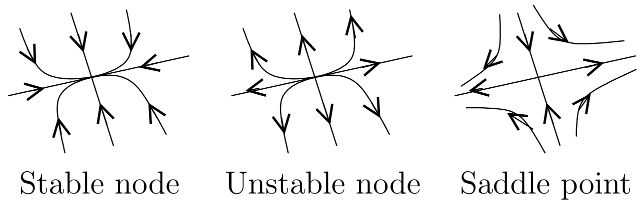
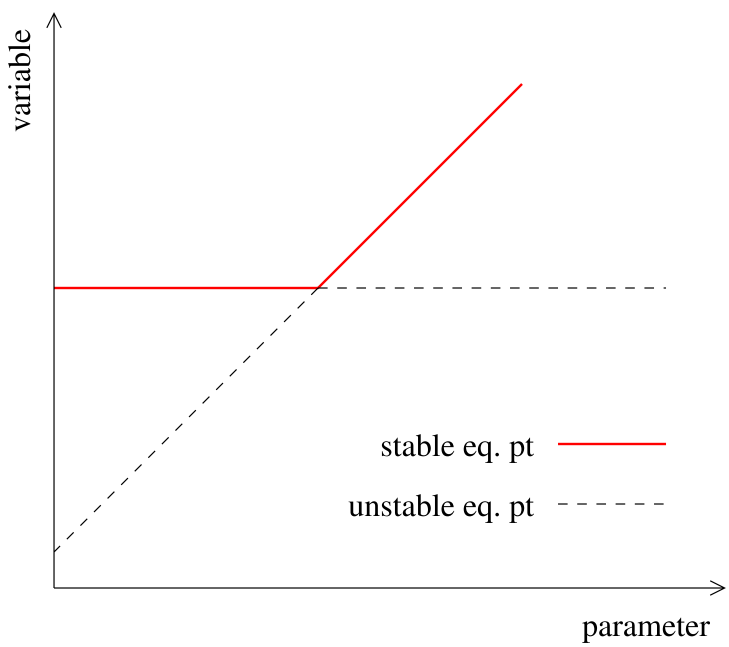
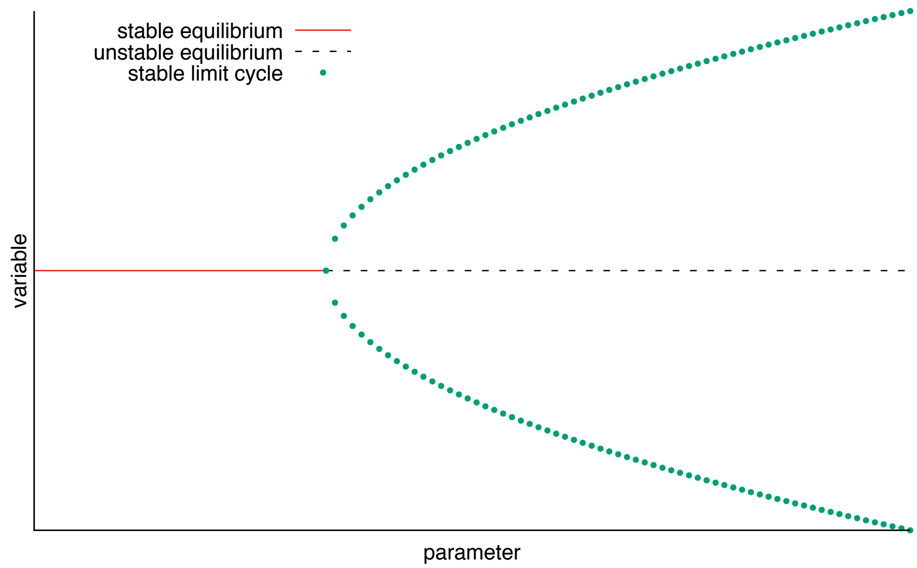
Chemistry 4010 Fall 2019
Test 1 solutions

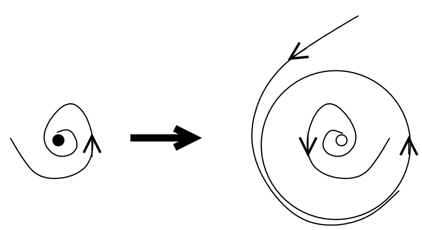
1. 

