On Approximate Linearized Triangular Decompositions

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Abstract. In this paper, we describe progress on the development of algorithms for triangular decomposition of approximate systems.

We begin with the treatment of linear, homogeneous systems with positive-dimensional solution spaces, and approximate coefficients. We use the Singular Value Decomposition to decompose such systems into a stable form, and discuss condition numbers for approximate triangular decompositions. Results from the linear case are used as the foundation of a discussion on the fully nonlinear case. We introduce linearized triangular sets, and show that we can obtain useful stability information about sets corresponding to different variable orderings. Examples are provided, experiments are described, and connections with the works of Sommese, Verschelde, and Wampler are made.

Keywords. Symbolic-numeric computation, triangular decomposition, singular value decomposition, linear system.

1. Introduction

Systems of polynomial equations frequently arise in applications, and it is often of interest to determine their triangular forms. Such representations enable the expression of some of the variables as functions of the remaining ("free") variables. Already, methods exist which are designed to compute triangular sets for exact systems whose varieties are of arbitrary dimension (43; 22; 28; 42). However, for real world problems, the systems under consideration frequently have approximate coefficients that are inferred from experimental data. This means that the stability of these triangular representations is a valid concern. To be more clear, we are not merely concerned with the sensitivity of the triangular representation to perturbations in the original data, but we also want the solution set to be stable under small changes in values taken by the free variables.

This work is supported by NSERC, MITACS, and Maplesoft, Canada.

In another paper, *On Approximate Triangular Decompositions I: Dimension Zero* (29), we gave a detailed treatment of approximate triangular decomposition for systems with finitely many roots (zero-dimensional systems). That work follows the equiprojectable decomposition presented in (9) and also makes use of the interpolation formulas recently proposed by Dahan and Schost (12). In this second paper, we study the simplest class of positive dimensional systems: linear homogeneous systems.

It is true that Gaussian elimination, with respect to a given variable ordering, will transform any exact linear system provided as input into a triangular solved form. Solutions are parameterized by free variables which are lower in the ordering than the remaining variables. However, in the case of approximate systems, neither replacement of floating point numbers with rational numbers nor use of Gaussian elimination with full pivoting can be guaranteed to give orderings which are ideal (see the standard text (21) for a discussion of these issues). Furthermore, such methods may lead to approximate triangular representations which are practically unstable, even in the case of exact systems.

The key idea for the portion of the current paper which deals with linear, homogeneous systems, is to use stable methods from Numerical Linear Algebra. Specifically we use the Singular Value Decomposition (SVD) to determine whether a stable approximate triangular set exists for some variable ordering. We will show that such a stable set and ordering always exists, but that a given ordering may lead to an unstable representation. Furthermore, an interpretation of this set is given in terms of an exact solution to some nearby (homogeneous) system.

From there we will further explore some local structure of nonlinear problems with Linearized Approximate Triangular Decompositions. Applying results from the treatment of linear problems to the linearization of nonlinear systems, variable orderings for locally-stable approximate triangular sets can be determined. To do this, we use the homotopy continuation methods of PHCpack (41) to generate generic points on each irreducible component of a given nonlinear polynomial system (32; 34; 35; 33). A collection of certain results on the decomposition of non-linear systems is also provided here. For example, for n variables, the interpolation methods of Sommese, Verschelde, and Wampler give approximate triangular representations of the $(n-1)$-dimensional components.

The above results, together with certain results using the equiprojectable decomposition (presented in our related work (29)), form an accessible bridge to the study of the fully non-linear case. This will be described in a forthcoming work.

2. Approximate Triangular Sets for Positive Dimensional Linear Systems

In this section we discuss triangular representations for linear systems. The foundation of our treatment is the Singular Value Decomposition, and techniques that have now become standard in Numerical Linear Algebra (21; 39).

2.1. The Singular Value Decomposition and Variable Orderings

Suppose we are given a system of m linear homogeneous equations in n variables, and that the solution space of the system has some positive dimension d. We wish to express the solution with $n - d$ variables in terms of d free variables.

Indeed, for reasons which will become clear, we worry that Gaussian elimination might produce an unstable (triangular) representation of the solution set. Instead of Gaussian elimination, our main tool will be the Singular Value Decomposition (SVD) of Numerical Linear Algebra.

Given $A \in \mathbb{F}^{m\times n}$ where $\mathbb{F}$ is $\mathbb{R}$ or $\mathbb{C}$ one can compute the SVD (21; 39):

$$A = U\Sigma V^t.$$

Here, Σ is a diagonal matrix with the same dimensions as A, both $U \in \mathbb{F}^{m\times m}$ and $V \in \mathbb{F}^{n\times n}$ are orthogonal matrices, and V^t denotes the transpose of V if $\mathbb{F} = \mathbb{R}$ or the complex conjugate transpose if $\mathbb{F} = \mathbb{C}$. If the rank of A is r, then the last $n - r$ columns of V form a basis for Null(A). The diagonal elements of Σ are real, and are called the *singular values* of A. Often, it is enough to take the number of nonzero singular values as the numerical rank of A. For later purposes, it is useful to mention that the singular values are the square roots of the eigenvalues of matrices A^tA and AA^t (where the transpose is the Hermitian transpose if $\mathbb{F} = \mathbb{C}$).

Let $P \in \mathbb{F}^{n\times d}$ be a matrix whose columns form a basis for Null(A). In particular, we can let P be composed of the last $n - r$ columns of V from the SVD of A and define $d := n - r$. Then

$$\begin{aligned} \mathbf{x} &= \alpha_1\mathbf{p}_1 + \alpha_2\mathbf{p}_2 + \ldots + \alpha_d\mathbf{p}_d \\ &= P\boldsymbol{\alpha}, \end{aligned} \tag{2.1}$$

with $\boldsymbol{\alpha} \in \mathbb{F}^d$. Furthermore, the matrix P is stable with respect to changes in the (approximate) coefficients of A. Indeed, adjoining $\alpha_1, \ldots, \alpha_d$ as new indeterminates we simply have the following:

Remark 2.1. Equation (2.1) is a (normalized) triangular set in any ordering ranking the variables $\{x_1, \ldots, x_n\}$ greater than the variables $\{\alpha_1, \ldots, \alpha_d\}$.

