Exercise Sheet 3: Bifurcations
Question 6 - Complete Solution

Methods of Applied Mathematics

Problem Statement

Consider the Brusselator system (a chemical reaction equation):

$$\dot{x} = a - bx + px^2y - qx$$
$$\dot{y} = bx - px^2y$$

Let $a = q = p = 1$ and consider what happens as b varies. In this problem b is a reaction rate so it is positive.

Tasks:

(a) Find any equilibria

(b) Find their stability

(c) Conjecture the bifurcation that occurs in the system, stating where (in x, y, and b) it happens, and sketch the bifurcation diagram

---

1 Step 1: Understand the Brusselator Model

Simplified system with $a = q = p = 1$

Substituting the parameter values:

$$\dot{x} = 1 - bx + x^2y - x = 1 - (b+1)x + x^2y$$
$$\dot{y} = bx - x^2y$$

Physical interpretation

The Brusselator models autocatalytic chemical reactions:

- x and y represent concentrations of chemical species
- The term x^2y represents an autocatalytic reaction (product catalyzes its own formation)
- Parameter b is a reaction rate controlling the conversion rate
- The opposite signs of x^2y in the two equations represent consumption in one reaction and production in another

XYZ Analysis of Model Structure

- **STAGE X (What we have):** A coupled nonlinear system with the autocatalytic term x^2y appearing with opposite signs. Similar structure to Question 5 but with different linear terms.
- **STAGE Y (Why this matters):** The Brusselator is a canonical example of a chemical oscillator. Key features:
  - The term x^2y couples the equations nonlinearly
  - It appears as $+x^2y$ in $\dot{x}$ (production of x) and $-x^2y$ in $\dot{y}$ (consumption of y)
  - The constant influx term $a = 1$ maintains the reaction
  - Parameter b controls the strength of the intermediate reaction

  Adding the equations: $\dot{x} + \dot{y} = 1 - x$, independent of b. This conservation-like property reflects the closed reaction scheme.
- **STAGE Z (What to expect):** The Brusselator is famous for exhibiting Hopf bifurcations - as reaction rate b increases, the system transitions from steady state to oscillatory behavior (chemical oscillations). This models real phenomena like the Belousov-Zhabotinsky reaction where concentrations oscillate periodically.

---

2 Step 2: Find Equilibria

Set up equilibrium conditions

For equilibria, we require $\dot{x} = 0$ and $\dot{y} = 0$:

$$1 - (b+1)x + x^2y = 0 \quad \cdots (1)$$
$$bx - x^2y = 0 \quad \cdots (2)$$

Solve systematically

From equation (2):

$$x(b - xy) = 0$$

This gives either $x = 0$ or $xy = b$.
Case 1: $x = 0$
Substitute into equation (1):

$$1 - 0 + 0 = 1 = 0 \quad \text{Contradiction!}$$

So $x = 0$ is not an equilibrium (the constant influx $a = 1$ prevents this).
Case 2: $xy = b$
This means $y = b/x$ (assuming $x \neq 0$).
Substitute into equation (1):

$$\begin{aligned} 1 - (b+1)x + x^2 \cdot \frac{b}{x} &= 0 \\ 1 - (b+1)x + xb &= 0 \\ 1 - bx - x + bx &= 0 \\ 1 - x &= 0 \end{aligned}$$

Therefore: $x = 1$
And: $y = b/1 = b$

Unique equilibrium

$$\boxed{(x^*, y^*) = (1, b)}$$

This equilibrium exists for all $b > 0$.

Verify equilibrium

Check equation (1): $1 - (b+1)(1) + (1)^2(b) = 1 - b - 1 + b = 0$
Check equation (2): $b(1) - (1)^2(b) = b - b = 0$

XYZ Analysis of Equilibrium

- **STAGE X (What we found):** Unique equilibrium at $(1, b)$ for all positive b. The x-coordinate is fixed at $x^* = 1$ while the y-coordinate equals the parameter: $y^* = b$.
- **STAGE Y (Why this structure):** From the equilibrium condition $bx = x^2y$, we have $y = b/x$. The first equation, after using this relation, becomes:

  $$1 - (b+1)x + xb = 1 - x = 0$$

  This forces $x = 1$ regardless of b. Then $y = b/1 = b$ follows automatically. The equilibrium position tracks the parameter vertically in the phase plane, moving along the line $x = 1$.
- **STAGE Z (What this means):** As b varies, the equilibrium slides along the vertical line $x = 1$. Unlike Question 5 where we proved a Hopf bifurcation exists, here we need to investigate whether changing b causes a similar stability transition. The equilibrium doesn't disappear or collide with others, so we expect either a Hopf bifurcation (oscillations emerge) or no bifurcation at all.

