UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

Diffusion-Driven Instability and Pattern Formation in Reaction-Diffusion-ODE Systems

Théo André

December 9, 2024

Heidelberg University

Table of contents

Motivation

Figure 1: Casually sitting Egyptian Goose

Figure 2: Close-up view of Egyptian Goose skin.

Figure 1: Casually sitting Egyptian Goose

Figure 2: Close-up view of Egyptian Goose skin.

Turing Pattern: stable, regular, spatially-heterogeneous, stationary solution to a Reaction-Diffusion (RD) equation, *e.g.*

$$\frac{\partial}{\partial t}u(t,x) = D_u \nabla^2 u(t,x) + f(u,v) \qquad t,x \in (0,T) \times \Omega$$

$$\frac{\partial}{\partial t}v(t,x) = D_v \nabla^2 v(t,x) + g(u,v) \qquad t,x \in (0,T) \times \Omega$$

$$+ \text{ Boundary and Initial Conditions}$$

Example: Gray-Scott model (1984)

$$\frac{\partial}{\partial t}u = D_u \nabla^2 u - uv^2 + F(1-u)$$
$$\frac{\partial}{\partial t}v = D_v \nabla^2 v + uv^2 - (F+k)v$$

$\Omega = (0,1)^2$ with zero-flux boundary condition.

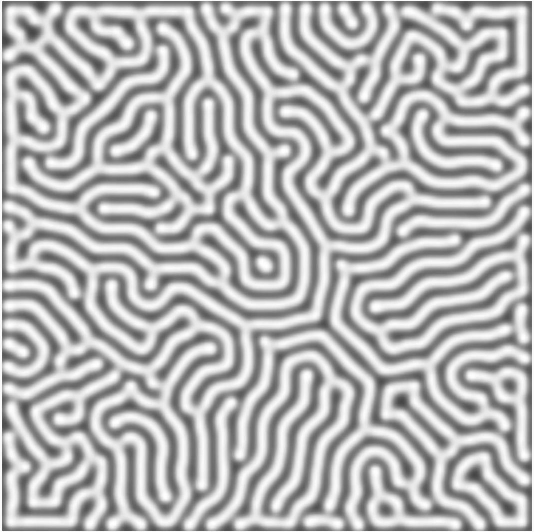


Figure 3: Simulation of the Gray-Scott model with feed parameter $F = 0.029$, and kill-rate $k = 0.057$

Example: Gray-Scott model (1984)

$$\frac{\partial}{\partial t} u = D_u \nabla^2 u - uv^2 + F(1-u)$$
$$\frac{\partial}{\partial t} v = D_v \nabla^2 v + uv^2 - (F+k) v$$

$\Omega = (0,1)^2$ with zero-flux boundary condition.

Method (DDI):

1. Find stable constant steady state $(\bar{u}, \bar{v})$ when $(D_u, D_v) = (0,0)$.
2. Linear stability analysis.
3. Find D_u, D_v making $(\bar{u}, \bar{v})$ unstable in presence of diffusion.
4. Solutions to the perturbed IVP with initial condition $(u_0, v_0) = (\bar{u} + \xi_1, \bar{v} + \xi_2)$ converge to patterned solution.

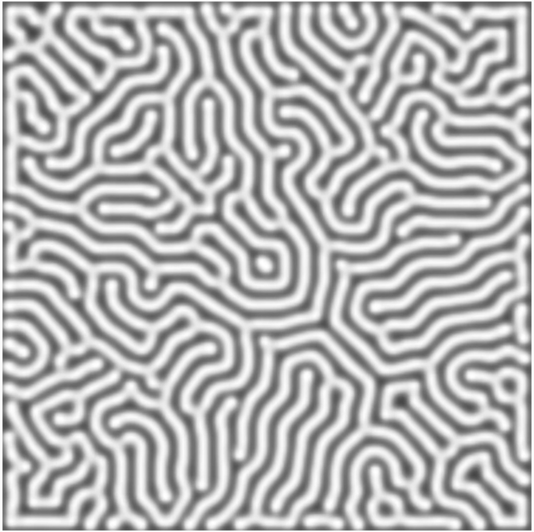
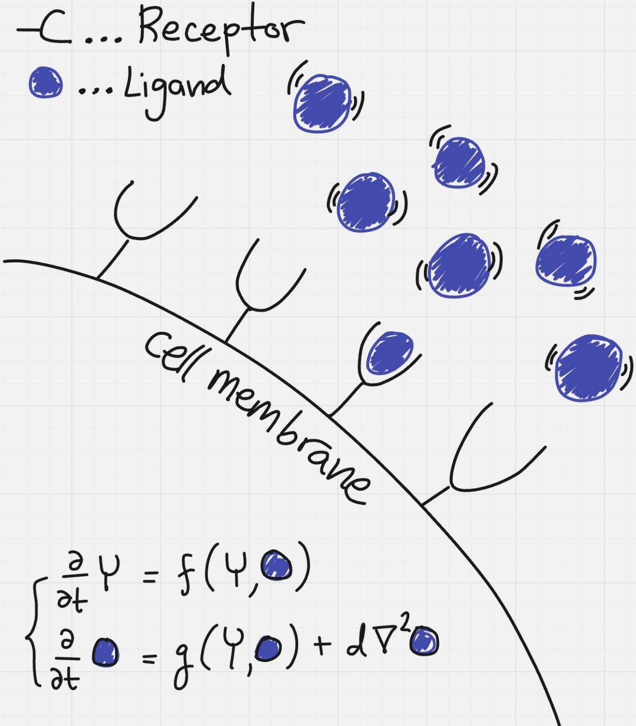


Figure 3: Simulation of the Gray-Scott model with feed parameter $F = 0.029$, and kill-rate $k = 0.057$

RD-ODE Systems:

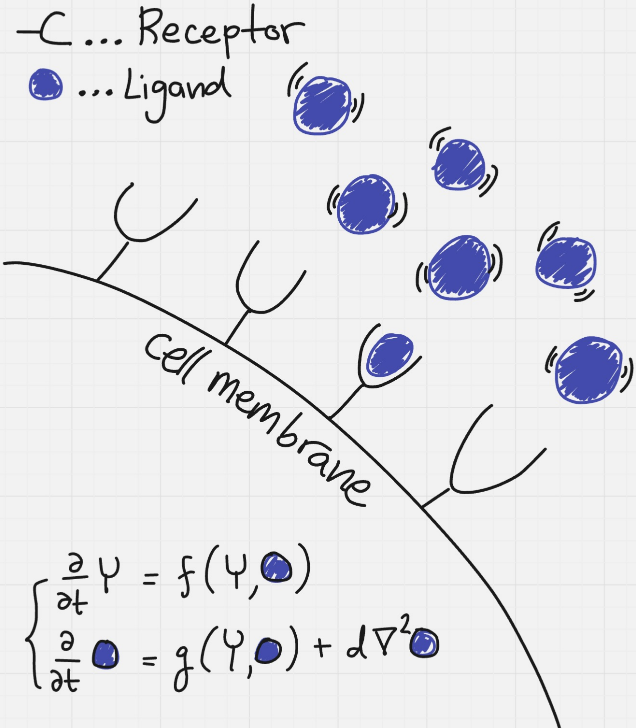
Sometimes in Biology, we are led to model systems featuring both diffusing and non-diffusing components.



