

Lecture 03: Dynamical Systems

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1 Introduction

In the previous lecture, we showed how to use Chemical Reaction Networks (CRNs) to represent biosystem dynamics.

Suppose x is the reactant concentration vector, and v is the rate of reactions concerned, we would have the dynamics of j th reactant x_j as:

$$\frac{dx_j}{dt} = \sum_i \gamma_{ij} v_i$$

We could write this in matrix form:

$$\frac{dx}{dt} = \Gamma v$$

where Γ denotes the matrix of reaction stoichiometry. Note that this gives the knowledge of $v \rightarrow x$: we update the reactant vector using the known reactions.

If we also know the detailed mechanisms (the elementary reactions), we could then write mass-action laws for the rate:

$$v_i = k_i [x_1]^{\alpha_{i1}} [x_2]^{\alpha_{i2}} \dots = k_i \prod_l [x_l]^{\alpha_{il}}$$

$$\frac{dx}{dt} = \Gamma v = \Gamma \wedge_k x^\alpha = \Gamma \begin{pmatrix} k_1 & & & \\ & k_2 & & \\ & & \ddots & \\ & & & k_n \end{pmatrix} \begin{bmatrix} x_1^{\alpha_{11}} & x_1^{\alpha_{21}} & \dots \\ x_2^{\alpha_{12}} & x_2^{\alpha_{22}} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

Note that mechanisms like the mass-action law here give us knowledge of $x \rightarrow v$, where we know the reaction rate based on current reactant vector.

So combining the understanding in both directions, we would have a closed-loop relationship of reactant x and rate v . It's now clear that $\frac{dx}{dt} = \Gamma v(x) = f(x)$, which means that the updating of x vector relies on itself. We call the system with $\frac{dx}{dt} = f(x)$ an **autonomous dynamical system**. We further need some methods or toolkits for us to conduct dynamical analysis upon the CRN that we've just defined, and that's what this lecture is basically about.

2 Dynamic Analysis

2.1 Dynamics of 1D Systems

We start from the simplest 1-dimension analysis, which is just a point moving along a line. The dynamics $\dot{x} = f(x)$ would tell us that when $f(x) > 0$, the point would move right; when $f(x) < 0$, the point would move left; and when $f(x) = 0$ the point doesn't move and would stay there.

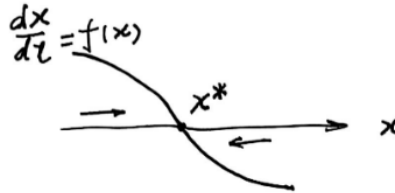


Figure 1

Figure 1 contains information sufficient to roughly determine the dynamics of state variable x , and provides us with a **geometric** way of reasoning about dynamics. It's essentially a diagram of state space with derivative on corresponding state points. We call this kind of diagram a “**phase portrait**”.

We could analyze the “stability” of point x^* that, if we start at x^* , then we would stay there forever. If we start from points other than x^* , it will always move towards x^* .

Definition 2.1. A **phase portrait** is a diagram that for every x , draws the derivative (essentially a vector field) $f(x) = \frac{dx}{dt}$.

Definition 2.2. A **fixed point** is x^* such that $f(x^*) = 0$.

Thus you can never cross a fixed point, since you would be trapped whenever you get there.

Definition 2.3. A fixed point x^* is **(locally) stable** if the starting point $x(0)$ is close to x^* , then $x(t) \rightarrow x^*$ as $t \rightarrow \infty$.

Apart from the phase portrait (Figure 1), we could also get intuitive understanding of stable fixed points using time trajectory plots (Figure 2).

