1) $y_{n+1} - y_n = h\left[\theta f_{n+1} + (1-\theta) f_n\right]$, $\theta \in [0, 1]$

(a) θ method to $y' = \lambda y$, $\lambda \in \mathbb{C}$. Show
$$y_{n+1} = \frac{1 + (1-\theta)z}{1-\theta z} y_n, \quad z = h\lambda.$$

Pf.

$$y_{n+1} = y_n + h\left[\theta f_{n+1} + (1-\theta) f_n\right]$$
$$= y_n + h\left[\theta \lambda y_{n+1} + (1-\theta)\lambda y_n\right]$$
$$\rightarrow y_{n+1} - h\theta\lambda y_{n+1} = y_n + h(1-\theta)\lambda y_n$$
$$\rightarrow y_{n+1}(1 - h\theta\lambda) = y_n + h(1-\theta)\lambda y_n$$
$$\rightarrow y_{n+1} = \frac{y_n(1 + h(1-\theta)\lambda)}{(1 - h\theta\lambda)}$$

where $z = h\lambda$
$$\rightarrow y_{n+1} = \frac{1 + (1-\theta)z}{1-\theta z} y_n$$

(b) Let $w = \dfrac{1 + (1-\theta)z}{1-\theta z}$. Show that
$$|w|^2 - 1 = \frac{(1-2\theta)|z|^2 + (z + \bar{z})}{|1-\theta z|^2}$$

Hence, deduce that
$$|w| < 1 \iff (1-2\theta)|z|^2 + (z+\bar{z}) < 0$$

* ($|w|^2 = w\bar{w} = \dfrac{1+(1-\theta)z}{1-\theta z} \dfrac{1+(1-\theta)\bar{z}}{1-\theta\bar{z}}$)

Pf.
$$|w|^2 = \frac{1 + (1-\theta)z + (1-\theta)\bar{z}(1 + (1-\theta)z)}{1 - \theta z - \theta\bar{z}(1-\theta z)}$$
$$= \frac{1 + (1-\theta)(z+\bar{z}) + (1-\theta)^2|z|^2}{1 - \theta(z+\bar{z}) + \theta^2|z|^2}$$
$$\rightarrow |w|^2 - 1 = \frac{\cancel{1} + (\cancel{1-\theta})(z+\bar{z}) + (\cancel{1-\theta})^2|z|^2}{1 - \theta(z+\bar{z}) + \theta^2|z|^2}$$
$$\frac{\cancel{-1} + \cancel{\theta(z+\bar{z})} - \cancel{\theta^2}|z|^2}{1 - \theta(z+\bar{z}) + \theta^2|z|^2}$$
$$= \frac{(z+\bar{z}) + |z|^2 - 2\theta|z|^2}{|1-\theta z|^2}$$
$$= \frac{(z+\bar{z}) + |z|^2(1-2\theta)}{|1-\theta z|^2}$$

For $|w| < 1 \rightarrow |w|^2 < 1$ as well,
$$\rightarrow \frac{(z+\bar{z}) + |z|^2(1-2\theta)}{|1-\theta z|^2} < 1 \quad (*)$$

Since $|1-\theta z|^2 > 0$, $(*)$ holds iff
$$(z+\bar{z}) + |z|^2(1-2\theta) < |1-\theta z|^2$$
For this to hold $\forall z, \theta$,
$$\rightarrow (z+\bar{z}) + |z|^2(1-2\theta) < 0$$
$$\rightarrow |w| < 1 \iff (1-2\theta)|z|^2 + (z+\bar{z}) < 0.$$

(c) Show that
$$(1-2\theta)|z|^2 + (z+\bar{z})$$
$$= (1-2\theta)\left|z + \frac{1}{1-2\theta}\right|^2 - \frac{1}{1-2\theta}$$

Pf.
RHS
$$= (1-2\theta)\left(z\bar{z} + \frac{z+\bar{z}}{1-2\theta} + \frac{1}{(1-2\theta)^2}\right) - \frac{1}{1-2\theta}$$
$$= (1-2\theta)|z|^2 + (z+\bar{z}) \quad \square$$

(d)(i) For $\theta \in (\frac{1}{2}, 1]$, show the stability region of θ method is given by $\left|z - \frac{1}{2\theta-1}\right| > \frac{1}{2\theta-1}$

