

On Global Identifiability for Arbitrary Model Parametrizations*

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Global identifiability is shown to be equivalent to the possibility to express the model structure as a linear regression. An explicit algorithm for testing this, based on differential algebra is also described.

Key Words—Differential algebra; excitation condition; global identifiability; nonlinear systems.

Abstract—It is a fundamental problem of identification to be able-even before the data have been analyzed-to decide if all the free parameters of a model structure can be uniquely recovered from data. This is the issue of global identifiability. In this contribution we show how global identifiability for an arbitrary model structure (basically with analytic nonlinearities) can be analyzed using concepts and algorithms from differential algebra. It is shown how the question of global structural identifiability is reduced to the question of whether the given model structure can be rearranged as a linear regression. An explicit algorithm to test this is also given. Furthermore, the question of 'persistent excitation' for the input can also be tested explicitly is a similar fashion. The algorithms involved are very well suited for implementation in computer algebra. One such implementation is also described

1. INTRODUCTION

Model structure identifiability is the question whether the parameters of a parametrized set of candidate models can be uniquely (globally or locally) determined from data. There are several reasons why such a question could be of utmost importance in various applications. The most obvious reason is that the model parameters have physical significance and we simply need to know if it is at all possible to determine their values from observed data. Another reason may be that numerical search procedures for the parameter estimates may suffer from problems when these are not unique.

Very pragmatically—we are going to be more formal later on—the problem can be described as follows for linear models: 'Let $G(s, \theta)$ be a parametrized transfer function model for a linear system. The variable θ is a d-dimensional vector containing the parameters. This model structure is globally identifiable at θ^* if the equations in θ that arise from the equivalence

$$G(s, \theta) \equiv G(s, \theta^*) \quad \forall s$$
 (1)

has the only solution

$$\theta = \theta^*. \tag{2}$$

The structure is locally identifiable at θ^* when (2) results when θ is constrained to a small enough neighborhood of θ^* . A further question is: Given that (1) implies that (2), what requirements will the input have to satisfy in order to allow the distinction between θ and θ^* for the actual data at hand? Such input requirements are typically called 'persistence of excitation'.

There is a substantial literature on identifiability and structural identifiability. Several different definitions, all variants on the theme $(1) \Rightarrow (2)$, have been given. An early reference is Bellman and Åström (1970). The books by Walter (1982), Walter (1987) and Godfrey (1983) treat the subject thoroughly. Recent surveys are given by Walter and Pronzato (1990) and by Chapell *et al.* (1990). Most efforts on structural identifiability have actually been related to biological applications.

The problem whether (1) implies (2) is a difficult one. Only for the case where the transfer function is parametrized in some 'canonical way'—and then also covering all systems of a given order—are there results of some generality. The book by Ljung (1987, Chapter 4), contains such results, which are of

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the character that the structures are globally identifiable at all θ^* where internal cancellations of dynamics cannot be done. For multivariable models this is difficult enough.

For models that are not parametrized in terms of canonical forms, the problem (1)–(2) has been treated on a case by case basis. For each given parametrization and each given value θ^* , (1) is a set of non-linear equations for θ . These can of course be examined with different tools, sometimes analytical. Computer algebra has allowed explicit treatment of more complex structures [e.g. Raksanyi et al. (1985); Chapell et al. (1990)].

In the current contribution we actually address a more general problem. We will allow the specification of the model structure to be in terms of a general differential-algebraic expression (formally restricted to polynomial nonlinearities—but this is not a severe constraint; see Remark 2 in Section 3). We also aim for a complete solution both for the problem of global structural identifiability and for the problem of what input properties will secure identifiability from actual data. The treatment is confined to continuous-time models, although a discrete-time counterpart to the theory can be developed, and to models that do not contain disturbances (which is common in this literature).

The solution is algorithmic in character. We derive an algorithm that converges in a finite number of steps and resolves all relevant questions about identifiability and persistence of excitation. We also describe an implementation of this algorithm in MAPLE.

Our solution is based on differential algebra (Ritt, 1950; Kolchin, 1973). Michel Fliess deserves the credit for drawing the control community's attention to these powerful tools for non-linear systems analysis (Fliess, 1987a, b 1989; Glad, 1990, 1989a). The current presentation does not assume (except in some technical parts of the proofs) that the reader is familiar with differential algebra.

It should be pointed out that identifiability can be seen as non-linear observability. There are several results on observability for non-linear systems (e.g. Fliess, 1987b). However, our results rely heavily upon the property that the parameters are time-invariant. This gives a particularly simple structure for the solution. Also, our approach is algorithmic in nature.

The paper is organized as follows. In Section 2 we briefly describe the problem of parameter estimation and in Section 3 we formulate the identifiability problem. Section 4 contains a conceptual description of the solution of the problem. The formal solution is presented in

Section 5. In Section 6 we discuss several aspects of the solution, and in Section 8 we describe a MAPLE implementation of the solution. Section 7 contains several examples.

A presentation that gives a more detailed account of the mathematical aspects of this problem is given in Glad and Ljung (1993). The conference papers by Glad and Ljung (1990a,b) and Ljung and Glad (1991) also contain complementary material.

2. MODEL SET PARAMETRIZATION

Consider a dynamical system, with input signals u(t) (an r-dimensional vector function of time), and output signals y(t) (m-dimensional). The dynamics of the system is not known to the user, but it is supposed that it belongs to a set of candidate descriptions, or models. If each is described in state space form we have

$$\dot{x}(t) = f(x(t), u(t), \theta), \quad x(0) = x_0$$
 (3)

$$y(t) = h(x(t), u(t), \theta). \tag{4}$$

Here θ is a d-dimensional parameter vector. For each given value of θ , equations (3) and (4) give a conventional state space description of the dynamics between the input u and the output y. The state variables or internal variables are thus x(t).

The parametrization in terms of θ may be of 'black box' character, in which case θ is just a vehicle to describe a sufficiently broad set of models in equations (3), (4). More often, in the non-linear case, θ corresponds to parameters with physical significance whose numerical values are unknown and need to be estimated.

