Application of Numerical Algebraic Geometry and Numerical Linear Algebra to PDE

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ABSTRACT

The computational difficulty of completing nonlinear PDE to involutive form by differential elimination algorithms is a significant obstacle in applications. We apply numerical methods to this problem which, unlike existing symbolic methods for exact systems, can be applied to approximate systems arising in applications.

We use Numerical Algebraic Geometry to process the lower order leading nonlinear parts of such PDE systems. The irreducible components of such systems are represented by certain generic points lying on each component and are computed by numerically following paths from exactly given points on components of a related system. To check the conditions for involutivity Numerical Linear Algebra techniques are applied to constant matrices which are the leading linear parts of such systems evaluated at the generic points. Representations for the constraints result from applying a method based on Polynomial Matrix Theory.

Examples to illustrate the new approach are given. The scope of the method, which applies to complexified problems, is discussed. Approximate ideal and differential ideal membership testing are also discussed.

Categories and Subject Descriptors: G.1.8 **General Terms:** Algorithms, Design

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1. INTRODUCTION

Over and under-determined (*non-square*) systems of ODE and PDE arise in applications such as constrained multibody mechanics and control systems. For example, differential-algebraic equations (DAE) arise from constrained Lagrangian mechanics (see [1] and the references therein).

Much progress has been made in exact differential elimination methods, theory and algorithms for polynomially nonlinear systems of PDE [3, 8, 14, 20, 19]. Such methods enable the identification of all hidden constraints of PDE systems and the computation of initial data and associated formal power series solutions in the neighborhood of a given point. Algorithmic membership tests (specifically in the radical of a differential ideal) can be given [3, 8]. They can ease the difficulty of numerical solution of DAE systems [1].

This paper is a sequel to [17] and [18] in which theory and methods are developed for using numerical homotopy continuation techniques in the differential elimination process. In [17] such methods were first introduced by combining the Cartan-Kuranishni approach with homotopy methods to identify missing constraints for PDE. Our tool to numerically solve polynomial systems is homotopy continuation. When applied to PDE we stress that the solutions obtained by Homtopy continuation are not graphs of solutions of the PDE but instead zeros of the functions defining the PDE. Homotopy methods define families of systems, embedding a system to be solved in a homotopy, connecting it to a start system whose solutions are known. Such methods track the paths defined by the homotopy, leading to the solutions.

In [23], a new field "Numerical Algebraic Geometry" was described which led to the development of homotopies to describe all irreducible components (all meaning: for all dimensions) of the solution set of a polynomial system. Witness Sets are the key data in a numerical irreducible decomposition. A *witness set* for a k-dimensional solution component consists of k random hyperplanes and all isolated solutions in the intersection of the component with those hyperplanes. The degree of the solution component equals the number of witness points. Witness sets are equivalent to lifting fibers in a geometric resolution [10].

During the application of the Cartan-Kuranishi approach all equations are differentiated up to the current highest derivative order, resulting in potentially large numbers of PDE. These PDE are treated as polynomial equations in jet space, and their large number implies that the number of continuation paths that must be tracked can be impractically large in a direct application of Homotopy methods.

A hybrid method is introduced in [18] to exploit the structure of such systems to make progress in dealing with the difficulty above. However the hybrid method uses exact linear algebra (Gaussian Elimination) to process the leading linear part of such systems, and so is not applicable to approximate systems since it is unstable. In this paper we instead use stable methods from Numerical Linear Algebra.

In particular we use a numerical version of the geometric Cartan-Kuranishi method. This yields a coordinate in-

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dependent split between leading linear and nonlinear systems, which grades only by total order of derivative, and not within derivatives of the same order. This independence aids numerical stability. Since the derivatives of leading nonlinear equations are leading linear with respect to highest order jet variables, the new PDE are viewed as linear equations corresponding to a coefficient matrix with polynomial entries. We apply the Singular Value Decomposition (a fundamental technique of Numerical Linear Algebra) to the null spaces of these polynomial matrices. This construction is based on a modification due to [2] of the classical criterion of involution for PDE (see [9, 15, 20] for the classical criterion).

2. PDE IN JET SPACE

There are several theoretical approaches to systems of PDE such as differential algebra, exterior differential systems and the so-called formal theory built on the jet bundle formalism. Jet space methods associate a given PDE system with a locus of points in a Jet space. Such methods concern the geometrical study of this locus and its relationship with the solutions of the differential equations [9, 20, 15].

2.1 Jet Space and Jet variety of a PDE

Our tools are applicable to systems of polynomially nonlinear PDE with complex-valued variables and solutions. Consider a polynomially nonlinear system of PDE $R = (R^1, \ldots, R^l) = 0$ with independent variables $x = (x_1, \ldots, x_r) \in \mathbb{C}^r$ and complex-valued dependent variables $u = (u^1, \ldots, u^s)$. We define a multi-index q as an r-tuple $[q_1, q_2, ..., q_r]$ with $q_i \in \mathbb{N}$. The order of the multi-index q, denoted $|q|$, is given by the sum of the q_i. As in [3, 20] solutions and derivatives are replaced by formal (jet) variables. In particular, denoting the p-th order jet variables corresponding to derivatives as $\underset{p}{u}$, the jet variety (locus) of a q-th order system in the jet space $J^q(\mathbb{C}^r, \mathbb{C}^s) \approx \mathbb{C}^{r_q}$ is

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

Here $r_q = r + s\binom{r+q}{q}$ is the number of independent variables, dependent variables and derivatives of order less than or equal to q. We will use the shorthand $J^q(\mathbb{C}^r, \mathbb{C}^s) \equiv J^q$.

EXAMPLE 2.1. *We use the following running example [16, 7]:*

$$\begin{aligned} \frac{\partial^2 u(x,y)}{\partial y^2} - \frac{\partial^2 u(x,y)}{\partial x \partial y} &= 0, \\ \left(\frac{\partial u(x,y)}{\partial x}\right)^2 + \frac{\partial u(x,y)}{\partial x} - u(x,y) &= 0 . \end{aligned} \quad (2)$$

This is a differential polynomial system $R = (u_{yy} - u_{xy}, u_x^2 + u_x - u) = 0$ in the jet space of second order $J^2 \approx \mathbb{C}^8$ and has jet variety $V(R) = \{(x,\ y,\ u,\ u_x,\ u_y,\ u_{xx},\ u_{xy},\ u_{yy}) \in J^2$: $u_{yy} - u_{xy} = 0,\ u_x^2 + u_x - u = 0\}$.

