Proceedings of the 2000 IEEE
International Conference on Control Applications
Anchorage, Alaska, USA • September 25-27, 2000

Identifiability of Hybrid System Models

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Abstract

Parameter estimation is an important tool in system modelling. However parameter estimation is difficult in many real-world application where continuous nonlinear dynamics interact with discrete-event dynamics. Nonlinear least-squares algorithms have been successfully applied. This paper establishes a connection between parameter identifiability and ill-conditioning of the least-squares algorithms. It is shown that a set of parameters is only identifiable if the trajectory sensitivities corresponding to those parameters are linearly independent. The importance of an appropriate choice of measurements is established.

1 Introduction

Parameter estimation is an important tool for developing and validating system models. Applications abound wherever it is important to match model predictions with observed behaviour. For example in power systems, system-wide measurements of disturbances are frequently used in post-mortem analysis to gain a better understanding of system behaviour [1, 2].

System identification concepts are well established for linear systems [3]. However, few real-world systems are linear. In fact, it is becoming more common to find applications where behaviour is governed by interactions between nonlinear continuous dynamics and discrete-event dynamics. Power systems again provide an important example. Components such as electric machines exhibit nonlinear continuous dynamics, whilst relay-driven components like tap-changing transformers display discrete-event behaviour. Such systems have become known as *hybrid systems.*

Parameter estimation for hybrid systems is a difficult task. A common approach has been to formulate the estimation problem as a nonlinear least-squares minimization [4], which is solved using the Gauss-Newton algorithm [5, 6, 7, 8]. That approach often works well, at least for finding local estimates of parameters. However it fails when the Jacobian, formed from trajectory sensitivities, is not full rank or is ill-conditioned. This paper establishes a connection between rank deficiency and parameter identifiability.

The paper is organized as follows. Section 2 provides background to a hybrid system model, and trajectory sensitivities. These sensitivities form the basis for a parameter estimation algorithm summarized in Section 3. The main results of the paper, on parameter identifiability, are presented in Section 4. Conclusions are given in Section 5.

2 Background

2.1 Model

Hybrid systems generally exhibit a mix of continuous time dynamics, discrete-time and discrete-event dynamics, switching action and jump phenomena. It is shown in [9] that such systems can be modelled by a set of switched differential-algebraic equations, coupled with equations to describe state resetting, i.e.,

$$\dot{\underline{x}} = \underline{f}(\underline{x}, y) \tag{1}$$

$$0 = g^{(0)}(\underline{x}, y) \tag{2}$$

$$0 = \begin{cases} g^{(i-)}(\underline{x}, y) & y_{d,i} < 0 \\ g^{(i+)}(\underline{x}, y) & y_{d,i} > 0 \end{cases} \quad i = 1, ..., d \tag{3}$$

$$\underline{x}^+ = \underline{h}_j(\underline{x}^-, y^-) \qquad y_{e,j} = 0 \quad j \in \{1, ..., e\} \tag{4}$$

where

$$\underline{x} = \begin{bmatrix} x \\ z \\ \lambda \end{bmatrix}, \qquad \underline{f} = \begin{bmatrix} f \\ 0 \\ 0 \end{bmatrix}, \qquad \underline{h}_j = \begin{bmatrix} x \\ h_j \\ \lambda \end{bmatrix}$$

and

- x are the continuous dynamic states,
- z are discrete dynamic states,
- y are algebraic states,
- λ are parameters.

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The model can capture complex behaviour such as hysteresis, non-windup limits and rule-based systems [9].

In this model, the parameters λ form part of the extended state $\underline{x}$. This allows a convenient development of trajectory sensitivities, which are used in the parameter estimation algorithm and described in Section 2.2. To ensure that parameters remain fixed at their initial values, the corresponding differential equations (1) are defined as $\dot{\lambda} = 0$.

Away from events, system dynamics evolve smoothly according to the familiar differential-algebraic model

$$\dot{\underline{x}} = \underline{f}(\underline{x}, y) \quad (5)$$
$$0 = g(\underline{x}, y) \quad (6)$$

where g is composed of $g^{(0)}$ together with appropriate choices of $g^{(i-)}$ or $g^{(i+)}$, depending on the signs of the corresponding elements of y_d. At switching events (3), some component equations of g change. To satisfy the new $g = 0$ equation, algebraic variables y may undergo a step change. Reset events (4) force a discrete change in elements of z. Algebraic variables may again step to ensure $g = 0$ is always satisfied.

