Rational parametrizations in differential algebra

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Overview

1. Algebraic Geometry
   - Rational parametrizations
   - Rational curves
2. Differential algebra
   - Implicitization
   - Algebro-geometric approach
   - Realizations
   - Results on realizations
3. Systems involving parameters
   - SEIR model
   - Identifiable functions
   - Reparametrization
   - Tsen's theorem
   - Witness variety

Motivation

The solutions $y(t)$ of the ODE-system

$$\Sigma = \begin{cases} x_1'(t) = x_2(t)^2, \\ x_2'(t) = x_1(t)\,u(t), \\ y(t) = x_2(t) \end{cases}$$

and that of $F = u(t)y''(t) - u(t)^2\,y(t)^2 - u'(t)\,y'(t) = 0$ are the same.

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Question

1. How to transform Σ into F and conversely, F into Σ?
2. Is this always possible? Under which assumptions for Σ (polynomiality, real coefficients etc.)?

Rational parametrizations $\mathcal{S} \to P$

Let $\mathcal{S} \subset K[y_0, \ldots, y_n]$ be a finite set of polynomials (over a field K with characteristic zero). We call

$$\mathbb{V}(\mathcal{S}) := \{P \in \overline{K}^{n+1} \mid \forall F \in \mathcal{S} : F(P) = 0\}$$

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the corresponding algebraic set. A tuple $P \in \overline{K}(x_1, \ldots, x_m)^{n+1} \setminus \overline{K}^{n+1}$ with $F(P) = 0$ for every $F \in \mathcal{S}$ is called a (rational) parametrization of $\mathbb{V}(F)$ iff the Jacobian $\mathcal{J}(P)$ of P w.r.t. $\mathbf{x} = (x_1, \ldots, x_m)$ has maximal rank.

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1. $P = (x^3, x^2)$ is a parametrization of the cusp $\mathbb{V}(y_0^2 - y_1^3)$.
2. The unit sphere $\mathbb{V}(y_0^2 + y_1^2 + y_2^2 - 1)$ has the parametrization

$$P = \left(\frac{2x_1}{x_1^2+x_2^2+1}, \frac{2x_2}{x_1^2+x_2^2+1}, \frac{x_1^2+x_2^2-1}{x_1^2+x_2^2+1} \right).$$

Rational curves

Characterization theorem

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2. Rational parametrizations of curves and surfaces can always be chosen birationally. As a consequence, all such rational parametrizations P, Q can be related by reparametrizations $P(x) = Q(s(x))$ with $s \in \overline{K}(x_1, \ldots, x_m)^m$ and invertible $\mathcal{J}(s)$, $m \in \{1, 2\}$.

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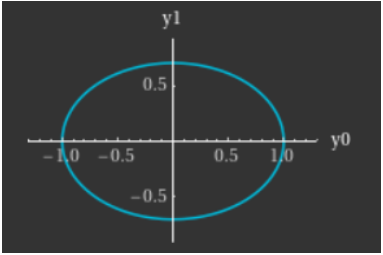
3. Rational parametrizations of curves $P \in L(x)^2$ can be found over optimal fields, i.e., with coefficients in a minimal field extension $K \subseteq L \subset \overline{K}$. In fact, $[L : K] \leq 2$.

Example 1

Let $F = y_0^2 + 2y_1^2 - 1$. Then $\mathbb{V}(F)$ admits the birational parametrization

$$P = \left(\frac{1-x^2}{1+x^2}, \frac{\sqrt{2}x}{1+x^2} \right)$$

over the optimal field of parametrization $\mathbb{Q}(\sqrt{2})$.



Implicitization $\mathcal{S} \leftarrow P$

Given $P = \left(\frac{p_0}{q}, \ldots, \frac{p_n}{q}\right) \in \overline{K}(x_1, \ldots, x_m)^{n+1}$, we can always find a system of algebraic polynomials $\mathcal{S}$ such that P is a rational parametrizations of $\mathbb{V}(\mathcal{S})$:

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$$\langle y_0\, q - p_0, \ldots, y_n\, q - p_n, q\, z - 1\rangle \cap \overline{K}[y_0, \ldots, y_n]$$

and the finite number of generators can be chosen as $\mathcal{S}$.

