Differential elimination for dynamical systems

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MEGA (Effective Methods in Algebraic Geometry)

June 10, 2021

Plan

I (Some) algebra of differential equations
Differential elimination: what and why?

II Elimination for dynamical system in theory & action

III Open problems and conclusions
Including very specific problems

Part I
(Some) Algebra of differential equations

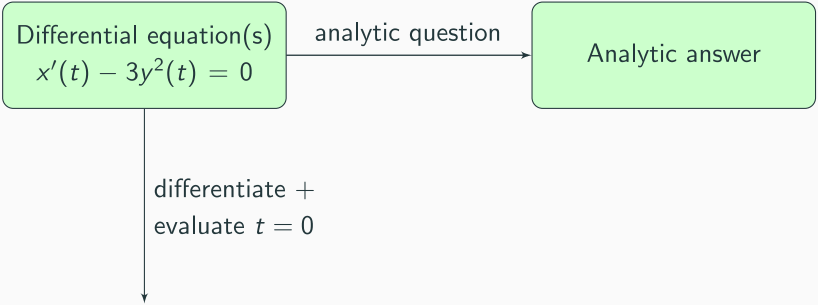
Differential equations meet algebraic geometry

Differential equation(s)
$x'(t) - 3y^2(t) = 0$

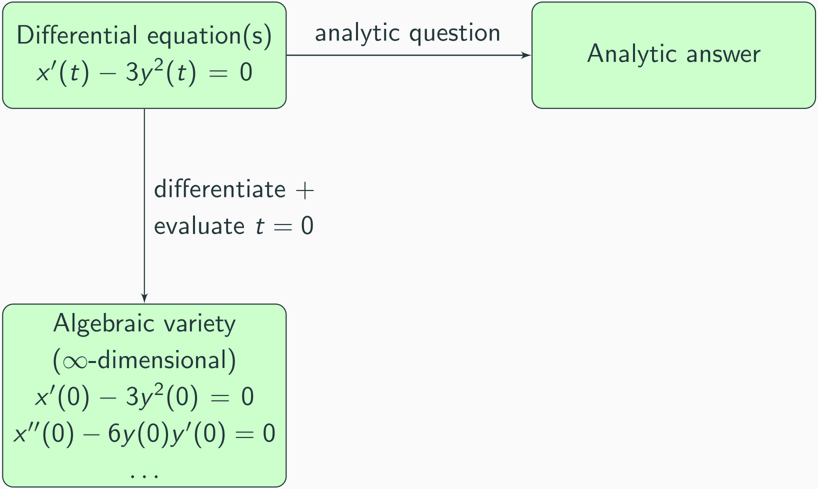
analytic question →

Analytic answer

Differential equations meet algebraic geometry



Differential equations meet algebraic geometry



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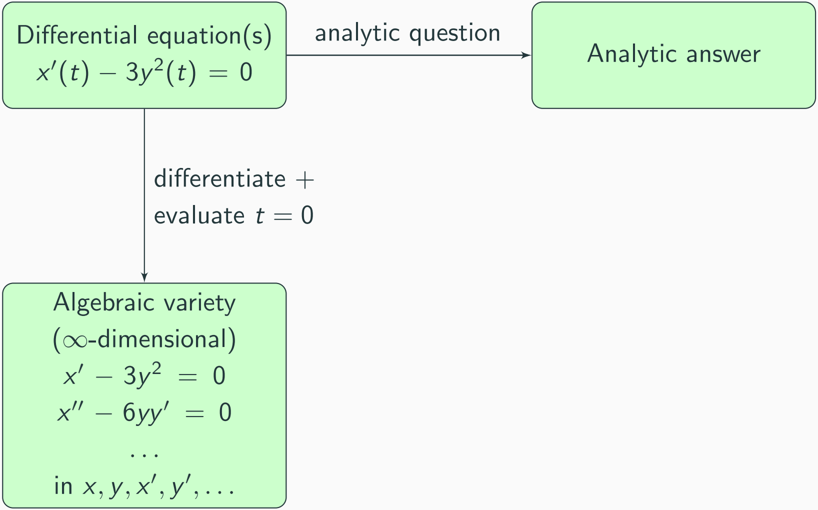