2.2 Prolongation and Projection

There are two fundamental operations, prolongation and projection, to manipulate the locus in Jet space. We give a brief description of them here. For details see [15]. Before we define prolongation of a PDE system, we introduce the operator of Formal Total Derivation

$$D_{x_j} = \frac{\partial}{\partial x_j} + \sum_{\ell=1}^{s} u^\ell_{x_j} \frac{\partial}{\partial u^\ell} + \cdots .$$

Given a list of equations $R = 0$, $\mathbf{D}(R)$ is the list of first order total derivatives of all equations of R with respect to all independent variables:

$$\mathbf{D}(R) := \{(x, u, \ldots, \underset{q+1}{u}) \in J^{q+1} : R = 0, D_{x_i} R_k = 0\} . \quad (3)$$

It forms a single prolongation of R.

For example, let $R = u_x^2 + u_x - u = 0$, then:
$\mathbf{D}(R) = \{(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}) \in J^2$:
$u_x^2 + u_x - u = 0,\ 2u_x u_{xx} + u_{xx} - u_x,\ 2u_x u_{xy} + u_{xy} - u_y\}$.
Prolongation extends the locus of a PDE system from lower order jet space to higher order space. An inverse operation, the so-called projection, maps the locus from higher to lower order jet space.

DEFINITION 2.1 (PROJECTION). *Given a jet variety R in J^q, a single projection is:*

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

Let $T_p V(R)$ denote the tangent space to $V(R)$ at a given point $p \in V(R)$ and $\mathcal{N}(p)$ be a neighborhood of p. We restrict to the case where $\dim \boldsymbol{\pi}^q(\mathcal{N}(p) \cap T_p V(R)) = r$, that is the r variables x are independent and dim is the dimension as a complex manifold. Here $\boldsymbol{\pi}^q : J^q \to \mathbb{C}^r$ is the projection onto the space of variables $x \in \mathbb{C}^r$.

2.3 Formally Integrable and Involutive Systems

The symbol of a system of PDE R of order q is the jacobian of its equations with respect to the highest derivatives:

$$\mathcal{S}R := \frac{\partial R}{\partial \underset{q}{u}} . \quad (4)$$

The computational characterization for the symbol being involutive is that in a δ-regular coordinate system

$$\operatorname{rank} \mathcal{S}DR = \sum_{k=1}^{r} k \beta_k^{(q)} . \quad (5)$$

Alternatively Spencer's involutivity test based on homology groups (and implementable using numerical linear algebra) can be used and this avoids the difficulty of δ-irregular coordinate systems. See [15, 20] for details and the definition of the characters $\beta_k^{(q)}$. The most important properties of an involutive system of PDE are that $\overline{\boldsymbol{\pi} \mathbf{D} R} = V(R)$ and the symbol of R is involutive. An involutive system is also a formally integrable system. That is for any $k \geqslant 0$:

$$\overline{(\boldsymbol{\pi}\mathbf{D})(\mathbf{D}^k R)} = V(\mathbf{D}^k R) . \quad (6)$$

REMARK 2.2. *In this paper $\overline{S}$ means the Zariski Closure of the set S which is the intersection of all varieties containing S. Since the projection of a variety may not be a variety, it is necessary to consider the Zariski closure. It is easy to show that $\boldsymbol{\pi} DR = V(R)$ implies $\overline{\boldsymbol{\pi} DR} = V(R)$.*

2.4 Cartan-Kuranishi Completion

The full geometric method to complete systems of partial differential equations is the Cartan-Kuranishni algorithm [19, 20]. This method prolongs the system to order $q + 1$, then projects to order q to test for the existence of new constraints. This is continued until no new constraints are found. If the symbol of the resulting q-th order system is involutive, then the method has terminated and the system is involutive. If the symbol is not involutive, the system is prolonged until its symbol becomes involutive. The system is again tested for the existence of constraints by prolongation and projection. See [19, 20] for the relevant definitions. In particular the main iteration involves comparing R and $\boldsymbol{\pi}\mathbf{D}(R)$. Note in general the locus of R contains that of $\boldsymbol{\pi}\mathbf{D}R$. A probabilistic method to check the involutivity of the symbol using Numerical Linear Algebra, and in particular the Singular Value Decomposition, is given in [26, Section 6]. Numerical difficulties can occur, if there are multiplicities, and that case is under investigation.

3. POLYNOMIAL MATRIX

In this section we will exploit the linearity of the PDE which always appears after prolongation. Suppose $R = (R^1, \ldots, R^l) = 0$ is a polynomially nonlinear system of PDE with independent variables $x = (x_1, \ldots, x_r)$ and dependent variables $u = (u^1, \ldots, u^s)$. If the order of R is q, then we can represent the prolongation of R as:

$$\mathbf{D}R = \{\mathcal{S} \cdot \underset{q+1}{u} + \mathbf{r}, R\} \tag{7}$$

where $\mathcal{S}$ is called the *Symbol Matrix* of $\mathbf{D}R$. The corresponding augmented matrix is denoted by $[\mathcal{S}, \mathbf{r}]$. Obviously they are matrices with polynomial coefficients.

We briefly review some polynomial matrix theory and the associated results on rank and null-space computation. We let $\mathcal{R}$ denote the polynomial ring $K[z]$ in this paper, where $z = (z_1, ..., z_s)$ and the field K can be $\mathbb{R}$ or $\mathbb{C}$. The ring $\mathcal{R}$ is an integral domain and also is a unique factorization domain. $Q(\mathcal{R})$ is the quotient field of $\mathcal{R}$ or say rational functions in the variables $z_1, ..., z_s$.

