

SBf12, Assignment 2 Solutions

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1 Problem 1



1.1 Part (a)

Let \mathbf{a} be the stoichiometric matrix,

$$\mathbf{a} = \begin{pmatrix} -2 \\ 1 \end{pmatrix} + \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (2)$$

$$= \begin{pmatrix} -1 \\ 1 \end{pmatrix}. \quad (3)$$

1.2 Part (b)

Let $K(\mathbf{v})$ be the kinetics vector (a scalar in this case),

$$K(\mathbf{v}) = v_x^2 v_y. \quad (4)$$

1.3 Part (c)

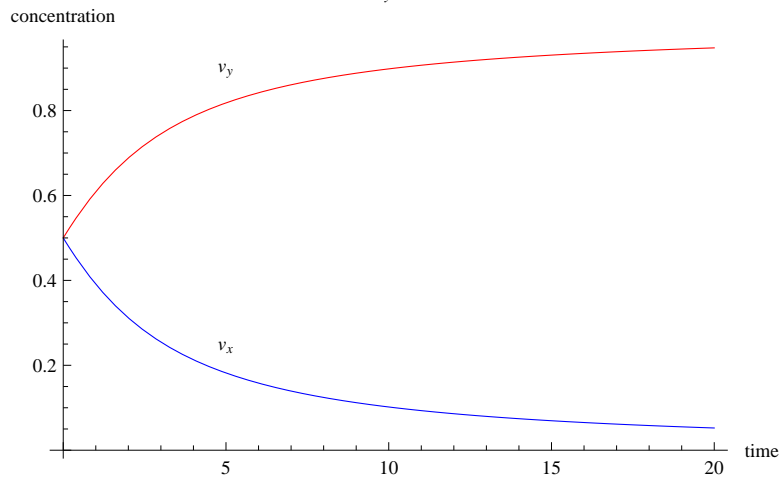
The ODE model is then,

$$\dot{\mathbf{v}} = \mathbf{a}K(\mathbf{v}) \quad (5)$$

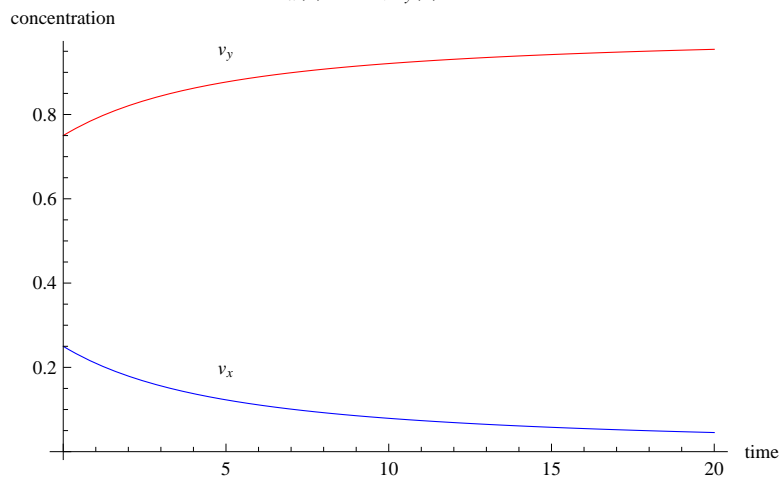
$$= \begin{pmatrix} -v_x^2 v_y \\ v_x^2 v_y \end{pmatrix}. \quad (6)$$

