Inversibility of Rational Mappings and Structural Identifiability in Control Theory

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Abstract: We investigate different methods to answer the membership problem for a finitely generated k-subalgebra or a subfield generated by a finite set of fractions and apply them for testing if a polynomial (resp. rational) map from k^n to k^m admits a polynomial (resp. rational) inverse. We recall the previously known method using "tag" variables and standard bases, and give then a new one, using "symmetrical" variables, which seems more efficient. In polynomial case one can also use canonical bases. But they are known to be possibly infinite, so we give new results and a conjecture providing finiteness conditions.

For testing inversibility, we prove two bounds on the maximal degree of polynomials calculated during the standard basis or canonical basis completion procedure.

We then illustrate the symmetrical variables method, with an application to stuctural identifiability in control theory. The implementation has been done in the IBM computer algebra system Scratchpad II.

0. Introduction

It is already known that such questions as testing whether a given polynomial Q belongs to $k[P_1, \ldots, P_m]$, where k denotes any field, can be solved by considering the reduction of Q with respect to the standard basis of the ideal $(P_i - T_i)$ in $k[X_1, \ldots, X_n, T_1, \ldots, T_m]$ for an ordering which eliminates X_1, \ldots, X_n . The technique of using m "tag" variables is attributed to SPEAR by David SHANNON and Moss SWEEDLER, who made an important work to apply it for testing membership to a finite subalgebra of a polynomial ring (see [SS1]), or of a field of fractions (see [SS2]).

Such a method can be used to test if $k[P_1, \ldots, P_m]$ is equal to $k[X_1, \ldots, X_n]$, which means that the polynomial map from k^n to k^m defined by the P_i admits a polynomial inverse. Shannon and Sweedler apply it also for testing whether the field of fractions $k(P_1, \ldots, P_n)$ is equal to $k(X_1, \ldots, X_n)$. In that case, the associated mapping is birational.

We will extend this result in order to get a similar one in the case of m rational fractions. We then prove in the birational case and for f polynomial a majoration on the degree of polynomials calculated during a standard basis computation, relying on a result of O. Gabber.

Our interest on this problems was originated by the problem of structural identifiability. It led us to investigate practical tests of inversibility for rational mappings, without caring much for an expression of the inverse. We were greatly influenced by preeceding works by E. Walter, Y. Lecourtier and A. Raksanyi who applied computer algebra to the study of structural properties in automatics (see [LE], [R] or [LW]). They already used only n additional "symmetrical" variables in the same way as we do. But their method relies on pseudo-divisions and is therefore related to Wu's one, which does not seem the most efficient in this case.

In fact, our method relies on a more precise result, which could be used to test whether a given fraction belongs to the subfield generated by a finite set of fractions. The ideal we associate to a subfield does not

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depend on the set of generators chosen. Furthermore, the preceding bound is still valid and a better one can be obtained under some assumption, related with the tame generators conjecture.

Our method also applies for testing the existence of a polynomial inverse if n = m. However it cannot be used to answer the membership problem for $k[P_1, \ldots, P_n]$.

Another method can be used in polynomial case. It relies on "canonical bases", which have been introduced a short time ago by L. ROBIANO, M. SWEEDLER, D. KAPPUR and K. MADLENER (see [RS] and [KM]). They play the same role for a k-algebra as standard bases do for an ideal, which means there is a reduction procedure such that all polynomials in a k-algebra are reduced to 0 by the canonical basis. Unfortunately, the completion procedure for canonical bases may nether stop. Nevertheless, they are often much faster to compute than the standard bases using tag variables.

We will state a conjecture and some results enlightening the connection between the canonical basis of a k-algebra and that of its integral closure.

The application to inversibility is easy and the bounds valid when using standard bases extend in this case, so that the completion procedure provides a algorithm in the situation of the jacobian conjecture.

The last part is devoted to applications, mostly to structural identifiability. We show here briefly how it can be reduced to an algebraic problem and then describe the algorithm as implemented in SCRATCHPAD. Two examples are then given, one of them being unsolved by RAKSANYI's algorithm.

The last example illustrate the efficiency in a purely rational case, where the extended tag variables method does not succeed.

1. Testing Inversibility with Standard Bases and Tag Variables

We will allow ourselves bellow, where no confusion can be done to write x^{α} for $x_1^{\alpha_1} \dots x_n^{\alpha_n}$, k[x] for $k[x_1, \dots, x_n]$ and $k(\frac{P}{Q})$ for $k(\frac{P_1}{Q_1}, \dots, \frac{P_m}{Q_m})$. Through all the paper k will denote any field.

When we consider a polynomial (resp. rational) mapping, we say it is inversible if it admits a polynomial (resp. rational) inverse. Otherwise, we will precise it, for example when dealing with a polynomial map with rational inverse.

1.1. The Polynomial Case

We consider a polynomial mapping

$$\begin{array}{cccc} f & : & k^n & \longrightarrow & k^m \\ & & (x_1, \dots, x_n) & \longrightarrow & (P_1(x_1, \dots, x_n), \dots, P_m(x_1, \dots, x_n)), \end{array}$$

and want to test whether it admits a polynomial inverse. It is obviously equivalent to test that $k[P_1, \ldots, P_m]$ is equal to $k[X_1, \ldots, X_n]$. So we will first investigate how the membership problem for a finite k-subalgebra can be solved. The method we give here is from Shannon and Sweedler (see [SS1]).

We give ourselves m additional "tag" variables t_1, \ldots, t_m , and consider the ideal \mathcal{I} generated by the m polynomials $P_i - t_i$ in $k[x_1, \ldots, x_n, t_1, \ldots, t_m]$. As it is the kernel of the ring homomorphism

$$\begin{array}{cccc} \phi & : & k[x_1,\ldots,x_n,t_1,\ldots,t_m] & \longrightarrow & k[x_1,\ldots,x_n] \\ & x_i & & \longrightarrow & x_i \\ & t_j & & \longrightarrow & P_j, \end{array}$$

 \mathcal{I} is prime. We will show that the reduced standard basis of \mathcal{I} with respect to some admissible orderings can be used to answer the membership problem.