Example 1

From $P = \left(\frac{1-x^2}{1+x^2}, \frac{\sqrt{2}x}{1+x^2}\right)$ we get the ideal generated by

$$(1+x^2)y_0 - (1-x^2),\ (1+x^2)y_1 - \sqrt{2}x,\ (1+x^2)z - 1.$$

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Its Groebner basis (w.r.t. $z > x > y_0 > y_1$) is

$$\mathcal{G} = \{y_0^2 + 2y_1^2 - 1,\ -\sqrt{2}xy_1 - y_0 + 1,\ -xy_0 - x + \sqrt{2}y_1,\ y_0 - 2z + 1\}$$

such that $F = y_0^2 + 2y_1^2 - 1$ is the only element in $\mathcal{G} \cap \overline{\mathbb{Q}}[y_0, y_1]$.

Main questions

Do we have counterparts of the previous concepts in differential algebra?

1. Parametrizations / Implicitization
2. Birationality
3. Optimal coefficient fields and computation with parameters
4. Is it algorithmic?

Differential algebra

Let us consider ODE models of the form

$$\Sigma = \begin{cases} \mathbf{x}' = \mathbf{f}(\mathbf{u}, \mathbf{x}), \\ \mathbf{y} = \mathbf{g}(\mathbf{u}, \mathbf{x}) \end{cases} \tag{1}$$

with the components of $\mathbf{f}, \mathbf{g}$ in $\overline{K}(\mathbf{u}, \mathbf{x})$.

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with the components of $\mathbf{f}, \mathbf{g}$ in $\overline{K}(\mathbf{u}, \mathbf{x})$. We define the (prime) differential ideal of Σ as

$$I_\Sigma = \left[q\,\mathbf{x}' - q\,\mathbf{f}, q\,\mathbf{y} - q\,\mathbf{g}\right] : q^\infty \subset \overline{K}[\mathbf{x}^{(\infty)}, \mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}],$$

where q is the common denominator of $\mathbf{f}$ and $\mathbf{g}$, and

$$I : a^\infty = \left\{ r \in R \mid \exists \ell \colon a^\ell r \in I \right\}.$$

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Important facts

1. The result is a finite number of (reduced) triangular sets with one essential component $\mathcal{G}$.
2. The general solution of $\mathcal{G}$ and that of I_Σ coincides.
3. Using the ordering $y_i', u_i' < x_i'$, the intersection ideal $I_\Sigma \cap \overline{K}[\mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}]$ is generated by $\mathcal{G} \cap \overline{K}[\mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}]$.

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Implicitization

$\mathcal{S} = \mathcal{G} \cap \overline{K}[\mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}]$ are called the IO-equations corresponding to Σ.

Example 2

Consider

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Then $y' = -3x^2 \cdot \frac{x^2-1}{3x^2} = -x^2 + 1$ and

$$\mathrm{Res}_x(y - x^3, y' + x^2 - 1) = y'^3 + y^2 - 3y'^2 + 3y' - 1$$

is the IO-equation of Σ.

Realization problem

Given $\mathcal{S} \subset K[\mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}]$, one can ask the question whether there is a system Σ as in (1) such that $\mathcal{S}$ are the IO-equations of Σ. In the affirmative case, Σ is called a realization of $\mathcal{S}$.

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Finding a realization is similar to the problem of finding a rational parametrizations of a given set algebraic set.

Algebro-geometric approach

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Parametrization

If $\mathcal{S}$ has a realization $\Sigma = \begin{cases} \mathbf{x}' = \mathbf{f}(u, \mathbf{x}), \\ y = g(u, \mathbf{x}), \end{cases}$ then

$$P = (g, \mathcal{L}_{\mathbf{f}}(g), \ldots, \mathcal{L}_{\mathbf{f}}^n(g)), \tag{2}$$

where $D_u(h) = \sum_{j \geq 0} u^{(j+1)} \cdot \partial_{u^{(j)}} h$ and $\mathcal{L}_{\mathbf{f}}(h) = \sum_{i=1}^n f_i \, \partial_{x_i} h + D_u(h)$ is the Lie-derivative of h w.r.t. $\mathbf{f}$, defines a rational parametrization of $\mathbb{V}(\mathcal{S})$.