Definition 2.2. A triangular representation of the form

$$\mathbf{x}_{\text{non-free}} = M\mathbf{x}_{\text{free}}, \tag{2.2}$$

where M is a matrix with entries in $\mathbb{F}$, is *practically stable* if the condition number of M is reasonable. Thus, small changes in the free variables of a practically stable solution will not induce huge changes in the non-free variables.

Remark 2.3. The triangular set (2.1) is practically stable. We write

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \|P\|\|P^\dagger\|\frac{\|\delta\boldsymbol{\alpha}\|}{\|\boldsymbol{\alpha}\|} \tag{2.3}$$

to estimate the sensitivity of the solution $\mathbf{x}$ (the non-free variables) to small perturbations of $\boldsymbol{\alpha}$ (the free variables), given the matrix P. Since P is not a square

matrix, the usual inverse has been replaced with the pseudo-inverse $P^\dagger$ (see Remark 2.8 for more details), and the condition number of the triangular solution (2.1) can still be expressed in terms of the singular values of P. Since the columns of P are orthogonal, the matrix P^tP is the identity matrix, whose eigenvalues are all equal to 1. Thus, every singular value of P is equal to 1, and so its condition number

$$\|P\|_2\|P^\dagger\|_2 = \sigma_1\frac{1}{\sigma_d} = 1. \tag{2.4}$$

This result is independent of the condition number of the given matrix A.

We will now further our development by investigating approximate linear triangular sets with respect to orderings of the variables $\{x_1, \ldots, x_n\}$ alone. It is natural to ask why we should investigate such sets, given that, by Remark 2.1, the SVD already directly yields the triangular set (2.1). One reason is that in applications we are often interested in expressing some variables in terms of others. Another, more mathematical, reason is that we wish to use the linear case as our guide in the study of the positive dimensional nonlinear case where such orderings on the variables $\{x_1, \ldots, x_n\}$ are often used.

To obtain triangular sets in the variables $\{x_1, \ldots, x_n\}$ alone, we need to eliminate the variables $\{\alpha_1, \ldots, \alpha_d\}$ in (2.1) in favor of d free variables suitably chosen from $\{x_1, \ldots, x_n\}$. The remaining $n - d$ variables will then be expressed as functions of these free variables instead of the α's. If we can find an invertible sub-matrix Q of P, then

$$\mathbf{x}_{\text{free}} = Q\boldsymbol{\alpha}, \tag{2.5}$$

and consequently

$$\boldsymbol{\alpha} = Q^{-1}\mathbf{x}_{\text{free}}. \tag{2.6}$$

Denoting by R the matrix composed of the $n - d$ rows of P that do not appear in Q, the remaining variables may be expressed as

$$\begin{aligned}\mathbf{x}_{\text{non-free}} &= R\boldsymbol{\alpha}\\ &= RQ^{-1}\mathbf{x}_{\text{free}}.\end{aligned} \tag{2.7}$$

Theorem 2.4. *For every $A \in \mathbb{F}^{m\times n}$ with dimension $d = n - r \neq 0$, there is always an ordering of the variables $\{x_1, x_2, \ldots, x_n\}$ which can be used to produce a stable triangular representation of the linear system $A\mathbf{x} = \mathbf{0}$.*

Proof. An invertible $d \times d$ sub-matrix of P will always exist since P has rank d. Moreover, the SVD guarantees that the computation of P is stable with respect to small perturbations in the coefficients of A. Thus, we will always have an ordering: $\{\mathbf{x}_{\text{non-free}}\} \succ \{\mathbf{x}_{\text{free}}\}$ with which we can write the solutions to $A\mathbf{x} = \mathbf{0}$ in the form of (2.7). (The practical stability of (2.7) will be discussed in Section 2.3.) □

2.2. Backward Error Analysis for Positive Dimensional Linear Homogeneous Systems

If the matrix A, with a positive dimensional null space, consists of entries which are approximate, a numerical solution to $A\mathbf{x} = 0$ will not likely solve this given problem exactly. However, it is standard to say that this solution exactly solves some nearby problem. We will present some such results on backward error analysis for the triangular solutions described in this paper. (For some interesting works on backward error analysis in both very general and applied settings, see (38) and references therein.)

If the solution that we find is $\mathbf{x}^*$, it does not make sense to say that we have solved $A\mathbf{x}^* = \mathbf{e}$ exactly for some nonzero vector of constants $\mathbf{e}$. Here are two reasons why:

(1) The residual is really of the form $\mathbf{e(x)}$, a vector which depends on all of the variables $\{x_1, x_2, \ldots, x_n\}$;
(2) Since our problem is homogeneous, the nearby problem which we have solved should also be homogeneous.

So, we want to say that we have solved $\tilde{A}\mathbf{x}^* = 0$ where $\mathbf{x}^* = X\mathbf{x}$, $X \in \mathbb{F}^{n\times n}$, and $\|A - \tilde{A}\|$ is small. In the context of the development in Section 2.1, we can find a *triangular* solution of the form $\mathbf{x}_{\text{non-free}} = RQ^{-1}\mathbf{x}_{\text{free}}$. So the problem that we have solved can be written as

$$A \begin{bmatrix} RQ^{-1} \\ \tilde{I} \end{bmatrix} \mathbf{x}_{\text{free}} = E\mathbf{x}_{\text{free}}. \tag{2.8}$$

Here the columns of A have simply been rearranged so that $\begin{bmatrix} RQ^{-1} \\ \tilde{I} \end{bmatrix}$ may be used to denote the $n \times d$ matrix with first (top) $n - d$ rows formed by the $n - d$ rows of RQ^{-1}, and the remaining (lowest) d rows are a suitable permutation of the identity matrix. The right hand side of (2.8) is non-zero because we are unlikely to find the exact solution to the original (approximate) problem. Presumably, there is some perturbation matrix δA with which we can write

$$(A - \delta A) \begin{bmatrix} RQ^{-1} \\ \tilde{I} \end{bmatrix} \mathbf{x}_{\text{free}} = \mathbf{0}. \tag{2.9}$$

