Symbolic Transformations of Dynamical Models

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LIX, CNRS, École Polytechnique, IP Paris

HDR defence, December 5th, 2024

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Françoise Point	Université de Mons
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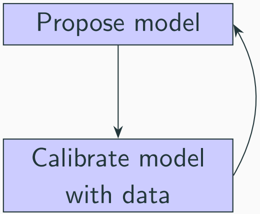
Bernd Sturmfels	Max Planck Institute
Jacques-Arthur Weil	Université de Limoges

Very simplified workflow



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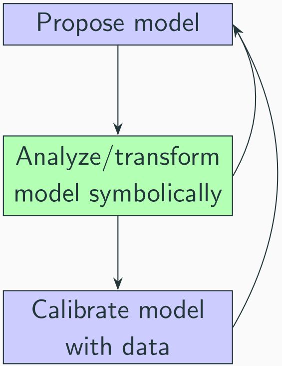

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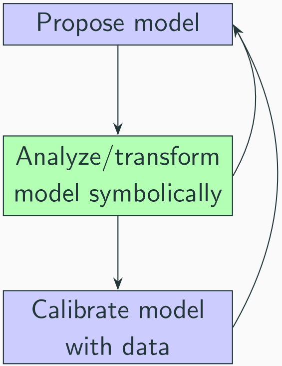

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1. Introduction
2. Differential and Difference Algebra
3. Differential/Difference Elimination
4. Structural Parameter Identifiability
5. Exact Model Reduction
6. Quadratization
7. Research Project

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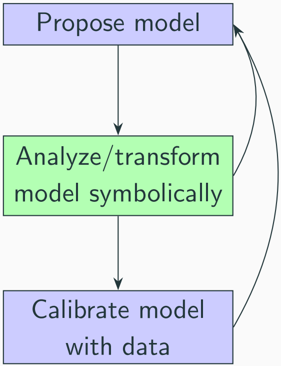

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- Started working on **Reduction** (supported by DIM RFSI) and **Quadratization** (supported by CNRS INS2I)
- New developments (including software) in **Identifiability** motivate revisiting **Elimination** (supported by ANR JCJC)

Plan of the talk

1. Elimination
   (focus on theory)
2. Parameter identifiability
   (focus on algorithms and software)
3. Future directions
   (with quadratization sneaking in)

Elimination: what and why?

General formulation

Given a system $\mathbf{f}(\mathbf{x}, \mathbf{y}) = 0$ in $\mathbf{x} = (x_1, \ldots, x_n)$, $\mathbf{y} = (y_1, \ldots, y_m)$

Find nontrivial $g(\mathbf{y}) = 0$ which hold on every solution

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Why?

- Get simpler equations
- Remove *latent* variables

Difference (discrete-time) equations

Setup

Solution space: two-sided sequences (signals) $(\ldots, a_{-1}, a_0, a_1, \ldots) \in \mathbb{C}^{\mathbb{Z}}$.

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Example

$$f_{n+2} = f_{n+1} + f_n \rightsquigarrow \sigma^2(F) = \sigma(F) + F$$

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(sharp contrast with the differential case!)

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Illustrating example

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Take the equations **and** a shift:

$$0 = (\underline{\sigma^2(X)} - \underset{\sim}{X} - Z) - \sigma(\underline{\sigma(X)} - \underline{\underline{X}} - Y) - (\underline{\underline{\sigma(X)}} - \underset{\sim}{X} - Y)$$

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1. Take several shifts of the original equations
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For differential case, done in (Ovchinnikov, P., Vo, 2019).

Difference elimination: Results

Theorem (Ovchinnikov, P., Scanlon, 2020)

There is an (explicit) function $B(n, d)$ such that,
for a system of dimension n and degree d:

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Idea: $\exists$ solution $\iff$ $\exists$ "periodic" solution
but need a correct notion of "periodic" !

