Delft University of Technology
Delft Center for Systems and Control

Technical report 10-022

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16 December 2009

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Identification of parameters in large scale physical model structures ⋆

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Abstract: When first principles models are used for model-based operations as monitoring, control and optimization, the estimation of accurate physical parameters is important in particular when the underlying dynamical model is nonlinear. If the models are the result of partial differential equations being discretized, they are often large-scale in terms of number of states and possibly also number of parameters. Estimating a large number of parameters from measurement data leads to problems of identifiability, and consequently to inaccurate identification results. 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 since also nearly unidentifiable model structures lead to poor parameter estimates, the questions is addressed how the model structure can be approximated so as to achieve local identifiability, while retaining the interpretation of the physical parameters. Appropriate attention is also given to the relevant scaling of parameters. The problem is addressed in a prediction error setting, and is illustrated with an example taken from oil reservoir engineering.

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

1. INTRODUCTION

Complex dynamical physical processes raise many challenges for model-based monitoring, control and optimization. On-line reconstruction of non-measurable variables, design of appropriate feedforward and feedback control strategies, as well as economic optimization of processes under appropriate operational constraints, generally require the availability of a reliable process model, preferably accompanied by a quantification of its reliability (uncertainty). If the dynamics of the considered process is linear, then a process model can be obtained by applying black-box system identification, which provides a well-studied set of tools for identifying linear models on the basis of experimental data Ljung [1999]. If there is a particular interest in the identification of physical parameters, this often does not raise any additional problems: one has to choose the right (physics-based) model structure and identify the parameters through one of the available (possibly non-convex) optimization methods. The only issue that has to be taken care of is that the physical model structure is identifiable, implying that the several physical parameters can be distinguished from each other on the basis of the model's input-output behavior.

In the situation that the process dynamics is nonlinear, it can often be linearized around an operating point (as e.g. in continuous-type industrial/chemical production processes) and the above mentioned linear approach can be followed leading to a linear (approximate) model. However when essential nonlinear dynamical phenomena are involved and the user needs to capture this dynamics in the model, it is much harder to come up with generic black-box techniques for identification. Although there are interesting attempts to capture the nonlinear phenomena in (black-box) model structures as Wiener and/or Hammerstein models, Bai [1998], Zhu [2002], and linear parameter-varying (LPV) models Verdult and Verhaegen [2002], Tóth et al. [2007], Tóth [2008], van Wingerden and Verhaegen [2009], information on the underlying physical structure of the nonlinearities is very often required for selection of an appropriate model structure.

In some processes it is desirable to capture the real underlying nonlinear dynamic structure of the process in order to make reliable long-term predictions. First-principles model then provide the structure of the model, while incorporated (physical) parameters have to be estimated on the basis of experimental data. Especially in situations where the first principles models are given by partial differential

⋆ The TU Delft authors acknowledge financial support from the Integrated Systems Approach to Petroleum Production (ISAPP) program, which is jointly sponsored by Shell International E&P, TNO and Delft University of Technology.

equations (pde's), the required step of discretizing the equations in space and time generally leads to complex models with a large number of states and possibly also a large number of unknown (physical) parameters. For an interesting example of this situation in a problem of (oil) reservoir engineering, the reader is referred to Jansen et al. [2008], where a model is handled with a number of states and parameters exceeding the order of 10^5.

Identifying extremely large number of parameters from measurement data leads to serious problems, and at least it leads to the question which model properties can be reliably estimated from the available measurement data. From a model-based operations point of view (monitoring, control, optimization) it makes sense to limit the complexity of an identified model to a level where the model can be reliably validated from data. If not, the parameter estimates might be highly determined by the -random- experiment that is done (overfit) leading to unreliable model predictions. In identification this problem is addressed by the notion of identifiability.