DEFINITION 1. The admissible ordering \prec on monomials of $k[x_1, \ldots, x_n, t_1, \ldots, t_m]$ is said to eliminate globally x_1, \ldots, x_n if for any two monomials $m_1 = x^{\alpha}$ and $m_2 = x^{\beta}$,

$$\sum_{i=1}^{n} \alpha_i < \sum_{i=1}^{n} \beta_i \Rightarrow m_1 \prec m_2.$$

It is known that for such an ordering, the set of polynomials in the standard basis of any ideal \mathcal{J} whose leading term depends only of the t_i form a standard basis of $\mathcal{J} \cap k[t]$.

PROPOSITION 1. Calling ST the standard basis of the ideal \mathcal{I} , defined as above, for any admissible ordering \prec which eliminates globally x_1, \ldots, x_n , and Q being any polynomial of k[x] the two following properties are equivalent:

- (i) Q belongs to k[P],
- (ii) the reduction of Q with respect to ST belongs to k[t].

Moreover, if Q is in k[P], the reduction of Q gives the expression of Q in function of P_1, \ldots, P_m .

PROOF. See [SS1]. ■

COROLLARY 1. If f admits a polynomial inverse, then ST contains n polynomials of the form $x_i - R_i(t)$ for i = 1, ..., n, and the R_i define an inverse of f.

PROOF. See [SS1]. ■

The last part is a simple consequence of the proposition.

The last corollary gives us a way of testing inversibility and getting the expression of an inverse.

COROLLARY 2. In the special case n=m, inversibility means that f is in fact one to one. Calling ψ the restriction of ϕ to k[t], ψ is also one to one and the polynomials R_i define its inverse. Furthermore ST is equal to $\{x_i - R_i(t)\}$

PROOF. See [SS1].

As this situation is related to the well known jacobian conjecture, many other "tests" have been proposed for it (see [B]). Many of them have a mere theoretical interest. K. Adjamagbo and A. van den Essen have recently proposed a differential test, relying on the same result of Gabber we are going to use in the next section (see [AE]).

REMARK 1. (About orderings) The lexicographic ordering on $x_1, \ldots, x_n, t_1, \ldots, t_m$ has obviously the wanted property.

Nevertheless, it is certainly not the most efficient. The elimination ordering of D. BAYER and M. STILL-MAN, used in their standard basis system MACAULAY would be a very better choice. Unfortunately, it is only available in a fiew computer algebra systems. We implemented it in SCRATCHPAD II where the only orderings available in the public system are the lexicographic and the degree ordering.

1.2. Inversibility in Rational Case

Let us come now to the case where

$$\begin{array}{cccc} f: & k^n & \longrightarrow & k^m \\ & (x_1, \dots, x_n) & \longrightarrow & \left(\frac{P_1(x_1, \dots, x_n)}{Q_1(x_1, \dots, x_n)}, \dots, \frac{P_m(x_1, \dots, x_n)}{Q_m(x_1, \dots, x_n)}\right) \end{array}$$

is a rational map. We state a general result, which extends a theorem that Shannon and Sweedler gave in the birational case and for f polynomial (see [SS1]). Again, we give ourselves m tag variables t_i and m more "inverse" variables u_i and consider the ideal \mathcal{I} of $k[u_1,\ldots,u_m,x_1,\ldots,x_n,t_1,\ldots,t_m]$, generated by the m polynomials $P_i-Q_it_i$ and the m other Q_iu_i-1 .

Proposition 1. The ideal \mathcal{I} is prime.

PROOF. Consider the ring homomorphism

$$\begin{array}{cccc} \psi: & k[u,x,t] & \longrightarrow & k(x) \\ & x_i & \longrightarrow & x_i \\ & u_j & \longrightarrow & Q_j^{-1} \\ & t_k & \longrightarrow & P_k Q_i^{-1}. \end{array}$$

We claim that \mathcal{I} is the kernel of ψ , which imply the proposition (see [SS2] for a more detailed proof).

DEFINITION 1. An admissible ordering \prec on monomials of k[u, x, t] is said to eliminate globally u_1, \ldots, u_m and successively x_1, \ldots, x_n if for any two monomials $m_1 = u^{\alpha} x^{\beta} t^{\gamma}$ and $m_2 = u^{\delta} x^{\varepsilon} t^{\zeta}$,

$$\begin{array}{lll} \sum_{i=1}^m \alpha_i < \sum_{i=1}^m \delta_i & \Rightarrow & m_1 \prec m_2 \\ & \sum_{i=1}^m \alpha_i = \sum_{i=1}^m \delta_i \\ & \text{and} & \exists \ 1 \leq i \leq n \ \beta_j = \varepsilon_j \ \text{for} \ j < i \ \text{and} \ \beta_i < \varepsilon_i & \Rightarrow & m_1 \prec m_2. \end{array}$$

PROPOSITION 2. In the situation given above, let \mathcal{I}' be the intersection of \mathcal{I} and k[x,t]. Then taking the reduced standard basis ST of \mathcal{I} for any admissible ordering \prec which eliminates globally the u_1, \ldots, u_m the polynomials in ST whose leading terms only depend of $x_1, \ldots, x_n, t_1, \ldots, t_m$ form a standard basis of \mathcal{I}' , and a fraction $R = \frac{M}{N}$ is in $k(\frac{P}{Q})$ iff there exist a reduced fraction $\frac{A}{B}$ of k(t) such that B does not belong to \mathcal{I}' , and MB - AN is in \mathcal{I}' .

PROOF. The first part is an easy result, using the property of \prec .

