5. Well-Stirred Reactors II

Lotka-Volterra model


original Lotka mechanism

\[ \begin{align*}
A + U & \xrightarrow{k_1} 2U \\
U + V & \xrightarrow{k_2} 2V \\
V & \xrightarrow{k_3} B
\end{align*} \]  

(R1)  

(R2)  

(R3)
modified Lotka mechanism

\[ A + U \xrightarrow{k_1} 2U \] \hspace{1cm} (R4)

\[ U + V \xrightarrow{k_2} 2V \] \hspace{1cm} (R5)

\[ V \xrightarrow{k_3} B \] \hspace{1cm} (R6)

\[ C + U \xrightarrow{k_4} D \] \hspace{1cm} (R7)

rate equations:

\[
\frac{du'}{dt'} = k_1 au' - k_4 cu' - k_2 u'v'
\]

\[
\frac{dv'}{dt'} = k_2 u'v' - k_3 v'
\]

non-dimensionalize the rate equations:

\[ t' = \tau t, \quad u' = \alpha u, \quad v' = \alpha v \]

\[
\frac{d(\alpha u)}{d(\tau t)} = (k_1 a - k_4 c) \alpha u - k_2 \alpha^2 u v
\]
\[
\frac{d(\alpha v)}{d(\tau t)} = k_2 \alpha^2 \nu \nu - k_3 \alpha v \\
\frac{du}{dt} = \tau (k_1 a - k_4 c) u - \tau k_2 \alpha u v \\
\frac{dv}{dt} = \tau k_2 \alpha u v - \tau k_3 v
\]

\[
\tau k_3 = 1 \\
\tau k_2 \alpha = 1
\]

\[
\tau = \frac{1}{k_3} \\
\alpha = \frac{k_3}{k_2} \\
\mu \equiv \frac{k_1 a - k_4 c}{k_3}
\]

non-dimensionalized Lotka-Volterra system

\[
\frac{du}{dt} = \mu u - uv \quad (1a) \\
\frac{dv}{dt} = uv - v \quad (1b)
\]
steady state:

\[ 0 = \frac{d\bar{u}}{dt} = \mu \bar{u} - \bar{u} \bar{v} \]
\[ 0 = \frac{d\bar{v}}{dt} = \bar{u} \bar{v} - \bar{v} \]
\[ \bar{u}(\mu - \bar{v}) = 0 \]
\[ \bar{v}(\bar{u} - 1) = 0 \]

\[ \Rightarrow \]
\[ (\bar{u}, \bar{v}) = 0, \quad \text{(complete extinction of both predator and prey)} \]
\[ (\bar{u}, \bar{v}) = (1, \mu) \text{ if } \mu > 0 \quad \text{(coexistence of predator and prey)} \]

linear stability analysis:

\[ u(t) = \bar{u} + \Delta u(t) \]
\[ v(t) = \bar{v} + \Delta v(t) \]
\[ \frac{d\Delta u}{dt} = \mu (\bar{u} + \Delta u) - (\bar{u} + \Delta u) (\bar{v} + \Delta v) \]
\[ \frac{d\Delta v}{dt} = (\bar{u} + \Delta u) (\bar{v} + \Delta v) - (\bar{v} + \Delta v) \]
\[
\frac{d\Delta u}{dt} = \mu \bar{u} + \mu \Delta u - (\bar{u} \bar{v} + \Delta u \bar{v} + \bar{u} \Delta v + \Delta u \Delta v)
\]

\[
\frac{d\Delta v}{dt} = (\bar{u} \bar{v} + \Delta u \bar{v} + \bar{u} \Delta v + \Delta u \Delta v) - \bar{v} - \Delta v
\]

\[
\frac{d\Delta u}{dt} = \mu \bar{u} - \bar{u} \bar{v} + \mu \Delta u - \bar{v} \Delta u - \bar{u} \Delta v - \Delta u \Delta v
\]

\[
\frac{d\Delta v}{dt} = \bar{u} \bar{v} - \bar{v} + \bar{v} \Delta u + \bar{u} \Delta v - \Delta v + \Delta u \Delta v
\]