In this paper the notion of identifiability will be evaluated in the scope of the high-complexity type of processes discussed above. Our argument will be that having an (locally) identifiable model structure will not be sufficient to provide reliable parameter estimates in large scale physical model structures. Methods will be presented that allow to reduce the parameter space to limited dimension, while being able to reliably estimate the reduced parameters and maintaining their physical interpretation. To this end the qualitative notion of (local) identifiability (with a yes/no answer) is generalized to a quantitative notion, removing that parameter subspace from the parametrization that can only be estimated with excessively large variance.

2. IDENTIFIABILITY - THE STARTING POINT

The notion of identifiability refers -roughly speaking- to the question whether parameter changes in the model can be observed in the model output signal (output identifiability) or in the model's input-output map or 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]. In its essence, identifiability properties are global properties, i.e. holding for the full parameter space. However restricting attention to a local analysis is often the only situation that is feasible in terms of computational complexity. As a result we will focus on local properties of (output) identifiability only.

Consider a nonlinear dynamical model that generates output predictions according to [1]:

$$\hat{\mathbf{y}} = h(\mathbf{u}, \theta; x_0), \tag{1}$$

where $\hat{\mathbf{y}}$ is a prediction of $\mathbf{y} := \begin{bmatrix} y_1^T & \dots & y_N^T \end{bmatrix}^T$ denoting output signal measurements $y_k \in \mathbb{R}^p$ stacked over time, $\theta \in \Theta \subset \mathbb{R}^q$ the parameter vector, $\mathbf{u} := \begin{bmatrix} u_1^T & \dots & u_N^T \end{bmatrix}^T$ the input vector $u_k \in \mathbb{R}^m$ stacked over time, and x_0 the initial state vector. Since the model (1) is parameterized it represents an input/output model structure.

The definition of local identifiability now is given as follows(Grewal and Glover [1976]):

Definition 1. An input/output model structure $h(\theta, \mathbf{u}; x_0) : \Theta \to \mathcal{H}$ is called locally identifiable in $\theta_m \in \Theta$ for a given $\mathbf{u}$ and x_0, if for all θ_1, θ_2 in the neighborhood of θ_m holds that

$$\{h(\mathbf{u}, \theta_1; x_0) = h(\mathbf{u}, \theta_2; x_0)\} \Rightarrow \theta_1 = \theta_2.$$

If we linearize the nonlinear process dynamics around a chosen operating point or trajectory, a linear dynamical system results. This system can be modelled by an LTI input-output model, represented by the transfer function G, leading to an output predictor

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

with q the shift operator $q u_k = u_{k+1}$.

In general identifiability questions are considered qualitatively, i.e. deciding whether a model structure is either identifiable or not. The tests required for this evaluation 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]. 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 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 Vajda et al. [1989] principal component analysis was applied to determine which parameters can be identified. Assessing identifiability can also be done a posteriori, after the identification of all parameters, by evaluating the parameter variance, see e.g. Hjalmarsson [2005].

3. TESTING LOCAL IDENTIFIABILITY IN IDENTIFICATION

3.1 Introduction

In a model identification framework we consider parameter estimation methods that are characterized by minimizing a cost function $V(\theta)$:

$$V(\theta) := \frac{1}{2} \boldsymbol{\epsilon}(\theta)^T P_v^{-1} \boldsymbol{\epsilon}(\theta), \tag{2}$$

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

$$\boldsymbol{\epsilon}(\theta) = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - h(\theta, \mathbf{u}; x_0), \tag{3}$$

where $\mathbf{y}$ denotes the measured output sequence and $\hat{\mathbf{y}}$ the predictor sequence, and P_v is a weighting matrix that could represent (an estimate of) the covariance matrix of the noise sequence $\mathbf{v}$ that is supposed to act on the measured output. In the rest of the chapter the shorthand notation $\hat{\mathbf{y}}(\theta)$ is used to indicate $h(\mathbf{u}, \theta; x_0)$.

