frac{1}{500} \begin{bmatrix} -501 & -1 \\ 500 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 2 \end{bmatrix}$$

$$= c_1 \begin{bmatrix} -e^{-t} \\ e^{-t} \end{bmatrix} + c_2 \begin{bmatrix} -e^{-500t} \\ 500e^{-500t} \end{bmatrix} - \frac{1}{500} \begin{bmatrix} -2 \\ 0 \end{bmatrix}$$

$$= c_1 \begin{bmatrix} -e^{-t} \\ e^{-t} \end{bmatrix} + c_2 \begin{bmatrix} -e^{-500t} \\ 500e^{-500t} \end{bmatrix} - \begin{bmatrix} -\frac{1}{250} \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ -1 \end{bmatrix} = c_1 \begin{bmatrix} -e^{-t} \\ e^{-t} \end{bmatrix} + c_2 \begin{bmatrix} -e^{-500t} \\ 500e^{-500t} \end{bmatrix} - \begin{bmatrix} -\frac{1}{250} \\ 0 \end{bmatrix} \Leftrightarrow \text{Applying initial condition}$$

$$1 = -c_1 e^{-t} - c_2 e^{-500t} + \frac{1}{250}$$

$$-1 = c_1 e^{-t} + c_2 e^{-500t}$$

$$\text{At } t = 0 \Rightarrow -c_1 - c_2 = 0.996$$

$$\text{At } t = 0 \Rightarrow -c_1 + 500 c_2 = -1$$

$$\begin{bmatrix} -1 & -1 \\ 1 & 500 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0.996 \\ -1 \end{bmatrix}$$

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \frac{1}{-499} \begin{bmatrix} 500 & 1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} 0.996 \\ -1 \end{bmatrix}$$

$$= \frac{1}{-499} \begin{bmatrix} 497 \\ 0.004 \end{bmatrix}$$

$$= \begin{bmatrix} -0.995 \\ -8.016 \times 10^{-6} \end{bmatrix}$$

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = -0.995 \begin{bmatrix} -e^t \\ e^t \end{bmatrix} + -8.016 \times 10^{-6} \begin{bmatrix} -e^{-500t} \\ 500e^{-500t} \end{bmatrix} - \begin{bmatrix} -\frac{1}{250} \\ 0 \end{bmatrix}$$

(v)

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$$\text{Stiffness ratio, SR} = \frac{|\mathbf{I}_{\max}|}{|\mathbf{I}_{\min}|} = \frac{|-500|}{|-1|} = 500$$

When  $\text{SR} = 100$  to  $100,000$ , the problem is classified as stiff. It encompasses a wide range of time scales. We need smaller time steps for numerical stability due to  $|\mathbf{I}_{\max}|$  and want larger time steps due to  $|\mathbf{I}_{\min}|$  to approach steady state.

$$\text{Maximum step size, } h_{\max} < \frac{2}{\mathbf{I}_{\max}}$$

$$h_{\max} < \frac{2}{500}$$

$$h_{\max} < 0.004$$

*Q 2.*

$$\begin{aligned} x' &= 1195x - 1995y, & x(0) &= 2 \\ y' &= 1197x - 1997y, & y(0) &= -2 \end{aligned}$$

$$\frac{d}{dt} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1195 & -1995 \\ 1197 & -1997 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 1195 & -1995 \\ 1197 & -1997 \end{bmatrix}$$

$$\begin{aligned} f(\mathbf{I}) &= \mathbf{I}^2 + 802\mathbf{I} + 1600 \\ 0 &= (\mathbf{I} + 800)(\mathbf{I} + 2) \end{aligned}$$

$$\mathbf{I}_1 = -2, \mathbf{I}_2 = -800$$

for  $\mathbf{I}_1 = -2$

$$\text{adj}(\mathbf{A} - \mathbf{I}_1\mathbf{I}) = \text{adj} \begin{bmatrix} 1197 & -1995 \\ 1197 & -1995 \end{bmatrix} = \begin{bmatrix} -1995 & 1995 \\ -1197 & 1197 \end{bmatrix} \Rightarrow \mathbf{v}_1 = \mathbf{a} \begin{bmatrix} 5 \\ 3 \end{bmatrix}$$

