Numeric-Geometric Techniques for Differential Equations I. Introduction

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1. Background and Motivation

- For a polynomially nonlinear PDE system, often need differentiation (*prolongation*) to cover all the system's constraints; and simplify them to check if they are "new" – *differential elimination*.
- Exact prolongation-elimination algorithms for exact polynomially nonlinear PDE are well studied in [1, 3, 4, **?**, **?**, **?**].
- Identify all hidden constraints and compute formal power series solutions in the neighborhood of a given point. Ready the system for numerical integration.

The Pendulum

Example (The Pendulum)

For the pendulum of unit mass, under constant gravity:

$$\begin{aligned} X_{tt} + \lambda X &= 0 \\ Y_{tt} + \lambda Y &= -g \\ X^2 + Y^2 &= 1. \end{aligned} \tag{1}$$

This DAE has singular Jacobian. Differentiate the third eqn. twice:

$$\begin{aligned} X X_t + Y Y_t &= 0 \quad \text{(velocity)} \\ X_t^2 + Y_t^2 + X X_{tt} + Y Y_{tt} &= 0 \quad \text{(acceleration)} \end{aligned}$$

- We need to differentiate the third eqn. twice to reduce this DAE to ODE. So for such differential systems, differentiation (Prolongation) is unavoidable.
- A major problem is the exploding size of prolongations, which causes huge non-linear systems with dramatically large Bezout numbers.

One PDE:

J^1

$u_x + v^3 = 0$

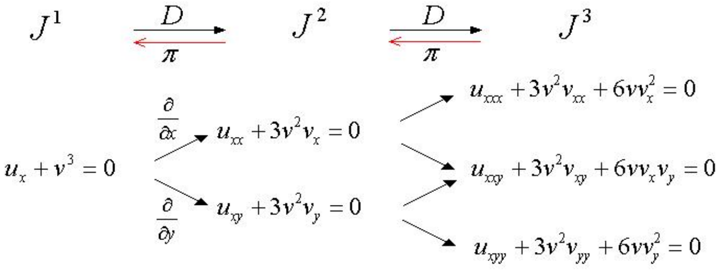
Prolongation once:

$$J^1 \underset{\pi}{\overset{D}{\rightleftarrows}} J^2$$

$$u_x + v^3 = 0 \quad \xrightarrow{\frac{\partial}{\partial x}} \quad u_{xx} + 3v^2 v_x = 0$$

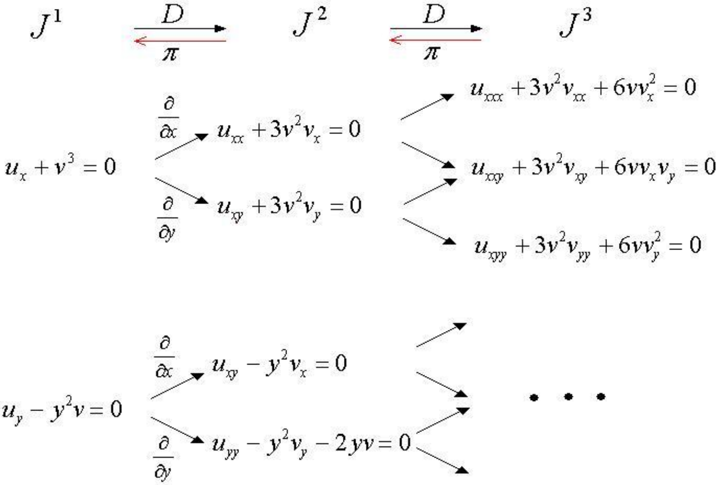
$$u_x + v^3 = 0 \quad \xrightarrow{\frac{\partial}{\partial y}} \quad u_{xy} + 3v^2 v_y = 0$$

Prolongation twice:

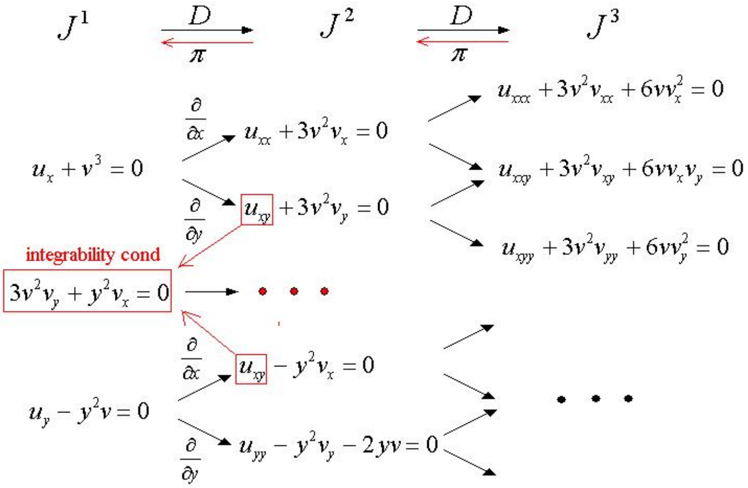


Total degree does not change, Bezout # increases exponentially.

