

Identifiability: from qualitative analysis to model structure approximation [★]

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Abstract: The question whether a physical model structure is identifiable is usually considered in a qualitative way, i.e. it is answered with a yes/no answer. However when considering parameters in large scale (nonlinear) physical models it is relevant to raise the question how the notion of identifiability can be quantified. This implies addressing the question how the model structure can be approximated so as to achieve identifiability, while retaining the interpretation of the physical parameters. In this paper this problem is addressed in a prediction error setting, and it is shown how the construction of best locally identifiable model structure approximations relates to notions of controllability and observability. Additionally the analysis in terms of an prediction error approach relates to iterative optimization algorithms (like Gauss-Newton and Steepest-Descent) and to Bayesian parameter estimation.

Keywords: identifiability; controllability; observability; structural identifiability; physical model structures; model structure approximation.

1. INTRODUCTION

When building dynamic models from physical first-principles relations model structures occur that are often large-scale in their dimensions (due to spatial discretization of pde's) and include a high number of physically interpretable parameters. If subsequently the model parameters have to be identified from measurement data with prediction error methods (PEM) or (extended) Kalman filtering methods the question occurs whether the parameters are identifiable. The notion of identifiability refers -roughly speaking- to the question whether parameter changes can be observed in the model output signal (output identifiability) or in the model's transfer function (structural identifiability).

The notion of output identifiability has been studied in e.g. Grewal and Glover [1976] and Ljung [1999]. The notion of structural identifiability was first stated by Bellman and Åström [1970] and has been extensively studied in the field of compartmental modeling [Godfrey, 1983, Norton, 1980]. State-space model parameterizations have been analyzed

by Glover and Willems [1974] and Walter [1987]. Lately there has been a renewed interest in structural identifiability analysis, with contributions from Stigter and Peeters [2007] and Van Doren et al. [2008].

In general identifiability questions are considered qualitatively, i.e. deciding whether a model structure is identifiable or not. The tests required for this decision are typically rank evaluations of matrices, as e.g. Fisher's information matrix, around a particular local operating point in the parameter space, see e.g. Dötsch and Van den Hof [1996]. Restricting attention to a local analysis is often the only situation that is feasible in terms of computational complexity. For issues around global properties see e.g. Ljung and Glad [1994] and Evans et al. [2002].

However, when considering parameters in large scale (nonlinear) physical models it is relevant to raise the question how the notion of local identifiability can be quantified. This implies addressing the question which part of the parameter space is best identifiable, and which part of the model structure can be approximated so as to achieve local identifiability, while retaining the interpretation of the physical parameters. For structural identifiability this question was preliminary addressed in Van Doren et al. [2008]. In Berntsen and Balchen [1973] the degree of identifiability was introduced. In Vajda et al. [1989] principal component analysis was applied to determine which parameters can be identified. McKelvey et al. [2004] introduced data driven local coordinates to overcome numerical disadvantages in identification of overparameterized state-

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space systems.

In this paper we will further investigate how the notions of identifiability can be quantified to allow for a reduction in the parameter space with physically interpretable parameters. The analysis will be restricted to the local case, considering (linearized) nonlinear dynamical models that are non-linear in the parameters. First the problem will be considered in the context of an off-line prediction error identification approach, while appropriate attention is given to the effect of parameter-scaling. Next the identifiable parameter space is related to controllability, observability and the mapping from a parameter perturbation to a state change (sensitivity). In Section 4.1 the analysis in terms of an off-line prediction error approach will be related to iterative optimization algorithms (like Gauss-Newton and Steepest-Descent) as well as to sequential (recursive) parameter estimation methods. Finally, in Section 5 structural identifiability is addressed and subsequently two small examples are presented.

2. IDENTIFIABILITY

In this section we describe how to quantify identifiability and how to approximate the model structure so as to guarantee identifiability. Additionally, we discuss the influence of parameter scaling on the model structure approximation.