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

$$\frac{\partial V(\theta)}{\partial \theta} = \frac{\partial \boldsymbol{\epsilon}(\theta)^T}{\partial \theta} P_v^{-1} \boldsymbol{\epsilon}(\theta) = -\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} P_v^{-1} \left(\mathbf{y} - \hat{\mathbf{y}}(\theta) \right). \tag{4}$$

[1] Without loss of generality we restrict attention to predictors that are not dependent on output measurements y, whch in an LTI-setting is referred to as Output Error predictors.

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

$$\frac{\partial^2 V(\theta)}{\partial \theta^2} = \frac{\partial \boldsymbol{\epsilon}(\theta)^T}{\partial \theta} P_v^{-1} \left(\frac{\partial \boldsymbol{\epsilon}(\theta)^T}{\partial \theta} \right)^T + S$$
$$= \frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} P_v^{-1} \left(\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} \right)^T + S, \qquad (5)$$

where S denotes the second-order information in $\frac{\partial^2 V(\theta)}{\partial \theta^2}$. The Jacobian and Hessian are for a given θ and a given operating point (given by $\mathbf{u}$ and x_0). Parameter estimation now consists in finding the parameter estimate as a minimizing argument of the cost function $V(\theta)$

$$\hat{\theta} := \arg\min_{\theta} V(\theta). \qquad (6)$$

At $\hat{\theta}$ the cost function $V(\theta)$ is minimized and the Jacobian (4) at $\hat{\theta}$ is zero, i.e. $\frac{\partial V(\theta)}{\partial \theta} = 0$ at $\hat{\theta}$.

3.2 Analyzing local identifiability in $\hat{\theta}$

Local identifiability in $\hat{\theta}$ is generally evaluated by the test whether the optimization problem (6) has a unique solution in the parameter space. By locally approximating the cost function $V(\theta)$ by a quadratic function [2] (and thus neglecting the second order term S in (5)), uniqueness of $\hat{\theta}$ is guaranteed if the Hessian at $\hat{\theta}$ is positive definite, i.e. $\frac{\partial^2 V(\theta)}{\partial \theta^2} > 0$ at $\hat{\theta}$, which in this case is equivalent to rank $\frac{\partial^2 V}{\partial \theta^2} = q$. This is a sufficient condition for local identifiability in $\hat{\theta}$.

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

$$\frac{\partial^2 V(\theta)}{\partial \theta^2} = U \Sigma V^T = [\, U_1 \; U_2 \,] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix},$$

where matrices U and V are unitary matrices, $\Sigma_1 = \mathrm{diag}(\sigma_1, \ldots, \sigma_p)$ with $\sigma_1 \geq \cdots \geq \sigma_p$.
If $p = q$ then identifiability is confirmed. If $p < q$ then the column space of U_1 represents the subspace of the parameter space that is identifiable, and the column space of 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 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 a reparametrization of the model structure by defining a reduced order parameter $\rho \in \mathbb{R}^p$ defined by

$$\theta = U_1 \rho \qquad (7)$$

leading to an identifiable model structure in the parameter ρ. The attractive feature of this mapping is that it allows to identify ρ while the estimated result $\hat{\rho}$ can be uniquely interpreted in terms of the original physical parameters θ through the mapping (7). The limitation of the approach is of course that only *linear* parameter transformations are considered.

[2] This is achieved by approximating $\hat{\mathbf{y}}(\theta)$ with a first-order Taylor expansion around $\hat{\theta}$.

3.3 Approximating the identifiable parameter space

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 correspond to directions in the parameter space in which the variance is (very) large. The Hessian evaluated at $\hat{\theta}$ is connected to the variance of $\hat{\theta}$, since for the Gaussian case (and provided that $\hat{\theta}$ is a consistent estimate) it follows that

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

with J the Fisher information matrix

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

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, as was also addressed in Vajda et al. [1989] for nonlinear parameter mappings, and in Lund and Foss [2008] for single parameters.