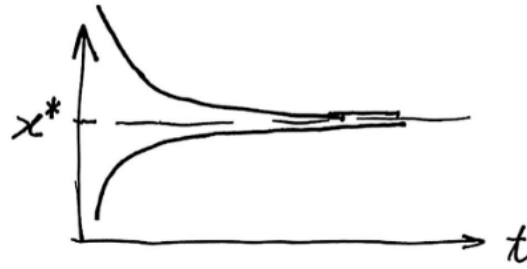


Figure 2

Example 1. Consider the dynamics(Figure 3):

$$\frac{dx}{dt} = f(x) = -x$$

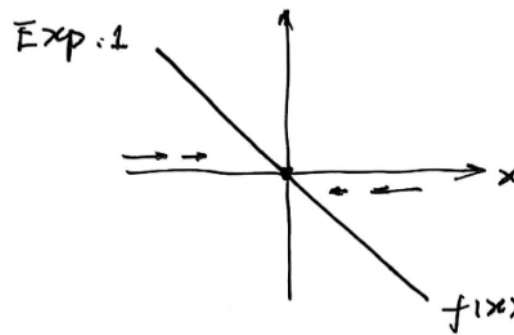


Figure 3

The dynamics of state variable in this case is so simple that we could even solve for the accurate dynamics first:

$$\begin{aligned} \frac{1}{x} \frac{dx}{dt} &= -1 \\ \frac{d \log x}{dt} &= -1 \\ \log x(t) &= -t + \log x(0) \\ x(t) &= x(0)e^{-t} \end{aligned}$$

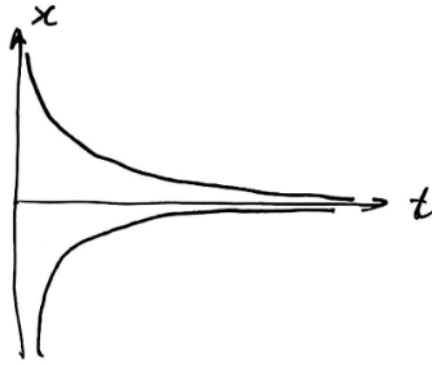


Figure 4

Thus $x = 0$ would be a stable fixed point.

△

Example 2. Consider the dynamics:

$$\frac{dx}{dt} = x^2$$

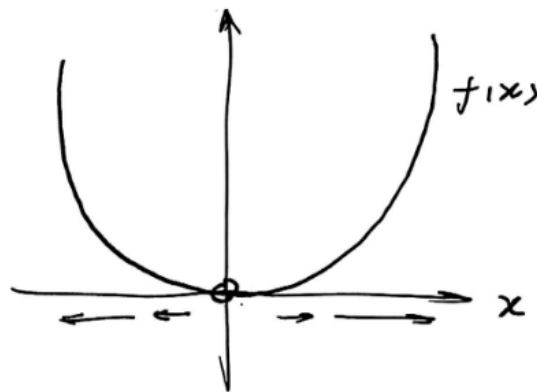


Figure 5

$$\begin{aligned}\frac{1}{x^2} \frac{dx}{dt} &= 1 \\ \frac{d(-\frac{1}{x})}{dt} &= 1 \\ -\frac{1}{x} &= t - \frac{1}{x(0)} \\ x(t) &= \frac{1}{\frac{1}{x(0)} - t} \\ x(t) &= \frac{x(0)}{1 - x(0)t}\end{aligned}$$

We see that $x = 0$ is also a fixed point, but no longer stable.

In fact from the detailed dynamics $x(t)$ that we worked out, the state x would blow up in **finite time** ($t = \frac{1}{x(0)}$). We couldn't get this information (finite-time blow up) by simply staring at the phase portrait. But this is indeed a pathological, unrealistic case. In normal regular cases the geometric thinking still does a good job.

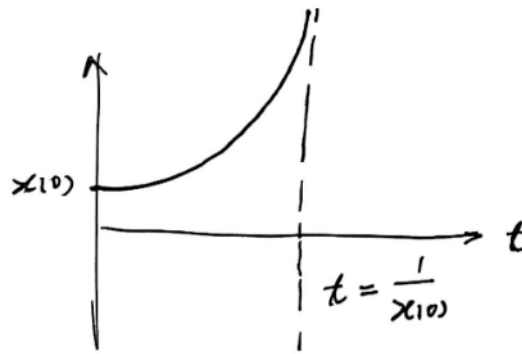


Figure 6

△

Example 3. Consider the dynamics:

$$\frac{dx}{dt} = x^2 - r$$

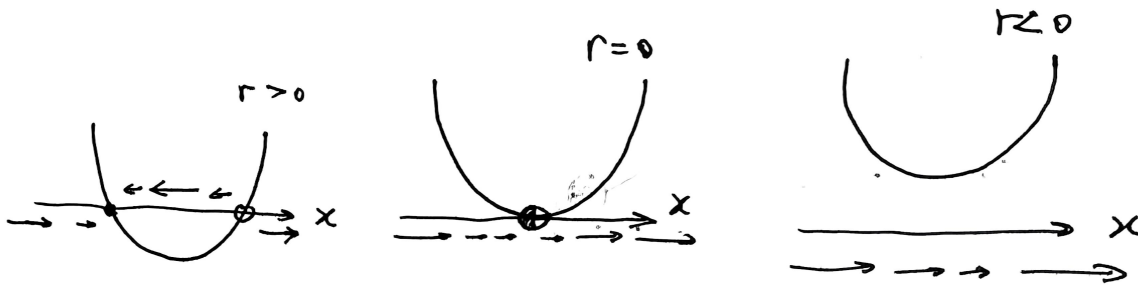


Figure 7

Depending on the specific parameters of dynamics, the stability would be different. We use open dots to indicate the unstable fixed points. Half-open dot in $r = 0$ indicates that only points starting from left plane would land onto $x = 0$, but the points starting from right plane would move on forever. So it's "half stable". $\triangle$

Example 4. We could even have infinitely many fixed points and use the geometric thinking to analyze dynamics. (ex. $f(x)$ is sinusoidal)

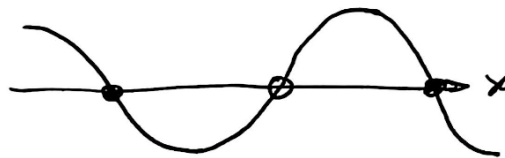


Figure 8

$\triangle$

Example 5. A point moving on a circle is also 1D, and the state variable now could be the rotation angle θ . The corresponding dynamics is the angular velocity $\dot{\theta}$. Simply $\dot{\theta} = -\theta$ would give us a fixed point in circular state space.

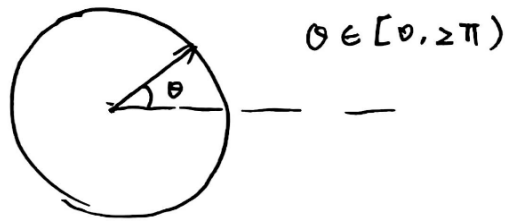


Figure 9

△

2.2 Dynamics of 2D Systems

We now move onto the 2D systems, with dynamics:

$$\dot{x}_1 = f_1(x), \quad \dot{x}_2 = f_2(x)$$

The phase portrait containing dynamical information of each point is now impossible to draw out completely. In this case we would have a two-dimensional space (x_1, x_2) and the corresponding velocity vector $(\dot{x}_1, \dot{x}_2)$ of each point (just like a directed compass accompanying every point on the 2D state space plane). But we actually don't require that much information! Our coarse-grained geometrical thinking needs just the sign of the dynamics (> 0 , < 0 or $= 0$), thus we explicitly draw the lines where $f_i = 0$ (we call them **nullclines**) and indicate $+$ or $-$ on either side.

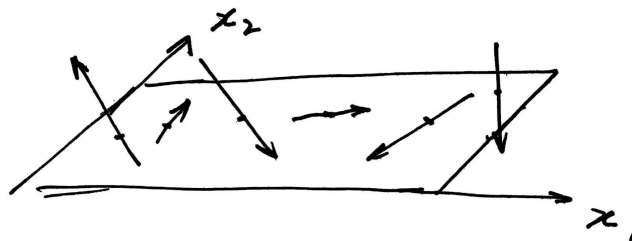


Figure 10

The fixed points discussed above would correspond to x^* such that $f_1(x^*) = f_2(x^*) = 0$.