We define the system *flow* as

$$\phi(\underline{x}_0, t) = \begin{bmatrix} \phi_{\underline{x}}(\underline{x}_0, t) \\ \phi_y(\underline{x}_0, t) \end{bmatrix} = \begin{bmatrix} \underline{x}(t) \\ y(t) \end{bmatrix} \quad (7)$$

where $\underline{x}(t)$ and $y(t)$ satisfy (1)-(4), along with initial conditions,

$$\phi_{\underline{x}}(\underline{x}_0, t_0) = \underline{x}_0 \quad (8)$$
$$g(\underline{x}_0, \phi_y(\underline{x}_0, t_0)) = 0. \quad (9)$$

2.2 Trajectory sensitivities

Trajectory sensitivities provide a way of quantifying the variation of a trajectory resulting from (small) changes to parameters and/or initial conditions [10]. To obtain the sensitivity of the flows $\phi_{\underline{x}}$ and ϕ_y to initial conditions $\underline{x}_0$, and hence to parameter variations, the Taylor series expansion of (7) is formed. Neglecting higher order terms gives

$$\Delta\underline{x}(t) = \frac{\partial \underline{x}(t)}{\partial \underline{x}_0}\Delta\underline{x}_0 \equiv \underline{x}_{\underline{x}_0}(t)\Delta\underline{x}_0 \quad (10)$$

$$\Delta y(t) = \frac{\partial y(t)}{\partial \underline{x}_0}\Delta\underline{x}_0 \equiv y_{\underline{x}_0}(t)\Delta\underline{x}_0. \quad (11)$$

It is important to keep in mind that $\underline{x}_0$ incorporates parameters λ, so sensitivity to $\underline{x}_0$ includes sensitivity to λ. Equations (10) and (11) describe the changes $\Delta\underline{x}(t)$ and $\Delta y(t)$ in a trajectory, at time t along the trajectory, for a given (small) change in initial conditions $\Delta\underline{x}_0 = [\Delta x_0^t \quad \Delta z_0^t \quad \Delta\lambda^t]^t$. The time-varying partial derivatives $\underline{x}_{\underline{x}_0}$ and $y_{\underline{x}_0}$ are known as *trajectory sensitivities*. A detailed investigation of these sensitivities can be found in [11].

3 Parameter Estimation

The algebraic state corresponding to a measurement sequence m will be denoted $\breve{y}$. The estimation process involves varying a subset of parameters θ to obtain the best match between the sequence m and the flow $\breve{y}(t)$ provided by the model (7).

The model produces the flow $\breve{y}(\theta, t)$ for all $t \geq t_0$. But the samples in the sequence m are measured at certain time instants. Therefore the model is sampled at each time instant t_k, $k = 0, 1, \ldots, q$, resulting in the sequence $\breve{y}_0(\theta), \breve{y}_1(\theta), \ldots, \breve{y}_q(\theta)$, where $\breve{y}_k(\theta) = \breve{y}(\theta, t_k)$. The aim is to determine the value of θ that makes the model response $\breve{y}_k(\theta)$ closest to the measured sample m_k for each k.

Let the mismatch between the measured value and the model output at each sample time be

$$e_k(\theta) = \breve{y}_k(\theta) - m_k \qquad k = 0, 1, \ldots, q$$

or in vector form

$$e(\theta) = \breve{y}(\theta) - m \quad (12)$$

where

$$e(\theta) = [e_0(\theta)\ e_1(\theta)\ \cdots e_q(\theta)]^t$$
$$\breve{y}(\theta) = [\breve{y}_0(\theta)\ \breve{y}_1(\theta)\ \cdots\ \breve{y}_q(\theta)]^t$$
$$m = [m_0\ m_1\ \cdots\ m_q]^t.$$

The desired value of θ minimizes the least squares cost

$$\mathcal{V}(\theta) = \frac{1}{2}\sum_{k=0}^{q} |e_k(\theta)|^2 = \frac{1}{2}\|e(\theta)\|_2^2. \quad (13)$$

The problem has been reduced to a nonlinear least squares formulation that can be solved using the Gauss-Newton method [4]. This is an iterative approach which is based on linearizing $e(\theta)$ around the point θ^j,

$$\tilde{e}(\theta, \theta^j) = e(\theta^j) + \frac{\partial e(\theta^j)}{\partial \theta}(\theta - \theta^j). \quad (14)$$