Definition 3.1. *The set of all $m \times n$ matrices with entries from $\mathcal{R}$ is denoted by $M^{m\times n}(\mathcal{R})$. Each member in $M^{m\times n}(\mathcal{R})$ is called a polynomial matrix over $\mathcal{R}$.*

3.1 Rank of Polynomial Matrix

Consider the column vectors of a polynomial matrix $A = (\alpha_1|\alpha_2|...|\alpha_n) \in M^{m\times n}(\mathcal{R})$ and assume $y_k \in \mathcal{R}$ for $k = 1, ..., n$. If $\sum_{k=1}^{m} y_k\alpha_k = 0^{m\times 1}$ implies $y_k = 0$ for $k = 1, ..., n$, then these vectors are said to be *linearly independent.* Otherwise these vectors are said to be *linearly dependent.*

Definition 3.2 (Rank). *The (column) rank of polynomial matrix $A \in M^{m\times n}(\mathcal{R})$ is the maximum number of linearly independent column vectors of A.*

Several other frequently used definitions of rank are equivalent to our definition over a polynomial ring $\mathcal{R}$ since it is an integral domain. For example in the book [4], (algebraic) rank is generalized to arbitrary commutative rings using ideals generated by the minors.

Theorem 3.3. *Let $A \in M^{m\times n}(\mathcal{R})$. Then* $\mathrm{rank}(A) = k$ *if and only if any $t \times t$ minor of A is zero when $t > k$ and there exist some $k \times k$ nonzero minors.*

By Theorem 3.3, the rank of a polynomial matrix with coefficient field $K = \mathbb{R}$ will not change when the K is extended to $\mathbb{C}$. Moreover the rank evaluation of a polynomial matrix can be reduced to a constant matrix by choosing a random point in $\mathbb{C}^s$. In Sommese and Wampler's book [23], the concept of a *generic point* over $\mathbb{C}$ is introduced, which plays an essential role in "Numerical Algebraic Geometry". Suppose some property P is satisfied everywhere except on a proper algebraic subset U of an irreducible variety V. We call the points in $V\backslash U$ generic points. Then $\dim V > \dim U$, so $V\backslash U$ is dense in V (with the standard Lebesgue measure 1). So we say P holds with *algebraic probability one* for a random point of V. The following proposition easily follows:

Proposition 3.4. *For any generic point $z_0 \in \mathbb{C}^s$ we have* $\mathrm{rank}(A) = \mathrm{rank}(A_{z_0})$.

Remark 3.5. *In Numerical Algebraic Geometry generic points in $\mathbb{C}^s$ can be produced by choosing points in $\mathbb{C}^s$ randomly. With probability* 1*, the rank of a polynomial matrix is equal to the rank of the matrix evaluated at some random point (actually this result is also valid in $\mathbb{R}$ by Schwartz-Zippel theorem). That is, this will fail only on some algebraic variety with standard Lebesgue measure* 0 *in the whole space. This reduces the cost of rank computation dramatically.*

The witness points of a variety V yield a finite number of generic points on each irreducible component of V. This set is denoted by $W(V)$. Note that the witness points of a polynomial system R is $W(V(R))$ and shortly we denote it by $W(R)$. A useful result in [18] is that each point in $W(V)$ is contained in another variety V' implies $V \subseteq V'$ with probability 1.

3.2 Computing the Null-space

Given a polynomial matrix $A \in M^{m\times n}(\mathcal{R})$, there exist $r = n - \mathrm{rank}(A)$ linearly independent polynomial vectors $\{f_i\}$ such that $Af_i = 0^{m\times 1}$. Let $F := [f_1, ..., f_r]$, then $AF = 0^{m\times r}$. In particular F generates a linear space of A over quotient field $Q(\mathcal{R})$, which is called the *null-space* of A over $Q(\mathcal{R})$ and is denoted by $NullSpace(A)$. F is called a *basis* of $NullSpace(A)$. Note that F may not be a module basis of the Syzygy module of A. In this section, we propose a method to compute F in $\mathcal{R}$ by using Sylvester Matrices (see [27] for more details).

There is a natural bijection: $M^{m\times n}(K[z]) \leftrightarrow M^{m\times n}(K)[z]$, where $K[z]$ is the polynomial ring $\mathcal{R}$ and $M^{m\times n}(K)$ is the matrix with entries in the field K. Hence, equivalently we can consider a polynomial matrix as a polynomial with matrix coefficients, a so-called *matrix polynomial.*

Let $T(d) = \binom{s+d}{d}$ (for notational simplification the parameter s, which is the number of variables in the polynomial ring, is omitted). The polynomial matrix A can be written in terms of increasing total degree order of monomials of z: $A(z) = \sum_{i=1}^{T(d_1)} A_i z^{\alpha_i}$. Here d_1 is the maximum total degree of the entries of A and $T(d_1)$ is maximum number of terms of $A(z)$. Assume $f \in N$ has degree d_2. Similarly we have $f(z) = \sum_{j=1}^{T(d_2)} f_j z^{\beta_j}$. Hence

$$A(z)f(z) = \sum_{k=1}^{T(d_1+d_2)} C_k z^{\gamma_k} = 0^{m\times 1} \tag{8}$$

where $C_k := \sum_{\alpha_i+\beta_j=\gamma_k} A_i f_j$. This equation is equivalent to each coefficient $C_k = 0$.

Naturally, we write the coefficients of $f(z)$ as a vector: $v_f := [f_1, ..., f_{T(d_2)}]^t$. It is not hard to find a matrix M_A whose entries are the coefficients of $A(z)$, such that

$$M_A^{mT(d_1+d_2)\times nT(d_2)} \cdot v_f^{nT(d_2)\times 1} = 0^{mT(d_1+d_2)\times 1}. \tag{9}$$

We call M_A the *Sylvester Matrix*. We make the relations above clear by a diagram:

$$f \xrightarrow{\phi} f(z) \xrightarrow{\psi} v_f, \qquad f \xrightarrow{\omega} v_f$$
$$A \xrightarrow{\phi} A(z) \xrightarrow{\psi} M_A, \qquad A \xrightarrow{\omega} M_A \tag{10}$$

where ϕ, ψ are bijections and $\omega = \psi \circ \phi$.