- (\Rightarrow) If R is in $k(\frac{P}{Q})$, then $\frac{M}{N} = \frac{A(\frac{P}{Q})}{B(\frac{P}{Q})}$ so that $M(x)B(\frac{P}{Q}) N(x)A(\frac{P}{Q}) = 0$. But this is $\psi(M(x)B(t) N(x)A(t))$. As \mathcal{I} is the kernel of ψ , M(x)B(t) N(x)A(t) is in \mathcal{I} . In the same way B(t) is not in \mathcal{I} for its image by ψ is not 0.
- (\Leftarrow) Now, if MB AN is in \mathcal{I}' , and B is not, we use another time the fact that \mathcal{I} is the kernel of ψ to conclude. ■

Sadly, we cannot use this to get the expression of R in $k(\frac{P}{Q})$, or even solve the membership problem, except if $k(\frac{P}{Q})$ is $k(x_1, \ldots, x_n)$, which is the aim of the next theorem. We will see in part 2.2. how to solve the membership problem with another method. The reader can refer to [SS2] to see how that technique can be used to solve the membership problem for $k[\frac{P}{Q}]$.

THEOREM 1. If f is defined as above and if ST is the standard basis of \mathcal{I} for an ordering which eliminates globally u_1, \ldots, u_m and successively x_1, \ldots, x_n , the two following properties are equivalent:

- (1) f admits an inverse,
- (2) for each i = 1, ..., n there exits in ST a polynomial of the form $B_i(t)x_i A_i(t)$.

Then the fractions $\frac{A_i}{B_i}$ give the expression of an inverse.

PROOF. (\Rightarrow) It suffices to apply the last proposition, to know that such polynomials are in \mathcal{I}' As the ordering eliminates successively x_1, \ldots, x_n , they must be in ST.

(\Leftarrow) Now, if such polynomials are in ST, B_i is not in \mathcal{I} for ST is reduced. We conclude as we did in prop. 2. ■

COROLLARY 1. If n = m, let \mathcal{J} be the ideal of k(t)[u, x] generated by the same polynomials as above, and ST the reduced standard basis of \mathcal{I} for an ordering which eliminates globally the u_i . Then the two following properties are equivalent:

- (i) f is birational,
- (ii) ST contains n polynomials of the form $x_i M_i(t)$.

The inverse is defined by the n fractions M_i .

PROOF. If f is birational, $\mathcal{I} \cap k[t]$ is (0), so that ψ extends to an morphism from k(t)[u, x] to k(x) whose kernel is generated by the same polynomials as \mathcal{I} . We use then the theorem.

REMARK 1. (About orderings) Another time, the lexicographic ordering satisfies the wanted property.

... But to use it is not the best we can do, for we do not need to eliminate successively all variables. Elimination is expensive (see [FGLM]), so that it is important to use it as few as possible. Anyway, even the elimination order does not match in that case. Such applications should lead to implement "general" orderings, allowing the user to eliminate sets of variables and/or variables one after each other, according to his needs.

1.3. A Bound for Birational Mappings

We have given so far necessary and sufficient conditions for inversibility, without caring much for complexity. But we know by experience that such calculations are much faster in the inversible case. So we need a bound to avoid useless calculations in "bad" cases. This is done in the birational case by using a theorem, proved by O. Gabber. So, until the end of this part, f will denote a rational map from k^n to k^n .

We would like to thank here Joos HEINTZ for his encouragements to search for such a result.

PROPOSITION 1. There is a one to one correspondence between rational maps (resp. birational maps) from k^n to k^n and rational (resp. birational) maps from P_n to P_n .

PROOF. See [H].

DEFINITION 1. Let F be a rational map from P_n to P_n , defined by

$$F(x_0,\ldots,x_n)=(R_0,\ldots,R_n),$$

where the R_i are n homogeneous polynomials without common factor. We call degree of F the common degree of the R_i . If f is a rational map from k^n to k^n , the degree of f is the degree of the corresponding homogeneous map.

PROPOSITION 2. If f is polynomial, its degree is the maximum degree of the P_i . In the general case, the degree of f is bounded by the maximum degree of the P_i and of the product of the Q_i .

PROPOSITION 3. (GABBER) If f is birational, then

$$\deg f^{-1} \le (\deg f)^{n-1}.$$

PROOF. See [B].

THEOREM 1. If f is a polynomial map of degree d, admitting a birational inverse, polynomials of th. 1.2.1 appear in the standard basis of \mathcal{I} where calculations are truncated in degree less than $d^n + 1$.

PROOF. The proof rests on a classical homogeneization argument (see [LA]). We first remark that in the polynomial case, we can forget the inverse variables and consider \mathcal{I} to be the ideal of k[x,t] generated by $P_x - t_i$. We define then a weight function p on variables $x_1, \ldots, x_n, t_1, \ldots, t_n$, such that $p(x_i) = 1$ and $p(t_i) = \deg P_i$. So we have a graduation \deg_p on monomials of k[x,t], such that $\deg_p(x^{\alpha}t^{\beta}) = \sum_{i=1}^n \alpha_i + \sum_{i=1}^n \beta_i p(t_i)$.

 $\deg P_i$. So we have a graduation \deg_p on monomials of k[x,t], such that $\deg_p(x^{\alpha}t^{\beta}) = \sum_{i=1}^n \alpha_i + \sum_{i=1}^n \beta_i p(t_i)$. We take then another variable x_0 of weight 1, and we homogenize \mathcal{I} for graduation \deg_p with respect to x_0 . We write \widetilde{S} the polynomial S homogenized, $\widetilde{\mathcal{I}}$ the ideal \mathcal{I} homogenized. $\widetilde{\mathcal{I}}$ is equal to $(\widetilde{P}_i - t_i)$ in $k[x_1, \ldots, x_n, t_1, \ldots, t_n, x_0]$. $\widetilde{\mathcal{I}}$ is obviously prime.

We further remark that we can extend any admissible ordering \prec on monomials of $k[t_1,\ldots,t_n]$ to an admissible ordering $\widetilde{\prec}$ on monomials of $k[x_1,\ldots,x_n,t_1,\ldots,t_n,x_0]$ of the same degree by evaluating x_0 to 1 and then applying \prec . So there is a one to one correspondence between standard basis calculations for any ideal $\mathcal J$ generated by S_1,\ldots,S_p in $k[x_1,\ldots,x_n,t_1,\ldots,t_n]$ with respect to \prec , and standard basis calculations for $\widetilde{\mathcal J}$, with respect to $\widetilde{\prec}$, if $\widetilde{\mathcal J}$ is generated by S_1,\ldots,S_p in $k[x_1,\ldots,x_n,t_1,\ldots,t_n,t_1,\ldots,t_n,x_0]$.