From (12) it follows that

$$\frac{\partial e(\theta^j)}{\partial \theta} = \frac{\partial \breve{y}(\theta^j)}{\partial \theta} = \begin{bmatrix} \breve{y}_\theta(\theta^j, t_0) \\ \breve{y}_\theta(\theta^j, t_1) \\ \vdots \\ \breve{y}_\theta(\theta^j, t_q) \end{bmatrix} \equiv S(\theta^j) \quad (15)$$

where $\breve{y}_\theta$ is composed of the columns of trajectory sensitivities $\breve{y}_{\underline{x}_0}$ that correspond to the subset of parameters θ. Because $S(\theta^j)$ is formed from $\breve{y}_\theta$, evaluated at time steps $t_0, t_1, \ldots, t_q$, it shall be referred to as the *sensitivity matrix.*

Assuming $S(\theta^j)^t S(\theta^j)$ is well-conditioned, Gauss-Newton minimization of (13) is achieved through the iterative scheme

$$\begin{aligned} S(\theta^j)^t S(\theta^j) v &= S(\theta^j)^t e(\theta^j) \\ &= S(\theta^j)^t (\breve{y}(\theta^j) - m) \qquad (16) \\ \theta^{j+1} &= \theta^j - \alpha^j v \qquad (17) \end{aligned}$$

where α^j is a scalar that determines the step size. The invertibility of $S^t S$ relates directly to identifiability, and is the subject of Section 4. Equation (16) could be solved by inverting $S^t S$, however algorithms that are faster and more numerically robust are available [12].

An estimate of θ which (locally) minimizes the cost function $\mathcal{V}(\theta)$ is obtained when $\Delta\theta^j = \theta^{j+1} - \theta^j$ is close to zero. Note that this procedure will only give local minima though, as it is based on a first-order approximation of $e(\theta)$. However if the initial guess for θ is good then a local minimum is sufficient.

4 Identifiability

The parameter estimation procedure (16)-(17) requires the matrix $S^t S$ to be invertible at each iteration. If $S^t S$ is not invertible, or equivalently if S does not have full rank, then estimation is not possible. This observation is now formalized in terms of model identifiability.

In discussing identifiability it is important to clearly define the concept of a model. If the hybrid system is described by the DAD representation (1)-(4) then the following definition can be stated:

Definition 1 (Models) *A model is a triple*

$$\begin{aligned} \mathcal{M} = &[\underline{f}(\underline{x}, y), \\ &\{g^{(0)}(\underline{x}, y), g^{(i-)}(\underline{x}, y), g^{(i+)}(\underline{x}, y), y_{d,i}, i = 1, ..., d\}, \\ &\{\underline{h}_j(\underline{x}, y), y_{e,j}, j = 1, ..., e\}]. \end{aligned}$$

Models are parameterized by initial conditions $\underline{x}_0$. Associated with each parameterized model $\mathcal{M}(\underline{x}_0)$ is the flow $\phi(\underline{x}_0, t)$. Model equality can therefore be defined as follows.

Definition 2 (Model equality) *Two models $\mathcal{M}^{(1)}$ and $\mathcal{M}^{(2)}$ are equal, i.e., $\mathcal{M}^{(1)}(\underline{x}_0^1) = \mathcal{M}^{(2)}(\underline{x}_0^2)$ if*

$$\phi^{(1)}(\underline{x}_0^1, t) = \phi^{(2)}(\underline{x}_0^2, t) \qquad \forall t \geq t_0.$$

Generally we are not interested in estimating all initial conditions $\underline{x}_0$. (Recall that the parameters λ are incorporated into $\underline{x}_0$.) More commonly only a subset θ of initial conditions (parameters) are required to be estimated. Thererfore we shall assume that models are parameterized only by θ, i.e., model $\mathcal{M}(\theta)$ gives rise to the flow $\phi(\theta, t)$. It is now appropriate to define the concept of local identifiability in terms of the unknown parameters θ.

Definition 3 (Local identifiability) *A model $\mathcal{M}$ is locally identifiable at θ^* if there exists an $\epsilon > 0$ such that*

$$\mathcal{M}(\theta) = \mathcal{M}(\theta^*), \quad \theta \in \beta(\theta, \epsilon) \quad \Rightarrow \quad \theta = \theta^*$$

where $\beta(\theta, \epsilon)$ denotes an ϵ-neighbourhood of θ^*.