for  $\mathbf{I}_1 = -800$

$$\text{adj}(\mathbf{A} - \mathbf{I}_2\mathbf{I}) = \text{adj} \begin{bmatrix} 1995 & -1995 \\ 1197 & -1197 \end{bmatrix} = \begin{bmatrix} -1197 & 1995 \\ -1197 & 1995 \end{bmatrix} \Rightarrow \mathbf{v}_2 = \mathbf{a} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} 5 & 1 \\ 3 & 1 \end{bmatrix}, \quad \mathbf{U}^{-1} = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -3 & 5 \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} -2 & 0 \\ 0 & -800 \end{bmatrix}$$

$$\begin{aligned} \begin{bmatrix} x \\ y \end{bmatrix} &= \begin{bmatrix} 5 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} e^{-2t} & 0 \\ 0 & e^{-800t} \end{bmatrix} \begin{bmatrix} 2 \\ -8 \end{bmatrix} \\ &= \begin{bmatrix} 5 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 2e^{-2t} \\ -8e^{-500t} \end{bmatrix} = \begin{bmatrix} 10e^{-2t} - 8e^{-500t} \\ 6e^{-2t} - 8e^{-500t} \end{bmatrix} \end{aligned}$$

(b) The steady state at  $x = 0, y = 0$

The steady state is stable since both eigenvalues have negative real part.

The steady state is unique since the equations are linear.

(c) Explicit Euler Method

$$y_{n+1} = y_n + hf(x_n, y_n)$$

$$\begin{aligned} y_1 &= y_0 + hf(x_0, y_0) \\ &= -2 + 0.1\{1197 \times 2 - 1997 \times (-2)\} \\ &= 636.8 \end{aligned}$$

$$\begin{aligned} x_1 &= x_0 + hf(x_0, y_0) \\ &= 2 + 0.1\{1195 \times 2 - 1995(-2)\} \\ &= 640 \end{aligned}$$

(d) Implicit Euler Method

$$h = 0.1$$

$$y_{n+1} = y_n + hf(x_{n+1}, y_{n+1})$$

$$x_1 = x_0 + hf(x_0, y_0)$$

$$y_1 = y_0 + hf(x_0, y_0)$$

$$\begin{aligned} x_1 &= 2 + 0.1(1195x_1 - 1995y_1) \leftarrow (1) \\ &= -118.5x_1 + 199.5y_1 = 2 \end{aligned}$$

$$\begin{aligned} y_1 &= -2 + 119.7x_1 - 199.7y_1 \\ &= -119.7x_1 + 200.7y_1 = -2 \end{aligned}$$


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$$\begin{bmatrix} -118.5 & 199.5 \\ -119.7 & 200.7 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \frac{1}{97.2} \begin{bmatrix} 200.7 & -199.54 \\ -119.7 & -118.5 \end{bmatrix} \begin{bmatrix} 2 \\ -2 \end{bmatrix}$$

$$= \frac{1}{97.2} \begin{bmatrix} 800.4 \\ 476.4 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} 8.23 \\ 4.9 \end{bmatrix}$$

(e) The exact solution is  $\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -8e^{-800t} + 10e^{-2t} \\ -8e^{-800t} + 6e^{-2t} \end{bmatrix}$

$$x = -8e^{-800t} + 10e^{-2t}$$

$$x(0.1) = -8e^{-800 \times 0.1} + 10e^{-2 \times 0.1} = 8.187$$

$$y = -8e^{-800t} + 6e^{-2t}$$

$$y(0.1) = -8e^{-80} + 6e^{-0.2} = 4.912$$

$$x(0.1) = 8.187$$

$$y(0.1) = 4.912$$

$$\left. \begin{array}{l} x(0.1) = 640 \\ y(0.1) = 636.8 \end{array} \right\} \text{Explicit Euler Method}$$

$$\left. \begin{array}{l} x(0.1) = 8.187 \\ y(0.1) = 4.912 \end{array} \right\} \text{Implicit Euler Method}$$

$\therefore$  Implicit Euler Method is good for moderately stiff equation.

(f)  $h_{\max} > \frac{2}{|\mathbf{I}_{\max}|}$

$$h_{\max} > \frac{2}{800}$$

$$h_{\max} > 0.0025$$

In order to compute a stable solution, maximum step size of 0.0025 can be used.

