Parameter identifiability through canonical bases

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State space models

An state space model is given by a system of ODEs

$$\dot{\boldsymbol{x}} = f(\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{u}) \tag{1}$$

$$\boldsymbol{y} = g(\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{u}) \tag{2}$$

and possibly a constraint

$$0 = h(\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{u}) \tag{3}$$

- $\boldsymbol{x}$ is a vector of state variables
- $\boldsymbol{u}$ is a vector of input variables
- $\boldsymbol{y}$ is a vector of output variables
- $\boldsymbol{\mu}$ is a vector of constants called the parameters
- For us, f, g, and h are vectors of rational functions with rational coefficient and will omit the constraint Equation 3.

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Identifiability

We will be interested in the parameter identification problem: can the parameters $\boldsymbol{\mu}$ be recovered from the output $\boldsymbol{y}$? If so, how? Sometimes, this problem goes under the name of system identification.

There are variants of this problem in which the input variables $\boldsymbol{u}$ are assumed to be known or not. There are related problems of determining the state $\boldsymbol{x}$ from the output $\boldsymbol{y}$ or even of inferring the input $\boldsymbol{u}$ from the output $\boldsymbol{y}$.

We shall interpret recovered from as expressed as a differential rational function of. Moreover, we shall ask $(\boldsymbol{x}, \boldsymbol{y})$ to be a generic solution of the equations for a sufficiently general (even generic) $\boldsymbol{u}$. So, given such generic solutions to Equations 1 and 2, we wish to compute $\mathbb{Q}(\boldsymbol{\mu}) \cap \mathbb{Q}\langle \boldsymbol{u}, \boldsymbol{y} \rangle$ and, in particular, wish to determine whether this intersection is $\mathbb{Q}(\boldsymbol{\mu})$.

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Canonical parameters

There may be obvious reasons why it is impossible to identify the parameters.

- For example, if some transcendental component of μ does not appear in Equation 1 at all, then it would be impossible to compute μ from $\boldsymbol{y}$.
- For a less trivial example, it may happen that the system is equivalent to one in which the coefficients are rational functions of μ. For example, our equations might be $\dot{x} = x^2 + \mu_1 + \mu_2$ and $y = x$.

At the very least, if we wish for the parameters to be indentifiable, then they need to be canonical parameters: any other choice of parameters would give an inequivalent system of equations.

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Canonical parameters, model theoretically

The canonical parameter is a standard notion of model theory.

We say that a formula $\phi(\boldsymbol{x}, \boldsymbol{y})$ has canonical parameters if for any two choices of parameters $\boldsymbol{c}$ and $\boldsymbol{d}$, we have that $(\forall \boldsymbol{x})(\phi(\boldsymbol{x}, \boldsymbol{c}) \leftrightarrow \phi(\boldsymbol{x}, \boldsymbol{d}))$ if and only if $\boldsymbol{c} = \boldsymbol{d}$. In this case, we would say that $\boldsymbol{c}$ is the canonical parameter for $\phi(\boldsymbol{x}, \boldsymbol{c})$.

We say that our theory eliminates imaginaries if for each formula $\phi(\boldsymbol{x}, \boldsymbol{y})$ there is some formula $\psi(\boldsymbol{x}, \boldsymbol{z})$ so that

- every instance of ϕ is equivalent to an instance of ψ: $(\forall \boldsymbol{y})(\exists \boldsymbol{z})(\forall \boldsymbol{x})(\phi(\boldsymbol{x}, \boldsymbol{y}) \leftrightarrow \psi(\boldsymbol{x}, \boldsymbol{z}))$
- every instance of ψ is equivalent to an instance of ϕ, and
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For us, the key point is that the theory of differentially closed fields of characteristic zero, DCF_0, eliminates imaginaries. So, every finite system of ODEs (and inequalities) is equivalent to one with canonical parameters.

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Canonical bases

There is a related, but more refined, notion of a canonical base of a type in a stable theory. We specialize the definition to the case of DCF_0.

Let (K, ∂) be a differential field, $k \subseteq K$ a differential subfield, and $\boldsymbol{a}$ a tuple from K. We write $I(\boldsymbol{a}/k) := \{f \in k\{\boldsymbol{x}\} \ : \ f(\boldsymbol{a}) = 0\}$ for the ideal of $\boldsymbol{a}$ over k.

- The type of $\boldsymbol{a}$ of k is stationary or just "$\boldsymbol{a}$ is stationary over k" if $I(\boldsymbol{a}/k)$ is absolutely prime. That is, the ideal generated by $I(\boldsymbol{a}/k)$ in $k^{\text{alg}}\{x\}$ is prime.
- Provided that $\boldsymbol{a}$ is stationary over k, the canonical base of $\boldsymbol{a}$ over k, written $\text{Cb}(\boldsymbol{a}/k)$, is the differential field of definition of $I(\boldsymbol{a}/k)$.

The canonical base $\text{Cb}(\boldsymbol{a}/k)$ may be realized as the differential field generated by the canonical parameters of a formula isolating the type of $\boldsymbol{a}$ over k up to dependence. Algebraically, it may be realized as the differential field generated by the coefficients of the monic differential polynomials in a characteristic generating set for $I(\boldsymbol{a}/k)$.