In terms of flows, this definition states that the model $\mathcal{M}$ is locally identifiable if

$$\phi(\theta, t) = \phi(\theta^*, t), \ \forall t \geq t_0 \quad \Rightarrow \quad \theta = \theta^*$$

or taking account of the local nature of the definition,

$$\begin{aligned} \phi(\theta, t) - \phi(\theta^*, t) = \Delta\phi(t) = 0 \quad \forall t \geq t_0 \\ \Rightarrow \theta - \theta^* = \Delta\theta = 0. \qquad (18) \end{aligned}$$

From (10)-(11) and (7) it can be seen that

$$\Delta\phi(t) = \begin{bmatrix} \Delta\underline{x}(t) \\ \Delta y(t) \end{bmatrix} = \begin{bmatrix} \underline{x}_\theta(t) \\ y_\theta(t) \end{bmatrix} \Delta\theta$$

where $\underline{x}_\theta$ and y_θ are appropriate columns of $\underline{x}_{\underline{x}_0}$ and $y_{\underline{x}_0}$ respectively. Consider sampling $\Delta\phi(t)$ at timesteps t_k, $k = 0,1,...,q$ and let

$$\Delta\bar{\phi} = \begin{bmatrix} \Delta\phi(t_0) \\ \Delta\phi(t_1) \\ \vdots \\ \Delta\phi(t_q) \end{bmatrix}.$$

Then

$$\Delta\bar{\phi} = \begin{bmatrix} \begin{bmatrix} \underline{x}_\theta(t_0) \\ y_\theta(t_0) \end{bmatrix} \\ \begin{bmatrix} \underline{x}_\theta(t_1) \\ y_\theta(t_1) \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \underline{x}_\theta(t_q) \\ y_\theta(t_q) \end{bmatrix} \end{bmatrix} \Delta\theta = \mathcal{S}\Delta\theta. \qquad (19)$$

A lemma regarding local identifiability follows directly.

Lemma 1 (Local identifiability)

$$\begin{aligned} &\text{“}\Delta\bar{\phi} = 0 \quad \Rightarrow \quad \Delta\theta = 0\text{”} \\ &\Leftrightarrow \quad \mathcal{S} \text{ has full rank.} \end{aligned}$$

Proof: Consider $\Delta\bar{\phi}^t \Delta\bar{\phi} = \Delta\theta^t \mathcal{S}^t \mathcal{S} \Delta\theta$.

$\Rightarrow$ If $\mathcal{S}^t\mathcal{S}$ is not full rank, then there exists a $\Delta\theta \neq 0$ such that $\Delta\theta^t\mathcal{S}^t\mathcal{S}\Delta\theta = 0$, i.e., $\Delta\bar{\phi} = 0$. Therefore, for $\Delta\bar{\phi} = 0 \Rightarrow \Delta\theta = 0$, $\mathcal{S}^t\mathcal{S}$ must be full rank. Hence $\mathcal{S}$ has full column rank.

$\Leftarrow$ If $\mathcal{S}$ has full column rank, then $\mathcal{S}^t\mathcal{S}$ has full rank. Hence $\Delta\theta^t\mathcal{S}^t\mathcal{S}\Delta\theta = 0$ if and only if $\Delta\theta = 0$. So if $\Delta\bar{\phi} = 0$ then $\Delta\theta = 0$.

□

The following theorem links the ideas together.

Theorem 1 (Local identifiability) *A model $\mathcal{M}$ is locally identifiable at θ^* iff $\mathcal{S}$ has full rank.*

Proof: Using (19) together with (18) and Lemma 1 proves the theorem.