Realization $\mathcal{S} \to \Sigma$

Necessary condition

A necessary condition for the existence of a realization of $\mathcal{S}$ is that $\mathbb{V}(\mathcal{S})$ admits a rational parametrization.

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Assume that $\mathbb{V}(\mathcal{S})$ with $\mathcal{S} \subset \overline{K}[y, \ldots, y^{(n)}, u^{(\infty)}]$ admits a rational parametrization $P = (P_0, \ldots, P_n) \in \overline{K(u^{(\infty)})}(\mathbf{x})^{n+1}$. Then we seek for a reparametrization $P(\mathbf{x}(\mathbf{t}))$ that additionally fulfills the differential relations

$$\mathcal{J}(P_0, \ldots, P_{n-1}) \cdot \mathbf{x}' = (P_1 - D_u(P_0), \ldots, P_n - D_u(P_{n-1})). \qquad (3)$$

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Correspondence theorem

$\mathcal{S}$ has a realization iff $\mathbb{V}(\mathcal{S})$ has a rational parametrization such that (3) is independent of derivatives of u.

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2. For a realization $\Sigma = \{\mathbf{x}' = \mathbf{f}(u, \mathbf{x}), y = g(u, \mathbf{x})$ and some $\mathbf{s} \in \overline{K}(\mathbf{x})^m$ with invertible Jacobi-matrix,

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The case when $P = (g, \mathcal{L}_{\mathbf{f}}(g), \ldots)$ is a birational parametrizations corresponds to the case when $\mathbf{x}$ is "globally observable" (important property in control theory).

Results on realizations in the curve case

Observability $\leftrightarrow$ Birationality

Let $F \in \overline{K}[u, u', y, y']$ be realizable. Then there is an observable realization of F.

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Real realizations

Let $F \in \mathbb{R}[u, u', y, y']$ be realizable with $\{x' = f(x, u), y = g(x, u)$ (over $\mathbb{C}$). Then there is a real realization of F iff there is a reparametrization $s \in \mathbb{C}(x)$ of $P = (f, \mathcal{L}_f(g))$ with $P(s) \in \mathbb{R}(u, u')(x)^2$.

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Polynomial realizations

Let $F \in \overline{K}[u, u', y, y']$ be realizable with $\{x' = f(u, x), y = g(u, x)$. Then there is a polynomial realization of F iff

- u does not effectively occur in any denominator of f or g; and
- the common denominator q of the coefficients of g, seen as polynomial in u, is of the form $a \cdot (x - b)^m$ for some $a, b \in \overline{K}$ with m greater or equal to the degrees of the numerators of f, g; and
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All these results are algorithmic and can be extended to the case of higher-dimensional corresponding algebraic sets $\mathbb{V}(\mathcal{S})$ as sufficient conditions.

Example 3

Let us consider the non-observable realization

$$\{x' = \tfrac{1-x}{2u},\ y = \tfrac{(1-x)^4}{u^2+(1-x)^6}$$

corresponding to the rational parametrization

$$P = \left(\tfrac{(1-x)^4}{u^2+(1-x)^6},\ \tfrac{-(4u^2(1-x)^3+2(1-x)^9+(u^2+(1-x)^6)uu')(1-x)^4}{(u^2+(1-x)^6)^3} \right).$$

We can choose the (algebraic) reparametrization $s := 1 + \sqrt{1-x}$ which leads to the realization

$$\{x' = \tfrac{1-x}{u},\ y = \tfrac{(1-x)^2}{u^2+(1-x)^3}.$$

Systems involving parameters

In a lot of applications there occur parameters that will be estimated from time-series data such as in the following commonly used SEIR epidemic model

$$\Sigma = \begin{cases} S'(t) = -\frac{bS(t)I(t)}{n}, \\ E'(t) = \frac{bS(t)I(t)}{n} - \nu E(t), \\ I'(t) = \nu E(t) - aI(t), \\ y_1(t) = I(t), \\ y_2(t) = n \end{cases} \tag{5}$$

with the coefficient field $K = \mathbb{C}(a, b, \nu, n)$.

