Semi-algebraic description of the equilibria of dynamical systems

Changbo Chen and Marc Moreno Maza

ORCCA, University of Western Ontario, Canada

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Outline

1. Motivation: a biochemical network
2. A new tool for solving parametric polynomial systems
3. Study the equilibria of dynamical systems symbolically

Outline

Mad cow disease

http://x-medic.net/infections/bovine-spongiform-encephalopathy/attachment/mad-cow-disease

A mad cow disease model (M. Laurent, 1996)

Hypothesis: the mad cow disease is spread by prion proteins.

The kinetic scheme

$$\begin{array}{l} \downarrow 1 \\ PrP^{C} \xrightarrow{3} PrP^{S_C} \xrightarrow{4} \text{Aggregates.} \\ \downarrow 2 \end{array}$$

- PrP^{C} (resp. PrP^{S_C}) is the normal (resp. infectious) form of prions
- Step 1 (resp. 2) : the synthesis (resp. degradation) of native PrP^{C}
- Step 3 : the transformation from PrP^{C} to PrP^{S_C}
- Step 4 : the formation of aggregates

Question: Can a *small amount of* PrP^{S_C} *cause prion disease?*

The dynamical system governing the reaction network

- Let x and y be respectively the concentrations of PrP^C and PrP^{S_C}.
- Let ν_i be the rate of Step i for $i = 1, \ldots, 4$.
- $\nu_1 = k_1$ for some constant k_1.
- $\nu_2 = k_2 x$ and $\nu_4 = k_4 y$.
- $\nu_3 = ax\frac{(1+by^n)}{1+cy^n}$.

$$\begin{array}{l} \downarrow 1 \\ PrP^C \quad \xrightarrow{3} PrP^{S_C} \xrightarrow{4} \text{Aggregates.} \\ \downarrow 2 \end{array} \qquad \left\{ \begin{array}{rcl} \frac{\mathrm{d}x}{\mathrm{d}t} & = & \nu_1 - \nu_2 - \nu_3 \\ \\ \frac{\mathrm{d}y}{\mathrm{d}t} & = & \nu_3 - \nu_4 \end{array} \right. \tag{1}$$

The simplified dynamical system by experimental values

Experiments (M. Laurent 96) suggest to set $b = 2$, $c = 1/20$, $n = 4$, $a = 1/10$, $k_4 = 50$ and $k_1 = 800$. Now we have:

$$\left\{ \begin{array}{rcl} \frac{\mathrm{d}x}{\mathrm{d}t} & = & f_1 \\ \frac{\mathrm{d}y}{\mathrm{d}t} & = & f_2 \end{array} \right. \quad \text{with} \quad \left\{ \begin{array}{rcl} f_1 & = & \frac{16000+800y^4-20k_2x-k_2xy^4-2x-4xy^4}{20+y^4} \\ f_2 & = & \frac{2(x+2xy^4-500y-25y^5)}{20+y^4} \end{array} \right. . \tag{2}$$

- x and y are unknowns and k_2 is the only parameter.
- A constant solution (x_0, y_0) of system (2) is called an equilibrium.
- (x_0, y_0) is called asymptotically stable if the solutions of system (2) starting out close to (x_0, y_0) become arbitrary close to it.
- (x_0, y_0) is called hyperbolic if all the eigenvalues of $\begin{pmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_2}{\partial x} \\ \frac{\partial f_1}{\partial y} & \frac{\partial f_2}{\partial y} \end{pmatrix}$ have nonzero real parts at (x_0, y_0).

The polynomial system to solve (CASC 2011)

Theorem: Routh-Hurwitz criterion

A hyperbolic equilibrium (x_0, y_0) is asymptotically stable if and only if

$$\Delta_1(x_0, y_0) := -\left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y}\right) > 0 \text{ and } \Delta_2(x_0, y_0) := \frac{\partial f_1}{\partial x} \cdot \frac{\partial f_2}{\partial y} - \frac{\partial f_1}{\partial y} \cdot \frac{\partial f_2}{\partial x} > 0.$$

The semi-algebraic systems encoding the equilibria

- Let p_1 (resp. p_2) be the numerator of f_1 (resp. f_2).
- The system $\mathcal{S}_1 : \{p_1 = p_2 = 0, x > 0, y > 0, k_2 > 0\}$ encodes the equilibria of (2).
- The system $\mathcal{S}_2 : \{p_1 = p_2 = 0, x > 0, y > 0, k_2 > 0, \Delta_1 > 0, \Delta_2 > 0\}$ encodes the asymptotically stable hyperbolic equilibria of (2).

