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# Finding identifiable parameter combinations in nonlinear ODE models and the rational reparameterization of their input-output equations

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# Abstract

When examining the structural identifiability properties of dynamic system models, some parameters can take on an infinite number of values and yet yield identical input-output data. These parameters and the model are then said to be unidentifiable. Finding identifiable combinations of parameters with which to reparameterize the model provides a means for quantifying the model and exercising its solutions. In this paper, we revisit and explore the properties of an algorithm for finding identifiable parameter combinations. We find conditions for the existence of a set of *M* algebraically independent identifiable parameter combinations and find sufficient conditions for rational reparameterization of the input-output equations derived from a given model. We also demonstrate the application of the procedure to a nonlinear biomodel.

Key words: Identifiability, Differential Algebra, Gröbner Basis, Reparameterization

# 1. Introduction

Parameter identifiability analysis for dynamic system ODE models addresses the question of which unknown parameters can be quantified from given input-output data. *Unidentifiable* parameters can take on arbitrary values and yet result in identical input-output data. In such cases, the model and its parameter vector **p** are underdetermined with respect to the input-output data. This indeterminacy can be removed by finding combinations of parameters that take on a unique or finite number of values, which are then used as candidates to reparameterize the model, rendering it *identifiable*. Thus the question becomes, how can identifiable parameter combinations be found?

This question has been partially answered for several model classes, under limited conditions. Evans and Chappell [1] and Gunn et al [2] adapt the Taylor series approach of Pohjanpalo [3] to find locally identifiable combinations. Chappell and Gunn [4] use the similarity transformation approach to generate locally identifiable reparameterizations. Thus, with these methods identifiability can only be guaranteed (at least) locally. The problem of finding identifiable parameter combinations has also been addressed using differential algebraic methods, as Denis-Vidal et al [5,6], Verdière et al [7], and Boulier [8] find globally identifiable combinations of parameters using an "inspection" method as discussed later in this paper. However, as shown by Meshkat et al [9], this method is difficult to implement as a fully

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automated computational procedure.

In [9], an algorithm was outlined for finding the 'simplest' set of globally identifiable parameter combinations for a practical class of nonlinear ODE models. This algorithm extended the method of Saccomani and coworkers [10] using a variation of the Gröbner basis approach. In this paper, we address several issues that arose in [9] regarding properties of the identifiable parameter combinations found, including algebraic independence and the existence of a rational reparameterization of the input-output equations. Although a rational reparameterization of the original nonlinear model cannot always be done (as shown in [1]), we prove here that a rational reparameterization of the input-output equations derived from the original nonlinear model can always be found over algebraically independent parameter combinations. In other words, we can always use the "normal canonical form" to reparameterize the input-output equations over identifiable parameter combinations. In addition to being useful in quantifying the model and exercising its solutions, we will show that the ability to rationally reparameterize the input-output equations leads to a rigorous proof of identifiability.

#### 2. Nonlinear ODE Model

The general form of the models under consideration is:

$$\dot{x}(t, p) = f(x(t, p), u(t), t; p), t \in [t_0, T]$$

$$y(t, p) = g(x(t, p); p)$$

$$x_0 = x(t_0, p)$$
(2.1)

Here x is a n-dimensional state variable,  $x_0$  is the initial state at time  $t_0$ , p is a P-dimensional parameter vector, u is the r-dimensional input vector, and y is the m-dimensional output vector. We assume f and g are rational polynomial functions of their arguments. Also, constraints reflecting known relationships among parameters, states, and/or inputs are assumed to be already included in (2.1), because they generally affect identifiability properties [11]. For example,  $p \ge 0$  is common.

#### 3. Identifiability and the Differential Algebra Approach

The question of *a priori structural identifiability* concerns finding one or more sets of solutions for the unknown parameters of a model from noise-free experimental data. Structural identifiability is a necessary condition for finding parameter values in the real "noisy" data problem, often called the *numerical identifiability* problem.

Structural identifiability can be expressed as an injectivity condition, as in [10]. Let  $y = \Phi(p, u)$  be the input-output map determined from (2.1) by eliminating the state variable x. Consider the equation  $\Phi(p, u) = \Phi(p^*, u)$ , where  $p^*$  is an arbitrary point in parameter space and u is the input function. If there exists only one solution  $p = p^*$ , then this corresponds to global identifiability. If there exists finitely many distinct solutions for p, then this corresponds to local identifiability. Infinitely many solutions for p corresponds to unidentifiability.

The *a priori structural identifiability* problem can be solved using the differential algebra approach of Saccomani et al [10], which follows methods developed by Ljung and Glad [12] and Ollivier [13,14]. Their program, DAISY, can be used to automatically check global identifiability of nonlinear dynamic models [15]. We summarize their approach below. A detailed description can be found in [9,15].

Using Ritt's pseudodivision algorithm, an input-output map can be determined in implicit form. The result of the pseudodivision algorithm is called the *characteristic set* [13], which is a "minimal" set of differential polynomials which generate the same differential ideal as the ideal generated by (2.1) [15]. The first m equations of the characteristic set are those independent of the state variables, and form the *input-output relations* [15]:

$$\Psi(\boldsymbol{y}, \boldsymbol{u}, \boldsymbol{p}) = \boldsymbol{0} \tag{3.1}$$

The characteristic set is in general non-unique, but the coefficients of the input-output equations can be fixed uniquely by normalizing the equations to make them monic [15].

The m equations of the input-output relations,  $\Psi(y, u, p) = 0$  are polynomial equations in the variables  $u, \dot{u}, \ddot{u}, ..., y, \dot{y}, \ddot{y}, ...$  with rational coefficients in the parameter vector p. Specifically, these equations involve polynomials from the differential ring R(p)[u, y], where R(p) is the field of rational functions over the real numbers in the parameter vector p. For each equation, we can write  $\Psi_j(y, u, p) = \sum_i c_i(p)\psi_i(u, y)$ , where  $c_i(p)$  is a rational function in the parameter vector p and  $\psi_i(u, y)$  is a monomial function in the variables  $u, \dot{u}, \ddot{u}, ..., y, \dot{y}, \ddot{y}, ...,$  etc. We call  $c_i(p)$  the coefficients of the input-output equations.

To form an injectivity condition, we set  $\Psi(\mathbf{y}, \mathbf{u}, \mathbf{p}) = \Psi(\mathbf{y}, \mathbf{u}, \mathbf{p}^*)$ . This becomes  $\sum_i (c_i(\mathbf{p}) - c_i(\mathbf{p}^*))\psi_i(\mathbf{u}, \mathbf{y}) = 0$  for each input-output equation. Since the characteristic set is computed from a prime ideal [16], then  $\sum_i (c_i(\mathbf{p}) - c_i(\mathbf{p}^*))\psi_i(\mathbf{u}, \mathbf{y}) = 0$  can be factored in such a way that  $\psi_i(\mathbf{u}, \mathbf{y})$  are linearly independent and global identifiability thus becomes injectivity of the map  $c(\mathbf{p})$  [15]. That is, identifiability is determined by the equations

$$\boldsymbol{c}(\boldsymbol{p}) = \boldsymbol{c}(\boldsymbol{p}^*) \tag{3.2}$$

for arbitrary  $p^*$  [15]. Thus, the model (2.1) is a priori globally identifiable if and only if  $c(p) = c(p^*)$ implies  $p = p^*$  for arbitrary  $p^*$  [15]. The equations  $c(p) = c(p^*)$  are called the *exhaustive summary* [13].