Two PDEs:


J^1
D
π
J^2
D
π
J^3
$u_x + v^3 = 0$
$\frac{\partial}{\partial x}$
$u_{xx} + 3v^2 v_x = 0$
$\frac{\partial}{\partial y}$
$u_{xy} + 3v^2 v_y = 0$
$u_{xxx} + 3v^2 v_{xx} + 6vv_x^2 = 0$
$u_{xxy} + 3v^2 v_{xy} + 6vv_x v_y = 0$
$u_{xyy} + 3v^2 v_{yy} + 6vv_y^2 = 0$
$u_y - y^2 v = 0$
$\frac{\partial}{\partial x}$
$u_{xy} - y^2 v_x = 0$
$\frac{\partial}{\partial y}$
$u_{yy} - y^2 v_y - 2yv = 0$
• • •

Integrability Cond.



Might need more prolongation (and differential elimination) to cover all the integrability conditions,

2. Fundamental Problem

Find numerically stable methods to identify all hidden constraints without prolongation explosion and complicated differential elimination?

Two streams of research:

- stable methods for general systems
- fast methods for certain generic systems

Special in our approach - geometry.

3. Key Ideas

We identify a certain class of PDE (called square t-dominated systems):

- Only prolongations w.r.t one variable are needed.
- No elimination is needed.
- Connection to Riquier Basis $\longrightarrow$ algebraic interpretation.
- Genericity– any system is t-dominated after a random change of coordinates.

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4. PDE in Jet Space

Consider q-th order PDE system $R = (R^1, ..., R^\ell) = 0$ with indep vars $x = (x_1, x_2, ..., x_n)$ and dep vars $u = (u^1, u^2, ..., u^m)$ in a field $\mathbb{F}$ ($\mathbb{R}$ or $\mathbb{C}$). Consider a set of indeterminates $\Omega = \{v^i_\alpha \mid \alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n, i = 1, \cdots, m\}$ where each member of Ω corresponds to a partial derivative by:

$$v^i_\alpha \leftrightarrow \mathbf{D}^\alpha u^i(x_1, \cdots, x_n) := (\mathbf{D}_{x_n})^{\alpha_n} \cdots (\mathbf{D}_{x_1})^{\alpha_1} u^i(x_1, \cdots, x_n) \, .$$

The total derivative $\mathbf{D}_{x_i}$ act on functions of $\{x\} \cup \Omega$ by:

$$\mathbf{D}_{x_i} = \frac{\partial}{\partial x_i} + \sum_{v \in \Omega} (\mathbf{D}_{x_i} v) \frac{\partial}{\partial v} \tag{2}$$

The PDE system R is associated with a **Jet Variety**

$$Z(R) := \{(x, v^i_\alpha) \in J^q(\mathbb{F}^n, \mathbb{F}^m) : R^k(x, v^i_\alpha) = 0, k = 1, ..., \ell\} \tag{3}$$

where $J^q(\mathbb{F}^n, \mathbb{F}^m)$ is the **Jet space** of order q.

4. PDE in Jet Space

Consider q-th order PDE system $R = (R^1, ..., R^k) = 0$ with indep vars $x = (x_1, x_2, ..., x_n)$ and dep vars $u(x) = (u^1(x), u^2(x), ..., u^m(x))$

Denoting $\underset{r}{u}$ as the formal (jet) variables corresponding to r-th order partial derivatives of $u(x)$ the jet variety is

$$V(R) := \{(x, u, \underset{1}{u}, ..., \underset{q}{u}) \in J^q : R(x, u, \underset{1}{u}, ..., \underset{q}{u}) = 0\}$$

Here $R^k : J^q \to \mathbb{C}$, $J^q = \mathbb{C}^{N_q}$ and $N_q = \#$ jet variables $\leq q$.

Example: $V(R) = \{(x, u, u_x) : u_x^2 + u^2 + x^2 = 1\}$

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Example: Extended Solutions lying in $V(R)$

Example (The Pendulum)

$$\begin{aligned} X_{tt} + \lambda X &= 0 \\ Y_{tt} + \lambda Y &= -g \\ X^2 + Y^2 &= 1. \end{aligned} \tag{4}$$

Here

$$Z(R) = \{(t, X, Y, \lambda, X_t, Y_t, \lambda_t, X_{tt}, Y_{tt}, \lambda_{tt}) \in J^2 : \\ X_{tt} + \lambda X = 0, Y_{tt} + \lambda Y + g = 0, X^2 + Y^2 - 1 = 0\}$$

is a 7 dimensional submanifold of $J^2 \simeq \mathbb{F}^{10}$.