With Equations (2.8) and (2.9), we can see that

$$\delta A \begin{bmatrix} RQ^{-1} \\ \tilde{I} \end{bmatrix} = E. \tag{2.10}$$

Proposition 2.5. *Given an approximate, linear, homogeneous equation $A\mathbf{x} = \mathbf{0}$, and a triangular representation for its solutions, there exists a perturbation to the coefficients of A so that this triangular solution exactly solves the perturbed system $(A - \delta A)$. Furthermore, we have $\|\delta A\| \leqslant \|E\|$.*

Proof. Transposing (2.10) gives

$$\left[RQ^{-1}|\tilde{I}\right] \delta A^t = E^t, \tag{2.11}$$

and we are free to choose the top $n-d$ rows of δA^t to be zero rows. The remaining d rows are then a permutation of E^t such that $\tilde{I}\tilde{E}^t = E$. With this choice, we have $\|\delta A\| = \|E\|$. There may also be alternative better choices of δA for which $\|\delta A\| < \|E\|$. □

2.3. Some Stability Results: in Theory and in Practice

In Section 2.1, we had claimed that there is an invertible $d \times d$ sub-matrix of P. However, this is a theoretical result which, in the approximate case, is rather subtle.

If P was exact, it would then contain exactly d linearly independent rows and $n - d$ linearly dependent rows. Furthermore, any particular row is linearly dependent on the other rows if and only if it is able to be expressed as an exact linear combination of them. In our case, the entries of P are approximate, and it is often quite unlikely that any row is an exact linear combination of the others. Thus, we cannot speak of having exactly d linearly independent and $n - d$ dependent rows. However, we are still guaranteed a $d \times d$ sub-matrix of P which is invertible, but there will likely be more than one such sub-matrix. So, our goal is to select for our Q the "best" $d \times d$ sub-matrix of P.

Theorem 2.6. *Given a matrix $A = U\Sigma V^t \in \mathbb{F}^{m\times n}$ with rank r, the closest singular matrix to A has rank $r-1$ and can be constructed as $\tilde{A} = U\tilde{\Sigma}V^t$, where $\tilde{\Sigma}$ is equal to Σ with σ_r replaced by zero. Furthermore, we have $\|A - \tilde{A}\|_2 = \sigma_r$.*

Proof. See Trefethen and Bau (39) for an even more general result and proof. □

Remark 2.7. The theorem about the approximation of a given matrix by another of lower rank is usually attributed to Eckart and Young (13), and is often called the Eckart-Young theorem. However, the theorem was first proved by Schmidt (1907) for integral operators, and was later generalized by Mirsky (1960) to all unitarily invariant norms.

This means that for any $d \times d$ sub-matrix Q with singular values $\{\sigma_1, \sigma_2, \ldots, \sigma_d\}$, there exists a singular matrix within distance σ_d of Q. In lieu of Theorem 2.6, our initial inclination was to claim that the "best" Q is the $d \times d$ sub-matrix of P which has the largest σ_d. Actually, the choice of the best Q is not quite that simple. It is true that we want a nonsingular Q, but, unfortunately, the Q which is farthest from singular may not give us the RQ^{-1} which is most practically stable.

Before going further, we wish to state some well-known results which will be used in an explanation of the conjecture which concludes this section.

Remark 2.8. It is well-known that for any given matrix $A = U\Sigma\mathrm{V}^t$, $\|A\|_2 = \sigma_1$. For any invertible matrix $A \in \mathbb{F}^{n\times n}$, we have $A^{-1} = V\Sigma^{-1}U$, and so the singular values of A^{-1} are $\{\frac{1}{\sigma_n}, \frac{1}{\sigma_{n-1}}, \ldots, \frac{1}{\sigma_1}\}$, and $\|A^{-1}\|_2 = \frac{1}{\sigma_n}$. If A is not square, then its pseudo-inverse $A^\dagger = V\Sigma^\dagger U^t$ can be computed instead of the inverse. For our purposes, we regard A as having full rank, and then the diagonal elements of $\Sigma^\dagger$ are still $\{\frac{1}{\sigma_n}, \frac{1}{\sigma_{n-1}}, \ldots, \frac{1}{\sigma_1}\}$. See, for example, (21) for more information on the pseudo-inverse.

Remark 2.9. Without proof we state the known result that if M is any sub-matrix of a given matrix A, then $\|M\|_p \leqslant \|A\|_p$ for any matrix p-norm.

A stable solution will have continuous dependence on its input data. However, it may be very sensitive to changes in the values substituted for the free variables. The acceptable magnitude of the condition number will depend on the particular application that is involved, and will determine if the triangular representation is practically stable. We introduce the notation: σ_Q and σ_R for the last (d^{th}) singular values of Q and R respectively. Simply, using Remarks 2.8 and 2.9, and the fact that $\|P\|_2 = 1$ (shown in Remark 2.3), we have the following bound for the condition number of RQ^{-1}:

$$\begin{aligned} \mathrm{Cond}(RQ^{-1}) &= \|RQ^{-1}\|_2 \|(RQ^{-1})^{-1}\|_2 \\ &\leqslant \|R\|_2 \|Q^{-1}\|_2 \|Q\|_2 \|R^{\dagger}\|_2 \\ &\leqslant \|P\|_2 \frac{1}{\sigma_Q} \|P\|_2 \frac{1}{\sigma_R} \\ &= \frac{1}{\sigma_Q} \cdot \frac{1}{\sigma_R}. \end{aligned} \tag{2.12}$$

By maximizing the product $\sigma_Q \cdot \sigma_R$, we will have minimized the bound on $\mathrm{Cond}(RQ^{-1})$. In our experiments, we have observed that choosing Q and R such that Q is non-singular, and $\sigma_Q \cdot \sigma_R$ is maximal, yielded a solution for which the condition number was minimal. Simply choosing Q such that it is the $d \times d$ sub-matrix which is farthest from singular does not guarantee the best solution (see the example in Section 3).