2.1 Preliminaries

Consider a nonlinear dynamical model that generates output predictions according to:

$$\hat{\mathbf{y}} = \mathbf{h}(\boldsymbol{\theta}, \mathbf{u}; \mathbf{x}_0), \quad (1)$$

where $\hat{\mathbf{y}}$ is a prediction of $\mathbf{y} := [\mathbf{y}_1^T \dots \mathbf{y}_N^T]^T$ denoting output signal measurements $\mathbf{y}_k \in \mathbb{R}^p$ stacked over time, $\boldsymbol{\theta} \in \Theta \subset \mathbb{R}^q$ the parameter vector, $\mathbf{u} := [\mathbf{u}_1^T \dots \mathbf{u}_N^T]^T$ the input vector $\mathbf{u}_k \in \mathbb{R}^m$ stacked over time, and \mathbf{x}_0 the initial state vector. Since the model (1) is parameterized it represents an input/output model structure.

First we give a definition of local identifiability [Grewal and Glover, 1976]:

Definition 1. An input/output model structure $\mathbf{h}(\boldsymbol{\theta}, \mathbf{u}; \mathbf{x}_0) : \Theta \rightarrow \mathcal{H}$ is called locally identifiable in $\boldsymbol{\theta}_m \in \Theta$ for a given \mathbf{u} and \mathbf{x}_0 , if for all $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2$ in the neighborhood of $\boldsymbol{\theta}_m$ holds that

$$\{\mathbf{h}(\mathbf{u}, \boldsymbol{\theta}_1; \mathbf{x}_0) = \mathbf{h}(\mathbf{u}, \boldsymbol{\theta}_2; \mathbf{x}_0)\} \Rightarrow \boldsymbol{\theta}_1 = \boldsymbol{\theta}_2.$$

After linearization of the dynamics in $\mathbf{h}(\boldsymbol{\theta}, \mathbf{u}; \mathbf{x}_0)$ around an operating point, a linear time-invariant model input-output model is obtained, denoted by the transfer function G , leading to an output predictor

$$\hat{\mathbf{y}}_k = G(q, \theta) \mathbf{u}_k,$$

with q the shift operator.

The notion of local structural identifiability [Glover and Willems, 1974] is then defined by considering the properties of the parameterized transfer function $G(q, \theta)$:

Definition 2. An input/output model structure $G : \Theta \rightarrow \mathcal{G}$ with $\Theta \subset \mathbb{R}^q$ and $\mathcal{G} \subset \mathbb{R}(z)^{p \times m}$ is called locally structural identifiable in $\boldsymbol{\theta}_m \in \Theta$ if for all $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2$ in the neighborhood of $\boldsymbol{\theta}_m$ holds that

$$\{G(z, \boldsymbol{\theta}_1) = G(z, \boldsymbol{\theta}_2)\} \Rightarrow \boldsymbol{\theta}_1 = \boldsymbol{\theta}_2. \quad (2)$$

Note that in contrast with (1) this notion does not include the input vector nor an initial state. Structural identifiability will be considered in Section 5, where a link is made between structural identifiability and identifiability.

In a prediction error framework we consider parameter estimation methods that are obtained by minimizing a cost function $V(\boldsymbol{\theta})$:

$$V(\boldsymbol{\theta}) := \frac{1}{2} \boldsymbol{\epsilon}(\boldsymbol{\theta})^T \mathbf{P}_v^{-1} \boldsymbol{\epsilon}(\boldsymbol{\theta}), \quad (3)$$

where the prediction error $\boldsymbol{\epsilon}$ is defined as

$$\boldsymbol{\epsilon}(\boldsymbol{\theta}) = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{h}(\boldsymbol{\theta}, \mathbf{u}; \mathbf{x}_0), \quad (4)$$

where \mathbf{y} denotes the measured outputs and $\hat{\mathbf{y}}$ the predictor, and \mathbf{P}_v is (an estimate of) the covariance matrix of the noise \mathbf{v} that is supposed to act on the measured output. In the rest of the paper the shorthand notation $\mathbf{h}(\boldsymbol{\theta})$ is used to indicate $\mathbf{h}(\boldsymbol{\theta}, \mathbf{u}; \mathbf{x}_0)$.