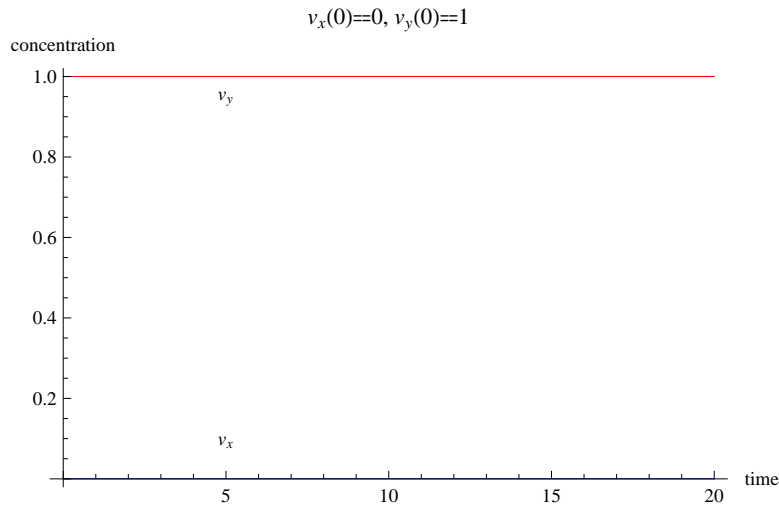
1.4 Part (d)

$$v_x(0) = v_y(0) = 0.5$$



$$v_x(0)=0.25, v_y(0)=0.75$$





1.5 Part (e)

Let \mathbf{m} be the mass vector. Suppose the system is conservative,

$$0 = \mathbf{m}^T \dot{\mathbf{v}} \quad (7)$$

$$= \mathbf{m}^T \mathbf{a}K(\mathbf{v}) \quad (8)$$

$$= \begin{pmatrix} m_x & m_y \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} K(\mathbf{v}) \quad (9)$$

$$m_x = m_y \quad (10)$$

The mass vector has a nontrivial solution, so the system is conservative.

1.6 Part (f)

To find the equilibria, solve for $\dot{\mathbf{v}} = 0$.

$$\dot{\mathbf{v}} = \begin{pmatrix} -v_x^2 v_y \\ v_x^2 v_y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (11)$$

$$v_x = 0 \quad \text{or} \quad v_y = 0 \quad (12)$$

The vector field associated with these ODEs is shown in Figure 1. Equilibrium points are plotted in orange, the vector field $\dot{\mathbf{v}}$ is plotted in blue, and a few sample trajectories are shown in black. You can see from this figure that equilibria along $v_x = 0$ are stable, and equilibria along $v_y = 0$ are unstable.

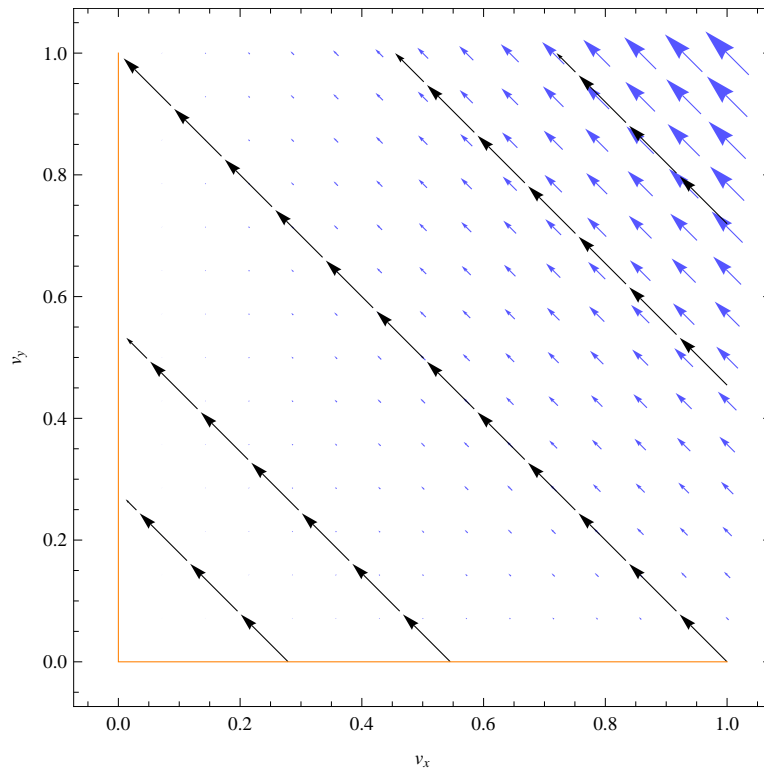


Figure 1: Vector field associated with $\dot{\mathbf{v}}$ in problem 1. Equilibrium points are shown in orange, the vector field is shown in blue, and a few sample trajectories are shown in black.