Pf.
Since $\theta > \frac{1}{2} \rightarrow (1-2\theta) < 0$,

The region is stable when
$$(1-2\theta)|z|^2 + (z+z) < 0$$
$$\rightarrow (1-2\theta)\left|z + \frac{1}{1-2\theta}\right|^2 - \frac{1}{1-2\theta} < 0$$
$$\rightarrow (1-2\theta)\left|z + \frac{1}{1-2\theta}\right|^2 < \frac{1}{1-2\theta}$$
(Δ)
Since $(1-2\theta) < 0$ for $\theta \in (\frac{1}{2}, 1]$
dividing reverses inequality
$$\rightarrow \left|z + \frac{1}{1-2\theta}\right|^2 > \frac{1}{(1-2\theta)^2}$$
$$\rightarrow \sqrt{\left|z + \frac{1}{1-2\theta}\right|^2} > \sqrt{\frac{1}{(1-2\theta)^2}}$$
$$\rightarrow \left|z - \frac{1}{2\theta-1}\right|^2 > \frac{1}{2\theta-1} \quad \square.$$

(d)(ii) For $\theta \in [0, \frac{1}{2})$ show stab. reg:
$$\left|z + \frac{1}{1-2\theta}\right| < \frac{1}{1-2\theta}$$
Since $(1-2\theta) > 0$ for $\theta \in [0, \frac{1}{2})$,
dividing doesn't reverse the inequality so we have:
$$\left|z + \frac{1}{1-2\theta}\right|^2 < \frac{1}{(1-2\theta)^2}$$
$$\rightarrow \left|z + \frac{1}{1-2\theta}\right| < \frac{1}{1-2\theta}$$

(d)(iii) if $\theta = \frac{1}{2}$, this corresponds to the trapezoidal method which is stable $\forall z \in \mathbb{C}$ such that the real part of z is negative.

② AB2

(a)

$$y_{n+2} - y_{n+1} = h\left(\frac{3}{2} f_{n+1} - \frac{1}{2} f_n\right)$$

$$\rightarrow y_{n+2} - y_{n+1} - \frac{3}{2} h\lambda y_{n+1} + \frac{1}{2} h\lambda y_n = 0$$

$$p(\xi) = \xi^2 - \left(1 + \frac{3}{2} h\lambda\right)\xi + \frac{1}{2} h\lambda$$

roots: $\xi_1 = \frac{1}{2} + \frac{\sqrt{3}}{2} i$, $\xi_2 = \frac{1}{2} - \frac{\sqrt{3}}{2} i$

$|\xi_1| = |\xi_2| = 1 \rightarrow$ strict root cond. not satisfied,

So the stability region is outside the locus.

(b) AM2

$$y_{n+2} - y_{n+1} = h\left(\frac{5}{12} f_{n+2} + \frac{8}{12} f_{n+1} - \frac{1}{12} f_n\right)$$

$$\rightarrow y_{n+2} - y_{n+1} - \frac{5}{12} h\lambda y_{n+2} - \frac{8}{12} h\lambda y_{n+1} + \frac{1}{12} h\lambda y_n = 0$$

$$\rightarrow p(\xi) = \xi^2 - \left(1 + \frac{8}{12} h\lambda\right)\xi + \frac{5}{12} h\xi^2 + \frac{1}{12} h\lambda$$

The roots: $\xi_1 = 1$, $\xi_2 = \frac{1}{2}$

Satisfy the strict root condition so the stability region is inside the locus.

