State Estimation Analysed as Inverse Problem

Luise Blank

NWF I - Mathematik, University of Regensburg, Germany luise.blank@mathematik.uni-regensburg.de

Summary. In dynamical processes states are only partly accessible by measurements. Most quantities must be determined via model based state estimation. Since in general only noisy data are given, this yields an ill-posed inverse problem. Observability guarantees a unique least squares solution. Well-posedness and observability are qualitative behaviours. The quantitative behaviour can be described using the concept of condition numbers. which we use to introduce an observability measure. For the linear case we show the connection to the well known observability Gramian. For state estimation regularization techniques concerning the initial data are commonly applied in addition. However, we show that the least squares formulation is well-posed, avoids otherwise possibly occuring bias and that the introduced observability measure gives a lower bound on the conditioning of this problem formulation.

Introducing possible model error functions we leave the finite dimensional setting. To analyse in detail the influence of the regularization parameters and of the coefficients of the model, we study, as a start, linear state equations as constraints, which appear nearly always as a subproblem of the nonlinear case. We show that state estimation formulated as optimization problem omitting regularization of the initial data leads to a well-posed problem with respect to L_2 - and L_{∞} - disturbances. If the introduced measure of observability is low, the arising condition numbers with respect to the L_2 norm can be arbitrarily large. Nevertheless, for the probably in praxis more relevant L_{∞} -norm perturbations yield errors in the initial data bounded independently of the system matrix.

1 Introduction

In application the state of a process has to be estimated given noisy data over a past time horizon. These data correspond only to a few state functions, so called output functions. The coupling with all remaining states is given by model equations. This inverse problem is in general ill-posed, since the measurements are noisy and the corresponding continuous signals do not fulfill the model equations. Hence, the existence requirement for well-posedness in the sense of Hadamard is violated. Considering the least squares solution the uniqueness is guaranteed by the observability of the system given by the model equation. The third requirement of well-posedness, namely stability, depends crucially on the norms, which are chosen to measure the disturbances. For state estimation stability may be present in some cases. However, as soon as model error functions are introduced

this is not any longer true. Additional regularization is required. Assuming now well-posedness, there arises the next question: how 'well' does the solution behave in case of disturbances? The corresponding question for the system itself is, how 'well' is the system observable?Both questions ask for the relation of the output error to the input error. Condition numbers is a general formulated mathematical concept for operators answering this question. Hence, we use this concept to derive a definition of observability measure. Alltogether, this paper discusses for state estimation the well-posedness of the regularized least squares problem formulation, the conditioning, i.e. error propagation, and the influencing observability measure. For all three issues the chosen norms play an important role.

The structure of the paper is the following. First we resume the definitions of well-posedness, the possibilities to overcome ill-posedness and the concept of condition numbers. We discuss for the system observability and introduce an observability measure based on condition numbers. For linear model equations and the L_2 -norm this observability measure depends on the observability Gramian. Then the well-posedness of the least squares formulation for linear estimation is shown requiring only observability.Additional regularization of the initial value yields unnecessary bias. In the following section we extend the model equations linearly by possible model error functions. The least squares problem formulation, now necessarily regularized with respect to the error functions, gives an optimization problem, for which we state the first order necessary condition. Then we restrict the analysis to linear state equations omitting inequality constraints. They appear usually as subproblems solving the nonlinear problem and their analysis enhances already some of the main features we face also for the nonlinear case. In particular, we study the influence of the measure of observability and of the regularization parameter. Omitting regularization of the initial data we derive well-posedness for the optimization formulation with respect to the L_2 -norm and with respect to the L_{∞} -norm. However, while for one state only we see that the problem is well-conditioned with respect to the L_{∞} -norm, a low observability measure may result into an ill-conditioned problem with respect to the L_2 -norm independent of the regularization parameter. In the last section we draw conclusions and emphasize the issue of the appropriate choice of norms concerning data errors and state errors.