The estimation of θ is typically carried out in the following conceptual way (see *e.g.* Ljung, 1987):

For each given value of θ , and for the given input sequence u(t), $0 \le t \le T$ the state equation (3) is solved giving the states $x(t, \theta)$. These are inserted into (4) giving

$$\hat{y}(t \mid \theta) = h(x(t, \theta), u(t), \theta). \tag{5}$$

Then

$$\varepsilon(t, \theta) = y(t) - \hat{y}(t \mid \theta) \tag{6}$$

is formed, where y(t) is the actually measured output, $0 \le t \le T$ and

$$V(\theta) = \int_0^T \varepsilon^2(t, \, \theta) \, \mathrm{d}t \tag{7}$$

is minimized with respect to θ .

Remark 1. It is often advantageous to feed back output observations into the calculation of the

states, as follows

$$\dot{x}(t,\,\theta) = F(x(t,\,\theta),\,u(t),\,y(t),\,\theta) \tag{8}$$

e.g. according to an observer structure

$$F(x, u, y, \theta) = f(x, u, \theta) + k(\theta)(y - h(x, u, \theta)).$$
(9)

The result is that $\hat{y}(t \mid \theta)$ in (5) will be a function of y(s), $0 \le s < T$, also.

Now there are two main issues in the minimization of (7). One is the numerical complexity of the problem: How much work is it to calculate, for each given θ , $V(\theta)$ and its derivatives? Do there exist local minima in addition to the sought global one? The other issue is the identifiability of θ : Is the global minimum of (7) unique or not?

Identifiability of parametric structures is discussed by many authors, such as Ljung (1987, Section 9.5), Söderström and Stoica (1989, Section 6.4), and Walter (1982). Basically global identifiability requires the following property of the model structure

$$\hat{y}(t \mid \theta') \equiv \hat{y}(t \mid \theta'') \Rightarrow \theta' = \theta''. \tag{10}$$

The issue (10) really contains two steps. These are discussed in detail for linear systems by Ljung (1987, Sections 4.5, 4.6 and 14.2). The first step is a property of the model structure itself: Is it at all possible to distinguish two given parameter values, provided we may choose the input in the best possible way? This is called model structure identifiability by Ljung (1987). The second step is to find out whether the actual input is 'informative enough' to allow this distinction. This leads to the requirement that the input be persistently exciting.

From this perspective it is an especially favorable situation when the model parametrization (5) is linear in θ :

$$\hat{y}(t \mid \theta) = \phi^{T}(t)\theta. \tag{11}$$

Here $\phi(t)$ is a matrix formed from y(s), u(s), $s \le t$. The structure (11) is known as a linear regression. It allows (7) to be solved explicitly by

$$\hat{\theta}_T = \left(\int_0^T \phi(t)\phi^T(t) dt\right)^{-1} \int_0^T \phi(t)y(t) dt. \quad (12)$$

Clearly this structure is always identifiable. Also the requirement on the input's persistence of excitation is resolved by examination of the indicated matrix inverse.

A slight generalization of (11) is

$$\psi(t) = \phi^{T}(t)\theta \tag{13}$$

where $\psi(t)$ like $\phi(t)$ is a matrix (vector), entirely formed from past values of y(t), u(t) (including their derivatives). This gives

$$V(\theta) = \int_0^T |\psi(t) - \phi^T(t)\theta|^2 dt \qquad (14)$$

and

$$\hat{\theta}_T = \left(\int_0^T \phi(t)\phi^T(t) dt\right)^{-1} \int_0^T \phi(t)\psi(t) dt. \quad (15)$$

3. PROBLEM FORMULATION

Here is the problem:

We write down all equations, that based on physics, chemistry (or whatever the application may be) are relevant for describing the system. This gives

$$g_i(u, y, x, \theta, p) = 0$$
 $i = 1, 2, ..., r$. (16)

Here u(t) and y(t) are the measured input and output signals (possibly vector valued) from the system. Moreover x(t) are auxiliary, non-measurable signals that we use to describe the system. We may think of them as state variables, but they could also have other interpretations. The vector θ contains all the unknown parameters that are used to describe the system. There are all time-invariant:

$$\dot{\theta} \equiv 0 \tag{17}$$

(which is a feature that distinguishes them from r^{\dagger})

Finally, p is the differentiation operator. The expressions (16) are thus differential-algebraic equations, *i.e.* algebraic relations between u(t), y(t), x(t), θ and their time derivatives of arbitrary order. These relations have to hold for all time instants t.

Remark 2. The formal development will require that the functions g_i in (16) are polynomial in u, y, x and θ and their derivatives. This is not so restrictive as it may seem. For example, the relation

$$x = \sin y$$

can also be written

$$\dot{x}^2 = \dot{y}^2 (1 - x^2).$$

The question now is: Suppose that we observe

$$u(t) \quad 0 \le t \le T$$

$$y(t) \quad 0 \le t \le T$$
(18)

is it then possible to uniquely determine the vector θ from (16)? In other words, do the given u, y in (18) satisfy the differential-algebraic relations (16) for only one unique value of θ ? In

that case the model structure defined by (16) would be globally identifiable.

4. A NAIVE DESCRIPTION OF THE SOLUTION

If a pair of signals (18) satisfies (16), they will also satisfy equations that are obtained by differentiating, adding, scaling and multiplying the left-hand sides of (16). That is, we may extend (16) with equations of the kind

$$p^{3} \cdot g_{2}(u, y, x, \theta, p) + 27\{p \cdot g_{3}(u, y, x, \theta, p)\} \cdot \{g_{31}(u, y, x, \theta, p)\} = 0 \quad (19)$$

and so on.

Clearly, an infinite amount of differentialalgebraic expressions can be formed from (16) in this way. We denote by

$$G$$
 (20)

the infinite set of all these expressions. Clearly, the solution u, y [i.e. those u, y that satisfy (16)] will still satisfy all equations in G.

It is also clear that it is sufficient to select a finite subset of G that has the same solution set. The original r equations (16) is one such set. One may ask if there are other such sets that make it easier to answer the question of Section 3

With an analogy from linear algebra we may think of linear spaces and bases. A finite dimensional basis is sufficient to describe the infinitely many vectors in the space. There are infinitely many bases, each of them defined by a finite set of vectors. Certain questions are more easily answered in one basis than another.

We are thus looking for a good 'basis' for G that can answer our question. To quantify what 'good' should mean we may list a number of wishes that would make it easier to decide upon the identifiability of G:

- 1. Expressions should not contain the variable x, since it is not known to us.
- 2. Expressions should not contain higher powers of θ , since this would make it more difficult to assess identifiability.
- 3. It is OK if the expressions contain powers and derivatives of u and y, since these anyway are known to us.