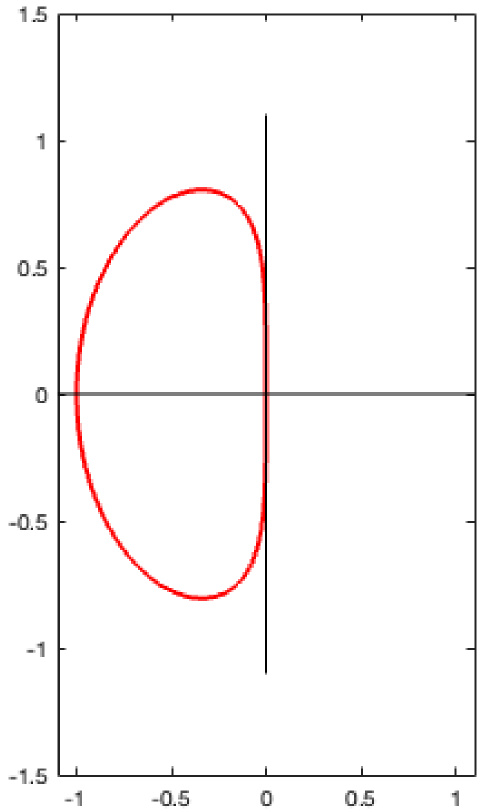
Table of Contents

Using boundary locus method to trace out the shape of stability region

```
% Clean workspace and command window, close all figures
clear ; clc ; close all ;
```

AB2 Method

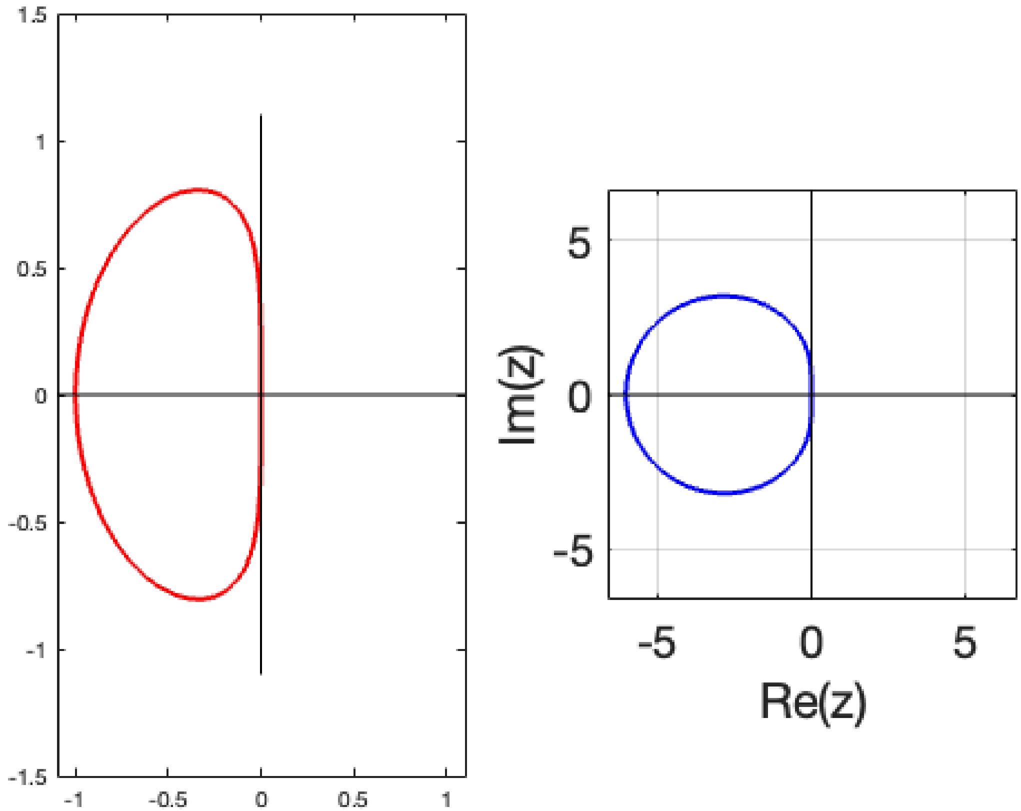
```
% Discretize theta space (0 to 2*pi)
thvec = linspace(0, 2*pi, 1000) ;

% Define 1st and 2nd characteristic polynomials for your LMM
rho_poly = @(r) r.^2 - r ;
sigma_poly = @(r) (3/2)*r - (1/2) ;

% Boundary locus
zvec = rho_poly(exp(1i*thvec)) ./ sigma_poly(exp(1i*thvec)) ; % 1i represents
 imaginary number

% Plot boundary of stability region in complex plane
figure(1) ; clf ;
% Plot boundary locus
subplot(1, 2, 1);
plot(zvec, 'r-', 'LineWidth', 2) ; hold on ;
% Plot axes
xmax = 1.1*max(abs(zvec)) ; ymax = 1.1*max(abs(zvec)) ;
plot([-xmax xmax], [0 0], 'k-', 'LineWidth', 0.5) ; % Real axis
plot([0 0], [-ymax, ymax], 'k-', 'LineWidth', 0.5) ; % Imaginary axis
```