2 Well-Posedness, Condition Number and Observability Measure

Typically the noisy measurements $z(t_i) \in \mathbb{R}^{n_y}$ at discrete times are preprocessed. Most algorithms are based on the assumption to have an underlying function corresponding to the discrete data, e.g. for many filtering techniques the Fourier transformation is used at some stage. Hence, it is appropriate to assume a preprocessing of the data on a horizon $[t_0, t_0 + H]$ to a still noisy function $z \in L_2([t_0, t_0 + H], \mathbb{R}^{n_y})$. These data z correspond to a few states, called output functions which we denote with y . The output functions y are coupled with all states x and their initial values $x_0 = x(t_0) \in \mathbb{R}^{n_x}$ by model equations. Usually

the number of output functions n_y is far less than the number of state functions n_x . Given the model equations one can determine from the initial values the states and therefore the outputs. Hence they define an operator $K: x_0 \to y$. In general we have $z \notin \mathcal{R}(K)$ (the range of K). This violates the first condition of well-posedness in the sense of Hadamard [8]:

2.1 Ill-Posed Problems, Regularization and Condition Numbers

Definition 1. *Given an operator* $K : X \to Y$ *where* X and Y are normed spaces, *then the equation* $Kx = y$ *is well-posed in the sense of Hadamard iff*

1. Existence: there exists for all $y \in Y$ *a solution* $x \in X$ *; (K surjective).*

- 2. Uniqueness: there is at most one solution $x \in X$; (K injective).
- *3. Stability:* x *depends continuously on* y*, i.e.*

 $||Kx_n - Kx||_{\mathbf{Y}} \to 0 \Rightarrow ||x_n - x||_{\mathbf{X}} \to 0;$ (*K*⁻¹ *continuous*).

The equation is ill-posed if one of these properties does not hold.

It is important to specify the spaces as well as the topologies of the spaces, i.e. the norms $\|\cdot\|_{\mathbf{X}}$ and $\|\cdot\|_{\mathbf{Y}}$. The problem can be well-posed using one set of norms and ill-posed in another set of norms. If the problem is ill-posed there are several remedies, of which we recall only some relevant in our context. Assume that X and Y are Hilbert-spaces (i.e. there exists a scalar product; e.g. the space L_2) and $K: X \to Y$ is linear and compact then x is called *least-squares solution* (best fit) if x is the solution of $\min_{\mathbf{x} \in \mathbf{X}} \|Kx - z\|_{\mathbf{Y}}$. Moreover, it holds: x is the least squares solution if and only if the *normal equation* $K^*Kx = K^*z$ holds, where K^* denotes the adjoint operator. In case of a finite-dimensional space X this ansatz overcomes the failure of existence. Uniqueness is not necessarily an issue in our context since we require observability of the system given by the model equations (see later). However, otherwise one can use the Moore-Penrose inverse, also called *generalized inverse*, which is the least squares solution of minimal norm $[8]$, if there exists a least squares solution. For finite-dimensional X the generalized inverse is given by $K^{\dagger} := (K^*K)^{-1}K^*$. However, the generalized inverse does not overcome the lack of continuity in general. Regularization techniques have to be applied. Here, we can distinguish roughly speaking three kinds of approaches, namely the Tikhonov regularization, which we consider here, iterative regularization methods and regularization by discretization (projection). An application of the latter in state estimation can be found i.e. in [3]. Tikhonov regularization shifts the spectrum of K∗K and leads to the *regularized generalized inverse* $R_d := (dI + K^*K)^{-1}K^*$, which is bounded, with a regularization parameter $d > 0$. Solving $R_d x = z$ is equivalent to the minimization problem

$$
\min_{\mathbf{x}\in\mathbf{X}} \|Kx-z\|_{\mathbf{Y}}^2 + d\|x\|_{\mathbf{X}}^2.
$$

The operator R_dK should converge pointwise to the identity for $d \to 0$. Moreover, the choice of the regularization parameter d should give the best compromise between data and regularization error, i.e. let $||z - z^{\delta}|| \leq \delta$ and $x^{d,\delta} = R_d z^{\delta}$ then $||x^{d,\delta} - x|| \le ||R_d(z^{\delta} - z)|| + ||R_d z - x|| \le ||R_d||\delta + ||R_d z - x||$, should be minimal. The first term is called data error and the second regularization error.

This is a non trivial task but will not be discussed in this paper, instead we refer to the literature, e.g. [8].

Now let us assume that $Kx = y$ is a well-posed problem. Then K^{-1} exists and is bounded with respect to the chosen norms. That means, the equation is stable, which is a qualitative statement. The mathematical concept of condition number is quantitative. It measures the possible error propagation with respect to the absolute or relative error [7].