We can use the SVD to compute the null-space of the Sylvester matrix M_A, denoted by N_A, then construct v_f and f from N_A. If f_i is in the null-space of A, then v_{f_i} must be in N_A. Note that $\dim N_A$ can be larger than r. First we choose lowest degree columns from N_A which are linearly independent vectors over the polynomial ring, denoted by F. Second we ascend from lower degree to higher degree columns to check the linear independency (using rank estimation). If a column is linearly independent it is included in F. Finally we obtain an updated F with rank r, which is a basis.

The remaining issue is the estimation of a degree bound for a null-space basis to guarantee the termination of the alogrithm. Henrion [6] gave a bound for such bases. Using the Laplace Theorem in [4] we also give a similar result which easily follows the standard linear algebra argument about the degree of the determinant of a polynomial matrix (or see [27] for the detail).

Proposition 3.6. *Suppose $A \in M^{m\times n}(\mathcal{R})$ is a polynomial matrix. Suppose $\mathrm{rank}(A) = k < n$, $r = n - k$, and $deg(Col_i(A))$ is the maximum degree of all the elements in the i-th column of A. We can always change the order of columns to satisfy $deg(Col_1(A)) \geqslant deg(Col_2(A)) \geqslant \cdots \geqslant deg(Col_n(A))$. Then there exists G which is a basis of the null-space of A, such that*

$$degree(G) \leq d_A = \sum_{i=1}^{k} deg(Col_i(A)) \ . \tag{11}$$

If each $deg_c(A_i) = d$, then $d_1 = d$ and $d_2 = (n-1)d$. So the maximum size of M_A is $m\binom{s+nd}{s} \times n\binom{s+nd-d}{s}$.

4. NUMERICAL COMPLETION METHODS

In this section we will present a numerical completion method based on polynomial matrix computation. In order to use generic points to ease our computation, we extend the coefficient field to $\mathbb{C}$. Note that the key step in completion of a PDE system is to determine whether R is equal to $\boldsymbol{\pi}\mathbf{D}R$ or not. The projection of a variety is not necessarily a variety. So we compute the *Zariski Closure* of the projection. But our method will fail to detect the singular cases of a PDE system when the Zariski closure has more points than the projection. Here we only consider the generic case and show that this problem can be reduced to rank computation.

To avoid the order dependence on the independent variables we propose a modified definition of leading linear part of PDE. An equation is *modified leading linear* (respectively, *modified leading nonlinear*) if it is linear (respectively, nonlinear) in the jet variables $\underset{q}{u}$, where q is the order of this equation (this (partial) ranking is: $\underset{0}{u} \prec \underset{1}{u} \prec \ldots \prec \underset{q}{u} \prec \ldots$).

The definition of modified leading linear and nonlinear PDE partitions R into two subsystems, the leading linear subsystem and the leading nonlinear subsystem respectively. Then we compute the witness sets of the leading nonlinear subsystem by (diagonal) homotopy continuation methods [22, 18]. The leading linear subsystem will be processed by numerical differential elimination methods using witness sets.

4.1 Using Witness Points

Here we first use witness points to detect whether there are some new constraints in lower order jet space. If they exist, then we find them by numerical differential elimination methods introduced in the next section. The advantage of this strategy is that it can avoid useless elimination of the strategy in [18] whose cost is much higher than checking the existence of new constraints.

Theorem 4.1. *For any $p \in W(R)$, $V(R) = \overline{\boldsymbol{\pi}\boldsymbol{D}R}$ if and only if $\mathrm{rank}(\mathcal{S}_p) = \mathrm{rank}([\mathcal{S}_p, \boldsymbol{r}_p])$.*

Proof: Suppose for any $p \in W(R)$, we have $\mathrm{rank}(\mathcal{S}_p) = \mathrm{rank}([\mathcal{S}_p, \mathbf{r}_p])$. At point p, there exists at least one solution u_p of $\mathcal{S}\cdot \underset{q+1}{u} + \mathbf{r} = 0$, so (p, u_p) must be in $V(\mathbf{D}R)$. Hence $p \in \overline{\boldsymbol{\pi}\mathbf{D}R}$. This is true for any generic point of R, so $V(R) \subseteq \overline{\boldsymbol{\pi}\mathbf{D}R}$. Consequently $V(R) = \overline{\boldsymbol{\pi}\mathbf{D}R}$.

Suppose $V(R) = \overline{\boldsymbol{\pi}\mathbf{D}R}$, then each $p \in W(R)$ must be in $\boldsymbol{\pi}\mathbf{D}R$ and $\boldsymbol{\pi}^{-1}p \in V(\mathbf{D}R)$. This means $\mathcal{S}\cdot \underset{q+1}{u} + \mathbf{r} = 0$ has at least one solution at point p, so $\mathrm{rank}(\mathcal{S}_p) = \mathrm{rank}([\mathcal{S}_p, \mathbf{r}_p])$.

4.2 Numerical Differential Elimination

Suppose there are some new constraints resulting from the leading linear equations of $\mathbf{D}R$ (7). Consider a polynomial vector f of order q, such that $f \cdot \mathcal{S} = 0$, then

$$f \cdot (\mathcal{S}\cdot \underset{q+1}{u} + \mathbf{r}) = f \cdot \mathbf{r} \tag{12}$$

which is a polynomial of order q. Obviously, this polynomial is also in the ideal generated by the leading linear part. To find all such polynomials in order to construct $\boldsymbol{\pi}\mathbf{D}R$, naturally leads us to consider the null-space of $\mathcal{S}^t$.