The corresponding constructible systems

- $\mathcal{C}_1 := \{p_1 = 0, p_2 = 0, x \neq 0, y \neq 0, k_2 \neq 0\}$ in $\mathbb{C}^3$.

Outline

Objectives

For a parametric polynomial system $F \subset \mathbf{k}[\mathbf{u}][\mathbf{x}]$, the following problems are of interest:

1. compute the values u of the parameters for which $F(u)$ has solutions, or has finitely many solutions.
2. compute the solutions of F as continuous functions of the parameters.
3. provide an automatic case analysis for the number (dimension) of solutions depending on the parameter values.

Related work

- (Comprehensive) Gröbner bases: (V. Weispfenning, 92, 02), (D. Kapur 93), (A. Montes, 02), (M. Manubens & A. Montes, 02), (A. Suzuki & Y. Sato, 03, 06), (D. Lazard & F. Rouillier, 07), (Y. Sun, D. Kapur & D. Wang, 10) and others.
- Triangular decompositions: (S.C. Chou & X.S. Gao 92), (X.S. Gao & D.K. Wang 03), (D. Kapur 93), (D.M. Wang 05), (L. Yang, X.R. Hou & B.C. Xia, 01), (R. Xiao, 09) and others.
- Cylindrical algebraic decompositions: (G.E. Collins 75), (H. Hong 90), (G.E. Collins, H. Hong 91), (S. McCallum 98), (A. Strzeboński 00), (C.W. Brown 01) and others.

A CASC story

At CASC 2007

- We investigated the specialization property of regular chains
- We introduced the concept of comprehensive triangular decomposition (CTD) of an algebraic variety.

At CASC 2011

- CTD of a parametric constructible set with application to complex root classification
- CTD of a parametric semi-algebraic system with application to real root classification

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Specialization

Definition

A (squarefree) regular chain T of $\mathbf{k}[\mathbf{u}, \mathbf{y}]$ specializes well at $u \in \mathbf{K}^d$ if $T(u)$ is a (squarefree) regular chain of $\mathbf{K}[\mathbf{y}]$ and $\mathrm{init}(T)(u) \neq 0$.

Example

$$T = \begin{cases} (s+1)z \\ (x+1)y + s \\ x^2 + x + s \end{cases} \quad \text{with} \quad s < x < y < z$$

does not specialize well at $s = 0$ or $s = -1$

$$T(0) = \begin{cases} z \\ (x+1)y \\ (x+1)x \end{cases} \quad T(1) = \begin{cases} 0z \\ (x+1)y - 1 \\ x^2 + x - 1 \end{cases}$$

Comprehensive Triangular Decomposition (CTD)

Definition

Let $F \subset \mathbf{k}[\mathbf{u}, \mathbf{y}]$. A CTD of $V(F)$ is given by :

- a finite partition $\mathcal{C}$ of the parameter space into constructible sets,
- above each $C \in \mathcal{C}$, there is a set of regular chains $\mathcal{T}_C$ such that
  - each regular chain $T \in \mathcal{T}_C$ specializes well at any $u \in C$ and
  - for any $u \in C$, we have $V(F(u)) = \bigcup_{T \in \mathcal{T}_C} W(T(u))$.

Example

A CTD of $F := \{x^2(1+y) - s, y^2(1+x) - s\}$ is as follows:

1. $s \neq 0 \longrightarrow \{T_1, T_2\}$
2. $s = 0 \longrightarrow \{T_2, T_3\}$

where

$$T_1 = \begin{cases} x^2y + x^2 - s \\ x^3 + x^2 - s \end{cases} \quad T_2 = \begin{cases} (x+1)y + x \\ x^2 - sx - s \end{cases} \quad T_3 = \begin{cases} y+1 \\ x+1 \\ s \end{cases}$$

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Disjoint squarefree comprehensive triangular decomposition (DSCTD)

Definition

Let $F \subset \mathbf{k}[\mathbf{u}, \mathbf{y}]$. A DSCTD of $V(F)$ is given by :

- a finite partition $\mathcal{C}$ of the parameter space,
- each cell $C \in \mathcal{C}$ is associated with a set of squarefree regular chains $\mathcal{T}_C$ such that
  - each squarefree regular chain $T \in \mathcal{T}_C$ specializes well at any $u \in C$ and
  - for any $u \in C$, $V(F(u)) = \uplus_{T \in \mathcal{T}_C} W(T(u))$. ($\uplus$ denotes disjoint union)

Example

1. $s \neq 0$, $s \neq 4/27$ and $s \neq -4 \longrightarrow \{T_1, T_2\}$
2. $s = -4 \longrightarrow \{T_1\}$
3. $s = 0 \longrightarrow \{T_3, T_4\}$
4. $s = 4/27 \longrightarrow \{T_2, T_5, T_6\}$

$$T_4 = \begin{cases} y \\ x \\ s \end{cases} \quad T_5 = \begin{cases} 3y - 1 \\ 3x - 1 \\ 27s - 4 \end{cases} \quad T_6 = \begin{cases} 3y + 2 \\ 3x + 2 \\ 27s - 4 \end{cases}$$

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Properties of CTD

Above each cell,

1. either there are no solutions
2. or finitely many solutions and the solutions are continuous functions of parameters
3. or infinitely many solutions, but the dimension is invariant.