---

3 Step 3: Compute Jacobian Matrix

Partial derivatives

For $f(x, y) = 1 - (b+1)x + x^2y$ and $g(x, y) = bx - x^2y$:

$$\frac{\partial f}{\partial x} = -(b+1) + 2xy$$
$$\frac{\partial f}{\partial y} = x^2$$
$$\frac{\partial g}{\partial x} = b - 2xy$$
$$\frac{\partial g}{\partial y} = -x^2$$

Jacobian at general point

$$J(x, y) = \begin{pmatrix} -(b+1) + 2xy & x^2 \\ b - 2xy & -x^2 \end{pmatrix}$$

Jacobian at equilibrium $(1, b)$

Substitute $x = 1, y = b$:

$$
\begin{aligned}
\left.\frac{\partial f}{\partial x}\right|_{(1,b)} &= -(b+1) + 2(1)(b) = -b - 1 + 2b = b - 1 \\
\left.\frac{\partial f}{\partial y}\right|_{(1,b)} &= (1)^2 = 1 \\
\left.\frac{\partial g}{\partial x}\right|_{(1,b)} &= b - 2(1)(b) = b - 2b = -b \\
\left.\frac{\partial g}{\partial y}\right|_{(1,b)} &= -(1)^2 = -1
\end{aligned}
$$

Therefore:

$$J(1, b) = \begin{pmatrix} b-1 & 1 \\ -b & -1 \end{pmatrix}$$

XYZ Analysis of Jacobian

- **STAGE X (What we have):** A 2×2 Jacobian where three of the four entries depend on parameter b. Compare with Question 5: identical structure!
- **STAGE Y (Why this structure):** Notice the Jacobian is exactly the same as Question 5 with $\mu = b$:

  $$J_{\text{Q5}}(1, \mu) = \begin{pmatrix} \mu-1 & 1 \\ -\mu & -1 \end{pmatrix}, \quad J_{\text{Q6}}(1, b) = \begin{pmatrix} b-1 & 1 \\ -b & -1 \end{pmatrix}$$

  This is not a coincidence! Both systems are from the same family of autocatalytic reaction models. The Brusselator and the system in Question 5 share the same local linearization structure at their equilibria, just with different parameter symbols. This means they'll have identical bifurcation behavior.
- **STAGE Z (What this means):** Since the Jacobians are identical (up to parameter naming), we can immediately import results from Question 5:
  - Trace: $\tau = b - 2$
  - Determinant: $\Delta = 1$
  - Eigenvalues follow same formula
  - Hopf bifurcation occurs at $b = 2$

  But let's work through it systematically to be thorough.

---

4 Step 4: Analyze Stability

Compute trace and determinant

$$
\begin{aligned}
\text{Trace: } \tau &= (b-1) + (-1) = b - 2 \\
\text{Determinant: } \Delta &= (b-1)(-1) - (1)(-b) \\
&= -b + 1 + b = 1
\end{aligned}
$$

Notice: $\Delta = 1 > 0$ for all b (constant!)

