Modeling Physics with Differential-Algebraic Equations

Lecture 4

Algebraic Methods: Elimination Theory and Invariant Sets

COMASIC (M2)

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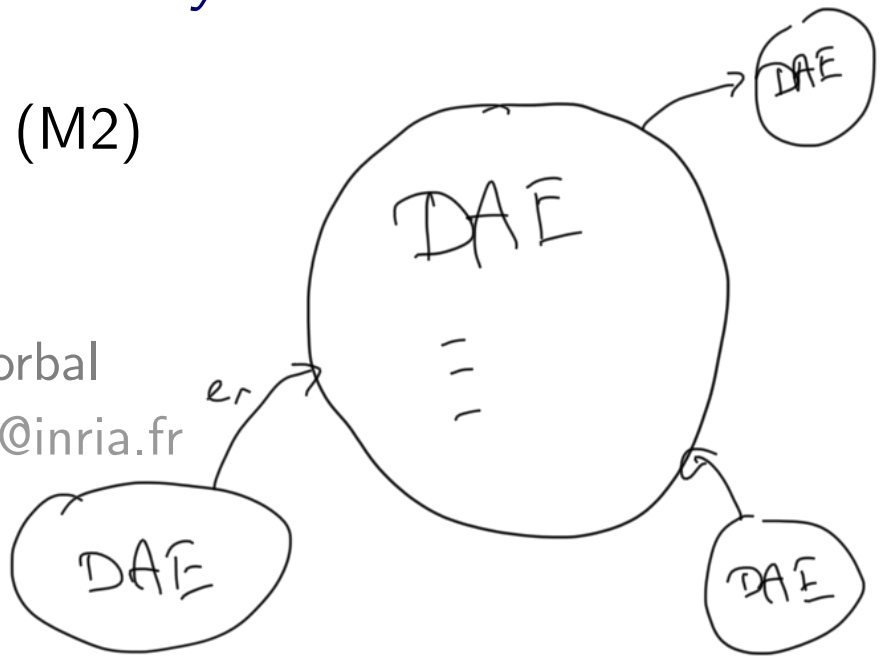


Outline

$\mathbb{C}$ $\mathbb{Q}$ $\mathbb{R}$ $\mathbb{Z}$

$2x^2 + x - 3 = 0$

$x^2 + 1 = 0$

- k denotes an $\boxed{\text{algebraically closed field}}$.
- $k[X] = k[X_1, \ldots, X_n]$: the ring of polynomials over k $\sum_i a_i \left(X_1^{\alpha_1} X_2^{\alpha_2} \cdots X_n^{\alpha_n} \right)_i$
- $I = (f_1, \ldots, f_s) \subset k[X]$ **ideal** generated by the f_i

$$I := \left\{ f \in k[X] \mid \exists \lambda_1, \ldots, \lambda_s \in k[X],\ f = \boxed{\sum_{i=1}^{s} \lambda_i f_i} \right\}$$

- The **Radical** of I, denoted $\sqrt{I}$, is an ideal of $k[X]$ defined as follows.

$$\sqrt{I} := \{ f \in k[X] \mid \exists m \in \mathbb{N}.\ f^m \in I \}$$

$I = (f_1, \ldots f_s)$ $s < +\infty$

Hilbert Basis Theorem

Every ideal of $k[X]$ is finitely generated.

$I = \langle x^2+y^2-1,\ x+y \rangle$

$\mathcal{V}(I) = \{(x,y) \in \mathbb{R}^2 \mid x^2+y^2-1=0 \wedge x+y=0\}$

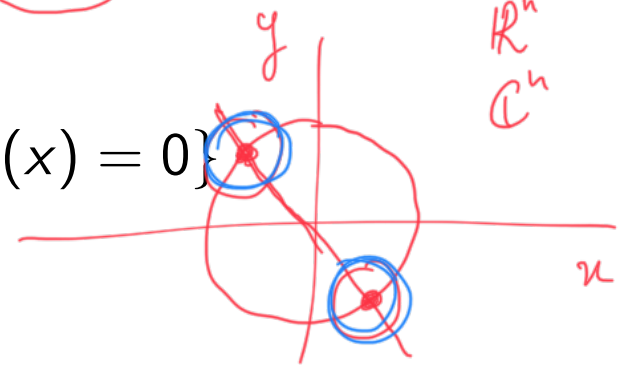
Definition: **Variety**

Let $I = (f_1, \ldots, f_s)$ be an ideal of $k[X]$. A *variety* $\mathcal{V}(I)$ is a $\boxed{\text{subset of } k^n}$ defined as follows.