On the frontier of decidability

Corollary (OPS, 2020)

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- check if a system $f_1 = \ldots = f_\ell = 0$, $g \neq 0$ has a solution $\mathbb{C}^{\mathbb{Z}}$ *i.e. radical ideal membership*
- check if a system $f_1 = \ldots = f_\ell = 0$ has a solution $\mathbb{C}^{\mathbb{Z}^2}$ *i.e. two shifts like in PDEs*

Concluding remarks

Summary

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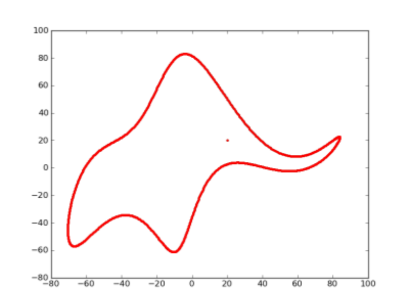
Not the end of the story

- Deciding $f_1 = \ldots = f_\ell = 0 \implies g = 0$ is important.
  Add restrictions to make decidable (e.g. existence of solutions)?
- Known hard cases come from "linear systems with switches".
  Study systematically and obtain lower bounds?

Parameter identifiability



from Mayer et al., 2009

With four parameters I can fit an elephant, and with five I can make him wiggle his trunk.

John von Neumann

Toy examples of non-identifiability

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Can such things naturally occur?

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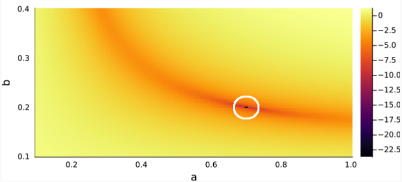
Heatmap of log of the minimal L^2 error for $(a, b) \in [0.1, 1.0] \times [0.1, 0.3]$



More realistic example

Simple ODE model:

$$\begin{cases} x_1'(t) = -ax_1(t) + bx_2(t), \\ x_2'(t) = -bx_2(t) \end{cases}$$

We have time series for x_1:

t	0.0	0.2	...	1.0
x_1	1.0	1.1	...	0.3

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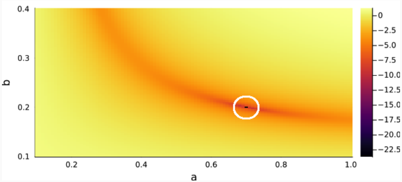
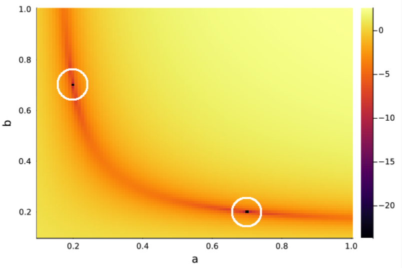


Zoom out:



Two perfect fits!

General setup

ODE model with rational rhs

$$\begin{cases} \mathbf{x}'(t) = \mathbf{f}(\mathbf{k}, \mathbf{x}(t), \mathbf{u}(t)), \\ \mathbf{y}(t) = \mathbf{g}(\mathbf{k}, \mathbf{x}(t), \mathbf{u}(t)) \end{cases}$$

$$\left.\begin{aligned} \mathbf{x}(t) &= \text{state variables} \\ \mathbf{k} &= \text{parameters} \end{aligned}\right\} \quad - \quad \text{unknown}$$

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Structural identifiability problem

A parameter k is identifiable if its value can be determined from $\mathbf{y}(t)$ and $\mathbf{u}(t)$ for generic values of $\mathbf{k}$ and initial conditions

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Lack of identifiability $\implies$ impossibility of reliable estimation

How to check: Taylor series approach

Goes back to Pohjanpalo in the 1970-s.

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k is identifiable $\iff$ k can be expressed via $\mathbf{y}(0), \mathbf{u}(0), \mathbf{y}'(0), \mathbf{u}'(0), \ldots$

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$$\begin{cases} x' = x + a, \\ y = x \end{cases} \implies a = y'(0) - y(0) \ \checkmark$$

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Goes back to PhD thesis of F. Ollivier (1990).

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Step 1 Eliminate states:

$$\begin{cases} x_1' = -ax_1 + bx_2, \\ x_2' = -bx_2, \\ y = x_1 \end{cases} \implies \underbrace{y'' + (a+b)y' + aby = 0}_{\text{input-output equation}}.$$

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Missing pieces

- Why correct?
- How eliminate efficiently?
- How check field membership efficiently?

Input-output equations: assembling the puzzle

Outline of the approach

1. Eliminate states
2. Check if the parameter belongs to the field of the coefficients

Missing piece #1: Why is this approach correct?