RD-ODE Systems:

Sometimes in Biology, we are led to model systems featuring both diffusing and non-diffusing components.

When that happens, the differential operator degenerates and complexity increases drastically.



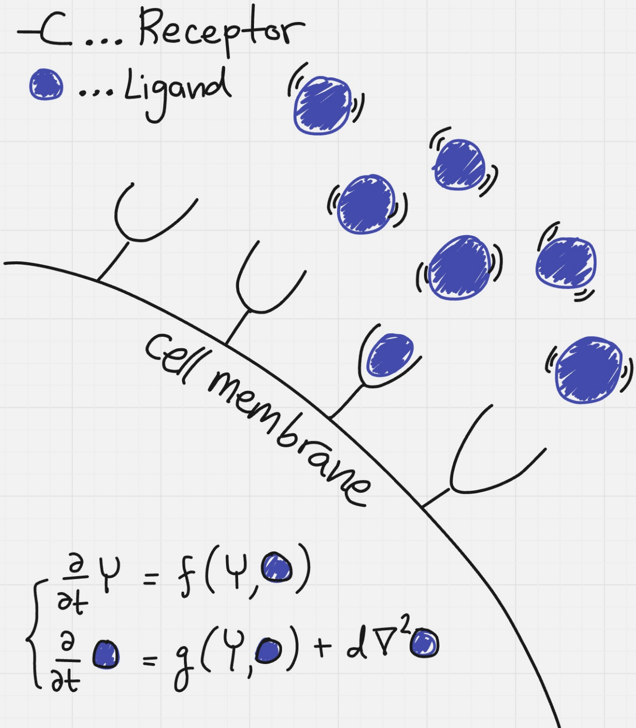
RD-ODE Systems:

Sometimes in Biology, we are led to model systems featuring both diffusing and non-diffusing components.

When that happens, the differential operator degenerates and complexity increases drastically.

A very natural question is the following:

“Can we still obtain patterns in systems of Reaction-Diffusion-ODE using the Turing mechanism (DDI)?



Patterned solutions in RD-ODE systems:

- *m* ODEs, 1 PDE: All regular solutions are unstable.
  But it is possible to construct stable
  far-from-equilibrium solutions to

$$\begin{cases} \frac{\partial}{\partial t}\boldsymbol{U} = \boldsymbol{f}(\boldsymbol{u}, V) \\ \frac{\partial}{\partial t}V = D\nabla^2 V + \boldsymbol{g}(\boldsymbol{u}, V) \end{cases}$$

Patterned solutions in RD-ODE systems:

- ***m* ODEs, 1 PDE:** All regular solutions are unstable. But it is possible to construct stable *far-from-equilibrium* solutions to

$$\begin{cases} \frac{\partial}{\partial t} \boldsymbol{U} = \boldsymbol{f}(\boldsymbol{u}, V) \\ \frac{\partial}{\partial t} V = D\nabla^2 V + \boldsymbol{g}(\boldsymbol{u}, V) \end{cases}$$

Idea:

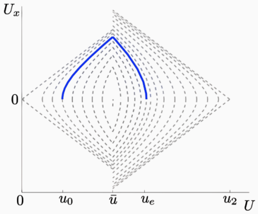
- Patterns are solution to

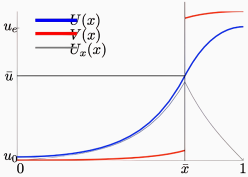
$$f(\boldsymbol{U}, V) = 0; \qquad d\nabla^2 V + g(\boldsymbol{U}, V) = 0$$

- Implicit function theorem: $\boldsymbol{U} = \boldsymbol{h}(V)$, thus

$$d\nabla^2 V + g\big(\boldsymbol{h}(V), V\big) = 0$$

- Phase portrait method:





Patterned solutions in RD-ODE systems:

- ***m* ODEs, 1 PDE:** All regular solutions are unstable. But it is possible to construct stable *far-from-equilibrium* solutions to

$$\begin{cases} \frac{\partial}{\partial t} U = \boldsymbol{f}(\boldsymbol{u}, V) \\ \frac{\partial}{\partial t} V = D\nabla^2 V + \boldsymbol{g}(\boldsymbol{u}, V) \end{cases}$$

- ***m* ODEs, *n* PDEs:** ???

Idea:

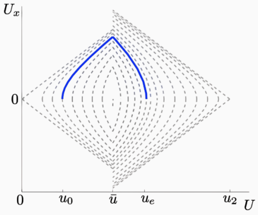
- Patterns are solution to

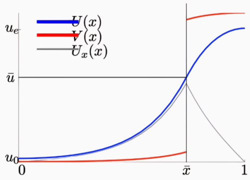
$$f(\boldsymbol{U}, V) = 0; \qquad d\nabla^2 V + g(\boldsymbol{U}, V) = 0$$

- Implicit function theorem: $\boldsymbol{U} = \boldsymbol{h}(V)$, thus

$$d\nabla^2 V + g\big(\boldsymbol{h}(V), V\big) = 0$$

- Phase portrait method:





Theory

Framework: Work on $\Omega \subset \mathbb{R}^p$ where zero-flux boundary conditions are assumed. Consider the system

$$\begin{cases} \dfrac{\partial}{\partial t} \boldsymbol{u} = \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{V}) & \text{(non-diffusing)} \\ \dfrac{\partial}{\partial t} \boldsymbol{V} = D\nabla^2 \boldsymbol{V} + \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{V}) & \text{(diffusing)} \end{cases}$$

Notation:

- $\boldsymbol{u}$: non-diffusive component $(\dim \boldsymbol{u} = m)$
- $\boldsymbol{V}$: diffusing component $(\dim \boldsymbol{V} = n)$
- $\boldsymbol{N} = (\boldsymbol{f}, \boldsymbol{g})$: reaction terms
- D: diffusion matrix $(\text{diag}(d_1, \ldots d_n))$

Framework: Work on $\Omega \subset \mathbb{R}^p$ where zero-flux boundary conditions are assumed. Consider the system

$$\begin{cases} \dfrac{\partial}{\partial t} u = f(u, V) & \text{(non-diffusing)} \\ \dfrac{\partial}{\partial t} V = D\nabla^2 V + g(u, V) & \text{(diffusing)} \end{cases}$$

Notation:

- u: non-diffusive component ($\dim u = m$)
- V: diffusing component ($\dim V = n$)
- $N = (f, g)$: reaction terms
- D: diffusion matrix ($\mathrm{diag}(d_1, \ldots d_n)$)

Framework: Work on $\Omega \subset \mathbb{R}^p$ where zero-flux boundary conditions are assumed. Consider the system

$$\begin{cases} \dfrac{\partial}{\partial t} u = f(u, V) & \text{(non-diffusing)} \\ \dfrac{\partial}{\partial t} v = D_1 \nabla^2 v + g(u, v, w) & \text{(slow-diffusing)} \\ \dfrac{\partial}{\partial t} w = D_2 \nabla^2 w + h(u, v, w) & \text{(fast-diffusing)} \end{cases}$$

Notation:

- u: non-diffusive component ($\mathbf{dim}\, u = m$)
- v: slow diffusive component ($\mathbf{dim}\, v = l$)
- w: fast diffusing component ($\mathbf{dim}\, w = k$)
- $N = (f, g\ h)$: reaction terms
- D_1: slow diffusion matrix ($\mathrm{diag}(d_1, \ldots, d_l)$)
- D_2: fast diffusion matrix ($\mathrm{diag}(d_{l+1}, \ldots, d_k)$)

Framework: Work on $\Omega \subset \mathbb{R}^p$ where zero-flux boundary conditions are assumed. Consider the system

$$\begin{cases} \dfrac{\partial}{\partial t} \boldsymbol{u} = \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{V}) & \text{(non-diffusing)} \\ \dfrac{\partial}{\partial t} \boldsymbol{v} = D_1 \nabla^2 \boldsymbol{v} + \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) & \text{(slow-diffusing)} \\ \dfrac{\partial}{\partial t} \boldsymbol{w} = D_2 \nabla^2 \boldsymbol{w} + \boldsymbol{h}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) & \text{(fast-diffusing)} \end{cases}$$

Notation:

- $\boldsymbol{u}$: non-diffusive component ($\mathbf{dim}\, \boldsymbol{u} = m$)
- $\boldsymbol{v}$: slow diffusive component ($\mathbf{dim}\, \boldsymbol{v} = l$)
- $\boldsymbol{w}$: fast diffusing component ($\mathbf{dim}\, \boldsymbol{w} = k$)
- $\boldsymbol{N} = (\boldsymbol{f}, \boldsymbol{g}\ \boldsymbol{h})$: reaction terms
- D_1: slow diffusion matrix ($\mathrm{diag}(d_1, \ldots, d_l)$)
- D_2: fast diffusion matrix ($\mathrm{diag}(d_{l+1}, \ldots, d_k)$)

Framework: Work on $\Omega \subset \mathbb{R}^p$ where zero-flux boundary conditions are assumed. Consider the system

$$\begin{cases} \frac{\partial}{\partial t}\mathbf{u} = \mathbf{f}(\mathbf{u}, \mathbf{V}) & \text{(non-diffusing)} \\ \frac{\partial}{\partial t}\mathbf{v} = D_1\nabla^2\mathbf{v} + \mathbf{g}(\mathbf{u}, \mathbf{v}, \mathbf{w}) & \text{(slow-diffusing)} \\ \frac{\partial}{\partial t}\mathbf{w} = D_2\nabla^2\mathbf{w} + \mathbf{h}(\mathbf{u}, \mathbf{v}, \mathbf{w}) & \text{(fast-diffusing)} \end{cases}$$

Notation:

- $\mathbf{u}$: non-diffusive component (**dim** $\mathbf{u} = m$)
- $\mathbf{v}$: slow diffusive component (**dim** $\mathbf{v} = l$)
- $\mathbf{w}$: fast diffusing component (**dim** $\mathbf{w} = k$)
- $\mathbf{N} = (\mathbf{f}, \mathbf{g}\ \mathbf{h})$: reaction terms
- D_1: slow diffusion matrix $(\text{diag}(d_1, \dots, d_l))$
- D_2: fast diffusion matrix $(\text{diag}(d_{l+1}, \dots, d_k))$

Question: What are sufficient and necessary conditions for DDI in the general system of Reation-Diffusion-ODE?

Framework: Work on $\Omega \subset \mathbb{R}^p$ where zero-flux boundary conditions are assumed. Consider the system

$$\begin{cases} \dfrac{\partial}{\partial t}\boldsymbol{u} = \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{V}) & \text{(non-diffusing)} \\ \dfrac{\partial}{\partial t}\boldsymbol{v} = D_1 \nabla^2 \boldsymbol{v} + \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) & \text{(slow-diffusing)} \\ \dfrac{\partial}{\partial t}\boldsymbol{w} = D_2 \nabla^2 \boldsymbol{w} + \boldsymbol{h}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) & \text{(fast-diffusing)} \end{cases}$$

Notation:

- $\boldsymbol{u}$: non-diffusive component ($\dim \boldsymbol{u} = m$)
- $\boldsymbol{v}$: slow diffusive component ($\dim \boldsymbol{v} = l$)
- $\boldsymbol{w}$: fast diffusing component ($\dim \boldsymbol{w} = k$)
- $\boldsymbol{N} = (\boldsymbol{f}, \boldsymbol{g}\ \boldsymbol{h})$: reaction terms
- D_1: slow diffusion matrix ($\mathrm{diag}(d_1, \ldots, d_l)$)
- D_2: fast diffusion matrix ($\mathrm{diag}(d_{l+1}, \ldots, d_k)$)

More notation (less standard):

- $X := (\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w})$: state variable
- $J(\cdot) := \nabla_{(\boldsymbol{u},\boldsymbol{v},\boldsymbol{w})}\boldsymbol{N}(\cdot)$: Jacobi matrix
- $J_{ij}(\cdot) := \begin{pmatrix} \partial_i \boldsymbol{N}^i(\cdot) & \partial_j \boldsymbol{N}^i(\cdot) \\ \partial_i \boldsymbol{N}^j(\cdot) & \partial_j \boldsymbol{N}^j(\cdot) \end{pmatrix}$: principal minor
- $s(\cdot) := \sup_{\lambda \in \sigma(\cdot)}\{\mathrm{Re}\lambda\}$ modulus of stability
- $\boldsymbol{\mathcal{L}}(\cdot) := D\nabla^2(\cdot) + J(\cdot)$: Linearized operator

Assumption: There exists a constant steady state $\bar{X}$

Assumption: There exists a constant steady state $\bar{X}$

Linearized operator around steady state $\bar{X}$:

$$\mathcal{L}_{D_1,D_2}[\boldsymbol{\xi}] = \underbrace{\begin{pmatrix} 0 & & \\ & D_1 & \\ & & D_2 \end{pmatrix}}_{D} \nabla^2 \boldsymbol{\xi} + J(\bar{X})\boldsymbol{\xi}$$