5. Ranking

We introduce ranking here only for theory and algebraic interpretation. In computation we use implicit form without elimination, so it is stable.

Definition (Ranking [?])

A positive ranking $\prec$ *of* Ω *is a total ordering on* Ω *which satisfies:*

$$U \prec V \Rightarrow D_{x_i} U \prec D_{x_i} V \tag{5}$$

$$v^j \prec D_{x_i} v^j \tag{6}$$

6. Signature Matrix of t-Dominated Systems

Start from a simple case: two indep vars (t, x). For each u^j, we choose a ranking (only need this partial ranking in computation):

$$u^j \prec u^j_x \prec u^j_{xx} \prec \cdots \prec u^j_t \prec u^j_{tx} \prec \cdots \tag{7}$$

Determine the leading derivative for each equation R_i w.r.t. each u^j using the ranking (7), denoted by $\mathrm{LD}(R_i, u^j)$.

We hide the details about the differential order of x by defining a weight map $\varphi : \Omega \to \mathbb{R}$ as follows:

$$\varphi(v^i_\alpha) := \begin{cases} \alpha_1, & \text{if } \alpha_p = 0, \text{ for any } p \neq 1 \text{ ;} \\ \alpha_1 + \epsilon, & \text{if there exists } p \neq 1,\ \alpha_p \neq 0 \end{cases} \tag{8}$$

where α_1 is the diff. order w.r.t. t and $\epsilon > 0$ but very close to zero.

Define the *signature matrix* of R (see Pryce [5] for ODE case) by

$$(\sigma_{i,j})(R) := \begin{cases} \varphi(\mathrm{LD}(R_i, u^j)), & \text{if } R_i \text{ depends on } u^j \text{ ;} \\ -\infty, & \text{otherwise .} \end{cases} \tag{9}$$

And define $\mathrm{LD}(R, u^j)$ to be the highest one of $\mathrm{LD}(R_i, u^j), i = 1, ..., \ell$, the *leading class* of derivatives $\mathrm{LCD}(R) := \{\mathrm{LD}(R, u^j)\}$, $1 \le j \le m$.

Definition

We say R is dominated by pure derivatives in the independent variable t if there is no ϵ appearing in $(\sigma_{i,j})(R)$. For notational simplicity, we also call R a t-dominated system.

7. Generalizing Pryce's Method to PDE

Let R be a square t-dominated system. Consider R as ODE (the only independent variable is t). Suppose R_i needs to be differentiated c_i times ($c_i \geq 0$) to find hidden local constraints. The new system after differentiation is denoted by $\mathbf{D}_t^c R$.

Suppose the highest order of w^j appear in $\mathbf{D}_t^c R$ is d_j. From the definition of $(\sigma_{i,j})$, clearly d_j is the largest of $c_i + \sigma_{ij}$, which implies that $d_j - c_i \geq \sigma_{ij}$, for all i, j.

There are $\sum d_j + m$ jet variables and $\sum c_i + m$ equations in $\mathbf{D}_t^c R$ (only count pure t-derivatives). If each equation drops the dimension of the zero set by one, then the dimension of $\mathbf{D}_t^c R$ is $\sum d_j - \sum c_i$. To find all the constraints means to minimize the dimension of $\mathbf{D}_t^c R$ (Geometric Interpretation).

8. Formulation of Linear Programming Problem

This can be formulated as an integer linear programming problem (LLP) in the variables $c = (c_1, ..., c_m)$ and $d = (d_1, ..., d_m)$:

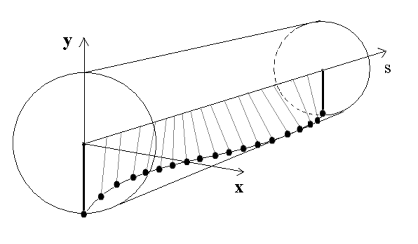
$$\left\{ \begin{array}{rl} \text{Minimize} & z = \sum d_j - \sum c_i, \\ \text{where} & d_j - c_i \geq \sigma_{ij}, \\ & c_i \geq 0 \end{array} \right. \tag{10}$$

The computation of c and d which only involves the information on differential order is consequently very fast. This problem is dual to the assignment problem [5].

Eric Schost pointed out that assignment problems can be done in $O(m^3)$ by using the Hungarian Method (Harold W. Kuhn, 1955).

Example

Consider a curtain made of many pendula hanging under gravity g as shown in Figure below.