Definition 2.4. The **nullcline** of x_i is the point set $\{x \in \mathbb{R}^2 : f_i(x) = 0\}$, $i = 1, 2$.

Consider single variable component at a time: suppose we consider the horizontal x_1 , then the nullcline $f_1(x) = 0$ indicates the places that we would be trapped when moving horizontally (just like the fixed points in 1D).

Using the intuition built in 1D, we could get the 2D dynamical behavior (around a fixed point) by simple combination of two 1D dynamics on different directions:

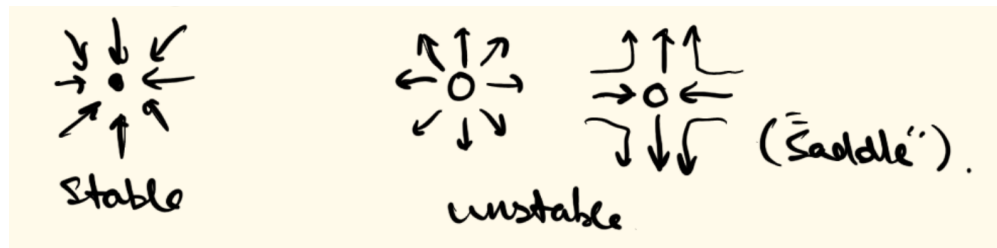


Figure 11

But we could also get some new behaviors:



Figure 12

2.3 2D System: Spiral and Radius

Example 6. See how we build up the dynamics by combining 1D dynamics: consider the system:

$$\begin{aligned}\dot{\theta} &= 1 \\ \dot{r} &= -r\end{aligned}$$

Intuitively, it's a constant-speed rotation with the shrinking radius movement.

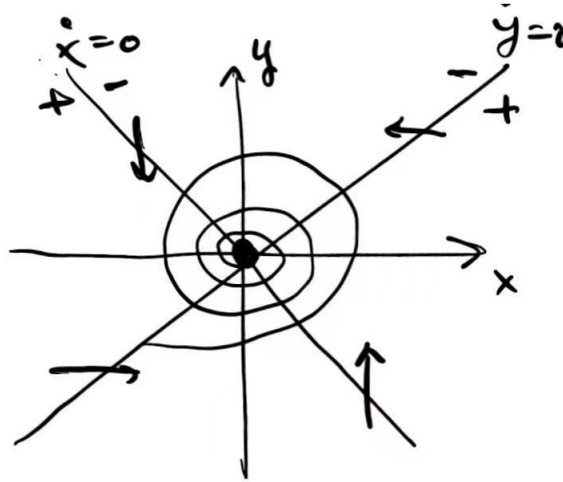


Figure 13

We can also try to convey the dynamics information using (x, y) coordinate ($x = r \cos \theta$ and $y = r \sin \theta$):

$$\begin{aligned}\dot{x} &= \dot{r} \cos \theta - r \sin \theta \cdot \dot{\theta} \\ &= -r \cos \theta - r \sin \theta \\ &= -x - y\end{aligned}$$

$$\begin{aligned}\dot{y} &= \dot{r} \sin \theta + r \cos \theta \cdot \dot{\theta} \\ &= -r \sin \theta + r \cos \theta \\ &= x - y\end{aligned}$$

In matrix form:

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

Notice that in (x, y) coordinate, the dynamics seems much more complicated: the dynamics of one state variables relies on the other. Whereas in the original polar coordinate, the dynamics are decomposed clearly. $\triangle$

Example 7. In the example above, if we let the radius remains constant:

$$\begin{aligned}\dot{\theta} &= 1 \\ \dot{r} &= 0\end{aligned}$$

then transform it into (x, y) coordinate gives:

$$\dot{x} = -r \sin(\theta) = -y$$

$$\dot{y} = r \cos(\theta) = x$$

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

This time the dynamics of one variable totally relies on the other one.