\[
\frac{d\Delta u}{dt} = (\mu - \bar{v}) \Delta u - \bar{u} \Delta v
\]

\[
\frac{d\Delta v}{dt} = \bar{v} \Delta u + (\bar{u} - 1) \Delta v
\]

in matrix form:

\[
\frac{d}{dt} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = \begin{pmatrix} \mu - \bar{v} & -\bar{u} \\ \bar{v} & \bar{u} - 1 \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}
\]

the matrix

\[
J = \begin{pmatrix} \mu - \bar{v} & -\bar{u} \\ \bar{v} & \bar{u} - 1 \end{pmatrix}
\]
is known as the Jacobian matrix of the system (1) ansatz:

\[
\begin{align*}
\Delta u(t) &= u_0 \exp(-\lambda t) \\
\Delta v(t) &= v_0 \exp(-\lambda t) \\
\frac{d\Delta u(t)}{dt} &= u_0 \lambda \exp(-\lambda t) = \lambda \Delta u(t) \\
\frac{d\Delta v(t)}{dt} &= v_0 \lambda \exp(-\lambda t) = \lambda \Delta v(t)
\end{align*}
\]

\[
\Rightarrow
\]

\[
\lambda \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = \begin{pmatrix} \mu - \bar{v} & -\bar{u} \\ \bar{v} & \bar{u} - 1 \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}
\]
eigenvalue problem

\[
J \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = \lambda \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}
\]

\[
\begin{pmatrix} \mu - \bar{v} - \lambda & -\bar{u} \\ \bar{v} & \bar{u} - 1 - \lambda \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = 0
\]
\[(J - \lambda l_2) \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = 0\]

\[I_n = n \times n \text{ identity matrix}\]

\[I_n = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix}\]

the eigenvalues \(\lambda\) are the roots of the characteristic equation

\[\det(J - \lambda l_2) = |J - \lambda l_2| = 0\]

\[\det \begin{pmatrix} J_{11} - \lambda & J_{12} \\ J_{21} & J_{22} - \lambda \end{pmatrix} = \begin{vmatrix} J_{11} - \lambda & J_{12} \\ J_{21} & J_{22} - \lambda \end{vmatrix} = 0\]

\[(J_{11} - \lambda)(J_{22} - \lambda) - J_{12}J_{21} = 0\]

\[\lambda^2 - (J_{11} + J_{22}) \lambda + J_{11}J_{22} - J_{12}J_{21} = 0\]

\[\lambda^2 - \text{tr} J \lambda + \det J = 0\]
\[ \text{tr} J = J_{11} + J_{22} \quad \text{trace} \]
\[ \lambda^2 - T\lambda + \Delta = 0 \]
\[ T \equiv \text{tr} J, \quad \Delta \equiv \det J \]
\[ \lambda_{1,2} = \frac{1}{2} \left[ T \pm \sqrt{T^2 - 4\Delta} \right] \quad (2) \]

the steady state is stable if both eigenvalues have a negative real part:

\[ \Re \lambda_i < 0 \]

Lotka-Volterra system, trivial steady state:

\[ (\overline{u}, \overline{v}) = 0 \]
\[ J = \begin{pmatrix} \mu & 0 \\ 0 & -1 \end{pmatrix} \]

the Jacobian is diagonal; no need to solve the characteristic equation; the eigenvalues are the diagonal elements

\[ \lambda_1 = \mu \]
\[ \lambda_2 = -1 \]

the trivial steady state is stable if \( \mu < 0 \): both eigenvalues are real and negative

such a steady state is known as a \textit{stable node}

the trivial steady state is unstable if \( \mu > 0 \): both eigenvalues are real, one is positive and one is negative

such a steady state is known as a \textit{saddle}; it has one stable direction and one unstable direction

specifically for the Lotka-Volterra model near the steady state \((0, 0)\):

\[
\begin{align*}
\frac{d\Delta u}{dt} &= \mu \Delta u \\
\frac{d\Delta v}{dt} &= -\Delta v \\
\Delta u(t) &= u_0 \exp(-\mu t) \\
\Delta v(t) &= v_0 \exp(-t)
\end{align*}
\]
perturbations in the $v$-direction always decay exponentially; perturbation in the $u$-direction grow exponentially if $\mu > 0$ [$\mu = 1.0$ in the figure below]

