

Solving Parametric Polynomial Systems by RealComprehensiveTriangularize

Changbo Chen¹ and Marc Moreno Maza²

¹ Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences
² ORCCA, University of Western Ontario

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Outline

- 1 An introductory example
- 2 Motivation: a biochemical network
- 3 A new tool for solving parametric polynomial systems
- 4 Study the equilibria of dynamical systems symbolically

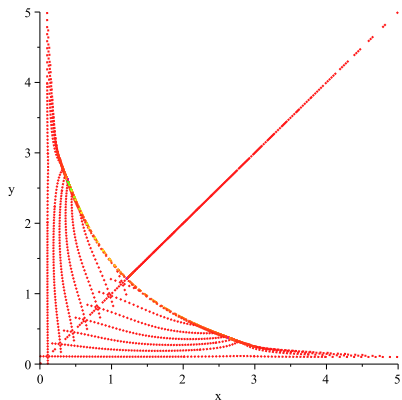
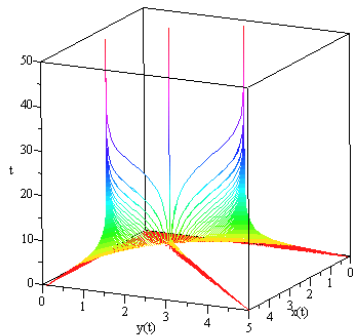
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Study of the stability of equilibria of a biological system

$$\frac{dx}{dt} = -x + \frac{s}{1+y^2}$$

$$\frac{dy}{dt} = -y + \frac{s}{1+x^2},$$



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$$\frac{dy}{dt} = -y + \frac{s}{1+x^2},$$

The biological system is described by the following system of differential equations.
Its right hand side encodes the equilibria:

```
> ode := {diff(x(t),t) = -x(t)+s/(1+y(t)^2), diff(y(t),t)=-y(t)+s/(1+x(t)^2)}:
F := [-x+s/(1+y^2), -y+s/(1+x^2)]:
```

The following two Hurwitz determinants determine the stability of the hyperbolic equilibria:

```
> D1 := -(diff(F[1],x)+diff(F[2],y)): #D1 is 2
D2 := diff(F[1],x)*diff(F[2],y)-diff(F[1],y)*diff(F[2],x):
```

The semi-algebraic system below encodes the asymptotically stable hyperbolic equilibria:

```
> P := [numer(normal(F[1]))=0, numer(normal(F[2]))=0, x>0, y>0, s>0, numer(D2)>0];
P:= [-y^2 x - x + s = 0, -y x^2 - y + s = 0, 0 < x, 0 < y, 0 < s, 0 < 1 + 2 x^2 + x^4 + 2 y^2 + 4 y^2 x^2 + 2 y^2 x^4 + y^4
+ 2 y^4 x^2 + y^4 x^4 - 4 y x s^2]
```

Figure: Study of the stability of equilibria of a biological system: problem set-up.

Compute a real comprehensive triangular decomposition of P w.r.t. the parameter s :

```
> R := PolynomialRing([y, x, s]); ctd := RealComprehensiveTriangularize(P, 1, R);
ctd := [[[1, squarefree_semi_algebraic_system], [2, squarefree_semi_algebraic_system]], [[semi_algebraic_set,
[ ]], [semi_algebraic_set, [1]], [semi_algebraic_set, [2]]]]
```

Derive the values of s such that P has 2 positive real solutions, that is the biological system is bistable:

```
> ctd2 := RealComprehensiveTriangularize(ctd, R, 2); Display(ctd2[2][1][1], R); Display(ctd2[1][1]
[2], R);
```

```
ctd2 := [[[1, squarefree_semi_algebraic_system]], [[semi_algebraic_set, [1]]]]
```

$$[2 < s]$$

$$xy - 1 = 0$$

$$x^2 - sx + 1 = 0$$

$$y > 0$$

$$x > 0$$

$$8xs^3 - 6xs^5 - 4s^2 + 5s^4 - s^6 + xs^7 > 0$$

Figure: Study of the stability of equilibria of biological system: solution with `RealComprehensiveTriangularize`.