1.7 Part (g)

Note that the systems is conservative, which reduces our system from two to one dimension. Let C be some constant,

$$C = v_x + v_y \quad (13)$$

$$\dot{v}_x = -\dot{v}_y \quad (14)$$

$$\dot{v}_x = -v_x^2 v_y \quad (15)$$

$$= -v_x^2 (C - v_x). \quad (16)$$

Let $f(v_x, v_y) = \dot{v}_x$. Linearizing this equation, we get

$$S = \partial f / \partial v_x \quad (17)$$

$$= v_x(3v_x - 2C). \quad (18)$$

Evaluating the eigenvalue of S at the equilibrium,

$$\lambda = v_x(3v_x - 2C) \quad (19)$$

$$\lambda|_{v_x=0} = 0 \quad (20)$$

$$\lambda|_{v_y=0} = \lambda|_{v_x=C} \quad (21)$$

$$= C^2. \quad (22)$$

Note that $C^2 = 0$ iff $v_x = 0$ and $v_y = 0$. This means that at $v_x = 0$ the system is marginally stable, and at $v_y = 0$ and $v_x > 0$ the system is unstable.

2 Problem 2

The CRN from the lecture 4 is as follows:



2.1 Part (a)

The stoichiometric matrix is then,

$$\mathbf{A} = \begin{pmatrix} 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (27)$$

$$= \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}. \quad (28)$$

2.2 Part (b)

The kinetics vector is as follows,

$$\mathbf{K}(\mathbf{v}) = \begin{pmatrix} \alpha_R \\ v_R \alpha_P \\ v_R \beta_R \\ v_P \beta_P \end{pmatrix}. \quad (29)$$

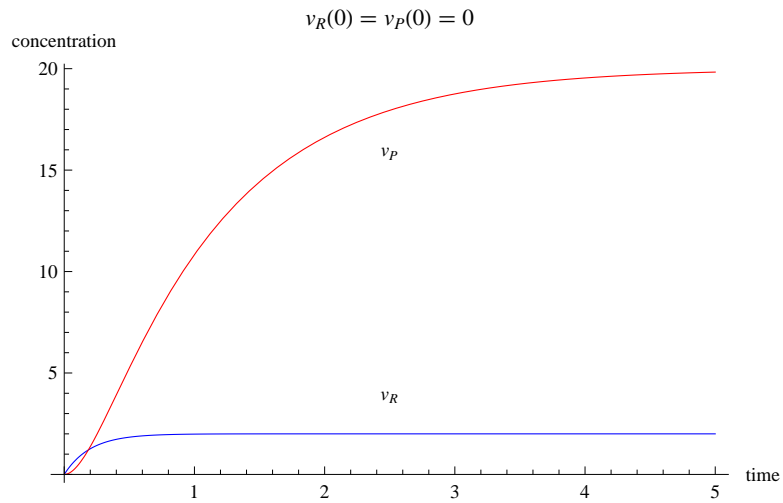
2.3 Part (c)