Lotka-Volterra system, non-trivial steady state:

$$(\bar{u}, \bar{v}) = (1, \mu), \quad \mu > 0$$

$$J = \begin{pmatrix} 0 & -1 \\ \mu & 0 \end{pmatrix}$$

characteristic equation:

$$\lambda^2 + \mu = 0$$
eigenvalues:

\[ \lambda_{1,2} = \pm \sqrt{-\mu} \]
\[ \lambda_{1,2} = \pm i \sqrt{\mu} \]

the eigenvalues are purely imaginary for all positive values of \( \mu \): \( \Re \lambda_{1,2} = 0 \implies \) marginal stability for all positive values of the bifurcation parameter near the non-trivial steady state:

\[
\frac{d\Delta u}{dt} = -\Delta v
\]
\[
\frac{d\Delta v}{dt} = \mu \Delta u
\]
\[
\frac{d^2 \Delta u}{dt^2} = -\frac{d\Delta v}{dt} = -\mu \Delta u
\]
\[
\frac{d^2 \Delta v}{dt^2} = \mu \frac{d\Delta u}{dt} = -\mu \Delta v
\]

both perturbations obey the ODE of a harmonic oscil-
lator with $\omega^2 = \mu$

$$\begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \exp(i\mu t)$$

circles around $(\overline{u}, \overline{v}) = (1, \mu)$, whose radius depends on $(u_0, v_0)$

however this is a linear analysis; we have neglected higher order terms

How is the knife’s edge situation of marginal stability resolved? What about finite-amplitude perturbations?

consider the quantity $H$:

$$H \equiv u + v - \ln u - \mu \ln v$$

$$\frac{dH}{dt} = \frac{du}{dt} + \frac{dv}{dt} - \frac{1}{u} \frac{du}{dt} - \mu \frac{1}{v} \frac{dv}{dt}$$

$$= \mu u - uv + uv - v - \frac{1}{u} (\mu u - uv) - \mu \frac{1}{v} (uv - v)$$

$$= \mu u - v - \mu + v - \mu u + \mu$$
\[ \frac{dH}{dt} = 0 \]

\( H \) is a constant of motion; characterizes closed trajectories

\( H \) is determined by \((u(0), v(0))\); a perturbation of a closed trajectory leads to a different value of \( H \) and a different closed trajectory; in other words perturbations of a closed trajectory do not decay and they also do not grow \( \Rightarrow \) these trajectories have neutral (marginal) stability \( \Rightarrow \) do not correspond to chemical oscillations [chemical oscillations are stable to small perturbations]

\[
H(\bar{u}, \bar{v}) = H(1, \mu) \\
= 1 + \mu - \ln 1 - \mu \ln \mu \\
= 1 + \mu (1 - \ln \mu)
\]

one can show that this is the minimum value of \( H \); as \( H \) increases, the size of the closed trajectory around \((1, \mu)\) increases
In the picture below, $\mu = 1$; so

$$(\overline{u}, \overline{v}) = (1, 1)$$

$H(1, 1) = 2$

Moving outwards from the steady state $(1, 1)$, marked by a crossmark, the closed trajectories correspond to:

$$(u(0), v(0)) = (1.1, 1), \quad H = 2.00469$$

$$(u(0), v(0)) = (1.5, 1), \quad H = 2.094535$$

$$(u(0), v(0)) = (2.0, 1), \quad H = 2.306853$$

$$(u(0), v(0)) = (3.0, 1), \quad H = 2.901388$$
\[(u(0), v(0)) = (4.5, 1), \quad H = 3.995923\]

\[(u(0), v(0)) = (6.0, 1), \quad H = 5.208241\]

the motion is counterclockwise

the trajectory for \((u(0), v(0)) = (2.0, 1), H = 2.306853\) is shown as a time series in the next figure [solid blue line = \(U\) (prey); dashed red line = \(V\) (predator)]