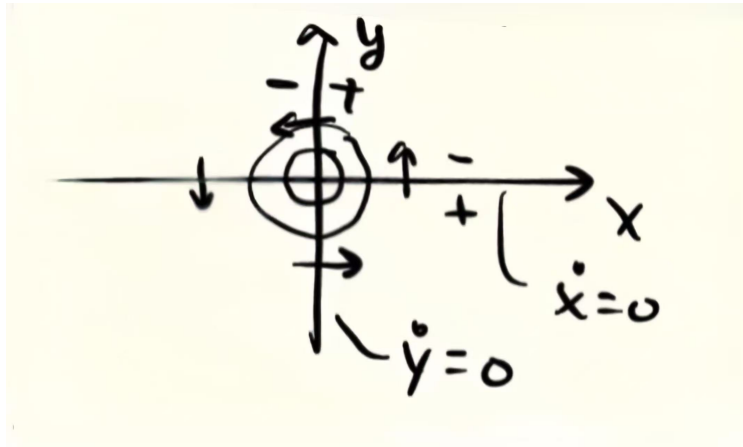


Figure 14

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2.4 2D System 'Center': Mass on a Spring

2.4.1 System Description

We consider an idealized spring-mass system with:

- A point mass m constrained to one-dimensional motion
- A linear spring with constant k (Hooke's law)
- No friction or external forces

Newton's second law yields:

$$m\ddot{x} + kx = 0 \tag{1}$$

where $x(t)$ is the displacement from equilibrium.

2.4.2 State Space Representation

Converting to first-order system with $x_1 = x$ and $x_2 = \dot{x}$:

$$\dot{x}_1 = x_2 \quad (2)$$

$$\dot{x}_2 = -\frac{k}{m}x_1 \quad (3)$$

Matrix form:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \mathbf{A}\mathbf{x} \quad (4)$$

2.4.3 Eigenvalue Analysis and Stability

The characteristic equation is:

$$\det(\mathbf{A} - \lambda\mathbf{I}) = \lambda^2 + \frac{k}{m} = 0 \quad (5)$$

Eigenvalues:

$$\lambda_{1,2} = \pm i\omega_0, \quad \omega_0 = \sqrt{\frac{k}{m}} \quad (6)$$

Stability criterion: Since $\text{Re}(\lambda) = 0$, the system is **marginally stable**. The equilibrium $(0, 0)$ is a **center** with closed orbital trajectories.

2.4.4 Energy Conservation

Total mechanical energy:

$$E = \frac{1}{2}mx_2^2 + \frac{1}{2}kx_1^2 \quad (7)$$

Time derivative:

$$\frac{dE}{dt} = mx_2\dot{x}_2 + kx_1\dot{x}_1 = mx_2\left(-\frac{k}{m}x_1\right) + kx_1x_2 = 0 \quad (8)$$

Energy conservation explains the closed orbital behavior: each trajectory lies on a constant energy ellipse.

2.5 3D and Beyond

In 1D systems, we cannot go back. In 2D systems, we cannot overlap with ourselves. But in 3D systems, limitations are seldom. (See Fig. Lines go across in 3D.)

For 1D systems, we have fixed points. For 2D systems, we have fixed points, nullclines, and limit cycles. For 3D or higher-dimensional systems, we need to reduce the dimension if we are lucky enough.