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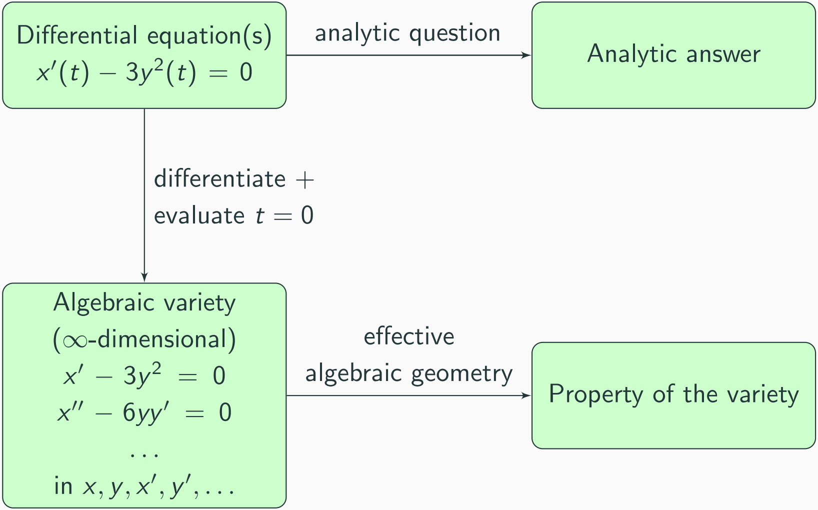

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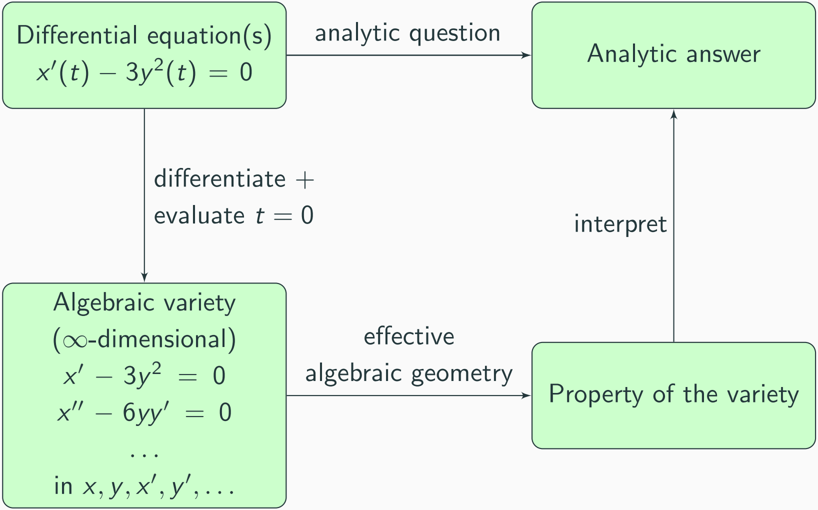

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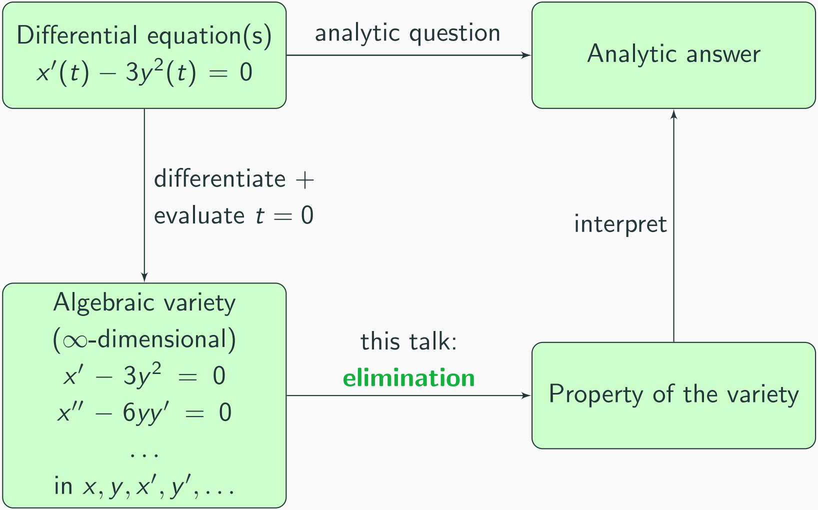


Differential equations meet algebraic geometry

Differential equation(s) $x'(t) - 3y^2(t) = 0$ → (analytic question) → Analytic answer

↓ differentiate + evaluate $t = 0$

Algebraic variety (∞-dimensional)