Assumption: There exists a constant steady state $\bar{X}$

Linearized operator around steady state $\bar{X}$:

$$\boldsymbol{\mathcal{L}}_{D_1,D_2}[\boldsymbol{\xi}] = \underbrace{\begin{pmatrix} 0 & & \\ & D_1 & \\ & & D_2 \end{pmatrix}}_{\boldsymbol{D}} \nabla^2 \boldsymbol{\xi} + J(\bar{X})\boldsymbol{\xi}$$

Spectrum on $L^2(\Omega)^{m+l+k}$: With "a little bit" of work, we split the spectrum for $D_1, D_2 > 0$

$$\sigma(\boldsymbol{\mathcal{L}}_{D_1,D_2}) = \{\sigma(\partial_{\boldsymbol{u}} \boldsymbol{f}(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j \boldsymbol{D} + J(\bar{X})\xi\right), \qquad \lambda_j \in \sigma(-\Delta_N^{\Omega})$$

Assumption: There exists a constant steady state $\bar{X}$

Linearized operator around steady state $\bar{X}$:

$$\mathcal{L}_{D_1,D_2}[\xi] = \underbrace{\begin{pmatrix} 0 & & \\ & D_1 & \\ & & D_2 \end{pmatrix}}_{\mathbf{D}} \nabla^2 \xi + J(\bar{X})\xi$$

Spectrum on $L^2(\Omega)^{m+l+k}$: With "a little bit" of work, we split the spectrum for $D_1, D_2 > 0$

$$\sigma(\mathcal{L}_{D_1,D_2}) = \underbrace{\{\sigma(\partial_u f(\bar{X}))\}}_{\substack{\text{spectrum} \\ \text{non-diffusing}}} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j \mathbf{D} + J(\bar{X})\xi\right), \qquad \lambda_j \in \sigma(-\Delta_N^\Omega)$$

Assumption: There exists a constant steady state $\bar{X}$

Linearized operator around steady state $\bar{X}$:

$$\boldsymbol{\mathcal{L}}_{D_1,D_2}[\boldsymbol{\xi}] = \underbrace{\begin{pmatrix} 0 & & \\ & D_1 & \\ & & D_2 \end{pmatrix}}_{\boldsymbol{D}} \nabla^2 \boldsymbol{\xi} + J(\bar{X})\boldsymbol{\xi}$$

Spectrum on $L^2(\Omega)^{m+l+k}$: With "a little bit" of work, we split the spectrum for $D_1, D_2 > 0$

$$\sigma(\boldsymbol{\mathcal{L}}_{D_1,D_2}) = \{\sigma(\partial_u \boldsymbol{f}(\bar{X}))\} \cup \underbrace{\bigcup_{j=0}^{\infty} \sigma\left(\lambda_j \boldsymbol{D} + J(\bar{X})\xi\right)}_{\substack{\text{spectrum} \\ \text{diffusing}}}, \qquad \lambda_j \in \sigma(-\Delta_N^{\Omega})$$

Assumption: There exists a constant steady state $\bar{X}$

Linearized operator around steady state $\bar{X}$:

$$\mathcal{L}_{D_1,D_2}[\boldsymbol{\xi}] = \underbrace{\begin{pmatrix} 0 & & \\ & D_1 & \\ & & D_2 \end{pmatrix}}_{\boldsymbol{D}} \nabla^2 \boldsymbol{\xi} + J(\bar{X})\boldsymbol{\xi}$$

Spectrum on $L^2(\Omega)^{m+l+k}$: With "a little bit" of work, we split the spectrum for $D_1, D_2 > 0$

$$\sigma(\mathcal{L}_{D_1,D_2}) = \{\sigma(\partial_{\boldsymbol{u}} \boldsymbol{f}(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j \boldsymbol{D} + J(\bar{X})\xi\right), \qquad \lambda_j \in \sigma(-\Delta_N^{\Omega})$$

Conditions for Diffusion-Driven Instability

We say the steady state $\bar{X}$ exhibits DDI as steady state of the system if

1. The spectral bound $s(\mathcal{L}_{0,0}) = s(J(\bar{X})) < 0$
2. The choice of $D_1, D_2 > 0$ is such that $s(\mathcal{L}_{D_1,D_2}) > 0$

Instability from the non-diffusing system: $\sigma(\boldsymbol{\mathcal{L}}_{D_1,D_2}) = \{\sigma(\partial_u \boldsymbol{f}(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j \boldsymbol{D} + J(\bar{X})\xi\right)$

Theorem 2.3: Autocatalysis condition

Suppose $s(J) < 0$. The condition $s(\partial_u \boldsymbol{f}(\bar{X})) > 0$ is called *autocatalysis*. If satisfied,

- $\bar{X}$ exhibits DDI independently from D_1, D_2
- Every stationary solution interesecting $\bar{X}$ is <u>unstable</u>

Instability from the non-diffusing system: $\sigma(\mathcal{L}_{D_1,D_2}) = \{\sigma(\partial_u f(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j D + J(\bar{X})\xi\right)$

Theorem 2.3: Autocatalysis condition

Suppose $s(J) < 0$. The condition $s(\partial_u f(\bar{X})) > 0$ is called *autocatalysis*. If satisfied,

- $\bar{X}$ exhibits DDI independently from D_1, D_2
- Every stationary solution interesecting $\bar{X}$ is unstable

Proof (1st point)

- Follows from $s(\mathcal{L}) \geq s(\partial_u f(\bar{X})) > 0$ $\quad$ ($\sup_{x \in A \cup B} \geq \sup_{x \in A}$) $\square$

Instability from the non-diffusing system: $\sigma(\mathcal{L}_{D_1,D_2}) = \{\sigma(\partial_u f(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j D + J(\bar{X})\xi\right)$

Theorem 2.3: Autocatalysis condition

Suppose $s(J) < 0$. The condition $s(\partial_u f(\bar{X})) > 0$ is called *autocatalysis*. If satisfied,

- $\bar{X}$ exhibits DDI independently from D_1, D_2
- Every stationary solution interesecting $\bar{X}$ is unstable

Proof (2nd point)

• Let $X^\star$ be a non-constant stationary solution intersecting $\bar{X}$ and $\mathcal{L}^\star := D\nabla^2 + J(X^\star)$ be the linearized operator around $X^\star$

Instability from the non-diffusing system: $\sigma(\mathcal{L}_{D_1,D_2}) = \{\sigma(\partial_u f(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j D + J(\bar{X})\xi\right)$

Theorem 2.3: Autocatalysis condition

Suppose $s(J) < 0$. The condition $s(\partial_u f(\bar{X})) > 0$ is called *autocatalysis*. If satisfied,

- $\bar{X}$ exhibits DDI independently from D_1, D_2
- Every stationary solution interesecting $\bar{X}$ is unstable