Characteristic equation

$$\lambda^2 - \tau\lambda + \Delta = 0$$
$$\lambda^2 - (b-2)\lambda + 1 = 0$$

Solve for eigenvalues

Using quadratic formula:

$$\lambda = \frac{(b-2) \pm \sqrt{(b-2)^2 - 4}}{2}$$

Analyze discriminant

Let $\Delta_{disc} = (b-2)^2 - 4$

$$\begin{aligned}
(b-2)^2 - 4 > 0 \quad &\Leftrightarrow \quad |b-2| > 2 \quad \Leftrightarrow \quad b < 0 \text{ or } b > 4 \\
(b-2)^2 - 4 = 0 \quad &\Leftrightarrow \quad b = 0 \text{ or } b = 4 \\
(b-2)^2 - 4 < 0 \quad &\Leftrightarrow \quad 0 < b < 4
\end{aligned}$$

Since $b > 0$ (positive reaction rate), we have:

- For $0 < b < 4$: $\Delta_{disc} < 0 \rightarrow$ complex eigenvalues
- For $b = 4$: $\Delta_{disc} = 0 \rightarrow$ repeated real eigenvalue
- For $b > 4$: $\Delta_{disc} > 0 \rightarrow$ distinct real eigenvalues

Complex eigenvalues for $0 < b < 4$

When eigenvalues are complex:

$$\lambda = \frac{b-2}{2} \pm i\frac{\sqrt{4-(b-2)^2}}{2}$$

Define:

$$\rho(b) = \mathrm{Re}(\lambda) = \frac{b-2}{2}$$
$$\omega(b) = \mathrm{Im}(\lambda) = \pm\frac{\sqrt{4-(b-2)^2}}{2}$$

Stability classification

Parameter Range	**Real Part**	**Stability**
$0 < b < 2$	$\rho = \frac{b-2}{2} < 0$	Stable spiral
$b = 2$	$\rho = 0$	Neutral (critical)
$2 < b < 4$	$\rho = \frac{b-2}{2} > 0$	Unstable spiral

XYZ Analysis of Stability

- **STAGE X (What we found):** The equilibrium $(1, b)$ transitions from stable spiral to unstable spiral as b increases through 2. The eigenvalues are complex for $0 < b < 4$, with real part changing sign at $b = 2$.
- **STAGE Y (Why this transition):** The constant determinant $\Delta = 1$ constrains eigenvalues to lie on the unit circle in the complex plane (for complex eigenvalues, $|\lambda|^2 = \rho^2 + \omega^2 = 1$). As b varies:
  - The trace $\tau = b - 2$ varies linearly
  - Real part $\rho = (b - 2)/2$ increases linearly with b
  - At $b = 2$: real part crosses zero while imaginary part $\omega = \sqrt{4 - 0}/2 = 1$ remains nonzero
  - For $b < 2$: negative real part $\to$ inward spiraling (stable)
  - For $b > 2$: positive real part $\to$ outward spiraling (unstable)
- **STAGE Z (What this indicates):** The sign change of the real part at $b = 2$ while the imaginary part remains nonzero is the signature of a Hopf bifurcation. The system transitions from damped oscillations (spiral to equilibrium) to growing oscillations (spiral away from equilibrium). The nonlinearity must stabilize the growing oscillations into a limit cycle.

---

5 Step 5: Identify Bifurcation Point

Critical parameter value

Real part is zero when:

$$\rho(b) = \frac{b-2}{2} = 0 \quad \Rightarrow \quad \boxed{b^* = 2}$$

Eigenvalues at critical point

At $b = 2$:

$$\lambda = 0 \pm i\frac{\sqrt{4-0}}{2} = \pm i$$

Equilibrium at bifurcation point

At $b = 2$, the equilibrium is:

$$(x^*, y^*) = (1, 2)$$

Check imaginary part

$$\omega(2) = 1 \neq 0 \quad \checkmark$$

Check transversality

$$\frac{d\rho}{db} = \frac{d}{db}\left[\frac{b-2}{2}\right] = \frac{1}{2} \neq 0 \quad \checkmark$$

The real part crosses zero with positive slope.

XYZ Analysis of Bifurcation Identification

- **STAGE X (What we verified):** At $b = 2$, the equilibrium $(1, 2)$ has purely imaginary eigenvalues $\lambda = \pm i$, and the real part crosses zero transversely.

- **STAGE Y (Why this is a Hopf bifurcation):** All the conditions are satisfied:

  - **(B1)** Equilibrium exists: $(1, 2)$
  - **(B2)** Purely imaginary eigenvalues: $\lambda = \pm i$
  - **(G1)** Nonzero imaginary part: $\omega = 1 \neq 0$
  - **(G2)** Transverse crossing: $d\rho/db = 1/2 > 0$

  The positive derivative means:

  - For $b < 2$: real part negative $\to$ stable
  - For $b > 2$: real part positive $\to$ unstable

  The crossing is not tangential or degenerate.

