Algebraic Constraints on Initial Values of Differential Equations

F. Leon Pritchard[†] and William Y. Sit[‡]

[†] Dept. of Math. and Comp. Sci., York College and Graduate Center, CUNY, U.S.A.
[‡] Dept. of Math., The City College of CUNY, U.S.A. (speaker)

June 25–28, 2009
Applications of Computer Algebra 2009

A Quotation from Gear, 2006

Interestingly, electrical networks were originally modelled with ODEs and a lot of sophisticated techniques were developed to reduce a network to ODEs. ...Initially these were index one problems, so did not present the DAE difficulties of higher index problems, but newer modelling approaches have lead [sic] to index two problems (e.g., [19]) and the problems have become so large and non-linear that some aspects of them, such as *finding consistent initial conditions, are extremely challenging*.

Mechanical systems with constraints usually lead to **index three problems** that cannot be solved directly. *The constraints in a DAE restrict the solution to a manifold and usually we cannot easily find the ODE on that manifold*.

Main Steps of Our Approach

We combined and modified approaches of **Thomas, Rabier and Rheinboldt** but **with no restrictions** on input form.

- transformations to quasi-linear systems
- the concepts of *essential degree* and *algebraic index* and algorithms to compute these
- algorithms for *prolongation and completion*
- **generalized concepts** of quasi-linearity
- **sufficient conditions for existence and uniqueness theorem**
- **algorithm** to compute constraints on initial conditions
- **algorithm** to compute explicit vector field
- examples and **implementation** in *Axiom*

Transformations to Quasi-linear Systems

By adding new variables and the chain rule, we can convert:

- an explicit system with rational right hand sides to a explicit **polynomial** system.
- a non-autonomous system to an **autonomous** system
- a high order system to a **first order** system
- an analytic system (with some limitation) to a **differential algebraic system**
- a non-linear system to a **quasi-linear system** (**quasi-linearization**)

(Non-linear) First Order DAE System

- Algebraic Indeterminates:

$$\begin{aligned} \mathbf{X} &= (X_1, \cdots, X_n), \\ \mathbf{P} &= (P_1, \cdots, P_n). \end{aligned}$$

  Polynomials $f_i(\mathbf{X}, \mathbf{P}) \in \mathbf{C}[\mathbf{X}, \mathbf{P}]$ for $1 \leqslant i \leqslant m$.

- Dependent Variables: $z = (z_1, \ldots, z_n)$
  First Order Derivatives: $\dot{z} = \dot{z}_1, \ldots, \dot{z}_n$ (with respect to t)

  Any system of first order ordinary DAE:

$$f_i(z_1, \cdots, z_n, \dot{z}_1, \cdots, \dot{z}_n) = 0, \quad 1 \leqslant i \leqslant m$$

  Initial conditions: $z(0) = \mathbf{x}_0$ where $\mathbf{x}_0 \in \mathbf{C}^n$.

Essential P-degree Basis and $\mathbf{P}$-Strong Basis

- The *essential* $\mathbf{P}$*-degree* d of a non-zero ideal J of $\mathbf{C}[\mathbf{X}, \mathbf{P}]$ is the least $\mathbf{P}$-degree of a finite set F generating J. Such an F is an *essential* $\mathbf{P}$*-degree basis*.

- A subset F of J is $\mathbf{P}$*-strong* if it generates all polynomials f in J of $\mathbf{P}$-degree $\leqslant d$ without involving cancellations of terms of $\mathbf{P}$-degree higher than the $\mathbf{P}$-degree of f.

- Specifically, $f = \sum_{j=1}^{N} h_j f_j$ with $h_j \in \mathbf{C}[\mathbf{X}, \mathbf{P}]$, $h_j \neq 0$, $f_j \in F$ and $\mathbf{P}$-deg $h_j f_j \leqslant \mathbf{P}$-deg f.

Algorithm for Essential P-Degree P-Strong Basis

- Using a **P**-degree compatible elimination term ordering where $\mathbf{X} < \mathbf{P}$, compute a Gröbner basis G of the ideal $J = (F)$.