Proof (2nd point)

• Let $X^\star$ be a non-constant stationary solution intersecting $\bar{X}$ and $\mathcal{L}^\star := D\nabla^2 + J(X^\star)$ be the linearized operator around $X^\star$

• There exists (at least one) $x_0 \in \Omega$ such that $X^\star(x_0) = \bar{X}$

Instability from the non-diffusing system: $\sigma(\mathcal{L}_{D_1,D_2}) = \{\sigma(\partial_u f(\bar{X}))\} \cup \bigcup_{j=0}^{\infty} \sigma\left(\lambda_j D + J(\bar{X})\xi\right)$

Theorem 2.3: Autocatalysis condition

Suppose $s(J) < 0$. The condition $s(\partial_u f(\bar{X})) > 0$ is called *autocatalysis*. If satisfied,

- $\bar{X}$ exhibits DDI independently from D_1, D_2
- Every stationary solution interesecting $\bar{X}$ is unstable

Proof (2nd point)

• Let $X^\star$ be a non-constant stationary solution intersecting $\bar{X}$ and $\mathcal{L}^\star := D\nabla^2 + J(X^\star)$ be the linearized operator around $X^\star$

• There exists (at least one) $x_0 \in \Omega$ such that $X^\star(x_0) = \bar{X}$

• So $s(\mathcal{L}^\star) \geq s(\partial_u f(X^\star)) \geq s(\partial_u f(X^\star(x_0))) \geq s(\partial_u f(\bar{X})) > 0$ $\square$

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently small ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently large (L large enough)

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently small ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently large (L large enough)

Proof sketch:

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently small ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently large (L large enough)

Proof sketch:

- Temporarily set $D_1 = \mathbf{0} = \mathrm{diag}(0, ..., 0)$

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently small ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently large (L large enough)

Proof sketch:

- Temporarily set $D_1 = \mathbf{0} = \mathrm{diag}(0, \ldots, 0)$
- For all $\nu \in \sigma(J_{12})$, there exists $\{\mu_j\}_{j \geq 0} \subset \sigma_p(\boldsymbol{\mathcal{L}}_{\mathbf{0}, D_2})$ such that $\mu_j \longrightarrow \nu$ (non-trivial)

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently <u>small</u> ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently <u>large</u> (L large enough)

Proof sketch:

- Temporarily set $D_1 = \mathbf{0} = \mathrm{diag}(0, ..., 0)$
- For all $\nu \in \sigma(J_{12})$, there exists $\{\mu_j\}_{j\geq 0} \subset \sigma_p(\mathcal{L}_{\mathbf{0},D_2})$ such that $\mu_j \longrightarrow \nu$ (non-trivial)
- The eigenvalues of $\mathcal{L}_{D_1,D_2}$ depend <u>continuously</u> on D_1

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently small ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently large (L large enough)

Proof sketch:

- Temporarily set $D_1 = \mathbf{0} = \text{diag}(0, ..., 0)$
- For all $\nu \in \sigma(J_{12})$, there exists $\{\mu_j\}_{j \geq 0} \subset \sigma_p(\boldsymbol{\mathcal{L}}_{\mathbf{0}, D_2})$ such that $\mu_j \longrightarrow \nu$ (non-trivial)
- The eigenvalues of $\boldsymbol{\mathcal{L}}_{D_1, D_2}$ depend continuously on D_1
- Result still holds when introducing a small $D_1 > 0$ $\square$

Instability from coupled sub-systems (non- and slow-diffusing):

Main result: DDI when J_{12} unstable

Suppose $s(J) < 0$ and $s(J_{12}) > 0$. Then, $\bar{X}$ exhibits DDI on the domain $(0, L)$ if

1. $\max\{d : d \in D_1\} \leq \tilde{d}$ for $\tilde{d}$ sufficiently small ($L = 1$)
2. $\inf\{d : d \in D_2\} \geq \hat{d}$ for $\hat{d}$ sufficiently large (L large enough)

Proof sketch:

- Temporarily set $D_1 = \mathbf{0} = \mathrm{diag}(0, ..., 0)$
- For all $\nu \in \sigma(J_{12})$, there exists $\{\mu_j\}_{j\geq 0} \subset \sigma_p(\boldsymbol{\mathcal{L}}_{\mathbf{0},D_2})$ such that $\mu_j \longrightarrow \nu$ (non-trivial)
- The eigenvalues of $\boldsymbol{\mathcal{L}}_{D_1,D_2}$ depend continuously on D_1
- Result still holds when introducing a small $D_1 > 0$ $\square$

Remark: The case D_2 large is proved by writing $D_2 = d\tilde{D}_2$, rescaling the domain $L = \dfrac{1}{\sqrt{d}}$ and letting $d \to \infty$.

The simplest case: $(m, l, k) = (1, 1, 1)$: Possible to list explicit sufficient conditions for DDI.

System:

$$\begin{cases} \dfrac{\partial}{\partial t} u = f(u, v, w) \\ \dfrac{\partial}{\partial t} v = d_1 \nabla^2 v + g(u, v, w) \\ \dfrac{\partial}{\partial t} w = d_2 \nabla^2 w + h(u, v, w) \end{cases}$$

The simplest case: $(m, l, k) = (1, 1, 1)$: Possible to list explicit sufficient conditions for DDI.

System:

$$\begin{cases} \dfrac{\partial}{\partial t} u = f(u, v, w) \\ \dfrac{\partial}{\partial t} v = d_1 \nabla^2 v + g(u, v, w) \\ \dfrac{\partial}{\partial t} w = d_2 \nabla^2 w + h(u, v, w) \end{cases}$$

Conditions for DDI

Suppose $\bar{X}$ steady state with $J(\bar{X}) < 0$. Then, $\bar{X}$ exhibits DDI on $\Omega = (0, L)$ if

- $s(\partial_u f(\bar{X})) > 0$, $d_1, d_2 > 0$ and $L = 1$ (autocatalysis)

The simplest case: $(m, l, k) = (1, 1, 1)$: Possible to list explicit sufficient conditions for DDI.

System:

$$\begin{cases} \frac{\partial}{\partial t} u = f(u, v, w) \\ \frac{\partial}{\partial t} v = d_1 \nabla^2 v + g(u, v, w) \\ \frac{\partial}{\partial t} w = d_2 \nabla^2 w + h(u, v, w) \end{cases}$$

Conditions for DDI

Suppose $\bar{X}$ steady state with $J(\bar{X}) < 0$. Then, $\bar{X}$ exhibits DDI on $\Omega = (0, L)$ if

- $s(\partial_u f(\bar{X})) > 0$, $d_1, d_2 > 0$ and $L = 1$ (autocatalysis)
- $s(J_{12}) > 0$, $d_1 \geq 0$ sufficiently small $d_2 > 0$, $L = 1$

The simplest case: $(m, l, k) = (1, 1, 1)$: Possible to list explicit sufficient conditions for DDI.