2.6 Eigenvalue Classification and Stability

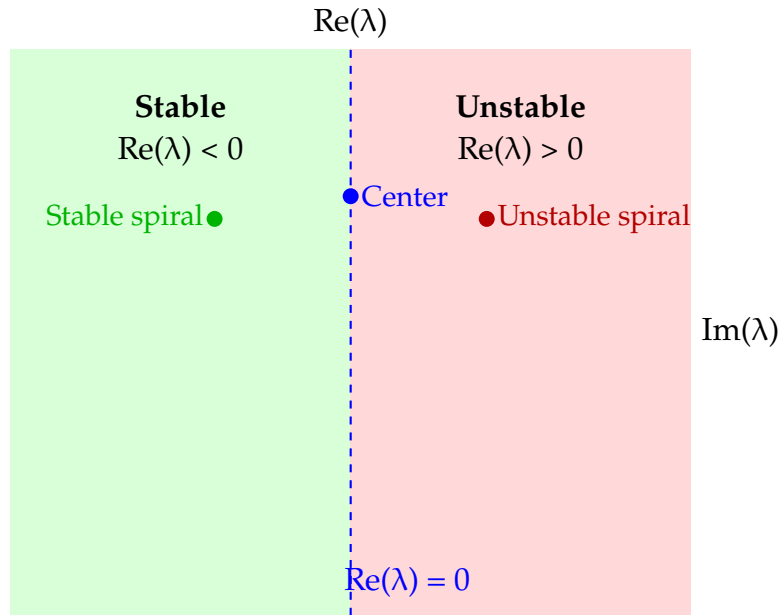
2.6.1 Routh-Hurwitz Stability Criterion for A

For linear systems $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$, stability is determined by eigenvalues of $\mathbf{A}$:

- **Asymptotically stable:** All $\text{Re}(\lambda) < 0$
 - Trajectories converge to equilibrium exponentially
 - Equilibrium is an **attractor**
 - Complex eigenvalues: **stable spiral/focus**
- **Unstable:** Any $\text{Re}(\lambda) > 0$
 - Trajectories diverge from equilibrium
 - Equilibrium is a **repeller**
 - Complex eigenvalues: **unstable spiral/focus**
- **Marginally stable:** All $\text{Re}(\lambda) = 0$ (purely imaginary)
 - Bounded oscillatory motion
 - Equilibrium is a **center**
 - Example: Conservative systems (spring-mass)

Routh-Hurwitz criterion: For polynomial $P(\lambda) = a_n\lambda^n + \dots + a_1\lambda + a_0$, all roots have $\text{Re}(\lambda) < 0$ if and only if all Routh-Hurwitz determinants are positive. For 2D systems, this simplifies to: $\text{tr}(\mathbf{A}) < 0$ and $\det(\mathbf{A}) > 0$.

2.6.2 Eigenvalue Plane Visualization



2.7 Linearization Around Fixed Points: The Jacobian Matrix J

2.7.1 From Nonlinear to Linear Analysis

Most biological systems are **nonlinear**. Unlike linear systems where dynamics can be described by a constant matrix A , nonlinear systems are governed by:

$$\frac{dx}{dt} = f(x) \quad (9)$$

where $x = [x_1, \dots, x_n]^T$ and $f(x) = [f_1(x), \dots, f_n(x)]^T$.

2.7.2 Linearization Around Fixed Points

A **fixed point** (equilibrium) x^* satisfies $f(x^*) = 0$.

Key idea: Near a fixed point, the nonlinear system behaves approximately like a linear system. We linearize by computing **partial derivatives (slopes)** of each component function with respect to each variable.

Taylor expansion around x^* :

$$f(x) \approx f(x^*) + J(x^*)(x - x^*) = J(x^*)(x - x^*) \quad (10)$$

The **Jacobian matrix** $J(x^*)$ contains all first-order partial derivatives (local slopes) evaluated at the fixed point:

$$\mathbf{J}(\mathbf{x}^*) = \left[\begin{array}{cccc} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_n} \end{array} \right] \bigg|_{\mathbf{x}=\mathbf{x}^*} \quad (11)$$

Physical interpretation: Each entry $J_{ij} = \frac{\partial f_i}{\partial x_j}$ represents how the rate of change of variable x_i responds to small changes in variable x_j near the fixed point.

2.7.3 Local Stability from Jacobian Eigenvalues

The linearized system is:

$$\frac{d(\mathbf{x} - \mathbf{x}^*)}{dt} \approx \mathbf{J}(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*) \quad (12)$$

Hartman-Grobman Theorem: If all eigenvalues of $\mathbf{J}(\mathbf{x}^*)$ have non-zero real parts (hyperbolic fixed point), the local behavior of the nonlinear system near $\mathbf{x}^*$ is topologically equivalent to the linearized system.