2. 

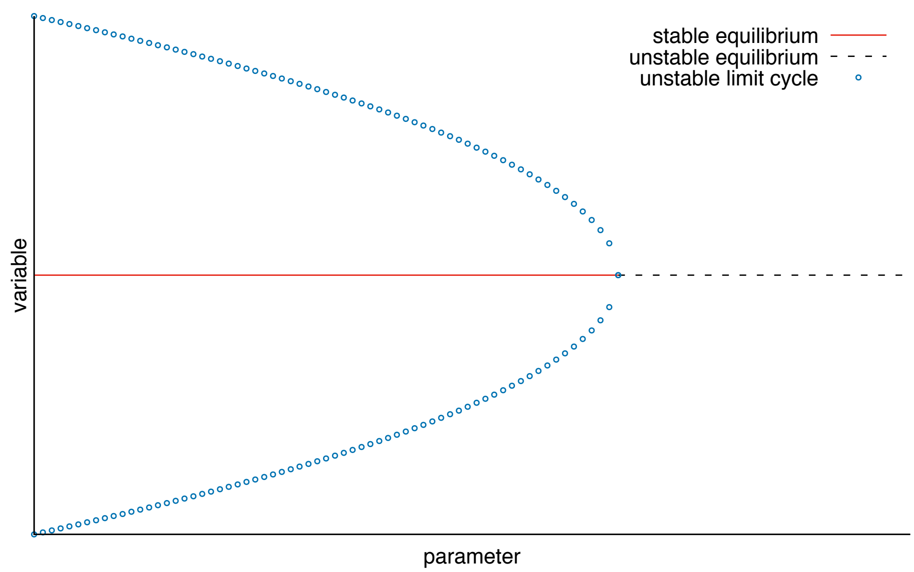
3. Sketch of the bifurcation diagram for a supercritical Andronov-Hopf bifurcation:



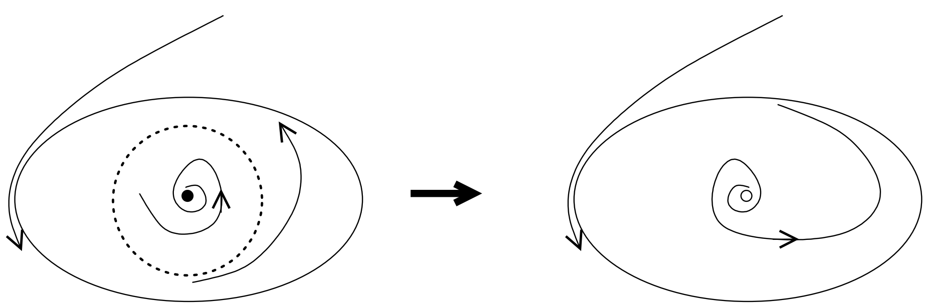
In a supercritical Andronov-Hopf bifurcation, the real part of a complex-conjugate pair of eigenvalues crosses zero. As the equilibrium point is destabilized, a stable limit cycle is born, which grows as we move away from the bifurcation point:



Sketch of the bifurcation diagram for a subcritical Andronov-Hopf bifurcation:



In a subcritical Andronov-Hopf bifurcation, an unstable limit cycle surrounding a stable focus shrinks until its radius goes to zero. At that point, the focus is destabilized, with the real part of a pair of complex-conjugate eigenvalues crossing zero.



In both cases, a stable focus loses stability and becomes an unstable focus. The difference is whether this loss of stability is accompanied by the creation of a stable limit cycle (supercritical case) or by the loss of an unstable limit cycle (subcritical).

