Differential Algebra : Applications, Software and Theory

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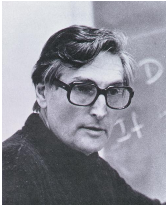
Differential Algebra



- Joseph Fels Ritt wrote *Differential Equations from an Algebraic Standpoint* (1932) and *Differential Algebra* (1950).
- Ellis Robert Kolchin wrote *Differential Algebra and Algebraic Groups* (1973).

The Problem

- Parametric version of a steering wheel model by Hairer, Wanner (1996). Nonlinear DAE has differentiation index 2.
- The ODE $\dot{z}(t) = \textit{something}$ is missing.

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

$$\begin{cases} \dot{x}(t) &= a\,y(t) + \sin(b\,z(t)) \\ \dot{y}(t) &= 2\,a\,x(t) + \cos(b\,z(t)) \\ 0 &= x(t)^2 + y(t)^2 - 1\,. \end{cases}$$

- The DAE implies the following constraint. Before numerical integration, one needs consistent initial values.

$$x(t)^4 = -\frac{2\cos(b\,z(t))}{3\,a}\left(x(t)^3 - x(t)\right) + \left(1 - \frac{1}{9\,a^2}\right)x(t)^2 + \frac{\cos(b\,z(t))^2}{9\,a^2}.$$

Differential Polynomial Reformulation

Define

$$s(t) = \sin(b\,z(t))\,, \qquad c(t) = \cos(b\,z(t))\,.$$

The two new unknown functions $s(t)$ and $c(t)$ are subject to :

$$\left\{\begin{array}{rcl} \dot{s}(t) & = & b\,\dot{z}(t)\,c(t)\,, \\ 1 & = & s(t)^2 + c(t)^2\,. \end{array}\right.$$

One gets a system of five differential polynomials :

$$\Sigma\ \left\{\begin{array}{rcl} \dot{x}(t) & = & a\,y(t) + s(t)\,, \\ \dot{y}(t) & = & 2\,a\,x(t) + c(t)\,, \\ \dot{s}(t) & = & b\,\dot{z}(t)\,c(t)\,, \\ 1 & = & x(t)^2 + y(t)^2\,, \\ 1 & = & s(t)^2 + c(t)^2\,. \end{array}\right.$$

Differential Polynomial (Rings)

A derivation over a ring $\mathscr{R}$ is a unary operation δ such that

$$\delta(a+b) = \delta(a) + \delta(b)\,, \quad \delta(a\,b) = a\,\delta(b) + \delta(a)\,b\,.$$

A ring (or a field) endowed with a derivation is a differential ring (or field). The equations of Σ can be viewed as having coefficients in

$$\mathscr{F} = \mathbb{Q}(a, b)\,.$$

They belong to the differential polynomial ring

$$\mathscr{R} = \mathscr{F}\{x, y, z, s, c\}$$

which is the ring of all polynomials in the infinite set of all derivatives of the differential indeterminates x, y, z, s, c, with coefficients rational fractions in a, b.

Differential Ideals (Motivation)

We have the following differential polynomials in Σ :

$$\begin{cases} \dot{s}(t) & = & b\,\dot{z}(t)\,c(t)\,, \\ 1 & = & s(t)^2 + c(t)^2\,. \end{cases}$$

But what about

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Substitute $\dot{s}(t) \to b\,\dot{z}(t)\,c(t)$:

$$0 = 2\,s(t)\,b\,\dot{z}(t)\,c(t) + 2\,c(t)\,\dot{c}(t)\,.$$

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Solve w.r.t. $\dot{c}(t)$:

$$\dot{c}(t) = -\frac{2\,s(t)\,b\,\dot{z}(t)\,c(t)}{2\,c(t)} = -b\,\dot{z}(t)\,s(t)\,.$$

Perfect Differential Ideals

Def. The perfect differential ideal $\{\Sigma\}$ generated by Σ :

$$\Sigma \subset \{\Sigma\}\,, \quad A,\, B \in \{\Sigma\} \Rightarrow A + B \in \{\Sigma\}\,, \quad A \in \{\Sigma\},\, B \in \mathscr{R} \Rightarrow A\,B \in \{\Sigma\}\,,$$
$$\exists\, n \in \mathbb{N},\, A^n \in \{\Sigma\} \Rightarrow A \in \{\Sigma\}\,, \quad A \in \{\Sigma\} \Rightarrow \dot{A} \in \{\Sigma\}$$

Thm of zeros. The ideal $\{\Sigma\}$ is the set of all differential polynomial (equations) that could be added to Σ without changing its analytic solutions.