Conjecture 2.10. For every $A \in \mathbb{F}^{m \times n}$ with dimension $d = n - r \neq 0$, we can write $\mathbf{x}_{\text{non-free}} = RQ^{-1}\mathbf{x}_{\text{free}}$. By choosing Q non-singular and such that $\sigma_Q \cdot \sigma_R$ is maximal, we will have found ordered sets $\{\mathbf{x}_{\text{non-free}}\} \succ \{\mathbf{x}_{\text{free}}\}$ for which the stable triangular representation of this linear system is most practically stable.

2.4. Some Notes on Computation

To find an invertible sub-matrix Q of P, and corresponding sub-matrix R, is one challenging step in computing a practically stable triangular representation. It is considerably more difficult still to find the "best" combination of Q and R. An ideal algorithm would be one which fulfills the following two criteria:

(1) The output variable ordering is optimal;
(2) The method is efficient.

This is not a straight-forward problem. Of course there exists an algorithm which will fulfill criterion (1): simply use brute force to try all $\binom{n}{d}$ combinations of d rows taken from P. This is a sensible strategy for small problems, but the expense of trying to solve systems which admit large P is unsatisfactory. We also note that there may be several optimal choices (e.g. consider $x + y + z = 0$, where every ordering is optimal).

Employing randomness can give us (2), but not necessarily (1). We can randomly select d rows from P. For large P, we are not likely to select the best Q

(and R), but we can also expect not to obtain the worst combination. For an even better solution, one could repeat this a number of times, and take the best result. For further study, one would like to know more about the distribution of the σ_d for all $d \times d$ and $n-d \times d$ sub-matrices of P. Furthermore, thought on this strategy raises another question: if we are not guaranteed an optimal solution, what may be accepted as a "sufficient" solution?

3. A Linear Example

In this example, we use the 10×15 Hilbert Matrix, which has full rank and has as each entry $h_{i,j} = \frac{1}{i+j}$. We will denote this exact matrix by H_e and its floating point approximation by H_f.

First, we want to point out that the issue of stability is encountered in both numerical and exact approaches. The stability of a triangular representation for the solutions of an *exact* system may also be ordering-dependent. Suppose that we are given a system of linear, homogeneous polynomials $P = \{p_1, \ldots, p_m\} \in \mathbb{Q} \in [x_1, \ldots, x_n]$, and that we want a triangularization of the solutions to $P\mathbf{x} = 0$ in the form of (2.7). The coefficients in the solution may be computed exactly (say, using exact Gaussian elimination). However, the solutions to the system are still real. The substitution of real values for the free variables admits the possibility of practical instability.

Using Gaussian elimination to solve $H_e\mathbf{x} = \mathbf{0}$ with $\mathbf{x} = (x_1, \ldots, x_{15})$, we achieve the variable ordering $\{x_{11}, x_{12}, x_{13}, x_{14}, x_{15}\} \prec \{x_1, x_2, \ldots, x_9, x_{10}\}$. This is as expected as H_e has (exactly) full rank. The condition number of this (triangular) solution is $\approx 2.66 \times 10^5$. Using the SVD, we can check that this solution corresponds to one for which $\sigma_Q \approx 0.11 \times 10^{-2}$, so Q is not singular. Also, we have $\sigma_R \approx 0.35 \times 10^{-2}$.

Another suitable solution strategy for linear polynomial solving is to use Gaussian elimination on the floating point system. This, instead of doing exact computation, can yield a considerable speed up, at least, due to a decrease in required storage and intermediate computations. With partial pivoting, Gaussian elimination does not re-order the columns of a given dimension$-d$ matrix A. Thus, generally, a solution will be achieved for which the free variables will be those associated with the last d columns of A. Gaussian elimination with full pivoting, however, will exchange the order of the columns. Although this strategy may consistently yield solutions for which the residual is small, the triangular representation may be unstable, or at least not guaranteed to be optimal.

Applying Gaussian elimination with full pivoting to solve $H_f\mathbf{x} = 0$, yields the ordering $\{x_2, x_3, x_4, x_5, x_6\} \prec \{x_1, x_7, \ldots, x_{14}, x_{15}\}$, and $\|E\|_F = 6.82 \times 10^{-15}$. So, at first glance, we appear to have found a good solution. However, the approximate triangular form is practically unstable, with computed condition number $\approx 1.29 \times 10^8$. Again using the SVD, we find that this corresponds to selecting a Q for which $\sigma_Q \approx 5.97 \times 10^{-9}$, and R such that $\sigma_R \approx 0.79$.

The solution for which Q is farthest from singular, with $\sigma_Q \approx 0.55$, has $\mathbf{x}_{\text{free}} = \{x_7, x_9, x_{11}, x_{12}, x_{14}\}$. Here, $\text{Cond}(RQ^{-1}) \approx 11.70$, so that this is close to the optimal solution, below.

There is (at least) one choice for Q and R such that $\text{Cond}(RQ^{-1})$ is minimized at ≈ 7.64. We have found one such partitioning with $\sigma_Q \approx 0.46$, $\sigma_R \approx 0.24$, and corresponding to $\mathbf{x}_{\text{free}} = \{x_6, x_8, x_{10}, x_{12}, x_{14}\}$.

We have seen that, for the purpose of finding practically stable triangular representations, both Gaussian elimination on exact systems and Gaussian elimination with full pivoting on approximate systems may indeed provide a poor variable ordering. Finally, it is interesting to note that, given an efficient and reliable method of computing an optimal ordering, one might think about using it to find practically stable triangular solutions even for exact systems.

4. Approximate Linearized Triangular Decompositions and Numerical Algebraic Geometry

In Section 4.1 we introduce triangular sets, linearized about points on the variety of a polynomial system (linearized triangular sets). The approximate points about which we linearize are computed using the methods of Numerical Algebraic Geometry due to Sommese, Verschelde, and Wampler. We discuss some background on this material in Section 4.2.