As \widetilde{I} must contain a polynomial of the form $(Q_i x_i - R_i) x_0^k$ (using th. 2.1.) and $x_0 \notin \widetilde{I}$, we deduce that \widetilde{I} contains $(Q_i x_i - R_i)$ whose degree \deg_p is less than $(\deg f)^n + 1$. Indeed we have two cases

$$\deg_p(Q_i\widetilde{x_i-R_i}) = \deg_p\widetilde{R}_i \leq \max_i \{p(Y_i)\} \deg R_i \leq \deg f \deg R_i$$

or

$$\deg_p(\widetilde{Q_ix_i-R_i}) = \deg_p\widetilde{Q}_ix_i \leq \max_i \{p(Y_i)\} \deg Q_i + 1$$

$$\leq \deg f \deg R_i + 1.$$

Then we only have to use the result of GABBER to show it is less or equal to $d^n + 1$.

 $\widetilde{\mathcal{I}}$ being homogeneous with respect to \deg_p , we can truncate the standard basis in degree $\deg_p \leq d^n + 1$. But as the ordinary degree is less or equal to \deg_p , we can a fortiori truncate it in degree $d^n + 1$.

Then, we evaluate x_0 to 1, which cannot increase the degree, and get the wanted result.

REMARK 1. We think a bound of the form $\varepsilon \deg(f)^{\alpha n}$ could be obtained for f rational. It should be only a technical problem to free the proof of the homogeneization argument.

2. Testing Inversibility with Standard Bases and Symmetrical Variables

2.1. Membership Problem and Inversibility in Rational Case

We return to the general case with another method. Instead of using m tag variables taking the place of P_i/Q_i , we take n "symmetrical" variables y_i taking the place of x_i . We associate to f the ideal \mathcal{J} of $k(y_1,\ldots,y_n)[u_1,\ldots,u_m,x_1,\ldots,x_n]$ generated by the 2m polynomials $Q_i(x)u_i-1$, and $P_i(x)-\frac{P_i(y)}{Q_i(y)}Q_i(x)$. We define the morphism:

$$\begin{array}{cccc} \phi: & k[u,x,t] & \longrightarrow & k(y)[u,x] \\ & x_i & \longrightarrow & x_i \\ & u_j & \longrightarrow & u_j \\ & t_k & \longrightarrow & \frac{P_k(y)}{Q_i(y)}. \end{array}$$

THEOREM 1. The fraction S = M/N belongs to k(P/Q) iff the polynomial $M(x) - M(y)N^{-1}(y)N(x)$ belongs to \mathcal{J} .

PROOF. (\Rightarrow) It is obvious that $\phi(\mathcal{I})$ is included in \mathcal{J} . We apply this to the polynomial of prop. 1.2.2. (\Leftarrow) Consider \mathcal{J}' generated in k(y)[u,x,t] by the same polynomials as \mathcal{J} and M(x)-N(x)t. $M(x)-M(y)N^{-1}(y)N(x)$ being in \mathcal{J} is equivalent to $t-M(y)N^{-1}(y)$ being in \mathcal{J}' . So we know that $t-M(y)N^{-1}(y)$ is in the reduced standard basis of \mathcal{J}' for some ordering eliminating u and x. By a classical argument, we know that any coefficient in a polynomial from the reduced standard basis is rational in the coefficients of the generating polynomials. So $M(y)N^{-1}(y)$ is in $k(\frac{P}{Q})$.

We now have an algorithm to solve the membership problem. All we have to do is calculate the standard basis of \mathcal{J} with respect to any ordering, and reduce $M(x) - M(y)N^{-1}(y)N(x)$.

COROLLARY 1. Let ST be the reduced standard basis of \mathcal{J} for any ordering, then the two following propositions are equivalent:

(i) f admits an inverse,

(ii)
$$ST = \{x_i - y_i, u_j - Q_j^{-1}(y)\}.$$

PROOF. We know that f admits an inverse iff k(P/Q) is equal to k(x). By the last theorem $x_i - y_i$ have to be in \mathcal{J} and so in ST. the property of the ordering imply they are in ST. Reducing $u_iQ_i(x) - 1$ with respect to these n polynomials, we find that $u_i - Q_i^{-1}(y)$ is in \mathcal{J} and so in ST.

Remark 1. If f is polynomial we can obviously forget the u_i .

PROPOSITION 1. If f is polynomial and if m equals n, the bound of th. 1.3.1. is still valid in this case. PROOF. It sufficies to use the morphism:

$$\begin{array}{cccc} \psi: & k[x,t,x_0] & \longrightarrow & k(y)[x,x_0] \\ & x_i & \longrightarrow & x_i \\ & t_k & \longrightarrow & P_k(y)x_0^{\deg P_k}, \end{array}$$

which satisfies $\deg_n R = \deg \psi(R)$.

REMARK 2. Of course we do not get the inverse of f by this method. We only know it exists. We sketch in [O2] a method to recover the inverse by tracing the operations performed in $k(\frac{P}{Q})$ during the standard basis calculation. We did not finish to implement it yet. We hope it could be better than the tag variables method for it avoids developping the inverse, which could be huge, and gives it rather as a "program computing the inverse".

REMARK 3. The ideal $\mathcal{I}' = \mathcal{I} \cap k[x]$ we associate to a subfield does not depend on the set of generators chosen. So we can test that two subfields are equal simply by cheking that the standard bases of the two corresponding ideals are.