AM2 Method

```
% Discretize theta space (0 to 2*pi)
thvec = linspace(0, 2*pi, 1000) ;

% Define 1st and 2nd characteristic polynomials for your LMM
rho_poly = @(r) r.^2 - r;
sigma_poly = @(r) (5/12)*r.^2 + (8/12)*r - (1/12);

% Boundary locus
zvec = rho_poly(exp(1i*thvec)) ./ sigma_poly(exp(1i*thvec)) ; % 1i represents
 imaginary number

% Plot boundary of stability region in complex plane
subplot(1, 2, 2);
% Plot boundary locus
plot(zvec, 'b-', 'LineWidth', 2) ; hold on ;
% Plot axes
xmax = 1.1*max(abs(zvec)) ; ymax = 1.1*max(abs(zvec)) ;
plot([-xmax xmax], [0 0], 'k-', 'LineWidth', 0.5) ; % Real axis
plot([0 0], [-ymax, ymax], 'k-', 'LineWidth', 0.5) ; % Imaginary axis
% Advanced plot settings
```

```
axis equal ; axis tight ; grid on ;
set(gca, 'FontSize', 20)
xlabel('Re(z)') ; ylabel('Im(z)') ;

saveas(gcf, 'AB2UAM2.png');
```



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(3)

(a) $k_1 = f(t_n, y_n)$
$k_2 = f(t_n + \frac{h}{2}, y_n + h\frac{k_1}{2}) = \lambda(y_n + \frac{h}{2}k_1)$
$y_{n+1} = y_n + hk_2$ $\quad = \lambda(y_n + \frac{h}{2}\lambda y_n)$

$\rightarrow y_{n+1} = y_n + h\lambda y_n + \frac{h^2}{2}\lambda^2 y_n$
$= y_n(1 + h\lambda + \frac{h^2}{2}\lambda^2)$

If $z = \lambda h$,
$y_{n+1} = y_n(1 + z + \frac{z^2}{2})$

(b)
$k_1 = f(t_n y_n) = \lambda y_n$
$k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1) = \lambda(y_n + \frac{h}{2}k_1)$
$k_3 = f(t_n + h, y_n - hk_1 + 2hk_2) = \lambda(y_n - hk_1 + 2hk_2)$
$y_{n+1} = y_n + h(\frac{1}{6}k_1 + \frac{4}{6}k_2 + \frac{1}{6}k_3)$

$\rightarrow y_{n+1} = y_n + \frac{h}{6}\lambda y_n + \frac{2h}{3}\lambda(y_n + \frac{h}{2}\lambda y_n)$
$+ \frac{h}{6}\lambda(y_n - h\lambda y_n + 2h\lambda(y_n + \frac{h}{2}\lambda y_n))$
$\rightarrow y_{n+1} = y_n + \frac{h}{6}\lambda y_n + \frac{2}{3}h\lambda y_n + \frac{h^2}{3}\lambda^2 y_n + \frac{h}{6}\lambda y_n + \frac{h^3}{6}\lambda^2 y_n$
$\rightarrow y_{n+1} = y_n(1 + h\lambda + \frac{h^2}{2}\lambda^2 + \frac{h^3}{6}\lambda^3)$

$\rightarrow y_{n+1} = y_n(1 + z + \frac{z^2}{2} + \frac{z^3}{6})$

(c) $k_1 = f(t_n y_n) = \lambda y_n$
$k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1)$
$k_3 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2)$
$k_4 = f(t_n + h, y_n + hk_3)$
$y_{n+1} = y_n + h(\frac{1}{6}k_1 + \frac{2}{6}k_2 + \frac{2}{6}k_3 + \frac{1}{6}k_4)$

$\rightarrow y_{n+1} = y_n + \frac{h}{6}\lambda y_n + \frac{h}{3}\lambda(y_n + \frac{h}{2}\lambda y_n)$
$+ \frac{h}{3}\lambda(y_n + \frac{h}{2}\lambda(y_n + \frac{h}{2}\lambda y_n))$
$+ \frac{h}{6}\lambda(y_n + h\lambda(y_n + \frac{h}{2}\lambda(y_n + \frac{h}{2}\lambda y_n)))$