Definition 2. *Considering the problem given* y *determining the solution* x *of* $Kx = y$ *and let* $\|\tilde{y} - y\|_{\mathbf{Y}} \to 0$:

1. the absolute condition number is the smallest number $\kappa_{abs}(y) > 0$ *with* $\|\tilde{x} - x\|_{\mathbf{X}} = \|K^{-1}\tilde{y} - K^{-1}y\|_{\mathbf{X}} \le \kappa_{abs}(y)\|\tilde{y} - y\|_{\mathbf{Y}} + o(\|\tilde{y} - y\|_{\mathbf{Y}}),$

2. the relative condition number is the smallest number $\kappa_{rel}(y) > 0$ with $\|\tilde{x} - x\|_{\mathbf{X}} / \|x\|_{\mathbf{X}} \leq \kappa_{rel}(y) \|\tilde{y} - y\|_{\mathbf{Y}} / \|y\|_{\mathbf{Y}} + o\left(\|\tilde{y} - y\|_{\mathbf{Y}} / \|y\|_{\mathbf{Y}}\right).$

The problem is called well-conditioned if κ is small and ill-conditioned for large κ . For linear K we have

 $\kappa_{abs}(y) \leq \|K^{-1}\|_{\mathbf{Y}\to\mathbf{X}}$ and $\kappa_{rel}(y) \leq \|K\|_{\mathbf{X}\to\mathbf{Y}} \|K^{-1}\|_{\mathbf{Y}\to\mathbf{X}}$.

If K is a matrix, the condition number is defined as the latter namely $cond(K) :=$ $||K|| ||K^{-1}||$, where commonly the l_2 -norms are used.

2.2 Observability Measure

For state estimation on the horizon $[t_0, t_0 + H]$ the operator $K : x_0 \mapsto y$ is given by the *model equations*:

State equations:
$$
G\dot{x} - f(x, u, p) = 0, \quad x(t_0) = x_0
$$
 (1)

Output equations:
$$
y - Cx = 0
$$
 (2)

The system $(1)-(2)$ is called *observable*, if for any given u and p the initial state x_0 can be uniquely determined from the output y [11]. Hence, $K : x_0 \longmapsto y$ is injective for fixed u, p and K^{-1} exists on $\mathcal{R}(K)$. The space X is the finitedimensional space \mathbb{R}^{n_x} . Observability is the qualitative behaviour that a difference in the states shall be seen in the outputs. The observability measure shall quantify this statement, hence we consider

$$
||y - \tilde{y}|| \ge c||x_0 - \tilde{x}_0||
$$

or a relative measurement independent of the scaling

$$
||y - \tilde{y}|| / ||y|| \ge c||x_0 - \tilde{x}_0|| / ||x_0||.
$$

As larger c as better the observability measure. This suggest the use of the condition number $\kappa = 1/c$ of the problem given y determining the solution of $Kx_0 = y$. The evaluation of the conditioning is mentioned also in [1] in preference to the yes/no answer of observability.

Definition 3. The absolute and the relative measure of observability of x_0 are *defined as* $1/\kappa_{abs}$ *and* $1/\kappa_{rel}$. *The system is called well observable for* x_0 *, if* κ = 1/c *is small, and has a low observability measure for large* κ*.*

For linear model equations the corresponding operator K is affine. Let us first consider linear K, i.e. the model equations are linear and p and $u = 0$. Without loss of generality we consider in the rest of the paper only the case $t_0 = 0$. Thus we have with

$$
\dot{x} - Ax = 0, \quad x(0) = x_0, \quad y - Cx = 0 \tag{3}
$$

$$
\Rightarrow Kx_0 = Ce^{\mathbf{A}t}x_0 \tag{4}
$$

Choosing now as norm on Y the $L_2([0, H])^{n_y}$ -norm we obtain

$$
||Kx_0||_{L_2}^2 = x_0^T \int_0^H (e^{At})^T C^T C e^{At} dt x_0 = x_0^T \mathcal{G}(H)x_0
$$

where the matrix $\mathcal{G}(H) \in \mathbb{R}^{n_x \times n_x}$ is the known finite time observability Gramian (e.g. [6, 11, 12]).

Lemma 1. *Let the system be observable, then:*

a.) The observability Gramian $\mathcal{G}(H) = \int_0^H (e^{\mathbf{A}t})^T C^T C e^{\mathbf{A}t} dt \in \mathbb{R}^{n_x \times n_x}$ is sym*metric positive definite, and therefore invertible.*

b.) Let v be a normed real eigenvalue of A to an eigenvalue $\alpha \in \mathbb{R}$. Then $\|\mathcal{G}(H)\|_2$ *is large for large* α *and for a long horizon* [0, H], while $\|\mathcal{G}(H)^{-1}\|_2$ *is large if* $-\alpha$ *is large or* $||Cv||_{l_2}$ *is small or if the horizon is short.*