4. (a)

$$\frac{dX}{dt} = k_x XY - d_x X$$
$$\frac{dY}{dt} = k_y XY - d_y Y$$

(b) To solve for the equilibrium points:

$$X\left(k_x Y - d_x\right) = 0 \tag{1}$$
$$Y\left(k_y X - d_y\right) = 0 \tag{2}$$

Equation 1 has two solutions: $X^\dagger = 0$ or $Y^* = d_x/k_x$. If we substitute $X^\dagger$ into equation 2, we get $Y^\dagger = 0$. On the other hand, since $Y^* \neq 0$, equation 2 gives $X^* = d_y/k_y$. We therefore have the two equilibrium points

$$(X^\dagger, Y^\dagger) = (0, 0)$$
$$(X^*, Y^*) = \left(\frac{d_y}{k_y}, \frac{d_x}{k_x}\right)$$

(c) **Phase-plane analysis:** Let us start by working out the nullclines. The X nullcline, which I will call $\mathcal{X}$, is obtained by setting $dX/dt = 0$. But as we saw above, this has two solutions. $\mathcal{X}$ is therefore the union of the following two lines in the phase plane:

$$\mathcal{X} = \bigcup\{X = 0, Y = Y^*\}.$$

Similarly, the Y nullcline, $\mathcal{Y}$, is

$$\mathcal{Y} = \bigcup\{Y = 0, X = X^*\}.$$

The nullclines are illustrated in Fig. 1.

Our job now is to sketch the vector field. On the Y axis, $dX/dt = 0$, and $dY/dt = -d_y Y < 0$. (This makes sense: if you don't have any females, you can't make any more, and the population dies off.) On the line $Y = Y^*$, we still have $dX/dt = 0$. As long as $X < X^*$, dY/dt must still be negative (since its sign can only change on the Y nullcline).

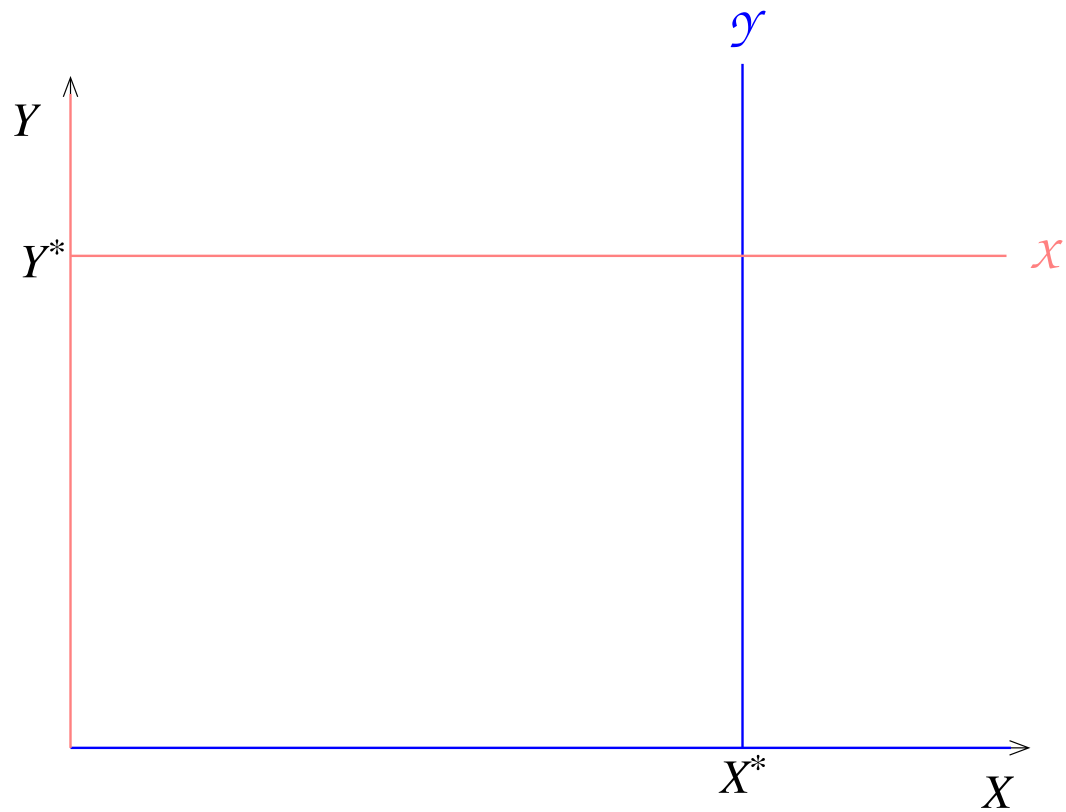


Figure 1: X and Y nullclines for the model of a sexually reproducing population. The X nullcline ($\mathcal{X}$) is in pink while the Y nullcline ($\mathcal{Y}$) is in blue. (And yes, I know that these are ridiculously stereotypical choices. I am hoping that they have some mnemonic value because of that.)