Theorem 4.2. *Let $F := NullSpace(\mathcal{S}^t)$, $P := \boldsymbol{r}^t \cdot F$ then*

1. *The inclusion $\boldsymbol{\pi}\boldsymbol{D}R \subseteq V(R) \cap V(P)$ holds, and*
2. *For all $p \in W(V(R) \cap V(P))$, $\mathrm{rank}(\mathcal{S}_p) = \mathrm{rank}([\mathcal{S}_p, \boldsymbol{r}_p])$ implies $\overline{\boldsymbol{\pi}\boldsymbol{D}R} = V(R) \cap V(P)$.*

Proof: (1) Because $F := NullSpace(\mathcal{S}^t)$ and $\mathcal{S}\cdot \underset{q+1}{u} + \mathbf{r} = 0$, $F^t \cdot (\mathcal{S}\cdot \underset{q+1}{u} + \mathbf{r}) = F^t \cdot \mathbf{r} = P^t = 0$. Hence $V(\mathbf{D}R) \subseteq V(P)$ and P only involves order q jet variables, so $\boldsymbol{\pi}\mathbf{D}R \subseteq V(P)$. And $\boldsymbol{\pi}\mathbf{D}R \subseteq V(R)$, hence (1) is proved.

(2) We only need to prove $V(R) \cap V(P) \subseteq \overline{\boldsymbol{\pi}\mathbf{D}R}$. Because for any $p \in W(V(R) \cap V(P))$, $\mathrm{rank}(\mathcal{S}_p) = \mathrm{rank}([\mathcal{S}_p, \mathbf{r}_p])$. At point p, there exists at least one solution u_p of $\mathcal{S}\cdot \underset{q+1}{u} + \mathbf{r} = 0$, so (p, u_p) must be in $V(\mathbf{D}R)$. Hence $p \in \overline{\boldsymbol{\pi}\mathbf{D}R}$. This is true for any generic point of $V(R) \cap V(P)$, so (2) is true.

5. SIMPLE EXAMPLES

Recall the simple illustrative system (2). At first differentiating R up to order 2 yields:

$$R^{(0)} = \{u_x^2 + u_x - u = 0, \qquad u_{yy} - u_{xy} = 0,$$
$$2u_x u_{xx} + u_{xx} - u_x = 0, \quad 2u_x u_{xy} + u_{xy} - uy = 0\} \ .$$

We can partition $R^{(0)}$ into a single leading nonlinear PDE $N^{(0)} = \{u_x^2 + u_x - u = 0\}$ and 3 leading linear PDE $L^{(0)}$:

$$\begin{pmatrix} 0 & (1+2u_x) & 0 \\ (1+2u_x) & 0 & 0 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{pmatrix} = \begin{pmatrix} u_y \\ u_x \\ 0 \end{pmatrix}. \tag{13}$$

Applying ***WitnessSet*** [18] to $N^{(0)}$ yields a witness set $W^{(0)}$ with two approximate generic points in $V(N^{(0)})$. Applying rank test at the witness points of $W^{(0)}$ shows that there are no new constraints arising from projection. Since symbol matrix has full rank, the algorithm has terminated.

Actually, for this example the second order jet variables, if desired, can be expressed in terms of lower order jet variables yielding the same answer as ***HybridRif*** [18] and the fully symbolic algorithm ***rifsimp*** [16]. However our goal is to obtain an involutive form rather than put the system into triangular solved form. The advantage is that we can avoid computing the inverse of a symbolic matrix which in some cases yields an unmanageably large polynomial matrix.

EXAMPLE 5.1 (USE OF ALL WITNESS POINTS). *The input system is $\langle u_t, v_t - u(u-1), u(v-1)\rangle$. First we prolong $u(v-1)$ once and obtain $D_t(u(v-1)) = (v-1)u_t + uv_t$. We write the system in matrix form as:*

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ (v-1) & u \end{pmatrix} \begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} 0 \\ u(u-1) \\ 0 \end{pmatrix} \tag{14}$$

with the constraint $u(v-1) = 0$. The witness set contains two points: $(0, \tilde{v})$ and $(\tilde{u}, 1)$, where $\tilde{u}, \tilde{v}$ are some random complex floating point numbers. At $(0, \tilde{v})$, the rank of symbol matrix is equal to the rank of the augmented matrix which indicates that there are no new constraints in this case. At $(\tilde{u}, 1)$, there exists a new constraint, since the ranks are not equal. We construct the projected polynomial by computing the null-space of the symbol matrix, which is $(1-v, -u, 1)$. So the new constraint is $(1-v, -u, 1)\cdot(0, u(u-1), 0)^t = -u^2(u-1)$. Appending the prolongation of the new equation $((3u^2 - 2u)u_t)$ to the system, we obtain a new system in matrix form:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ (v-1) & u \\ (3u^2-2u) & 0 \end{pmatrix} \begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} 0 \\ u(u-1) \\ 0 \\ 0 \end{pmatrix} \tag{15}$$

with constraints $\{u(v-1) = 0, u^2(u-1) = 0\}$. This implies two cases: $u = 0$ which was found before and $(u, v) = (1, 1)$. In this case the rank test shows that there are no new constraints. Hence our algorithm terminates.

6. PHYSICAL EXAMPLE

Systems such as the DAE below, often arise in applications. Such systems of higher index can become very challenging for symbolic differential elimination algorithms such as **rifsimp**. Such algorithms attempt to triangularize the systems, and expression swell, from the inversion of densely filled symbolic matrices can follow. We briefly mention that the size of these matrices below can be sharply reduced when a strategy is applied to detect constant full rank submatrices and reduce the number of variables by elimination.

EXAMPLE 6.1 (DISTILLATION STAGES [25]). *Let us consider the square DAE system:*

$$\begin{aligned} z_t^1 - f_1(z^1, u, t) &= 0, \quad z_t^2 - f_2(z^1, z^2, t) = 0, \\ z_t^3 - f_3(z^2, z^3, t) &= 0, \quad z_t^4 - f_4(z^3, z^4, t) = 0, \\ z^4 - out(t) &= 0 \end{aligned} \tag{16}$$