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A CTD of $F := \{x^2(1+y)-s, y^2(1+x)-s\}$ is as follows:

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where

$$T_1 = \begin{cases} x^2y + x^2 - s \\ x^3 + x^2 - s \end{cases} \quad T_2 = \begin{cases} (x+1)y + x \\ x^2 - sx - s \end{cases} \quad T_3 = \begin{cases} y+1 \\ x+1 \\ s \end{cases}$$

Additional properties of DSCTD

Above each cell, where the system has finitely many solutions

1. the graphs of functions are disjoint
2. the number of distinct complex solutions is constant

Example

1. $s \neq 0$, $s \neq 4/27$ and $s \neq -4 \longrightarrow \{T_1, T_2\}$
2. $s = -4 \longrightarrow \{T_1\}$
3. $s = 0 \longrightarrow \{T_3, T_4\}$
4. $s = 4/27 \longrightarrow \{T_2, T_5, T_6\}$

$$T_1 = \begin{cases} x^2y + x^2 - s \\ x^3 + x^2 - s \end{cases} \quad T_2 = \begin{cases} (x+1)y + x \\ x^2 - sx - s \end{cases}$$

$$T_3 = \begin{cases} y+1 \\ x+1 \\ s \end{cases} \quad T_4 = \begin{cases} y \\ x \\ s \end{cases} \quad T_5 = \begin{cases} 3y-1 \\ 3x-1 \\ 27s-4 \end{cases} \quad T_6 = \begin{cases} 3y+2 \\ 3x+2 \\ 27s-4 \end{cases}$$

Comprehensive triangular decomposition of semi-algebraic systems?

Related concepts

- Cylindrical algebraic decomposition (CAD by G.E. Collins 75)
- Border polynomial (BP by L. Yang, X.R. Hou & B.C. Xia, 01)
- Discriminant variety (DV by D. Lazard & F. Rouillier, 07)

Why we want more?

- CAD does too much work when used for the purpose of solving semi-algebraic systems.
- BP and DV are only about the parameter space.
- Algorithm based on BP or DV focus on the components of maximal dimension in the parameter space.

Comprehensive triangular decomposition of semi-algebraic systems

Input

A parametric semi-algebraic system $S \subset \mathbb{Q}[\mathbf{u}][\mathbf{y}]$.

Output

- A partition of the whole parameter space into connected cells, such that above each cell
  1. either the corresponding constructible system of S has infinitely many complex solutions,
  2. or S has no real solutions
  3. or S has finitely many real solutions which are continuous functions of parameters with disjoint graphs
- A description of the solutions of S as functions of parameters by triangular systems in case of finitely many complex solutions.

How to compute a RCTD?

Specifications

- Input: a parametric semi-algebraic system S
- Output: a RCTD of S, that is, parameter space partition + triangular systems.

Algorithm

For simplicity, we assume S consists of only equations.

(1) Compute a DSCTD $(\mathcal{C}, (\mathcal{T}_C, C \in \mathcal{C}))$ of S.

(2) Refine each constructible set cell $C \in \mathcal{C}$ into connected semi-algebraic sets by CAD.

(3) Let C be a connected cell above which S has finitely many complex solutions.
Compute the number of real solutions of $T \in \mathcal{T}_C$ at a sample point u of C.
Remove those Ts which have no real solutions at u.

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Outline

Equilibria of mad cow disease model

Recall the dynamical system

$$\left\{\begin{array}{rcl} \frac{\mathrm{d}x}{\mathrm{d}t} & = & f_1 \\ \frac{\mathrm{d}y}{\mathrm{d}t} & = & f_2 \end{array}\right. \quad \text{with} \quad \left\{\begin{array}{rcl} f_1 & = & \frac{16000+800y^4-20k_2x-k_2xy^4-2x-4xy^4}{20+y^4} \\ f_2 & = & \frac{2(x+2xy^4-500y-25y^5)}{20+y^4} \end{array}\right. .$$

Let p_1 (resp. p_2) be the numerator of f_1 (resp. f_2).

$$\begin{array}{rcl} p_1 & := & (-20k_2 - k_2y^4 - 2 - 4y^4)x + 16000 + 800y^4 \\ p_2 & := & (2y^4+1)x - 500y - 25y^5 \end{array}$$

The system $\mathcal{S}_1 : \{p_1 = p_2 = 0, x > 0, y > 0, k_2 > 0\}$ encode the equilibria.