Proof: a.) Symmetry is obvious. Given $v \neq 0$ then $y(t) = Ce^{\mathbf{A}t}v \neq 0$ since the system is observable. Hence, $v^T G v = \int_0^H y^T(t)y(t) dt = ||y||^2_{L_2} > 0.$ b.) Let v and α fulfill the assumption, then

$$
v^T \mathcal{G} v = \|e^{\alpha t}\|_{L_2(0,H)}^2 \|Cv\|_{l_2}^2 = \frac{e^{2\alpha H} - 1}{2\alpha} \|Cv\|_{l_2}^2.
$$
 (5)

With $||\mathcal{G}||_2 = \max_{v \in \mathbb{R}^{n_x}} (v^T \mathcal{G}v) / (v^T v), ||\mathcal{G}^{-1}||_2 = \max_{v \in \mathbb{R}^{n_x}} (v^T v) / (v^T \mathcal{G}v)$ follows the assertion.

Using the l_2 -norm for $X = \mathbb{R}^{n_x}$ it follows for K:

$$
||K||_{l_2 \to L_2}^2 = \sup_{\mathbf{x}_0 \in \mathbb{R}^{n_x}} \frac{||Kx_0||_{L_2}^2}{||x_0||_{l_2}^2} = \sup_{\mathbf{x}_0 \in \mathbb{R}^{n_x}} \frac{x_0^T \mathcal{G} x_0}{x_0^T \mathcal{G} x_0} = ||\mathcal{G}||_2
$$
(6)

$$
\|(K\left|_{\mathcal{R}(K)}\right)^{-1}\|_{L_2\to L_2}^2 = \sup_{\mathbf{x}_0 \in \mathbb{R}^{n_x}} \frac{\|x_0\|_{L_2}^2}{\|Kx_0\|_{L_2}^2} = ||\mathcal{G}^{-1}||_2 \tag{7}
$$

For linear systems with not necessarily p and $u = 0$ we need to consider for the condition numbers $||K\tilde{x_0} - Kx_0||_{L_2}^2 = (\tilde{x_0} - x_0)^T \mathcal{G}(\tilde{x_0} - x_0)$. Hence, having $\sqrt{\|\mathcal{G}^{-1}\|_2}\|y-\tilde{y}\|_{L_2} \ge \|x_0-\tilde{x}_0\|_{L_2}$ for all x_0 , we can define for linear systems -like condition numbers for matrices- a observability measure independent of the state x_0 :

Definition 4. *The absolute, respectively the relative observability measure with respect to the* l_2 *and* L_2 *-norms for linear systems is given by* $1/\sqrt{||\mathcal{G}^{-1}||_2}$ respectively $1/\sqrt{cond(\mathcal{G})}$.

This definition is in agreement with the Gramian based measure in [13], where one considers a infinite horizon. There, several measures are proposed and compared, which are all rather based on the various tests for observability than motivated by error propagation.

Lemma 1 immediately shows that long horizons are better for observability reasons. It also reassures that the eigenvectors of system matrix A should not be close to the null-space of the output matrix C . For rapidly decaying systems it is confirmed that it is difficult to determine the initial value exactly, while for the forward problem K the value at the end point is sensitive to $\alpha \gg 0$.

2.3 State Estimation as a Least Squares Problem

Going back to the inverse problem of state estimation we obtain

Theorem 1. *For a observable system the problem formulation on* [0, H]

$$
\min \|y - z\|_{L_2}^2 + d\|x_0 - x_0^{ref}\|_{L_2}^2 \ s.t. \ \dot{x} - Ax = u, x(0) = x_0, y - Cx = 0 \tag{8}
$$

is well-posed for all $d \geq 0$ *, and the solution is given by*

$$
x_0 = (G(H) + dI)^{-1} \left[\int_0^H e^{\mathbf{A}^T t} C^T \{ z(t) - Ce^{\mathbf{A}t} \int_0^t e^{-As} u(s) \, ds \} \, dt + dx_0^{ref} \right]. \tag{9}
$$

Regularization of the initial data $(d \neq 0)$ *is not necessary, and leads to bias if inexact reference values are used.*

Proof: Setting $\hat{z} = z - C \int_0^t e^{\mathbf{A}(t-s)} u(s) ds$ we have

 $\min_{z} \|y - z\|_{L_2} + d\|x_0 - x_0^{ref}\|_{l_2}^2 = \min_{z} \|\hat{y} - \hat{z}\|_{L_2} + d\|x_0 - x_0^{ref}\|_{l_2}^2$ where \hat{y} fulfills the model equations with $\hat{u} = 0$. Then, dropping for convenience the $\hat{ }$ we have the equivalence of (8) to the normal equation:

 $(K*K + dI)x_0 = K^*z + dx_0^{ref}$ with $K^*z = \int_0^H e^{\mathbf{A}^T t} C^T z(t) dt$ since $(\xi_0, K^*y)_{l_2} =$ $(K\xi_0, y)_{L_2} = \xi_0^T \int_0^H (e^{At})^T C^T y(t) dt$. Hence $\mathcal{G} = K^*K$ which is invertible for observable systems, and we obtain (9) . Moreover, since $\mathcal G$ is finite-dimensional it has a bounded inverse. Therefore, (8) is a well-posed problem even for $d = 0$, i.e. without regularizing the initial value. Given a noise free signal z , there exists a unique x_0^{exact} s.t. $Kx_0^{exact} = z$. We obtain

$$
x_0 = x_0^{exact} + (\mathcal{G} + dI)^{-1} d(x_0^{ref} - x_0^{exact})
$$
\n(10)

which answers the question of bias.

(Remark: the result concerning the bias is not in contrast to the probabilistic ansatz leading to the Kalman filter, since there one would choose also $d = 0$ for noise free signals [10]. If one may wish to include a priori knowledge about a linear process appropriate priors and consequently possible choices for d with a small influence on the solution can be found e.g. in [5]. For $d = 0$ see also [6] for extension to time varying systems and the connection to the Kalman filter.)

While the least squares formulation is well-posed, it is not necessarily wellconditioned.

Corollary 1. *The condition number of (8) with* $d = 0$ *, i.e. of the least squares problem* $K^{\dagger} = \mathcal{G}^{-1} K^*$ *with respect to the* l_2 *and* L_2 *-norms obeys*

$$
\kappa_{abs} \geq ||(K|_{\mathcal{R}(\mathbf{K})})^{-1}||_{L_2 \to l_2}^2 = \sqrt{||\mathcal{G}^{-1}||_2} \quad \text{and} \quad \kappa_{rel} \geq \sqrt{cond(\mathcal{G})}.
$$

Proof: Let v be the normed eigenvector to the smallest eigenvalue of \mathcal{G} , then $\|\mathcal{G}^{-1}\|_2 = \|\mathcal{G}^{-1}v\|_2$. For $z(t) = kCe^{At}\mathcal{G}^{-1}v$ and $u = 0$ we have $x_0 = k\mathcal{G}^{-1}v$. Furthermore, $||z||_{L_2}^2 = k^2 ||\mathcal{G}^{-1}||_2$ and therefore $||x_0|| = ||z||_{L_2} \sqrt{||\mathcal{G}^{-1}||_2}$. With (6) and (7) the assertion holds.

Consequently, a low observability measure leads to an ill-conditioned least squares formulation, even though observability provides well-posedness. E.g. we may face large error propagation if the assumptions of Lemma 1b.) hold.

3 Inclusion of Model Error Functions

3.1 Optimality Conditions

 \overline{H}

In the following we include linearly possible model error functions w in the model equations. With this step we leave the finite dimensional setting. Considering only the least squares solution does not guarantee stability any longer, as the example of the signal $z(t) = \delta \sin \frac{n}{\delta} t$ with the model equations $\dot{x} = ax + w$ and $y = x$ shows for $n \to \infty$. Regularization with respect to w is necessary. As regularization parameters we employ now matrices instead of scalars. For the mathematical consideration it is at this point no issue to distinguish the given parameters p and the controls u . We summarize them to u . Equation (1) for the initial condition can be omitted, since it does not contain any information. Additional inequality constraints reflect safety constraints as well as model verification. Summarized we consider in the following the Tikhonov-type regularized least squares solution of:

$$
\min \int_{0}^{H} (y - z)^{T} Q(y - z) + w^{T} R_{w} w dt + ||D^{1/2}(x(0) - x_{0}^{ref})||_{l_{2}}^{2}
$$
 (11)

s.t.
$$
G\dot{x} - f(x, u) - Ww = 0
$$
, $y - Cx = 0$, $c(x, u) \ge 0$. (12)

