Differential Algebra, Regular Chains and Modeling

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Abstract

- Differential Algebra provides algorithmic tools for dealing with DAE (index reduction, computation of the variety of constraints and the missing relations)
- We will demonstrate an example from modeling in biochemistry
- Regular Chains (or equivalently characteristic sets) are the fundametal objects of Differential Algebra.
- Moreover, regular chains provide a bridge from Differential Algebra to Polynomial Algebra. As a consequence, any improvement on one side benefits to the other.
- The co-authors of this talk have developed various algorithms (`RosenfeldGroebner`, `Triade`, `Pardi`, `VCA`) and software `DifferentialAlgebra`, `MABSys`, `Modpn`, `RegularChains` for computing with algebraic and differential regular chains.

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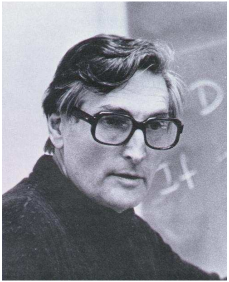
Differential algebra

A mathematical theory (Ritt, Kolchin) which permits to process systems of differential equations symbolically, without integrating them.



Regular Chains

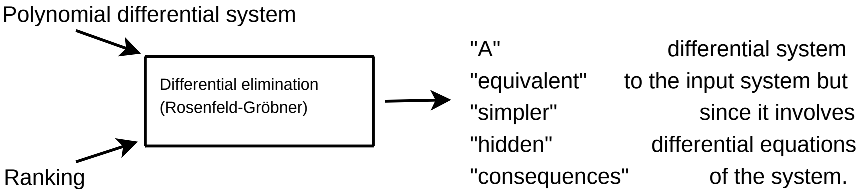
For the following input polynomial system :

$$F : \begin{cases} x^2 + y + z = 1 \\ x + y^2 + z = 1 \\ x + y + z^2 = 1 \end{cases}$$

The following regular chains describe its solutions :

$$\begin{cases} z = 0 \\ y = 1 \\ x = 0 \end{cases} \cup \begin{cases} z = 0 \\ y = 0 \\ x = 1 \end{cases} \cup \begin{cases} z = 1 \\ y = 0 \\ x = 0 \end{cases} \cup \begin{cases} z^2 + 2z - 1 = 0 \\ y = z \\ x = z \end{cases}$$

Differential elimination



"The" output system is a list of regular differential chains or differential characteristic sets.

Rankings indicate the sort of sought differential equations.

Technically, a ranking is an "admissible" total ordering on the derivatives of the dependent variables.
In the case of ODE in two dep. vars. $u(t)$ and $v(t)$ it might be :

$$\cdots > \ddot{u} > \dot{v} > \dot{u} > v > u.$$

Bibliography

E. R. Kolchin.
Differential Algebra and Algebraic Groups.
Academic Press (1973).

J. F. Ritt.
Differential Algebra.
Dover Publ. Inc. (1950).
http://www.ams.org/online_bks/coll33.

M. Kalkbrener
Three contributions to elimination theory
Johannes Kepler University, Linz (1991)

W.-T. Wu.
On the foundation of algebraic differential geometry.
MM, research preprints (1989).

Example : a DAE (Hairer, Wanner)

The unknowns are three functions $x(t)$, $y(t)$ and $z(t)$.

$$\left\{ \begin{array}{rcl} \dot{x}(t) & = & 0.7 \cdot y(t) + \sin(2.5 \cdot z(t)) \\ \dot{y}(t) & = & 1.4 \cdot x(t) + \cos(2.5 \cdot z(t)) \\ 1 & = & x^2(t) + y^2(t). \end{array} \right.$$

Differential elimination helps integrating the DAE by computing

- the underlying ODE $\dot{z}(t) = \textit{something}$
- a complete set of constraints on initial values

Demo using *DifferentialAlgebra*

- Convert the DAE into a polynomial DAE

$$\left\{\begin{array}{rclcrcl} \dot{x}(t) & = & 0.7\cdot y(t)+s(t) & \quad & \dot{s}(t) & = & 2.5\cdot \dot{z}(t)\cdot c(t) \\ \dot{y}(t) & = & 1.4\cdot x(t)+c(t) & & \dot{c}(t) & = & -2.5\cdot \dot{z}(t)\cdot s(t) \\ 1 & = & x^2(t)+y^2(t) & & 1 & = & s^2(t)+c^2(t). \end{array}\right.$$

- Use *DifferentialRing* to set the ranking.
- Use *RosenfeldGroebner* to perform differential elimination.
- *DifferentialAlgebra* is just an interface MAPLE package for the BLAD libraries (open source, LGPL, C language, 40000 lines)

The set of equations "consequences" of the DAE

This set has the structure of a (radical) differential ideal.