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Canonical base and parameter identifiability

Let us restrict to a simple case where our equation takes the form

$$\dot{\boldsymbol{x}} = f(\boldsymbol{x}, \boldsymbol{\mu})$$

$$\boldsymbol{y} = \boldsymbol{x}$$

so that there are no input variables and the state and output variables are identical.

If we set $k = \mathbb{Q}(\mu)$ and let $\boldsymbol{a}$ be a generic solution, then the type of $\boldsymbol{a}$ over k is stationary.

If μ is a canonical parameter for the formula $\dot{\boldsymbol{x}} = f(\boldsymbol{x}, \mu)$, then $k = \mathrm{Cb}(\boldsymbol{a}/k)$.

So, the parameter identifiability problem reduces to asking whether the canonical base $\mathrm{Cb}(\boldsymbol{a}/k)$ is contained in the differential field generated by $\boldsymbol{a}$, or in more model theoretic terms, in the definable closure of a realization of the generic type of this system.

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Computing the canonical base over the full field of constants

Parameters are always identifiable over the full field of constants.

Proposition

Let K be a differentially closed field, $C = \{x \in K : \partial(x) = 0\}$ its field of constants and $\boldsymbol{a}$ a tuple from K. Then $\mathrm{Cb}(\boldsymbol{a}/C) = \mathbb{Q}\langle \boldsymbol{a} \rangle \cap C$

Proof.

- Extending K if need be, we may arrange that $\mathbb{Q}\langle \boldsymbol{a} \rangle$ is the fixed field of the group $G_{\boldsymbol{a}}$ of differential field automorphisms of K fixing $\boldsymbol{a}$.
- If $\sigma \in \mathrm{Aut}(K)$, then σ fixes C setwise.
- Thus, if $f \in I(\boldsymbol{a}/C)$ and $\sigma \in G_{\boldsymbol{a}}$, we have $f^\sigma \in I(\boldsymbol{a}/C)$. Therefore, $\mathrm{Cb}(\boldsymbol{a}/C) \subseteq \mathbb{Q}\langle \boldsymbol{a} \rangle \cap C$.
- On the other hand, if $b \in \mathbb{Q}\langle \boldsymbol{a} \rangle \cap C \smallsetminus \mathrm{Cb}(\boldsymbol{a}/C)$, it cannot be algebraic over $\mathrm{Cb}(\boldsymbol{a}/C)$ (as this would violate stationarity) and it cannot be transcendental because then $\boldsymbol{a}$ would depend on b over $\mathrm{Cb}(\boldsymbol{a}/C)$ violating the defining property of the canonical base.

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□

Reducing to the canonical base over the full field of constants

Proposition

With the notation as above, if $k \subseteq C$ is a field of constants, $\mathbf{a}$ is stationary over k, and $\mathbf{c}$ is a tuple generating $\mathrm{Cb}(\mathbf{a}/C)$, then $\mathrm{Cb}(\mathbf{a}/k) = \mathrm{Cb}(\mathbf{c}/k)$ and $\mathbb{Q}\langle \mathbf{a} \rangle \cap k = \mathbb{Q}(\mathbf{c}) \cap k$.

Abstract failure of single experiment identifiability

- In general stable theories it is “rare” for the canonical base of a type to be definable (or even algebraic) from a single realization.
- Theories where this always happens are (provably) degenerate or closely related to linear algebra.
- Even for algebraically closed field, if $f(\boldsymbol{x}, \boldsymbol{y})$ is a monic polynomial over $\mathbb{Q}$ for which $f(\boldsymbol{x}, \boldsymbol{b})$ is always absolutely irreducible, then a generic solution to $f(\boldsymbol{a}, \boldsymbol{b}) = 0$ will be stationary over $\mathbb{Q}(\boldsymbol{b}) = \mathrm{Cb}(\boldsymbol{a}/\mathbb{Q}(\boldsymbol{b}))$. If $\boldsymbol{x} = (x_1, \ldots, x_n)$ has $n > 2$, then it is not possible to compute $\boldsymbol{b}$ from $\boldsymbol{a}$.

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A failure of single-experiment identifiability

Let $b, c, d \in C$ be three algebraically independent elements. Set $e := bd + c$ and let $k = \mathbb{Q}(d, e)$.

Since the ideal $I((b, c)/k)$ is generated by $x_2 + dx_1 - e$, $\mathrm{Cb}((b, c)/k) = k$.

In particular, $\mathrm{Cb}((b, c)/k) \not\subseteq \mathbb{Q}(b, c)$.

Consider a satisfying $\partial(a) = ba + c$. A simple computation shows that (a, b) is the generic solution to the following system.

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Multi-experiment identifiability

Given an input-output system

$$\begin{aligned} \dot{\boldsymbol{x}} &= f(\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{u}) \\ \boldsymbol{y} &= g(\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{u}) \end{aligned}$$

one might ask whether the parameters $\boldsymbol{\mu}$ are identifiable from multiple independent experiments.