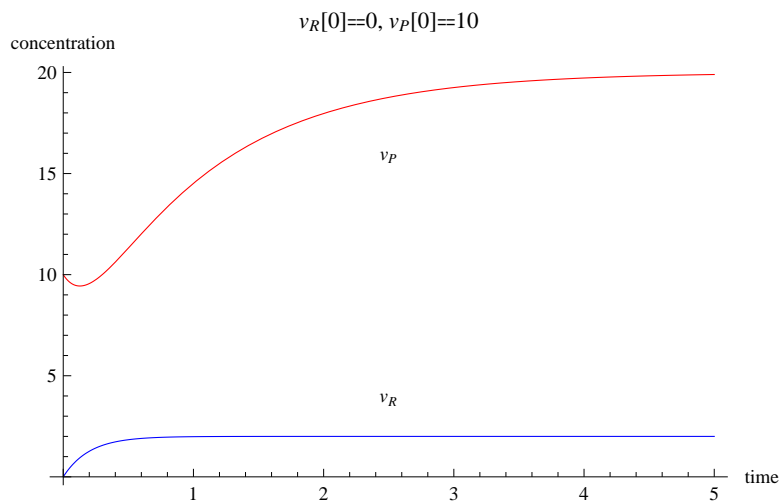
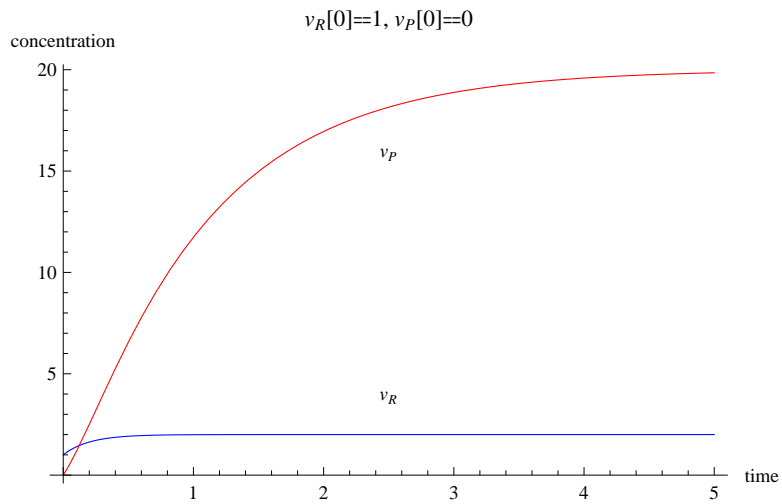
The ODEs are,

$$\dot{\mathbf{v}} = \mathbf{A}\mathbf{v} \quad (30)$$

$$= \begin{pmatrix} \alpha_R - v_R \beta_R \\ v_R \alpha_P - v_P \beta_P \end{pmatrix} \quad (31)$$

2.4 Part (d)





2.5 Part (e)

Let \mathbf{m} be the mass vector. Suppose the system is conservative,

$$0 = \mathbf{m}^T \dot{\mathbf{v}} \quad (32)$$

$$= \mathbf{m}^T \mathbf{a}K(\mathbf{v}) \quad (33)$$

The mass vector has only the trivial solution, so the system is not conservative.