Inference rules applied by Rosenfeld-Gröbner

Let a, b be two differential polynomials

1. $a = 0$ and $b = 0 \Rightarrow a + b = 0$
2. $a = 0$ and $b = ? \Rightarrow a\, b = 0$
3. $a = 0 \Rightarrow \delta a = 0$
4. $a\, b = 0 \Rightarrow a = 0$ or $b = 0$

A word on rankings

Let I be the differential ideal associated to the DAE.

```
R := DifferentialRing (derivations = [t], blocks = [[x,y,s,c,z]])
RosenfeldGroebner (DAE, R) ;
```

regchain

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regchain

- The ranking is orderly.
- The *regchain* involves the elements of I of lowest order in all dep. vars.

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```

regchain

- The ranking eliminates x w.r.t y, s, c, z.
  It eliminates y w.r.t. s, c, z and so on ...
- The *regchain* involves the element of I of lowest order in z, which only depends on z.
- It also involves the element of I of lowest order in c, which only depends on c and z.
- And so on ...

A word on rankings

Let I be the differential ideal associated to the DAE.

R := DifferentialRing (derivations = [t], blocks = [[x,y],[s,c,z]])
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A word on rankings

Let I be the differential ideal associated to the DAE.

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regchain

- The ranking eliminates (x, y) w.r.t. (s, c, z).
  It is a block elimination ranking.
- The *regchain* involves the element of I of lowest order in s, c, z which only depend on s, c, z.
- It also involves the element of I of lowest order in x, y which depend on all the dep. vars.

Implicitizations, Ranking Conversions

For $\mathcal{R} = x > y > z > s > t$ and $\overline{\mathcal{R}} = t > s > z > y > x$:

$$\text{convert}(\begin{cases} x - t^3 \\ y - s^2 - 1 \\ z - s\,t \end{cases}, \mathcal{R}, \overline{\mathcal{R}}) = \begin{cases} s\,t - z \\ (x\,y + x)s - z^3 \\ z^6 - x^2y^3 - 3x^2y^2 - 3x^2y - x^2 \end{cases}$$

For $\mathcal{R} = \cdots > v_{xx} > v_{xy} > \cdots > u_{xy} > u_{yy} > v_x > v_y > u_x > u_y > v > u$ and
$\overline{\mathcal{R}} = \cdots u_x > u_y > u > \cdots > v_{xx} > v_{xy} > v_{yy} > v_x > v_y > v$:

$$\text{convert}(\begin{cases} v_{xx} - u_x \\ 4\,u\,v_y - (u_x\,u_y + u_x\,u_y\,u) \\ u_x^2 - 4\,u \\ u_y^2 - 2\,u \end{cases} \mathcal{R}, \overline{\mathcal{R}}) = \begin{cases} u - v_{yy}^2 \\ v_{xx} - 2\,v_{yy} \\ v_y\,v_{xy} - v_{yy}^3 + v_{yy} \\ v_{yy}^4 - 2\,v_{yy}^2 - 2\,v_y^2 + \end{cases}$$

Bibliography

F. Boulier, D. Lazard, F. Ollivier, M. Petitot.
Representations for the radical of a finitely generated differential ideal
Proc. ISSAC. 1995.

F. Boulier, F. Lemaire, M. Moreno Maza.
PARDI!
ISSAC (2001).

E. Hairer, G. Wanner.
Solving ordinary differential equations II. Stiff and Differential–Algebraic Problems
Springer-Verlag. 1996.

How does Rosenfeld-Gröbner work ?

- The Rosenfeld-Gröbner algorithm computes a triangular decomposition of the input system into differential regular chains.
- This algorithm relies on three key routines : differentiation, pseudo-division and GCD modulo **algebraic** regular chains.
- The same holds for the Pardi algorithm.
- Hence, improvements on the algebraic side benefit to the differential side.
- Therefore, there is today a great potential of algebraic technology transfert !

Modular Methods

$$
\begin{array}{ccc}
F \subset \mathbb{Q}[x_1, \ldots, x_n] \\ p \text{ prime}, \; p > A(F) & \longrightarrow & Eq.D._{\mathbb{Q}}(F) \\
\Big\downarrow \text{Triang.}(F \mod p) & & \Big\uparrow \textit{Lifting} \\
\{T^1, \ldots, T^s\} \\ \subset \mathbb{F}_p[x_1, \ldots, x_n] & \xrightarrow{\textbf{Split + Merge}} & Eq.D._{\mathbb{F}_p}(F)
\end{array}
$$

- $A(F) := 2n^2 d^{2n+1}(3h + 7\log(n+1) + 5n \log d + 10)$ where h and d upper bound coeff. sizes and total degrees for $f \in F$. Assumes F square and generates a 0-dimensional radical ideal.
- In practice we choose p much smaller with a probability of success, i.e. $> 99\%$ with $p \approx ln(A(F))$.

Modular Methods

$F \subset \mathbb{Q}[x_1, \ldots, x_n]$
p prime, $p > A(F)$ $\longrightarrow$ $Eq.D._{\mathbb{Q}}(F)$

Triang.$(F \mod p)$ $\downarrow$ $\qquad$ $\uparrow$ *Lifting*

$\{T^1, \ldots, T^s\}$
$\subset \mathbb{F}_p[x_1, \ldots, x_n]$ $\xrightarrow{\textbf{Split} + \textbf{Merge}}$ $Eq.D._{\mathbb{F}_p}(F)$

- $A(F) := 2n^2 d^{2n+1}(3h + 7\log(n+1) + 5n \log d + 10)$ where h and d upper bound coeff. sizes and total degrees for $f \in F$. Assumes F square and generates a 0-dimensional radical ideal.
- In practice we choose p much smaller with a probability of success, i.e. $> 99\%$ with $p \approx ln(A(F))$.