Stability determination:

- All $\text{Re}(\lambda_i) < 0 \Rightarrow$ fixed point is **locally asymptotically stable**
- Any $\text{Re}(\lambda_i) > 0 \Rightarrow$ fixed point is **unstable**
- All $\text{Re}(\lambda_i) = 0 \Rightarrow$ linearization inconclusive (requires nonlinear analysis)

2.7.4 Example: Predator-Prey System

Consider the Lotka-Volterra model:

$$\frac{dx}{dt} = ax - bxy = f_1(x, y) \quad (13)$$

$$\frac{dy}{dt} = -cy + dxy = f_2(x, y) \quad (14)$$

Fixed points: $(0, 0)$ and $(\frac{c}{d}, \frac{a}{b})$.

Computing partial derivatives:

$$\mathbf{J}(x, y) = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix} = \begin{bmatrix} a - by & -bx \\ dy & -c + dx \end{bmatrix} \quad (15)$$

At coexistence equilibrium $(\frac{c}{d}, \frac{a}{b})$:

$$\mathbf{J}\left(\frac{c}{d}, \frac{a}{b}\right) = \begin{bmatrix} 0 & -\frac{bc}{d} \\ \frac{da}{b} & 0 \end{bmatrix} \quad (16)$$

Eigenvalues: $\lambda_{1,2} = \pm i\sqrt{ac}$ (purely imaginary).

The linearization predicts a center, but nonlinear effects may produce limit cycles or more complex dynamics.

2.7.5 Limitations of Linear Analysis

- Valid only near fixed points (local analysis)
- Cannot capture global phenomena (bifurcations, limit cycles, chaos)
- Fails at non-hyperbolic equilibria ($\text{Re}(\lambda) = 0$)
- Misses nonlinear effects (multistability, hysteresis)

3 Chemical Reaction Network Related

3.1 Constraints Rules for CRN

Now that we've learned how to analyze dynamics, let's look at dynamical systems that arise from **Chemical Reaction Networks (CRNs)**. These systems have further structure.

$$\dot{x} = \Gamma v(x) = \Gamma \Lambda_k x^\alpha = f^+(x) - f^-(x)$$

Rule [P]: Positivity

- Variables x_j are positive.
- Fluxes $v_i(x)$ are positive.

Rule [PU]: Parameter Uncertainty

Reaction rate constants satisfy $k_i \neq k_{i'}$ for different reactions $i \neq i'$. This means we **cannot perfectly match** different processes.

Both the increase and decrease of x_j arise from comparison between its production and degradation terms:

$$\dot{x}_j = f_j = f_j^+ - f_j^-$$

Example:

$$\dot{x} = \mu - \gamma x$$

Here, the production rate μ and the degradation rate γx are two different processes. Thus, the fixed point is:

$$x^* = \frac{\mu}{\gamma}$$

This steady state results from two processes pushing against each other. Therefore, x^* is not structural—it is **uncertain** and may “shake” due to fluctuations in parameters.

Rule [CP]: Constructural Polynomial Dynamics

Positivity implies a constraint on polynomial dynamics:

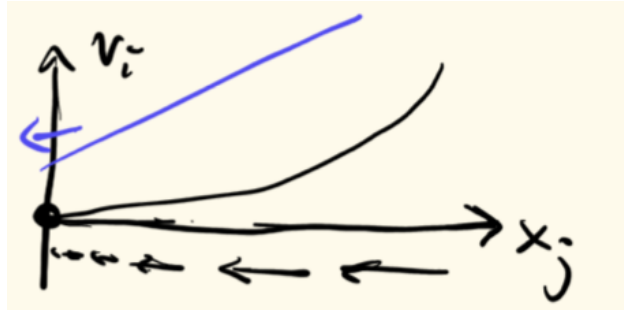
$$\dot{x}_j = \sum_{i: v_{ij} > 0} v_{ij} v_i - \sum_{i: v_{ij} < 0} |v_{ij}| v_i$$

where each flux term follows:

$$v_i = k_i x_1^{\alpha_{i1}} x_2^{\alpha_{i2}} \dots x_n^{\alpha_{in}}$$

Summary

- CRNs can be viewed as structured polynomial dynamical systems.
- Positivity and parameter uncertainty govern their qualitative behavior.
- Steady states may not be structurally stable due to distinct production and degradation processes.