The system R is:

$$X_{tt} + \lambda X = \kappa X_{ss} \quad (11)$$

$$Y_{tt} + \lambda Y + g = \kappa Y_{ss} \quad (12)$$

$$\Phi = \frac{1}{2}(X^2 + Y^2 - 1) = 0 \quad (13)$$

It is t-dominated (and also s-dominated).

The signature matrix: $(\sigma_{i,j})(R) = \begin{pmatrix} 2 & -\infty & 0 \\ -\infty & 2 & 0 \\ 0 & 0 & -\infty \end{pmatrix}$.

And

$$LPP: \begin{cases} \text{Minimize} & z = d_1 + d_2 + d_3 - c_1 - c_2 - c_3, \\ \text{where} & d_1 - c_1 \geq 2, \quad d_1 - c_2 \geq -\infty, \quad d_1 - c_3 \geq 0, \\ & d_2 - c_1 \geq -\infty, \quad d_2 - c_2 \geq 2, \quad d_2 - c_3 \geq 0, \\ & d_3 - c_1 \geq 0, \quad d_3 - c_2 \geq 0, \quad d_3 - c_3 \geq -\infty, \\ & c_1 \geq 0, \quad c_2 \geq 0, \quad c_3 \geq 0 \end{cases}$$

Solving this integer LPP by LPSolve in the Optimization package of Maple10, we obtain

$$c_1 = 0, \quad c_2 = 0, \quad c_3 = 2; \tag{14}$$

$$d_1 = 2, \quad d_2 = 2, \quad d_3 = 0. \tag{15}$$

9. Jacobian Criterion for Termination

Assume $c_1 \geq c_2 \geq \cdots \geq c_m$, and let $k_c = c_1$. Then we can partition $\mathbf{D}_t^c R$ into $k_c + 1$ parts,

B_0	B_1	$\cdots$	B_{k_c-1}	B_{k_c}
$R_1^{(0)}$	$R_1^{(1)}$	$\cdots$	$R_1^{(c_1-1)}$	$R_1^{(c_1)}$
	$R_2^{(0)}$	$\cdots$	$R_2^{(c_2-1)}$	$R_2^{(c_2)}$
		$\vdots$	$\vdots$	$\vdots$
		$R_m^{(0)}$	$\cdots$	$R_m^{(c_m)}$

Table: The triangular block structure of $\mathbf{D}_t^c R$, B_{i+1} involves more jet variables than B_i.

For each $B_i, 0 \leq i \leq k_c$, let $U_i := \text{LCD}(B_i)$ and define the *Jacobian Matrix*

$$\text{Jac}_i := \left(\frac{\partial B_i}{\partial U_i}\right). \qquad (16)$$

9. Jacobian Criterion for Termination

To apply the Riquier Existence Theorem, we need to refine the partial ranking (7) to a positive ranking.

Proposition

Let $\mathrm{LCD}(R) = \{\theta_1, ..., \theta_m\}$ *and let* B *be the set of all the other derivatives of* R*. Then there exists a positive ranking* $\prec$ *which satisfies the partial ranking (7) and* $\theta_1 \prec \theta_2 \prec \cdots \prec \theta_m$ *and each* θ_i *is greater than any* $b \in B$*.*

By Implicit Function Theorem and properties of analytic functions, we can show the Analytic Interpretation:

Theorem (Jacobian Criterion)

Let R *be a square analytic* t*-dominated system of* PDE *and* $\mathbf{D}_t^c R$ *be the system of* t*-prolongation by solving LPP (10). If* Jac_{k_c} *is nonsingular at some point* p *in* $Z(\mathbf{D}_t^c R)$*, then* $\mathbf{D}_t^c R$ *is an implicit Riquier Basis at* p *with a ranking given by Proposition 1.*

The t-prolongation procedure for ODE and PDE was implemented in Maple10 with polynomial solver PHCPack [?]. The integer linear programming involved using Maple10's LPSolve command. We applied our maple program to a Test Set of Visconti [?] containing 27 DAE with index ranging from 1 to 6.

- The procedure identified index consistent with Visconti's results.
- The LP problems were solved in less than one second.
- Our 6 failures were due to: 3 non-square system; 3 systems with singular Jacobians.
- Like other standard DAE approaches, Visconti required an initial guess for a consistent initial point, but we use homotopy continuation method to compute initial points.

11. Conclusion

We introduce a new concept: t-dominated PDE systems.

- Prolongations with respect to a single independent variable t are needed.
- No differential elimination for generic systems.
- Generalized Pryce's technique in the framework of Riquier Bases.
- Disadvantages: its limitation to square and t-dominated systems; a local method; not a universal method and does not pursue all singular cases.
- Future work: to investigate PDE models and extend the method to non-square systems.

Acknowledgment

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