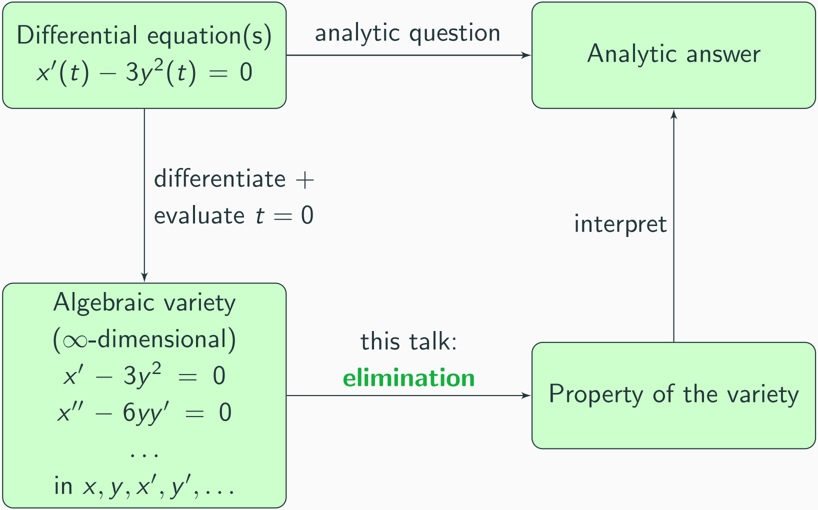
$$x' - 3y^2 = 0$$
$$x'' - 6yy' = 0$$
$$\ldots$$

in $x, y, x', y', \ldots$

→ (this talk: **elimination**) → Property of the variety → (interpret) → Analytic answer

Convergence questions: talk by S. Falkensteiner, J. Cano, R. Sendra on Tuesday

Differential equations meet algebraic geometry



Other connections of algebra and differential equations: talk by D. Agostini, C. Fevola, Y. Mandelshtam, B. Sturmfels on Friday

Differential elimination: general

Fix a ground field k.

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Semantic: Relations satisfied by the **y**-component of any power series solution of $f_1 = f_2 = \ldots = f_s = 0$.

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Toy example

$$\begin{cases} f_1 = x' - y, \\ f_2 = y' - x \end{cases} \implies y^{(2)} - y = (x' - y) + (y' - x)' \in \langle f_1, f_1', \ldots, f_2, f_2', \ldots \rangle$$

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Moreover $\langle f_1, f_1', \ldots, f_2, f_2', \ldots \rangle \cap k[y^{(\infty)}] = \langle y^{(2)} - y, y^{(3)} - y', \ldots \rangle$.

Differential elimination: why?

- Eliminate non-observable variables from models.

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- Eliminate auxiliary (non-important) variables.

State of the art: general-purpose algorithms

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For every elimination method X there exists at least one "differential X".

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Their relative standing is different, e.g:

- differential Gröbner bases are not so popular (may be infinite)

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- in practice, characteristic sets are the most popular
  BLAD library by F. Boulier, available in MAPLE

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So the problem is solved, no?

Existing algorithms are general $\implies$
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efficient computation in practice is still a challenge.

And the plan is?

Restrict to dynamical systems and use Effective Algebraic Geometry.

Part II

Elimination for dynamical systems: in theory and in action

What do we mean by dynamical system?

System

$$\begin{cases} x_1' = f_1(x_1, \ldots, x_n), \\ \ldots \\ x_n' = f_n(x_1, \ldots, x_n), \end{cases}$$

where $f_1, \ldots, f_n \in k[x_1, \ldots, x_n]$.

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Corresponding ideal

$$\mathcal{I} := \langle \mathbf{x}' - \mathbf{f}, \mathbf{x}^{(2)} - \mathbf{f}', \ldots \rangle \subset k[\mathbf{x}^{(\infty)}].$$

Algebraic properties

- $\mathcal{I}$ is prime
- generators $\rightarrow$ Gröbner basis
- the variety is rational (parameters = initial conditions)

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Notation fixed for the rest of the section: n, $\mathcal{I}$

Elimination in dynamical systems: setup

Input:

- dynamical system

$$\begin{cases} x_1' = f_1(x_1, \ldots, x_n), \\ \ldots \\ x_n' = f_n(x_1, \ldots, x_n). \end{cases}$$

- integer $1 \leqslant s \leqslant n$

("to keep $x_1, \ldots, x_s$")

Output:

A description of

$$\mathcal{I}_{\text{elim}} := \mathcal{I} \cap k[x_1^{(\infty)}, \ldots, x_s^{(\infty)}]$$

(recall $\mathcal{I} := \langle \mathbf{x}' - \mathbf{f}, \mathbf{x}^{(2)} - \mathbf{f}', \ldots \rangle$)

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What kind of description? $\Longleftarrow$ depends on the questions we ask!