RCTD of $\mathcal{S}_1$

Let $0 < \alpha_1 < \alpha_2$ be the two positive real roots of the following polynomial

$$\begin{aligned} r \quad := \quad & 100000k_2^8 + 1250000k_2^7 + 5410000k_2^6 + 8921000k_2^5 - 9161219950k_2^4 \\ - \quad & 5038824999k_2^3 - 1665203348k_2^2 - 882897744k_2 + 1099528405056. \end{aligned}$$

The isolating intervals for α_1 and α_2 are respectively $[3.175933838, 3.175941467]$ and $[14.49724579, 14.49725342]$.
A RCTD of S_1 is as follows.

$$\begin{cases} \{\ \} & k_2 \le 0 \\ \{B_1\} & 0 < k_2 < \alpha_1 \\ \{B_2\} & k_2 = \alpha_1 \\ \{B_1\} & \alpha_1 < k_2 < \alpha_2 \\ \{B_2\} & k_2 = \alpha_2 \\ \{B_1\} & k_2 > \alpha_2 \end{cases} \qquad \begin{cases} 0 & k_2 \le 0 \\ 1 & 0 < k_2 < \alpha_1 \\ 2 & k_2 = \alpha_1 \\ 3 & \alpha_1 < k_2 < \alpha_2 \\ 2 & k_2 = \alpha_2 \\ 1 & k_2 > \alpha_2 \end{cases}$$

Theorem

If $0 < k_2 < \alpha_1$ or $k_2 > \alpha_2$, then the dynamical system has 1 equilibrium;
if $k_2 = \alpha_1$ or $k_2 = \alpha_2$, then the dynamical system has 2 equilibria;
if $\alpha_1 < k_2 < \alpha_2$, then dynamical system has 3 equilibria.

Hurwitz determinants and hyperbolicity

- Let (x, y) be an equilibrium of the dynamical system
- Let J be the Jacobian matrix of the dynamical system at (x, y)
- Then the characteristic polynomial of J is $\lambda^2 + \Delta_1 \lambda + \Delta_2$.
- Let λ_1 and λ_2 be the two eigenvalues of J
- Then we have $\lambda_1 + \lambda_2 = -\Delta_1$ and $\lambda_1 \lambda_2 = \Delta_2$

Thus

- $\mathsf{S}_1 := \{p_1 = p_2 = 0, x > 0, y > 0, k_2 > 0\}$ encodes the equilibria.
- $\mathsf{S}_2 := \{\mathsf{S}_1, \Delta_1 = \Delta_2 = 0\}$ encodes the nonhyperbolic equilibria with zero as eigenvalue of multiplicity two.
- $\mathsf{S}_3 := \{\mathsf{S}_1, \Delta_1 \neq 0, \Delta_2 = 0\}$ encodes the nonhyperbolic equilibria with zero as eigenvalue of multiplicity one.
- $\mathsf{S}_4 := \{\mathsf{S}_1, \Delta_1 = 0, \Delta_2 > 0\}$ encodes the nonhyperbolic equilibria with a pair of pure imaginary eigenvalues, that is, a Hopf bifurcation.
- $\mathsf{S}_5 := \{\mathsf{S}_1, \Delta_1 > 0, \Delta_2 > 0\}$ encodes the asymptotically stable hyperbolic equilibria.

Stability and bifurcation analysis (I)

- RCTD(S_1) shows that the system has
  - one equilibrium if and only if $k_2 < \alpha_1$ or $k_2 > \alpha_2$;
  - two equilibria if and only if $k_2 = \alpha_1$ or $k_2 = \alpha_2$;
  - three equilibria if and only if $k_2 > \alpha_1$ and $k_2 < \alpha_2$.
- RCTD(S_2) and RCTD(S_4) show that neither S_2 nor S_4 have real solutions.
- RCTD(S_3) show that the system has
  - one nonhyperbolic equilibria with zero eigenvalue of multiplicity one if and only if $k_2 = \alpha_1$ or $k_2 = \alpha_2$.
- RCTD(S_5) show that the system has
  - one asymptotically stable hyperbolic equilibria if and only if $k_2 \leq \alpha_1$ or $k_2 \geq \alpha_2$;
  - two asymptotically stable hyperbolic equilibria if and only if $k_2 > \alpha_1$ and $k_2 < \alpha_2$.