$\mathbb{R}^n$

$\mathbb{C}^n$

$$\mathcal{V}(I) := \{x \in k^n \mid f_1(x) = 0, \ldots, f_s(x) = 0\}$$



$\mathcal{I}(\mathcal{V}(I)) = I \iff I = \sqrt{I} \neq \sqrt[\mathbb{R}]{I}$

Definition: **Vanishing ideal**

Let S be a subset of k^n. A *Vanishing ideal* $\mathcal{I}(S)$ is an ideal of $k[X]$ defined as follows.

$$\mathcal{I}(S) := \{f \in k[X] \mid \forall x \in S, f(x) = 0\}$$

$P_1 P_2 = 0$

$P_1 = 0 \vee P_2 = 0$

$P_1 = 0$ $\quad (x^2+y^2-1) = 0$

$P_2 = 0$ $\quad (x+y) = 0$

$2x^2-1=0 \quad y=-x$

$I = \langle P_1, P_2 \rangle$

$P_1(x) = P_2(x) = 0$

$\forall f \in I \quad f^m(x) = 0$

- A monomial is an element of $k[X]$ of the form $X_1^{\alpha_1} \cdots X_n^{\alpha_n}$.
- Notation: $\boxed{X^\alpha}$, $\alpha := (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$.

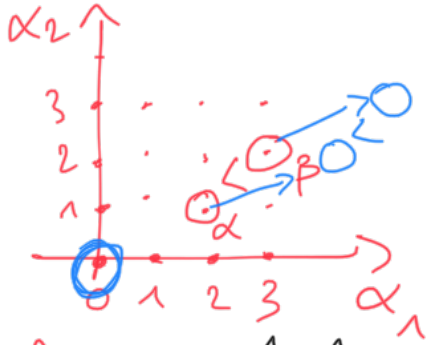
$X^3 - 2X^2 + 1 = 0$

$-2X^2 + 1 + X^3 = 0$

Definition: **Monomial Order**

Total order on the set of monomials satisfying:

1. For all $\gamma \in \mathbb{N}^n$, $X^\alpha < X^\beta$ implies $X^\alpha X^\gamma < X^\beta X^\gamma$,
2. For all $\alpha \in \mathbb{N}^n$, $X^\alpha > 1$, so 1 is the minimal element.



$X = \{X_1, X_2\}$ $\quad X_1^{\alpha_1} X_2^{\alpha_2}$

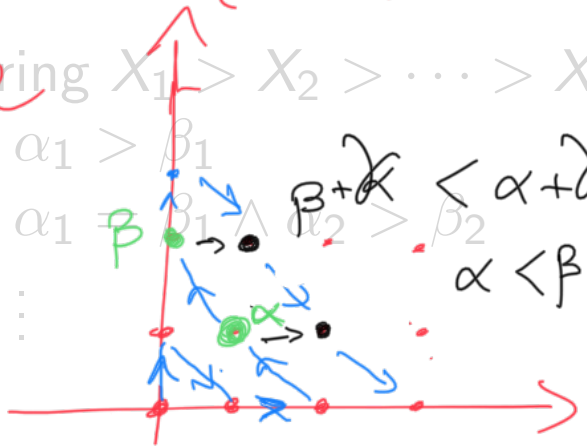
Example: Lex Ordering

Extends the lexicographic ordering $X_1 > X_2 > \cdots > X_n$ as follows:

$X^\alpha > X^\beta$ if and only if $\begin{cases} \alpha_1 > \beta_1 \\ \text{or} \quad \alpha_1 = \beta_1 \wedge \alpha_2 > \beta_2 \\ \text{or} \quad \vdots \end{cases}$

$\alpha_1 = 1$, $\alpha_2 = 1$ $\quad \beta_1 = 0$, $\beta_2 = 2$

$\gamma = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad \alpha < \beta$



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$\alpha_i, \beta_i \in \mathbb{N}$

$X_1^2 X_2^1 > X_1^1 X_2^4$

Leading Terms, Monomials and Coefficients

For a fixed monomial order ($>$), one can write any polynomial $f \in k[X]$ as follows:

$$f = cX^{\alpha} + \sum_{i=1}^{s} a_i X^{\beta_i}$$

such that $c \neq 0$ and X^{α} is bigger than any other monomial with a nonzero coefficient (formally, for all $i = 1, \ldots, s$: $a_i \neq 0$ implies $X^{\alpha} > X^{\beta_i}$).

Definitions

- $\mathrm{LT}(f) = cX^{\alpha}$: **Leading Term** of f — cX^{α}
- $\mathrm{LM}(f) = X^{\alpha}$: **Leading Monomial** of f — X^{α}
- $\mathrm{LC}(f) = c$: **Leading Coefficient** of f — c

depend on $>$

Theorem

Given non zero polynomials $f, f_1, \ldots, f_s \in k[X]$ and a monomial ordering $(>)$, there exists $r, q_1, \ldots, q_s \in k[X]$ such that

- $f = (\sum_1^s q_i f_i) + r$
- No term in r is divisible by any $\mathrm{LT}(f_i)$
- $\mathrm{LT}(f) = \max_{>}\{\mathrm{LT}(q_i)\mathrm{LT}(f_i) \mid q_i \neq 0\}$

$f \mid g =$

$$\begin{array}{l|l} f \quad X^3 - 2X^2 + 1 & X - 1 \\ \hline -X^3 - X^2 & X^2 - X - 1 \\ \hline -X^2 + 1 & \\ -X^2 + X & \\ \hline -X + 1 & \\ -X + 1 & \\ \hline 0 & \end{array}$$

$X^3 - 2X^2 + 1 = (X^2 - X - 1)(X - 1)$

Given I an ideal of $k[X]$, the **leading terms ideal** of I is defined by

$$\mathrm{LT}(I) = (\{\mathrm{LT}(f) \mid f \in I\})$$

That is, the ideal generated by all the LT of all the polynomials in I. By definition the following inclusion of ideals holds

$$(\mathrm{LT}(f_1), \ldots, \mathrm{LT}(f_s)) \subset \mathrm{LT}(I)$$

$f = q + r$

$\deg r < \deg q$

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$\mathrm{LT}(I) = (\mathrm{LT}(f_1), \mathrm{LT}(f_2), \mathrm{LT}(f_s))$

$$(\mathrm{LT}(f_1), \ldots, \mathrm{LT}(f_s)) \subset \mathrm{LT}(I)$$

$=$ Grobner Basis ideal

$\neq$

- $\mathrm{LT}(I)$ is "bigger" than $(\mathrm{LT}(f_1), \ldots, \mathrm{LT}(f_s))$
- $X > Y$: $f_1 = X^2 + X$; $f_2 = X^2 + Y$
- $(\mathrm{LT}(f_1), \mathrm{LT}(f_2)) = (X^2, X^2) = (X^2)$
- $f_1 - f_2 = X - Y \in I := (f_1, f_2)$
- $\mathrm{LT}(\underbrace{X - Y}_{f_1 - f_2}) = X$ is in $(\mathrm{LT}(I))$. Clearly $X \notin (X^2)$

(f_1, f_2) is not a Gröbner Basis

$\mathrm{LT}(I) \not\subseteq (\mathrm{LT}(f_1), \mathrm{LT}(f_2))$

Definition: **Gröbner Bases**

Fix the monomial order $(>)$. Let I be an ideal of $k[X]$. G is a *Gröbner Basis* for I with respect to $(>)$ if and only if

$$(\mathrm{LT}(g) \mid g \in G) = (\mathrm{LT}(I)) \ .$$

In words: The leading terms ideal of G is generated by the leading terms of the generators of G.