4.1. Approximate Linearized Triangular Decompositions

In this section we will make use of the results from our study of the linear case to introduce Linearized Triangular Sets. Suppose that we are given a nonlinear polynomial system $p = \{p_1, p_2, \ldots, p_m\}$ in n variables $\mathbf{x} = (x_1, \ldots, x_n)$. Then the affine variety of the system over $\mathbb{C}$ is defined as

$$V(p) = \{x \in \mathbb{C}^n : p(x) = 0\}. \tag{4.1}$$

The key idea of this section is to linearize about some given nonsingular point $\mathbf{x}^0 = (x_1^0, \ldots, x_n^0)$ on the variety of the system and let $\mathbf{v} = (x_1 - x_1^0, \ldots, x_n - x_n^0)^t$. This will yield the linear system

$$\frac{\partial p_j}{\partial x_k}\left(\mathbf{x}^0\right)\mathbf{v} = \mathbf{0}. \tag{4.2}$$

If p generates a radical ideal, it is easy to show that this linearized system is the tangent space of $V(p)$ at $\mathbf{x}^0$ (7). We know the tangent space has the same dimension as the variety at this point. To avoid rank deficiency, the condition number of the Jacobian matrix at $\mathbf{x}^0$ must be considered. An extremely large condition number will either mean that this point is a multiple root, or that the polynomial system is ill-conditioned.

It is natural to use this linearization to study the fully non-linear positive dimensional case.

4.2. Numerical Algebraic Geometry

In order to achieve the linearization above we need to determine points $\mathbf{x}^0 \in V(p)$. The tools we use to determine approximations of such so-called "witness" points are the homotopy continuation methods of Sommese, Verschelde, and Wampler (37; 33).

In (37), Sommese and Wampler outlined the development of a new field "Numerical Algebraic Geometry," which led to the development of homotopies to describe all irreducible (or the weaker equidimensional) components of the solution set of a polynomial system.

An *irreducible affine variety* V is an affine variety that can not be expressed as a finite union of proper sub-varieties. A well-known result is that that any affine variety can be expressed uniquely as a union of finitely many irreducible affine varieties. The dimension of these irreducible components can vary from 0 to $n-1$:

$$V(p) = Z = \bigcup_{i=0}^{n-1} Z_i = \bigcup_{i=0}^{n-1} \bigcup_{j \in \mathcal{I}_i} Z_{ij}, \tag{4.3}$$

where Z_i is the union of all i-dimensional components, Z_{ij} are the irreducible components and $\mathcal{I}_i$ are index sets with finitely many entries. See Section 5 for an example.

Definition 4.1. Given a polynomial system $p(x) = 0$ having a decomposition Z into irreducible components Z_{ij} or more weakly into equidimensional components Z_i in (4.3), a witness set W is a set of points of the form

$$W := \bigcup_{i=0}^{n-1} W_i = \bigcup_{i=0}^{n-1} \bigcup_{j \in \mathcal{I}_i} W_{ij}, \tag{4.4}$$

where

1. W_{ij} is a finite sub-set of Z_{ij} (i.e. $W_{ij} \subset Z_{ij}$),
2. W_{ij} contains no points from any other $Z_{k\ell}$ (i.e. $W_{ij} \cap Z_{k\ell} = \emptyset$ for $(i,j) \neq (k,\ell)$),
3. W_{ij} contains $\deg Z_{ij}$ points, each occurring ν_{ij} times for some integer $\nu_{ij} \geq \mu_{ij}$ where μ_{ij} is the multiplicity of Z_{ij} as an irreducible component of $p^{-1}(0)$. Moreover, if $\mu_{ij} = 1$ then $\nu_{ij} = 1$.

See Section 5 for an example. The W_i above are the witness sets for the equidimensional decomposition and W_{ij} are the witness sets for the irreducible decomposition. Approximate points for these can be determined by numerical homotopy continuation methods. It is important to note that the witness sets for an equidimensional decomposition can be computed more cheaply than that for the irreducible decomposition.

4.3. Results for Approximate Triangular Decomposition

Examples illustrating the results of this section can be found in Section 5.

Since the witness points computed for the zero-dimensional case each have the form $x_1 = a_1, x_2 = a_2, \ldots, x_n = a_n$, it follows that:

Remark 4.2. For an exactly given input system of polynomials over $\mathbb{C}$, the (exact) witness point representation of the set of isolated points Z_0 is a collection of triangular representations over $\mathbb{C}$.

The homotopy continuation methods of (33) give a method for approximating all such isolated points, provided a small enough tolerance is used, which rely for their stability on Bernstein's theorem (1). Certification that the tolerance is small enough for Newton's method using approximate arithmetic to be certified as converging to an exact solution of the original exact system requires use, for example, of Shub and Smale's γ theory (2). We note that the case of approximate input systems is more involved, and is the subject of current research.

In our previous paper, we reassembled this collection of approximate triangular representations to give an approximate equiprojectable decomposition of the Z_0 (which is an equidimensional decomposition). That triangular decomposition can be regarded as an approximation of the decomposition that is obtained by exact methods.

For the positive $(n-1)$-dimensional case, the witness set characterization (33) can be regarded as an exact, probability 1, non-algorithmic construction using exact complex arithmetic. In addition an exact interpolation process can be given, leading us to:

Remark 4.3. For systems with n variables, each such interpolating polynomial for each irreducible component of dimension $n-1$ constitutes a triangular representation for that irreducible component. In the equi $(n-1)$-dimensional case the single interpolation polynomial is also a triangular representation.

The methods of Sommese, Verschelde, and Wampler, regarded exactly, generate enough generic points to exactly interpolate each such irreducible component by a *single* polynomial in the variables x_1, x_2, $\ldots$, x_n. In addition, by these methods a single interpolation polynomial can be obtained for Z_{n-1}, ie. for the components of dimension $n-1$ in the equidimensional decomposition. In the case of approximate arithmetic, the zero-dimensional systems arising in the above process again require certification for convergence, and algorithmic certification (in the sense of Shub and Smale) is an interesting topic of current research.