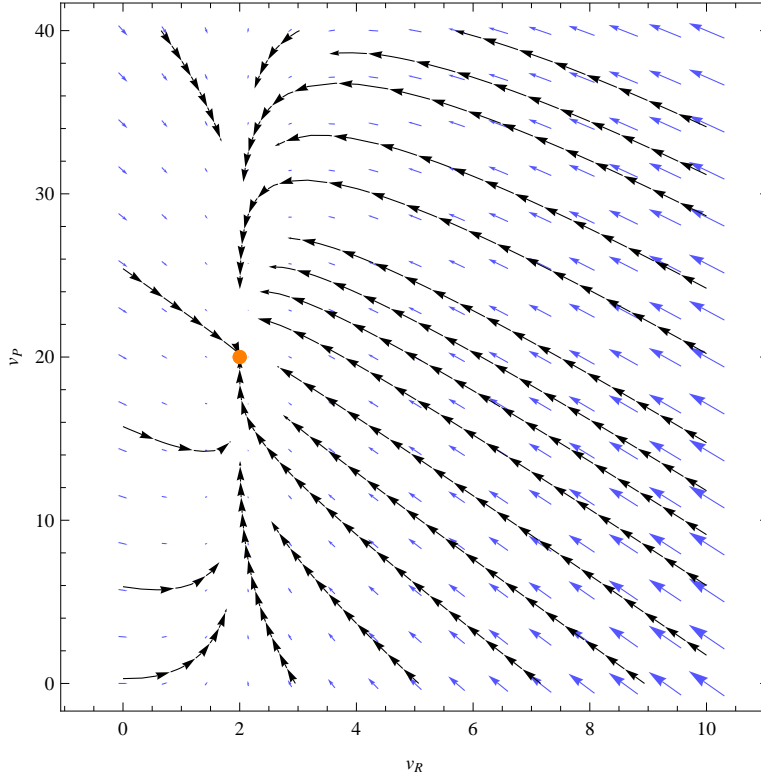


Figure 2: Vector field associated with $\dot{\mathbf{v}}$ in problem 2. The equilibrium point is shown in orange, the vector field is shown in blue, and a few sample trajectories are shown in black.

2.6 Part (f)

Solving for the equilibria,

$$0 = \dot{\mathbf{v}} \quad (34)$$

$$= \begin{pmatrix} \alpha_R - \beta_R v_R \\ \alpha_P v_R - \beta_P v_P \end{pmatrix} \quad (35)$$

$$v_R = \frac{\alpha_R}{\beta_R} \quad \text{and} \quad v_P = \frac{\alpha_R \alpha_P}{\beta_R \beta_P}. \quad (36)$$

. The vector field along with some sample trajectories and the equilibrium point are shown in Figure 2. From the vector field, this appears to be a stable equilibrium point.

2.7 Part (g)

Let $f_1(v_r, v_P) = v_r$ and $f_2(v_R, v_P) = v_P$. Linearizing the ODEs,

$$\mathbf{S} = \begin{pmatrix} \frac{\partial f_1}{\partial v_R} & \frac{\partial f_1}{\partial v_P} \\ \frac{\partial f_2}{\partial v_R} & \frac{\partial f_2}{\partial v_P} \end{pmatrix} \quad (37)$$

$$= \begin{pmatrix} -\beta_R & 0 \\ \alpha_P & -\beta_P \end{pmatrix}. \quad (38)$$

Solving for the eigenvalues of \mathbf{S} ,

$$\lambda_1 = -\beta_P \quad (39)$$

$$\lambda_2 = -\beta_R. \quad (40)$$

Clearly both eigenvalues are negative (rates can only be positive), so the system is stable.

3 Problem 3

Let \mathbf{A} be the stoichiometric matrix,

$$\mathbf{A} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}. \quad (41)$$

Let $\mathbf{K}(\mathbf{v})$ be the kinetics vector,

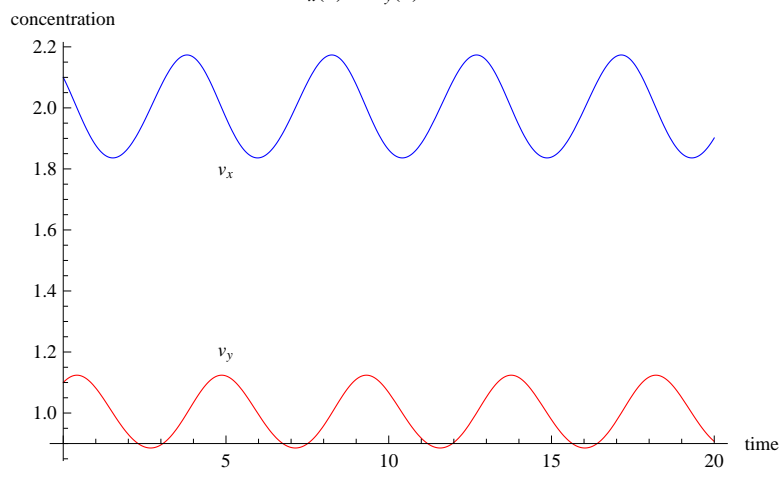
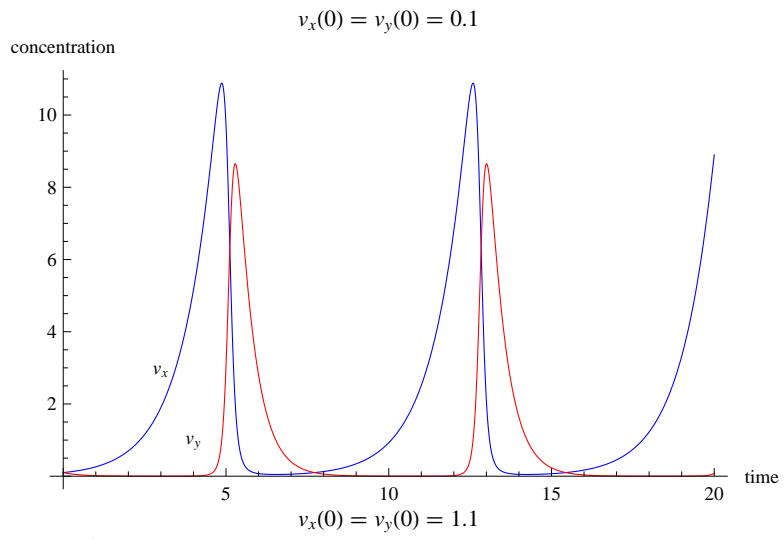
$$\mathbf{K}(\mathbf{v}) = \begin{pmatrix} v_X \\ v_X v_Y \\ 2v_Y \end{pmatrix}. \quad (42)$$