Obviously, we can substitute y by Cx and reduce the system by y, the output equations and avoid Lagrange multipliers for these. In addition, setting up the necessary first order equations we see w can be eliminated by the Lagrange multiplier with resp. to the DAE's, namely $w = R_w^{-1} W^T \lambda$. This is a major reduction in size since $w(t)$ may be in \mathbb{R}^{n_x} . Defining $\overline{R} := WR_w^{-1}W^T$ we obtain the following *necessary conditions* (for details see [4], for the linear case without inequality constraints see [10], where also the connection to the Kalman filter is given):

$$
G\dot{x} - f(x, u) - R\lambda = 0 \tag{13}
$$

$$
-\frac{d}{dt}(G^T\lambda) - (\frac{\partial}{\partial x}f(x,u))^T\lambda + C^TQCx + (\frac{\partial}{\partial x}c(x,u))^T\nu = C^TQz
$$
 (14)

$$
(G^T \lambda)(0) = D(x(0) - x_0^{ref}) \quad \text{and} \quad (G^T \lambda)(H) = 0 \tag{15}
$$

$$
\nu^T c(x, u) = 0 \quad c(x, u) \le 0 \quad \nu \ge 0. \tag{16}
$$

In case of ODE's as state constraints with no regularization of the initial state, this yields $w \in H^1$, where H^1 denotes the Sobolev-space of weakly differentiable functions in L_2 , and $w = 0$ at the end points. If model error functions are present in all state equations, the Lagrange parameter λ can be eliminated too with $\lambda = R^{-1} (G\dot{x} - f(x, u))$. Then, the necessary conditions reduce to a second order DAE system with mixed boundary constraints for the state x only and the equations (16) for the inequality constraints.

3.2 Analysis for Linear ODE's

In the solution process for a nonlinear problem with inequality constraints nearly always optimization problems with linear model equations and without inequality constraints (or an equivalent linear equation system) appear as subproblems. Although for the linear case, in particular with regularization of the initial data, efficient methods as the Kalman filter are well established [10, 11], these methods and its extensions cannot be applied or do not perform sufficiently in the presence of nonlinearity and inequality constraints [9]. However, the study of linear model equations without inequality constraints enhances already some of the main features we face for the treatment of the optimization formulation of the nonlinear state estimation. The goal of the study here is to iluminate the influence of the eigenvalues of the system matrix, the influence of the observability measure and the influence of the regularization parameters. As a start we assume possible model error functions in all state equations. We consider the following problem:

$$
\min_{0} \int_{0}^{H} (Cx - z)^{T} Q(Cx - z) + w^{T} R_{w} w dt + ||D^{1/2}(x(0) - x_{0}^{ref})||_{l_{2}}^{2}
$$
 (17)
s.t. $\dot{x} - Ax - w = u$.

A detailed analysis of this problem and its results can be found in [4], where they are presented for $H = 1$ and $D = 0$. With a few modifications they can be extended to any $H > 0$. In this paper we summarize some of the main results. To study the properties we choose one of the following three equivalent formulation, which derive from elimination of the error function w using the state equation or from the necessary conditions eliminating the Lagrange parameter λ . The boundary value problem and its weak formulation are not only necessary but also sufficient condition, which is shown later (Theorem 4): *Optimization problem:*

$$
\min_{\mathbf{x}\in H^1} \left\{ \|Q^{\frac{1}{2}} \left(Cx - z \right)\|_{L_2}^2 + \|R^{-\frac{1}{2}} \left(\dot{x} - Ax - u \right)\|_{L_2}^2 + \|D^{\frac{1}{2}} (x(0) - x_0^{ref})\|_{L_2}^2 \right\}.
$$
\n(18)

Second order BVP:

$$
-R^{-1}\ddot{x} + (R^{-1}A - A^{T}R^{-1})\dot{x} + (A^{T}R^{-1}A + R^{-1}\dot{A} + C^{T}QC)x
$$

$$
= C^{T}Qz - R^{-1}\dot{u} - A^{T}R^{-1}u
$$
(19)

with boundary conditions $\dot{x}(0) - (A + RD)x(0) = u(0) - RDx_0^{ref}$ and $\dot{x}(H) - Ax(H) = u(H).$ *Weak Formulation:*

$$
\langle \dot{\zeta} - A\zeta, R^{-1} (\dot{x} - Ax) \rangle + \langle C\zeta, QCx \rangle + \zeta^T (0) D(x(0) - x_0^{ref}) \qquad (20)
$$

= $\langle C\zeta, Qz \rangle + \langle \dot{\zeta} - A\zeta, R^{-1}u \rangle$ for all $\zeta \in H^1$.