- Of course, as before we must assume that the parameters $\boldsymbol{\mu}$ are canonical.
- If the answer is yes, then we would like to compute a bound on the number of experiments needed.
- The bounds may depend on whether we vary the input variable or not between the various experiments.

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Shelah reflection principle

There is a very general model theoretic result which says that multi-experiment parameter identification is always possible, even if we allow our parameters to be nonconstant.

Theorem

In any totally transcendental theory if $\mathbf{a}$ is a tuple which is stationary over B, then there is a number N so that if $\mathbf{a}_1, \ldots, \mathbf{a}_N$ is a sequence of independent realizations of the type of $\mathbf{a}$ over B, then $\mathrm{Cb}(\mathbf{a}/B)$ is definable from $\langle \mathbf{a}_1, \ldots, \mathbf{a}_N \rangle$. Moreover, if $\mathbf{b}$ is a tuple from which $\mathrm{Cb}(\mathbf{a}/B)$ is definable and the Lascar rank of $\mathbf{b}$ is $s < \omega$, then it suffices to take $N = s + 1$.

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Interpreting the general theorem for systems of ODEs

- The theory of differentially closed fields of characteristic zero is the quintessential example of a totally transcendental theory.
- Independence may be defined differential algebraically: if $\boldsymbol{a}$ is stationary over the differential field L and M is an differential extension field, then $\boldsymbol{a}$ is independent from L over M if $I(\boldsymbol{a}/M)$ generates $I(\boldsymbol{a}/L)$. A sequence $\langle \boldsymbol{a}_1, \ldots, \boldsymbol{a}_n \rangle$ is independent over the differential field M if for each $i < n$, $\boldsymbol{a}_{i+1}$ is stationary over M and independent from $M\langle \boldsymbol{a}_1, \ldots, \boldsymbol{a}_i \rangle$ over M.
- In a differentially closed field, an element c is definable from some tuple $\boldsymbol{b}$ just in case $c \in \mathbb{Q}\langle \boldsymbol{b} \rangle$.
- The Lascar rank is a dimension defined using (in)dependence. For us, the main point is that the Lascar rank of a tuple $\boldsymbol{b}$ is bounded above by $\operatorname{tr.deg} \mathbb{Q}\langle \boldsymbol{b} \rangle$ and when $\boldsymbol{b}$ is a tuple of constants, the Lascar rank is equal to this transcendence degree.

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Differential algebraic approach to multi-experiment identifiability

The Shelah reflection principle is really an abstract version of the method of Lagrange interpolation or undetermined coefficients.

From such an interpretation, we can produce an explicit algorithm to compute the the canonical base from a small number of experiments.

Differential algebraic multi-experiment identifiability with one variable

For the sake of illustration, we discuss the one-variable case. That is, we presume that a is stationary over k, a field of constants. We wish to compute a bound N and then to compute $\mathrm{Cb}(a/k)$ from some finite sequence $a_1, \ldots, a_N$ of independent copies of a, that is, $I(a/k) = I(a_i/k)$.

In this one-variable case, $I(a/k) = [f] : S_f^\infty$ where $f \in k\{x\}$ is a monic differential polynomial of minimal order-degree with $f(a) = 0$ and S_f is the separant of f. Our task is to recover the coefficients of f.

The most natural approach would be to express $f = \sum_{\alpha \in S} c_\alpha x^\alpha$ and then aim to compute the vector $(c_\alpha)_{\alpha \in S}$. Here α is a multi-index, $x^\alpha = \prod (x^{(n)})^{\alpha_n}$, S is a finite set, $c_\alpha \in k$, and $c_{\alpha_0} = 1$ for some $\alpha_0 \in S$.

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Differential algebraic multi-experiment identifiability with one variable, continued

The vector $(c_\alpha)_{\alpha \in S}$ is then a solution to the linear equations

$$\sum_{\alpha \in S} (a_i)^\alpha Y_\alpha = 0$$

Via basic linear algebra, one sees that these equations together with $Y_{\alpha_0} = 1$ determine $(c_\alpha)_{\alpha \in S}$ provided that $N \gg 0$ ($N > |S|$ would work).

We improve the bounds, and thereby reduce the size of the linear algebraic problem to be solved, by taking into account differential algebraic relations, specifically by considering the rank of the Wronskian of $(a^\alpha)_{\alpha \in S}$

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Further considerations for the differential algebraic multi-experiment identifiability

- In the case of several variables, we express the problem of computing $\mathrm{Cb}(\boldsymbol{a}/k)$ as that of finding the coefficients of the polynomials in a *characteristic presentation* $\{p_1, \ldots, p_m\}$ of $I(\boldsymbol{a}/k)$.
- It can be useful to use some other finite set $\mathscr{S}_j$ of linearly independent differential polynomials over $\mathbb{Q}$ in place of the monomials and to express $p_i = \sum_{g \in \mathscr{S}_i} c_g g$ with $c_g \in k$.

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- The general results from model theory we have described work equally well for PDEs, but what specific consequences they have and the computational approach remain to be investigated.
- Extensions to difference equations and difference-differential equations should be possible, but here the model theory is somewhat more complicated.

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The end

Thanks again to the program committee for this invitation to speak and to all of you for your attention.