$\rightarrow y_{n+1} = y_n + \frac{h}{6}\lambda y_n + \frac{h}{3}\lambda y_n + \frac{h^2}{6}\lambda^2 y_n + \frac{h^3}{12}\lambda^3 y_n + \frac{h}{6}\lambda y_n$
$+ \frac{h^2}{6}\lambda^2 y_n + \frac{h^3}{12}\lambda^3 y_n + \frac{h^4}{24}\lambda^4 y_n$

$\rightarrow y_{n+1} = y_n(1 + h\lambda + \frac{h^2}{2}\lambda^2 + \frac{h^5}{6}\lambda^3 + \frac{h^4}{24}\lambda^4)$
$\rightarrow y_{n+1} = y_n(1 + z + \frac{z^2}{2} + \frac{z^3}{6} + \frac{z^4}{24})$

(d) The size of the stability region increases for higher order methods.

```
% specify range in x and y for plot below, and number of points
```

Construct two-dimensional mesh

```
xv = linspace(-3, 3, 301);
yv = linspace(-3, 3, 301);
[xx, yy] = meshgrid(xv, yv);            % x and y each are NxN arrays to be
                                       % used in the call to 'contour' below

% calculate z
zz = xx + 1i*yy;         % notice the imaginary number i is written 1i


%%%%%%%%%%%%%%% Uncomment below and begin your edits %%%%%%%%%%%%%%%%%%%%%%


% Define Q for second-order RK (Explicit Midpoint)
Q_rk2 = 1 + zz + zz.^2 / 2;

% Define Q for third-order RK
Q_rk3 = 1 + zz + zz.^2 / 2 + zz.^3 / 6;

% Define Q for fourth-order RK (Classical RK4)
Q_rk4 = 1 + zz + zz.^2 / 2 + zz.^3 / 6 + zz.^4 / 24;


%%%%%%%%%%%%%%%%%%%%%%%%%% End of your edits %%%%%%%%%%%%%%%%%%%%%%%%%%%%%


% compute complex modulus of Q
Q_rk2_mag = abs(Q_rk2);
Q_rk3_mag = abs(Q_rk3);
Q_rk4_mag = abs(Q_rk4);
```