□

It is important to note that the definition of local identifiability says that

$$\left.\begin{array}{lccc} & \phi_1(\theta,t) & = & \phi_1(\theta^*,t) \\ \text{and} & \phi_2(\theta,t) & = & \phi_2(\theta^*,t) \\ \text{and} & \vdots & \vdots & \vdots \\ \text{and} & \phi_{n+m}(\theta,t) & = & \phi_{n+m}(\theta^*,t) \end{array}\right\} \Rightarrow \quad \theta = \theta^*$$

where ϕ_i refers to the ith component of ϕ. The contrapositive of the definition is that

$$\theta \neq \theta^* \quad \Rightarrow \quad \left\{\begin{array}{lccc} & \phi_1(\theta,t) & \neq & \phi_1(\theta^*,t) \\ \text{or} & \phi_2(\theta,t) & \neq & \phi_2(\theta^*,t) \\ \text{or} & \vdots & \vdots & \vdots \\ \text{or} & \phi_{n+m}(\theta,t) & \neq & \phi_{n+m}(\theta^*,t). \end{array}\right.$$

Hence it is possible for a locally identifiable model to have $\phi_i(\theta,t) = \phi_i(\theta^*,t)$ when $\theta \neq \theta^*$ for one or more i, provided $\phi_j(\theta,t) \neq \phi_j(\theta^*,t)$ for at least one j. In other words, some components of the flow may be completely uninfluenced by the parameters θ. However for the model to be identifiable there must be at least one component that is influenced by θ.

This concept is important because it confirms that model identifiability does not guarantee identifiability based on any arbitrary set of measurements. (Recall that measurements correspond to components of the flow ϕ). However it does guarantee that a set of measurements can be found such that the model is identifiable from those measurements.

The states (or components of ϕ) corresponding to measurements are given by $\breve{y}$. Therefore, referring to (15),

$$\Delta\bar{\phi}_{\breve{y}} = \Delta\breve{y} = S\Delta\theta$$

where S is constructed from appropriate rows of $\mathcal{S}$, with each component of $\breve{y}$, i.e., each measurement, introducing $q+1$ rows into S. Earlier it was shown that model identifiability was associated with the rank of $\mathcal{S}$. In the same way, identifiability from measurements is related to the rank of S.

Theorem 2 (Identifiability from measurements) *A model $\mathcal{M}$ is locally identifiable at θ^* from measurements $\breve{y}$ iff S has full rank.*

Proof: Follows the same argument as the proof of Theorem 1.

□

This allows another useful result.

Lemma 2 (Identifiability from measurements) *If a model $\mathcal{M}$ is not locally identifiable at θ^* then it is not identifiable from any set of measurements.*

Proof: If a model $\mathcal{M}$ is not locally identifiable then $\mathcal{S}$ does not have full rank. But S is constructed from rows of $\mathcal{S}$ so S cannot have higher rank than that of $\mathcal{S}$, no matter which rows (measurements) are chosen. Hence S cannot have full rank. By Theorem 2, the model is not identifiable for any choice of measurements.

□

These results indicate the importance of the choice of measurements. An inappropriate choice could result in the model not being identifiable, in which case the parameter estimation process will fail. (This failure appears as a very small pivot when attempting to factorize the singular matrix S^tS.)

This discussion of identifiability also highlights the case where a parameter may have only a small influence on the flow corresponding to a measurement. In that case S may have full rank, but S^tS is ill-conditioned. This problem can often be overcome by a better choice of measurements. However if the measurement set cannot be adjusted, numerically robust algorithms for factorizing the nearly singular S^tS should be used [12].

Theorem 2 motivates the use of trajectory sensitivities in selecting an appropriate measurement set. The Jacobian S is composed of sampled trajectory sensitivities, which are available from simulation. The conditioning of S can be maximized, i.e., the best measurement set chosen, by selectively adding (or removing) trajectory sensitivities that correspond to available measurements. This same process can assist in determining new measurements that would further improve identifiability. These ideas are explored in [13].

Note that the discussion of identifiability is limited to local identifiability. This is a consequence of Gauss-Newton minimization ignoring the higher order terms in the Taylor series expansion of ϕ. As justification, it

is assumed that the initial guesses for unknown parameters are close to their actual values. We cannot however reach any conclusions regarding global identifiability.

5 Conclusions

Parameter estimation of hybrid system models can be formulated as a nonlinear least-squares minimization. Solution of this minimization using Gauss-Newton involves the (effective) inversion of a Jacobian matrix formed from trajectory sensitivities.

It is shown in the paper that the Jacobian will be full rank (nonsingular) if the model is identifiable from available measurements. Parameter estimation is therefore possible (though convergence is not guaranteed.) However if the model is not identifiable from available measurements, then the Jacobian will be singular, and the estimation process will fail.

Trajectory sensitivities can be used to guide the selection of measurements that maximize the conditioning of the estimation process.

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