The interpolation procedure applied in Remark 4.3 incrementally increases the interpolation degree from 1 until the minimum degree where interpolation is successful is obtained, and yields triangular representations which generate radical ideals.

From Remarks 4.2 and 4.3 we have:

Remark 4.4. Approximate triangular representations can be obtained for each irreducible (and each equidimensional) component of a bivariate system of polynomials.

An easy consequence of Remark 2.4 is:

Remark 4.5. Given $\mathbf{x}^0 \in V(p)$, an ordering of the variables can be determined so that there is a stable linearized triangular representation of the polynomial system about $\mathbf{x}^0$.

Such linearized triangular systems give information on the existence and construction of associated nonlinear triangular systems. Again we add the cautionary remarks that the above statements are true as exact statements of $\mathbb{C}$, and care must be taken in approximate counterparts of such statements.

5. An Example of Sommese, Verschelde and Wampler

Consider the system, which is used as an illustrative example by (33):

$$p = \begin{bmatrix} (y-x^2)(x^2+y^2+z^2-1)(x-0.5) \\ (z-x^3)(x^2+y^2+z^2-1)(y-0.5) \\ (y-x^2)(z-x^3)(x^2+y^2+z^2-1)(z-0.5) \end{bmatrix} = 0. \tag{5.1}$$

In this illustrative example, it is easy to find the decomposition

$$V(p) = Z_2 \cup Z_1 \cup Z_0 = \{Z_{21}\} \cup \{Z_{11} \cup Z_{12} \cup Z_{13} \cup Z_{14}\} \cup \{Z_{01}\}, \tag{5.2}$$

where

1. Z_{21} is the sphere $x^2+y^2+z^2-1=0$,
2. Z_{11} is the line $(x=0.5, z=0.5^3)$,
3. Z_{12} is the line $(x=\sqrt{0.5}, y=0.5)$,
4. Z_{13} is the line $(x=-\sqrt{0.5}, y=0.5)$,
5. Z_{14} is the twisted cubic $(y-x^2=0, z-x^3=0)$,
6. Z_{01} is the point $(x=0.5, y=0.5, z=0.5)$.

For the example above, which is executed by the algorithm IrreducibleDecomposition in (33), the witness set W, the degrees d_{ij} and multiplicity bounds ν_{ij} are

$$W = W_2 \cup W_1 \cup W_0 = \{W_{21}\} \cup \{W_{11} \cup W_{12} \cup W_{13} \cup W_{14}\} \cup \{W_{01}\}, \tag{5.3}$$

where

1. W_{21} contains 2 points, $d_{21}=2$ and $\nu_{21}=1$,
2. W_{11} contains 1 point, $d_{11}=1$ and $\nu_{11}=1$,
3. W_{12} contains 1 point, $d_{12}=1$ and $\nu_{12}=1$,
4. W_{13} contains 1 point, $d_{13}=1$ and $\nu_{13}=1$,
5. W_{14} contains 3 points, $d_{14}=3$ and $\nu_{14}=1$,
6. W_{01} is a non-singular point.

See Section 7.2 of (33) for the execution summary of this example.

Consider the system p from (5.1), with decomposition (5.2), and the description of the witness points and their degrees given above. As previously noted, the possible dimensions of the irreducible components are 0, 1, and $n-1=2$.

Zero-Dimensional Components: Using the methods of (33) yields one single isolated point of degree 1: $x = 0.5$, $y = 0.5$, $z = 0.5$. This, of course, is a triangular set (and is also equiprojectable).

One-Dimensional Components: The methods of (33) predict 3 one-dimensional degree 1 (linear) components, and 1 one-dimensional degree 3 component. Immediately, the linearized triangular set method of Section 4.1 can be applied to approximate the linear one-dimensional components. Here is a sketch of the details.

First, from (33), we can determine an approximate generic point, $\mathbf{x}^0$, on each linear component: $\mathbf{a} \in Z_{11}$, $\mathbf{b} \in Z_{12}$, $\mathbf{c} \in Z_{13}$. Then, we can make use of the SVD to achieve linearized triangular representations of the form

$$\mathbf{x} = \mathbf{x}^0 + \alpha \mathbf{w}, \qquad \alpha \in \mathbb{C}, \tag{5.4}$$

where $\mathbf{x}^0 \in \{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ and $\mathbf{w} \in \{\mathbf{w}_a, \mathbf{w}_b, \mathbf{w}_c\}$ are the corresponding basis vectors given by the SVD. Here, α is regarded as an additional indeterminate with $\{x, y, z\} \succ \alpha$. Recalling (2.7), if $w_k \neq 0$ we can choose x_k as a free variable and rewrite (5.4) as

$$x_j = x_j^0 + \frac{w_j}{w_k}\left(x_k - x_k^0\right), \tag{5.5}$$

where all other x_j $(j \neq k)$ are the two non-free variables.

We used for $\mathbf{x}^0$ (respectively for each of the 3 linear 1-dimensional components):

$$\begin{aligned}
\tilde{\mathbf{a}} &\approx \left[0.50 + 2.08 \times 10^{-11} i, 1.00 + 1.64 \times 10^{-11} i, 0.125 - 7.13 \times 10^{-11} i\right]^t, \\
\tilde{\mathbf{b}} &\approx \left[0.71 + 4.10 \times 10^{-11} i, 0.50 - 9.30 \times 10^{-11} i, 1.00 + 2.92 \times 10^{-11} i\right]^t, \\
\tilde{\mathbf{c}} &\approx \left[-0.71 - 9.68 \times 10^{-11} i, 0.50 - 4.28 \times 10^{-11} i, 1.00 - 8.51 \times 10^{-11} i\right]^t.
\end{aligned}$$

The corresponding vectors $\mathbf{w}$ obtained by applying the SVD to the linearized systems about $\mathbf{x}^0$ are

$$\begin{aligned}
\mathbf{w}_a &\approx [-2.50 \times 10^{-10} - 0.i, 0.68 + 0.74i, 3.37 \times 10^{-10} - 6.32 \times 10^{-10} i]^t, \\
\mathbf{w}_b &\approx [-5.22 \times 10^{-10} + 0.i, 1.73 \times 10^{-10} + 3.54 \times 10^{-10} i, -0.85 + 0.53i]^t, \\
\mathbf{w}_c &\approx [1.51 \times 10^{-10} + 0.i, 1.39 \times 10^{-11} + 3.64 \times 10^{-10} i, -0.73 - 0.69i]^t,
\end{aligned}$$

where we have rounded the above results to two decimal places (and $0.i$ is used to denote floating point zero). The next step is to find the stable orderings of $\{x, y, z\}$ on each linear component.