That is, among all the expressions in G we should 'look for' ones with these properties. We could, in principle, 'rank' all the expressions according to how well they satisfy our wishes. The 'best' element in G would be something like

$$\psi_0(y, u, p) = 0 \tag{21}$$

i.e. an arbitrary differential-algebraic expression in u and y only. The next best one would be of

the form

$$\phi_1(y, u, p) + \theta \psi_1(y, u, p) = 0 \tag{22}$$

if such an expression exists within G, and so on. If indeed we find an expression (22) within G, we may conclude that we can uniquely determine the value of θ if only the function

$$\psi_1(y, u, p) \tag{23}$$

has full rank. This is a condition on the input (of a 'persistency of excitation' type).

Conversely, and this is a bit more tricky, if there is no expression of the type (22) in G, then it actually follows that θ cannot be uniquely determined in the space of \mathscr{C}^d ($d=\dim\theta$). This takes a few lines to prove, but the basic argument goes as follows (let θ be scalar for simplicity): The ranked set of expressions will appear in a triangular structure as follows:

$$\phi_0(y, u, p) = 0.$$

$$\phi_1(y, u, \theta, p) = 0$$

$$\phi_2(y, u, \theta, x_1, p) = 0$$

$$\phi_3(y, u, \theta, x_1, x_2, p) = 0.$$
:

The second expression is then not linear in θ by assumption. We can then always, for given u, y, choose 'the other θ -root' of ϕ_1 and adjust x_i in the later equations accordingly, and thus satisfy all the basic expressions with this 'other' value of θ . Then all of G is satisfied for this θ , and lack of global identifiability follows.

Note that this discussion relates to the full space of complex valued parameters $\mathcal{D}_{\mathcal{M}} = \mathcal{C}^d$. With physical insights some roots of θ could be excluded (by being complex or negative or whatever is not physically feasible in the application in question). This means that in fact $\mathcal{D}_{\mathcal{M}}$ is less than \mathcal{C}^d and that global identifiability with respect to $\mathcal{D}_{\mathcal{M}}$ indeed could be at hand in this case.

Now, how do we decide if G has an element (22)? Basically we search over G with a procedure that resembles the Gram-Schmidt or Gauss-elimination algorithm: Take an arbitrary element. If it contains unwanted features, try to eliminate them by the allowed algebraic manipulations (addition or multiplication of another element or its derivative). By this procedure 'a better' element is created in each step, and finally (after a finite number of 'reductions') we will find if (22) exists or not. Formally this is 'Ritt's algorithm' (Ritt, 1950; see the next section).

5. A FORMAL DESCRIPTION OF THE SOLUTION

5.1. Some conditions on the model structure

Since the model (16) is very general, some of the solutions to these equations might be of a degenerate character. Therefore we introduce the concept of a non-degenerate solution as a solution of (16) such that

$$h_k(y, u, x, \theta) \neq 0, \quad k = 1, ..., s$$
 (24)

where the h_k , the non-degeneracy conditions, are differential algebraic equations of the same type as (16).

For the set (16) we introduce the following regularity conditions.

- A.1 For each parameter value θ and for each input signal u_i , $i=1,\ldots,m$ the differential equations (16) and (24) define sets of non-degenerate solutions $\bar{x}(\theta,u)$, $\bar{y}(\theta,u)$. (Since initial conditions are not specified, there will in general be a set of solutions corresponding to the given θ , u.)
- A.2 The control signals u_i , i = 1, ..., m can be chosen independently, *i.e.* they are not constrained by (16).

Remark 3. The precise formulation of these conditions is as follows (Kolchin 1957, 1973):

AA.1 y and x are differentially algebraic over $\mathscr{F}\langle u, \theta \rangle$ by (16). [This is equivalent to saying that x, y are differentially algebraic over $\mathscr{F}\langle u \rangle$, since θ is differentially algebraic over \mathscr{F} from (17).]

AA.2 u is differentially transcendent in (16).

A set of parametrized equations (16) subject to A.1 will be called a model structure and generically denoted by \mathcal{M} .

We can now state the general definition of identifiability (the set $\mathcal{D}_{\mathcal{M}}$ below is assumed to be a subset of the real or complex numbers):

Definition 1. A model structure \mathcal{M} is said to be globally identifiable at θ_* with respect to $\mathcal{D}_{\mathcal{M}}$ if there exists an input signal u_* such that $\bar{y}(\theta_*, u_*) \neq \emptyset$ and

$$\bar{y}(\theta_*, u_*) \cap \bar{y}(\theta, u_*) \neq \emptyset, \quad \theta \in \mathcal{D}_{\mathcal{M}} \Rightarrow \theta_* = \theta.$$
 (25)

This definition is well in line with the traditional definitions of global identifiability. The possibility that the solutions may be non-unique forces us to consider the intersection of the solution sets. Otherwise we would have the usual formulation

$$\bar{y}(\theta_*, u_*) \equiv \bar{y}(\theta, u_*) \quad \theta \in \mathcal{D}_{\mathcal{M}} \Rightarrow \theta_* = \theta.$$
 (26)

It is now straightforward to define local

identifiability:

Definition 2. A model structure \mathcal{M} is said to be locally identifiable at θ_* if there exists an open neighborhood $\mathcal{D}_{\mathcal{M}}$ of θ_* such that \mathcal{M} is globally identifiable at θ_* with respect to $\mathcal{D}_{\mathcal{M}}$.

We shall now also define a generalized version of the concept of persistence of excitation.

Definition 3. Consider a model structure \mathcal{M} that is globally identifiable at θ_* with respect to $\mathcal{D}_{\mathcal{M}}$. The input signal u_* is said to be persistently exciting with respect to \mathcal{M} , $\mathcal{D}_{\mathcal{M}}$ at θ_* if (25) holds.