$I = (X^2+X,\ X^2+Y)$

$= (\underbrace{Y+Y^2}_{g_1},\ \underbrace{X-Y}_{g_2})$

$LT(I) = (LT(g_1), LT(g_2))$

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In words: The leading terms ideal of G is generated by the leading terms of the generators of G.

$G = (g_1, \ldots, g_m)$ is **reduced** if for every $i = 1, \ldots, m$, $\mathrm{LC}(g_i) = 1$ and $\mathrm{LT}(g_i)$ does not divide any term of any g_j, $j \neq i$.

$X + Y^2 + (-Y)Y = X \in G$

Example

- $G = (X + Y^2, Y)$ is a non reduced Gröbner basis.
- (X, Y) is a reduced Gröbner basis.

Theorem

Every ideal has a unique reduced Gröbner Basis representation (up to the fixed monomial order).

k is algebraically closed.

Theorem: **Hilbert's Nullstellensatz**

- Strong: $\mathcal{I}(\mathcal{V}(I)) = \overset{\mathbb{R}}{\sqrt{I}}$
- Weak: $\mathcal{V}(I) = \emptyset$ if and only if $1 \in I$

Alg $\quad$ Geo

$I \longrightarrow S = \mathcal{V}(I) \subseteq k^n$

$\mathcal{I}(S) \longleftarrow$

$\mathcal{I}(\mathcal{V}(I)) = I \iff I = \sqrt{I}$

Corollaries: Solvability and Gröbner Bases

I is an ideal of $k[X]$. The following statements are equivalent:

- $I \neq k[X]$
- $1 \notin I$
- $\mathcal{V}(I) \neq \emptyset$
- I has a Gröbner Basis having nonconstant polynomials
- The reduced Gröbner Basis of I is different from $\{1\}$

$\boxed{1 \in (p_1, \dots, p_n)}$?!

$\begin{cases} p_1 = 0 \\ p_2 = 0 \\ \vdots \\ p_m = 0 \end{cases}$ $\quad X_1 \dots X_n$ $\quad \emptyset$

k is algebraically closed.

$$\begin{cases} p_1 = 0 \\ \vdots \\ p_n = 0 \end{cases} \qquad p_i \in k[X]$$

Theorem: **Hilbert's Nullstellensatz**

- Strong: $\mathcal{I}(\mathcal{V}(I)) = \sqrt{I}$
- Weak: $\mathcal{V}(I) = \emptyset$ if and only if $1 \in I$

$p_i \in k\{X\}$

$k[X_1, X_1', \ldots, X_2, X_2', \ldots]$

decidable

Corollaries: Solvability and Gröbner Bases

I is an ideal of $k[X]$. The following statements are equivalent:

- $I \neq k[X]$ (I proper)
- $1 \notin I$
- $\mathcal{V}(I) \neq \emptyset$
- I has a Gröbner Basis having nonconstant polynomials
- The reduced Gröbner Basis of I is different from $\{1\}$

$\boxed{1 \in (f_1 \cdots f_s)}$

$(f_1 \cdots f_s) \longrightarrow G = (g_1 \cdots g_m) = (f_1 \cdots f_s)$

$\exists i$ tq $1 = g_i$

$G = (1)$

The Finiteness Theorem

Let I be an ideal of $k[X]$. The following statements are equivalent.

- $\mathcal{V}(I)$ is finite (finite set of points in k^n)
- $k[X]/I$ is a finite-dimensional vector space over k
- Only a finite number of monomials are not in $\mathrm{LT}(I)$

In addition $\dim_k k[X]/I$ gives exactly the number of solutions (counted with their multiplicities) of the system defined by I.