Our computations proved (straightforward) that

$$2\, s(t)\, b\, \dot{z}(t)\, c(t) + 2\, c(t)\, \dot{c}(t) \in \{\Sigma\}\,.$$

But what about the division by $2\, c(t)$?

$$s(t)\, b\, \dot{z}(t) + \dot{c}(t) \overset{?}{\in} \{\Sigma\}\,.$$

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Indeed,

$$s(t)\, b\, \dot{z}(t) + \dot{c}(t) \in \{\Sigma\}$$

but this does not come from the definition of ideals : one can prove that $2\,c(t)$ is not a zero-divisor modulo $\{\Sigma\}$. Had it been a zero-divisor, it would have been convenient to split cases and study :

$$\{\Sigma\} = \underbrace{\{\Sigma\} : c^\infty}_{c \text{ does not divide zero here}} \cap \underbrace{\{\Sigma,\, c\}}_{c \text{ is zero here}} \,.$$

Rankings

During computations, new equations regularly show up e.g.

$$\dot{s}(t) - b\,\dot{z}(t)\,c(t) = 0\,.$$

There are three derivatives w.r.t which solving and substituting :

$$\dot{s}(t) \to b\,\dot{z}(t)\,c(t)\,, \quad \dot{z}(t) \to \frac{\dot{s}(t)}{b\,c(t)}\,, \quad c(t) \to \frac{\dot{s}(t)}{b\,\dot{z}(t)}\,.$$

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Which one ? The choice is done by fixing a ranking.

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Ex. W.r.t. the following ranking

$$\cdots > \dot{s}(t) > \dot{z}(t) > \dot{c}(t) > s(t) > z(t) > c(t) > a > b$$

the subtitution is :

$$\dot{s}(t) \to b\,\dot{z}(t)\,c(t)\,.$$

Rankings (exercises and software notation)

Question. A DAE Σ depends on differential indeterminates

$$\{x(t), y(t), z(t), c(t), s(t)\}.$$

You are looking for its variety of constraints, i.e the order zero differential polynomial which belong to $\{\Sigma\}$. Which ranking do you provide to the simplifier ?

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You are looking for its variety of constraints, i.e the order zero differential polynomial which belong to $\{\Sigma\}$. Which ranking do you provide to the simplifier ?

Answer. A ranking such that order zero derivatives are lower than nonzero order ones.

Such orderly rankings are denoted using two levels of square brackets. Here is an example :

$$[[x, y, z, c, s]]\,.$$

Rankings (exercises and software notation)

Question. A dynamical system depends on state variables $x_1(t)$ and $x_2(t)$, an input $u(t)$ and an output $y(t)$. You are looking for the IO equation, i.e. an equation that binds $u(t), y(t)$ and their derivatives but is free of the state variables. Which ranking do you provide to the simplifier ?

Rankings (exercises and software notation)

Question. A dynamical system depends on state variables $x_1(t)$ and $x_2(t)$, an input $u(t)$ and an output $y(t)$. You are looking for the IO equation, i.e. an equation that binds $u(t), y(t)$ and their derivatives but is free of the state variables. Which ranking do you provide to the simplifier ?

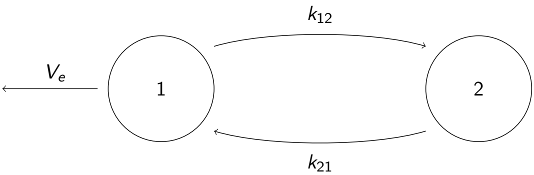
Answer. A ranking such that any derivative of $y(t)$ and $u(t)$ is lower than any derivative of the state variables.

An example of such a block elimination ranking can be denoted :

$$[[x1, x2], [y, u]] \, .$$

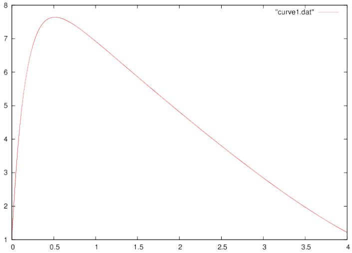
An Academic Nonlinear Dynamical System

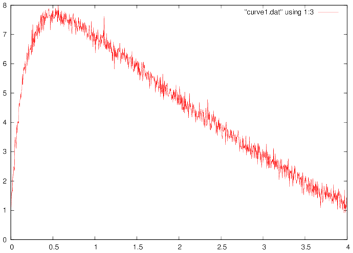
Three parameters k_{12}, k_{21}, V_e to be estimated.



$$
\begin{aligned}
\dot{x}_1(t) &= -k_{12}\, x_1(t) + k_{21}\, x_2(t) - \frac{V_e\, x_1(t)}{1 + x_1(t)}\,, \\
\dot{x}_2(t) &= k_{12}\, x_1(t) - k_{21}\, x_2(t)\,, \\
y(t) &= x_1(t)\,.
\end{aligned}
$$

The Estimation Problem





The leftmost curve is obtained by numerically integrating the model equations for $t = [0, 4]$, with

$$(x_1(0), x_2(0), k_{12}, k_{21}, V_e) = (1, 10, 1, 5, 3)\,.$$

The rightmost one is obtained by adding to it a white Gaussian noise with standard deviation $\sigma = 0.2$.