The trajectory for \((u(0), v(0)) = (6.0, 1), H = 5.208241\) is shown as a time series in the next figure [solid blue line = \(U\) (prey); dashed red line = \(V\) (predator)]
besides having infinitely many, neutrally stable closed trajectories around \((1, \mu)\) for positive \(\mu\), the Lotka-Volterra model has another shortcoming: it is \textit{structurally unstable}.

If we include the back reaction of R4, then the non-dimensionalized rate equations read,

\[
\frac{du}{dt} = \mu u - uv - \epsilon u^2 \tag{3a}
\]
\[
\frac{dv}{dt} = uv - v \tag{3b}
\]

in an ecological context, predator-prey model, this
corresponds to introducing a large, but finite carrying capacity $K$ for the prey, $\epsilon \propto 1/K$

the steady states are

$$(\bar{u}, \bar{v})_0 = (0, 0) \text{ (complete extinction)}$$

$$(\bar{u}, \bar{v})_1 = (\mu/\epsilon, 0) \text{ if } \mu > 0 \text{ (predator extinction)}$$

$$(\bar{u}, \bar{v})_2 = (1, \mu - \epsilon) \text{ if } \mu > \epsilon \text{ (coexistence)}$$

[an additional steady state appears, $(\bar{u}, \bar{v}) = (\mu/\epsilon, 0)$; this state moves in, so to speak, from infinity $(\infty, 0)$; in the original Lotka-Volterra model the prey undergoes simple Malthusian (first-order) growth in the absence of a predator, i.e., the prey population will explode; if we replace Malthusian growth, $\dot{u} = \mu u$, by logistic growth, $\dot{u} = \mu u - \epsilon u^2$, then the prey population will saturate at $\bar{u} = \mu/\epsilon$]

the Jacobian is

$$J = \begin{pmatrix} \mu - \bar{v} - 2\epsilon \bar{u} & -\bar{u} \\ \bar{v} & \bar{u} - 1 \end{pmatrix}$$
for the trivial steady state \((\bar{u}, \bar{v})_0 = 0\):

\[
J = \begin{pmatrix} \mu & 0 \\ 0 & -1 \end{pmatrix}
\]

i.e, the back reaction does not affect the stability of the trivial steady state and the behavior of small perturbations for \((\bar{u}, \bar{v})_1 = (\mu/\epsilon, 0)\):

\[
J = \begin{pmatrix} -\mu & -\frac{\mu}{\epsilon} \\ 0 & \frac{\mu}{\epsilon} - 1 \end{pmatrix}
\]

the eigenvalues are, see (2),

\[
\lambda_{1,2} = \frac{1}{2} \left[ T \pm \sqrt{T^2 - 4\Delta} \right]
\]

\[
T = -\mu + \frac{\mu}{\epsilon} - 1
\]

\[
\Delta = \mu - \frac{\mu^2}{\epsilon}
\]

\[
T = 0: \mu = \frac{\epsilon}{1 - \epsilon}
\]
\( \Delta = 0: \mu = 0 \) or \( \mu = \epsilon \)

\( \epsilon < \frac{\epsilon}{1 - \epsilon} \)

\( T^2 - 4\Delta = 0: \mu = \frac{\epsilon}{1 + \epsilon} \) (double root)

so for \( 0 < \mu < \epsilon \), we have \( T < 0, \Delta > 0 \), and \( T^2 - 4\Delta \geq 0 \), i.e., both eigenvalues are real and negative [the two eigenvalues coincide at \( \mu = \epsilon/(1 + \epsilon) \)]; at \( \mu = \epsilon \): \( \lambda_1 = 0, \lambda_2 < 0 \), and for \( \epsilon < \mu < \epsilon/(1 - \epsilon) \): \( \lambda_1 > 0, \lambda_2 < 0 \); in other words, the steady state \((\overline{u}, \overline{v}) = (\mu/\epsilon, 0)\) becomes unstable at \( \mu = \epsilon \), turns from a stable node into a saddle