The essential information on the SVD of the Hessian is now obtained from:

$$\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} P_v^{-\frac{1}{2}} = [\, U_1 \; U_2 \,] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} \qquad (9)$$

where the separation between Σ_1 and Σ_2 is chosen in such a way that the singular values in Σ_2 are considerably smaller than those in Σ_1.
If we now reparametrize the model structure by employing the reduced parameter ρ determined by $\theta = U_1 \rho$, we have realized a model structure approximation, in which the parameters to be identified are well identifiable with a limited variance and the physical interpretation of the parameters remains untouched. The singular vectors that occur as the columns in U_1 actually can be seen as basis functions in the parameter space.

With the SVD (9) it follows that the sample estimate of the covariance matrix of $\hat{\theta}$ becomes:

$$cov(\hat{\theta}) = \begin{cases} [\, U_1 \; U_2 \,] \begin{bmatrix} \Sigma_1^{-2} & 0 \\ 0 & \Sigma_2^{-2} \end{bmatrix} \begin{bmatrix} U_1^T \\ U_2^T \end{bmatrix} & \text{for } \mathrm{trace}(\Sigma_2) > 0 \\ \infty & \text{for } \Sigma_2 = 0 \end{cases} \qquad (10)$$

while the sample estimate of the covariance matrix of the reparametrized parameter estimate $U_1 \hat{\rho}$ is given by

$$cov(U_1 \hat{\rho}) = U_1 \Sigma_1^{-2} U_1^T. \qquad (11)$$

This shows that if $\Sigma_2 = 0$ there is no benefit of the reparametrization in terms of variance of the estimated parameter $\hat{\theta}$. However if nonzero singular values are discarded in Σ_2, i.e. if $\mathrm{trace}(\Sigma_2) > 0$ then

$$cov(\hat{\theta}) > cov(U_1 \hat{\rho})$$

showing a covariance that is reduced by the reparametrization. This reduction is particularly interesting if Σ_2 contains a (very) large number of small singular values.

4. PARAMETER SCALING IN IDENTIFIABILITY

The notions of identifiability are defined in such a way that the result is independent of any particular scaling of parameters. A scaling happens when choosing a particular physical unit for a particular parameter, as e.g. using either [nm] or [m] as measure of distance. While the analysis and test in section (3.2) is independent of parameter scaling, this scaling does influence the analysis of of section (3.3) where the numerical values that occur in Σ_1, Σ_2 vary with parameter scaling.

It appears that in the approach presented above the absolute variance of parameters is used as a measure for selection through the Fisher matrix. A scaling invariant analysis results if instead we consider the relative variance of parameters, i.e.

$$cov\ (\Gamma_{\hat{\theta}}^{-1}\hat{\theta})$$

where $\Gamma_{\hat{\theta}} = \text{diag}\left(\,|\hat{\theta}_1|\ \ldots\ |\hat{\theta}_q|\,\right)$. This motivates the analysis of a scaled Hessian

$$\Gamma_{\hat{\theta}}\ \frac{\partial^2 V(\theta)}{\partial \theta^2}\bigg|_{\hat{\theta}}\ \Gamma_{\hat{\theta}}, \tag{12}$$

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

$$\tilde{J} = \mathbb{E}\left[\Gamma_{\hat{\theta}}\ \frac{\partial^2 V(\theta)}{\partial \theta^2}\bigg|_{\hat{\theta}}\ \Gamma_{\hat{\theta}}\right]. \tag{13}$$

Note that the evaluation of the relative variance of parameter estimates for model structure selection is also done in classical methods when considering the standard deviation of an estimated parameter related to the parameter value itself, see e.g. Ljung [1999] and Hjalmarsson [2005]. However usually the analysis is performed for parameters separately (e.g. is zero included in the parameter confidence interval?). In the analysis presented here linear combinations of parameters are evaluated, thus focussing on the ratio between the lengths of the principle axes of the uncertainty ellipsoids representing the parameter confidence bounds for $\hat{\theta}$.