The Jacobian of $V(\boldsymbol{\theta})$ with respect to the parameters is

$$\begin{aligned} \frac{\partial V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} &= \frac{\partial \boldsymbol{\epsilon}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \mathbf{P}_v^{-1} \boldsymbol{\epsilon}(\boldsymbol{\theta}) = \\ &\quad - \frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \mathbf{P}_v^{-1} (\mathbf{y} - \mathbf{h}(\boldsymbol{\theta})). \end{aligned} \quad (5)$$

The Hessian of $V(\boldsymbol{\theta})$ with respect to the parameters is

$$\begin{aligned} \frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} &= \frac{\partial \boldsymbol{\epsilon}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \mathbf{P}_v^{-1} \left(\frac{\partial \boldsymbol{\epsilon}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \right)^T + \mathbf{S} = \\ &\quad \frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \mathbf{P}_v^{-1} \left(\frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \right)^T + \mathbf{S}, \end{aligned} \quad (6)$$

where \mathbf{S} denotes the second-order information in $\frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2}$. The Jacobian and Hessian are for a given $\boldsymbol{\theta}$ and operating point. Parameter estimation then consists in finding a parameter estimate as a minimizing argument of the cost function $V(\boldsymbol{\theta})$

$$\hat{\boldsymbol{\theta}} := \arg \min_{\boldsymbol{\theta}} V(\boldsymbol{\theta}). \quad (7)$$

At $\hat{\boldsymbol{\theta}}$ the cost function $V(\boldsymbol{\theta})$ is minimized and the Jacobian (5) at $\hat{\boldsymbol{\theta}}$ is zero, i.e. $\frac{\partial V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \mathbf{0}$ at $\hat{\boldsymbol{\theta}}$.

2.2 Analyzing local identifiability

Local identifiability in $\hat{\boldsymbol{\theta}}$ is generally evaluated by the test whether the optimization problem (7) has an unique solution in the parameter space. By locally approximating the cost function $V(\boldsymbol{\theta})$ by a quadratic function¹, and thus neglecting the second order term \mathbf{S} in (6), uniqueness of $\hat{\boldsymbol{\theta}}$ is guaranteed if the Hessian at $\hat{\boldsymbol{\theta}}$ is positive definite, i.e. $\frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} > 0$ at $\hat{\boldsymbol{\theta}}$, which in this case is equivalent to $\text{rank} \frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} = q$. This is a sufficient condition for local identifiability in $\hat{\boldsymbol{\theta}}$, see e.g. Bellman and Åström [1970], Glover and Willems [1974] and Ljung [1999].

The considered rank test is naturally performed by applying a singular value decomposition (SVD):

$$\frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^T = [\mathbf{U}_1 \ \mathbf{U}_2] \begin{bmatrix} \boldsymbol{\Sigma}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V}_1^T \\ \mathbf{V}_2^T \end{bmatrix},$$

where matrices \mathbf{U} and \mathbf{V} are unitary matrices, $\boldsymbol{\Sigma}_1 = \text{diag}(\sigma_1, \dots, \sigma_p)$ with $\sigma_1 \geq \dots \geq \sigma_p$. If $p = q$ then

¹ This is achieved by approximating $\mathbf{h}(\boldsymbol{\theta})$ with a first-order Taylor expansion around $\hat{\boldsymbol{\theta}}$

identifiability is confirmed. If $p < q$ then the column space of \mathbf{U}_1 represents the subspace of the parameter space that is identifiable, and the column space of \mathbf{U}_2 is its orthogonal complement, characterizing the subspace that is not identifiable.

As a result, the SVD of the Hessian can be used to extend the qualitative treatment of the question whether or not a particular model structure is identifiable, to a quantitative property of specifying the identifiable parameter space. The columns of \mathbf{U}_1 basically act as basis functions in the parameter space, determining the linear combinations of the original parameters that will be identifiable from the measurements. Differently formulated, this would point to reparameterize the model structure by defining a reduced order parameter $\boldsymbol{\rho} \in \mathbb{R}^p$ defined by

$$\boldsymbol{\theta} = \mathbf{U}_1 \boldsymbol{\rho}$$

leading to an identifiable model structure in the parameter $\boldsymbol{\rho}$.

2.3 Model structure approximation

When in the SVD of the Hessian singular values are found that are (very) small, this points to directions in the parameter space that have very limited (but nonzero) influence on the cost function V .