Z_{11}: For the one-dimensional case, we do want to find the invertible $d \times d$ sub-matrix Q of $\mathbf{w}_a$ which has greatest d^{th} singular value. Since here we have $d = 1$, the singular values of each of the three 1×1 sub-matrix of $\mathbf{w}_a$ are simply the magnitudes of each complex entry itself. This means that we are looking for the entry of $\mathbf{w}_a$ with greatest magnitude, and this will tell us which of $\{x, y, z\}$ will be the best free-variable. We find a single stable choice:

$$\begin{aligned}
\mathbf{x}_{\text{free}} &= \{y\}, \\
\mathbf{x}_{\text{non-free}} &= \{x, z\},
\end{aligned}$$

which corresponds to either of the orderings: $y \prec x \prec z$, or $y \prec z \prec x$.

Geometrically, this can be interpreted as follows: the linear component Z_{11} is exactly a line perpendicular to the xz-plane. Because the numerical approximation to this component contains errors (due in part to the inexact point $\tilde{\mathbf{a}}$), it is a line which is not exactly perpendicular to the xz-plane. Solving for y, z in terms of x, or x, y in terms of z, are unstable choices. A small change in x would then cause a change in y roughly on the order of 10^9 (in the first case), or a change in z would cause a change in y which would also be around the order of 10^9 (in the second case).

The (only) stable approximate linearized triangular representation is

$$\begin{aligned} x &= \tilde{a}_x - (1.69 \times 10^{-10} - 1.84 \times 10^{-10} i)(y - \tilde{a}_y), \\ z &= \tilde{a}_z - (2.37 \times 10^{-10} + 6.76 \times 10^{-10} i)(y - \tilde{a}_y). \end{aligned}$$

Z_{12}: As for Z_{11}, we find just one stable choice of free variables:

$$\begin{aligned} \mathbf{x}_{\text{free}} &= \{z\}, \\ \mathbf{x}_{\text{non-free}} &= \{x, y\}, \end{aligned}$$

which corresponds to either of the orderings: $z \prec x \prec y$, or $z \prec y \prec x$. This corresponds to the approximate solution

$$\begin{aligned} x &= \tilde{b}_x + (4.43 \times 10^{-10} + 2.76 \times 10^{-10} i)(z - \tilde{b}_z), \\ y &= \tilde{b}_y + (4.07 \times 10^{-11} - 3.92 \times 10^{-10} i)(z - \tilde{b}_z). \end{aligned}$$

Z_{13}: Here the stable choice of free variables is

$$\begin{aligned} \mathbf{x}_{\text{free}} &= \{z\}, \\ \mathbf{x}_{\text{non-free}} &= \{x, y\}, \end{aligned}$$

which corresponds to either of the orderings: $z \prec x \prec y$, or $z \prec y \prec x$. The stable approximate solution is

$$\begin{aligned} x &= \tilde{c}_x - (1.10 \times 10^{-10} - 1.04 \times 10^{-10} i)(z - \tilde{c}_z), \\ y &= \tilde{c}_y - (2.60 \times 10^{-10} + 2.55 \times 10^{-10} i)(z - \tilde{c}_z), \end{aligned}$$

It is both interesting and important to note that for exact triangular decomposition, one can set a single order for the entire computation. However, here there is no single stable choice of $\{\mathbf{x}_{\text{non-free}}\}$ and $\{\mathbf{x}_{\text{free}}\}$ which covers all three cases (Z_{11}, Z_{12}, and Z_{13}).

Z_{14} (*Twisted Cubic*): Consider the linearization of p about the (random) point $\mathbf{x}^0$ on the twisted cubic given by

$$\tilde{\mathbf{d}} \approx [0.50 + 4.16 \times 10^{-11} i, 0.25 + 3.41 \times 10^{-11} i, 0.125 + 9.63 \times 10^{-11} i]^t.$$

Applying the SVD to the linearization of the system about $\mathbf{x}^0 = \mathbf{d}$ yields $\mathbf{w}$ given by

$$\mathbf{w}_d \approx [0.48 + 0.i, 0.80 + 0.10i, 0.36 - 4.30 \times 10^{-10} i]^t.$$

Then the method above yields the most stable choice

$$\begin{aligned} \mathbf{x}_{\text{free}} &= \{y\}, \\ \mathbf{x}_{\text{non-free}} &= \{x, z\}, \end{aligned}$$

which corresponds to either $y \prec x \prec z$, or $y \prec z \prec x$. We obtain the following linearized triangular decomposition:

$$\begin{aligned} x &= \tilde{d}_x - (5.90 \times 10^{-1} - 0.76 \times 10^{-1} i)(y - \tilde{d}_y), \\ z &= \tilde{d}_z - (4.43 \times 10^{-1} - 0.57 \times 10^{-1} i)(y - \tilde{d}_y). \end{aligned}$$

However, we are more interested in what can be said about the triangular decomposition of the original non-linear problem.