5. COST FUNCTION MINIMIZATION IN IDENTIFICATION

If we iteratively solve for a parameter estimate $\hat{\theta}$ by minimizing a cost function $V(\theta)$, the general update rule in step m of a Newton-type algorithm is given by

$$\hat{\theta}_{m+1} = \hat{\theta}_m - \gamma \left(\frac{\partial^2 V}{\partial \theta^2}\right)^{-1} \frac{\partial V}{\partial \theta}, \tag{14}$$

where γ denotes a scalar damping factor. Note that in this expression the partial derivatives are evaluated in the local parameter $\hat{\theta}_m$. In contrast with the analysis in the previous section this local parameter does not necessarily reflect a (local) minimum of the cost function V.

If we consider the prediction error cost function as used before, then for the model structure considered and after linearization of $\hat{\mathbf{y}}(\theta)$ around parameter θ_m the update rule becomes

$$\hat{\theta}_{m+1} = \hat{\theta}_m + \gamma \left(\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta}\left(\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta}\right)^T\right)^{-1} \frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta}\left(\mathbf{y} - \hat{\mathbf{y}}(\theta)\right). \tag{15}$$

where P_v is considered identity for notational simplicity. The parameter update (15) is actually a Gauss-Newton step, employing a first order Taylor expansion of $\hat{\mathbf{y}}(\theta)$ around θ_m, similar to the approximation in section 3.3.

If the model structure is not identifiable in $\hat{\theta}_m$ the matrix inverse in (15) will not exist. Although this is often indicated as a serious problem for iterative optimization algorithms it can simply be overcome by restricting the update rule to make steps only in that part of the parameter space that does influence the output predictor, see e.g. McKelvey et al. [2004]. This actually comes down to utilizing the pseudo-inverse of the Jacobian in (15), on the basis of the SVD:

$$\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} = [\,U_1\ U_2\,] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} \tag{16}$$

with $\Sigma_1 \in \mathbb{R}^{p\times p}$. If $\Sigma_2 = 0$, the update rule for the Gauss-Newton iteration can then be replaced by

$$\hat{\theta}_{m+1} = \hat{\theta}_m + \gamma U_1 \Sigma_1^{-1} V_1^T (\mathbf{y} - \hat{\mathbf{y}}(\theta)).$$

The algorithm updates the parameter only in the subspace that is determined by the column space of U_1, being the locally identifiable subspace of the parameter space in the local point $\hat{\theta}_m$.

Similar to the analysis in the previous sections the rank reduction of the Jacobian, as represented in (16) can of course be enforced if the SVD shows a large number of small singular values in Σ_2, and the Jacobian is approximated by setting $\Sigma_2 = 0$.

A similar approach of Jacobian reduction is employed in the fully parametrized state-space model identification using so-called data-driven local coordinates of McKelvey et al. [2004] as well as in subspace identification Verdult [2002], where search directions are chosen to be orthogonal to the tangent space of the manifold representing equivalent models. See also Wills and Ninness [2008] for a further comparison of methods. If the main interest of the modelling procedure is to identify (linear) system dynamics, these approaches are attractive as they simply use the parameters as vehicles to arrive at an appropriate system model. However, in this paper we aim at preserving the physical interpretation of the parameters and therefore are more focussing on the uniqueness of the parameters estimates in order to obtain reliable long-term (non-linear) model predictions.

6. A BAYESIAN APPROACH

Lack of identifiability of a model structure and the subsequent non-uniqueness of parameters that are estimated on the basis of measurement data, can be dealt with in different ways. One way is to reduce the parameter space in the model structure, as indicated in the previous sections. Alternatively additional prior information can be added to the identification problem. In those situations where a parameter estimate may not be uniquely identifiable from the data, a regularization term can be added to the cost function that takes account of prior knowledge of the parameters to be estimated. In this setting an alternative (Bayesian) cost function is considered:

$$V_p(\theta) := V(\theta) + \frac{1}{2}(\theta - \theta_p) P_{\theta_p}^{-1} (\theta - \theta_p), \tag{17}$$

where the second term represents the weighted mismatch between the parameter vector and the prior parameter vector θ_p with covariance P_{θ_p}. When again the model output $\hat{\mathbf{y}}(\theta)$ is approximated using a first-order Taylor expansion around θ_p, the Hessian of (17) becomes:

$$\frac{\partial^2 V_p(\theta)}{\partial \theta^2} = \frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} P_v^{-1} \left(\frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} \right)^T + P_{\theta_p}^{-1}. \tag{18}$$