Questions: identifiability

Given: parametric dynamical system

$$\text{observed}\begin{cases} x_1' = f_1(\boldsymbol{\mu}, \mathbf{x}), \\ \ldots \\ x_s' = f_s(\boldsymbol{\mu}, \mathbf{x}) \end{cases}$$

$$\text{hidden}\begin{cases} x_{s+1}' = f_{s+1}(\boldsymbol{\mu}, \mathbf{x}), \\ \ldots \\ x_n' = f_n(\boldsymbol{\mu}, \mathbf{x}), \end{cases}$$

$\boldsymbol{\mu}$: unknown scalar parameters
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Informal definition

μ_1 is identifiable if (generically) μ_1 is uniquely determined by functions $x_1(t), \ldots, x_s(t)$.

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Example: $s = 1$

$$\begin{cases} x_1' = x_2,\\ x_2' = \mu x_1.\end{cases} \implies \text{YES } \left(\mu = \frac{x_1''}{x_1}\right)$$

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Algebraic characterization

(Ollivier'90)

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$\mu_1 \in$ the field of definition of $\mathcal{I}_{\text{elim}}$

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Algebraic characterization (Ollivier'90)

μ_1 is identifiable $\iff$ $\mu_1 \in$ the field of definition of $\mathcal{I}_{\text{elim}}$ *(under a mild condition, more in Ovchinnikov, Pillay,* ***P.****, Scanlon'20)*

Assessing identifiability via elimination

Joint with Ruiwen Dong, Christian Goodbrake, and Heather Harrington.

Overall: we compute the field of definition of $\mathcal{I}_{\mathsf{elim}}$.

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In the next slides

- How we represent $\mathcal{I}_{\mathsf{elim}}$?
- How we compute the representation?
- How we extract the field of definition?
- Performance

Representation: infinite $\to$ finite

How many Taylor coefficients are enough?

A tuple $(h_1, \ldots, h_s) \in \mathbb{Z}^s$ is called profile if

- $x_1^{(<h_1)}, \ldots, x_s^{(<h_s)}$ are algebraically independent modulo $\mathcal{I}$, *where* $x_j^{(<i)} := (x_j, x_j', \ldots, x_j^{(i-1)})$

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- $(h_1, \ldots, h_s)$ is maximal with this property.

Intuition: $x_1^{(<h_1)}(0), \ldots, x_s^{(<h_s)}(0)$ define $x_1(t), \ldots, x_s(t)$ up to finitely many choices (generically).

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Example

$$\begin{cases} x_1' = -x_2, \\ x_2' = x_1 \end{cases} \quad \& \quad s = 1 \implies h_1 = 2$$

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Propositions on profiles

- *(Hong, Ovchinnikov,* **P.***, Yap, 2020)* $x_1^{(\leqslant h_1)}, \ldots, x_s^{(\leqslant h_s)}$ generate the fraction field of $k[x_1^{(\infty)}, \ldots, x_s^{(\infty)}]/\mathcal{I}_{\text{elim}}$.
(used for assessing identifiability and observability)

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- *(Dong, Goodbrake, Harrington,* **P.**, *2021)* The fields of definition of $\mathcal{I}_{\text{elim}}$ and $\mathcal{I}_{\text{elim}} \cap k[x_1^{(\leqslant h_1)}, \ldots, x_s^{(\leqslant h_s)}]$ are the same.

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  Talk about this now!

Representation: profiles + projections

Representation

- Profile: $(h_1, \ldots, h_s) \in \mathbb{Z}^s$ such that
  - $x_1^{(<h_1)}, \ldots, x_s^{(<h_s)}$ are algebraically independent modulo $\mathcal{I}_{\mathrm{elim}}$.
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  - $(h_1, \ldots, h_s)$ is maximal with this property.
- Projections: for every $1 \leqslant i \leqslant s$, the generator of the principal ideal

$$\mathcal{I}_{\text{elim}} \cap \mathbb{C}(\boldsymbol{\mu})[x_1^{(<h_1)}, \ldots, x_i^{(\leqslant h_i)}, \ldots, x_s^{(<h_s)}]$$

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$$\mathcal{I}_{\text{elim}} \cap \mathbb{C}(\boldsymbol{\mu})[x_1^{(<h_1)}, \ldots, x_i^{(\leqslant h_i)}, \ldots, x_s^{(<h_s)}]$$

Example (contd.)

$$\begin{cases} x_1' = -x_2, \\ x_2' = x_1 \end{cases} \quad \& \quad s = 1 \quad \& \quad h_1 = 2 \implies \text{Projection: } x_1'' + x_1$$

Representation: profiles + projections

Representation

- Profile: $(h_1, \ldots, h_s) \in \mathbb{Z}^s$ such that
  - $x_1^{(<h_1)}, \ldots, x_s^{(<h_s)}$ are algebraically independent modulo $\mathcal{I}_{\text{elim}}$.
  - $(h_1, \ldots, h_s)$ is maximal with this property.
- Projections: for every $1 \leqslant i \leqslant s$, the generator of the principal ideal

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Observation

Original system is already in this form with $s = n$ and $h_1 = \ldots = h_n = 1$.