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  Correct but for a different problem *(multi-experiment identifiability)*
- (Dong, Goodbrake, Harrington, P., 2023)
  Efficient correctness check $\Longrightarrow$ in practice, almost always correct

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$\Longrightarrow$ outperforms general purpose elimination algorithms by orders

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Missing piece #3: How check membership efficiently?

Answer (DGHP, 2023): Randomized algorithm to check

Voilà: StructuralIdentifiability.jl

Resulted in Julia package StructuralIdentifiability.jl.

Model	DAISY	SIAN	SI.jl
SIWR model	OOM	> 5 h.	18 s.
SIWR model - 2	OOM	213 s.	0.7 s.
Pharmacokinetics	> 5 h.	> 5 h.	406 s.
MAPK pathway - 1	OOM	31 s.	39.5 s.
MAPK pathway - 2	> 5 h.	> 5 h.	58 s.
MAPK pathway - 3	> 5 h.	35 s.	1084 s.
SEAIJRC model	OOM	> 5 h.	131.3 s.
Akt pathway	182 s.	28 s.	5 s.
NFκB	> 5 h.	2018 s.	> 5 h.
Mass-action	> 5 h.	3 s.	0.5 s.
SIRS w. forcing	OOM	5 s.	30.3 s.

Ça marche !

PNAS nexus

PNAS Nexus, 2024, 3, 1–15
https://doi.org/10.1093/pnasnexus/pgae031
Advance access publication 20 January 2024
Biological, Health, and Medical Sciences

Signaling-biophysical modeling unravels mechanistic control of red blood cell phagocytosis by macrophages in sickle cell disease

Yu Zhang[a,*,1], Yuhao Qiang[b,1], He Li[c], Guansheng Li[d], Lu Lu[e], Ming Dao[b], George E. Karniadakis[d], Aleksander S. Popel[a,*] and Chen Zhao[f,*]

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[b]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
[c]School of Chemical, Materials and Biomedical Engineering, University of Georgia, Athens, GA 30602, USA
[d]School of Engineering, Brown University, Providence, RI 02912, USA
[e]Department of Statistics and Data Science, Yale University, New Haven, CT 06520, USA
[f]School of Pharmacy, Nanjing Medical University, Nanjing, Jiangsu 210029, China
*To whom correspondence should be addressed: Email: zhangyu@jhmi.edu (Y.Z.); Email: apopel@jhu.edu (A.S.P); Email: zcshinchon4677@outlook.com (C.Z.)
[1]Co-first authors.
Edited By: Dennis Discher

Neural Networks 180 (2024) 106732

Contents lists available at ScienceDirect

Neural Networks

journal homepage: www.elsevier.com/locate/neunet

ELSEVIER

Full Length Article

Coagulo-Net: Enhancing the mathematical modeling of blood coagulation using physics-informed neural networks

Ying Qian[a,1], Ge Zhu[b,1], Zhen Zhang[c,1], Susree Modepalli[d], Yihao Zheng[e], Xiaoning Zheng[f], Galit Frydman[g,h], He Li[a,*]

[a] School of Chemical, Materials and Biomedical Engineering, University of Georgia, Athens, USA
[b] Department of Biomedical Engineering, Worcester Polytechnic Institute, Worcester, USA
[c] Division of Applied Mathematics, Brown University, Providence, RI, USA
[d] School of Medicine, Georgetown University, Washington DC, USA
[e] Department of Mechanical and Material Engineering, Worcester Polytechnic Institute, Worcester, USA
[f] Department of Mathematics, College of Information Science & Technology, Jinan University, Guangzhou, Guangdong, 510632, China
[g] Division of Trauma, Emergency Surgery and Surgical Critical Care at the Massachusetts General Hospital, Boston, MA, USA
[h] Division of Comparative Medicine, Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA

Contents lists available at ScienceDirect

Journal of Theoretical Biology

journal homepage: www.elsevier.com/locate/yjtbi

ELSEVIER

Journal of Theoretical Biology

Modeling the CD8+ T cell immune response to influenza infection in adult and aged mice

Benjamin Whipple[a,b], Tanya A. Miura[b,c,d], Esteban A. Hernandez-Vargas[a,b,d,*]