Fast Computation of Normal Froms

- Normal form computations are used for simplification and equality test of algebraic expressions modulo a set of relations.

$$y^3x + yx^2 \equiv 1 - y \mod x^2 + 1, y^3 + x$$

- By extending the fast division trick (Cook 1966) (Sieveking 72) (Kung 74) we have obtained “nearly optimal” algorithms when the numbers of rules and variables are equal
- Relaxing this constraint and adapting to differential normal forms is work in progress.

Bibliography

X. Li, M. Moreno Maza and W. Pan
Computations modulo regular chains
In proc. of ISSAC 2009.

X. Dahan, M. Moreno Maza, É. Schost, W. Wu and Y. Xie
Lifting techniques for triangular decompositions
In proc. ISSAC'05

M. Moreno Maza and Y. Xie
Balanced Dense Polynomial Multiplication on Multicores.

O. Golubitsky, M. Kondratieva, M. Moreno Maza and A. Ovchinnikov
A bound for the Rosenfeld-Gröbner Algorithm
Journal of Symbolic Computation, 2007

The Michaelis-Menten reduction revisited

The basic enzymatic reaction system

$$E + S \underset{k_2}{\overset{k_1}{\rightleftarrows}} C \xrightarrow{k_3} E + P$$

Basic differential model :

$$\begin{aligned} \dot{E} &= k_3\, C - k_1\, E\, S + k_2\, C\,, \\ \dot{S} &= -k_1\, E\, S + k_2\, C\,, \\ \dot{C} &= -k_3\, C + k_1\, E\, S - k_2\, C\,, \\ \dot{P} &= k_3\, C\,. \end{aligned}$$

The approximation, assuming mainly : $k_1,\ k_2 \gg k_3$

$$\dot{S} = -\frac{V_{\max}\, S}{K + S}$$

$V_{\max}$ and K being parameters.

The Michaelis-Menten reduction revisited

$$E + S \underset{k_2}{\overset{k_1}{\rightleftarrows}} C \xrightarrow{k_3} E + P$$

Red terms are the contributions of the fast reaction.

$$\begin{aligned}
\dot{E} &= k_3\, C - (k_1\, E\, S - k_2\, C)\,,\\
\dot{S} &= -(k_1\, E\, S - k_2\, C)\,,\\
\dot{C} &= -k_3\, C + k_1\, E\, S - k_2\, C\,,\\
\dot{P} &= k_3\, C\,.
\end{aligned}$$

The Michaelis-Menten reduction revisited

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_3} E + P$$

- Encode the conservation of the flow by replacing the contribution of the fast reaction by a new symbol F_1.

$$\begin{aligned} \dot{E} &= k_3\, C - F_1\,, \\ \dot{S} &= -F_1\,, \\ \dot{C} &= -k_3\, C + F_1\,, \\ \dot{P} &= k_3\, C\,. \end{aligned}$$

The Michaelis-Menten reduction revisited

$$E + S \underset{k_2}{\overset{k_1}{\rightleftarrows}} C \xrightarrow{k_3} E + P$$

- Encode the conservation of the flow by replacing the contribution of the fast reaction by a new symbol F_1.
- Encode the speed by adding the equilibrium equation.

$$\begin{aligned}
\dot{E} &= k_3\,C - F_1\,,\\
\dot{S} &= -F_1\,,\\
\dot{C} &= -k_3\,C + F_1\,,\\
\dot{P} &= k_3\,C\,,\\
0 &= k_1\,E\,S - k_2\,C\,.
\end{aligned}$$

The Michaelis-Menten reduction revisited

$$E + S \underset{k_2}{\overset{k_1}{\rightleftarrows}} C \xrightarrow{k_3} E + P$$

- Encode the conservation of the flow by replacing the contribution of the fast reaction by a new symbol F_1.
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- Raw formula by eliminating F_1 from Lemaire's DAE.

$$\dot{S} = -\frac{k_1^2\, k_3\, E\, S^2 + k_1\, k_2\, k_3\, E\, S}{k_1\, k_2\,(E+S) + k_2^2}.$$

Bibliography

V. Van Breusegem, G. Bastin.
Reduced order dynamical modelling of reaction systems : a singular perturbation approach
30th IEEE Conf. on Decision and Control. (1991).

N. Vora, P. Daoutidis.
Nonlinear model reduction of chemical reaction systems.
AIChE Journal vol. 47 (2001).

F. Boulier, M. Lefranc, F. Lemaire, P.-E. Morant.
Model Reduction of Chemical Reaction Systems using Elimination.
MACIS (2007). Submitted to MCS.
http://hal.archives-ouvertes.fr/hal-00184558