- **The essential P-degree d is the least k such that the elements P-degree $\leqslant k$ in G generates J.**

- **The set E_d of those elements of G is a P-strong essential P-degree basis of J.**

Prolongation of an Ideal

- *prolongation*: For arbitrary $h \in \mathbf{C}[\mathbf{X}]$, let $\nabla h = \sum_{j=1}^{n} \frac{\partial h}{\partial X_j} P_j$ in $\mathbf{C}[\mathbf{X}, \mathbf{P}]$.

- The *prolongation ideal* J^* of an ideal J is the ideal generated by J, R, and ∇R, where $R = \sqrt{J \cap \mathbf{C}[\mathbf{X}]}$

- **Algorithm for Prolongation**:
  The prolongation ideal can be computed from any generating set of J. We need only to prolong generators of R, which can be computed.

- Prolongation only introduces polynomials of $\mathbf{P}$-degree $\leqslant 1$.

Completion Ideal and Algebraic Index

- An ideal J is *complete* if $J = J^*$.
  The intersection of complete ideals of $\mathbf{C}[\mathbf{X}, \mathbf{P}]$ is complete.
  The *completion ideal* of J is the smallest complete ideal $\widetilde{J}$ containing J.

- **Algorithm for Completion**: Just keep prolonging till it stops at $\widetilde{J}$.
  The *algebraic index* p is the smallest number of prolongation to obtain a complete ideal.

- Use of an essential $\mathbf{P}$-degree basis for J keeps $\mathbf{P}$-degree low.

Geometric Property

- *first jet domain* V = algebraic set of zeros of J
  initial domain W = algebraic set of zeros of $J \cap \mathbf{C}[\mathbf{X}]$
  = algebraic set of zeros of R
  projection $\pi : V \longrightarrow W$
  an open subset $W^0 = \{\mathbf{x} \mid \pi^{-1}(\mathbf{x}) \ \ \textbf{is finite}\}$

- *tangent variety* $T(W)$ = algebraic set of zeros in $\mathbf{C}^{2n}$ of
  $(R \cup \nabla R)$

- J **complete implies** $V \subseteq T(W)$

Quasi-Linearities and Associated Quasi-linear Ideal

- An ideal J of $\mathbf{C}[\mathbf{X}, \mathbf{P}]$
  (a) is (essentially) *quasi-linear* if $\mathrm{edeg}_{\mathbf{P}}(J) \leqslant 1$.
  (b) is *eventually quasi-linear* if its completion $\widetilde{J}$ is quasi-linear.

- Every J has an *associated quasi-linear ideal* J^{ℓ}, which is generated by the set of all polynomials of $\mathbf{P}$-degree at most 1 in J.
  If E a P-strong subset of J, then J^{ℓ} is generated by E_1, the subset of E of P-degree $\leqslant 1$.

Properties

- **Properties**:(i) J quasi-linear implies $\widetilde{J}$ quasi-linear;
(iiı) $V \subseteq V^{\ell}$ and $W = W^{\ell}$ (hence $T(W) = T(W^{\ell})$)
(iii) J is complete if and only if J^{ℓ} is complete
(iv) ind $J^{\ell} \leqslant$ ind J.

- All are concepts: essential **P**-degree, prolongation, completion, quasi-linearities are ideal-theoretic, yet all algorithms are simple in an intuitive way, providing flexibility in implementation.

Existence and Uniquenss Theorems Summary

- Given arbitrary system of first order DAEs (or an ideal J), we can compute a Zariski-closed subset M of $\mathbf{C}^n$ and find an **open subset M^0 as a finite irredundant union of non-empty Zariski open sets U_k.**
- The solution to the initial value problem for any $\mathbf{x}_0 \in U_k$ can be uniquely defined by a **vector field:** $\dot{\psi}_{\mathbf{x}}(t) = \mathbf{r}_k(\psi_{\mathbf{x}}(t))$, where $\mathbf{r}_k$ is a vector of rational functions in $\mathbf{C}(\mathbf{X})^n$ defined on U_k.
- Furthermore, for any **$\mathbf{x} \notin M$, the initial value problem $(J, \mathbf{x})$ does not admit a solution** on interval $(-\epsilon, \epsilon)$ in $\mathbf{C}^n$ for any $\epsilon > 0$.
- Note: the theorem, due to its generality, **allows for degenerate situations** such as M^0 is empty.