for the coexistence steady state we find

\[ (\overline{u}, \overline{v})_2 = (1, \mu - \epsilon); \quad \mu > \epsilon, \]

\[ J = \begin{pmatrix} -\epsilon & -1 \\ \mu - \epsilon & 0 \end{pmatrix} \]

the characteristic equation is

\[ \lambda^2 + \epsilon \lambda + \mu - \epsilon = 0 \]
and the eigenvalues are

\[ \lambda_{1,2} = \frac{-1}{2} \epsilon \pm \sqrt{\frac{1}{4} \epsilon^2 - \mu - \epsilon} \]

consider the case \( \epsilon \ll 1 \); then

\[ \lambda_{1,2} \approx \frac{-1}{2} \epsilon \pm \sqrt{-\mu} \]

\[ = \frac{1}{2} \epsilon \pm i \sqrt{\mu} \]

in other words, even for \( \epsilon \) very small, the eigenvalues have a negative real part:

\[ \Re \lambda_{1,2} = -\frac{1}{2} \epsilon \]

i.e., the coexistence steady state is stable

even a very small backward rate constant for reaction R4 destroys the closed trajectories and renders the non-trivial steady state stable

trajectory for \((u(0), v(0)) = (6.0, 1), \mu = 1, \epsilon = 0.1, (\bar{u}, \bar{v})_2 = (1, 0.9); (\bar{u}, \bar{v})_1 = (10.0, 0)\)
the trajectory spirals counterclockwise into the non-trivial steady state

trajectory for \((u(0), v(0)) = (20.0, 0.001), \mu = 1, \epsilon = 0.1, (\bar{u}, \bar{v})_2 = (1, 0.9); (\bar{u}, \bar{v})_1 = (10.0, 0)\)
Brusselator


mechanism

\[ A \xrightarrow{k_1} U \quad \text{(R8)} \]
\[ B + U \xrightarrow{k_2} V + C \quad \text{(R9)} \]
\[ 2U + V \xrightarrow{k_3} 3U \quad \text{(R10)} \]
\[ U \xrightarrow{k_4} D \quad \text{(R11)} \]

non-dimensionalize:

\[ t = k_4 t' \]
\[ u = \sqrt{\frac{k_3}{k_4}} u' \]
\[ v = \sqrt{\frac{k_3}{k_4}} v' \]
\[ a = \sqrt{\frac{k_1^2 k_3}{k_4^3}} a' \]

\[ b = \frac{k_2}{k_4} b' \]

non-dimensionalized Brusselator

\[ \frac{du}{dt} = a - (b + 1) u + u^2 v \quad (4a) \]

\[ \frac{dv}{dt} = b u - u^2 v \quad (4b) \]

steady state

\[ 0 = \frac{d\bar{u}}{dt} = a - (b + 1) \bar{u} + \bar{u}^2 \bar{v} \]

\[ 0 = \frac{d\bar{v}}{dt} = b \bar{u} - \bar{u}^2 \bar{v} \]

\[ \bar{v} = \frac{b}{\bar{u}} \quad [1\text{st equation} \implies \bar{u} \neq 0] \]

\[ 0 = a - (b + 1) \bar{u} + \bar{u}^2 \cdot \frac{b}{\bar{u}} \]

\[ 0 = a - (b + 1) \bar{u} + b \bar{u} \]
\[ \bar{u} = a \]
\[ \bar{v} = \frac{b}{a} \]