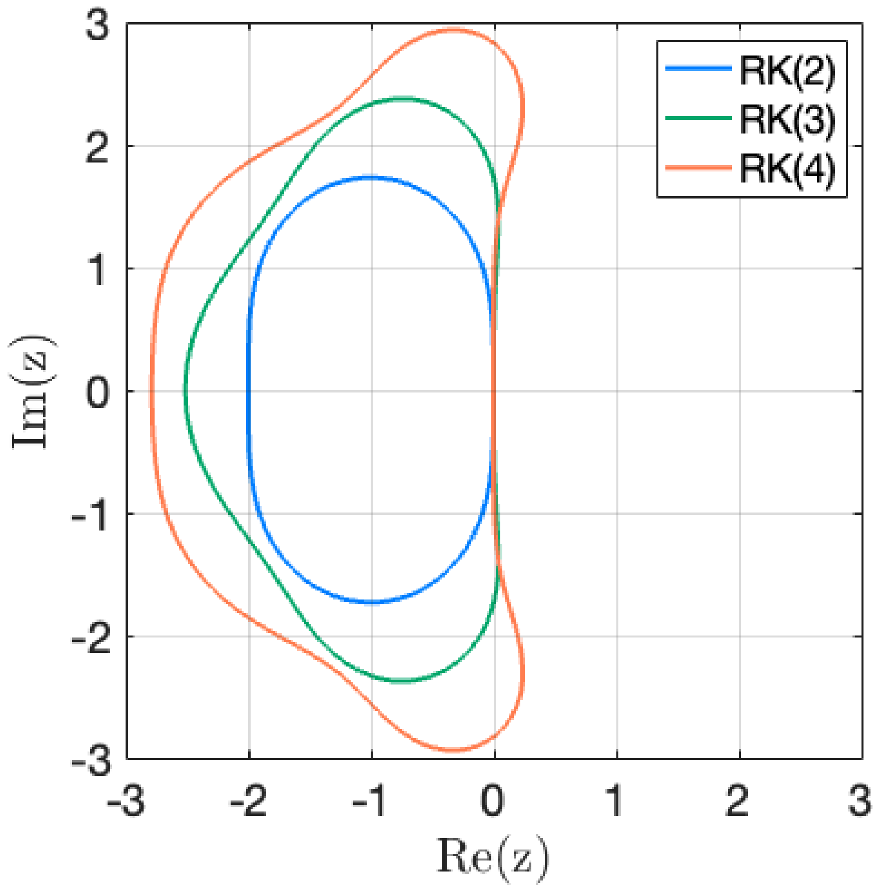
Plot contours--these plot the contour lines Q(z) = 1; since the region

```
               of absolute stability is defined to be when |Q(z)| < 1,
               this means everything ~inside~ the curves is the stable
               region, and everything outside is unstable.

% Define "good-looking" color for plotting
azure = [0, 128, 255]/255 ;
jade = [0, 168, 107]/255 ;
coral = [255, 127, 80]/255 ;

figure(1) ; clf ;
contour(xx, yy, Q_rk2_mag, [1 1], '-', 'LineWidth', 2, 'Color', azure) ;
 hold on ;
contour(xx, yy, Q_rk3_mag, [1 1], '-', 'LineWidth', 2, 'Color', jade)
```

```
contour(xx, yy, Q_rk4_mag, [1 1], '-', 'LineWidth', 2, 'Color', coral)
axis([-3, 3, -3, 3]);
axis('square')
set(gcf, 'defaultTextInterpreter', 'Latex')
set(gca, 'FontSize', 20)
xlabel('Re(z)') ;  ylabel('Im(z)') ; grid on ;
legend('RK(2)', 'RK(3)', 'RK(4)')
```



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4

(a) ~~Ve~~ Verify a steady state $(y' = 0)$ is given by $y_e = (0,0,1)^T$.

$$y_1' = -\alpha y_1 + \beta y_2 y_3$$
$$y_2' = \alpha y_1 - \beta y_2 y_3 - \gamma y_2^2$$
$$y_3' = \gamma \cdot y_2^2$$

Substitute $y_e = (0,0,1)^T$:

$$y_1' = -\alpha(0) + \beta(0)(1) = 0$$
$$y_2' = \alpha(0) - \beta(0)(1) - \gamma(0)^2 = 0$$
$$y_3' = \gamma(0)^2 = 0$$

$\rightarrow$ y_e is a steady state.

HW5 Problem 4: simulation a stiff chemical reaction system

Table of Contents

Initial value

```
y0 = [1 ; 0 ; 0] ;


%%%%%%%%%%%%%%%%%%%%%%%%%%%% Begin your edits %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

Time span for simulating chemical reaction