Methods for E&U Theorems

- The theorem for E&U of analytic solutions is **first proved** for any given initial value problem defined by a **complete quasi-linear ideal**, using a classical E&U theorem and a result on parametric linear systems.
- The computations of algebraic constraints and equivalent vector fields are made effective by introducing the *linear rank at a point*, proving its relation to matrix rank, obtaining an algorithm to compute this rank, and characterizing the **set of points with maximum linear rank** as precisely W^0 for quasi-linear ideals.
- The theorem is then **generalized to a quasi-linear ideal**, and by passing to the associated quasi-linear ideal, **further to an arbitrary ideal**, again "**effectively**."

Algorithm for the General Case

- Given J, an ideal in $\mathbf{C}[\mathbf{X}, \mathbf{P}]$.
  Compute its completion ideal $\widetilde{J}$.
- Compute a **P**-strong essential **P**-degree basis $f_1, \ldots, f_m$ of the associated quasi-linear ideal $\widetilde{J}^\ell$ of $\widetilde{J}$.
- Compute an irredundant set of Zariski open sets $U_1, \ldots, U_\nu$ whose union is $M^0 = \widetilde{W}^0 = (\widetilde{W}^\ell)^0$.
- For $1 \leqslant k \leqslant \nu$, compute the **vectors of rational functions** $\mathbf{r}_k$ on U_k using Cramer's Rule (or other algorithms for parametric linear system).
- For any initial condition $\mathbf{x}_0$, use any U_k containing $\mathbf{x}_0$ to (numerically) **integrate the vector field** defined by $\mathbf{r}_k$.
- The symbolic part of the algorithm is implemented in Axiom.

Non Quasi-Linear Example

- $x(t), y(t)$ functions of t
- $p(t), q(t)$ their derivatives with respect to t

$$\begin{array}{rcrcl} & & pq & = & xy \\ -yp & + & 3xq & = & 3x^2+6 \\ & & 4q^2 & = & 9x^2 \\ & & p^2 & = & x^2-4 \end{array}$$

- The ideal J corresponding to this system is complete and has essential **P**-degree 2.

Illustration of the Algorithm

- An **essential P-degree basis** gives another presentation:

$$\begin{array}{rcrcl} & & q^2 & = & y^2+9, \\ 27p & + & 6xyq & = & 4y^3+54y, \\ & & (4y^2+54)q & = & 6xy^2+81x, \\ & & 0 & = & 9x^2-4y^2-36. \end{array}$$

- *Associated quasi-linear ideal*: Retaining only the quasi-linear equations: $\mathrm{rank}\,(J,\mathbf{x})=2$ whenever $27(4y^2+54)\neq 0$.
- The **explicit system** is

$$\mathbf{v}: p=\frac{2y}{3}, \qquad q=\frac{3x}{2}.$$

- The **integral curve** for $\mathbf{v}$ satisfying $x(0)=x_0, y(0)=y_0$ is

$$x=x_0\cosh(t)+\frac{2}{3}y_0\sinh(t), \qquad y=y_0\cosh(t)+\frac{3}{2}x_0\sinh(t).$$

Comments on Example

- This solution exists and lies on the (complex) **hyperbola** $9x^2 - 4y^2 - 36 = 0$ whenever (x_0, y_0) does.
- The solution satisfies $q^2(t) = y^2(t) + 9$ for all t.
- When $2y_0^2 + 27 = 0$, we have $x_0^2 + 2 = 0$.
- The 4 points $(\pm\sqrt{-2}, \pm 3\sqrt{-3/2})$ are **equilibrium solutions** of J^ℓ.
- They are *not* solutions of J, nor are equilibrium points of $\mathbf{v}$.
- At each of these 4 initial conditions, $(J^\ell, \mathbf{x})$ **does not have unique solutions**, but $(J, \mathbf{x})$ **does**.
- The sets of solutions for J^ℓ and J are not the same.