(g) The maximum step size for which the solution does not change when h is decreased.

$$h_{opt} \leq h_{max}$$

But it can only be determined observing how computed solution varies as  $h$  is decreased. For accuracy one must use smaller step size than the step size required for just maintaining the numerically stable.

$$(h) \quad SR = \frac{|I_{max}|}{|I_{min}|} = \frac{800}{2} = 400$$

Since  $40 < SR < 100,000$  it is moderately stiff, meaning it encompasses a wide range of time steps. We need smaller time steps for numerical stability due to  $|I_{max}|$  but want larger time steps due to  $|I_{min}|$  in order to approach the steady state.

- (i) Implicit Euler Method is always numerically stable. Only thing to worry is accuracy. In general, one could take time step which are as large as desired without risking numerical instability. Accuracy, however, would still depend on the size of the time step taken.
- (j) If the computer requires  $1 \times 10^{-6}$  sec of CPU time to do the computation with explicit method, it requires  $4 \times 10^{-6}$  sec of the 4<sup>th</sup> order R.K method was used instead.

Q 3.

$$x' = 1.2x - 0.6xy, \quad x(0) = 2$$

$$y' = -0.8y + 0.2xy \quad y(0) = 1$$

$$x' = f(x, y) \quad x(0) = 2$$

$$y' = g(x, y) \quad y(0) = 1$$

$$J = \begin{bmatrix} \frac{df}{dx} & \frac{df}{dy} \\ \frac{dg}{dx} & \frac{dg}{dy} \end{bmatrix}$$

$$J = \begin{bmatrix} 1.2 - 0.6y & -0.6x \\ 0.2y & -0.8 + 0.2x \end{bmatrix}$$

At steady state, steady state 1

$$x_s = 0 \quad y_s = 0$$

$$J = \begin{bmatrix} 1.2 & 0 \\ 0 & -0.8 \end{bmatrix}$$

$$\Rightarrow \mathbf{I} = 1.2, -0.8$$

$$y = \sum_{i=1}^n e^{a_i t} [C_i \sin b_i t + D_i \cos b_i t]$$

$$x = ae^{-0.8t} + be^{1.2t}$$

$$y = ce^{-0.8t} + de^{1.2t}$$

at  $t \rightarrow \infty$ ,  $x$  &  $y \rightarrow \infty$  because of  $(\mathbf{I} = 1.2)e^{1.2t}$

The system is conditionally stable

Steady state 2

$$x_s = 4, \quad y_s = 2$$

$$J = \begin{bmatrix} 0 & -2.4 \\ 0.4 & 0 \end{bmatrix}$$

$$F(\mathbf{I}) = \mathbf{I}^2 + 0.96 = 0 \Rightarrow \mathbf{I} = \pm 0.96i$$

$$x = e^{0t} [a \sin 0.98t + b \cos 0.98t]$$

$$y = e^{at} [a \sin 0.98t + d \cos 0.98t]$$

- (b) The function F and g are non-linear. Therefore, Jacobin matrix is changing with time, eigenvalues of Jacobin matrix is changing with time and the stability also changes with time.
- (c) For explicit (Forward Euler) method to maintain numerical stability (i.e, obtaining bounded numerical solution for function with bounded exact solution), the maximum step size that can be used is given by

$$h_{\max} \leq \frac{2}{|\mathbf{I}_{\max}|}$$

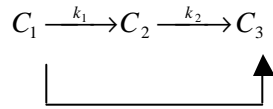
For accuracy, one must use smaller step size than the step size required for just maintaining the numerical stability.

Implicit (Backward Euler Method) is always numerically stable. Therefore, one could use as large a step size as desired without taking numerical instability. However, for accuracy one must use small step sizes.

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Q 4.



$$\frac{dy_1}{dx} = -\frac{[k_1 + k_3]}{S} \mathbf{j} y^2, y_1(0) = 1$$

$$\frac{dy_2}{dx} = y^2 - \frac{k_2}{S} \mathbf{j} y_2, y_2(0) = 0$$

$$k_1 = 18.1 \text{ hr}^{-1}$$

$$k_2 = 1.7 \text{ hr}^{-1}$$

$$k_3 = 4.8 \text{ hr}^{-1}$$

$$\mathbf{j} = \exp(-\mathbf{a}x)$$

$$S = 20, 50 \text{ \& } 100 \text{ hr}^{-1}$$

$$\mathbf{a} = 0, 1, 2$$

Solve the problem by using 4<sup>th</sup> Order Runge-Kutta method,

$$S = 20, \mathbf{a} = 0$$

$$\frac{dy_1}{dx} = \frac{(k_1 + k_2)}{S} \mathbf{j} y^2 = \frac{-(18.1 + 4.8)}{20} \exp(-0 \times x) y^2$$