The model (2.1) is locally identifiable if and only if there are finitely many distinct solutions for p. The model (2.1) is unidentifiable if and only if there are infinitely many solutions for p, that is, the solution for p is expressed in terms of one or more free variables. Thus, determining structural identifiability is reduced to the nature of the solutions to  $c(p) = c(p^*)$ , which is typically solved by finding a Gröbner Basis and using elimination [15].

#### 4. Some methods for finding identifiable parameter combinations

We focus on the case when (3.2) has infinitely many solutions (unidentifiability) in this paper. Unidentifiable models cannot be quantified from input-output data. A useful alternative is to find identifiable parameter combinations which can always be determined from input-output data, and attempt to reparameterize our model (2.1) in terms of these new parameters. Before we revisit our method for finding identifiable parameter combinations [9], we briefly present two other methods for finding identifiable parameter combinations. Both of these procedures rely on using the exhaustive summary  $c(p) = c(p^*)$  to find parameter combinations that are either uniquely or finitely determined by  $p^*$ .

Let *s* be the number of free parameters, defined as the number of total parameters *P* minus the number of equations *M* in a solution of  $c(p) = c(p^*)$ . That is, there are *s* free parameters and *M* "non-free" parameters, where P = M + s. Sometimes identifiable combinations can be found directly from the solutions to the equations  $c(p) = c(p^*)$ , by algebraically manipulating their solutions to form M = P - s parameter combinations in terms of  $p^*$  only. For example, if the solution to  $c(p) = c(p^*)$  is of the following form:

$$p_1 = \frac{p_1^* p_2^*}{p_2}$$
$$p_3 = p_3^*$$

Then clearly  $\{p_1p_2, p_3\}$  are uniquely determined by  $p^*$  because we can move the parameter vector p all to one side of the equation. To verify global identifiability, one would then reparameterize  $c(p) = c(p^*)$  over these parameter combinations  $\{p_1p_2, p_3\}$  and check the injectivity condition.

However, this ability to "move all parameters to one side of the equation" and thus "decouple" our parameter solution cannot always be done, as demonstrated in the example below:

$$p_1 = \frac{p_2 - p_2^*}{p_1^*}$$
$$p_3 = p_3^*$$

Here we see that we cannot put the first equation in the form  $g(\mathbf{p}) = g(\mathbf{p}^*)$ .

Why is this the case? The solutions to  $c(p) = c(p^*)$  can be found by solving for a Gröbner Basis, which is basically a way of simplifying the equations to be solved to a "triangular form" where we attempt to eliminate some parameters, based on a chosen ranking. Thus no attempt to keep the p and  $p^*$ parameters separated is made during the elimination process, so it is simply fortuitous if this occurs! Several examples of models whose parameter solutions cannot be decoupled can be found in [9].

The other way to find identifiable combinations is through the process called "inspection" [8]. The coefficients  $c_i(\mathbf{p})$  of the input-output equations are assumed to be identifiable [17]. The process of "inspection" involves adding/subtracting/multiplying/dividing the coefficients  $c_i(\mathbf{p})$  amongst each other

to form simpler identifiable combinations, which are always of the form  $g(\mathbf{p}) = g(\mathbf{p}^*)$ . For example, if the coefficients are:

$$c_1(\boldsymbol{p}) = p_1 p_2 p_3$$
$$c_2(\boldsymbol{p}) = p_2$$

Then it is obvious that the combinations  $\{p_1p_2, p_3\}$  are also uniquely determined by  $p^*$  and by reparameterizing c(p) over these combinations, one could verify injectivity and thus global identifiability.

However, if we instead have the following as coefficients:

$$c_1(\mathbf{p}) = p_1 + p_2 + p_3 + p_4$$
$$c_2(\mathbf{p}) = p_1 p_3 + p_1 p_4 + p_2 p_3 + p_2 p_4$$

then it is not so easy to simplify these coefficients amongst each other to form simpler identifiable combinations. If we solve  $c(p) = c(p^*)$ , then we discover that  $\{p_1 + p_2, p_3 + p_4\}$  have two distinct sets of solutions:  $\{p_1^* + p_2^*, p_3^* + p_4^*\}$  and  $\{p_3^* + p_4^*, p_1^* + p_2^*\}$  and thus can be shown to be locally identifiable. There are some examples of models in [9] where inspection gets trickier, primarily in examples where there a finite number of distinct solutions for p, expressed in terms of one or more free variables. This is where a Gröbner Basis can come to the rescue.

#### 5. Method for finding identifiable parameter combinations

Our algorithm for finding identifiable combinations is based on the principle that a Gröbner Basis is in a sense a "simpler form" of  $c(p) = c(p^*)$ . When testing for identifiability using the differential algebra approach of [15], we are solving the system  $c(p) = c(p^*)$  by finding a Gröbner Basis and then by elimination, finding a solution for p in terms of  $p^*$  and possibly free parameters. Since a Gröbner Basis helps solve the system  $c(p) = c(p^*)$ , by reducing it to a simpler (triangular) form, then we speculated and consequently demonstrated in [9] that the Gröbner Basis can find identifiable combinations that are 'simpler' than c(p).

There are at least M coefficients of the input-output equations, by definition. Thus, the ideal generated by  $c(p) = c(p^*)$  is composed of at least M equations. From the exhaustive summary,  $c(p) = c(p^*)$ , we construct a Gröbner Basis in the form  $G = \{G_1(p, p^*), ..., G_k(p, p^*)\}$ , where  $G_i$  is a polynomial function with  $k \ge M$ , depending on the ranking of parameters. Our goal is to find M terms of the form

$$q_i(\mathbf{p}) - q_i(\mathbf{p}^*)$$
 (5.1)

appearing either as an element by itself or as a factor of an element in a Gröbner Basis, since when set to zero this means  $q_i(\mathbf{p})$  has either a unique or finite number of solutions, respectively. In other words,  $G_i(\mathbf{p}, \mathbf{p}^*)$  is "decoupled" into a polynomial in  $\mathbf{p}$  minus the same polynomial in  $\mathbf{p}^*$ .

For example, if there is a Gröbner Basis element  $p_1p_2 - p_1^*p_2^*$ , this means  $p_1p_2$  has a unique solution. Or we may have  $(p_3p_4 - p_3^*p_4^*)(p_3p_4 - p_5^*p_6^*)$  and  $(p_5p_6 - p_3^*p_4^*)(p_5p_6 - p_5^*p_6^*)$  as elements, which means that  $p_3p_4$  and  $p_5p_6$  have a finite number of distinct solutions.

Note that instead of (5.1), we may have elements scaled by an arbitrary polynomial function  $\tilde{f}(\boldsymbol{p}^*)$ ,

$$\tilde{f}(\boldsymbol{p}^*)q_i(\boldsymbol{p}) - \tilde{f}(\boldsymbol{p}^*)q_i(\boldsymbol{p}^*)$$

whose solution reduces to the simplified form (5.1). For example,  $p_1^*p_2p_3 - p_1^*p_2^*p_3^*$  reduces to  $p_2p_3 - p_2^*p_3^*$ .