REMARK 4. (About inverse variables) If all or part of the fractions are in fact polynomials, so that some Q_i are equal to 1, one can obviously forget all about u_i . As pointed out in [SS2], we can only use one inverse variable u and replace u_iQ_i-1 by $uQ_1...Q_m-1$. We can also use more variables and lower the degree by taking all the factors of the Q_i . We think it is better in most cases to keep the maximum degree of the generating polynomial small, even if that increases the number of variables. This could look strange, but it is true for many examples (see 4.3. ex. 3.).

2.2. The Polynomial Case

f is now a polynomial map from k^n to k^n , defined by n polynomials P_i . We associate to it an ideal \mathcal{I} of $k[x_1,\ldots,x_n,y_1,\ldots,y_n]$, generated by the n polynomials $P_i(x)-P_i(y)$.

PROPOSITION 1. Let ST be the reduced standard basis of \mathcal{I} for any ordering \prec with $x_i \prec y_j$, then f admits a polynomial inverse iff ST equals $\{x_i - y_i\}$ and the standard basis calculation can be truncated in degree $d^n + 1$.

PROOF. (\Rightarrow) If f admits a polynomial inverse, defined by n polynomials Q_i , $Q_i(f(x)) - Q_i(f(y))$ belongs to \mathcal{I} and is equal to $x_i - y_i$. We use then the property of the ordering which implies that those n polynomials form the standard basis. The bound on the degree follows from the same argument as in prop. 1.1.

 (\Leftarrow) We can suppose k is algebraically closed by replacing it by its algebraic closure. We deduce from the form of the standard basis that f is injective. The standard basis of the ideal generated by the same polynomials in k(y)[x] whould be the same, so using cor. 2.1.1. we know that f is birational. Suppose the inverse of f is not polynomial. It is then defined by n reduced fractions $\frac{R_i}{S_i}$, where S_i is not 1 for some i. The set defined by $S_i(P)$ is nonempty for k is algebraically closed and its irreducible components are of dimension n-1. But the image of any point in this set is in the set defined by the ideal (R_i, S_i) , whose irreducible components are of dimension n-2 at most, for $\frac{R_i}{S_i}$ is reduced. This contadicts the fact that f is injective. So its inverse is polynomial. \blacksquare

The proposition does not extend in the situation where f is from k^n to k^m with m > n.

EXAMPLE 1. If we take $f(x_1, x_2) = (x_1, x_1x_2, x_1x_2^2 + x_2)$, it is easy to check that \mathcal{I} is equal to $\{x_1 - y_1, x_2 - y_2\}$ which means that f is univalent, but $k[x_1, x_1x_2, x_1x_2^2 + x_2]$ is different from $k[x_1, x_2]$. So f admits no polynomial inverse.

REMARK 1. We do not know in this case how to recover the inverse, even by tracing the standard basis calculation.

2.3. A Bound for De JONQUIÈRE's Maps

We will show that some assumption on the form of f, a polynomial map defined by P_1, \ldots, P_m , allow us to majorate the degree in the standard basis calculation with a better bound. It has been conjectured by Segre that if f is a polynomial map from k^n to k^n admitting a polynomial inverse, it can be obtained as a composition of one to one linear maps and maps of DE Jonquière, of the form: $g(x_1, \ldots, x_n) = (\rho_1(x_1, \ldots, x_n), \ldots, \rho_n(x_1, \ldots, x_n))$, where

$$\begin{array}{rcl}
\rho_1 & = & x_1 \\
\rho_2 & = & x_2 \\
& \vdots \\
\rho_{n-1} & = & x_{n-1} \\
\rho_n & = & x_n + P_n(x_1, \dots, x_{n-1}).
\end{array}$$

This is known as the "tame generators" conjecture and it is in fact a theorem, proved by H. Jung, if n is 2 (see [B], [J]).

We will suppose that f is a polynomial map from k^n to k^m which can be obtained as a composition of one to one linear maps and maps of the two following forms:

(i)
$$g_i(x_1, ..., x_r) = (\rho_1(x_1, ..., x_r), ..., \rho_r(x_1, ..., x_r))$$
 with

$$\rho_{i,1} = x_1
\rho_{i,2} = x_2
\vdots
\rho_{i,r-1} = x_{r-1}
\rho_{i,r} = Q_i(x_1, \dots, x_{r-1})x_r + P_i(x_1, \dots, x_{r-1}),$$

(ii)
$$g_i(x_1, ..., x_r) = (\rho_1(x_1, ..., x_r), ..., \rho_{r+1}(x_1, ..., x_r))$$
 with
$$\begin{array}{rcl} \rho_{i,1} & = & x_1 \\ \rho_{i,2} & = & x_2 \\ & \vdots \\ \rho_{i,r} & = & x_r \\ \rho_{i,r+1} & = & P_i(x_1, ..., x_r). \end{array}$$

DEFINITION 1. If a map f satisfies our assumption, it is said to admit an extended Segre form.

DEFINITION 2. If f admits an extended Segre form, let $g_h \circ \ldots \circ g_1$ be an expression of f as in prop 1. and $g_i \circ \ldots \circ g_1$ be defined by r_i polynomials $\mu_{i,j}$. $\mu_{0,j}$ is taken to be x_j by convention. We take $mon_{i,j,k}$; $k = 1, \ldots, s_{i,j}$ to be all the monomials occurring in the expression of $\rho_{i,j}$. Then we call upper degree of f with respect to that extended Segre form the value

$$\max_{i=1}^{h} \max_{j=1}^{r_i} \max_{k=1}^{s_{i,j}} \deg \ mon_{i,j,k}(\mu_{i-1})$$

and the upper degree of f the minimum of the upper degrees for all possible extended Segre forms of f.

DEFINITION 3. Let $A = \{Q_1, \ldots, Q_k\}$ be a finite set of polynomials of $k[x_1, \ldots, x_n]$. An admissible ordering been given, any of them can be considered as a rewrite rule $\xrightarrow{Q_i}$. Then we call a *chain of reduction* from A, a finite list of polynomials T_1, \ldots, T_q such that T_i is equal to Q_i for $i = 1, \ldots, k$ and for each $i = k + 1, \ldots, q$ there exist j, j' < i such that

$$T_j \xrightarrow{T_{j'}} T_i$$
 or $T_j \xleftarrow{T_{j'}} T_i$.