*The unknown functions $\{f_1, f_2, f_3, f_4, out\}$ are replaced with random polynomials with degree 2. The system is prolonged to order 1 to obtain 5 equations in J^1 and one equation in J^0. These 5 equations are written in matrix form and the rank test shows there are new constraints. We construct them by null-space computation. In the next iteration, the new equations are prolonged to order 1 and the matrix updated and so on. After 5 iterations, our algorithm stops and finds 5 constraints in J^0. There are 11 equations in J^1. The singular values of the symbol matrix are $[158.7, 65.1, 54.1, 25.9, .316]$. So it has full rank. The largest matrix processed in this example is 1120×210. Since the symbol matrix has an identity sub-matrix, the size of Sylvester matrix can be reduced by solving the corresponding sub-system first. We also applied **rifsimp** to this problem using Maple 10, on a 1.5 GHZ Pentium M, with 512 MB of RAM, running under Windows XP. After 2 hours the computation exhausted RAM and failed.*

7. RANDOM PDE EXAMPLES

In this section we use random systems of PDE to illustrate the methods developed in this paper. By their generic form, one would expect integrability conditions to impose new algebraic conditions in Jet space, cascading until such systems became algebraically inconsistent. However, we have:

THEOREM 7.1. *Consider a system of s random PDE: $\{R^1, R^2, ..., R^s\}$ in $\mathbb{C}[x, u, \underset{1}{u}, ..., \underset{q}{u}]$ with s dependent variables $u^1, u^2, \ldots, u^s$ and r independent variables $x_1, ..., x_r$ where each PDE has order q. Then with probability 1 the system is involutive.*

Outline of Proof: The proof follows directly from the definitions in the Cartan-Kuranishi approach.

Consider the s so-called highest class order q jet variables w corresponding to $\left(\frac{\partial}{\partial x_r}\right)^q u^k$ and denote the remaining order q jet variables by z (see [15, 20] for the definition of the class of a jet variable). Then $\mathcal{S}R = \left(\ \frac{\partial R}{\partial w} \mid \frac{\partial R}{\partial z}\ \right)$ and randomness implies that $\det\left(\frac{\partial R}{\partial w}\right) \neq 0$ and $\operatorname{rank}\left(\frac{\partial R}{\partial w}\right) = s$ on $V(R)$ with probability 1.

Then by the definition of class of a jet variable $\beta_r^{(q)} = s$, $\beta_{r-1}^{(q)} = \cdots = \beta_1^{(q)} = 0$. In addition it easily follows from $\det\left(\frac{\partial R}{\partial w}\right) \neq 0$ that $\operatorname{rank}(\mathcal{S}\mathbf{D}R) = rs$. As a consequence (5) is satisfied and $\operatorname{rank}(\mathcal{S}\mathbf{D}R) = rs = \sum_1^r k\beta_k^{(q)}$. Thus the symbol of the system is involutive. Then $\mathbf{D}R$ is easily seen to be of maximal rank, and hence there are no projected conditions and the system is involutive.

EXAMPLE 7.1 (RANDOM SQUARE PDE). *We generate a PDE system R' randomly as follows. First generate two random polynomial PDE with degree 2:*

$$R = \{R^1(u_x, u_y, v_x, v_y, u, v), R^2(u_x, u_y, v_x, v_y, u, v)\}$$

Note that R is involutive by Theorem 7.1. This implies the prolongation $\boldsymbol{D}R$ is also involutive. Then we obtain our test *system R' (6 equations with order 2) using random linear combination of $\boldsymbol{D}R$. Since R' has the same variety as $\boldsymbol{D}R$ it is also an involutive system (in disguise). We show that our method can determine the involutivity of R'.*

First we verify $\boldsymbol{\pi}\boldsymbol{D}R' = R'$, which requires tracing 2^6 homotopy paths to compute the witness set of $V(R')$ (if the degree is 5, this number will be 15625!). Applying the rank test at generic points in J^2 space shows there are no new constraints. The test (5) shows that the symbol is involutive since $\sum_{k=1}^{2} k\beta_k = 2 \times 2 + 1 \times 2 = 6$ and the rank of the symbol matrix of $\boldsymbol{D}R'$ is 6. This means R' is involutive.

Actually R' is leading linear, which motivates us to compute $\boldsymbol{\pi}R'$. Applying the rank test at generic points in J^1 space shows there are new constraints. We use our algorithm to construct the projected equations S^1, S^2 in J^1. They have degree 2, which means only 4 (when the degree is 5, it is 25) homotopy paths need to be traced and this is much more efficient. Let $H = \{R', \boldsymbol{D}(S^1), \boldsymbol{D}(S^2), S^1, S^2\}$. Similarly we can check that H is involutive. Using PHCpack [24] we verify $V(S^1, S^2) = V(R^1, R^2)$, which shows our algorithm finds the projected equations correctly.

*When symbolic methods such as **rifsimp** are applied to R', they can explode in memory as a result of trying to triangularize (or invert) complicated high degree polynomial matrices. Here **rifsimp** failed to terminate on the above systems with degree ≥ 2, while the method of this paper easily handled systems up to degree 5 in a few minutes of CPU time.*

8. EXPERIMENTS WITH APPROXIMATE IDEAL MEMBERSHIP TESTING

It is natural to wonder how some sort of approximate ideal membership testing might be done with the output of symbolic-numeric methods. Simply following the same strategy of exact membership testing, reducing first to a Gröbner Basis, then finding a normal form of an expression h to test its ideal membership, will usually be unstable.

To test membership of an expression h in a differential ideal generated by R, instead of finding a normal form for R we use the tables of dimensions $\dim \boldsymbol{\pi}^\ell \mathbf{D}^k R$. If done exactly, when $\boldsymbol{\pi}^\ell \mathbf{D}^k R$ is involutive, this information encodes the differential Hilbert function of the differential ideal. See [20] for a discussion of the Hilbert function of involutive systems. If an expression is not in the differential ideal, then it must change the Hilbert function (a measure of the indeterminancy in the formal power series solutions of the system). Thus, in our approach, if applied exactly, we would first determine ℓ and k such that $\boldsymbol{\pi}^\ell \mathbf{D}^k R$ satisfies the involutive dimension criteria. Then, exact involution would be applied to the system R, h. If any of the dimensions, determining the Hilbert function, at involution, change, then h is not in the differential ideal generated by R. We follow a similar strategy in the approximate case.