5.2. Ranking

As mentioned above we deal with polynomials in several variables and their derivatives. The nth derivative of v is denoted $v^{(n)}$. As usual the lowest derivatives are also denoted \dot{v} , \ddot{v} . We let $\deg_v A$ denote the degree of the variable v in the polynomial A. The ranking is a total ordering of all the variables and their derivatives. It must have the property that, for all non-negative integers μ , ν , σ and all positive integers τ

$$u^{(v)} < u^{(v+\tau)}, \quad u^{(v)} < v^{(\mu)} \Rightarrow u^{(v+\sigma)} < v^{(\mu+\sigma)}$$
(27)

where < means 'is ranked lower than'. Examples of rankings of the variables u_1 and u_2 are

$$u_1 < \dot{u}_1 < \ddot{u}_1 < \dots < u_2 < \dot{u}_2 < \ddot{u}_2 < \dots$$

 $u_1 < u_2 < \dot{u}_1 < \dot{u}_2 < \ddot{u}_1 < \ddot{u}_2 < \dots$

The leader of a polynomial is the highest ranking derivative of that polynomial (it might be a derivative of order zero). The corresponding variable is called the leading variable. The ranking concept now carries over to differential polynomials: the differential polynomial A with leader v_A ranks lower than B with leader v_B , if v_A ranks lower than v_B or if $v_A = v_B$ and $\deg_{v_A} A < \deg_{v_A} B$.

Let the leader of the polynomial A be v_A . The polynomial F is partially reduced with respect to A if there is no proper derivative of v_A in F. If F is partially reduced with respect to A and the degree of v_A in F is less than the degree of v_A in A, then F is said to be reduced with respect to A. A set of polynomials that are all reduced with respect to each other, is called an autoreduced set.

Two autoreduced sets, $\mathbf{A} = A_1, \dots, A_r$ and $\mathbf{B} = B_1, \dots, B_s$ are ranked according to the following principle. If there is an integer k,

 $0 \le k \le \min(s, r)$ such that

 $\operatorname{rank} A_i = \operatorname{rank} B_i,$

$$j = 0, \ldots, k - 1$$
, rank $A_k < \text{rank } B_k$

then **A** is said to be of lower rank than **B**. If r > s and

$$\operatorname{rank} A_i = \operatorname{rank} B_i, \quad j = 0, \ldots, s$$

then A is also said to be lower. A lowest autoreduced set that can be formed among a given set of differential polynomials, is called a characteristic set.

The coefficient of the highest power of the leader in a polynomial is called the initial. The derivative with respect to the leader is called the separant.

5.3. Differential ideals

Consider a set of differential polynomials

$$\Phi = \{\phi_1, \ldots, \phi_n\}. \tag{28}$$

The differential ideal generated by Φ is denoted $[\Phi]$ and consists of all differential polynomials that can be formed of elements in Φ by multiplication with arbitrary polynomials, addition and differentiation. This corresponds to the set G in (20). If also all polynomials p such that $p^m \in [\Phi]$ are included, we have the perfect differential ideal described by Φ , denoted by $\sqrt{[\Phi]}$. The reason for our interest in these objects is that a solution to the elements of Φ will also be a solution to all elements in $[\Phi]$ and $\sqrt{[\Phi]}$. A differential ideal Π is called prime when $pq \in \Pi$ implies that either $p \in \Pi$ or $q \in \Pi$.

5.4. Ritt's algorithm

The objects introduced in the previous sections can be used in computational procedures. Of interest here is an algorithm indicated by Ritt (Ritt, 1950; Kolchin, 1973), which takes a set of differential polynomials, like (28) and computes a set of characteristic sets A_1, \ldots, A_p of prime differential ideals Π_1, \ldots, Π_p so that

$$\sqrt{|\Phi|} = \Pi_1 \cap \Pi_2 \cap \dots \cap \Pi_p. \tag{29}$$

The use of this algorithm in control applications is discussed in Glad (1989a,b).

5.5. Identifiability and characteristic sets

$$\Phi = \{g_k : k = 1, \dots, r, \, \dot{\theta}_j : j = 1, \dots, d\} \quad (30)$$

i.e. the differential polynomials making up the left-hand side of (16) and (17).

Now suppose we want to examine the identifiability of θ . Then introduce a ranking

such that:

$$u^{(\mu)} < y_j^{(\nu)} < \theta_1 < \dot{\theta}_1 < \cdots$$
$$< \theta_d < \dot{\theta}_d < \cdots x_k^{(\sigma)} \quad (31)$$

for all indices $1 \le i \le m$, $1 \le j \le p$, $1 \le k \le n$ and all derivative orders μ , ν and σ .

To simplify things we will assume that $[\Phi]$ is prime, so that $\sqrt{[\Phi]} = [\Phi]$. This is for instance the case if we start with a state space description. In the general case, the reasoning below has to be applied to each component of the decomposition (29). We now have

Proposition 1. With the ranking (31), $[\Phi]$ has a characteristic set of the following form

$$A_1(u, y), \ldots, A_p(u, y), B_1(u, y, \theta_1),$$

 $B_2(u, y, \theta_1, \theta_2) \cdots B_d(u, y, \theta_1, \theta_2, \ldots, \theta_d),$
 $C_1(u, y, \theta, x) \cdots C_n(u, y, \theta, x).$ (32)

Here the leaders of the A_i are derivatives of the y_j , each y_j being the leading variable of precisely one A_i . B_i is either $\dot{\theta}_i$ or a polynomial containing no derivatives of the θ -variables.

Proof. Let **A** be a characteristic set of $[\Phi]$. There cannot be any differential polynomial containing only u in $[\Phi]$, since that would imply differential algebraic dependence among the u, contradicting (AA.2). Since the u_i are ranked lowest, there can be no polynomials in A, having a u_i as the leading variable. Now suppose that y_k is not the leading variable of any element of A. Since y_k is differentially algebraic over $\mathcal{F}\langle u \rangle$, (AA.1), there exists some differential polynomial $A(u, y_k)$ in $[\Phi]$. It is then possible to make a lower autoreduced set than A, by taking those elements of A that have lower leaders than $A(u, y_k)$ and then placing $A(u, y_k)$ or its remainder with respect to the previous $A(u, y_i)$ as the last polynomial. This contradiction shows that every y_i must be the leading variable of some element in A. Since the y_i are ranked lower than the θ_i and x_i , those elements must contain only u and y as variables and be placed first in A. Since it is a general property of autoreduced sets that different elements have different leading variables, there must be precisely p such polynomials. $[\Phi]$ contains the differential polynomials $\dot{\theta}_i$. The B_i must then be those differential polynomials or something that is ranked lower, which can only be a polynomial containing no derivative of θ_i . Since it must be reduced with respect to the preceding polynomials, there can be no derivatives of the other θ -variables either.

From the identification point of view there are three different situations that can arise in (32).