Degradation Reactions and Forward Invariance

For a reaction degrading x_j , we require:

$$v_{ij} < 0.$$

Since $\alpha_{ij} \geq 0$ and $\beta_{ij} \geq 0$, this requires:

$$\alpha_{ij} \geq 1.$$

Hence, the flux follows:

$$v_i \propto x_j^{\alpha_{ij}}, \quad \text{with } \alpha_{ij} \geq 1.$$

Reasoning from Positivity:

$$v_i = 0 \quad \text{when} \quad x_j = 0.$$

Otherwise, x_j would become negative — which is physically impossible.

This constraint ensures that the **positive orthant** is **forward invariant**, meaning that trajectories starting with $x_j > 0$ will remain in the positive domain.

Examples of Constrained Polynomial Dynamics in CRNs

1. $\dot{x} = x - \mu$

Is this possible? *No*, because the degradation term $-\mu$ is constant and does not vanish when $x = 0$. Thus, positivity is violated.

2.
$$\begin{cases} \dot{x}_1 = \mu_1 - x_2 \\ \dot{x}_2 = x_1 - \mu_2 \end{cases}$$

or equivalently,

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Question: Is this possible? Here, both equations depend on variables that vanish at zero, ensuring positivity consistency — but such a structure may not correspond to an actual CRN unless stoichiometric coefficients and rate laws align.

Conclusion:

- Degradation reactions require $\alpha_{ij} \geq 1$ to preserve positivity.
- The positive orthant remains forward invariant — states cannot cross into negative concentrations.
- Not all polynomial systems satisfy CRN constraints; each term must obey physical positivity rules.

3.2 Methods to Circumvent Polynomial Constraints

3.2.1 Dual Rail Representation

Coordinate transformation approach:

$$x = x_+ - x_-, \quad \dot{x}_+ = f^+ - \eta x_+ x_-, \quad \dot{x}_- = f^- - \eta x_+ x_- \quad (17)$$

Limitation: For $\dot{x} = \mu - kx$, decomposition requires:

$$\mu - k(x_+ - x_-) = \mu + kx_- - kx_+ \quad (18)$$

This introduces two separate rate constants, violating parameter independence.

3.2.2 Time-Scale Separation in Enzymatic Reactions

Standard enzymatic reaction:



Typical rate constants:

- Binding: $k_{\text{on}} \sim 10^8 \text{ M}^{-1}\text{s}^{-1}$, effective rate $k_{\text{on}}[S] \sim 10^5 \text{ s}^{-1}$ at $[S] \sim 1 \text{ mM}$
- Catalysis: $k_{\text{cat}} \sim 10^1\text{--}10^2 \text{ s}^{-1}$

Time-scale separation: Binding ($\sim \mu\text{s}$) is much faster than catalysis ($\sim \text{ms}$), enabling quasi-equilibrium approximation and Michaelis-Menten kinetics.

Advantages over coordinate transformation:

- Preserves physical meaning
- Maintains parameter independence
- Based on real biophysical processes
- Enables multi-scale modeling

4 Credit

Contributor	Sections
Xinyu Wang	• Introduction • 2.1 Dynamics of 1D Systems • 2.2 Dynamics of 2D Systems • 2.3 2D System: Spiral and Radius
Shuo Wang	• 2.4 2D System 'Center': Mass on a Spring • 2.6 Eigenvalue Classification and Stability • 2.7 Linearization Around Fixed Points: The Jacobian Matrix • 3.2 Methods to Circumvent Polynomial Constraints
Shaocong Fang	• 2.5 3D and beyond • 2.6 Eigenvalue Classification and Stability • 3.1 Constraints Rules for CRN