Example

- $I = (X^2 + 1)$
- $k[X]/I$ is isomorphic, as a vector space, to k^2: elements of $k[X]/I$ are of the form $a + bX$ where $a, b \in k$
- When k is algebraically closed, $X^2 + 1$ has two roots since it is of degree 2

Computational Aspects

- Gröbner Bases are akin to Standard Bases by Hironaka (1964).
- The name Gröbner was introduced by Buchberger in his thesis (1965) where he gives a procedure to compute such bases.
- The coefficients of the intermediate (S) polynomials computed while generating a basis could be very large, likewise their polynomial degrees can be as large as n^2 if one starts with polynomials of degree n.
- The fastest known implementation if Fougere's F4 and F5 packages (available in Maple), they are however limited in the size of X and the total degrees of the f_i.
- Almost all computer algebra systems have an implementation the Buchberger algorithm (possibly with different optimizations and heuristics).

Practical Applications

This classical correspondence between Algebra and Geometry, together with the existence of procedures to compute Gröbner Bases in many practically relevant cases have many applications:

- Solvability of a system of polynomial equations
- Finite solutions test
- Ideal membership test
- Polynomial reduction (division)
- Elimination theory (next section)

Outline

- $k[X, Y] = k[X_1, \ldots, X_s, Y_{s+1}, \ldots, Y_n]$
- A monomial in $k[X, Y]$ has the form $X^\alpha Y^\gamma$
- Let I be an ideal of $k[X, Y]$

Elimination Order

A monomial ordering eliminates X if $X^\alpha > X^\beta$ implies $X^\alpha Y^\gamma > X^\beta Y^\delta$ for every Y^γ and Y^δ. (For instance, the lex monomial ordering is an elimination order.)

Elimination Ideal

$I \cap k[Y]$ is the *elimination ideal* of I that eliminates X.

Elimination Theorem

Let G be a Gröbner basis of I for a monomial order $(>)$ that eliminates X. Then $G \cap k[Y]$ is a Gröbner Basis of the elimination ideal $I \cap k[Y]$ for the monomial order on $k[Y]$ induced by $(>)$.

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Given the coordinates $x_1, \ldots, x_s, y_{s+1}, \ldots, y_n$, let

$$\pi_s : \mathbb{A}^n \to \mathbb{A}^{n-s}$$

denote the projection onto the last $n - s$ coordinates.

Variety of Partial Solutions

$$\pi_s(\mathcal{V}(I)) \subseteq \mathcal{V}(I \cap k[Y]) \ .$$

Moreover, $\mathcal{V}(I \cap k[Y])$ is the Zariski Closure of the projection, that is the *s*mallest variety containing the set $\pi_s(\mathcal{V}(I))$.

Example

$I = (XY - 1, Z - Y)$, with respect to the lex order $(X > Y > Z)$, the generator of I form a Gröbner Basis. Thus $I \cap k[Y, Z] = (Z - Y)$. So $(y, z) = (0, 0)$ is in $\mathcal{V}(I \cap k[Y])$ but not in $\pi_s(\mathcal{V}(I))$.

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Solving by Triangulation

- $f_1, \ldots, f_s \in k[X_1, \ldots, X_n]$
- Use the lex order $X_1 > \cdots > X_n$ which is an elimination order for each X_i
- Compute a Gröbner Basis G with respect to that order
- Then $G \cap k[X_n]$ is a principal ideal, thus one gets a univariate polynomial in X_n to solve
- Now compute $G \cap k[X_{n-1}, X_n]$, knowing the X_n, this gives a univariate polynomial in X_{n-1} alone
- Keep iterating till solving the entire system

Order $X > Y > Z$.