The degree of the chain is the maximum degree of the T_i .

PROPOSITION 1. If f admits an extended Segre form, then it admits a rational inverse and the standard basis of the ideal \mathcal{I} of k(y)[x] generated by the n polynomials $P_i(x) - P_i(y)$, which is $\{x_i - y_i\}$, can be calculated in degree less or equal to the upper degree of f.

PROOF. f obviously admits a rational inverse, for each ρ_i does. Now, we know than the standard basis is of the wanted form from cor 1. of th. 2.1. To prove it can be obtained by a standard basis calculation in degree less than $\deg f$, we use the following two lemmas.

LEMMA 1. Let $\mu_{i,j}$ to be defined as in def. 2. Then for all i < h and all $j = 1, \ldots, m_{i-1}, \mu_{i-1,j}(x) - \mu_{i-1,j}(y)$ appears in a chain of reductions of degree d from $\{\mu_{i,j}(x) - \mu_{i,j}(y)\}$.

PROOF. If g_i is linear or of form (ii), it is immediate. Now, if g_i if of form (i), we just remark that the μ_{i-1} are equal to the μ_i , except for one of them and that

$$\prod_{j=1}^{m_{i-1}} \mu_{i-1,j}^{\alpha_j}(x) - \prod_{j=1}^{m_{i-1}} \mu_{i-1,j}^{\alpha_j}(y) = \sum_{j=1}^{m_{i-1}} A_j (\mu_{i-1,j}(x) - \mu_{i-1,j}(y)),$$

where the maximum degree of all terms in the sum is equal to the degree of the products.

This implies that $x_i - y_i$ appears in a chain of reductions of degree the upper degree of f from $\{P_i(x) - P_i(y)\}$. We use then the second lemma.

LEMMA 2. If the polynomial R appears in a chain of reductions T_1, \ldots, T_q of degree d from $\{Q_1, \ldots, Q_k\}$, R is reduced to 0 by the set of polynomials S calculated during a standard basis calculation of the ideal \mathcal{J} generated by Q_1, \ldots, Q_k , truncated in degree d.

PROOF. Obviously, the Q_i appear in a chain of reductions from S. So that we can take $\{Q_1, \ldots, Q_k\}$ to be S. Now the property is true for T_1, \ldots, T_k . Suppose it is true for all $1 \leq j \leq j_0$. Then $T_{j_0+1} = T_k + cx^{\alpha}T_l$ with k and l less or equal to j_0 . So that T_k and $cx^{\alpha}T_l$ are reduced to 0 by S. As the chain of reductions is of degree d, the degree of these two polynomials is bounded by d. So, if T_{j_0+1} were not reduced to 0 by S.

there would still be a critical pair of degree d at most from polynomials of S to compute, which contadicts our assumption. \blacksquare

The second lemma implies that $x_i - y_i$ appears during a standard basis calculation truncated in the upper degree of f.

If we take k to be \mathbf{R} or \mathbf{C} , and the c_j of prop 1. to be random constants, then the upper degree of f will be the degree of f. So that our calculations are done in degree less than deg f for "almost all" f admitting an extended Segre form. But it is easy to build examples where the upper degree is more than deg f, even for f one to one.

Furthermore, certainly not all f admitting an inverse admits an extended Segre form. Nevertheless, it is so for all examples of practical interest we have encountered so far. This is an explanation a posteriori for the small time of computation.

3. Testing Inversibility of Polynomial Maps with Canonical Bases.

We will briefly give the definition of canonical bases, and their main properties. More details can be found in [KM]. A will now denote the k-subalgebra of $k[x_1, \ldots, x_n]$ generated by P_1, \ldots, P_m . \prec will denote an admissible ordering on monomials of $k[x_1, \ldots, x_n]$.

DEFINITION 1. We call leading monomial of a polynomial p the monomial $x_1^{\alpha_1} \dots x_x^{\alpha_n}$ corresponding to its leading term with respect to \prec . The multidegree of p (mdeg(p)) will be the n-uple $(\alpha_1, \ldots, \alpha_n)$ of \mathbf{N}^n . The leading coefficient of p will be written $\mathrm{lc}(p)$. S being any subset of $k[x_1, \ldots, x_n]$, we call monoid associated to S (MonS), the submonoid of \mathbf{N}^n generated by the multidegrees of polynomials in S.

We can now introduce a reduction relation and a reduction process, by considering polynomials as rules.

DEFINITION 2. S being any subset of $k[x_1, \ldots, x_n]$, p and q two polynomials, we say that p is reduced to q by S ($p \xrightarrow{S} q$) if $mdeg(p) = \sum_{r \in S} d_r \; mdeg(r) \in MonS$ and $q = p - lc(p) \prod_{r \in S} lc(r)^{-d_r} \prod_{r \in S} r^{d_r}$. We can now define a reduction process consisting to reduce a polynomial with respect to S while its multidegree is in MonS. It is said then to be reduced with respect to S. If no monomial from P is in MonS, P is said to be strongly reduced.

We remark that we cannot reduce a part of a monomial as it is done for standard bases; we have to reduce the whole of it.

Remark 1. Constant polynomials are reduced to 0 with respect to any set.

Proposition 1. The reduction process allways terminates

PROOF. See [KM]. ■

We give a definition for canonical bases, enlighting their similarities with standard bases, for we can define them in the same way by replacing "k-algebra" by "ideal" and "monoid" by "monoideal" (or e-set).

DEFINITION 3. A subset S of A is a canonical basis of A if MonS = MonA. There is a unique canonical basis S such that the mutidegrees of polynomials in S form a minimal set of generators of MonA and each R in S is monic and strongly reduced with respect to $S \setminus \{R\}$. It is called the reduced canonical basis of A.

We have again a notion of S-polynomials. The main difference is that it can involve more than two polynomials.