Additionally, sometimes the Gröbner Basis element or factor can be rewritten in decoupled form in order to get an identifiable expression. For example, an element  $p_2^*p_1 - p_1^*p_2$  can be decoupled as  $\frac{p_1}{p_2} - \frac{p_1^*}{p_2^*}.$ 

Determination of additional expressions of the type (5.1) depends upon the choice of ranking of parameters when constructing the Gröbner Basis. The combinations we seek may not all appear in a single Gröbner Basis, hence the need for several rankings of parameters. One technique described in [9] is to try all P shifts of the parameter vector p, since this forces each parameter to have the highest ranking, and thus be eliminated in that order. However, this may not give all M decoupled terms, thus different permutations of the parameter vector  $\boldsymbol{p}$  may also need to be tested [9].

More than M decoupled elements can appear in the Gröbner Bases, so as stated in [9], we look for the M 'simplest' algebraically independent combinations that as a set span all P parameters. We note that if the model is reducible, i.e. if one or more parameters in the model equations do not appear in the input-output equations, then we rename P to the number of parameters appearing in the input-output By 'simplest', we mean the lowest degree and fewest number of terms. Algebraic equations. independence will be defined in Section 8. We called the M simplest terms of the form (5.1) the canonical set [9]. It is important to note that the canonical set is not necessarily unique, as discussed in [9]. We called the polynomials in the canonical set of the form  $q_i(\mathbf{p})$  the simplified canonical set [9].

To formally check identifiability, one attempts to reparameterize the coefficients c(p) of the inputoutput equations over the terms  $q = q_i(\mathbf{p})$  in the simplified canonical set. If a rational reparameterization  $\tilde{c}(q)$  exists, then injectivity of  $\tilde{c}(q)$  is tested, i.e. if  $\tilde{c}(q) = \tilde{c}(q^*)$ , does  $q = q^*$ ? We found in [9] that if  $q_i(\mathbf{p}) - q_i(\mathbf{p}^*)$  appeared as an element in a Gröbner Basis, then global identifiability results, whereas if  $q_i(\mathbf{p}) - q_i(\mathbf{p}^*)$  appeared as a factor in a Gröbner Basis, then local identifiability results.

A more detailed explanation of our algorithm can be found in [9]. Here, we summarize it as three basic steps:

Step 1: Search through all relevant rankings and determine elements of the Gröbner Bases (or factors, as needed) that *can be simplified* to the decoupled form  $q_i(\mathbf{p}) - q_i(\mathbf{p}^*)$ .

Step 2: Select the M 'simplest' algebraically independent combinations. By 'simplest', we mean the lowest degree and fewest number of terms. The set of M combinations must span all P parameters.

Step 3: Verify the injectivity condition of the model, that is, reparameterize c(p) as  $\tilde{c}(q)$  and then test if  $\tilde{c}(q) = \tilde{c}(q^*)$  implies that q has a unique or finite number of solutions.

It should be noted that the method used in the DAISY program is capable of handling nonzero initial conditions [15, 18], and once the input-output equations are generated, the algorithm described in this paper can still be used to find identifiable combinations.

#### 6. Example of finding decoupled combinations

We now demonstrate our algorithm on a classic 2-compartment model that has been made nonlinear.

$$\dot{x}_1 = k_{12}x_2 - (k_{01} + k_{21})x_1^2 + b_1u$$
$$\dot{x}_2 = k_{21}x_1^2 - (k_{02} + k_{12})x_2$$
$$y = c_1x_1$$

Definitions:

 $x_1, x_2$  state variables

*u* input

y output

 $k_{12}, k_{21}, k_{01}, k_{02}, b_1, c_1$  unknown parameters

Figure 1.

Let  $p = \{k_{12}, k_{21}, k_{01}, k_{02}, b_1, c_1\}$  and  $p^* = \{\alpha, \beta, \gamma, \delta, \epsilon, \theta\}$ .

The input-output equation determined by Ritt's pseudodivision algorithm is:

$$-b_1c_1^2\dot{u} + c_1\ddot{y} + (k_{02} + k_{12})c_1\dot{y} + 2(k_{01} + k_{21})y\dot{y} - (k_{02} + k_{12})b_1c_1^2u + (k_{01}k_{02} + k_{01}k_{12} + k_{02}k_{21})y^2 = 0$$

We normalize the equation to make it monic by diving by  $b_1c_1^2$  [15]. The coefficients c(p) are:

$$\frac{1}{b_1 c_1}$$
$$\frac{k_{02} + k_{12}}{b_1 c_1}$$
$$\frac{2(k_{01} + k_{21})}{b_1 c_1^2}$$

$$\frac{-(k_{02} + k_{12})}{\frac{k_{01}k_{02} + k_{01}k_{12} + k_{02}k_{21}}{b_1c_1^2}}$$

Notice there are 5 coefficients, but only 4 of them are algebraically independent. Thus, we only use the first, third, fourth, and fifth coefficients. We will address this in more detail in section 9 of this paper.

We solve  $c(p) = c(p^*)$ :

$$\begin{split} b_{1}c_{1} - \epsilon\theta \\ b_{1}c_{1}^{2}(\beta + \gamma) - (k_{01} + k_{21})\epsilon\theta^{2} \\ k_{02} + k_{12} - \alpha - \delta \\ b_{1}c_{1}^{2}(\alpha\gamma + \beta\delta + \gamma\delta) - (k_{01}k_{02} + k_{01}k_{12} + k_{02}k_{21})\epsilon\theta^{2} \end{split}$$

To get:

$$k_{12} = \frac{c_1 \alpha \beta}{c_1 \beta + c_1 \gamma - k_{01} \theta}$$
$$k_{21} = \frac{c_1 \beta + c_1 \gamma - k_{01} \theta}{\theta}$$
$$k_{02} = \frac{c_1 \alpha \gamma + c_1 \beta \delta + c_1 \gamma \delta - k_{01} \alpha \theta - k_{01} \delta \theta}{c_1 \beta + c_1 \gamma - k_{01} \theta}$$
$$b_1 = \frac{\epsilon \theta}{c_1}$$

Thus not all of the identifiable combinations are obvious from this solution.

From the Gröbner Basis with ranking  $\{k_{01}, k_{02}, b_1, c_1, k_{12}, k_{21}\}$ , we have:

$$\begin{cases} -\epsilon\theta(c_1\alpha\beta - k_{12}k_{21}\theta), & \epsilon\theta^2(b_1k_{12}k_{21} - \alpha\beta\epsilon), & b_1c_1 - \epsilon\theta, & k_{02} + k_{12} - \alpha - \delta, \\ & \epsilon\theta(c_1\beta + c_1\gamma - k_{01}\theta - k_{21}\theta) \end{cases}$$

Notice there are 5 decoupled terms to choose from, but we only need M = P - s = 5 - 1 = 4 terms. Thus we pick the following algebraically independent decoupled combinations, which we also call our *simplified canonical set*:

$$b_{1}c_{1}$$

$$k_{02} + k_{12}$$

$$\frac{k_{01} + k_{21}}{c_{1}}$$

$$\frac{k_{12}k_{21}}{c_1}$$

Which we call:  $q_1, q_2, q_3, q_4$ 

We can reparameterize our coefficients as:

$$\frac{1}{q_1}$$
$$\frac{q_2}{q_1}$$
$$\frac{2q_3}{q_1}$$
$$-q_2$$
$$\frac{q_2q_3 - q_4}{q_1}$$

Thus we have found a rational reparameterization of the input-output equation. Then, when we set  $\tilde{c}(q) = \tilde{c}(q^*)$ , we get  $q = q^*$ , which means that our decoupled combinations q are globally identifiable.