```
T = 40000 ; % Edit this for (d)
tspan = [0, T] ;
```

Parameters

```
alpha = 0.04;
beta = 1e4;
gamma = 3e7;
```

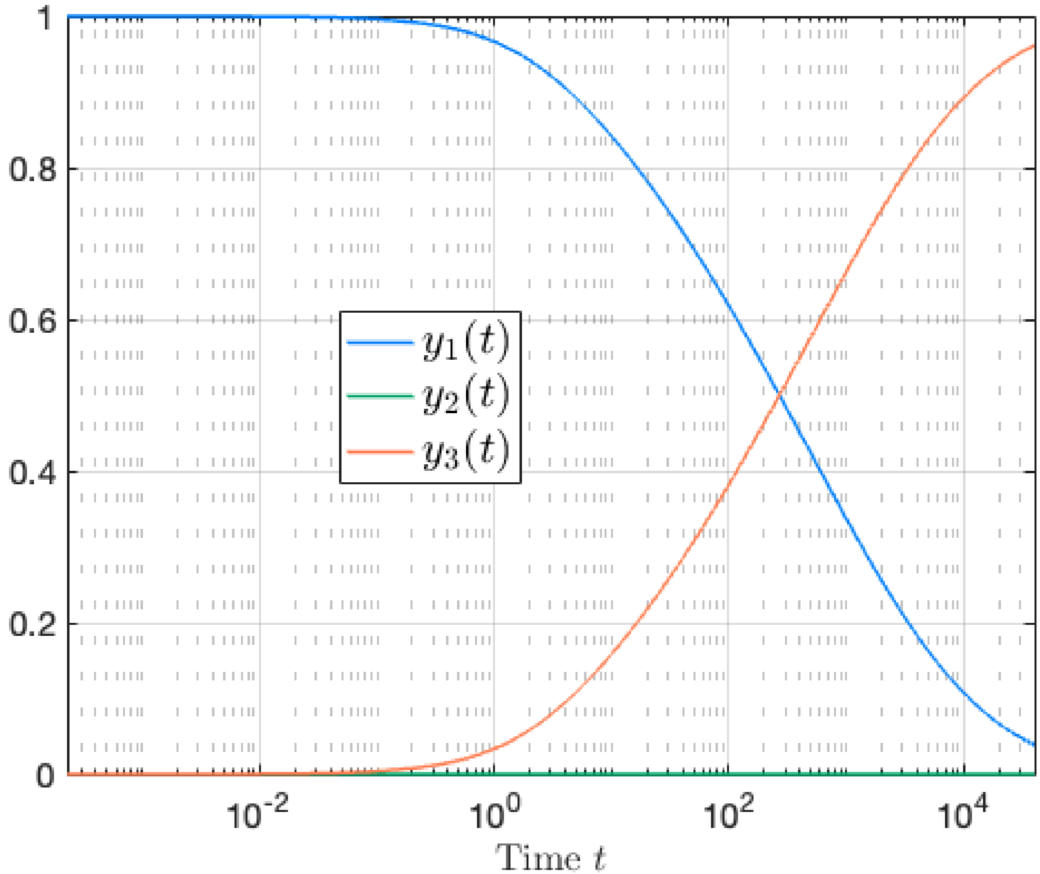
Solve IVP with ode45/ode15s

```
% Don't uncomment both (run one each time)

% [t,y] = ode45(@(t,y) [-alpha*y(1) + beta*y(2)*y(3);
%                        alpha*y(1) - beta*y(2)*y(3) - gamma*y(2)^2;
%                        gamma*y(2)^2], tspan, y0);

[t,y]= ode15s(@(t,y) [-alpha*y(1) + beta*y(2)*y(3);
                      alpha*y(1) - beta*y(2)*y(3) - gamma*y(2)^2;
                      gamma*y(2)^2], tspan, y0);


% % You may report your findings for (b), (c) and (d) here:
```

```
% (b): It appears that y1 is decreasing to 0, y2 is staying at 0, and y3 is
% increasing towards 1, which is approaching the steady state (0,0,1).
% Although our solution is not close to the steady state after just 3
% steps.

% (c): The approach seems similar to (b) in that after 3 steps the values
% are nearly identical yet are not yet near the steady state.

% (d): It is interesting, there was rapid convergence towards 1/2 for both
% y1 and y3, yet after passing 1/2 both decreased their absolute rate of
% change. Increaing T by magnitudes of 10 incrementally edged the solution
% towards the steady state. I found T to be around 40000 for y3 to be
% around 0.95.

%%%%%%%%%%%%%%%%%%%%%%%% End of your edits %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

Plot

```
% Define "good-looking" color for plotting
azure = [0, 128, 255]/255 ;
jade = [0, 168, 107]/255 ;
coral = [255, 127, 80]/255 ;

figure(1) ; clf ;
semilogx(t, y(:,1), '-', 'LineWidth', 1.5, 'Color', azure) ; hold on ;
semilogx(t, y(:,2), 'r-', 'LineWidth', 1.5, 'Color', jade) ;
semilogx(t, y(:,3), 'b-', 'LineWidth', 1.5, 'Color', coral)
set(gca, 'FontSize', 15) ;
set(gcf, 'defaultTextInterpreter', 'Latex') ;
xlabel('Time $t$') ; xlim([t(1), t(end)]) ; grid on ;
leg = legend('$y_1(t)$', '$y_2(t)$', '$y_3(t)$') ;
set(leg, 'Interpreter', 'Latex', 'FontSize', 20, 'Location', 'Best')
```



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