Original System

$$f_1 = X^2 + Y + Z - 1$$
$$f_2 = X + Y^2 + Z - 1$$
$$f_3 = X + Y + Z^2 - 1$$

Gröbner Basis

$$g_1 = X + Y + Z^2 - 1$$
$$g_2 = Y^2 - Y - Z^2 + Z$$
$$g_3 = 2YZ^2 + Z^4 - Z^2$$
$$g_4 = Z^6 - 4Z^4 + 4Z^3 - Z^2$$

Elimination Ideals

$$I_1 = G \cap k[Z] = (g_4)$$
$$I_2 = G \cap k[Y, Z] = (g_2, g_3, g_4)$$
$$I_3 = G \cap k[X, Y, Z] = (g_1, g_2, g_3, g_4)$$

Outline

Given a polynomial ordinary differential equation $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$.

Initial Value Problem

$$\mathbf{x}(t), t \in U \text{ solution of the Cauchy problem } \left(\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(\mathbf{x}), \mathbf{x}(0) = \mathbf{x}_0 \right)$$

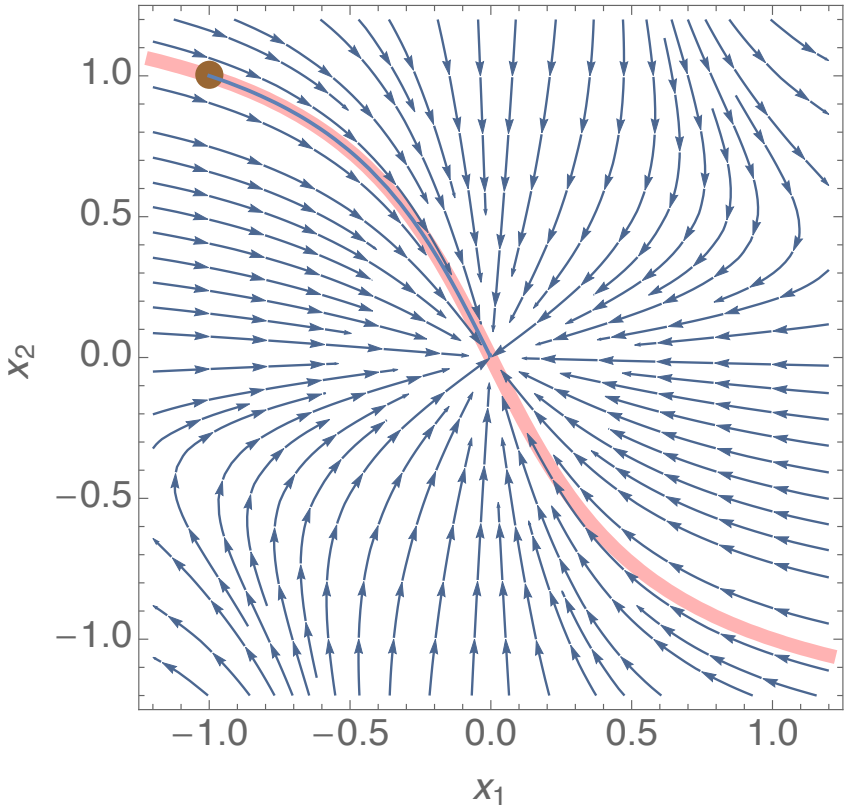
Orbit

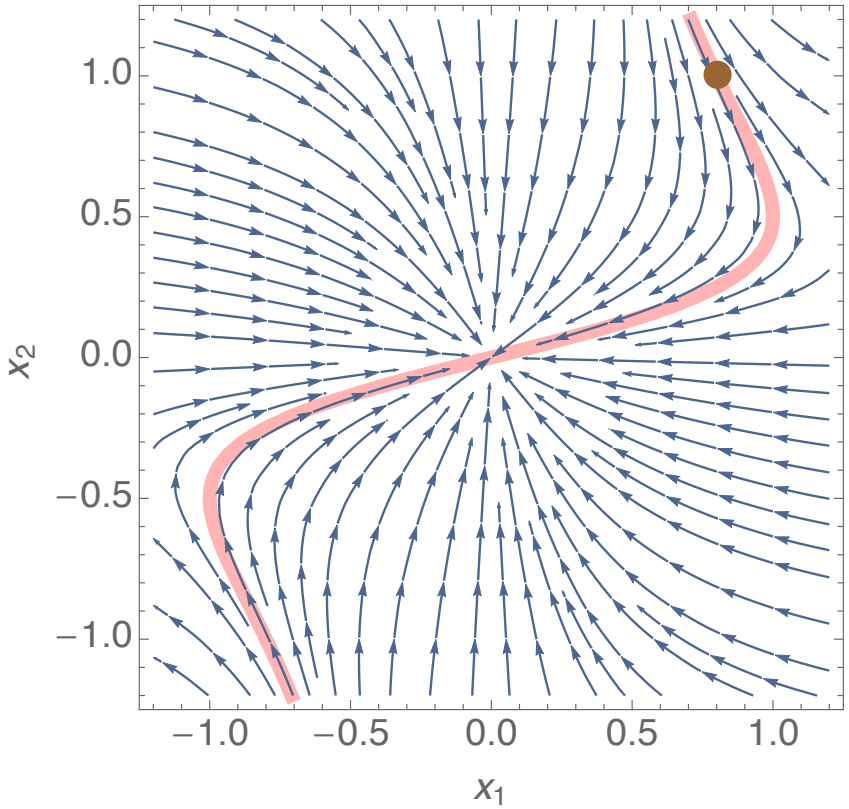
$$\mathcal{O}_{\mathbf{x}_0} := \{\mathbf{x}(t) \mid t \in U\} = \{\mathbf{x} \in \mathbb{R}^n \mid \exists t \in \mathbb{R}, \mathbf{x} = \varphi_t(\mathbf{x}_0)\} \subset \mathbb{R}^n$$

Invariant Region $S \subset \mathbb{R}^n$

$$\forall \mathbf{x}_0 \in S, \forall t \in U, \mathbf{x}(t) \in S$$

$$\mathbf{f} = (-x_1 - 2x_1^2 x_2, -x_2),$$





$$p(x_1, x_2) = (x_2(0) - x_1(0)x_2(0)^2)x_1 - x_1(0)(x_2 - x_1 x_2^2) = 0$$

Gradient

$$\nabla p := \left(\frac{\partial p}{\partial x_1}, \ldots, \frac{\partial p}{\partial x_n} \right)$$

Lie Derivation