- **STAGE Z (What this means):** By the Hopf Bifurcation Theorem, a limit cycle emerges for b near 2. The question is whether it's supercritical (stable limit cycle for $b > 2$) or subcritical (unstable limit cycle for $b < 2$). For the Brusselator with these parameters, it's known to be supercritical, meaning stable oscillations emerge for $b > 2$.

---

6 Step 6: Conjecture Bifurcation Type

Observed characteristics

1. Unique equilibrium for all $b > 0$
2. Equilibrium stable for $b < 2$, unstable for $b > 2$
3. Eigenvalues cross imaginary axis at $b = 2$
4. Imaginary part nonzero at crossing ($\omega = 1$)
5. No other equilibria created or destroyed
6. Complex eigenvalues indicate oscillatory behavior

Bifurcation conjecture

$$\boxed{\text{HOPF BIFURCATION at } b = 2, \text{ equilibrium } (x, y, b) = (1, 2, 2)}$$

Expected behavior:

- For $b < 2$: Stable equilibrium, no oscillations
- For $b \gtrsim 2$: Unstable equilibrium, stable limit cycle (periodic oscillations)
- Amplitude of limit cycle grows like $\sqrt{b - 2}$ near bifurcation

Physical interpretation

In the chemical reaction context:

- For low reaction rate ($b < 2$): System reaches steady-state concentrations
- For high reaction rate ($b > 2$): Concentrations oscillate periodically
- Critical rate $b = 2$: Threshold for sustained chemical oscillations

XYZ Analysis of Bifurcation Type

- **STAGE X (What we conjecture):** A supercritical Hopf bifurcation creating a stable limit cycle for $b > 2$.
- **STAGE Y (Why Hopf and not others):**
  - **Not fold**: No equilibria annihilate; one equilibrium exists throughout
  - **Not transcritical**: No second equilibrium passing through; equilibrium position moves but doesn't interact with another
  - **Not pitchfork**: No equilibrium splitting into three; no reflectional symmetry
  - **Hopf**: Eigenvalues cross imaginary axis, creating periodic behavior where there was none

  The distinguishing feature: emergence of periodic orbits from a fixed point as stability changes. Before bifurcation, trajectories spiral inward to equilibrium. After bifurcation, they spiral outward until nonlinearity creates a stable closed orbit.
- **STAGE Z (What this represents):** The Brusselator Hopf bifurcation models real chemical oscillators like the Belousov-Zhabotinsky reaction:
  - Reactants are continuously supplied (the constant $a = 1$ term)
  - Autocatalytic reactions (x^2y term) provide positive feedback
  - Varying reaction rate b controls system behavior
  - Above threshold: concentrations oscillate in a limit cycle (visible as periodic color changes in BZ reaction)

  This is one of the most famous examples of spontaneous oscillations in chemistry, demonstrating that far-from-equilibrium systems can self-organize into periodic behavior.

---

7 Step 7: Bifurcation Diagram

What to plot

For a Hopf bifurcation, the bifurcation diagram typically shows:

- Horizontal axis: bifurcation parameter (b)
- Vertical axis: amplitude or coordinates of attractors
- Equilibrium branch: x vs b or y vs b
- Limit cycle branches: maximum and minimum values of x or y on limit cycle