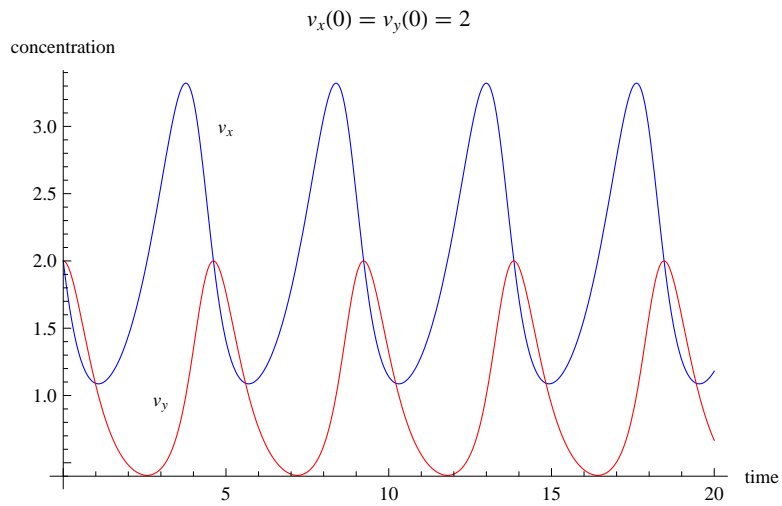
The the ODE model is,

$$\dot{\mathbf{v}} = \mathbf{A}\mathbf{K}(\mathbf{v}) \quad (43)$$

$$= \begin{pmatrix} v_x - v_x v_y \\ v_x v_y - 2v_y \end{pmatrix}. \quad (44)$$

Some sample trajectories are show below.