In the following we concentrate only on the case $D = 0$, i.e. on the least squares formulation without regularization of the initial data. Among other things we show its well-posedness. With regularization of the initial data this can be studied in the framework of Tikhonov regularization.

For one state function only $(A = \alpha, C = \delta, Q = q, R^{-1} = r)$ one can use the BVP to derive an explicit formula for the solution. Analysing this solution we obtain the following theorem.

Theorem 2

- 1. The regularized problem formulation (17) (with $D = 0$), *i.e.* given z deter*mining* x⁰ *and* w*, is well-posed.*
- *2. Small perturbation of* z *in the* L2*-norm may lead to large error propagation in the initial data* x_0 *independently of* r and q *if* −α *is large.*
- *3. For perturbations of* z *in the* L∞*-norm we have bounds for the errors in* x_0 *and* w *independently of* α *.*

For several state functions we use the weak formulation to show well-posedness. As a first step we again study first the case of one state function where observability is not an issue and extend then the result to several state functions. Let us define the symmetric bilinear form $a: H^1(0, H) \times H^1(0, H) \to \mathbb{R}$

$$
a(\zeta, x) = \langle \dot{\zeta} - A\zeta, R^{-1}(\dot{x} - Ax) \rangle + \langle C\zeta, QCx \rangle \tag{21}
$$

If $A, C \in \mathbb{R}$ then a is positive definite if $R^{-1}, Q > 0$. Hence it defines an operator $S: H^1(0, H) \longrightarrow (H^1(0, H))'$ with $(\zeta, S_x) := a(\zeta, x)$ and the weak formulation (20) is equivalent to $(\zeta, \mathcal{S}x) = \langle C\zeta, Qz \rangle + \langle \zeta - A\zeta, R^{-1}u \rangle$ for all $\zeta \in H^1$. We would like to remark that, not only for the well-posedness it is of interest to study the properties of $\mathcal S$ but also for the numerical solution approaches. If we use a Galerkin discretization of (17) then the properties of S govern to a large extend also the numerical method. For example the condition number of the discretization matrix is influenced by the condition number of S . Using methods of functional analysis one can show the following result in the case of one state function:

Theorem 3. S *is a linear isomorphism and with the real values* $A = \alpha, C = \delta$, $Q = q, R^{-1} = r$ *we have*

$$
\min(4r, q\delta^2) \le ||\mathcal{S}||_{H^1 \to (H^1)'} \le 2r \max(1, \alpha^2) + q\delta^2,\tag{22}
$$

$$
\frac{c(\alpha)}{q\delta^2} \le ||\mathcal{S}^{-1}||_{(H^1)' \to H^1} \le \max\left\{\frac{2}{r}, \frac{2\alpha^2 + 1}{q\delta^2}\right\},\tag{23}
$$

with $c(\alpha) \approx |\alpha|^{3/2} \sqrt{\frac{e^{2H}-1}{2(e^{2H}+1)}}$ *for large* $|\alpha|$ *. Hence for fixed regularization pa* $rameters \ r \ and \ q \ cond(\mathcal{S}) = ||\mathcal{S}||_{H^1 \to (H^1)'} ||\mathcal{S}^{-1}||_{(H^1)' \to H^1}$ *is bounded but tends to infinity with* $|\alpha| \to \infty$ *.*

The exact value of $c(\alpha) := || \exp(\alpha \cdot) ||_{H^1} / || \exp(\alpha \cdot) ||_{(H^1)'}$ is $c^2(\alpha) = \frac{(1+\alpha^2)(\alpha+1)^2(\alpha-1)^2(e^H-e^{-H})(e^{2\alpha H}-1)}{(2\alpha+1)(\alpha-1)^2(e^H-e^{-H})(e^{2\alpha H}-1)+4\alpha^3e^{-H}(e^{\alpha H}-e^H)^2}.$

Considering several state functions one has to take into account observability to show positive definiteness and herewith continuity and coercivity of a. We shortly sketch this step while refering for the other arguments to [4]. Given $a(x, x)=0$ then x is the solution of the system $\dot{x} - Ax \equiv 0$, $x(0) = x_0$ and $(y \equiv)Cx \equiv 0$. Since the system is observable $y \equiv 0$ yields $x_0 = 0$ and consequently $x \equiv 0$. Hence, $a(x, x) > 0$ for $x \neq 0$. Then continuity and coercivity of a yield

Theorem 4. For any $z, u \in L_2$ the solution x of the weak formulation (20) *determines the unique solution of the minimization problem (18).*