- 1. For some *i* one has $B_i = \dot{\theta}_i$.
- 2. All B_i are of order 0 and degree 1 in θ_i .
- 3. All B_i are of order 0 in θ_i , and some B_j is of degree > 1 in θ_i .

We will see that essentially these cases correspond to unidentifiability, global identifiability, and local identifiability respectively. The simplest case is the first one. (Recall that 'separant' and 'initial' were defined in Section 5.2.)

Theorem 1. Let the nondegeneracy conditions be that no separant or initial of (32) is zero. If the characteristic set (32) has the form of case 1 above, then the model structure is not locally identifiable at any θ^* .

Proof. Let k be the lowest index such that $B_k = \dot{\theta}_k$. Take any θ^* and any u_* . Assume that the model structure is identifiable at θ^* . Then there exists a non-degenerate solution $(y_*, u_*, x_*, \theta_*)$ of (16), which is then a solution of (32) such that all separants and initials are non-zero. Now take a value θ , such that

$$\theta_i = \theta_{*i}, \quad i = 1, \ldots, k-1$$

$$\theta_k \neq \theta_{*k}$$

 u_* , y_* will then together with θ still satisfy A_i , $i=1,\ldots,p$ and B_j , $j=1,\ldots,k-1$. It is possible to take θ and \dot{x} such that the rest of the elements of the characteristic set are zeroed and all separants and initials are non-zero. This will then give a solution also of the original equations (16) which is non-degenerate, has the same input—output pair, but different values of θ , contradicting the identifiability of θ_* .

Theorem 2. Let the non-degeneracy conditions be that no separant or initial of (32) is zero. Let θ_* be such that there exists some non-degenerate solution (y, u, θ_*, x) . Then, if the characteristic set (32) has the form of case 2 above, the model structure is globally identifiable at θ_* for any \mathcal{D}_{μ} .

Proof. If each B_i is of degree one in θ_i , then it must be independent of the other θ_j for (32) to be autoreduced. Each B_i then has the form

$$P_i(u, y)\theta_i - Q_i(u, y). \tag{33}$$

Since we look at non-degenerate solutions, it is then possible to solve for each θ_i :

$$\theta_i = \frac{Q_i(u, y)}{P_i(u, y)} \tag{34}$$

and the identifiability is obvious. This means that

 θ_i belongs to $\mathcal{F}(u, y)$ i.e. it is rationally identifiable according to Diop and Fliess (1991).

Theorem 3. Let the non-degeneracy conditions be that no separant or initial of (32) is zero and let θ_* be such that there exists some non-degenerate solution (y, u, θ_*, x) . Then, if the characteristic set of (32) has the form of case 3 above, the model structure is locally identifiable at θ_* .

Proof. B_1 can be regarded as a function of θ_1 with coefficients depending on u and y. Since $\partial B_1/\partial \theta_1$ is non-zero, the implicit function theorem guarantees a locally unique θ_1 . Inductively, when θ_1 through θ_i have been determined locally uniquely, θ_{i+1} is determined locally uniquely by $B_{i+1}(u, y, \theta_1, \ldots, \theta_{i+1}) = 0$, since $\partial B_{i+1}/\partial \theta_{i+1}$ is non-zero at θ_* .

This case is one where θ is algebraic over $\mathcal{F}\langle u, y \rangle$, which is called algebraic identifiability in Diop and Fliess (1991). See also Glad and Ljung (1993) for a more complete account of the technical aspects of the problem.

6. ASPECTS ON THE SOLUTION

6.1. Rearrangement to a linear regression

A striking, and somewhat surprising aspect of the solution is that the structure is globally identifiable with respect to \mathcal{C}^d if and only if we can rearrange the original equations so that we obtain—parameter by parameter—linear regressions (33):

$$P_i(u, y)\theta_i - Q_i(u, y) = 0$$
 $i = 1, \ldots, d$.

This suggests that the parameter θ_i can easily be estimated by

$$\hat{\theta}_{i} = \int_{0}^{T} P_{i}(u(t), y(t)) Q_{i}(u(t), y(t)) dt / \int_{0}^{T} P_{i}^{2}(u(t), y(t)) dt.$$
 (35)

With (35) rather than (34) we utilize the redundancy that stems from our observation record $0 \le t \le T$.

Now, one must be aware of the fact that in practice P and Q may be very complex functions of u and y and involve quite high order derivatives. This means that we would need to use well matched differentiating signal filters. Nevertheless (35) may provide an interesting and new way to find initial parameter estimates for more sophisticated methods such as maximum likelihood. A rather remarkable fact is that we in this way circumvent problems with local minima of the criterion functions.

6.2. Testing the usefulness of the model structure

Note that, according to Proposition 1, the first expressions that the algorithm constructs are θ -and y-independent [see (32)]:

$$A_i(u, y) = 0$$
 $i = 1, ..., p.$ (36)

This means that any signal pair (u, y) that satisfies our model for any value of θ must also satisfy (36)! We can thus test whether our structure is at all capable of describing the data by checking if (36) holds without ever estimating any parameters!

6.3. Persistence of excitation

Suppose now that the structure is globally identifiable, so that each of the $P_i(u, y)$ in (33) came out to be non-identically zero. It may still happen that for a particular input u^* and the corresponding output y^* we have that

$$P_i(u^*, y^*) = 0. (37)$$

To check which u^* (37) holds for, we adjoin $P_i(u, y)$ to the original model equations to see if $P_i(u, y) = 0$ at the same time as the model equations are satisfied. We now seek an expression, preferably only in u and its derivatives, that characterizes this situation. We may have to accept that the expression also involves the parameters, *i.e.* that the exact condition on persistence of excitation actually depends on the true system. Therefore we change the ranking from (31) to

$$u_i^{(\mu)} < \theta_i^{(\nu)} < y_k^{(\sigma)} < x_i^{(\eta)}$$
 (38)

and run Ritt's algorithm again. Ideally, the first returned expression will then contain u and its derivatives:

$$R(u) = 0. (39)$$

This means that if (39) holds, $P_i(u, y)$ will be zero and θ_i cannot be estimated. Conversely if u does not obey any of the (39) that result when each of the $P_i(u, y)$ are adjoined to the model equations, we have an input that is persistently exciting for the structure in question.

We must also be prepared for the situation that the simplest returned expression is not of the form (39), but also contains the parameters:

$$R(u, \theta) = 0. (40)$$

In these cases the conditions for persistence of excitation depend on the parameter values that describe the actually resulting model.