Equilibrium branch

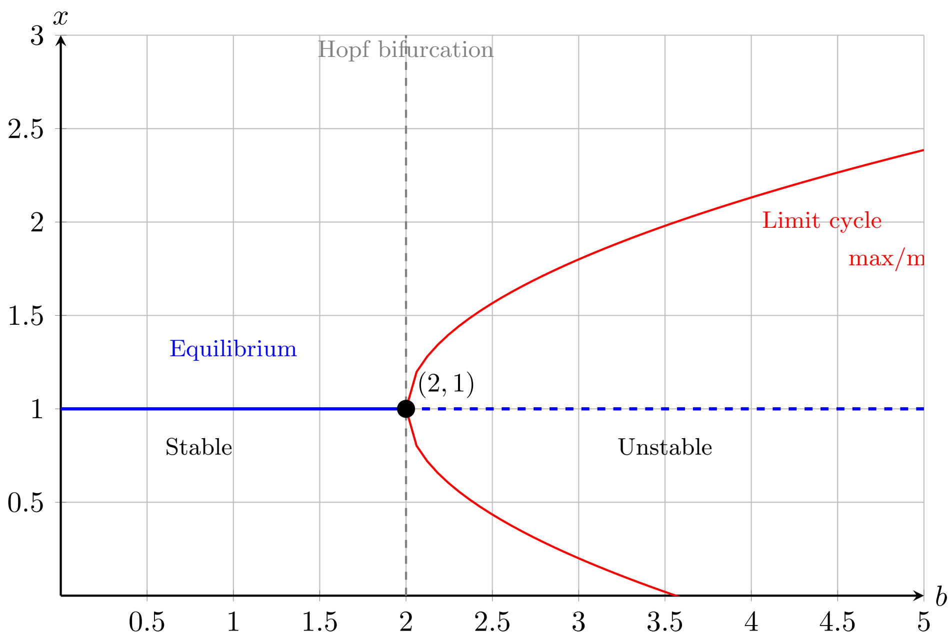
The equilibrium $(1, b)$ gives:

- In (b, x) space: horizontal line $x = 1$ (stable for $b < 2$, unstable for $b > 2$)
- In (b, y) space: diagonal line $y = b$ (stable for $b < 2$, unstable for $b > 2$)

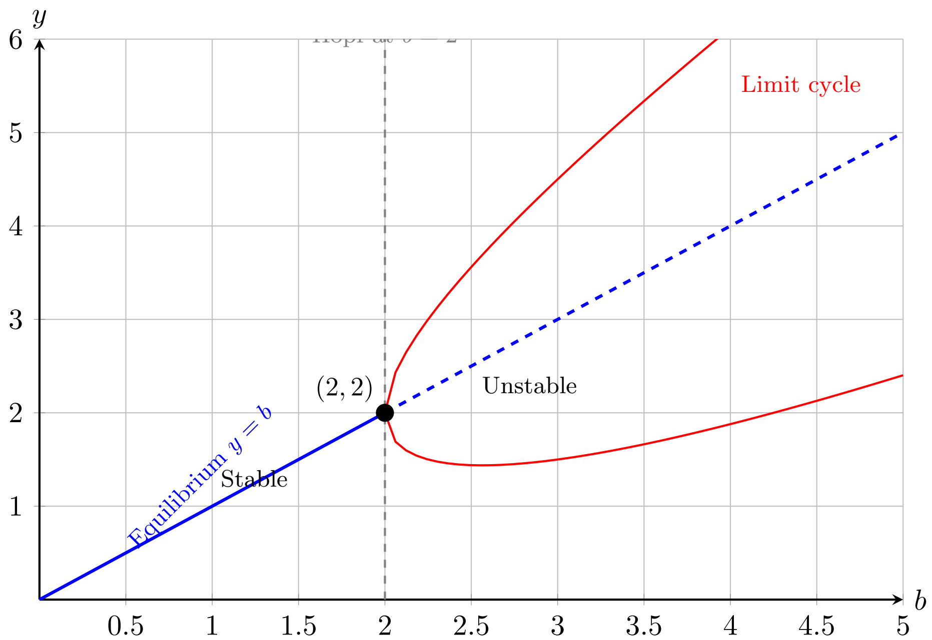
Limit cycle branches

For $b > 2$ (just above bifurcation), a small-amplitude limit cycle emerges. As b increases, the amplitude grows. The limit cycle oscillates around $(1, b)$.