System:

$$\begin{cases} \dfrac{\partial}{\partial t} u = f(u, v, w) \\ \dfrac{\partial}{\partial t} v = d_1 \nabla^2 v + g(u, v, w) \\ \dfrac{\partial}{\partial t} w = d_2 \nabla^2 w + h(u, v, w) \end{cases}$$

Conditions for DDI

Suppose $\bar{X}$ steady state with $J(\bar{X}) < 0$. Then, $\bar{X}$ exhibits DDI on $\Omega = (0, L)$ if

- $s(\partial_u f(\bar{X})) > 0$, $d_1, d_2 > 0$ and $L = 1$ (autocatalysis)
- $s(J_{12}) > 0$, $d_1 \geq 0$ sufficiently small $d_2 > 0$, $L = 1$
- $s(J_{12}) > 0$, $d_1 > 0$, $d_2 \geq 0$ sufficiently large, $L \geq 1$ sufficiently large

The simplest case: $(m, l, k) = (1, 1, 1)$: Possible to list explicit sufficient conditions for DDI.

System:

$$\begin{cases} \frac{\partial}{\partial t} u = f(u, v, w) \\ \frac{\partial}{\partial t} v = d_1 \nabla^2 v + g(u, v, w) \\ \frac{\partial}{\partial t} w = d_2 \nabla^2 w + h(u, v, w) \end{cases}$$

Conditions for DDI

Suppose $\bar{X}$ steady state with $J(\bar{X}) < 0$. Then, $\bar{X}$ exhibits DDI on $\Omega = (0, L)$ if

- $s(\partial_u f(\bar{X})) > 0$, $d_1, d_2 > 0$ and $L = 1$ (autocatalysis)
- $s(J_{12}) > 0$, $d_1 \geq 0$ sufficiently small $d_2 > 0$, $L = 1$
- $s(J_{12}) > 0$, $d_1 > 0$, $d_2 \geq 0$ sufficiently large, $L \geq 1$ sufficiently large
- $s(J_{13}) > 0$, $d_1 > 0$, $d_2 \geq 0$ sufficiently small, $L = 1$

The simplest case: $(m, l, k) = (1, 1, 1)$: Possible to list explicit sufficient conditions for DDI.

System:

$$\begin{cases} \frac{\partial}{\partial t} u = f(u, v, w) \\ \frac{\partial}{\partial t} v = d_1 \nabla^2 v + g(u, v, w) \\ \frac{\partial}{\partial t} w = d_2 \nabla^2 w + h(u, v, w) \end{cases}$$

Conditions for DDI

Suppose $\bar{X}$ steady state with $J(\bar{X}) < 0$. Then, $\bar{X}$ exhibits DDI on $\Omega = (0, L)$ if

- $s(\partial_u f(\bar{X})) > 0$, $d_1, d_2 > 0$ and $L = 1$ (autocatalysis)
- $s(J_{12}) > 0$, $d_1 \geq 0$ sufficiently small $d_2 > 0$, $L = 1$
- $s(J_{12}) > 0$, $d_1 > 0$, $d_2 \geq 0$ sufficiently large, $L \geq 1$ sufficiently large
- $s(J_{13}) > 0$, $d_1 > 0$, $d_2 \geq 0$ sufficiently small, $L = 1$
- $s(J_{13}) > 0$, $d_1 \geq 0$ sufficiently large, $d_2 > 0$, $L \geq 1$ sufficiently large

Application: Pattern Formation in receptor-based model

Consider the problem:

- Domain: $\Omega = (0, L), L > 0$, and Zero-flux boundary conditions
- Parameters: $\mu_f, \mu_l, \mu_b, \mu_e, m_1, m_2, m_3 > 0$
- Equations:

$$\begin{cases} \dfrac{\partial}{\partial t} u = -\mu_f u + m_1 \dfrac{uv}{1+uv} - \mu_b uv \\ \dfrac{\partial}{\partial t} v = d_1 \nabla^2 v - \mu_l v + m_2 \dfrac{uv}{1+uv} - \mu_b uv - vw \\ \dfrac{\partial}{\partial t} w = d_2 \nabla^2 w - \mu_e w + m_3 \dfrac{uv}{1+uv} \end{cases}$$

Consider the problem:

- Domain: $\Omega = (0, L), L > 0$, and Zero-flux boundary conditions
- Parameters: $\mu_f, \mu_l, \mu_b, \mu_e, m_1, m_2, m_3 > 0$
- Equations:

$$\begin{cases} \dfrac{\partial}{\partial t} u = -\mu_f u + m_1 \dfrac{uv}{1+uv} - \mu_b uv \\ \dfrac{\partial}{\partial t} v = d_1 \nabla^2 v - \mu_l v + m_2 \dfrac{uv}{1+uv} - \mu_b uv - vw \\ \dfrac{\partial}{\partial t} w = d_2 \nabla^2 w - \mu_e w + m_3 \dfrac{uv}{1+uv} \end{cases}$$

Well-posedness of the problem

Let $X_0 = (u_0, v_0, w_0) \in L^\infty(\Omega)^3$ be an initial condition such that

$$X_0 \in \left\{ X \in \mathbb{R}^3 \;:\; 0 \le u_0 \le \frac{m_1}{\min\{\mu_f, \mu_b\}}, \quad 0 \le v_0 \le \frac{m_2}{\min\{\mu_l, \mu_b, 1\}}, \quad 0 \le w_0 \le \frac{m_3}{\mu_e} \right\}.$$

Then, the associated IVP has a unique, non-negative, uniformly-bounded, global solution on $\mathbb{R}_{\ge 0} \times \Omega$

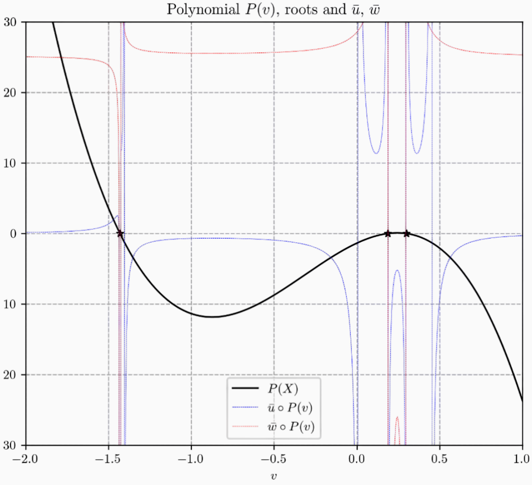
Proof: The region defined above is a Bounded Invariant Rectangle $\square$.