Thus, we can reparameterize our nonlinear model using the normal canonical form, i.e. reduction to a first order system. Let  $y = v_1$ ,  $\dot{y} = \dot{v}_1 = v_2$ ,  $u = u_1$ ,  $\dot{u}_1 = u_2$ . Then the input-output equations become:

$$\dot{v}_1 = v_2$$
  
$$\dot{v}_2 = -\frac{q_2}{q_1}v_2 - \frac{2q_3}{q_1}v_1v_2 + q_2u_1 - \frac{q_2q_3 - q_4}{q_1}v_1^2 + \frac{1}{q_1}u_2$$

where  $q_1, q_2, q_3, q_4$  are all globally identifiable.

Note that in this case, the identifiable combinations could be found from a single Gröbner basis, but this is not true in general, as seen in [9]. Additionally, the "inspection" method could have been used to find the identifiable parameter combinations we found, but we note that this method is not easily automatable.

Using these q, we seek to reparameterize the original model. In this case, this can be done by using the scaling:  $X_1 = c_1 x_1$  and  $X_2 = k_{12} c_1 x_2$ 

$$\dot{X}_1 = X_2 - q_3 X_1^2 + q_1 u$$
  
 $\dot{X}_2 = q_4 X_1^2 - q_2 X_2$   
 $y = X_1$ 

# 7. Theoretical Considerations

As discussed above, there are 3 steps in our approach. First, we find parameter combinations q(p) from the Gröbner Bases of the exhaustive summary. Second, we reparameterize c(p) over q(p) to get  $\tilde{c}(q)$ . Third, we show that  $\tilde{c}(q) = \tilde{c}(q^*)$  implies that q has a unique or finite number of solutions, and thus we have rigorously proved identifiability.

The main objective of the theoretical work is to show that the Gröbner Bases formed from the exhaustive summary  $c(p) = c(p^*)$  always provide a set of M combinations q(p) such that there exists a unique rational reparameterization of c(p) over q(p). To establish this, we show:

- I. A set of exactly M algebraically independent combinations q(p) can always be obtained from the Gröbner Bases of the exhaustive summary or from the exhaustive summary itself (Theorem 1).
- II. For such a set of *M* combinations, there exists a unique rational reparameterization of c(p) over q(p), i.e.  $\tilde{c}(q)$  (Theorem 2).
- III. By construction of the q(p), we have that  $\tilde{c}(q) = \tilde{c}(q^*)$  will yield that the combinations q(p) are either globally or locally identifiable, depending on whether they had a unique or finite number of solutions in the Gröbner Bases of the exhaustive summary (Theorem 3).

We address (I) in section 8 and we prove that there are at least M algebraically independent decoupled combinations q(p) in the Gröbner Bases of the exhaustive summary (adjoined with the exhaustive summary).

We address (II) in section 9 and we prove that if a decoupled term is contained in the ideal of other decoupled terms (thus "redundant"), then it is a polynomial or rational combination of these terms. We will show any term  $c_i(\mathbf{p}) - c_i(\mathbf{p}^*)$  is "redundant" with respect to the ideal generated by  $(q_1(\mathbf{p}) - q_1(\mathbf{p}^*), q_2(\mathbf{p}) - q_2(\mathbf{p}^*), ..., q_M(\mathbf{p}) - q_M(\mathbf{p}^*))$ . We also show there are at most M algebraically independent decoupled combinations, thus there are exactly M. We combine these results to get that there is a unique rational reparameterization of the input-output equations over our M algebraically independent decoupled combinations

We address (III) in section 10 and we show that a unique rational reparameterization of the coefficients of input-output equations over our M algebraically independent decoupled combinations implies that these combinations are in fact identifiable.

Before we address the algebraic independence of q(p), one must first show that the Gröbner Bases generate enough (that is, M) decoupled combinations that as a set span all P parameters. A simple explanation is that even in the pathological case where the Gröbner Bases do not generate enough combinations, we always have at least M coefficients c(p) of the input-output equations, which are known to be identifiable [17] and must span all P parameters, by definition. Thus, there is no possibility of not finding enough identifiable combinations to reparameterize c(p), i.e. we can trivially reparameterize c(p) over itself. The point of using a Gröbner Basis is that we can form 'simpler' parameter combinations. However, in the case that no new ones are generated, this suggests the c(p) were "simple enough"! Thus, from now on, when we refer to decoupled combinations q(p), we are referring to the decoupled combinations found in the Gröbner Bases of  $c(p) = c(p^*)$ , and in the pathological case where not enough are generated, then q(p) possibly includes terms in c(p).

In our previous work [9], we referred to a decoupled combination found in the Gröbner Basis of (3.2) as "identifiable". We refrain from preemptively calling the decoupled combinations "identifiable" here, since the goal is to find the conditions to rationally reparameterize c(p) over q(p) and thus get identifiability in the rigorous sense, i.e. the injectivity definition. We will see that a sufficient condition for finding a rational reparameterization is that our M parameter combinations q(p) are algebraically independent.

#### 8. Algebraic Independence

**Definition**: A subset  $S = \{\alpha_1, ..., \alpha_n\}$  of a field *L* is *algebraically dependent* over a subfield *K* if there exists a nonzero polynomial *P* of *n* variables with coefficients in *K* such that

 $P(\alpha_1, \dots, \alpha_n) = 0 \quad (*)$ 

**Definition:** If S is not algebraically dependent, i.e. if there exists no nonzero polynomial P such that (\*) holds, then S is algebraically independent [19].

In this paper,  $L = R(\mathbf{p})$  and K = R. Thus, S is a subset of polynomials in  $R(\mathbf{p})$ .

Algebraic independence can be tested in the following way. Let our polynomials be  $r_1(\mathbf{p}), r_2(\mathbf{p}), ..., r_n(\mathbf{p})$ . We let  $\hat{\mathbf{r}}$  be a tag variable, i.e. a variable introduced in order to eliminate other variables [9]. Then we take the Gröbner Basis of the set  $\{\hat{r}_1 - r_1(\mathbf{p}), \hat{r}_2 - r_2(\mathbf{p}), ..., \hat{r}_n - r_n(\mathbf{p})\}$  with the ranking  $\{p_1, ..., p_P, \hat{r}_1, ..., \hat{r}_n\}$ . A polynomial in only  $\hat{r}_1, ..., \hat{r}_n$  will result if and only if the set is algebraically dependent. If no such polynomial results, then the set is algebraically independent [19].

We now show that if there exist M algebraically independent c(p) (which we will discuss in section 9), then there exists M algebraically independent q(p). To prove this, we show that if there were less than M algebraically independent q(p), for instance, M - 1, then these M - 1  $q_j(p)$  elements cannot be algebraically dependent with each of the M original coefficients  $c_i(p)$  because then the original M coefficients would also be dependent. This contradiction implies that we can adjoin a subset of the algebraically independent c(p) to our set of algebraically independent  $q_j(p)$  to obtain M algebraically independent q(p).

**Theorem 1:** Assume that there are (at least) M decoupled q(p) terms over P parameters. Assume there are exactly M algebraically independent coefficients  $c_i(p)$ . Then there exist (at least) M algebraically independent q(p).

Proof: We want to show that there exists a set of M algebraically independent q(p). Assume every set of M elements chosen is algebraically dependent. In other words, the largest set of algebraically independent elements is less than M, say M - 1 (proof follows similarly if any number less than or equal to M - 1 is chosen).