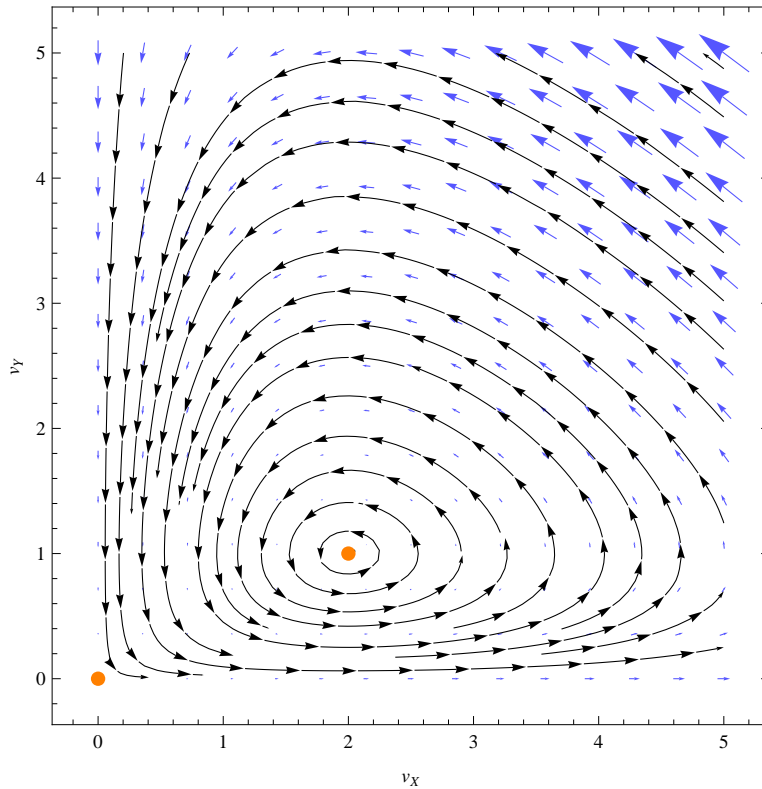
Note that $\text{Ker}(\mathbf{A}^T) = \emptyset$. This system does not admit a nontrivial mass vector, so the system is not conservative.

Solving for the equilibria,

$$0 = v_x - v_x v_y \quad (45)$$

$$0 = v_x v_y - 2v_y \quad (46)$$

$$v_x = v_y = 0 \quad \text{or} \quad v_x = 2, v_y = 1. \quad (47)$$



Linearizing the ODEs,

$$\mathbf{S} = \begin{pmatrix} 1 - v_y & -v_x \\ v_y & v_x - 2 \end{pmatrix} \quad (48)$$

$$\{\lambda_1, \lambda_2\}|_{v_x=v_y=0} = \{-2, 1\} \quad (49)$$

$$\{\lambda_1, \lambda_2\}|_{v_x=v_y=1} = \{-i\sqrt{2}, i\sqrt{2}\} \quad (50)$$

Since there is a positive eigenvalue at $v_x = v_y = 0$, and the eigenvalues at $\{v_x, v_y\} = \{2, 1\}$ have zero real part, we can tell that the system is unstable at $v_x = v_y = 0$ and marginally stable at $\{v_x, v_y\} = \{2, 1\}$.

4 Problem 4

For this problem I used the following `gro` code:

```
include gro
set("dt",0.01);
alphaR := 2.0;
```

```

alphaP := 3.0;
betaR := 0.1;

outfile := fopen("a2.csv","w");

program p() := {
  gfp := 0;
  RNA := 0;
  r := [t := 0, s := 0];

  rate (alphaR * volume)      : { RNA := RNA + 1 }
  rate (alphaP * RNA)         : { gfp := gfp + 1 }
  rate (betaR * RNA)          : { RNA := RNA-1 }

  id = 0 & r.s >= 1.0 : {
    fprintf(outfile, r.t, ",", gfp, ",", RNA, ",", volume, "\n"),
    r.s := 0;
  }
  true : {
    r.t := r.t + dt,
    r.s := r.s + dt
  }
};

ecoli ([], program p());

```

5 Problem 5

Let r be RNA concentration and p be GFP concentration. I used the following ODEs to simulate the concentration dynamics in a cell where δ is the dilution rate:

$$\dot{r} = \alpha_r - (\beta_r + \delta)r \quad (51)$$

$$\dot{p} = \alpha_p r - \delta p. \quad (52)$$

A reasonably good fit was achieved with the following parameters,

$$\alpha_r = 2 \quad (53)$$

$$\alpha_p = 3 \quad (54)$$

$$\beta_r = 0.1 \quad (55)$$

$$\delta = 0.0346574. \quad (56)$$

The trajectories found using these ODEs are overlaid on data obtained from gro simulation in Figure 3.