In identification terms this corresponds to directions in the parameter space in which the variance is large. The Hessian evaluated at $\hat{\boldsymbol{\theta}}$ is connected with the variance of $\hat{\boldsymbol{\theta}}$, since for the Gaussian case (and provided that $\hat{\boldsymbol{\theta}} = \boldsymbol{\theta}_0$) it follows that

$$\text{cov}(\hat{\boldsymbol{\theta}}) = J^{-1}$$

with J the Fisher information matrix

$$J = \mathbb{E} \left[\frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} \Bigg|_{\hat{\boldsymbol{\theta}}} \right], \quad (8)$$

where \mathbb{E} denotes expectation [Ljung, 1999].

We are interested in specifying that part of the parameter space that is best identifiable by removing the subspace that has only a very small influence on the cost function V . This reasoning would point to removing those parameter (combinations) from the model structure for which the variance is very large (and the corresponding singular value is very small), as also addressed in Vajda et al. [1989]. However it appears that when using absolute variance as a measure of selection, the selected parameter space will become dependent on the scaling of parameters, as e.g. the choice of physical units in which we represent the parameters. In order to arrive at a selection mechanism that is scaling independent, the relative variance of parameters should be used, i.e.

$$\text{cov}(\boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}}^{-1} \hat{\boldsymbol{\theta}})$$

where $\boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}} = \text{diag}(|\hat{\boldsymbol{\theta}}_1| \dots |\hat{\boldsymbol{\theta}}_q|)$. This motivates the analysis of a scaled Hessian

$$\boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}} \frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} \Bigg|_{\hat{\boldsymbol{\theta}}} \boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}}, \quad (9)$$

related to the scaled Fisher information matrix \tilde{J} :

$$\tilde{J} = \mathbb{E} \left[\boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}} \frac{\partial^2 V(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} \Bigg|_{\hat{\boldsymbol{\theta}}} \boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}} \right]. \quad (10)$$

Consequences of this parameter scaling are illustrated later on for some simple examples in Section 6.

The essential information on the SVD of the scaled Hessian (9) is now obtained from:

$$\boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}} \frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \mathbf{P}_v^{-\frac{1}{2}} = [\mathbf{U}_1 \ \mathbf{U}_2] \begin{bmatrix} \boldsymbol{\Sigma}_1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_2 \end{bmatrix} \begin{bmatrix} \mathbf{V}_1^T \\ \mathbf{V}_2^T \end{bmatrix} \quad (11)$$

where the separation between $\boldsymbol{\Sigma}_1$ and $\boldsymbol{\Sigma}_2$ is chosen in such a way that the singular values in $\boldsymbol{\Sigma}_2$ are considerably smaller than those in $\boldsymbol{\Sigma}_1$. If we now reparameterize the model structure by employing the reduced parameter $\boldsymbol{\rho}$ determined by $\boldsymbol{\theta} = \mathbf{U}_1 \boldsymbol{\rho}$, we have realized a model structure approximation, in which the parameters to be identified are well identifiable and the physical interpretation of the parameters remains untouched. Specifically in the case of parameters in spatially distributed systems with all parameters having the same physical unit, the singular vectors can be seen as basis functions in the parameter space.

3. RELATION WITH CONTROLLABILITY AND OBSERVABILITY

In this section we will show how the identifiable parameter space that results from (11) is related to properties of controllability and observability. Since we like to consider controllability and observability we consider the strictly proper deterministic linear time-varying (LTV) model in discrete-time state-space form, that could result from linearizing a nonlinear model in the vicinity of the nominal trajectory. The model is