$$y_1' = -1.145 y^2$$

$$\text{Let } u' = y_1' = -1.145 u^2, u(0) = 1$$

$$\frac{dy_2}{dx} = y_1^2 - \frac{k_2}{S} \mathbf{j} y_2, y_2(0) = 0$$

$$= y_1^2 - \frac{1.7}{20} (\exp - (0 \times x)) y_2$$

$$y_2' = y_1^2 - 0.085 y_2$$

$$\text{Let } y_2 = w$$

$$y_2' = w' = u' - 0.085 w, w(0) = 0$$

By RK-4 method,

$$u_{n+1} = u_n + \frac{1}{6} [K_1 + 2K_2 + 2K_3 + K_4]$$

$$w_{n+1} = w_n + \frac{1}{6} [L_1 + 2L_2 + 2L_3 + L_4]$$

$$u = f(t, u)$$

$$\mathbf{w} = g(t, u, \mathbf{w})$$

$$\text{At } n = 0, h = 0.2$$

$$\begin{aligned} K_1 &= hf(t_n, u_n) \\ &= 0.2(-1.145e^{-x}u^2) \\ &= -0.229 \end{aligned}$$

$$\begin{aligned} L_1 &= hg(t_n, u_n, \mathbf{w}_n) \\ &= 0.2(u_0^2 - 0.085e^{-o}\mathbf{w}_0) \\ &= 0.2 \end{aligned}$$

$$\begin{aligned} K_2 &= h + \left[ t_n + \frac{h}{2}, u_n + \frac{K_1}{2} \right] \\ &= 0.2f[0.1, 0.9542] \\ &= -0.1796 \end{aligned}$$

$$\begin{aligned} L_2 &= 0.2g[0.1, 0.9542, 0.1] \\ &= 0.2[(0.9542)^2 - 0.034e^{-0.1}(0.1)] \\ &= 0.1551 \end{aligned}$$

$$\begin{aligned} K_3 &= hf \left[ t_n + \frac{h}{2}, u_n + \frac{K_2}{2} \right] \\ &= 0.2f[0.1, 0.96225] \\ &= -0.1897 \end{aligned}$$

$$\begin{aligned} L_3 &= 0.2g[0.1, 0.96225, 0.09075] \\ &= 0.2[(0.96225)^2 - 0.034e^{-0.1} \times 0.09075] \\ &= 0.1644 \end{aligned}$$

$$\begin{aligned} K_4 &= hf[t_n + h, u_n + K_3] \\ &= 0.2f[0.1, 0.9233] \\ &= 0.2[-0.458e^{-0.1}(0.9233)^2] \\ &= -0.1504 \end{aligned}$$

$$\begin{aligned} L_4 &= 0.2g[0.1, 0.9233, 0.0923] \\ &= 0.2[(0.9233)^2 - 0.034e^{-0.1} \times 0.0923] \\ &= 0.1285 \end{aligned}$$

$$\begin{aligned}
u_{n+1} &= u_1 = u_0 + \frac{1}{6}[K_1 + 2K_2 + 2K_3K_4] \\
&= 1 + \frac{1}{6}[(-0.229) + 2(-0.1796) + 2(-0.1897) + (-0.1507)] \\
&= 0.8134
\end{aligned}$$

$$\begin{aligned}
w_{n+1} &= w_1 = 0 + \frac{1}{6}[0.2 + 2(0.1551) + 2(0.1644) + 0.1285] \\
&= 0.16125
\end{aligned}$$

$$y_1^{(1)} = u_1 = 0.8134$$

$$y_2^{(2)} = w = 0.16125$$

$$S = 50, \mathbf{a} = 1$$

$$\frac{dy_1}{dx} = \frac{(k_1 + k_2)}{S} \mathbf{j} y^2 = \frac{-(18.1 + 4.8)}{20} \exp(-1 \times x) y^2$$