[a] Department of Mathematics and Statistical Science, University of Idaho, Moscow, ID, 83844, United States
[b] Bioinformatics and Computational Biology Program, University of Idaho, Moscow, ID, 83844, United States
[c] Department of Biological Sciences, University of Idaho, Moscow, ID, 83844, United States
[d] Institute for Modeling Collaboration and Innovation, University of Idaho, Moscow, ID, 83844, United States

ARTICLE INFO

Keywords:
Mathematical model
Influenza
Aging
CD8+ T cells
Murine model

ABSTRACT

The CD8+ T cell response is the main determinant of viral clearance during influenza infection. However, influenza viral dynamics and the respective immune responses are affected by the host's age. To investigate age-related differences in the CD8+ T cell immune response dynamics, we propose 16 ordinary differential equation models of existing experimental data. These data consist of viral titer and CD8+ T cell counts collected periodically over a period of 19 days from adult and aged mice infected with influenza A/Puerto Rico/8/34 (H1N1). We use the corrected Akaike Information Criterion to identify the models which best represent the

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https://doi.org/10.1007/s41109-023-00578-z

Applied Network Science

RESEARCH Open Access

Modeling self-propagating malware with epidemiological models

Alesia Chernikova[1*], Nicolò Gozzi[2], Nicola Perra[3], Simona Boboila[1], Tina Eliassi-Rad[1] and Alina Oprea[1]

*Correspondence: chernikova.a@northeastern.edu
[1] Northeastern University, Boston, MA, USA
[2] ISI Foundation, Turin, Italy
[3] School of Mathematical Sciences, Queen Mary University of London, London, UK

Abstract

Self-propagating malware (SPM) is responsible for large financial losses and major data breaches with devastating social impacts that cannot be understated. Well-known campaigns such as WannaCry and Colonial Pipeline have been able to propagate rapidly on the Internet and cause widespread service disruptions. To date, the propagation behavior of SPM is still not well understood. As result, our ability to defend against these cyber threats is still limited. Here, we address this gap by performing a comprehensive analysis of a newly proposed epidemiological-inspired model for SPM propagation, the *Susceptible-Infected-Infected Dormant-Recovered* (SIIDR) model. We

Concluding remarks

Summary

- Algebra in action $\implies$ two state-of-the-art software tools

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- Efficient elimination via change of representation
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Research project

Transformation for learning

Scientific Machine Learning

model calibration $\rightsquigarrow$ learning (a part of) model from data

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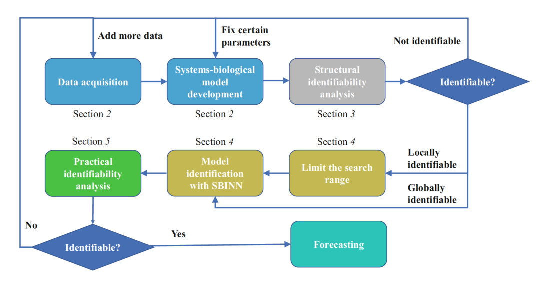
Use-case #1: structural parameter identifiability

Identifiability assessment as a preprocessing for PINNs.



Systems Biology: Identifiability Analysis and Parameter Identification via Systems-Biology-Informed Neural Networks, Daneker et al., 2023

Transformation for learning

Use-case #2: quadratization for model reduction

Model order reduction: replace an ODE model with a smaller one.

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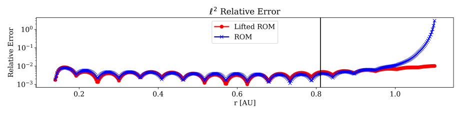

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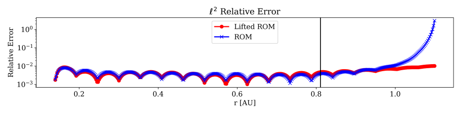
- (Olivieri, P., Kramer, 2024+)
  Algorithm for PDEs



Transformation for learning

Scientific Machine Learning

model calibration $\rightsquigarrow$ learning (a part of) model from data

General research question

How to compute "convenient" coordinates for learning?
(e.g., identifiable reparametrizations, quadratizations for PDEs, etc.)

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  Something in the middle?

  Based on algebraic version from (Ait El Manssour, P., 2022, 2024)

All these adventures made possible by

- my teachers
- my postdoc mentors
- my collaborators
- my students
- my colleagues
- and my family

Thank you!