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{A}_k(\boldsymbol{\theta}) \mathbf{x}_k + \mathbf{B}_k(\boldsymbol{\theta}) \mathbf{u}_k \\ \mathbf{h}(\boldsymbol{\theta})_k &= \mathbf{C}_k(\boldsymbol{\theta}) \mathbf{x}_k, \end{aligned}$$

where subscript k denotes the time index. The sensitivity of the predicted outputs with respect to the parameter vector $\boldsymbol{\theta}$ is element-wise given by

$$\frac{\partial \mathbf{h}(\boldsymbol{\theta})_k}{\partial \boldsymbol{\theta}(i)} = \mathbf{C}_k(\boldsymbol{\theta}) \frac{\partial \mathbf{x}_k}{\partial \boldsymbol{\theta}(i)} + \frac{\partial \mathbf{C}_k(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(i)} \mathbf{x}_k,$$

where $\frac{\partial \mathbf{x}_k}{\partial \boldsymbol{\theta}(i)}$ is determined by

$$\frac{\partial \mathbf{x}_{k+1}}{\partial \boldsymbol{\theta}(i)} = \mathbf{A}_k(\boldsymbol{\theta}) \frac{\partial \mathbf{x}_k}{\partial \boldsymbol{\theta}(i)} + \underbrace{\frac{\partial \mathbf{A}_k(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(i)} \mathbf{x}_k + \frac{\partial \mathbf{B}_k(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(i)} \mathbf{u}_k}_{:= \tilde{\mathbf{u}}_k^{\boldsymbol{\theta}(i)}}. \quad (12)$$

Without loss of generality we can assume that $\frac{\partial \mathbf{C}_k}{\partial \boldsymbol{\theta}(i)} = \mathbf{0}$, since \mathbf{C}_k can be made independent of $\boldsymbol{\theta}$ by redefining the state. Note that the effect of a parameter change is weighted by the value of current state and input, i.e. in (12) $\frac{\partial \mathbf{A}_k(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(i)}$ is weighted by \mathbf{x}_k and $\frac{\partial \mathbf{B}_k(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(i)}$ is weighted by \mathbf{u}_k . This means that given a specific model structure, outputs are more sensitive to parameters associated with states that have a large value. In stacked form we can write

$\mathbf{h}(\boldsymbol{\theta})$ is approximated using a first-order Taylor expansion around $\boldsymbol{\theta}_p$. The Hessian is given by

$$\frac{\partial^2 V_p(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2} = \frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \mathbf{P}_v^{-1} \left(\frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} \right)^T + \mathbf{P}_\theta^{-1}. \quad (18)$$

Note that the Hessian can be scaled with covariance matrix \mathbf{P}_θ as is done in Tavakoli and Reynolds [2009]. In (18) the first term is positive and the second term \mathbf{P}_θ^{-1} is positive definite by construction. Therefore, the Hessian in has full rank and the parameter estimate is unique. However, that estimate is possibly strongly influenced by the prior knowledge in \mathbf{P}_θ . If prior knowledge is not included, then there will be adaptations in the identifiable parameter space only, while leaving the remainder of the space completely untouched. Furthermore, when the non-identifiable directions in \mathbf{U}_2 are made explicit, other sources of information can freely be applied when projected onto the non-identifiable directions.

5. STRUCTURAL IDENTIFIABILITY

The question whether parameters can be uniquely identified from data basically consists of two parts. The first part concerns the model structure: is it possible at all to distinguish two given parameters, provided that the input is chosen in the best possible way? This property is called structural identifiability of a model structure. The second part concerns the issue whether the actual input is informative enough to allow this distinction. In the previous sections both parts were considered simultaneously. In this section only the first part is investigated. Consider Definition 2 on structural identifiability. Without loss of generality, but for ease of notations, we will limit attention to the SISO case. Note that $G(z, \boldsymbol{\theta})$ can be written as:

$$G(z, \boldsymbol{\theta}) = \sum_{k=1}^{\infty} \mathbf{M}(k, \boldsymbol{\theta}) z^{-k}, \quad (19)$$

where $\mathbf{M}(k, \boldsymbol{\theta})$ are the Markov parameters. Based on (19) we argue that equality of $G(z, \boldsymbol{\theta}_1)$ and $G(z, \boldsymbol{\theta}_2)$ is related to equality of the Markov parameters of $G(z, \boldsymbol{\theta}_1)$ and $G(z, \boldsymbol{\theta}_2)$. We now present Lemma 3 on injective maps, which will lead together with Definition 2 to Proposition 4 [see also Glover and Willems, 1974, Grewal and Glover, 1976, Norton, 1980, Van Doren et al., 2008]:

Lemma 3. Let Ω be an open set in \mathbb{R}^n and $f : \Omega \rightarrow \mathbb{R}^m$ be a k -times continuously differentiable map with $k \geq 1$. If $\frac{\partial f(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$ has constant rank l in a neighborhood of $\boldsymbol{\theta}_m$, then f is locally injective at $\boldsymbol{\theta}_m$ if and only if $l = n$.