$$\mathfrak{D}_{\mathbf{f}}(p) := \frac{dp(\mathbf{x}(t))}{dt} = \nabla p \cdot \mathbf{f} \qquad (\dot{\mathbf{x}} = \mathbf{f})$$

Closure (Zariski Topology)

$$\bar{\mathcal{O}}_{\mathbf{x}_0} := \mathcal{V}(\mathcal{I}(\mathcal{O}_{\mathbf{x}_0}))$$

Proposition1: Dimension and Integrability

$\mathcal{O}_{\mathbf{x}_0} \subset \bar{\mathcal{O}}_{\mathbf{x}_0}$

Proposition2: Stability under Lie derivation

$\mathcal{I}(\mathcal{O}(\mathbf{x}_0))$ is a (proper) *differential ideal* for $\mathfrak{D}_{\mathbf{f}}$, that is, $\mathfrak{D}_{\mathbf{f}}(p) \in \mathcal{I}(\mathcal{O}(\mathbf{x}_0))$ for all $p \in \mathcal{I}(\mathcal{O}(\mathbf{x}_0))$

Example: Zariski Dense Varieties

$\dot{x} = x \rightsquigarrow \mathcal{O}(\mathbf{x}_0) = [0, \infty[\rightsquigarrow I = \langle 0 \rangle \rightsquigarrow \bar{\mathcal{O}}_{\mathbf{x}_0} = \mathcal{V}(\mathcal{I}(\mathcal{O}(\mathbf{x}_0))) = \mathbb{R}$

Definition: Differential Order

The *differential order* of $p \in \mathbb{R}[\mathbf{x}]$ denotes the length of the chain of ideals

$$\langle p \rangle \subset \langle p, \mathfrak{D}_{\mathbf{f}}(p) \rangle \subset \cdots \subset \left\langle p, \mathfrak{D}_{\mathbf{f}}(p), \ldots, \mathfrak{D}_{\mathbf{f}}^{(N_p-1)}(p) \right\rangle =: \partial p.$$

$N_p = \mathrm{card}(\partial p)$ ($< \infty$ since $\mathbb{R}$ is Notherian).