Only one steady state

Linear stability analysis

\[ u = \bar{u} + \Delta u \]
\[ v = \bar{v} + \Delta v \]

\[ \frac{d\Delta u}{dt} = a - (b + 1)(\bar{u} + \Delta u) + (\bar{u} + \Delta u)^2(\bar{v} + \Delta v) \]
\[ \frac{d\Delta v}{dt} = b(\bar{u} + \Delta u) - (\bar{u} + \Delta u)^2(\bar{v} + \Delta v) \]

\[ \frac{d\Delta u}{dt} = a - (b + 1)\bar{u} - (b + 1)\Delta u + \bar{u}^2\bar{v} + \bar{u}^2\Delta v + 2\bar{u}\bar{v}\Delta u + \text{h.o.t} \]
\[ \frac{d\Delta v}{dt} = b\bar{u} + b\Delta u - \bar{u}^2\bar{v} - \bar{u}^2\Delta v - 2\bar{u}\bar{v}\Delta u + \text{h.o.t} \]

\[ \frac{d\Delta u}{dt} = -(b + 1)\Delta u + 2\bar{u}\bar{v}\Delta u + \bar{u}^2\Delta v \]
\[ \frac{d\Delta v}{dt} = b\Delta u - 2\bar{u}\bar{v}\Delta u - \bar{u}^2\Delta v \]
\[
\frac{d\Delta u}{dt} = -(b+1)\Delta u + 2a\frac{b}{a}\Delta u + a^2\Delta v
\]

\[
\frac{d\Delta v}{dt} = b\Delta u - 2a\frac{b}{a}\Delta u - a^2\Delta v
\]

\[
\frac{d\Delta u}{dt} = (b-1)\Delta u + a^2\Delta v
\]

\[
\frac{d\Delta v}{dt} = -b\Delta u - a^2\Delta v
\]

\[
\frac{d}{dt} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}
\]

Jacobian

\[
J = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix}
\]

(5)

trace

\[
T = b - 1 - a^2
\]

determinant

\[
\Delta = a^2
\]
eigenvalues, see (2),

\[
\lambda_{1,2} = \frac{1}{2} \left[ T \pm \sqrt{T^2 - 4\Delta} \right]
\]

\[
\lambda_{1,2} = \frac{1}{2} \left[ b - 1 - a^2 \pm \sqrt{(b - 1 - a^2)^2 - 4a^2} \right]
\]

If \( b < 1 + a^2 \), i.e., \( T < 0 \), then either (i) \( \lambda_{1,2} < 0 \), if the discriminant \( (b - 1 - a^2)^2 - 4a^2 \) is positive, which is the case for \( b < (a - 1)^2 \), and the steady state is a stable node, or (ii) \( \Re \lambda_{1,2} < 0 \), if the discriminant \( (b - 1 - a^2)^2 - 4a^2 \) is negative \( [(a - 1)^2 < b < (a + 1)^2] \), then the concentrations display damped oscillations and the system spirals into the steady state: stable focus

if \( T = 0 \), then \( \Re \lambda_{1,2} = 0 \), i.e., the steady state of the Brusselator becomes unstable at

\[
b = b_H = 1 + a^2
\]

where

\[
\lambda_{1,2} = \pm \sqrt{-a^2} = \pm ia = \pm i\omega
\]
at $b = b_H$ oscillations set in

for $b > 1 + a^2$, we have $\Re \lambda_{1,2} > 0$, and the trajectories of the Brusselator spiral away from the steady state

one can show that explosion, i.e.,

$$\sqrt{u^2(t) + v^2(t)} \rightarrow \infty \quad t \rightarrow \infty$$

cannot occur in the Brusselator, no matter what the initial condition $(u(0), v(0))$

for $b > b_H$, the trajectory spirals away from the steady state $(\bar{u}, \bar{v})$ and converges to a **limit cycle**

limit cycle = isolated closed trajectory, i.e., nearby trajectories are not closed and either spiral towards the limit cycle or spiral away from the limit cycle