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Question

1. Is (5) a good model for estimating parameters?
2. If not, do we find an equivalent, better, model?

Identifiable parameters (informal)

Consider the ODE system Σ (over $\mathbb{C}(\mathbf{c})$) as in (1). Assume that $\mathbf{x}(0), \mathbf{x}'(0), \mathbf{u}(0) \to \mathbf{y}(0)$ (maybe even $\mathbf{x}''(0), \ldots, \mathbf{u}'(0), \ldots, \mathbf{y}'(0), \ldots$) are known.

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- If c_i is uniquely given from the resulting equations, then c_i is called a (globally) identifiable parameter.
- If c_i can have infinitely many values, it is called non-identifiable.
- Otherwise, c_i is called locally identifiable and can obtain finitely many values given by a polynomial function.

Identifiable functions

The smallest field $\mathbb{C} \subset \mathbb{K} \subset \mathbb{C}(\mathbf{c})$ such that $I_\Sigma \cap \mathbb{C}(\mathbf{c})[\mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}]$ is generated as an ideal by $I_\Sigma \cap \mathbb{K}[\mathbf{y}^{(\infty)}, \mathbf{u}^{(\infty)}]$ is called the field of identifiable functions of Σ. $h \in \mathbb{C}(\mathbf{c})$ is called identifiable if $h \in \mathbb{K}$ and locally identifiable if $h \in \overline{\mathbb{K}}$.

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Rule of thumb

The identifiable functions are the rational expressions generated by the coefficients of the IO-equations.

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The identifiable functions are the rational expressions generated by the coefficients of the IO-equations.

The identifiable parameters are that which are identifiable functions themselves.

SEIR model

The corresponding IO-equations are

$$ny_1y_1''' + (-ny_1' + y_1(by_1 + n(a+\nu)))y_1'' - n(a+\nu)y_1'^2 + by_1^2(a+\nu)y_1' + ab\nu y_1^3,$$
$$y_2 - n$$

with $\mathbb{K} = \mathbb{C}(n, b, h_1 := a+\nu, h_2 := a\nu)$ as the field of identifiable functions.

Reparametrization

Given an ODE-system Σ with the IO-equations $\mathcal{S}$ and the field of identifiable functions $\mathbb{C}(\mathbf{h}(\mathbf{c}))$, we seek for another realization Σ_0 of $\mathcal{S}$ over $\mathbb{C}(\mathbf{h})$. Thus, $\mathbf{h}$ can then be used as a new set of parameters that are identifiable and Σ_0 replaces Σ as model.

SEIR model

The parametrization corresponding to Σ is

$$P = \Big(I,\ \nu E - aI,\ \tfrac{b\nu SI - an\nu E - n\nu^2 E + a^2 nI}{n},\\ \tfrac{bn\nu^2 SE - b^2\nu SI^2 - 2abn\nu SI - bn\nu^2 SI + a^2 n^2\nu E + an^2\nu^2 E + n^2\nu^3 E - a^3 n^2 I}{n^2},\ n\Big).$$

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a is a root of the polynomial

$$X^2 - (a+\nu)X + a\nu \in= X^2 - h_1 X + h_2\mathbb{K}[X].$$

We substitute

$$S = z_{1,0} + a\, z_{1,1}, E = z_{2,0} + a\, z_{2,1}, I = z_{3,0} + a\, z_{3,1}$$

into P, expand, and set the coefficients of a to zero. The resulting variety (called witness variety) is given by

$$W := \mathbb{V}(z_{1,0}, z_{3,1}, z_{3,0} + z_{2,0}) \cup \mathbb{V}(z_{2,0}, z_{2,1}, z_{3,0}, z_{3,1}).$$

SEIR model

W has the birational parametrization

$$\phi = (0, z_1, -z_3, z_2, z_3, 0).$$

Then the resulting change of variables

$$\begin{cases} S = az_1, \\ E = -z_3 + az_2, \\ I = z_3, \end{cases}$$

leads to the equivalent system (over $\mathbb{C}(n, b, h_1 = a + \nu, h_2 = a\nu)$)

$$\Sigma_0 = \begin{cases} z_1'(t) = -\frac{bz_1(t)I(t)}{n}, \\ z_2'(t) = -\frac{I(t)(n - bz_1(t))}{n}, \\ I'(t) = a\nu z_2(t) - (a + \nu)I(t) = h_2 z_2(t) - h_1 I(t), \\ y_1(t) = I(t), \\ y_2(t) = n. \end{cases}$$

Tsen's theorem

Question

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Tsen's theorem

If $\mathbb{V}(F)$ is rational (over $\overline{K}$), then there is a rational parametrization over K.