When Φ is enlarged with $P_i(u, y)$ it is possible that, although $[\Phi]$ is prime, the ideal $\sqrt{[\Phi, P_i]}$ will not be prime. Then there will be a decomposition so that $\sqrt{[\Phi, P_i]}$ is an intersection of prime differential ideals, like (29). Ritt's

algorithm will return a characteristic set for each of these. There will then be characteristic sets

$$\mathbf{A}_{1}: R_{11}(u), R_{12}(u), \ldots, R_{1j_{1}}(u, \theta), \ldots$$

$$\mathbf{A}_{2}: R_{21}(u), R_{22}(u), \ldots, R_{2j_{2}}(u, \theta), \ldots$$

$$\vdots$$

$$\mathbf{A}_{a}: R_{a1}(u), R_{a2}(u), \ldots, R_{aj_{a}}(u, \theta), \ldots$$

A solution of Φ and P; will then be a solution of some \mathbf{A}_i . The excitation condition is then that some polynomial in each \mathbf{A}_i has to be non-zero. A typical situation is something like

$$\mathbf{A}_1: R_{11}(u), \ldots$$
$$\mathbf{A}_2: R_{21}(\theta), \ldots$$

An excitation condition is then $R_{11}(u) \neq$ and $R_{21}(\theta) \neq 0$. See Glad and Ljung (1993) for a further discussion on this.

6.4. Known initial conditions

Let us return to our definition of global identifiability, (25) in Definition 1. Note that we have said nothing about the initial conditions for the various differential equations involved. The solution sets \bar{y} correspond, as remarked under A.1, to all possible initial conditions. The consequence is that if two different θ with two different initial values for the differential equations give identical solutions, we deem the structure non-identifiable. This means that in our definition of global identifiability we regard the initial conditions for the underlying differential conditions to be unknown. This would also correspond to the most natural situation in practice.

However, there may be closely monitored experiments where we know the initial conditions of the states. This is not uncommon in biological and biomedical applications. Knowledge of the initial values could then resolve lack of identifiability.

To deal with known initial values in our approach we could proceed as follows. If we have an unmeasured state variable x_i with known initial value $x_i(0)$, we would choose a ranking such that Ritt's algorithm searches for low order expressions involving only x_i , u and y. If we find a first order (highest derivative of x_i being 1) differential expression

$$L(x_i, u, y) = 0$$

that does not involve θ , we may regard x_i as a known variable, since $x_i(0)$ and u and y are known. This variable x_i can then be given a ranking together with u and y and before θ in (31) and we could then proceed as described. See Example 5 below.

6.5. Some user aspects

As a user of the theory we proceed as follows:

- 1. Enter the model structure expressions (16).
- 2. Specify the ranking (31).
- 3. The computer returns A_i and B_i as specified in Proposition 1.
- 4. Examine the B_i s to decide what identifiability properties we have, as described in Theorems 1-3.
- 5. To investigate what are the persistence of excitation conditions, adjoin each of the $P_i(u, y)$ (one at a time) in (33) to the model equations as described in Section 6.3.

7. EXAMPLES

Example 1. Goodwin's Napkin example. Consider the homogeneous equation

$$\ddot{y} + 2\theta \dot{y} + \theta^2 y = 0. \tag{41}$$

We observe y and have a single unknown parameter θ . This parameter seems to be globally identifiable, but how on earth can the structure be written as a linear regression in θ ? (G. Goodwin, pers. comm.) Some fairly simple direct manipulations will reveal how our algorithm thinks (G. Goodwin, pers. comm.). Differentiate (41):

$$y^{(3)} + 2\theta \ddot{y} + \theta^2 \dot{y} = 0. \tag{42}$$

Now multiply (41) by \dot{y} and (42) by y and subtract the expressions:

$$(\dot{y}\ddot{y} - yy^{(3)}) + 2\theta(\dot{y}^2 - y\ddot{y}) = 0.$$
 (43)

This is the linear regression that reveals that the structure is globally identifiable. This is also what Ritt's algorithm returns to us. In addition it provides as its lowest ranked expression

$$4y\ddot{y}^{3} - 3\dot{y}^{2} \cdot \ddot{y}^{2} - 6yy^{(3)}\dot{y}\ddot{y} + 4y^{(3)}\dot{y}^{3} + y^{2}y^{(3)2} = 0$$
(44)

which is the differential equation any y(t) must satisfy that obeys (41) for any value of θ .

Ritt's algorithm also returns the following alternative to (43)-(44):

$$\begin{cases} \dot{y} = 0 \\ \dot{\theta} = 0 \end{cases} \tag{45}$$

which points out that θ is not identifiable if y is identically zero.

Example 2. A non-linear model. Consider the system defined by

$$\dot{x}_1 = \theta x_2^2$$

$$\dot{x}_2 = u$$

$$v = x_1.$$

With the ranking (31) Ritt's algorithm returns in order the expressions

$$2u\dot{y}y^{(3)} - u\ddot{y}^2 - 2\dot{u}\dot{y}\ddot{y} = 0 \tag{46}$$

$$\ddot{y}^2 - 4\theta u^2 \dot{y} = 0. {47}$$

Here (46) corresponds to A(u, y) and (47) to $B(u, y, \theta)$ in Proposition 1. We see from (47) that the model structure is globally identifiable. To check the conditions for persistence of excitation we adjoin

$$u^2\dot{y}$$

to the model equations, change the ranking to (38) and run Ritt's algorithm. This gives the expressions

$$u = 0$$

$$\theta = 0$$

so that any non-zero u is persistently exciting with respect to $\theta_* \neq 0$, giving global identifiability. (A closer look at the characteristic set reveals that the global identifiability actually applies to all θ_* .)