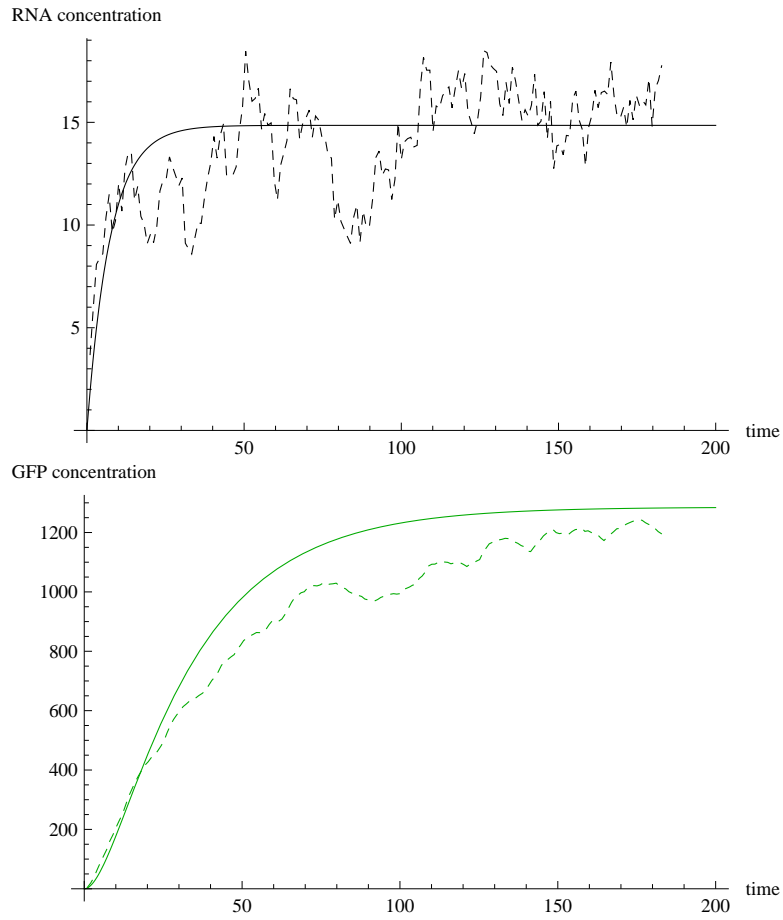


Figure 3: `gro` simulation data overlaid with ODEs simulated in Mathematica. `gro` data for RNA and GFP concentration are shown as dashed lines, the simulated ODEs are shown as solid lines.

6 Problem 6

The following gro code prints the RNA and GFP count, and volume for each cell every second of simulation time:

```
program main() := {
  t := 0;
  s := 0;
  L := {};
  s >= 1 : {
    L := maptocells {id,gfp,rna,volume} end;
    foreach q in L do
      fprintf(outfile,q[0],"",t,"",q[1],"",q[2],"",q[3],"\\n")
    end;
    s := 0;
  }
  true : {s := s + dt, t := t + dt}
};
```

The following Mathematica code imports and plots the collected data:

```
data = Import["a2-2.csv", "CSV"];
{id, time, gfp, rna, volume} = Transpose[data];
data = Transpose[{id, time, gfp/volume, rna/volume}];
idSplit = SplitBy[SortBy[data, First], First];
idSplit = Function[{x}, SortBy[x, #[[2]] &]] /@ idSplit;

GFPplots =
  Table[ListLinePlot[#[[{2, 3}]] & /@ idSplit [[i]],
    PlotStyle -> Hue[i/Length@idSplit]], {i, Length@idSplit}];
RNAplots =
  Table[ListLinePlot[#[[{2, 4}]] & /@ idSplit [[i]],
    PlotStyle -> Hue[i/Length@idSplit]], {i, Length@idSplit}];

p1 = Show[RNAplots, PlotRange -> All,
  AxesLabel -> {"time", "RNA_concentration"}]
p2 = Show[GFPplots, PlotRange -> All,
  AxesLabel -> {"time", "GFP_concentration"}]
```