Consequently, if there is just one parameter c in a given ODE system Σ, then there is an equivalent realization Σ_0 in an identifiable parameter $h(c)$.

Example 4

Let $F = a_2 y_0^2 + y_1^2 - a_1^2$.

$$P = \left(\frac{a_1}{\sqrt{a_2}} \cdot \frac{1-x^2}{1+x^2}, \frac{2a_1 x}{1+x^2} \right) \in \mathbb{Q}(a_1, \sqrt{a_2})(x)^2$$

is a rational parametrization of $\mathbb{V}(F)$. By elementary reasoning it can be shown that $\mathbb{V}(F)$ cannot be parametrized over $\mathbb{Q}(a_1, a_2)$.

Example 4

$$\Sigma = \begin{cases} x' = -c_2(1+x^2)/2, \\ y = \frac{c_1}{c_2} \cdot \frac{1-x^2}{1+x^2} \end{cases}$$

has for $c_1 = a_1, c_2 = a_2^2$ the corresponding parametrization P. The IO-equation

$$F = c_2^2 y_0^2 + y_1^2 - c_1^2$$

has the identifiable functions $h_1 = c_1^2, h_2 = c_2^2$. Since there is no rational parametrization of $\mathbb{V}(F)$ with coefficients in $\mathbb{C}(h_1, h_2)$, there is no realization equivalent to Σ with just identifiable parameters.

Witness variety

Assume that the ODE system $\Sigma = \{\mathbf{x}' = \mathbf{f}(\mathbf{u}, \mathbf{x}), \mathbf{y} = \mathbf{g}(\mathbf{u}, \mathbf{x})$ with corresponding rational parametrization P has a coefficient field that is algebraic over $\mathbb{C}(\mathbf{h})$ of degree n, where $\mathbf{h}$ are the identifiable functions. Substitute each x_i by

$$x_i = z_{i,0} + z_{i,1}\alpha + \cdots + z_{i,m-1}\alpha^{m-1},$$

where $z_{i,j}$ are new variables and α is the primitive element of the algebraic field extension. Write

$$P = \left(\sum_{j=0}^{m-1} \frac{H_{1,j}(\mathbf{z})}{\delta(\mathbf{z})} \alpha^j, \ldots, \sum_{j=0}^{m-1} \frac{H_{n,j}(\mathbf{z})}{\delta(\mathbf{z})} \alpha^j \right).$$

Define the witness variety W (associated to P and α) as the Zariski closure of $\mathbb{V}(\{H_{i,j}(\mathbf{z})\}_{1 \le i \le n, 1 \le j \le m-1}) \setminus \mathbb{V}(\delta(\mathbf{z}))$.

Identifiable functions

Assume that W has a component of dimension $\dim(\mathbb{V}(\mathcal{S}))$ with a birational parametrization $(s_0, \ldots, s_{n-1}) \in \mathbb{C}(\mathbf{h})(\mathbf{z})^n$. Then we can use the reparametrization

$$s = s_0(\mathbf{z}) + \cdots + s_{n-1}(\mathbf{z}) \cdot \alpha^{n-1}$$

to obtain the realization

$$\Sigma_0 = \begin{cases} \mathbf{z}' = \mathcal{J}(\mathbf{s})^{-1} \cdot \mathbf{f}(\mathbf{u}, \mathbf{s}), \\ \mathbf{y} = \mathbf{g}(\mathbf{u}, \mathbf{s}). \end{cases}$$

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1. In the case of $\dim(\mathbb{V}(\mathcal{S})) = 1$, the existence of such a birational parametrization is equivalent to W having a component that is a hypercircle parametrizable over $\mathbb{C}(\mathbf{c})$.
2. If P and the reparametrization are assumed to be polynomial, then W has to have a component that is a line (over $\mathbb{C}(\mathbf{c})$).

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