Computation of the IO Equation

Applying differential elimination over the model equations and a block elimination ranking such as

$$[[x_1, x_2], y, [k_{12}, k_{21}, V_e]]$$

one gets $(\mathrm{IO})_{\mathrm{diff}}$:

$$\begin{aligned}\ddot{y}(t)\, y(t)^2 + 2\,\ddot{y}(t)\, y(t) + \ddot{y}(t) & \\ + \dot{y}(t)\, y(t)^2\, \theta_2 + 2\,\dot{y}(t)\, y(t)\, \theta_2 & \\ + \dot{y}(t)\, \theta_3 + y(t)^2\, \theta_1 + y(t)\, \theta_1 &= 0\end{aligned}$$

where the θ_i stand for the blocks of parameters :

$$\theta_1 = k_{21}\, V_e\,, \quad \theta_2 = k_{12} + k_{21}\,, \quad \theta_3 = k_{12} + k_{21} + V_e\,.$$

Where Does [BLRR13] Apply ?

By collecting and factoring coefficients, one even gets $(\mathrm{IO})_{\mathrm{diff}}$:

$$
\begin{aligned}
k_{21}\, V_e\, \frac{y(t)}{y(t)+1} \\
+ (k_{12}+k_{21})\, \frac{y(t)\,\dot{y}(t)\,(y(t)+2)}{(y(t)+1)^2} \\
+ (k_{12}+k_{21}+V_e)\, \frac{\dot{y}(t)}{(y(t)+1)^2} &\quad = \quad -\ddot{y}(t)
\end{aligned}
$$

But one can do better than that !

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Our [BLRR13] algorithm rewrites it as :

$$\begin{aligned} & k_{21}\, V_e\, \frac{y(t)}{y(t)+1} \\ + & (k_{12}+k_{21})\, \frac{\mathrm{d}}{\mathrm{d}t}\, \frac{y(t)^2}{y(t)+1} \\ - & (k_{12}+k_{21}+V_e)\, \frac{\mathrm{d}}{\mathrm{d}t}\, \frac{1}{y(t)+1} \quad = \quad -\frac{\mathrm{d}^2}{\mathrm{d}t^2}\, y(t) \end{aligned}$$

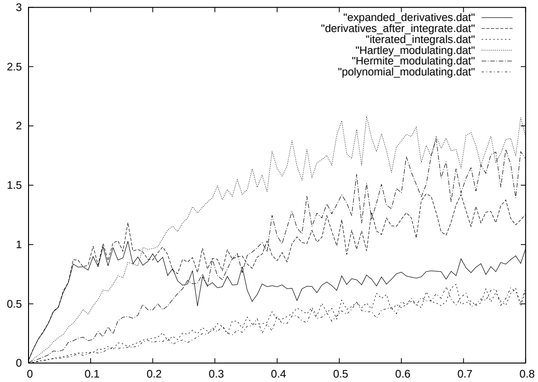
Where Does [BKLPPU14] Apply ?

Because the $\frac{\mathrm{d}}{\mathrm{d}t}$ operator is factored out it is easy to convert the differential equation $(\mathrm{IO})_{\mathrm{diff}}$ into the integral equation $(\mathrm{IO})_{\mathrm{int}}$:

$$\begin{aligned} k_{21}\,V_e \int_0^t \int_0^t \frac{y(t)}{y(t)+1}\,\mathrm{d}t\,\mathrm{d}t & \\ +\,(k_{12}+k_{21})\left(\int_0^t \frac{y(t)^2}{y(t)+1}\,\mathrm{d}t - \frac{y(0)^2}{y(0)+1}\,t\right) & \\ -\,(k_{12}+k_{21}+V_e)\left(\int_0^t \frac{1}{y(t)+1}\,\mathrm{d}t - \frac{1}{y(0)+1}\,t\right) & \\ -\,\dot{y}(0)\,t &= -y(t)+y(0) \end{aligned}$$

Viewing $\dot{y}(0)$ as a parameter, no derivative of $y(t)$ occurs anymore.

Results From [BKLPPU14]



Abscissa : the standard deviation σ used to produce the noise.
Ordinate : the relative error of estimated blocks of parameters.
Experiments using plain integral equations, modulating functions,

On the Integration Algorithm

A ranking is a total ordering on the derivatives, satisfying some axioms (compatibility conditions with differentiation).

Def. The leader of a differential fraction F is the highest derivative v such that $\partial F / \partial v \neq 0$.

By the axioms of rankings

$$\dot{F} = \underbrace{\left(\frac{\partial F}{\partial v}\right)}_{\text{leader of } F} \underbrace{\dot{v}}_{\text{degree } 1} + \underbrace{\cdots}_{\text{derivatives less than } \dot{v}}$$

The Integrate algorithm starts from a fraction G and tries to recover F such that $G = \dot{F}$ by pattern matching.

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$$\dot{F} = \left(\frac{\partial F}{\partial v}\right) \dot{v} + \cdots$$

leader of F

degree 1

derivatives less than $\dot{v}$

If G does not match, the Integrate algorithm removes the "smallest" part which prevents the pattern matching.

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The Integrate algorithm is easy for polynomials, difficult for fractions. A flaw in [BLRR13] was fixed in [BKLPPU14].

Conclusion

Long Term Goal. Have differential algebra methods present in major scientific computation software.

Software. These methods must be provided in a good software library.

- Simple Programming Interface
- Portability
- Reliability

Speed is not a major concern.

The open source BLAD library is already available.

A new project for a complete redesign and implementation has been started. Temporary nickname : BLATTE.