Computing the representation: reprofiling!

Profile point of view on elimination

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$$\left.\begin{array}{l}(\ldots, \underbrace{h}_{x_i,\ i\leqslant s}, \ldots, \underbrace{1}_{x_j,\ j>s}, \ldots) \\ \text{the projection for } x_i \text{ involves } x_j\end{array}\right\}$$

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- profile **h** is built dynamically by the socoban algorithm (and can be chosen in a more efficient way)
- special variable change to simplify resultant computation.

How to find the field of definition?

Subtlety

The coefficients of the projections belong to the field of definition but not necessarily generate it.

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The coefficients of the projections belong to the field of definition but not necessarily generate it.

Solution

Taking coefficients of one more projection on a generic plane is enough (but typically not needed and can be avoided)

Performance

The resulting algorithm is implemented in **julia** using OSCAR library

`https://github.com/pogudingleb/StructuralIdentifiability.jl`

Runtimes below are on a laptop, 16 GB RAM, 1.6 GHz.

Elimination

Model	Maple	Our
Cholera	$>$ 5 h.	3 s.
Pharm	OOM	18 s.
MAPK	OOM	28 s.
SEAIJRC	OOM	29 s.

Identifiability

Model	DAISY	SIAN	Our
Cholera	OOM	$>$ 5 h.	18 s.
Pharm	$>$ 5 h.	$>$ 5h.	7 min.
MAPK	$>$ 5 h.	$>$ 5h.	1 min.
SEAIJRC	OOM	$>$ 5 h.	2 min.
NFκB	OOM	33 min.	$>$ 5 h.

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SIAN (Hong, Ovchinnikov, **P.**, Yap, 2020) is also based in elimination for dynamical systems!

Part III
Open problems and conclusions

Problem 1: Degree of a prolongation variety

Consider a variety V_1

$$\begin{cases} x_1' = x_2^2, \\ x_2' = x_1^2 \end{cases}$$

$\deg V_1 = ?$

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deg V_m	4	7	16	25	34	49	64	79

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$$\deg V_m = \begin{cases} (m+1)^2, \text{ if } m \equiv 0, 1 \pmod 3, \\ (m+1)^2 - 2, \text{ if } m \equiv 2 \pmod 3 \end{cases}$$

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Why mod 3???

Similar to Jan Draisma's talk at the NASO seminar...

Problem 2: Computing the support

Predator-prey model

$$\begin{cases} x_1' = a_1 x_1 - a_2 x_1 x_2, \\ x_2' = -a_3 x_2 + a_4 x_1 x_2. \end{cases}$$

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Implicit hypersurface in the $(a_1, \ldots, a_4,\, x_1,\, x_1',\, x_1^{(2)})$-space.

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Result: $a_1 a_4 x_1^3 - a_4 x_1^2 x_1' - a_1 a_3 x_1^2 + a_3 x_1 x_1' + x_1 x_1^{(2)} - (x_1')^2 = 0$

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Tropical methods $\Longrightarrow$ Newton polytope of the implicit equation

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$$a_1 a_4 x_1^3 - a_4 x_1^2 x_1' + 7 a_1^2 x_1^2 + 3 a_1 a_3 x_1^2 - 7 a_1 x_1 x_1' - 3 a_3 x_1 x_1' - x_1 x_1'' + 2 (x_1')^2 = 0$$

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Problem
For a system

$$\begin{cases} x_1' = f(\boldsymbol{\mu}, x_1, x_2), \\ x_2' = g(\boldsymbol{\mu}, x_1, x_2), \end{cases}$$

where $f, g \in \mathbb{C}[\boldsymbol{\mu}, x_1, x_2]$, given Newton polytopes of f and g, predict the Newton polytope of the minimal differential equation for x_1.

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- Commutative algebra and algebraic geometry provide a view on differential equations which is coherent and complementary to the analytic one.

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- Equations defining dynamical systems are ubiquitous in applications and have interesting and useful geometry.
- Although differential elimination has been studied for ~ 100 years, one can still compute much more.
- Open problems in effective algebraic geometry of practical interest.

Acknowledgements

This work was partially supported by the Paris Ile-de-France Region and National Science Foundation.