EXAMPLE 8.1 (DIFFERENTIAL IDEAL MEMBERSHIP). *Consider the* ODE

$$y_{xx} + 5\,y_x - 6\,y^2 + 6\,y = 0\,. \tag{17}$$

The symmetry vector fields $\xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y}$ generating Lie symmetries leaving its solution set invariant, have coefficients satisfying the linear homogeneous system of PDE *[13]. Most computer algebra systems have programs for automatically generating such systems. The symmetry defining*

	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
$\ell=0$	8	8	6	4	3	2	2
$\ell=1$	6	8	6	4	3	2	2
$\ell=2$			6	4	3	2	2
$\ell=3$				4	3	2	2
$\ell=4$					3	2	2
$\ell=5$						$\boxed{2}$	2
$\ell=6$						2	2

Figure 1: Table of $\dim \boldsymbol{\pi}^\ell \mathbf{D}^k R$ for (18) with SVD tolerance 10^{-7}. The location of the passing of the involution test, is indicated by the box.

system R associated with ODE *(17) is:*

$$\begin{aligned} \xi_{yy} = 0\,, \quad 10\xi_y - 2\xi_{xy} + \eta_{yy} = 0 \qquad (18) \\ (6-12y)\eta + (6y^2-6y)(\eta_y - 2\xi_x) + 5\eta_x + \eta_{xx} &= 0 \\ 5\xi_x + 18(y-y^2)\xi_y - \xi_{xx} + 2\eta_{xy} &= 0 \end{aligned}$$

Consider the problem of testing whether h lies in the differential ideal generated by (18) where:

$$h := x(\eta_{xx} - \eta_x) + y(2y\xi_{xx} + \eta_x) + (x+2)(y^2\eta_{yy} - y\eta_y + \eta_{xy})$$

Reduction of R to a (linear) differential Gröbner Basis easily yields $\eta_x - \eta, \xi_x + \frac{1}{2y}\eta, \eta_y - \frac{1}{y}\eta, \xi_y$ in a ranking dominated by total order of derivative. Reducing h with respect to this basis yields 0, and so h lies in the differential ideal.

Instead of following this standard procedure, we first applied our symbolic-numeric projective involutive form method [2]. We observed that the system $\boldsymbol{\pi}^5\boldsymbol{D}^5 R$ approximately satisfies the dimension criteria for projective involution (see Figure 1). Next, a perturbation of order 10^{-9} was added to h to form $\widetilde{h}$. An SVD tolerance 10^{-7} was used to test approximate involution, but this time for the system $R, \widetilde{h}$. We found that the relevant dimensions at involution did not change. If these results were obtained exactly then $\widetilde{h}$ would be in the ideal generated by R. However since the computations are approximate they only offer some evidence that some nearby exact $\hat{R}$, $\hat{h}$ has $\hat{h}$ in the ideal generated by $\hat{R}$.

Suppose we have approximate $\widetilde{R}, \widetilde{h}$ where the Hilbert dimensions for $\widetilde{R}, \widetilde{h}$ at involution are the same as those for $\widetilde{R}$, using some reasonable tolerance. We then use refinement processes to attempt to construct nearby systems $\hat{R}$, $\hat{h}$ which exactly satisfy all of the dimension criteria for (exact) ideal membership.

EXAMPLE 8.2 (POLYNOMIAL IDEAL MEMBERSHIP). *Consider the system of polynomials in $\mathbb{Q}[x,y]$*

$$\begin{aligned} p &= x^3 - y^3, \quad q = (x^2+y+1)(x-y), \qquad (19) \\ f &= -5\,y^3x + 7\,x^2y^3 + xy^4 + 12\,y^4 - 8\,y^5 - 3\,y^2x - 7\,y^2x^2 \\ &\quad -12\,y^3 + 3\,x^2 + 7\,x^3 + 8\,x^2y - 4\,y^2 - 4\,x + yx + 4\,y \end{aligned}$$

It is easily exactly verified by Gröbner Basis computation that $\langle p, q\rangle$ is positive dimensional and that $f \in \langle p, q\rangle$.

To apply our approximate differential elimination methods, we exploit the well-known bijection between PDE *and polynomials where monomials in x, y are mapped to monomials in the differential operators $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$.*

We form $\tilde{p} = p + \delta p$, $\tilde{q} = q + \delta q$ and $\tilde{f} = f + \delta f$ where the perturbations δp, δq, δf are randomly generated degree 3 dense polynomials with random coefficients of order 10^{-9}.

	$d=3$	$d=4$	$d=5$	$d=6$
	$k=0$	$k=1$	$k=2$	$k=3$
$\ell=0$	8	$\boxed{9}$	10	11
$\ell=1$	6	8	9	10
$\ell=2$	3	6	8	9
$\ell=3$	1	3	6	8

Figure 2: Table of $\dim \boldsymbol{\pi}^\ell \mathbf{D}^k R$ for R, which is of degree $d = 3$, given by $\tilde{p}$, $\tilde{q}$ in (19) SVD tolerance 10^{-7} (& also for $\hat{p}, \hat{q}$ with tolerance 10^{-13}). The box gives the location of the passing of the involution test.

	$d=5$	$d=6$	$d=7$	$d=8$
	$k=0$	$k=1$	$k=2$	$k=3$
$\ell=0$	$\boxed{10}$	11	12	13
$\ell=1$	9	10	11	12
$\ell=2$	8	9	10	11
$\ell=3$	6	8	9	10
$\ell=4$	3	6	8	9
$\ell=5$	1	3	6	8

Figure 3: Table of $\dim \boldsymbol{\pi}^\ell \mathbf{D}^k R$ for R, which is of degree $d = 5$, given by $\hat{p}$, $\hat{q}$, $\tilde{f}$ with tolerance 10^{-5} (& also for $\hat{p}$, $\hat{q}$, $\hat{f}$ with tolerance 10^{-13}).The box gives the location of the passing of the involution test.