Since $P_{\theta_p}^{-1}$ is positive definite by construction and the first term is positive semi-definite, the Hessian has full rank and the parameter estimate

$$\hat{\theta}_{bayes} = \arg\min_{\theta} V_p(\theta)$$

is unique. This uniqueness is guaranteed by the prior information that has been added to the problem. Formally there can still be lack of identifiability, however it is not any more reflected in a non-unique parameter estimate. A consequence of this approach is that the obtained parameter estimate may be highly influenced by the prior information, and less by the measurement data.

The covariance matrix of the Bayesian parameter estimate can also be analyzed using the classical prediction error theory, see Ljung [1999]. Under ideal circumstances (consistent estimation and $\theta_p = \theta_0$ (!)) it can be shown that

$$cov(\hat{\theta}_{bayes}) = \left[\mathbb{E} \left. \frac{\partial^2 V_p(\theta)}{\partial \theta^2} \right|_{\theta_0} \right]^{-1}. \tag{19}$$

In other words, the inverse of the Hessian of the identification criterion remains to play the role of (sample estimate of) the parameter covariance matrix, and the same considerations as discussed in the earlier sections can be applied to the SVD analysis of this Hessian. By appropriately operating on the expression for the Hessian (18), it can be shown that a relevant SVD analysis for dimension reduction can now be applied to

$$P_{\theta_p}^{\frac{T}{2}} \frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} P_v^{-\frac{1}{2}},$$

which in Tavakoli and Reynolds [2009] is referred to as the dimensionless sensitivity matrix.

It may be clear that the parameter estimate becomes highly dependent on the prior information, and that bias will occur when the parameter prior θ_p is not correct.

It has to be noted that this Bayesian approach is typically followed when using sequential estimation algorithms for joint parameter and state estimation, as in Extended Kalman Filters and variations thereof, such as the Ensemble Kalman Filter, see e.g. Evensen [2007].

7. EXAMPLE FROM RESERVOIR ENGINEERING

Petroleum reservoir engineering is concerned with maximizing the oil and gas production from subsurface reservoirs. A common way to increase the production is to inject water in the reservoir via injection wells to drive the oil via production wells towards the subsurface. However, due to strong heterogeneities in the porous reservoir rock the resulting oil-water front is not progressing uniformly and a large part of the oil is bypassed and not produced. This can be partly counteracted by manipulating the injection and production settings in the wells. The dynamic control strategy that maximizes the production is calculated based on a model of the reservoir.

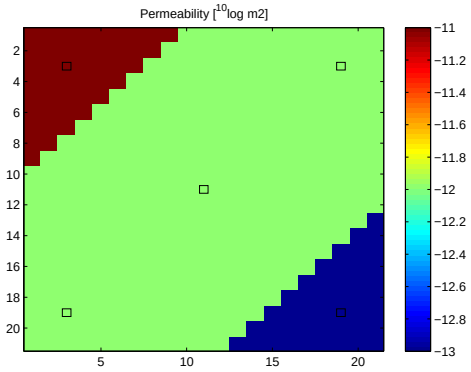

Fig. 1. Permeability distribution (top view) for MIMO example. Rectangles indicate well positions.