Bifurcation diagram: b vs x



Bifurcation diagram: b vs y



XYZ Analysis of Bifurcation Diagrams

- **STAGE X (What the diagrams show):** A single equilibrium branch that changes from solid (stable) to dashed (unstable) at $b = 2$. For $b > 2$, two additional curves emerge representing the maximum and minimum values of oscillations on the limit cycle.
- **STAGE Y (Why this structure):**
  - **Equilibrium branch**: Shows the fixed point position. In (b, x) space, it's horizontal at $x = 1$ because $x^* = 1$ is independent of b. In (b, y) space, it's diagonal $y = b$ because $y^* = b$ increases with parameter.
  - **Limit cycle envelope**: After bifurcation, trajectories don't settle to equilibrium but instead approach a periodic orbit. The envelope shows the range of oscillation - how far from equilibrium the system swings. Near $b = 2$, amplitude is small (envelope close to equilibrium). As b increases, amplitude grows roughly like $\sqrt{b-2}$ (typical for supercritical Hopf).
  - **Pitchfork-like appearance in y diagram**: The diagram in (b, y) space resembles a supercritical pitchfork, but it's not - the outer branches represent extrema of a single periodic orbit, not separate equilibria. This visual similarity sometimes causes confusion.
- **STAGE Z (What dynamics look like):**
  - **Below bifurcation ($b < 2$)**: Trajectories spiral inward to $(1, b)$ and stay there (steady state)
  - **At bifurcation ($b = 2$)**: Critical point; trajectories slowly circulate near $(1, 2)$ but don't quite settle
  - **Above bifurcation ($b > 2$)**: Trajectories spiral outward from $(1, b)$ until reaching the limit cycle, then circulate on it indefinitely (sustained oscillations)
  - **Far above ($b \gg 2$)**: Large-amplitude oscillations; concentrations swing widely between max and min values

  The bifurcation represents the onset of oscillatory behavior - a qualitative change from monotonic approach to periodic cycling.

---

8 Step 8: Summary of Brusselator Behavior

System parameters

With $a = q = p = 1$:

$$\dot{x} = 1 - (b+1)x + x^2 y$$
$$\dot{y} = bx - x^2 y$$

Part (a): Equilibrium

$$\boxed{(x^*, y^*) = (1, b)} \quad \text{for all } b > 0$$

Unique equilibrium exists for all positive reaction rates.

Part (b): Stability

Jacobian:

$$J(1,b) = \begin{pmatrix} b-1 & 1 \\ -b & -1 \end{pmatrix}$$

Eigenvalues:

$$\begin{aligned} \tau &= b-2 \\ \Delta &= 1 \\ \lambda &= \frac{b-2}{2} \pm i\frac{\sqrt{4-(b-2)^2}}{2} \quad \text{for } 0 < b < 4 \end{aligned}$$

Stability classification:

- $0 < b < 2$: Stable spiral (equilibrium attracts)
- $b = 2$: Neutral, purely imaginary eigenvalues $\lambda = \pm i$
- $2 < b < 4$: Unstable spiral (equilibrium repels)
- $b \geq 4$: Unstable (real eigenvalues)

Part (c): Bifurcation

$$\boxed{\text{HOPF BIFURCATION}}$$

Location:

$$b = 2, \quad (x,y) = (1,2), \quad \text{i.e., } (x,y,b) = (1,2,2)$$

Characteristics:

- Supercritical type (stable limit cycle emerges for $b > 2$)
- Oscillation frequency at bifurcation: $\omega = 1$ (period $T = 2\pi$)
- Amplitude near bifurcation: $A \propto \sqrt{b-2}$

Physical interpretation:

- Below threshold ($b < 2$): Chemical reaction reaches steady-state concentrations
- Above threshold ($b > 2$): Chemical oscillator - concentrations vary periodically
- Critical value ($b = 2$): Onset of spontaneous oscillations

Bifurcation diagrams:

- In (b,x) space: Horizontal equilibrium line at $x = 1$ with limit cycle envelope growing from $b = 2$
- In (b,y) space: Diagonal equilibrium line $y = b$ with limit cycle envelope (resembles pitchfork but represents oscillation amplitudes)

Connection to real chemistry

The Brusselator models reactions like the Belousov-Zhabotinsky reaction where:

- Multiple chemical species interact autocatalytically
- Continuous supply of reactants maintains far-from-equilibrium conditions
- Concentrations spontaneously oscillate with visible color changes
- Oscillation onset occurs when reaction rates exceed critical threshold

The Hopf bifurcation at $b = 2$ represents the transition from chemical equilibrium to chemical oscillations - a beautiful example of self-organization in nonlinear dynamics.