On the X axis, $dY/dt = 0$, and $dX/dt = -d_x X < 0$. On the line $X = X^*$, we have the same pattern of signs provided we are below the X nullcline, where the sign of dX/dt will change.

The signs of the two velocity components will be the same everywhere inside the rectangle whose opposite corners are $(X^\dagger, Y^\dagger)$ and (X^*, Y^*). For the sake of argument then, suppose that we consider a point with small values of both X and Y. Then $(dX/dt, dY/dt) \approx (-d_x X, -d_y Y)$, so both derivatives are negative. We can now use this information and the fact that the signs of the corresponding velocity components change on the nullclines to sketch the vector field, which is shown in Fig. 2.

Finally, we can sketch trajectories. My sketch is shown in Fig. 3. We see that the origin is a locally stable equilibrium point. However, trajectories that start from sufficiently far away from the origin, and in particular all trajectories that start from the region $X > X^*$, $Y > Y^*$, diverge to infinity. Thus, small populations become extinct, while large populations explode.

Linear stability analysis: This analysis starts like the phase plane analysis, by finding the two equilibrium points.

We then compute the Jacobian:

$$\mathbf{J} = \begin{bmatrix} k_x Y - d_x & k_x X \\ k_y Y & k_y X - d_y \end{bmatrix}$$

We start by analyzing the stability of the origin. We have

$$\mathbf{J}^\dagger = \begin{bmatrix} -d_x & 0 \\ 0 & -d_y \end{bmatrix}$$

The eigenvalues of this matrix are $-d_x$ and $-d_y$, so the origin is a stable equilibrium point.

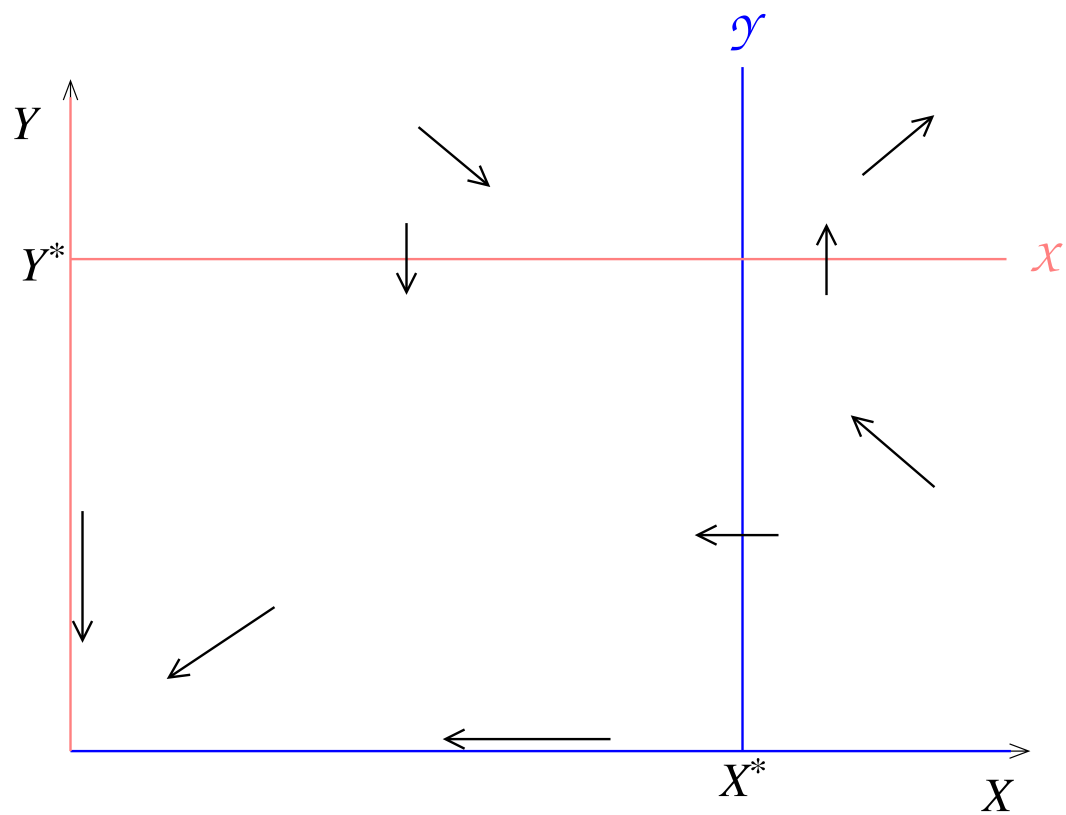


Figure 2: Sketch of the vector field for the model of a sexually reproducing population.