A reservoir model describes the fluid flow in a porous medium in time and space. The model basically is determined by a non-linear pde, which after discretization in space and time yield the following state-space ordinary differential equation in discrete time

$$\mathbf{p}(k+1) = \mathbf{A}(\boldsymbol{\theta})\mathbf{p}(k) + \mathbf{B}\mathbf{u}(k), \quad \mathbf{p}(0) = \mathbf{p}_0 \tag{20}$$

$$\mathbf{y}(k) = \mathbf{C}\mathbf{p}(k), \tag{21}$$

A model typically contains 10^5 to 10^6 states in $\mathbf{p}$, which are composed of the fluid pressure and fluid saturations in each grid block. The input variables $\mathbf{u} \in \mathbb{R}^m$ denote control settings such as injection or production rates or pressures in grid blocks containing wells. The output variables $\mathbf{y} \in \mathbb{R}^p$ denote flow rates in grid blocks containing wells. In the most simple model, the parameters represent the permeability in each grid block which determines how easily fluids flow through the porous medium. Because the permeability in each grid block directly influences the flow, it is vital to estimate this parameter vector using the available measurements in order to obtain reliable model predictions and control strategies.

The simple example that we consider here reflects a 2D reservoir with five wells in a characteristic five-spot pattern, indicated in Figure 1 by grey squares. There is one injection well in the center and four production wells in the four corners. The reservoir model is discretized in 441 grid blocks and therefore also has 441 parameters. The permeability distribution consists of three zones: the upper left corner has a high permeability, the lower right corner a low permeability, and the intermediate zone an intermediate permeability. As inputs we use the injection flow rate in the injection well and four bottom hole pressures in the production wells. The input signals $\mathbf{u}$ are depicted in Figure 2. As measurements we have used the oil and water flow rates in the four production wells, where we note that water breakthrough has occurred in all wells.

In our identifiability analysis we have chosen $\boldsymbol{\Gamma}_{\hat{\theta}} = \text{diag}(^{10}\log \boldsymbol{\theta})$ and $\mathbf{P}_v^{-\frac{1}{2}} = \mathbf{I}$ in our SVD analysis of the expression

$$\boldsymbol{\Gamma}_{\hat{\theta}} \frac{\partial \hat{\mathbf{y}}(\theta)^T}{\partial \theta} P_v^{-\frac{1}{2}}. \tag{22}$$

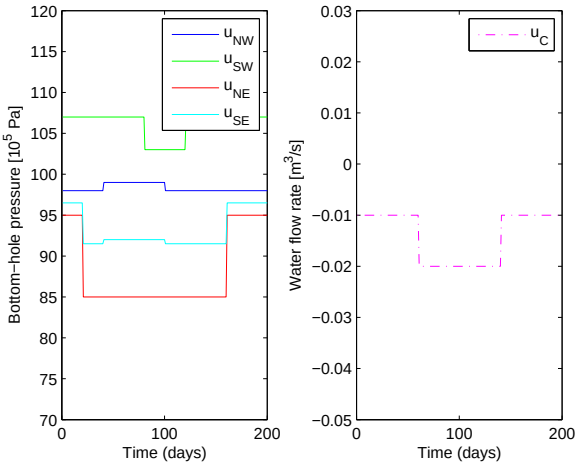

Fig. 2. Input signals as function of time that are used to excite the two-phase reservoir model. Liquid flow rates (right) and bottom-hole pressures (left).

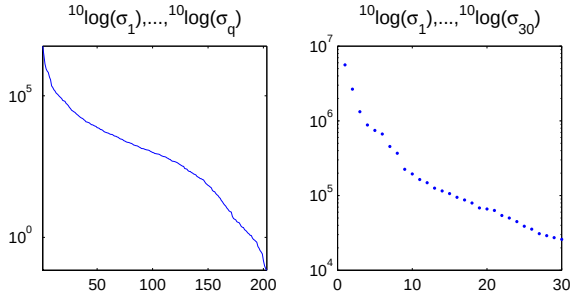

Fig. 3. All singular values (left) and 30 largest singular values (right) of (22) using the permeability distribution depicted in Figure 1.