Assume for a contradiction that these M - 1 elements  $q_j(\mathbf{p})$  are algebraically dependent with each of the M original coefficients  $c_i(\mathbf{p})$  (taken individually). Then we have the following polynomials:

$$\begin{split} f_1(q_1(p), q_2(p), \dots, q_{M-1}(p), c_1(p)) &= 0 \\ f_2(q_1(p), q_2(p), \dots, q_{M-1}(p), c_2(p)) &= 0 \\ & \dots \\ f_M(q_1(p), q_2(p), \dots, q_{M-1}(p), c_M(p)) &= 0 \end{split}$$

Where each  $f_i$  includes  $c_i$  and one or more  $q_i$ .

Then since each  $f_i, 1 \le i \le M$  must include some  $q_j, 1 \le j \le M - 1$ , then this means the  $f_i$  cannot be disjoint, i.e. they overlap in some  $q_j$ . Since there are M such  $f_i$ , using elimination we can form a polynomial  $g(c_1(p), c_2(p), ..., c_M(p)) = 0$  [19]. This implies that the  $c_i(p)$  are algebraically dependent, thus we have a contradiction.

Thus, these M - 1 elements  $q_j(\mathbf{p})$  must be algebraically independent with (at least) one of the M original coefficients, say  $c_i(\mathbf{p})$ . Thus, we adjoin  $c_i(\mathbf{p})$  to the set of M - 1 algebraically independent  $q_j(\mathbf{p})$  to get a total of M algebraically independent decoupled combinations (which is, of course, a simpler set of decoupled combinations than the original  $c(\mathbf{p})$  we started with). Thus, in the pathological case where there are not M algebraically independent  $q(\mathbf{p})$ , we can adjoin a subset of the M algebraically independent coefficients  $c(\mathbf{p})$  to get the "simplest set" of algebraically independent decoupled terms.

Thus, in addition to looking for the 'simplest' identifiable combinations, we look for M algebraically independent ones. As described above, we take the Gröbner Basis of the set  $\{\hat{q}_1 - q_1(\boldsymbol{p}), \hat{q}_2 - q_2(\boldsymbol{p}), \dots, \hat{q}_m - q_m(\boldsymbol{p})\}$  with the ranking  $\{p_1, \dots, p_P, \hat{q}_1, \dots, \hat{q}_m\}$  to test if our set of  $\boldsymbol{q}(\boldsymbol{p})$  is algebraically independent.

The algebraic independence of q(p) is important for the reparameterization the input-output equations and the original state-space equations. If a rational reparameterization over algebraically independent q(p) is possible (which we prove), then algebraic independence implies the reparameterization is unique, since if another reparameterization existed, then this would imply dependence amongst the q(p).

#### 9. Rational Reparameterization

We now will prove that a unique rational reparameterization of c(p) over algebraically independent q(p) always exists. To do this, we prove that it is sufficient to show that  $c_i(p) - c_i(p^*)$  is "redundant" with respect to the ideal generated by  $(q_1(p) - q_1(p^*), q_2(p) - q_2(p^*), ..., q_M(p) - q_M(p^*))$ , because we will show this implies that  $c_i(p)$  is a polynomial or rational combination of  $q_1(p), q_2(p), ..., q_M(p)$ .

9.1 Redundancy

When we consider solving a system of equations  $\{c(p) = c(p^*)\}\)$ , an interesting question arises: do we need every equation  $c_i(p) = c_i(p^*)$ , or are some of these equations redundant? Redundant means that the solution space of some equation contains the intersection of the solution spaces of other equations in the set. In the language of ideals, redundancy means one ideal is contained in the ideal generated by the intersection of other ideals. The question of redundancy can be reduced to the question of algebraic dependence. Thus, we examine a more general space of the form  $\{r(p) = \hat{r}\}\)$  for an arbitrary tag variable  $\hat{r}$ . We now show that a redundant system, i.e. a system where one ideal is contained in the intersection of other ideals, implies that the polynomials are algebraically dependent.

**Lemma 1:** Let  $c_i(\mathbf{p}) - \hat{c}_i$ ,  $q_1(\mathbf{p}) - \hat{q}_1$ ,  $q_2(\mathbf{p}) - \hat{q}_2$ , ...,  $q_M(\mathbf{p}) - \hat{q}_M$  be polynomials of the decoupled form  $\mathbf{r}(\mathbf{p}) - \hat{\mathbf{r}}$ . If  $c_i(\mathbf{p}) - \hat{c}_i$  is contained in the ideal  $(q_1(\mathbf{p}) - \hat{q}_1, q_2(\mathbf{p}) - \hat{q}_2, ..., q_M(\mathbf{p}) - \hat{q}_M)$ , then  $c_i(\mathbf{p})$  must be a polynomial/rational combination of  $q_1(\mathbf{p}), q_2(\mathbf{p}), ..., q_M(\mathbf{p})$  and  $c_i(\mathbf{p}), q_1(\mathbf{p}), q_2(\mathbf{p}), ..., q_M(\mathbf{p})$  are algebraically dependent.

Proof: Let  $c_i(\boldsymbol{p}) - \hat{c}_i$  be contained in the ideal  $(q_1(\boldsymbol{p}) - \hat{q}_1, q_2(\boldsymbol{p}) - \hat{q}_2, \dots, q_M(\boldsymbol{p}) - \hat{q}_M)$ .

This means that the solution space of  $c_i(\mathbf{p}) - \hat{c}_i$  contains the solution space of  $(q_1(\mathbf{p}) - \hat{q}_1, q_2(\mathbf{p}) - \hat{q}_2, ..., q_M(\mathbf{p}) - \hat{q}_M)$ , so this means:

There exists a  $\boldsymbol{p}$  such that  $\{q_1(\boldsymbol{p}) = \hat{q}_1, q_2(\boldsymbol{p}) = \hat{q}_2, \dots, q_M(\boldsymbol{p}) = \hat{q}_M\}$  must satisfy  $c_i(\boldsymbol{p}) - \hat{c}_i = 0$ .

This means that if we solve for  $\boldsymbol{p}$  in the equations  $q_1(\boldsymbol{p}) = \hat{q}_1, q_2(\boldsymbol{p}) = \hat{q}_2, \dots, q_M(\boldsymbol{p}) = \hat{q}_M$  and substitute into  $c_i(\boldsymbol{p}) - \hat{c}_i$ , it identically vanishes. In other words, find a Gröbner Basis of  $\{q_1(\boldsymbol{p}) = \hat{q}_1, q_2(\boldsymbol{p}) = \hat{q}_2, \dots, q_M(\boldsymbol{p}) = \hat{q}_M\}$  and use it to substitute into  $c_i(\boldsymbol{p}) - \hat{c}_i$ . Since  $\hat{c}_i$  is a tag variable and not a function of  $\boldsymbol{p}$ , then this means  $\hat{c}_i$  must be only a function of  $\hat{q}_1, \hat{q}_2, \dots, \hat{q}_M$ . Since  $c_i(\boldsymbol{p}) - \hat{c}_i$  is contained in the ideal  $(q_1(\boldsymbol{p}) - \hat{q}_1, q_2(\boldsymbol{p}) - \hat{q}_2, \dots, q_M(\boldsymbol{p}) - \hat{q}_M)$ , then this means  $\hat{c}_i$  must be a *polynomial* or *rational* function of  $\hat{q}_1, \hat{q}_2, \dots, \hat{q}_M$ . Thus,  $c_i(\boldsymbol{p}), q_1(\boldsymbol{p}), q_2(\boldsymbol{p}), \dots, q_M(\boldsymbol{p})$  are algebraically dependent.