Example 3. The model structure of Dasgupta et al. (1991). Dasgupta et al. (1991) considered the following model structure

$$\dot{y} = \varphi(y)^{\mathrm{T}}\theta + m(y) + \sum_{i=1}^{l} g_i(y)u^i$$
 (48)

where φ , m and g are known polynomials in y. The vector θ contains all the unknowns. Let us for simplicity introduce the known differential polynomial

$$n(y, u) = \dot{y} - m(y) - \sum_{i=1}^{l} g_i(y)u^i$$
 (49)

so that we have

$$n(y, u) = \varphi(y)^{\mathrm{T}} \theta. \tag{50}$$

This is already in linear regression form, but Ritt's algorithm will provide linear regressions for each individual parameter. This means that we will obtain by successive differentiations

$$n(y, u) = \varphi(y)^{\mathrm{T}} \theta$$

$$\frac{\mathrm{d}}{\mathrm{d}t} n(y, u) = \frac{\mathrm{d}}{\mathrm{d}t} \varphi(y)^{\mathrm{T}} \theta = \frac{\mathrm{d}}{\mathrm{d}y} \varphi(y)^{\mathrm{T}} \dot{y} \theta$$

$$\vdots \qquad (51)$$

$$\frac{\mathrm{d}^r}{\mathrm{d}t^r}n(y,u) = \frac{\mathrm{d}^r}{\mathrm{d}v^r}\varphi(y)^{\mathrm{T}}(\dot{y})^r\theta + h(y)\cdot\theta$$

where h(y) is of the form

$$\sum_{k=1}^{r-1} c_k \frac{d^k}{dy^k} \varphi(y)^T y^{(j_1)} y^{(j_2)} \cdots y^{(j_r)}.$$

Thus $h(y)\theta$ is just a linear combination of the rows above. Therefore, if and only if the matrix

$$\left[\varphi(y)\frac{d}{dy}\varphi(y)\dot{y},\ldots,\frac{d'}{dy'}\varphi(y)\cdot(\dot{y})'\right]$$

has full row rank for some r, we can solve for the components of θ in (51). Ritt's algorithm will thus provide the following conditions for global identifiability and persistence of excitation:

$$\begin{cases} \dot{y} \neq 0 \\ \left[\varphi(y) \frac{d}{dy} \varphi(y), \dots, \frac{d^r}{dy^r} \varphi(y) \right] \end{cases}$$
 (52)
has full row rank for some r .

These are the same conditions as derived in Dasgupta et al. (1991).

Example 4. Compartmental models: Unknown initial conditions. Chapell et al. (1990) studied the following example

$$\begin{cases} \dot{x}(t) = -\frac{V_{\text{m}}x(t)}{k_{\text{m}} + x(t)} - k_{01}x(t) \\ x(0) = D \\ y(t) = cx(t). \end{cases}$$
 (53)

D is here a known constant, while we shall investigate the identifiability of $V_{\rm m}$, $k_{\rm m}$, $k_{\rm 01}$ and c.

Let us first ignore the known initial value D and run the standard analysis. Our algorithm gives, in addition to some degenerate cases, like $x \equiv 0$, the following set of equations:

$$-3y^{2}\ddot{y}^{4} + 2y^{2}\dot{y}y^{(3)}\ddot{y}^{2} - 2y^{2}\dot{y}^{2}y^{(4)}\ddot{y} + 3y^{2}\dot{y}^{2}y^{(3)^{2}} + 12y\dot{y}^{2}\ddot{y}^{3} - 14y\dot{y}^{3}y^{(3)}\ddot{y} + 2y\dot{y}^{4}y^{(4)} - 6\dot{y}^{4}\ddot{y}^{2} + 6\dot{y}^{5}y^{(3)} = 0 \quad (54)$$

$$\dot{V}_{m} = 0 \quad (55)$$

$$(4V_{m}\dot{y}^{8} - 8yV_{m}\ddot{y}\dot{y}^{6} + 4\dot{y}^{5}y^{2}y^{(3)}V_{m} - 4\dot{y}^{3}y^{3}y^{(3)}\ddot{y}V_{m} + \dot{y}^{2}y^{(3)^{2}}V_{m}y^{4} + 4\dot{y}^{2}\ddot{y}^{3}V_{m}y^{3} - 2y^{(3)}\ddot{y}^{2}V_{m}y^{4}\dot{y} + \ddot{y}^{4}V_{m}y^{4})c + 4\dot{y}^{9} - 12y\ddot{y}\dot{y}^{7} + 12\ddot{y}^{2}y^{2}\dot{y}^{5} - 4\ddot{y}^{3}y^{3}\dot{y}^{3} = 0 \quad (56)$$

$$(y^{2}y^{(3)}\dot{y} - y^{2}\ddot{y}^{2} - 2y\dot{y}^{2}\ddot{y} + 2\dot{y}^{4})k_{01} + y\dot{y}^{2}y^{(3)} - 3y\dot{y}\ddot{y}^{2} + 2\dot{y}^{3}\ddot{y} = 0 \quad (57)$$

$$(4\dot{y}^{9} - 12\ddot{y}y\dot{y}^{7} + 12\dot{y}^{5}y^{2}\ddot{y}^{2} - 4\dot{y}^{3}y^{3}\ddot{y}^{3})k_{m} + 2\dot{y}^{3}y^{4}\ddot{y}y^{(3)}V_{m} - 2\dot{y}^{5}y^{3}y^{(3)}V_{m} + 2y^{3}\ddot{y}^{2}V_{m}\dot{y}^{4} - \dot{y}^{2}y^{(3)^{2}}V_{m}\dot{y}^{5} - 2\dot{y}^{2}y^{4}\ddot{y}^{3}V_{m} + 2\ddot{y}^{2}y^{5}y^{(3)}V_{m}\dot{y}$$

Despite the somewhat lengthy expressions the information about identifiability is easy to see:

 $-\ddot{v}^4 v^5 V_{\rm m} = 0. \quad (58)$

1. The structure is neither globally nor locally

- identifiable, due to the expression (55) (See Theorem 1).
- 2. Nevertheless the parameter k_{01} is globally identifiable from (57).
- 3. Now, if $V_{\rm m}$ indeed were known, we see from (56) that c would be globally identifiable. The excitation conditions would then follow by analysis of

$$\begin{split} 4V_{\rm m}\dot{y}^8 - 8yV_{\rm m}\ddot{y}\dot{y}^6 + 4\dot{y}^5y^2y^{(3)}V_{\rm m} \\ - 4\dot{y}^3y^3y^{(3)}\ddot{y}V_{\rm m} + \dot{y}^2y^{(3)^2}V_{\rm m}y^4 + 4\dot{y}^2\ddot{y}^3V_{\rm m}y^3 \\ - 2y^{(3)}\ddot{y}^2V_{\rm m}y^4\dot{y} + \ddot{y}^4V_{\rm m}y^4 = 0. \end{split}$$

A similar statement holds for $k_{\rm m}$ from (58).