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Mad cow disease

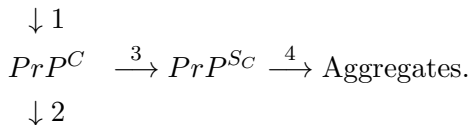


[http://x-medic.net/infections/
bovine-spongiform-encephalopathy/attachment/mad-cow-disease](http://x-medic.net/infections/bovine-spongiform-encephalopathy/attachment/mad-cow-disease)

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

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

The kinetic scheme

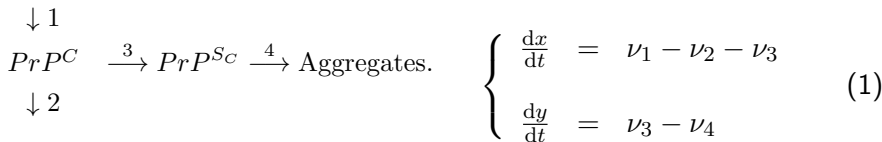


- PrP^C (resp. PrP^{Sc}) is the normal (resp. infectious) form of prions
- Step 1 (resp. 2) : the synthesis (resp. degradation) of native PrP^C
- Step 3 : the transformation from PrP^C to PrP^{Sc}
- Step 4 : the formation of aggregates

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

The dynamical system governing the reaction network

- Let x and y be respectively the concentrations of PrP^C and PrP^{Sc} .
- Let ν_i be the rate of Step i for $i = 1, \dots, 4$.
- $\nu_1 = k_1$ for some constant k_1 .
- $\nu_2 = k_2x$ and $\nu_4 = k_4y$.
- $\nu_3 = ax \frac{(1+by^n)}{1+cy^n}$.



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:

$$\begin{cases} \frac{dx}{dt} = f_1 \\ \frac{dy}{dt} = f_2 \end{cases} \quad \text{with} \quad \begin{cases} f_1 = \frac{16000 + 800y^4 - 20k_2x - k_2xy^4 - 2x - 4xy^4}{20 + y^4} \\ f_2 = \frac{2(x + 2xy^4 - 500y - 25y^5)}{20 + y^4} \end{cases} \quad (2)$$

- 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

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

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 .

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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.

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 $\text{init}(T)(u) \neq 0$.

Example

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

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 $u \in C$, $V(F(u)) = \cup_{T \in \mathcal{T}_C} W(T(u))$. (\cup denotes **disjoint** union)

Example

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

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

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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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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 $s \neq -4 \rightarrow \{T_1, T_2\}$
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 \end{array}
 \quad
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 \end{array}$$

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 T s which have no real solutions at u .

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Equilibria of mad cow disease model

Recall the dynamical system

$$\begin{cases} \frac{dx}{dt} = f_1 \\ \frac{dy}{dt} = f_2 \end{cases} \quad \text{with} \quad \begin{cases} f_1 = \frac{16000 + 800y^4 - 20k_2x - k_2xy^4 - 2x - 4xy^4}{20 + y^4} \\ f_2 = \frac{2(x + 2xy^4 - 500y - 25y^5)}{20 + y^4} \end{cases} .$$

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

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

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

RCTD of S_1

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

$$r := 100000k_2^8 + 1250000k_2^7 + 5410000k_2^6 + 8921000k_2^5 - 9161219950k_2^4 - 5038824999k_2^3 - 1665203348k_2^2 - 882897744k_2 + 1099528405056.$$

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.

$$\left\{ \begin{array}{ll} \{ \} & k_2 \leq 0 \\ \{B_1\} & 0 < k_2 < \alpha_1 \\ \{B_2\} & k_2 = \alpha_1 \\ \{B_1\} & \alpha_1 < k_2 < \alpha_2 \\ \{B_2\} & k_2 = \alpha_2 \\ \{B_1\} & k_2 > \alpha_2 \end{array} \right. \quad \left\{ \begin{array}{ll} 0 & k_2 \leq 0 \\ 1 & 0 < k_2 < \alpha_1 \\ 2 & k_2 = \alpha_1 \\ 3 & \alpha_1 < k_2 < \alpha_2 \\ 2 & k_2 = \alpha_2 \\ 1 & k_2 > \alpha_2 \end{array} \right.$$