First, we mention that the methods of (33) interpolate this one-dimensional curve as the intersection of $n + 1 = 4$ hyper-surfaces, which are in fact ruled surfaces. These ruled surfaces correspond to random (generic) projections. Lemma 5.3 in (33) expresses the fact that the irreducible component, corresponding to this one-dimensional curve, is precisely cut out by the intersection of these 4 ruled hyper-surfaces. Equivalently in terms of generic coordinates X, Y, Z, which are random linear combinations of x, y, z, the irreducible component is defined in terms of 4 polynomials in X, Y, Z. Three of the polynomials are bivariate polynomials (of (X, Y), (X, Z), and (Y, Z) respectively) and correspond to projections onto the generic coordinate hyperplanes. Triangular decomposition of this one-dimensional curve should require only 2 rather than 4 polynomials. However, approximate triangular representations in the generic coordinates can be extracted by choosing subsystems of 2 polynomials from the 3 bivariate polynomials. Note that, in general, such triangular representations will have excess components (removed by intersection with the remaining polynomials). In some cases, excess components do not occur (a fact that can be checked in a number of ways, e.g. by numerical membership testing, or testing numerically for irreducibility). In this case, a tight generic triangular representation is determined.

We now briefly discuss the task of finding triangular decompositions in terms of the original coordinates x, y, z, rather than the generic coordinates. It is clear from our comments above, in the linear case, that we need an ordering of the variables that is numerically stable, and should be applicable even in the non-linear case. Here, we require a projection that maps the nonlinear curve onto one which has the same dimension. The linearization shows that any projection will have this property. This projection can be interpolated, so the degree of the interpolated curve is important. The approach of (33) determines that the degree of the curve is 3, and this can only drop upon projection. So a second obvious property for a 'good' projection is that this degree not be diminished.

A possible alternative approach is to bootstrap from the zero-dimensional case. The general idea of reducing a positive dimensional system to a zero-dimensional one goes back to Van der Waerden (40) for primary decomposition, and was later made algorithmic by Gianni, Trager, and Zacharias (17), among others. The

most recent work is due to Schost (31) and Dahan, et al. (11), where triangular decompositions are obtained for exact positive dimensional systems.

It is interesting to investigate how these methods might be adapted to approximate systems. Here is a sketch of this method. First, the numerical irreducible decomposition would be performed, and each irreducible component would be treated separately. The witness points for a component would be used to determine a stable ordering for the linearized system. Setting the free variables to random values yields a zero-dimensional system, to which the approximate equiprojectable decomposition (29) would be applied. The triangular sets so-obtained involve only the non-free variables. The dependence on the free variables could be determined, through choosing different random values for them, by interpolation. However, we caution that there are serious stability issues that need to be resolved, and also note that the interpolation process involving rational function reconstruction needs to be developed before such an approach can be realized.

Two-Dimensional Components: There is one single component of p, predicted by (33) which has dimension $n - 1 = 2$ and degree 2. Homotopy continuation can be used to generate enough points from which a single polynomial of degree 2 in x, y, z can be interpolated. This interpolation can be carried out automatically by PHCPack (41). This is a triangular set for the component. Note also that the minimality of the degree ensures that the ideal is radical (one property of a triangular set). It is equivalent to a multiple of $x^2 + y^2 + z^2 - 1 = 0$, which is easily seen independently here, but, of course, the method will work on examples where such a property and an expression cannot be so easily extracted.

6. Discussion

Exact triangular decomposition methods for representing exact polynomials systems (see for example (43; 24; 28; 22; 42)) have proved valuable in applications (5; 23; 14; 31; 16), and there are well-developed algorithms (28; 9) for their construction. There have also been considerable recent improvements (12; 10) in the complexity of algorithms for their construction. Such representations are desirable, not only because of their triangular solved-form structure, but also because (in comparison with other exact methods) they give the minimum number of polynomials required to form a description of the equidimensional decomposition components of such systems.

The goal of our research is to extend such methods to approximate systems of polynomials. Our previous paper (29) gave a detailed treatment of zero-dimensional systems, and in this current paper we have studied linear positive dimensional systems using methods from Numerical Linear Algebra.

The methods of (33) enable approximate generic points on the solution components of polynomial systems to be computed by numerical homotopy continuation. These witness points give the layout of the decomposition as well as the number of witness points on a component, which is its degree. As we indicate in

this paper, the zero-dimensional components, computed by the methods of (33) are a solved form (explicitly giving the coordinates of the zero sets), and constitute a collection of triangular sets (each being an isolated root). However, these sets do not directly correspond to the triangular representation computed by exact methods. Also, if n is the number of variables, each irreducible component of dimension $n-1$ (hyper-surfaces) can have additional generic points generated by homotopy continuation, and interpolated by a single polynomial. This representation, which is automatically generated by PHCPack of (41; 33), is again, as we note, trivially, a triangular set.

In the d-dimensional case where $0 < d < n-1$, the methods of (33) also generate additional points on each irreducible component, and give interpolating polynomials to represent the component. Each interpolating polynomial corresponds to a random projection of the component in $\mathbb{C}^n$ to a $(d+1)$-dimensional affine space. In general, $n+1$ generic projections (and $n+1$ interpolating polynomials) are used in that approach to precisely describe the component (see especially Lemma 5.3 of (33) for the theoretical justification). Such a representation is not triangular, since a triangular representation would only require $n-d$ polynomials. However, a triangular sub-system of $n-d$ polynomials can be extracted in generic coordinates (e.g. as discussed for the twisted cubic example). Although a numerical test for irreducibility can be applied, such generic triangular sub-systems are not generally irreducible. Their chance of irreducibility can be enhanced by adding random linear combinations of the remaining $d+1$ polynomials to the triangular system, while maintaining its triangular structure.

Given a point $\mathbf{x}^0$ on a d-dimensional irreducible component of a polynomial system computed using SVW, we compute a local linearization of the form $\mathbf{x} = \mathbf{x}^0 + P\boldsymbol{\alpha}$, where P is computed using the SVD, and the $\boldsymbol{\alpha}$'s are d newly introduced parameters. In the case of linear varieties this is actually a triangular representation. Secondly, by eliminating $\boldsymbol{\alpha}$, and provided certain stability-invertibility properties are satisfied, stable triangular representations in the variables $\mathbf{x}$ can be obtained for the linearization. We note that both of these representations involve $n-d$ linear polynomials. For linear components, (33) gives a non-triangular representation, also only requiring $n-d$ linear polynomials.

In future work, we will extend the results of this paper and (29) to the construction of triangular sets for positive dimensional systems of polynomials.

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