Thus we have shown that if  $c_i(\mathbf{p}) - c_i(\mathbf{p}^*)$  is contained in the intersection of  $q_1(\mathbf{p}) - q_1(\mathbf{p}^*), \dots, q_M(\mathbf{p}) - q_M(\mathbf{p}^*)$ , then  $c_i(\mathbf{p})$  must be a *polynomial* or *rational* function of  $q_1(\mathbf{p}), \dots, q_M(\mathbf{p})$ , which means that  $c_i(\mathbf{p})$  and  $q_1(\mathbf{p}), \dots, q_M(\mathbf{p})$  are algebraically dependent.

**Corollary to Lemma 1**: Assume there are *M* algebraically independent terms  $c_1(\mathbf{p}), ..., c_M(\mathbf{p})$ . Then the set  $\{c_1(\mathbf{p}) - \hat{c}_1, ..., c_M(\mathbf{p}) - \hat{c}_M\}$  contains no redundant elements.

Proof: This is the contra-positive to Lemma 1, thus it is proven. ■

We have just found that a sufficient condition for M non-redundant equations  $c(p) = c(p^*)$  is that there are M algebraically independent coefficients c(p). In other words, the number of algebraically independent coefficients c(p) determines the number of non-redundant equations and thus the number of non-free parameters in the solution set to  $c(p) = c(p^*)$ . So another definition for M is the number of algebraically independent terms. This means if there are more than M coefficients of the input-output equations, then we only need to choose M coefficients that are algebraically independent to be used in the exhaustive summary  $c(p) = c(p^*)$ . Thus, we pick M algebraically independent c(p)amongst the original coefficients and obtain M non-free parameters and s free parameters. As discussed earlier, algebraic independence can be easily checked by taking a Gröbner Basis of  $\{c(p) - \hat{c}\}$ .

### 9.2 Solution space

We now seek to prove that  $c_i(\mathbf{p}) - c_i(\mathbf{p}^*)$  is in fact redundant with respect to the ideal generated by  $(q_1(\mathbf{p}) - q_1(\mathbf{p}^*), q_2(\mathbf{p}) - q_2(\mathbf{p}^*), \dots, q_M(\mathbf{p}) - q_M(\mathbf{p}^*))$  which will immediately prove  $c_i(\mathbf{p})$  can be rationally reparameterized over  $q(\mathbf{p})$ . To do this, we examine the solution space generated the exhaustive summary  $c(\mathbf{p}) = c(\mathbf{p}^*)$  and the solution space generated by  $\{q_1(\mathbf{p}) = q_1(\mathbf{p}^*), q_2(\mathbf{p}) = q_2(\mathbf{p}^*), \dots, q_M(\mathbf{p}) = q_M(\mathbf{p}^*)\}$ .

By the **p**-solution (or simply solution space) of a polynomial set of  $\{f_1(\mathbf{p}), f_2(\mathbf{p}), \dots, f_M(\mathbf{p})\}\)$ , we mean the set of values of p's where each polynomial vanishes. This is also known as an algebraic set or variety, which we call  $V_p(f)$ .

**Definition:** A variety  $V_p(f)$  is *irreducible* if whenever  $V_p(f)$  is written in the form  $V_p(f) = V_1 \cup V_2$  where  $V_1$  and  $V_2$  are varieties, then either  $V_p(f) = V_1$  or  $V_p(f) = V_2$  [19].

For example,  $V_p(p_1 - p_1^*)$  is irreducible, but  $V_p(p_1^2 - p_1^{*2})$  is not irreducible. The varieties we examine will be irreducible, and this will be useful in proving Lemma 3.

There are two cases for the form of the solution to the exhaustive summary  $c(p) = c(p^*)$  in the unidentifiable case:

In case 1, the solution can be written as M non-free parameters in terms of s free parameters (described as  $\tilde{p}$ ) with only 1 solution branch:

$$\{p_1 = f_1(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*), p_2 = f_2(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*), \dots, p_M = f_M(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*)\}$$

In case 2, the solution can be written as M non-free parameters in terms of s free parameters with multiple branches of solutions:

$$\{p_{1} = g_{1}^{1}(\widetilde{p}, p^{*}), p_{2} = g_{2}^{1}(\widetilde{p}, p^{*}), \dots, p_{M} = g_{M}^{1}(\widetilde{p}, p^{*})\}$$
$$\{p_{1} = g_{1}^{2}(\widetilde{p}, p^{*}), p_{2} = g_{2}^{2}(\widetilde{p}, p^{*}), \dots, p_{M} = g_{M}^{2}(\widetilde{p}, p^{*})\}$$
$$\dots$$

$$\{p_1 = g_1^{\eta}(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*), p_2 = g_2^{\eta}(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*), \dots, p_M = g_M^{\eta}(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*)\}$$

Where  $\eta$  equals the number of distinct solutions in p. In this case, we describe the algebraic set of

$$\{p_1 = g_1^i(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*), p_2 = g_2^i(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*), \dots, p_M = g_M^i(\widetilde{\boldsymbol{p}}, \boldsymbol{p}^*)\}$$

as the sub-variety  $V_p^i(\mathbf{c})$ . So we have that  $V_p(\mathbf{c}) = \bigcup_{i=1}^{\eta} V_p^i(\mathbf{c})$ . Note that there are only two cases because when solving polynomial equations there cannot be an infinite number of branches in the solution.

Let  $\{q_1(\mathbf{p}), q_2(\mathbf{p}), ..., q_M(\mathbf{p})\}$  be a set of algebraically independent parameter combinations found from decoupled terms/factors in the Gröbner Bases of (3.2). As mentioned above, there are two cases for  $q_i(\mathbf{p})$ .

In case 1,  $q_j(\mathbf{p})$  appears in some Gröbner Basis as  $q_j(\mathbf{p}) - q_j(\mathbf{p}^*)$ , i.e. by itself.

In case 2,  $q_j(\mathbf{p})$  appears as a factor of a Gröbner Basis element, i.e. in the form  $(q_j(\mathbf{p}) - f_{j_1}(\mathbf{p}^*))(q_j(\mathbf{p}) - f_{j_2}(\mathbf{p}^*)) \dots (q_j(\mathbf{p}) - f_{j_{N_j}}(\mathbf{p}^*))$  where  $N_j$  is the multiplicity of  $q_j(\mathbf{p})$ . We know that for each  $q_j(\mathbf{p})$ , one of the  $f_{j_{\alpha}}(\mathbf{p}^*)$  must be  $q_j(\mathbf{p}^*)$  since this represents the trivial solution.

Let the elements  $q_j(\mathbf{p})$ , where  $j \in S$ , S is a subset of the indicies  $\{1, 2, ..., M\}$ , be the elements of  $q(\mathbf{p})$  which belong to case 2, i.e. those that appear as a factor in a Gröbner Basis. Thus, the elements  $q_j(\mathbf{p})$ , where  $j \notin S$ , are the elements of  $q(\mathbf{p})$  which belong to case 1.