**stable limit cycle**: attracts all nearby trajectories

**unstable limit cycle**: repels all nearby trajectories

the bifurcation of the Brusselator is an example of a **Hopf bifurcation**
the Hopf bifurcation in the Brusselator is supercritical and the amplitude of the oscillations $\propto \sqrt{b - b_H}$; the limit cycle appears with a finite frequency $\omega = a$

in the following figures $a = 1$, which yields $b_H = 2.0$

initial conditions $(u(0), v(0) = (0.9, 0.9)$

$u$: black; $v$: red
initial condition on the limit cycle \((u(0), v(0)) = (0.9259388, 2.169121)\)
growth of limit cycle

the motion in the phase plane is clockwise
Summing Up

two-variable systems

rate equations:

\[
\frac{du}{dt} = f_u(u, v) \quad (6a)
\]

\[
\frac{dv}{dt} = f_v(u, v) \quad (6b)
\]

stationary states:

\[f_u(\bar{u}, \bar{v}) = f_v(\bar{u}, \bar{v}) = 0\]

stability: determined by eigenvalues of the Jacobian

\[
J = \begin{pmatrix}
J_{11} & J_{12} \\
J_{21} & J_{22}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial f_u(u, v)}{\partial u} \bigg|_{(\bar{u}, \bar{v})} & \frac{\partial f_u(u, v)}{\partial v} \bigg|_{(\bar{u}, \bar{v})} \\
\frac{\partial f_v(u, v)}{\partial u} \bigg|_{(\bar{u}, \bar{v})} & \frac{\partial f_v(u, v)}{\partial v} \bigg|_{(\bar{u}, \bar{v})}
\end{pmatrix}
\]
system (6) is said to be of the pure activator-inhibitor type if the Jacobian has the sign structure

$$J = \begin{pmatrix} + & - \\ + & - \end{pmatrix}$$

i.e.,

$$J_{11} > 0, J_{22} < 0, J_{12} < 0, J_{21} > 0$$

system (6) is said to be of the cross activator-inhibitor type if the Jacobian has the sign structure

$$J = \begin{pmatrix} + & + \\ - & - \end{pmatrix}$$

i.e.,

$$J_{11} > 0, J_{22} < 0, J_{12} > 0, J_{21} < 0$$

it follows from (5) that the Brusselator is a cross activator-inhibitor system for $$b > 1$$
some authors call pure activator-inhibitor systems simply activator-inhibitor systems and call cross activator-inhibitor systems by the name activator-substrate-depletion systems.

characteristic polynomial for a two-variable system:

$$\lambda^2 - T\lambda + \Delta = 0$$

with

$$T = \text{tr} J = J_{11} + J_{22}, \quad \Delta = \det J = J_{11}J_{22} - J_{12}J_{21}$$

roots of the characteristic polynomial, i.e., the eigenvalues of the Jacobian, are given by

$$\lambda_{1,2} = \frac{1}{2} \left[ T \pm \sqrt{T^2 - 4\Delta} \right]$$

stationary state is stable, i.e., $\Re \lambda_{1,2} < 0$, if

$$T < 0$$

$$\Delta > 0$$
detailed analysis of the behavior of the eigenvalues:

Case (I): $T < 0$, $\Delta > 0$, and the discriminant is positive, $T^2 - 4\Delta > 0$: both eigenvalues are real and negative; all perturbations to the steady state decay monotonically and the steady state is a \textit{stable node}.

Case (II): $T < 0$, $\Delta > 0$, and the discriminant is negative, $T^2 - 4\Delta < 0$: the eigenvalues form a pair of complex conjugate numbers, $\lambda_{1,2} = \lambda \pm i\omega$, with $\lambda = T/2$ and $\omega = \sqrt{4\Delta - T^2}/2$; the real part is negative and perturbations of the steady state decay; presence of a non-zero imaginary part implies that the perturbations decrease in an oscillatory manner. The trajectory approaches the steady state spiraling into it. The steady state is a \textit{stable focus}.

Case (III): $T > 0$, $\Delta > 0$, and the discriminant is negative, $T^2 - 4\Delta < 0$: eigenvalues are complex conjugate with a positive real part, $\lambda = T/2$; the steady state is unstable. Due to the presence of a non-zero imaginary part, perturbations grow in an oscillatory manner and spiral away from the steady state. The steady state is a \textit{unstable focus}.