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

- $S_1 := \{p_1 = p_2 = 0, x > 0, y > 0, k_2 > 0\}$ encodes the equilibria.
- $S_2 := \{S_1, \Delta_1 = \Delta_2 = 0\}$ encodes the nonhyperbolic equilibria with zero as eigenvalue of multiplicity two.
- $S_3 := \{S_1, \Delta_1 \neq 0, \Delta_2 = 0\}$ encodes the nonhyperbolic equilibria with zero as eigenvalue of multiplicity one.
- $S_4 := \{S_1, \Delta_1 = 0, \Delta_2 > 0\}$ encodes the nonhyperbolic equilibria with a pair of pure imaginary eigenvalues, that is, a Hopf bifurcation.
- $S_5 := \{S_1, \Delta_1 > 0, \Delta_2 > 0\}$ 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

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

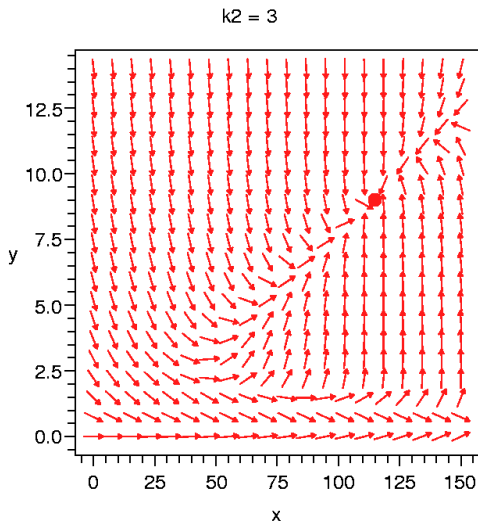


Figure: Vector field for $k_2 = 3$ ($x : PrP^C$, $y : PrP^{Sc}$)

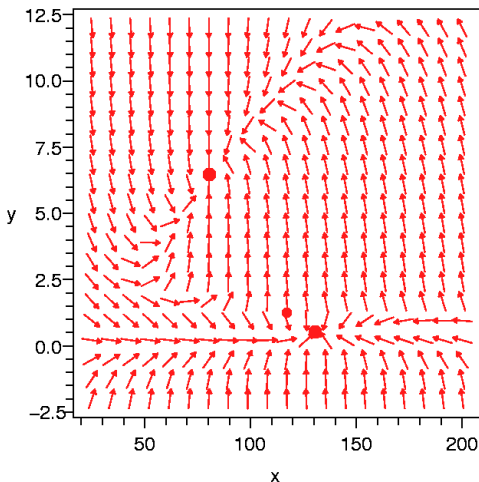
Can a small amount of PrP^{Sc} cause prion disease? (II) $k_2 = 8$ 

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

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

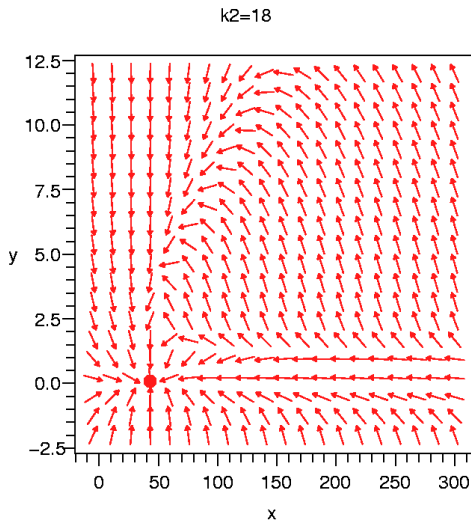


Figure: Vector field for $k_2 = 18$ ($x : PrP^C$, $y : PrP^{Sc}$)