We are now going to relate the variety  $V_p(q)$  to the variety  $V_p(c)$ . The variety  $V_p(c)$  corresponding to equations  $c(p) = c(p^*)$  is an intersection of varieties formed by its Gröbner Basis elements. If one of the Gröbner Basis elements factorizes non-trivially, then a solution is formed by taking one of the factors and again intersecting it with other elements or factors of other elements in the Gröbner Basis. Thus, the variety generated by each element in a Gröbner Basis contains the variety  $V_p(c)$ . So this means the variety of a Gröbner Basis element  $q_j(p) - q_j(p^*)$  contains the variety  $V_p(c)$ . (\*)

For a Gröbner Basis element  $(q_j(\mathbf{p}) - f_{j_1}(\mathbf{p}^*))(q_j(\mathbf{p}) - f_{j_2}(\mathbf{p}^*))...(q_j(\mathbf{p}) - f_{j_{N_j}}(\mathbf{p}^*))$ , the variety of each  $q_j(\mathbf{p}) - f_{j_\alpha}(\mathbf{p}^*)$  factor contains one or more sub-varieties  $V_p^i(\mathbf{c})$ . Since each element of a Gröbner Basis contains the solution space generated by the whole Gröbner Basis, then the union of the varieties of  $q_j(\mathbf{p}) - f_{j_1}(\mathbf{p}^*), ..., q_j(\mathbf{p}) - f_{j_{N_j}}(\mathbf{p}^*)$  contains the union of  $V_p^i(\mathbf{c})$ , i.e.  $V_p(\mathbf{c})$ . Thus, for every  $V_p^i(\mathbf{c})$ , there exists some factor  $q_j(\mathbf{p}) - f_{j_\alpha}(\mathbf{p}^*)$  whose variety contains  $V_p^i(\mathbf{c})$  (for all  $j \in S$ , for some  $\alpha$ ). (\*\*)

We call  $V_p^k(\boldsymbol{q})$  the sub-variety formed by the variety of  $\{q_j(\boldsymbol{p}) - f_{j_\alpha}(\boldsymbol{p}^*) \text{ for all } j \in S$ , for some  $\alpha$ , where  $1 \leq \alpha \leq N_j\}$ , together with  $\{q_j(\boldsymbol{p}) - q_j(\boldsymbol{p}^*) \text{ for } j \notin S\}$ . In other words,  $V_p^k(\boldsymbol{q})$  is generated by choosing a factor from elements like  $(q_j(\boldsymbol{p}) - f_{j_1}(\boldsymbol{p}^*))(q_j(\boldsymbol{p}) - f_{j_2}(\boldsymbol{p}^*)) \dots (q_j(\boldsymbol{p}) - f_{j_{N_j}}(\boldsymbol{p}^*))$  where  $j \in S$  and combining it with elements  $q_j(\boldsymbol{p}) - q_j(\boldsymbol{p}^*)$  for  $j \notin S$ , and then finding the algebraic set of zeroes of this set. Here  $1 \leq k \leq \mu$ , where  $\mu$  is the product of the multiplicities of all  $q_j(\boldsymbol{p})$ , i.e.  $\mu = \prod_{j \in S} N_j$ . Combining (\*) and (\*\*), we get that some  $V_p^k(\boldsymbol{q})$  contains  $V_p^i(\boldsymbol{c})$ .

Loosely speaking, the dimension of a variety is the number of parameters that can vary freely [20]. We will employ the dimension of a variety to prove the next two lemmas, by using the following fact: If  $V_p^k(q)$  contains  $V_p^i(c)$ , then this means the dimension of  $V_p^k(q)$  is greater than or equal to the dimension of  $V_p^i(c)$ , thus  $V_p^k(q)$  has equal or more free parameters than  $V_p^i(c)$ . Before we examine

when this containment becomes equality, we first prove that there are exactly M algebraically independent q(p).

**Lemma 2**: Assume there are at least M q(p) terms over P parameters in the Gröbner Bases of the exhaustive summary (3.2). There are exactly M algebraically independent q(p).

Proof: Theorem 2 showed that there are at least M algebraically independent q(p). We now show there are at most M algebraically independent q(p).

Assume there are more than M algebraically independent parameter combinations q(p) in the Gröbner Bases, i.e. there are more than M terms of the form  $q_j(p) - q_j(p^*)$  or  $q_j(p) - f_{j_\alpha}(p^*)$  where  $q_j(p)$ are algebraically independent. As described above, the variety  $V_p^k(q)$  contains  $V_p^i(c)$ . Thus, a variety  $V_p^k(q)$  generated by more than M terms of the form  $q_j(p) - q_j(p^*)$  or  $q_j(p) - f_{j_\alpha}(p^*)$  still contains  $V_p^i(c)$ . This implies that  $V_p^k(q)$  has equal or more free parameters than  $V_p^i(c)$ . Since there are more than M algebraically independent q(p) (by assumption) but exactly M algebraically independent c(p), then Corollary to Lemma 1 implies that there are more non-redundant constraints, thus more non-free parameters that form  $V_p^k(q)$  than form  $V_p^i(c)$ . Thus  $V_p^k(q)$  will contain fewer free parameters than  $V_p^i(c)$ . However, this contradicts  $V_p^k(q)$  containing  $V_p^i(c)$ . Thus, there are exactly M algebraically independent q(p).

**Lemma 3**: When the solution to (3.2) can be written as M non-free parameters in terms of s free parameters with only 1 solution branch (case 1), then  $V_p(q)$  equals  $V_p(c)$ .

When the solution to (3.2) can be written as M non-free parameters in terms of s free parameters with multiple branches of solutions (case 2), some union of  $\eta$  different sub-varieties  $V_p^k(q)$  equals the union of sub-varieties  $V_p^i(c)$  for  $1 \le i \le \eta$ .

Proof:

First we examine case 1, where there is a single solution branch where non-free parameters can be written in terms of the free parameters in  $V_p(c)$ . As mentioned above, the variety  $V_p(q)$  contains the variety  $V_p(c)$  since the variety of each element  $q_j(p) - q_j(p^*)$  contains the solution to  $c(p) = c(p^*)$ . By Lemma 2, both of the ideals generated by  $q(p) - q(p^*)$  and  $c(p) - c(p^*)$  contain M algebraically independent elements, thus by Corollary to Lemma 1, none of the elements that generate the ideals are redundant. This means the solutions to  $c(p) = c(p^*)$  and  $q(p) = q(p^*)$  can be solved for (over the complex numbers) in terms of M non-free parameters in s free parameters [19]. This means that both of the varieties  $V_p(q)$  and  $V_p(c)$  are spanned by s free parameters. Thus, since each of the varieties can be parameterized in terms of s free parameters, then the dimensions for each of these varieties is the same. Since we are in case 1 and the variety  $V_p(q)$  is formed by taking irreducible elements in the Gröbner Bases, then the varieties  $V_p(q)$  and  $V_p(c)$  themselves are irreducible. Thus, the fact that  $V_p(q)$  contains  $V_p(c)$  but the dimensions are the same implies that  $V_p(q)$  equals  $V_p(c)$  [21]. Next, we examine case 2, where the non-free parameters are written in terms of the free parameters in a finite number of distinct ways in  $V_p(\mathbf{c})$ . As mentioned above, some  $V_p^k(\mathbf{q})$  contains  $V_p^i(\mathbf{c})$  since for every  $V_p^i(\mathbf{c})$ , there exists some factor  $q_j(\mathbf{p}) - f_{j_\alpha}(\mathbf{p}^*)$  whose variety contains  $V_p^i(\mathbf{c})$  (for all  $j \in S$ , for some  $\alpha$ ) and the variety of each element  $q_j(\mathbf{p}) - q_j(\mathbf{p}^*)$  contains  $V_p^i(\mathbf{c})$  (for  $j \notin S$ ). We want to show that some  $V_p^k(\mathbf{q})$  will result in some  $V_p^i(\mathbf{c})$ . Again, these varieties are irreducible since they are formed by taking irreducible factors. Again, the dimensions of  $V_p^k(\mathbf{q})$  and  $V_p^i(\mathbf{c})$  must be the same due to the number of free parameters, but  $V_p^k(\mathbf{q})$  containing  $V_p^i(\mathbf{c})$  implies that some  $V_p^k(\mathbf{q})$  equals some  $V_p^i(\mathbf{c})$ [21]. Thus, some union of  $\eta$  different  $V_p^k(\mathbf{q})$  equals  $V_p(\mathbf{c})$ .