Equilibria

Constant steady states of the system are the points

$$\mathbf{0} = (0,0,0), \qquad \bar{X} = \left(\frac{m_1}{(\mu_f + \mu_b \varrho_i)} - \frac{1}{\varrho_i}, \;\; \varrho_i, \;\; \frac{m_3}{\mu_e}\left(1 - \frac{\mu_f + \mu_b \varrho_i}{m_1 \varrho_i}\right)\right)$$

where ϱ_i are the (up to three) roots of a degree-three polynomial P.

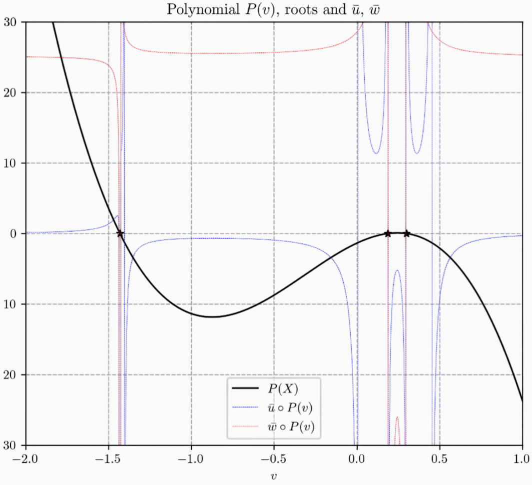


Equilibria

Constant steady states of the system are the points

$$\mathbf{0} = (0,0,0), \qquad \bar{X} = \left(\frac{m_1}{(\mu_f + \mu_b \varrho_i)} - \frac{1}{\varrho_i},\ \ \varrho_i,\ \ \frac{m_3}{\mu_e}\left(1 - \frac{\mu_f + \mu_b \varrho_i}{m_1 \varrho_i}\right)\right)$$

where ϱ_i are the (up to three) roots of a degree-three polynomial P.



Proposition: If parameters belong to

$$\Pi := \Big\{ \theta \in \mathbb{R}^7 \ : \mu_f, \mu_b, \mu_l, \mu_e \in (0,1),$$
$$m_1, m_2, m_3 \in (2, \infty),$$
$$m_2 - \frac{m_3 \mu_f}{m_1 \mu_e} - 2\sqrt{\mu_f \mu_l \frac{m_2}{m_1}} > 0 \Big\}$$

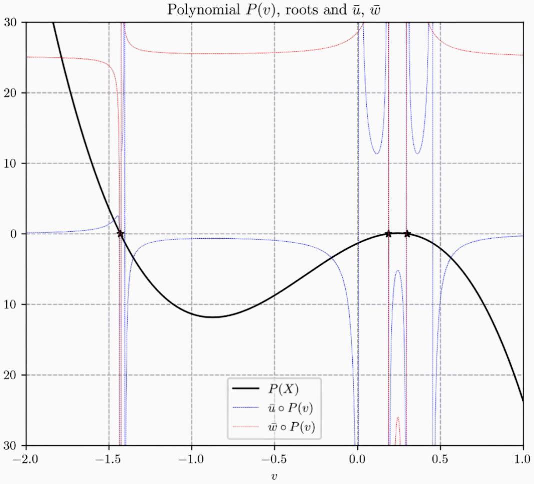
then steady states are $(\mathbf{0}, \bar{X}_1, \bar{X}_2)$.

Equilibria

Constant steady states of the system are the points

$$\mathbf{0} = (0,0,0), \qquad \bar{X} = \left(\frac{m_1}{(\mu_f + \mu_b \varrho_i)} - \frac{1}{\varrho_i}, \ \ \varrho_i, \ \ \frac{m_3}{\mu_e}\left(1 - \frac{\mu_f + \mu_b \varrho_i}{m_1 \varrho_i}\right)\right)$$

where ϱ_i are the (up to three) roots of a degree-three polynomial P.



Proposition: If parameters belong to

$$\Pi := \Big\{ \theta \in \mathbb{R}^7 \ : \mu_f, \mu_b, \mu_l, \mu_e \in (0,1), \\ m_1, m_2, m_3 \in (2, \infty), \\ m_2 - \frac{m_3 \mu_f}{m_1 \mu_e} - 2\sqrt{\mu_f \mu_l \frac{m_2}{m_1}} > 0 \Big\}$$

then steady states are $(\mathbf{0}, \bar{X}_1, \bar{X}_2)$.

Moreover, if $-\mathrm{tr}(J) \sum_{i<j} \mathbf{det}(J_{ij}) + \mathbf{det}(J) > 0$,
then the system is bi-stable and we write $\bar{X} := \bar{X}_2$.

Remark: We can show $s(\partial_u f(\bar{X})) < 0$ and that $s(J_{13}) < 0$ too. Thus, DDI can occur if and only if $s(J_{12}) > 0$. This occurs when parameters satisfy the additional relation:

$$\Gamma := \left\{ \theta \in \mathbb{R}^7 \ : \ 2\mu_l^2 - m_2\mu_l + \left(\frac{m_3\mu_f}{m_1\mu_e}\right)^2 + (3\mu_l - m_2)\frac{m_3\mu_f}{m_1\mu_e} > 0 \right\}$$

Remark: We can show $s(\partial_u f(\bar{X})) < 0$ and that $s(J_{13}) < 0$ too. Thus, DDI can occur if and only if $s(J_{12}) > 0$. This occurs when parameters satisfy the additional relation:

$$\Gamma := \left\{ \theta \in \mathbb{R}^7 \;:\; 2\mu_l^2 - m_2\mu_l + \left(\frac{m_3\mu_f}{m_1\mu_e}\right)^2 + (3\mu_l - m_2)\frac{m_3\mu_f}{m_1\mu_e} > 0 \right\}$$

Theorem: Exact conditions for DDI

On the domain $\Omega = (0, L)$, $\bar{X}$ exhibits DDI if parameters θ are in $\Pi \cap \Gamma$ and

1. $L > 0$, the diffusion coefficient $d_2 > 0$ is fixed and

$$\exists j \in \mathbb{N} \;:\; \qquad 0 < d_1 < \frac{\det(J) - \det(J_{12})\, d_2\lambda_j}{\lambda_j\left(\det(J_{13}) - J_1\, d_2\lambda_j\right)}$$

