Identifiability of parameters in ODEs with differential algebra

Alexey Ovchinnikov

Results are from joint work with Hoon Hong, Gleb Pogudin, Peter Thompson, and Chee Yap

Implementation is available here:
`https://github.com/pogudingleb/SIAN`

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Structural identifiability analysis addresses this issue.

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- Applied math aspects:
  - unexpected appearance of pure math techniques in applications
  - significantly improved algorithms/methodology for scientists to replace guessing by rigorous reasoning
  - randomized computing to increase the efficiency

Part I: Theory

Differential algebra: elimination problem

General question about systems of equations: for given $F = f_1, f_2$ in x_1, x_2, check the following:

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– see MAPLE example.

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  – see Maple example.
- **Challenge**: instead of 2, we might have 100 – efficiency

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Part II: Applications

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$$\begin{array}{c}\text{impossible to eliminate } k_2 \\ \text{in } \dot{x} = x + k_1 + k_2\end{array} \implies \text{impossible to find } k_1$$

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Applying elimination: joint work with H. Hong, G. Pogudin, and C. Yap

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Lotka-Volterra system (predator-prey model)

$$\begin{cases} \dot{x} = ax - bxy, \\ \dot{y} = -cy + dxy, \end{cases}$$

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We checked parameter identifiability without solving the system – see MAPLE and next slide (Wronskians).

Wronskian

Using Wronskian matrix

For analytic functions f_1, f_2, f_3, define

$$\mathrm{Wr}(f_1, f_2, f_3) := \begin{pmatrix} f_1 & f_2 & f_3 \\ f_1' & f_2' & f_3' \\ f_1'' & f_2'' & f_3'' \end{pmatrix}.$$

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Suppose that

$$af_1 + bf_2 + cf_3 = f_4$$

holds for some constants a, b, c and analytic functions f_1, f_2, f_3, f_4. If $\det \mathrm{Wr}(f_1, f_2, f_3) \neq 0$, then

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \mathrm{Wr}(f_1, f_2, f_3)^{-1} \cdot \begin{pmatrix} f_4 \\ f_4' \\ f_4'' \end{pmatrix}.$$

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and verify (in Maple) that

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$$c = A, \quad d = B, \quad ad = C, \quad ac = D$$

and solve:

$$a = C/B, \quad c = A, \quad d = B.$$

Applications: Identifiability of parameters

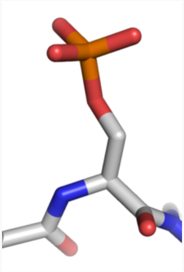
Chemistry (Phosphorylation)

$$A + B \underset{\mu_2}{\overset{\mu_1}{\rightleftharpoons}} AB \xrightarrow{\mu_3} C + B$$

$$C + D \underset{\mu_5}{\overset{\mu_6}{\rightleftharpoons}} CD \xrightarrow{\mu_4} A + D,$$

Amounts of B and C can be measured.

Q: Are $\mu_1, \dots, \mu_6$ identifiable?



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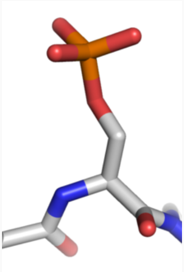

Differential equations

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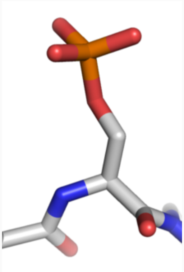

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Result: $\mu_1, \ldots, \mu_6$ are identifiable (probability $> 99\%$)

Time: seconds – see MAPLE

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Analysis of ODEs: first integrals – obstacles.

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Theorem *(Ovchinnikov, Pogudin, Thompson)*. Practical sufficient conditions for $\det \mathrm{Wr} \neq 0$ (so, no issue): e.g., linear systems of any size with one measured variable.

Part III

Monte Carlo algorithm to speed up checking if elimination is possible

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Let a be sampled uniformly from 0 to 99:

$$\Pr[a \neq 0] = 1 - 1/100 = 0.99.$$

Thus, the above test is correct with probability 99% for such a sampling.

Randomization and elimination. Toy example 2

Can we eliminate x from this system?

$$\begin{cases} x + y = 0 \\ y = 0 \end{cases} \tag{2}$$

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DeMillo-Lipton-Schwartz-Zippel lemma

Theorem
Let

- $P(x_1, \ldots, x_n)$ be a non-zero polynomial of degree d
- N be a positive integer
- $r_1, r_2, \ldots, r_n$ be selected at random independently and uniformly from $\{0, 1, \ldots, N-1\}$.

Then

$$\Pr[P(r_1, r_2, \ldots, r_n) \neq 0] \geqslant 1 - \frac{d}{N}.$$

Randomization and elimination. Result

Proposition
Let

- $f_1, \ldots, f_r \subset k[x_1, \ldots, x_n, y_1, \ldots, y_m]$ be polynomials, $\deg f_i \leqslant d$,

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Proposition
Let

- $f_1, \ldots, f_r \subset k[x_1, \ldots, x_n, y_1, \ldots, y_m]$ be polynomials, $\deg f_i \leqslant d$,
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Example. Checking elimination for an epidemiology model that took 40 minutes, now takes 1 second (probability at least 99.9%).