Thus we have shown that the **p**-solution space generated by  $c(p) = c(p^*)$  is the same as the **p**-solution space generated by (a subset of) the union of the solutions of M q(p) terms. Mathematically, this is interesting because it means that our space  $c(p) = c(p^*)$  can be represented by the solution spaces associated with the simpler combinations q(p) instead. Thus, even though q(p) may not all come from a single Gröbner Basis, the decoupled combinations of the form  $q_j(p) - q_j(p^*)$  or  $q_j(p) - f_{j_{\alpha}}(p^*)$  still behave like a basis for the ideal generated by the exhaustive summary.

9.3 Reparameterization of c(p) over q(p)

In [9], we showed that when a rational reparameterization of c(p) over q(p) exists, then the ideal generated by  $c(p) - c(p^*)$  is congruent to the ideal generated by  $q(p) - q(p^*)$ , i.e. that  $V_p(q)$  equals  $V_p(c)$ . Now we show the converse is also true.

We show that Lemma 3 implies that each  $c_i(\mathbf{p}) - c_i(\mathbf{p}^*)$  is redundant with respect to the ideal generated by  $(q_1(\mathbf{p}) - q_1(\mathbf{p}^*), q_2(\mathbf{p}) - q_2(\mathbf{p}^*), \dots, q_M(\mathbf{p}) - q_M(\mathbf{p}^*))$ . Then by Lemma 1 we have that each  $c_i(\mathbf{p})$  is an rational combination of  $q(\mathbf{p})$ . Thus we always have a rational reparameterization of  $c(\mathbf{p})$  over  $q(\mathbf{p})$ :

**Theorem 2**: Assume there exists a set of *M* algebraically independent identifiable combinations c(p) in the input-output equations. Then we can form a simpler set of *M* algebraically independent decoupled combinations (called q(p)) by using the Gröbner Bases of (3.2) and the original c(p). Then there exists a unique rational reparameterization of c(p) over q(p), call it  $\tilde{c}(q)$ .

Proof: From Lemma 2, we have that there exists a set of M algebraically independent decoupled combinations q(p). Lemma 3 implies that:

 $c_i(\mathbf{p}) - c_i(\mathbf{p}^*)$  is contained in the ideal generated by  $(q_1(\mathbf{p}) - q_1(\mathbf{p}^*), q_2(\mathbf{p}) - q_2(\mathbf{p}^*), ..., q_M(\mathbf{p}) - q_M(\mathbf{p}^*))$  (\*\*\*)

since  $V_p(q)$  equals  $V_p(c)$  in case 1 or some  $V_p^k(q)$  equals some  $V_p^i(c)$  in case 2.

From Lemma 1, if  $c_i(\mathbf{p}) - \hat{c}_i$  is contained in the ideal generated by  $(q_1(\mathbf{p}) - \hat{q}_1, q_2(\mathbf{p}) - \hat{q}_2, ..., q_M(\mathbf{p}) - \hat{q}_M)$ , then  $\hat{c}_i$  equals a polynomial or rational function of  $\hat{q}_1, \hat{q}_2, ..., \hat{q}_M$ . Applying this to (\*\*\*), we have that  $\hat{c}_i$  is a polynomial or rational function of  $\hat{q}_1, \hat{q}_2, ..., \hat{q}_M$ , or in other words, each coefficient  $c_i(\mathbf{p})$  is equal to a rational combination of  $\mathbf{q}(\mathbf{p})$ . This reparameterization is unique, since if there were two

distinct reparameterizations  $\tilde{c}(q)$  and  $\hat{c}(q)$ , then since  $c(p) = \tilde{c}(q(p)) = \hat{c}(q(p))$ , this implies dependence amongst the q(p), a contradiction.

To find the rational reparameterization of c(p) over q(p), one finds the Gröbner Basis of  $\{\hat{c}_i - c_i(p_1, ..., p_P), \hat{q}_1 - q_1(p_1, ..., p_P), ..., \hat{q}_M - q_M(p_1, ..., p_P)\}$  over the ranking  $\{p_1, ..., p_P, \hat{q}_1, ..., \hat{q}_M, \hat{c}_i\}$  for each coefficient  $c_i(p)$ . As discussed in [9], a linear polynomial  $f(\hat{q}_1, ..., \hat{q}_M) - g(\hat{q}_1, ..., \hat{q}_M)\hat{c}_i$  will result.

#### **10.** Global or Local Identifiability

**Theorem 3**: Assume there exists a unique rational reparameterization of c(p) over q(p), call it  $\tilde{c}(q)$ . Then q is either globally or locally identifiable.

Proof:

Since each q(p) has at most a finite number of solutions in the Gröbner Basis of (3.2), then solving  $\tilde{c}(q) = \tilde{c}(q^*)$  gives that each q = q(p) is either globally or locally identifiable, depending on whether each  $q_j(p)$  has a unique (case 1) or finite number (case 2) of solutions. In other words, if the q(p) only appeared as elements  $q_j(p) - q_j(p^*)$  in the Gröbner Bases, then global identifiability results, and if at least one  $q_j(p)$  appears as a factor  $q_j(p) - f_{j_{\alpha}}(p^*)$  in a Gröbner Basis, then local identifiability results.

This means we can take for granted that a set of algebraically independent q(p) are identifiable and thus the  $\tilde{c}(q)$  reparameterization step mentioned is truly a mathematical formality, as predicted in [9].

In addition, this means the reparameterization of the input-output equations via the "normal canonical form" will always result in polynomial or rational functions.

#### 11. Conclusion

In this paper, we have shown that the Gröbner Bases formed from the exhaustive summary can be used, in conjunction with the exhaustive summary, to provide a set of M algebraically independent parameter combinations q(p) to uniquely reparameterize the coefficients of the input-output equations as rational terms. These parameter combinations are found by searching for "decoupled" terms or factors in the Gröbner Bases of the exhaustive summary. A unique rational reparameterization over these parameter combinations immediately implies global identifiability when decoupled terms are used and local identifiability when decoupled factors are used. Thus, the algebraic independence of q(p) is a sufficient condition for a rational reparameterization of the input-output equations. We have thus provided a class of nonlinear models for which a "normal canonical form" always exists to rationally reparameterize the input-output equations over identifiable parameter combinations. One practical consequence of this work is the result that when seeking q(p) one need not only consider those arising from a single Gröbner Basis, but can consider q(p) arising from any ordering. This freedom to use q(p) from any ordering means that one may need to search through a large number of Gröbner Bases, at most P!. In the future, we hope to find a more efficient method to find these algebraically independent identifiable parameter combinations.

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