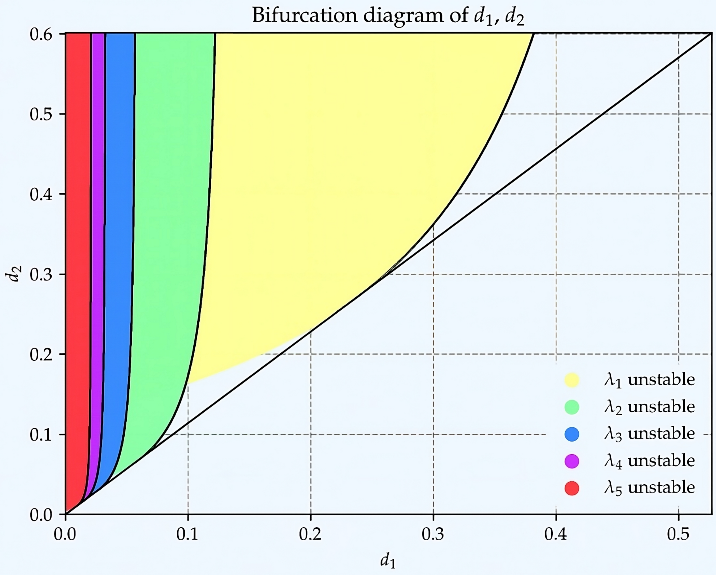
2. $d_1 > 0$ fixed, and

$$\exists j \in \mathbb{N} \;:\; \qquad L > \pi j\sqrt{\frac{J_1\, d_1}{\det(J_{12})}}, \qquad d_2 > \frac{\det(J) - \det(J_{13})\, d_1\lambda_j}{\lambda_j(\det(J_{12}) - J_1\, d_1\lambda_j)} > 0$$

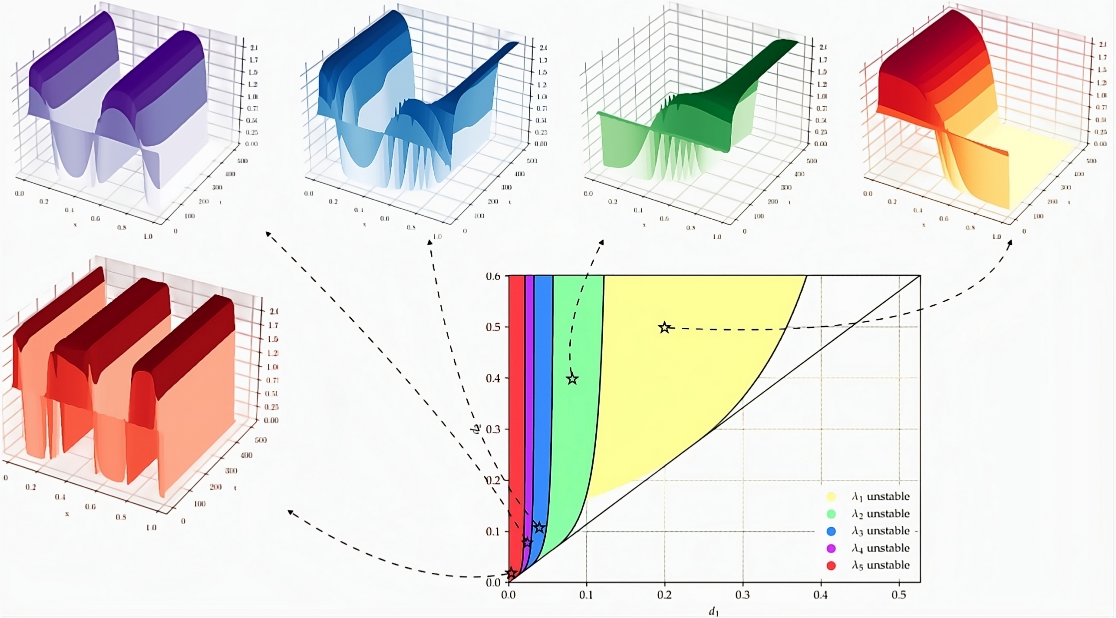
Bifurcation diagram:

Plotting values of d_1, d_2 such that $\bar{X}$ exhibits DDI.

The patterned solution depend on the area the point(d_1, d_2) lies within.



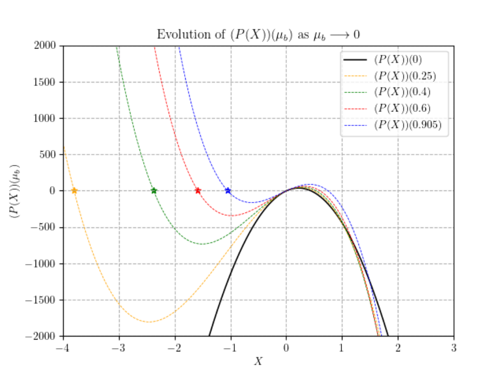
Numerical simulations:



Thank you for you attention!

Questions?

Additional Slides



Why $(\star)$: $\quad m_2 - \dfrac{m_3\mu_f}{m_1\mu_e} - 2\sqrt{\mu_f\mu_l\dfrac{m_2}{m_1}} > 0$?

- When $\mu_b \to 0$, P converges to an upside-down parabola Q.
- Condition $(\star)$ ensures two things:
  1. $\Delta_Q > 0$, so Q has two roots
  2. These roots are both positive and are $\mathcal{O}(\mu_b)$−close to the roots of P [1]
- Introduce $\mu_b > 0$ again, then P has three roots $\varrho_1 < 0 < \varrho_2 < \varrho_3$
- ϱ_2, ϱ_3 define two additional nonnegative steady state besides the origin.

Why $(\star\star)$: $-tr(J)\sum_{i<j}\mathbf{det}(J_{ij}) + \mathbf{det}(J) > 0$?

- Ensures $\bar{X}(\varrho_3)$ is stable $\implies$ system is bistable.

[1] See next slide for proof of this claim.

Proof: The two positive roots of Q are $\mathcal{O}(\mu_b)$—close to ϱ_2, ϱ_3, while $\varrho_1 \to -\infty$ as $\mu_b \to 0$

- Write the roots $\varrho_i := \sum_{k \geq k_0} a_k \mu_b^{k/d}$ for some $d \geq 0$ and $k \in \mathbb{Z}$
- Newton Polygon yields

$$\varrho_1 = \frac{a_{-1}}{\mu_b} + C_1 + \mathcal{O}(\mu_b), \qquad \varrho_2 = C_2 + \mathcal{O}(\mu_b), \qquad \varrho_3 = C_3 + \mathcal{O}(\mu_b)$$

- Factorization $P(v) := p_3 \prod_i (v - \varrho_i)$ and expansion $P(v) := \sum_i p_i v^i$. By power indentification:

$$p_2 = -K\left(a_{-1} + \mu_b \sum_i C_i + \mathcal{O}(\mu_b^2)\right), \qquad K > 0$$

- Hence, when $\mu_b \to 0$, we find $a_{-1} = -p_2/K$
- Therefore, the roots ϱ_2, ϱ_3 are $\mathcal{O}(\mu_b)$ and ϱ_1 is singular, in the sense

$$\varrho_1 = -\frac{p_2}{K}\frac{1}{\mu_b} + C_1 + \mathcal{O}(\mu_b) \quad \xrightarrow{\mu_b \to 0} \quad -\infty$$