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Theorem

The polynomial p is in $I(\mathcal{O}(\mathbf{x}_0))$ if and only if $\mathfrak{D}_{\mathbf{f}}^{(i)}(p)(\mathbf{x}_0) = 0$, for all $i = 0, \ldots, N_p - 1$.

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$N_p = \mathrm{card}(\partial p)$ ($< \infty$ since $\mathbb{R}$ is Notherian).

Theorem

The polynomial p is in $I(\mathcal{O}(\mathbf{x}_0))$ if and only if $\mathfrak{D}_{\mathbf{f}}^{(i)}(p)(\mathbf{x}_0) = 0$, for all $i = 0, \ldots, N_p - 1$.

Proof Sketch

$\leftarrow$: Since $\mathbf{x}(t)$ is analytic, $p(\mathbf{x}(t))$ is also analytic. Thus for a nonempty open neighborhood $V \subset U$ around 0, the null Taylor series of $p(t)$ is equal to p, thus $p = 0$ for all U.

Corollary1

An algebraic set $\mathcal{V}(\langle p \rangle)$ is invariant for $\mathbf{f}$ if and only if

$$\partial p \subset \mathcal{I}(\mathcal{V}(\langle p \rangle)) \ .$$

Corollary2

For each $\mathbf{x}_0$, there exists a unique (up to multiplication by a constant and rearrangement of its factors) $p \in \mathbb{R}[\mathbf{x}]$ such that

$$\partial p = \mathcal{I}(\mathcal{O}(\mathbf{x}_0)) \ .$$

Decidability: $\partial p \subset \mathcal{I}(\mathcal{V}(\langle p \rangle))$

Given $\mathbf{f}$ and $p \in \mathbb{R}[\mathbf{x}]$, the invariance of $\mathcal{V}(\langle p \rangle)$ is decidable.

$$\frac{\begin{array}{c} \mathfrak{D}_{\mathbf{f}}^{(N_p)}(p) = \sum_{i=0}^{N_p-1} \lambda_i \mathfrak{D}_{\mathbf{f}}^{(i)}(p) \ (\lambda_i \in \mathbb{R}[\mathbf{x}]) \ \wedge \ p = 0 \rightarrow \bigwedge_{i=1}^{N_p-1} \mathfrak{D}_{\mathbf{f}}^{(i)}(p) = 0 \\ \cdots \\ \mathfrak{D}_{\mathbf{f}}^{(3)}(p) = \sum_{i=0}^{2} \lambda_i \mathfrak{D}_{\mathbf{f}}^{(i)}(p) \ (\lambda_i \in \mathbb{R}[\mathbf{x}]) \ \wedge \ p = 0 \rightarrow \bigwedge_{i=1}^{2} \mathfrak{D}_{\mathbf{f}}^{(i)}(p) = 0 \\ \mathfrak{D}_{\mathbf{f}}^{(2)}(p) = \lambda_0 p + \lambda_1 \mathfrak{D}_{\mathbf{f}}(p) \ (\lambda_i \in \mathbb{R}[\mathbf{x}]) \ \wedge \ p = 0 \rightarrow \mathfrak{D}_{\mathbf{f}}(p) = 0 \\ \mathfrak{D}_{\mathbf{f}}(p) = \lambda p \ (\lambda \in \mathbb{R}[\mathbf{x}]) \end{array}}{V(\langle p \rangle) \text{ is an invariant algebraic set}}$$

- Existence of λ_i: Gröbner Basis
- $p = 0 \rightarrow \mathfrak{D}_{\mathbf{f}}^{(i)}(p) = 0$: (Universal) Quantifier Elimination

Decidability: $\partial p \subset \mathcal{I}(\mathcal{V}(\langle p \rangle))$

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