Case (IV): $T > 0$, $\Delta > 0$, and the discriminant is posi-
tive, $T^2 - 4\Delta > 0$: eigenvalues are both real and positive; all perturbations grow exponentially. The steady state is a *unstable node*.

Case (V): $\Delta < 0$: the discriminant is always positive, $T^2 - 4\Delta > 0$, and both eigenvalues are real; one is positive and the other is negative. Trajectories approach the steady state along the eigenvector corresponding to the negative eigenvalue, but move away along the eigenvector corresponding to the positive eigenvalue. The steady state has one stable and one unstable direction. It is therefore unstable and called a *saddle*.

The cases are summarized in the following stability classification for two-variable systems:
two generic local instabilities for a two-variable system:

(i) a real eigenvalue passes through zero as a parameter $\mu$ of the system is varied: *stationary bifurcation* occurs when the determinant of the Jacobian changes sign:

$$\mu = \mu_{st} : \quad \Delta = \det J = 0$$
$$\lambda_1 = 0$$
$$\lambda_2 = T < 0$$

(ii) a pair of complex conjugate eigenvalues crosses the imaginary axis as a parameter $\mu$ of the system is varied: *Hopf bifurcation*
occurs when the trace of the Jacobian changes sign:

\[ \mu = \mu_H : \quad T = \text{tr} J = 0 \]

\[ \lambda_1 = +i\omega_H \]

\[ \lambda_2 = -i\omega_H \]

\[ \omega_H = \sqrt{\Delta} \]

the stationary bifurcation and the Hopf bifurcation typically occur as one parameter of the system is varied: \textit{codimension-one} bifurcations

sometimes possible to make the stationary and Hopf instability threshold coalesce, \( \mu_{st} = \mu_H \), by varying
two parameters: *codimension-two* bifurcation (fine-tuning of two parameters)

\[ T = \Delta = 0 \]

Takens-Bogdanov bifurcation or double-zero bifurcation

\[ \lambda_1 = \lambda_2 = 0 \]

*limit cycles* in *two-variable* systems

1. The region bounded by a limit cycle contains at least one steady state.

2. *Poincaré-Bendixson Theorem*: If \( D \) denotes an annular region bounded by two closed curves \( C' \) and \( C'' \) and if (1) no steady state exists in the closure of \( D \) and (2) the trajectories through points on \( C' \) and \( C'' \) all extend into \( D \) either for \( t \) increasing or \( t \) decreasing, then \( D \) contains at least one limit cycle.
3. **Bendixson’s negative criterion:** If

\[
\frac{\partial f_u(u, v)}{\partial u} + \frac{\partial f_v(u, v)}{\partial v}
\]

has the same sign throughout a simply connected domain \( D \) [i.e., region without holes], then there are no cycles wholly contained in \( D \).

4. If \( f_u(u, v) \) and \( f_v(u, v) \) are polynomials without a common factor, which in particular implies that the nullclines \( \dot{u} = f_u(u, v) = 0 \) and \( \dot{v} = f_v(u, v) = 0 \) have only isolated intersections, then more can be said about the asymptotic states [states attained as \( t \to \infty \)] of the system. We further assume that the system is structurally stable.

(a) As \( t \to \infty \), the trajectory \((u(t), v(t))\) can approach only a stable focus, a stable node, a saddle point, or a limit cycle. Trajectories tending to saddle points are such that none join two saddle points.

(b) There exists at most a finite number of limit cycles. We have the following estimate: If
$f_u(u, v)$ and $f_v(u, v)$ are polynomials of degree $n$, then the number of limit cycles does not exceed $(6n^3 - 7n^2 + n + 4)/2$ if $n$ is even and $(6n^3 - 7n^2 - 11n + 6)/2$ if $n$ is odd. For $n = 2$, we have the sharper result that the maximum number of limit cycles does not exceed 3, and there are systems with exactly 3 limit cycles.


Conclusion: The only asymptotic states of a structurally stable two-variable system are steady states and limit cycles. [$f_u(u, v)$ and $f_v(u, v)$ need not be polynomials for this to be true.]