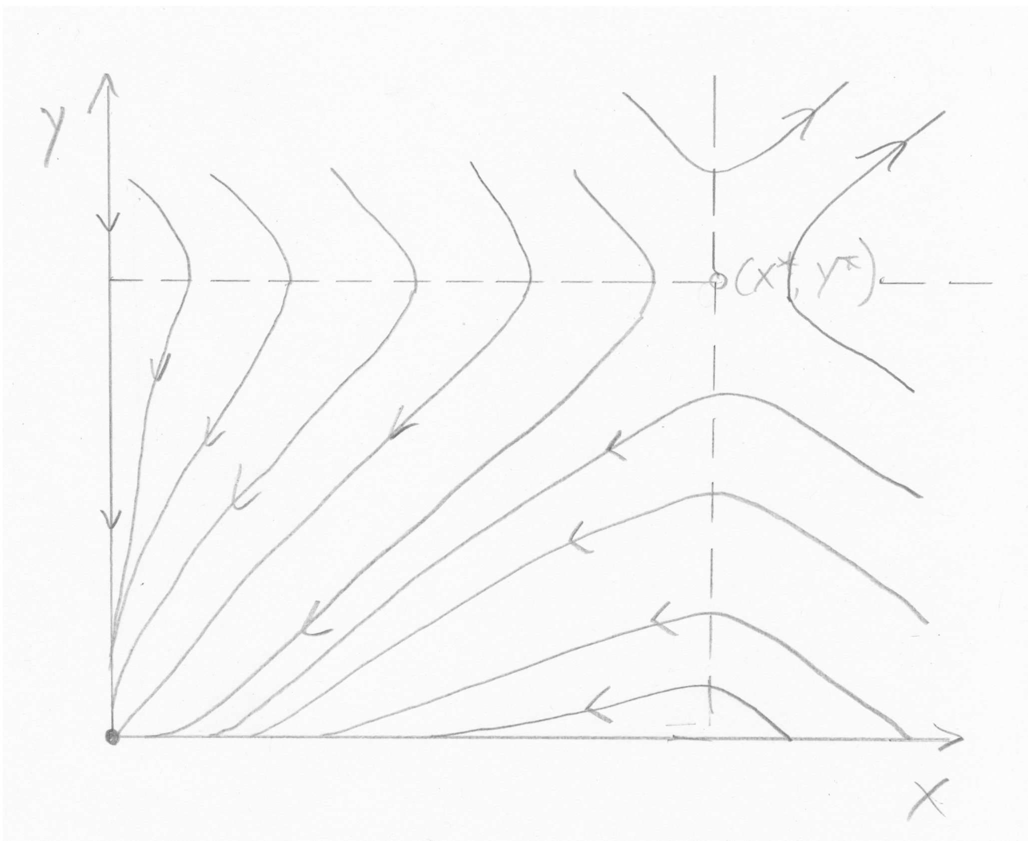


Figure 3: Sketch of the trajectories in the X-Y phase plane.

For the other equilibrium point, we have

$$\begin{aligned}
\mathbf{J}^* &= \begin{bmatrix} 0 & k_x d_y/k_y \\ k_y d_x/k_x & 0 \end{bmatrix} \\
\therefore |\lambda \mathbf{I} - \mathbf{J}^*| &= \begin{vmatrix} \lambda & -k_x d_y/k_y \\ -k_y d_x/k_x & \lambda \end{vmatrix} \\
&= \lambda^2 - d_x d_y = 0 \\
\therefore \lambda = \pm\sqrt{d_x/d_y}.
\end{aligned}$$

(X^*, Y^*) is therefore a saddle point.
From this analysis alone, we can conclude that the origin is a stable equilibrium point, i.e. that extinction is a possible long-term fate of such a population. We know that there does not exist a stable non-extinction equilibrium. However, the population explosion trajectories we saw in the phase-plane analysis are not evident from the linear stability analysis alone.