$$\frac{dy_1}{dx} = -0.458 e^{-x} y^2$$

$$y_1' = -0.458 e^{-x} y_1^2$$

$$\text{Let } u = y_1$$

$$u' = y_1'$$

$$u' = -0.458 e^{-x} y^2$$

$$\frac{dy_2}{dx} = y_1^2 - \frac{k_2}{s} \mathbf{j} y_2$$

$$y_2' = y_1^2 - \frac{1.7}{50} e^{-x} y_2$$

$$\text{Let } w = y_2 \Rightarrow w' = y_2'$$

$$w = u^2 - 0.034 e^{-x} w$$

Assume  $x = \frac{l}{l_0} = 0$  at initial condition,

By RK-4 method,

$$u = f(t, u)$$

$$w = g(t, u, w)$$

$$\text{At } n = 0, h = 0.2$$

$$u_{n+1} = u_n + \frac{1}{6}[K_1 + 2K_2 + 2K_3 + K_4]$$

$$\mathbf{w}_{n+1} = \mathbf{w}_n + \frac{1}{6}[L_1 + 2L_2 + 2L_3 + L_4]$$

$$\begin{aligned}K_1 &= hf(t_n, u_n) \\ &= 0.2(-0.458e^{-x}u^2) \\ &= -0.0916\end{aligned}$$

$$\begin{aligned}L_1 &= hg(t_n, u_n, \mathbf{w}_n) \\ &= 0.2(u_0^2 - 0.034e^{-o}\mathbf{w}_0) \\ &= 0.2\end{aligned}$$

$$\begin{aligned}K_2 &= h + \left[ t_n + \frac{h}{2}, u_n + \frac{K_1}{2} \right] \\ &= 0.2f[0.1, 0.9542] \\ &= -0.0755\end{aligned}$$

$$\begin{aligned}L_2 &= 0.2g[0.1, 0.9542, 0.1] \\ &= 0.2[(0.9542)^2 - 0.034e^{-0.1}(0.1)] \\ &= 0.1815\end{aligned}$$

$$\begin{aligned}K_3 &= hf\left[ t_n + \frac{h}{2}, u_n + \frac{K_2}{2} \right] \\ &= 0.2f[0.1, 0.96225] \\ &= -0.0767\end{aligned}$$

$$\begin{aligned}L_3 &= 0.2g[0.1, 0.96225, 0.09075] \\ &= 0.2[(0.96225)^2 - 0.034e^{-0.1} \times 0.09075] \\ &= 0.1846\end{aligned}$$

$$\begin{aligned}K_4 &= hf[t_n + h, u_n + K_3] \\ &= 0.2f[0.1, 0.9233] \\ &= 0.2[-0.458e^{-0.1}(0.9233)^2] \\ &= -0.0707\end{aligned}$$

$$\begin{aligned}L_4 &= 0.2g[0.1, 0.9233, 0.0923] \\ &= 0.2[(0.9233)^2 - 0.034e^{-0.1} \times 0.0923] \\ &= 0.1699\end{aligned}$$

$$\begin{aligned}
u_{n+1} &= u_1 = u_0 + \frac{1}{6}[K_1 + 2K_2 + 2K_3K_4] \\
&= 1 + \frac{1}{6}[(-0.0916) + 2(-0.0755) + 2(-0.0767) + 9 - 0.0707] \\
&= 0.9222 \\
w_{n+1} &= w_1 = 0 + \frac{1}{6}[0.2 + 2(0.1815) + 2(0.1846) + 0.1699] \\
&= 0.1837 \\
y_1^{(1)} &= u_1 = 0.9222 \\
y_2^{(1)} &= w_1 = 0.1837
\end{aligned}$$

Q 5.

- (a) Since the slope of the data in *circle* has slope of 1, the numerical method used should be Forward Euler Method, Backward Euler Method.

Since the slope of the data in *square* has the slope of 4, the numerical method used should be Forth-order Runge-Kutta Method.

- (b) The step size is quit large at the point A, so truncating error come into play and resulting error larger than slope of 1.

- (c) The step size is quit small at the point C, so round-off error come into play and resulting error larger than slope of 4.

(d) 
$$\frac{\log[E_t(y(t_f))]|_E - \log[E_t(y(t_f))]|_D}{\log(h)|_E - \log(h)|_D} = 4$$

$$\log \frac{[E_t(y(t_f))]|_E}{[E_t(y(t_f))]|_D} = \log \left( \frac{(h)|_E}{(h)|_D} \right)^4$$

$$\frac{[E_t(y(t_f))]|_E}{[E_t(y(t_f))]|_D} = 2^4$$

$$[E_t(y(t_f))]|_E = 16[E_t(y(t_f))]|_D$$

- (e) CPU time of D is 8 times longer than E.  
Forth-order Runge-Kutta Method is assumed.

- (f) CPU time of B is 2 times longer than C.  
Forward Euler Method is assumed.
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