Stability and bifurcation analysis

Combining several RCTDs

- $\mathsf{RCTD}(\mathcal{S}_1)$: equilibria.
- $\mathsf{RCTD}(\mathcal{S}_1, \Delta_1 = \Delta_2 = 0)$, $\mathsf{RCTD}(\mathcal{S}_1, \Delta_1 \neq 0, \Delta_2 = 0)$, and $\mathsf{RCTD}(\mathcal{S}_1, \Delta_1 = 0, \Delta_2 > 0)$: nonhyperbolic equilibria.
- $\mathsf{RCTD}(\mathcal{S}_1, \Delta_1 > 0, \Delta_2 > 0)$: asymptotically stable hyperbolic equilibria.

Theorem

- $0 < k_2 < \alpha_1$ or $k_2 > \alpha_2 \longrightarrow$ the system has 1 equilibrium, which is hyperbolic and asymptotically stable
- $k_2 = \alpha_1$ or $k_2 = \alpha_2 \longrightarrow$ the system has 2 equilibria, one is nonhyperbolic, another one is hyperbolic and asymptotically stable
- $\alpha_1 < k_2 < \alpha_2 \longrightarrow$ the system has 3 equilibria, two are hyperbolic and asymptotically stable, one is hyperbolic and non-stable.
- the system experiences a bifurcation at $k_2 = \alpha_1$ or $k_2 = \alpha_2$

Can a small amount of PrP^{Sc} cause prion disease? (I)

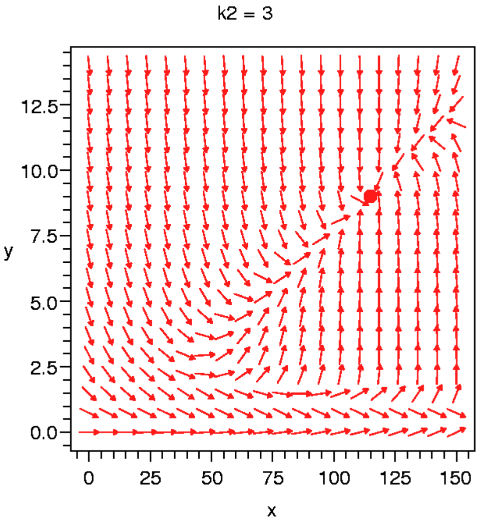

Figure: Vector field for $k_2 = 3$ ($x : PrP^C$, $y : PrP^{Sc}$)

Can a small amount of PrP^{Sc} cause prion disease? (II)

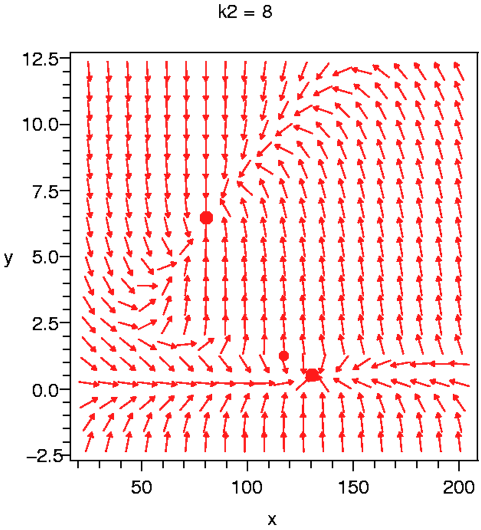

Figure: Vector field for $k_2 = 8$ ($x : PrP^C$, $y : PrP^{Sc}$)

Can a small amount of PrP^{Sc} cause prion disease? (III)

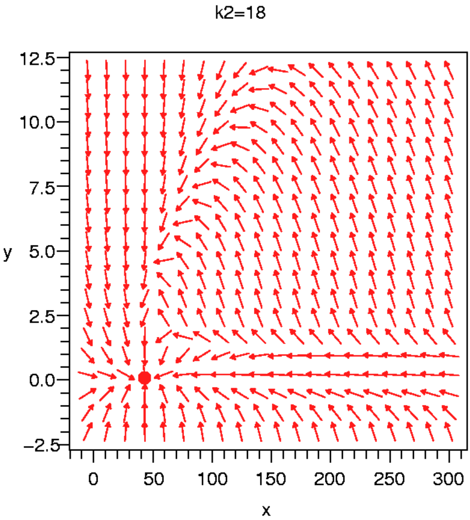

Figure: Vector field for $k_2 = 18$ ($x : PrP^C$, $y : PrP^{Sc}$)