DEFINITION 4. S being any subset of $k[x_1, \ldots, x_n]$, a superposition of polynomials in S is a 4-uple $(S', S'', (d_r \ r \in S'), (e_r \ r \in S''))$ S' and S'' being finite subsets of S with void intersection, and the d_r and e_r being positive integers, such that $\sum_{r \in S'} d_r \operatorname{mdeg}(r) = \sum_{r \in S''} e_r \operatorname{mdeg}(r)$. The S-polynomial associated to the superposition is

$$\prod_{r \in S^{\prime\prime}} lc(r)^{e_r} \prod_{r \in S^\prime} r^{d_r} - \prod_{r \in S^\prime} lc(r)^{d_r} \prod_{r \in S^{\prime\prime}} r^{e_R}.$$

The similarities extend with the following theorem.

THEOREM 1. The three following propositions are equivalent:

- (i) S is a canonical basis of A,
- (ii) for every P in A, P is reduced to 0 by S,
- (iii) for every superposition of polynomials in S, the associated S-polynomial is reduced to 0 by S.

PROOF. A sketch of the proof for $(ii) \Leftrightarrow (iii)$ is given in [KM]. The equivalence between (i) and (ii) is easy.

The part (ii) of the theorem shows that canonical bases can be used to answer the membership problem for k-algebras as part (iii) gives a process to test that a set is a canonical basis, and allows to build canonical basis by completion.

```
COMPLETION PROCEDURE

(i) S := (P_1, ..., P_m)

(ii) 1Sup := list of superpositions of polynomials in S

(iii) S2:= (); for Sup in 1Sup repeat

if (Pred:= reduire S-Pol (Sup)) \neq 0 then S2:= cons(Pred,S2)

(iv) if S2 \neq () then

S:= append(S,S2); go to (ii)

else return S
```

Proposition 2. The completion procedure stops iff the canonical basis of $A = k[P_1, \ldots, P_m]$ is finite.

Unfortunately, there are cases where it is not so.

EXAMPLE 1. (Robiano) Take A to be $\mathbf{Q}[x,xy-y^2,xy^2]$ and \prec to be such that $y \prec x$, then the canonical basis of A is infinite. Indeed it contains the polynomials xy^{2n} for $n \in \mathbf{N}$. We can remark three facts about this example. First, the k-algebra generated by the same polynomials for k of characteristic p > 0 is finite. The second fact is that A is not integrally closed, its integral closure being $\mathbf{Q}[x,y]$. The last is that the canonical basis is finite if we take $y \prec x$.

We need then finiteness conditions for canonical bases.

DEFINITION 5. We call cone associated to a submonoid Mon of \mathbf{N}^n ($\mathcal{C}(Mon)$), the convex cone of \mathbf{R}^n_+ with vertex at the origin generated by the elements of Mon considered as elements of \mathbf{R}^n_+ . We say that such a cone is polyhedral, if its topological closure is generated by a finite number of points of \mathbf{N}^n .

PROPOSITION 3. The k-algebra A has a finite canonical basis iff $\mathcal{C}(\operatorname{Mon}A)$ is polyhedral and closed. \overline{A} being the integral closure of A (in its field of fractions), $\mathcal{C}(\operatorname{Mon}A)$ is included in $\mathcal{C}(\operatorname{Mon}\overline{A})$ and $\mathcal{C}(\operatorname{Mon}\overline{A})$ is included in the topological closure of $\mathcal{C}(\operatorname{Mon}A)$, which means that if the canonical basis of A is finite, the canonical basis of \overline{A} is finite.

Conjecture — If A is finitely generated and integraly closed, its canonical basis is finite.

We have implemented the completion procedure in SCRATCHPAD II. It seams much more efficient than the tag variables, or symetrical variables method in many cases. The following proposition shows that we can use it to test polynomial inversibility, with the same bounds on the degrees of calculations as those given above for tag variables of symetric variables methods.

PROPOSITION 4. Let $A = k[P_1, ..., P_m]$, then the application $f: k^n \mapsto k^m$ defined by the P_i admits a polynomial inverse iff the canonical basis of A for any order is $\{x_1, ..., x_n\}$.

Furthermore, if m = n, the calculation during the canonical basis procedure can be trunctated in degree $deg(f)^n + 1$.

If f can be obtained as a composition of maps of de Jonquière, its upper degree Δ being defined as in def. 2.3.2., the calculations can be truncated in degree Δ .

Another interesting property is that the canonical basis procedure can be traced, in order to get an expression of the inverse as a composition of maps... being in most cases DE JONQUIÈRE's maps.

4. Application to Global Indentifiability and Other Problems

4.1. Some Control Theory

We will be interested in linear state space structures with zero initial conditions. Such a structure M is a set of models $M(\theta)$ defined by:

$$\begin{array}{rcl} dX/dt & = & A(\theta)X + B(\theta)u(t) \\ Y & = & C(\theta)X \\ X(0) & = & 0, \end{array}$$

where the input function $u(t) \in U$ denotes the action of the experimentator (U is generally the set of piecewise-continuous functions), the state vector $X \in \mathbf{R}^q$ denotes the internal state of the physical or chemical system described by the model, the output vector $Y \in \mathbf{R}^r$ denotes the values measured during the experiment, and $\theta \in D \subset \mathbf{R}^n$ denotes internal parameters of the system.

We will now state some formal definitions.

DEFINITION 1. A property is said to be structural if it is valid for almost all models of a structure.

Definition 2. A model $M(\theta)$ is globally identifiable if for all $u \in U$, for all $\theta' \in D$

$$Y(t, \theta', u) = Y(t, \theta, u) \Rightarrow \theta' = \theta.$$

DEFINITION 3. According to the preceding definitions, a structure M is said to be globally identifiable if almost all model $M(\theta)$; $\theta \in D$ is.

In practice this means that we want to know a priori if we have a probability 1 to determine a unique value of θ and a unique model, from the experimental results. Such definitions could be given for structures described by other kinds of differential systems. But the considered case has the nice property that we can summarize its input-output behaviour with a polynomial function of the coefficient of A, B and C, by taking the coefficients of the transfer matrix, or the Markov parameters. We suppose for now on that the coefficients of A, B and C are polynomials in θ . So we only have to test the structural injectivity of a polynomial map $f(\theta)$. The reader can refer to [LE], [R] or [LW] for more details.