Example 5. Compartmental models: Known initial conditions. Let us now turn to the case studied by Chapell et al. (1990) where the initial values x(0) = D are known. We then follow the discussion in Section 6.4 and rank, tentatively, x(t) as a known variable; that is to say it is ranked after y but before the parameter θ . Our algorithm then gives the following expressions: First expression = (54)

$$x\dot{y} - y\dot{x} = 0 \tag{59}$$

$$y - cx = 0 \tag{60}$$

$$(2\dot{y}^4 - y^2\ddot{y}^2 - 2y\dot{y}^2\ddot{y} + y^2\dot{y}y^{(3)})k_{01} - 3y\dot{y}\ddot{y}^2 + 2\dot{y}^3\ddot{y} + y\dot{y}^2y^{(3)} = 0$$
 (61)

$$(y^2\dot{y}y^{(3)} - 2\dot{y}^2y\ddot{y} + 2\dot{y}^4 - y^2\ddot{y}^2)k_{\rm m} - y^2x\ddot{y}^2 + y^2\dot{y}y^{(3)}x = 0$$
 (62)

$$(y^{5}\ddot{y}^{4} + 4y^{4}\ddot{y}^{3}\dot{y}^{2} - 2y^{5}\ddot{y}^{2}\dot{y}y^{(3)} + 4y\dot{y}^{8} - 8\dot{y}^{6}y^{2}\ddot{y} + 4\dot{y}^{5}y^{3}y^{(3)} - 4y^{4}\dot{y}^{3}\ddot{y}y^{(3)} + y^{5}\dot{y}^{2}y^{(3)^{2}})V_{m} + 12x\dot{y}^{5}y^{2}\ddot{y}^{2} - 4x\dot{y}^{3}y^{3}\ddot{y}^{3} - 12x\dot{y}^{7}y\ddot{y} + 4x\dot{y}^{9} = 0.$$
(63)

Here we readily see from (59) that x can indeed be regarded as a known signal if only x(0) is known (we can then solve the first order differential equation (59) uniquely for given y, \dot{y}). Then we see from (60)-(63) that the model structure is globally identifiable, since all expressions are linear in the sought parameters.

8. SOFTWARE ISSUES

An important and pleasant aspect of our global identifiability test is that it can be coded in computer algebra languages, such as MACSYMA and MAPLE.

The dominating part of the test is Ritt's algorithm. S. T. Glad (1992) gives a discussion of how to implement Ritt's algorithm in symbolic algebra. He also describes an implementation in MAPLE that is quite efficient.

Based on this code we have written software

that implements our algorithm for testing identifiability. The user aspects are quite straightforward: we give the dialog for Example 1 in Section 7.

1. Inform the program which symbols are functions of time.

```
vars := [y(t), th(t)];
```

2. Enter the given equations:

```
eql:= [diff(diff(y, t), t)+2*th *diff(y, t)+th*th*y];
```

eq2 := th;

3. Give the ranking:

rank := [y, th];

- Run Ritt's algorithm idRitt([eq1,eq2],vars, rank);
- 5. The computer will now return the expressions A_i and B_i according to Proposition 1. Sometimes there may be separate possibilities corresponding to special cases. All possibilities are then listed separately. For Example 1, idRitt returns two lists of expressions:

```
results = [[1, 2], [3, 4]]

1 = y

2 = \theta

3 = 4y\ddot{y}^3 - 3\dot{y}^2\ddot{y}^2 - 6yy^{(3)}\dot{y}\ddot{y} + 4y^{(3)}\dot{y}^3 + y^2y^{(3)2}

4 = -yy^{(3)} - 2y\ddot{y}\theta + \dot{y}\ddot{y} + 2\theta\dot{y}^2.
```

This corresponds to the solution described in Section 7, Example 1.

It will be interesting and useful to work further with the software to provide a more sophisticated user interface. It is of particular interest to arrange this interface so that the software can be used without detailed knowledge of the underlying theory. In essence we only have to look for how the parameters enter the final differential algebraic expressions. The exact form of the expressions is immaterial. Adjoining proper coefficient expressions to the original equations, changing the ranking and rerunning the algorithm for checking persistence of excitation conditions, could all be done automatically.

9. CONCLUSIONS

We have studied the problem of global and local identifiability for quite arbitrary model structures. We have shown how tools from differential algebra, in particular Ritt's algorithm for computing characteristic sets, provide a fairly complete solution to this problem.

The solution also sheds some light on the identification problem from a somewhat different angle than the usual one. It will be interesting to further pursue several ideas that have been brought out in this way:

Checking the validity of a model structure without ever estimating any parameters. This

was mentioned in Section 6.2. Can this be a practical tool?

Simple linear least squares procedures for providing initial parameter estimates. It is a notoriously difficult problem to find good initial parameter values for iterative estimation schemes for physically parameterized systems. This is true also for linear systems (but non-linearly parametrized) for which very efficient, maximum likelihood-based, local numerical estimation schemes exist. Can procedures like (35) solve this problem also in practice?

Developing explicit identifiability conditions. The solution is algorithmic in nature. However, the insight into what produces identifiable structures can also be used to derive explicit identifiability conditions for classes of model structures. We saw one such case in Example 3. What more can be done on this theme?

Making non-identifiable structures identifiable. Our solution procedure does not only give an unqualified answer 'yes' or 'no' to the identifiability question. The returned expressions indeed contain information about the nature of possible lack of identifiability. We saw in Example 4 how this could be interpreted. Identifiability can, basically, be recovered by fixing certain parameters or by extending the set of observed variables ('making some x:s y'). Our procedure allows easy tests of this. How can it be made explicit to the user?

Efficient implementations of the algorithm. We have derived an algorithm which converges in as finite number of steps, and we have implemented it in Maple, Macsyma and Mathematica. Honestly, it must be added that the actual complexity of this algorithm increases very rapidly with the size of the problem. Our current implementations have difficulties when the sum of the number of parameters and the number of states exceeds 10 or so. On the other hand, the algorithm has an ambitious goal. The identifiability question can be answered without a complete characteristic set. It is an important challenge to find practical implementations that are more efficient than our current ones.

Finally we should remark that we have studied the identifiability problem in a deterministic setting. This is also the most natural approach, since the nature of the matter is whether the observed signals indeed contain sufficient information about parameters of interest. Adding noise to the observations can never improve this situation. Neither will it, typically, deteriorate the situation—but we may suffer from worse accuracy.

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