Hence for well-posedness only the question of stability has still to be answered. Using the Riesz representation theorem [2] and considering like for one state only and Lemma 1b.) the exponential function we obtain

Theorem 5. $S: H^1 \to (H^1)'$ is bounded, has a bounded inverse and

$$
0 < 2/\|R\| \le \|\mathcal{S}\|_{H^1 \to (H^1)'} \le 2\|R\|^{-1} \max(1, \|A\|^2) + \|C^T Q C\|,\tag{24}
$$

$$
\max\{c(\alpha)/\|C^TQCv\|_{l_2}\} \le \|\mathcal{S}^{-1}\|_{(H^1)'\to H^1}.\tag{25}
$$

for all normed $v \in \mathbb{R}^{n_x}$ *eigenvectors of* A *with real eigenvalue* α *. In (24) the lower bound is valid if there exists an* $\alpha^2 > 1$ *. Observability guarantees* $Cv \neq 0$ *.*

As a consequence of Theorem 5 and Lemma 1b.) we have:

Corollary 2. *For any fixed regularization* cond(S) *is large, if there exists an in modulo large real eigenvalue of* A *or if there exists a real eigenvector* v *of* A *which is close to the null space of* C*. If this is the case then the observability measure is low too.*

Nevertheless, the boundedness of the inverse S^{-1} and the compact inbedding $H^1 \hookrightarrow C^0$ yields

Corollary 3. *Linear state estimation formulated as least squares problem* $\min \frac{1}{2} \int_0^H (y - z)^T Q(y - z) + w^T R_{\bm{w}} w \, dt$

s.t. $\dot{x} - Ax - w = u$ $y - Cx = 0$ *is well-posed, i.e.* $||x - x^{\delta}||_{H^1} \le c||z - z^{\delta}||_{(H^1)'}$ and, consequently, with a generic *constant* c, $\max_{\delta} \{|x_0 - x_0^{\delta}|, \|w - w^{\delta}\|_{L_2}\} \le c \|z - z^{\delta}\|_{L_2}$ and $||x - x^{\delta}||_{C^{0}} \leq c||z - z^{\delta}||_{L_{2}} \leq c||z - z^{\delta}||_{L_{\infty}}.$

4 Conclusions and Questions Concerning the Appropriate Norms

Observability is like well-posedness a qualitative property. Condition numbers quantify the error propagation. We used this concept to define an observability measure. For linear systems we derived the use of the inverse of observability Gramian G. With \mathcal{G}^{-1} one can estimate the minimal difference in the outputs which can be seen for given different initial data. Also we showed that regularization of initial data is not necessary for stability, hence the least squares formulation for state estimation is well-posed. Regularization of initial data would lead to bias. However, a low observability measure leads to an ill-conditioned least squares problem.

Introducing linearly model error functions we leave the finite dimensional setting. For this case we stated the first order necessary condition and reduced them by several variables and equations. Analysing them for linear systems we showed that the least squares problem formulation without regularizing the initial data is well-posed not only with respect to the L_2 -norm but also for the L_∞ -norm. However, the error propagation with respect to L_2 -errors may be large for low observability measures independent of the regularization parameter for the model errors. Considering L_{∞} -errors the behaviour is different. Then, in case of one state only, we have bounds independent of the stiffness of state equations.

As seen it is fundamental to discuss in which norms the data errors are bounded and what output is of interest. In my opinion one has not only the L_2 -norm of the data error bounded, but one can assume $||z^{\delta}||_{L_2(t_0,t_0+H)} \leq \delta \sqrt{H}$ and $||z^{\delta}||_{\infty} \leq c$. Hence, one has additional information about the error which should be taken into account, and the error would depend on the length of the horizon. The question concerning the outputs depends on the application of state estimation. Which output is of interest should be stated together with the problem formulation. For example, employing state estimation to obtain the current state required for the main issue of controling a process should have the focus on $x(t_0 + H)$, the filtered state. Then the L_2 -norm of the state on $[t_0, t_0 + H]$ is less adequate than measuring the error of $x(t_0 + H)$. If one is interested on the state over the whole horizon, also called smoothed state, one may consider a weighted L_2 -norm putting more weight on the current state than on the past state. Or, is the L_{∞} - norm over the whole horizon more adequate than the L_2 -norm? The answers of these question do not only influence the theoretical analysis but should also affect the numerical studies. In particular, as soon as adaptivity concerning the underlying discretization grid is introduced it is of greatest importance to know which error shall be finally small to obtain greatest efficency.

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