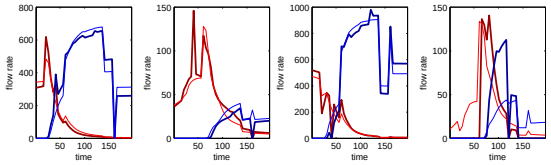

Fig. 4. Measured and predicted water (blue) and oil (red) flow rates.

As can be clearly seen the singular values in Figure 3 drop steeply. Since the identifiable parametrization partly depends on the parameter value we use an iterative procedure. Starting from an initial parameter vector an (locally) identifiable parametrization is determined. With this parametrization a new parameter vector is estimated, and the procedure is repeated. The iteration is stopped when no substantial improvement of the cost function is obtained.

Perfect measurements $\mathbf{y}$ are generated by simulating the two-phase reservoir model for 200 days in the in-house reservoir simulator with the so-called real permeability distribution (see left plot in Figure 5), initial pressure $\mathbf{p}_0 = 100 \times 10^5$Pa and initial oil saturation $\mathbf{s}_0 = 0.2$ in every grid block. As input we have used the pressures in the production wells and the injection flow rate in the injection well (see Figure 2 for the signals). As measurements we have used the oil and water flow rates in the four production wells (see Figure 4 for the signals).

As initial guess a homogeneous permeability distribution is chosen with the value $\boldsymbol{\theta}_{\text{init}} = -13.3$ which is equivalent to a permeability value of $5 \times 10^{-13}\text{m}^2$. This permeability distribution is depicted in the middle of Figure 5. The corresponding value of the objective function is $V(\boldsymbol{\theta}_{\text{init}}) = 135$. Based on $\boldsymbol{\theta}_{\text{init}}$ the model structure is approximated using the SVD of (22) keeping only the first 15 singular values. To estimate the grid block permeability we have used the Gauss-Newton update rule. In this example the best result is obtained in case the model structure is approximated after each update. The estimate has converged after 30 iterations to the permeability distribution depicted in the right of Figure 5. The value of the objective function has decreased to $V = 5.93$. From the estimated permeability distribution we see that the largest changes have occurred in the grid blocks which are penetrated by production wells. Although the real permeability distribution is not recognizable anymore, the flow relevant features are apparently estimated since the objective function has decreased significantly, and the fluid flow rates predicted by the model according to Figure 4 are very well matching the measurements.

The example shows that the premeability is only identifiable in the grid blocks that are in the direct neighborhood of wells.

8. CONCLUSIONS

The question whether a large scale (nonlinear) physical model structure is identifiable, is usually considered in a qualitative way. In this chapter 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 chapter this question has been addressed in a prediction error setting. The analysis has been related to Bayesian estimation, and has been illustrated for an example from oil reservoir engineering, in which lack of identifiability has been illustrated.

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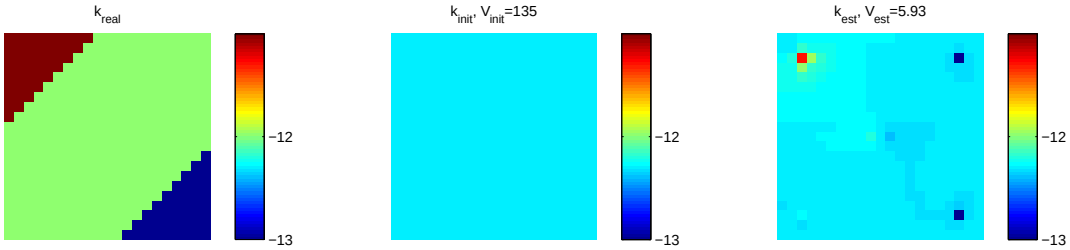

Fig. 5. Real permeability distribution (left), initial permeability distribution (middle) and estimated permeability distribution (right) obtained with the identifiable parameterization in a two-phase reservoir model.

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