So the problem is now to test whether there exist a subset E of D such that f restricted to $D \setminus E$ is injective. In practice the answer can often been given by considering only the complex case.

PROPOSITION 1. Let f from \mathbb{C}^n to \mathbb{C}^m be a polynomial map. Then, there exist a domain E of zero measure such that f restricted to $\mathbb{C}^n \setminus E$ is an one to one iff f admits a rational inverse.

This property allows us to use cor 1. of th. 2.2.1. where we can forget the u_i for f is polynomial. If f admits no inverse, we can use the standard basis calculated to get more precise information. For example, if the set of solution is of dimension greater than zero, we know that the structure f is not structurally identifiable even in real case.

4.2. An Implementation in Scratchpad II

The implementation we made in SCRATCHPAD II contains two main parts. The first is the domain STRUCTLS, whose elements represent linear structures with zero initial conditions. They are mostly represented as a record of three matrix. It allows the calculation of classical summaries as Markov parameters or coefficients of the transfer matrix. Other "special" summaries could be calculated with existing functions of SCRATCHPAD II. We have developed many functions to store information about the structure in order not to repeat calculations. Structures can also easily be stored on disk, for further use.

The package IDPACK realize the test of inversibility. It builds the list of polynomials $P_i(x) - P_i(y)$ and then calls the standard basis package of SCRATCHPAD II. It answers **True** if the standard basis has the form of cor. 1. of th. 2.1.1. and **False** in all other cases. Of course, in this case we cannot be sure of it, except if the dimension of the ideal is greater than zero. In general, the user can recover the result of the standard basis calculations which has been stored. As we use degree ordering, we cannot solve the system yet. But, the package implemented by J.C. FAUGÈRE in SCRATCHPAD (see [FGLM]) allow us to get easily

the standard basis for lexicographic ordering. In this form, we can try to define extra solutions and check if they can or not be in D. This part of work has not yet been developed in our implementation.

Another function deals with the case where f is rational, which we do not need yet for structural identifiability. We will see an application for it with the last example.

4.3. Examples

EXAMPLE 1. ([LE] p. 105) For this example, already solved by LECOURTIER, we show a part of SCRATCHPAD session, as an illustration of our implementation.

struct

Parametres internes = [th1,th2,th3,th4,th6,th7]

Type: STRUCTLS

identifiable?(struct, "Transfert")

(6) false

Type: B
$$.06 (IN) + .247 (EV) + .023 (OT) = .33 sec$$

It is easy to deduce from the form of the standard basis that there is an extra solution given by:

$$\begin{array}{lcl} \theta_1 & = & \theta_3' - \theta_2' \\ \theta_2 & = & \theta_2' \\ \theta_3 & = & \theta_1' + \theta_2' \\ \theta_4 & = & \theta_4' \\ \theta_6 & = & \theta_1' \theta_6' / (\theta_3' - \theta_2') \\ \theta_7 & = & \theta_7'. \end{array}$$

Even in that case, where the summary mapping admits no inverse, the standard basis is calculated in degree 3, which is the degree of the mapping.

EXAMPLE 2. ([R] p. 115) We consider the structure defined by the three matrix:

$$A = \begin{pmatrix} -f_1(v_{3,1} + v_{2,1} + v_{0,1}) & f_1v_{1,2} & f_1v_{1,3} & 0 & 0 \\ f_2v_{2,1} & -f_2(v_{3,2} + v_{2,1}) & f_2v_{2,3} & 0 & 0 \\ f_3v_{3,1} & f_3v_{3,2} & -f_3(v_{4,3} + v_{2,3} + v_{1,3}) & f_3v_{3,4} & 0 \\ 0 & 0 & f_4v_{4,3} & -f_4(v_{5,4} + v_{3,4}) & f_4v_{4,5} \\ 0 & 0 & 0 & f_5v_{5,4} & -f_5(v_{4,5} + v_{0,5}) \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} .$$

In this example, ordinary summaries would be too great to be computed. But the form of the structure allowed RAKSANYI to find a smaller one, which we have recomputed in SCRATCHPAD II. It takes 140.431

sec. to our program to find it is not identifiable. Indeed there is again one extra solution. Raksanyi's program does not succed in this case. It stops by lack of memory after many hours of calculation. Some unfortunate mistake made Raksany believe at one time that it was identifiable as it is said in [R].

EXAMPLE 3. The last example has no connection with identifiability. We want to test whether f from \mathbb{C}^9 to \mathbb{C}^{12} defined by the 12 polynomials $\rho_{i,j,k}$; i,j,k=1,2,3 $j\neq i$ $k\neq i$ in the 9 variables $s_{l,m}$; l,m=1,2,3:

$$\rho_{i,j,k} = s_{j,k} + \frac{s_{j,i}s_{i,k}}{g_i - s_{i,i}},$$

where the gi are known constants, admits a rational inverse. We give a part of the scratchpad session, where lp is the list of polynomials defining \mathcal{I} . As there is only three different denomianators, we only need three inverse variables.

groebner lp

loading GB LISPLIB K1 for package GroebnerPackage loading GBINTERN LISPLIB K1 for package GroebnerInternalPackage

Type:

L NDMP([s11,s12,s13,s21,s22,s23,s31,s32,s33,u1,u2,u3],QF P[S11,S12,S13,S21,S22,S23,S31,S32,S33,G1,G2,G3]I) 1.907 (IN) + 34.772 (EV) + 1.614 (OT) + 5.218 (GC) = 43.512 sec

We have simulated the tag variable method of th. 1.2.1. with MACAULAY by trying to eliminate globally the u_i . We used MACAULAY because it is much more powerfull for standard basis, than the package of SCRATCHPAD even in a small computer SPS7 BULL. It stops by lack of memory after about a day of calculations.

If we use only one inverse variable u, it takes 247.62 sec to compute the standard basis.

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