5. (a) Units of the variables and parameters:

S:	M
t:	s
S_0:	M
Q:	s^{-1}
V:	s^{-1}
K_M:	M
K_I:	M

I choose the following dimensionless variables:

$$\begin{aligned}
\tau &= Vt \\
s &= S/S_0
\end{aligned}$$

Replacing the original variables by my scaled variables, I get

$$\begin{aligned}
S_0 V \frac{ds}{d\tau} &= Q(S_0 - S_0 s) - \frac{V S_0 s}{1 + \frac{S_0 s}{K_M} + \frac{S_0^2 s^2}{K_M K_I}} \\
\therefore \dot{s} &= \frac{Q}{V}(1 - s) - \frac{s}{1 + \frac{S_0 s}{K_M} + \frac{S_0^2 s^2}{K_M K_I}}.
\end{aligned}$$

Define the dimensionless parameters

$$q = Q/V$$
$$\alpha = S_0/K_M$$
$$\beta = S_0/K_I$$

The dimensionless differential equation is therefore

$$\dot{s} = q(1-s) - \frac{s}{1 + \alpha s + \alpha\beta s^2}.$$

(b) When $q = 0$, we have the equilibrium point $s = 0$.

(c) To set up my XPPAUT input file, I need to calculate the equivalent values of my parameters:

$$\alpha = S_0/K_M = 10\,\mu\text{M}/1\,\mu\text{M} = 10$$
$$\beta = S_0/K_I = 10\,\mu\text{M}/0.5\,\mu\text{M} = 20$$

My XPPAUT input file is pretty simple:

```
# Xppaut input file for Degn's model of the
#       peroxidase-oxidase reaction

ds/dt=q*(1-s) - s/(1 + alpha*s + alpha*beta*s^2)

param q=0, alpha=10, beta=20

done
```

After a small amount of experimentation to set appropriate axes and step sizes, I got the bifurcation diagram shown in Fig. 4. We see that there is a range of bistability between the saddle-node bifurcations at $q = 0.018$ and 0.028.

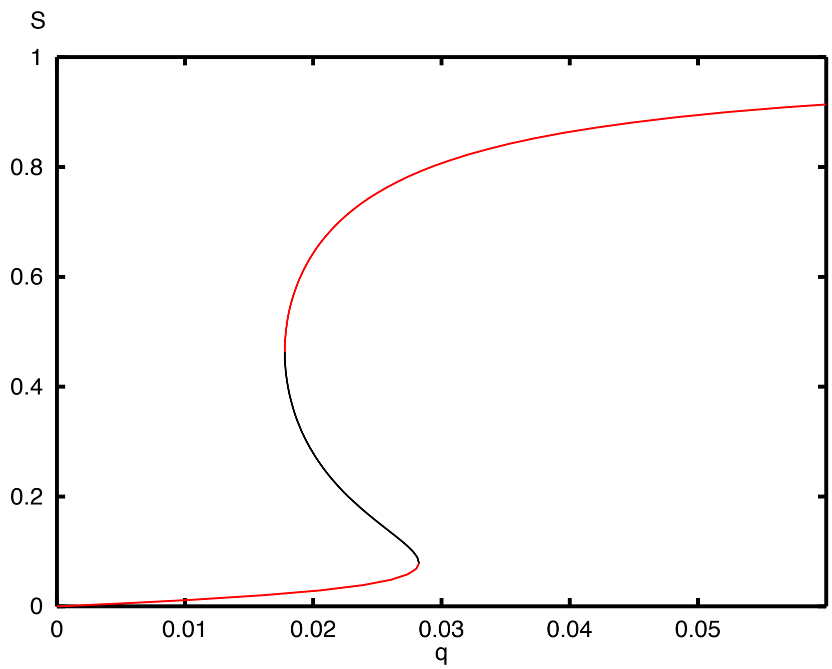


Figure 4: Bifurcation diagram for the peroxidase-oxidase model