Proposition 4. Consider the map $\mathbf{S}_N(\boldsymbol{\theta}) : \Theta \subset \mathbb{R}^q \rightarrow \mathbb{R}^N$ defined by:

$$\mathbf{S}_N(\boldsymbol{\theta}) := [\mathbf{M}(1, \boldsymbol{\theta}) \dots \mathbf{M}(N, \boldsymbol{\theta})]^T. \quad (20)$$

Then the model structure is locally structural identifiable in $\boldsymbol{\theta}_m$ if $\text{rank} \left(\frac{\partial \mathbf{S}_N^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right) = q$ in $\boldsymbol{\theta} = \boldsymbol{\theta}_m$.

Both the qualitative question of structural identifiability, and the determination of the “best” structurally identifiable subspace of parameters can now be examined by applying an SVD to the matrix

$$\frac{\partial \mathbf{S}_N^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \quad (21)$$

and examining the column space of this matrix, see Van Doren et al. [2008]. However also in this problem we

need to take care that our (approximate) identifiability test is not dependent on user-chosen parameter scaling, and so we need a premultiplication of (21) with the scaling matrix $\boldsymbol{\Gamma}_{\theta_m}$. If a parameter has high impact on a particular Markov parameter, but the Markov parameter itself has a very small value, the considered parameter is still a good candidate to be removed in our model structure approximation problem. Therefore an additional weighting of (21) is desired that takes account of the values of the Markov parameters. As a result we consider the column space of the matrix

$$\boldsymbol{\Gamma}_{\theta_m} \frac{\partial \mathbf{S}_N^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \boldsymbol{\Gamma}_S \quad (22)$$

where for the SISO case $\boldsymbol{\Gamma}_S := \text{diag}(|M_1| \dots |M_N|)$. The consequence is that Markov parameters that have a high value are considered to be more important to include than Markov parameters with a small value. The column space of (22) that relates to the dominant singular values of the matrix, now is a representation of the parameter space of the approximated model structure. The structurally identifiable problem and the identifiability problem are of course closely related to each other. This can be observed by realizing that

$$\frac{\partial \mathbf{h}(\boldsymbol{\theta})^T}{\partial \boldsymbol{\theta}} = \frac{\partial \mathbf{S}_N^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \boldsymbol{\Phi}_N, \quad (23)$$

where $\boldsymbol{\Phi}_N$ is given by

$$\boldsymbol{\Phi}_N = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_N \\ & \mathbf{u}_1 & & \vdots \\ & & \ddots & \\ & & & \mathbf{u}_1 \end{bmatrix} \quad (24)$$

and the derivatives are evaluated at $\boldsymbol{\theta} = \boldsymbol{\theta}_m$. Note that the matrix $\boldsymbol{\Phi}_N$ with input signals acts as a weighting matrix in (23) in a similar way as the weighting matrix $\boldsymbol{\Gamma}_S$ does in (22).

6. EXAMPLES

In order to illustrate the concepts, and in particular the role of the scaling/weighting functions, we will now discuss two examples where we have chosen a very simple SISO finite impulse response (FIR) model. The model structure will be approximated using the previously discussed identifiability analysis, where we assume that $\mathbf{P}_v = \mathbf{I}$.