We apply the approximate projective involution method to $\tilde{p}$, $\tilde{q}$, with an SVD tolerance of 10^{-7} and obtain the results given in Figure 2. This gives some evidence of the possibility of a nearby projectively involutive system. To give stronger evidence, we actually now search for an exact such nearby system. We set our search space as the following symbolic class of polynomials in which $\tilde{p}$, $\tilde{q}$ is embedded (this is a step where there are often many choices):

$$P(a) = \sum_{j+k=0}^{3} a_{j,k}\, x^j y^k, \quad Q(b) = \sum_{j+k=0}^{3} b_{j,k}\, x^j y^k \;. \quad (20)$$

So $\tilde{p} = P(a^{(0)})$, $\tilde{q} = Q(b^{(0)})$ where $a^{(0)}$, $b^{(0)}$ is the list of $10 + 10 = 20$ coefficients defining $\tilde{p}$, $\tilde{q}$.

Scott's STLS (Structured Total Least Squares) implementation in Maple of the method [11] is applied to $\tilde{p}$, $\tilde{q}$. In 2 iterations, it converges to a nearby system, $\{\hat{p} = P(a^{(0)} + \delta a), \hat{q} = Q(b^{(0)} + \delta b)\}$ (ie. δa and δb were computed numerically). Now, with the obtained $\hat{p}$ and $\hat{q}$, the dimensions in the table in Figure 2 can be recovered with tolerances roughly equal to working precision.

We apply the approximate projective involution method to $\hat{p}$, $\hat{q}$, $\tilde{f}$ with an SVD tolerance of 10^{-5} and obtain the results given in Figure 3. This gives some evidence of the possible existence of a nearby projectively involutive system. The nearby system was chosen to consist of $\hat{p}$, $\hat{q}$ and $F(c)$. Here the forms of $\hat{p}$, $\hat{q}$ are fixed as $\hat{p} = P(a^{(0)} + \delta a)$, $\hat{q} = Q(b^{(0)} + \delta b)$ and $F(c)$ is a member of the class of polynomials:

$$F(c) = \sum_{j+k=0}^{5} c_{j,k}\, x^j y^k \;. \quad (21)$$

So, $\tilde{f} = F(c^{(0)})$ where $c^{(0)}$ is the initial list of its 21 defining coefficients, while the 20 coefficients of $\hat{p}$, $\hat{q}$ will not be altered in the following refinement step.

This time, instead of STLS, Scott's structured Newton in Maple is applied to $\hat{p}$, $\hat{q}$, $\tilde{f}$ and converges to a nearby system $\{\hat{p}, \hat{q}, \hat{f} = F(c^{(0)} + \delta c)\}$ in 1 iteration. This new system is exactly projectively involutive (to within working precision). Now, with tolerances about working precision, the dimensions of Figure 3 can be recovered.

With the exact systems $\{\hat{p}, \hat{q}\}$ and $\{\hat{p}, \hat{q}, \hat{f}\}$ in mind, Figure 2 and 3 can be compared. Note that the pattern of dimensions is the same in both tables and implies that these two systems have the same Hilbert Function. Thus $\hat{f} \in \langle \hat{p}, \hat{q} \rangle$.

9. DISCUSSION

Our method applies to inexact systems of polynomially nonlinear PDE and relies on splitting the system into a leading linear subsystem and its complement. A new numerical differential elimination method based on polynomial matrix solving is applied to the leading linear part of the system. The success of this strategy enables the shrinking of the number of genuinely nonlinear equations that are dealt with by the numerical continuation methods.

A shortcoming of the new differential elimination method is that the size of matrices we need to process can be very large (see Example 6). Let us consider a polynomial matrix $A \in M^{m\times n}(\mathcal{R})$, if each $deg(Col_i(A)) = d$ and rank of A is k, then $d_1 = d$ and $d_A = kd$. So the maximum size of M_A is $m\binom{s+d+kd}{s} \times n\binom{s+kd}{s}$. Assume $m \approx n$ and $kd \gg s$, the size of this matrix is bounded by $n(k+1)^s d^s$. We know $k < n$, so the bound is $n^{s+1}d^s$. When $s = 1$, a symbolic complexity result in [21] reports that the cost to compute the rank and null-space is the same as the cost of multiplication of matrices $\tilde{O}(n^{2.7}d)$, where $\tilde{O}$ indicates missing logarithmic factors $\alpha(\log n)^\beta(\log d)^\gamma$ for three positive real constants α, β, γ. Since the Sylvester matrix M_A is always sparse with block Toeplitz structure [28] gives a numerical algorithm with complexity $O(n^3 d)$ using block LQ factorization. However when $s > 1$, the block Toeplitz structure of M_A is much more complicated and further study is required.

In general, when the size, degree and number of unknowns of the symbol matrix are large, it is unrealistic to solve the corresponding matrix M_A. However, in many applications (e.g. multi-link pendula and Example 6) the symbol matrix has a very special structure, enabling the easy solution of subsystems. If we solve such sub-systems first, then the projected relations can be obtained directly without polynomial matrix solving. Hence our strategy is to find well-conditioned constant sub-matrices and substitute the corresponding solutions into the original system.

Geometric approaches have the advantage that they apply to both real ($\mathbb{F} = \mathbb{R}$) and and complex ($\mathbb{F} = \mathbb{C}$) smooth manifolds. One of our main tools, numerical algebraic geometry, depends on $\mathbb{F}$ being algebraically closed (so that a polynomial over $\mathbb{F}$ always has a root in $\mathbb{F}$). Indeed many of the main tools of (exact) algebraic geometry, although algorithmically powerful suffer from the same restriction. To apply our approach to a real system, the PDE, the problem is first complexified, and the results for the real case, checked heuristically on a case by case basis. However progress in making numerical algebraic geometric techniques algorithmic for the real case is reported in [12].

Our experimental approach for testing approximate ideal membership differs radically from Gröbner type approaches, that utilize normal forms and reductions which are not numerically stable. In some sense, we are going back in history, to Macaulay and Hilbert's initial studies. In particular we are framing ideal membership, in terms of the dimensions that determine the Hilbert function of an ideal. Analogously, the new methods of Numerical Algebraic Geometry, in some sense go back to a more primitive notion of geometry – that of a point on a variety.

This paper belongs to a series initiated in [26], continued in [17], [7] and [18] aimed at developing "Numerical Jet Geometry", based on "Numerical Algebraic Geometry".

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