A Quasi-Linear Example

- $z_1(t), z_2(t), z_3(t)$ are functions of t
  $\dot{z}_1(t), \dot{z}_2(t), \dot{z}_3(t)$ are their derivatives with respect to t

$$\begin{array}{rcrcrcr} & - & z_2\dot{z}_2 & + & z_1\dot{z}_3 & = & z_1^4 \\ -z_2\dot{z}_1 & & & + & 2\dot{z}_3 & = & 5z_3 \\ z_3\dot{z}_1 & + & z_1^2\dot{z}_2 & & & = & 3z_2^2 \\ & - & z_1\dot{z}_2 & + & \dot{z}_3 & = & z_3 \end{array}$$

- **Algebraic constraints** found by symbolic computation:

$$z_1^2 = z_2, z_1^3 = z_3.$$

Explicit representation found by symbolic computation:

$$\dot{z}_1 = \frac{z_3}{z_2}, \quad \dot{z}_2 = 2z_2, \quad \dot{z}_3 = 3z_3, \quad z_2 \neq 0.$$

Some Statistics on the Example

- J contains an algebraic constraint of total degree 7 in $\mathbf{X}$. An essential **P**-degree basis of the completion ideal consists of 7 binomials of **P**-degree 1 and 4 binomial algebraic constraints.
- The ideal has index 3.

$X_1 > X_2 > X_3$	first prolongation	second prolongation
max deg in algebraic constraints	36	10
max coefficient in constraints	95 digits	30 digits
max **P**-degree in system	4	4

Maple (dsolve) ran out of memory on a PC with 2GB DRAM. Mathematica (DSolve) does not accept overdetermined systems. The same PC runs the Axiom algorithm.

Unconstrained and Underdetermined Ideals

- An ideal J in $\mathbf{C}[\mathbf{X}, \mathbf{P}]$ is *unconstrained* if $J \cap \mathbf{C}[\mathbf{X}] = (0)$. Unconstrained implies complete.

- J is *underdetermined* if $(\widetilde{W^\ell})^0 = \emptyset$.
Intuitively, underdetermined means there is no initial conditions $\mathbf{x}_0$ that will guarantee a unique solution. Either some dependent variable will be arbitrary, or there are multiple integral curves through $\mathbf{x}_0$.

- **These properties are algorithmically decidable.**

Underdetermined Quasi-Linear Example

- System (complete system, index 0):

$$\begin{array}{rcrcrcl} (-x+y)\dot{x} & + & x\dot{y} & + & (x^2-1)\dot{z} & = & 0 \\ y\dot{x} & + & (x^2+1)\dot{y} & + & x^3\dot{z} & = & 0 \end{array}$$

- Solutions: Every constant point is an **equilibrium solution**. Explicit System: **No algebraic constraints**. k arbitrary.

$$\begin{array}{rcl} \dot{x} & = & k \\ \dot{y} & = & k(x^4-(x^3+x^2-1)y) \\ \dot{z} & = & k(-x^3-x+(x^2-x+1)y) \end{array}$$

We can obtain unique solution by adding any quasi-linear equation $g(\mathbf{X}, \mathbf{P}) = 0$, for example $\dot{x} = 1$.

Conclusions

- Approach is ideal theoretic, providing maximum flexibility in implementation
- Applies to all eventually quasi-linear systems without any transformation
- Applies to overdetermined as well as underdetermined systems
- Applies to non-linear systems either by a transformation or by dropping some non-linear equations
- Any system may be completed with no *a priori* conditions.
- Existence and Uniqueness theorem holds for computed initial conditions
- Provides equivalent explicit form ready for numerical methods and dynamical analysis