Example 5. Consider the data-generating system

$$y(t) = \alpha_0 u(t-1) + \beta_0 u(t-2)$$

with $\alpha_0 = 10^6$ and $\beta_0 = 10^{-6}$, and $\boldsymbol{\theta}_0 := [\alpha_0 \ \beta_0]^T$. Consider the input/output model structure

$$y(t, \boldsymbol{\theta}) = \alpha u(t-1) + \beta u(t-2), \quad \boldsymbol{\theta} := [\alpha \ \beta]^T.$$

The scaled Fisher information matrix \tilde{J} of (10) for a local analysis around $\boldsymbol{\theta}_0$ is

$$N \begin{bmatrix} \alpha_0 & 0 \\ 0 & \beta_0 \end{bmatrix} \begin{bmatrix} R_u(0) & R_u(1) \\ R_u(1) & R_u(0) \end{bmatrix} \begin{bmatrix} \alpha_0 & 0 \\ 0 & \beta_0 \end{bmatrix},$$

where $R_u(\tau) = \mathbb{E}[u(t)u(t-\tau)]$. The relative parameter variance is indicated by \tilde{J}^{-1} . In the case of a unit variance white noise input, it follows that

$$\tilde{J} = N \begin{bmatrix} 10^{12} & 0 \\ 0 & 10^{-12} \end{bmatrix},$$

while the unscaled Fisher information matrix satisfies $J = N\mathbf{I}$. Analysis of \tilde{J} shows that the second parameter can very well be neglected, leading to an approximate model structure $y(t) = \alpha u(t - 1)$.

Structural identifiability analysis without scaling shows that both parameters are structurally identifiable, since $\frac{\partial \mathbf{S}_N^T(\theta)}{\partial \theta} = \mathbf{I}$. However, including both scaling matrices Γ_θ and Γ_S , we obtain

$$\Gamma_\theta \frac{\partial \mathbf{S}_N^T(\theta)}{\partial \theta} \Gamma_S = \begin{bmatrix} 10^{12} & 0 \\ 0 & 10^{-12} \end{bmatrix},$$

also showing that the second parameter can be very well neglected. In light of Section 3 we remark that in $\theta = \theta_0$ this model is poorly observable/controllable and as a result it is also poorly identifiable.

Example 6. In this example the same data-generating system as in the previous example is considered. Consider the input/output model structure

$$y(t, \theta) = \alpha u(t - 1) + 10^{-6} \gamma u(t - 2), \quad \theta := [\alpha \ \gamma]^T.$$

where $\gamma_0 = 1$. The scaled Fisher information matrix \tilde{J} of (10) is

$$N \begin{bmatrix} \alpha_0 & 0 \\ 0 & \gamma_0 \end{bmatrix} \begin{bmatrix} R_u(0) & 10^{-6} R_u(1) \\ 10^{-6} R_u(1) & 10^{-12} R_u(0) \end{bmatrix} \begin{bmatrix} \alpha_0 & 0 \\ 0 & \gamma_0 \end{bmatrix}.$$

Under the same input conditions it follows that

$$\tilde{J} = N \begin{bmatrix} 10^{12} & 0 \\ 0 & 10^{-12} \end{bmatrix},$$

while the unscaled Fisher information matrix is

$$J = N \begin{bmatrix} 1 & 0 \\ 0 & 10^{-12} \end{bmatrix}.$$

Whereas the unscaled matrix is essentially different from the previous example, the scaled analysis shows again that the second parameter can be very well neglected and that the model structure can be approximated with $y(t) = \alpha u(t - 1)$.

Structural identifiability analysis without scaling shows that α is structurally best identifiable, since

$$\frac{\partial \mathbf{S}_N^T(\theta)}{\partial \theta} = \begin{bmatrix} 1 & 0 \\ 0 & 10^{-6} \end{bmatrix}.$$

Including both scaling matrices Γ_θ and Γ_S , we obtain in quadratic form

$$\Gamma_\theta \frac{\partial \mathbf{S}_N^T(\theta)}{\partial \theta} \Gamma_S = \begin{bmatrix} 10^{12} & 0 \\ 0 & 10^{-12} \end{bmatrix},$$

being exactly the same as matrix as in the previous example, meaning that the structural identifiability analysis is now-scaling invariant.

7. CONCLUSIONS

The question whether a large scale (nonlinear) physical model structure is identifiable, is usually considered in a qualitative way. In this paper the notion of identifiability is quantified and it is shown how the model structure can be approximated so as to achieve identifiability, while retaining the interpretation of the physical parameters. In this paper this question has been addressed in a prediction error setting, and it is shown how the construction of best identifiable model structure approximations relates to notions of controllability and observability. Additionally the analysis has been related to iterative optimization algorithms (like Gauss-Newton and Steepest-Descent).

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