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ANALYTICAL CONSIDERATIONS OF STATE ESTIMATION: REGULARIZATION AND ERROR PROPAGATION

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Abstract - Monitoring dynamical processes requires the estimation of the entire state, which is only partly accessible by measurements. Most quantities must be determined via model based state estimation, which in general is an ill-posed inverse problem. Regularization techniques have to be applied. In most of the literature the initial data are also regularized. However, the initial data are typically unknown and only a rough guess is provided by experience or from the previous time window. Hence, to avoid undesired bias we omit the regularization of the initial data. The purpose of this paper is to analyse the effects of this problem formulation.

We shortly deduce the problem formulation of state estimation with incorporated model error functions, discuss the ill-posedness and introduce the applied regularization. Then the first order necessary conditions are presented and the optimization problem is reduced by several variables. Hence, e.g. one otherwise necessary regularization parameter is dispensable.

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. We show that the regularized inverse problem is well-posed with respect to L_2-perturbations. However, a large spectral radius of the system matrix can lead to a large condition number and small disturbances in the measurements may propagate to large errors in the initial data. Moreover the issue of observability comes into play, since also eigenvectors of the system matrix which are close to the null space of the output election matrix can cause arbitrary large norms. From the engineering side the perhaps more interesting case of disturbances in the supremum-norm leads to bounds only dependent on the regularization parameters.

1. INTRODUCTION

State estimation is the task of determining from a few given, typically noisy measurements over a past time horizon all state functions, which are involved e.g. into a chemical process. The measurements correspond only to a few states. The others have to be estimated using the coupling of the states via model equations. State estimation can be viewed in general as an ill-posed inverse problem. Then, regularization techniques have to be applied. In most of the literature the initial data are also regularized (see e.g.[1, 15, 16, 18]). In this case the resulting optimization formulation coincides widely with a corresponding control problem, where the initial data are given. Control problems are analysed by many authors and numerical methods are available. However, in state estimation the initial data are typically unknown. Sometimes experiences provide a rough guess for the initial data, or state estimation on one horizon provides guesses for a forwardly moved time horizon, which are then used as reference values for regularization, though precise values are not available. Hence, to avoid bias we omit the regularization of the initial data (for further discussion see [3]). The purpose of this paper is to analyse this problem formulation.

We shortly deduce in Section 2 the problem formulation of state estimation with incorporated model error functions, discuss the ill-posedness and introduce the applied regularization. In Section 3 we derive the first order optimality conditions for the resulting optimization problem. As a consequence we can reduce the optimization problem by several variables and avoid the choice of one otherwise necessary regularization parameter. Section 4 is concerned with the study of well-posedness of the formulation, with the error propagation and the analysis of the resulting solution operator. As a start we restricted these considerations to the linear case with time independent coefficient. Of particular interest is here the influence of the regularization parameters and the influence of the model equations with their observability and their model matrices.

2. DERIVATION OF THE PROBLEM FORMULATION

In [3] the mathematical formulation of the estimation problem is discussed and its engineering interpretation is given in detail. In this paper we concentrate on the more mathematical approach, arguing with the mathematical features of the variables and equations. We state the model equations and their extension by model error functions and then discuss shortly the regularization of the problem.

2.1. Model Equations

The quantities of interest in process monitoring can be summarized in the state functions $\boldsymbol{x}$, the output functions $\boldsymbol{y}$, the control variables $\boldsymbol{u}$ and parameters $\boldsymbol{p}$. For the particular case of state estimation the controls $\boldsymbol{u}$ and the parameters $\boldsymbol{p}$ are known variables. Then, the mathematical description of the state equations of the process is assumed to be given by the differential algebraic equations (DAE's)

$$\boldsymbol{G}\dot{\boldsymbol{x}} - \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) = \boldsymbol{0} \tag{1}$$

with a possibly time dependent matrix $\boldsymbol{G}$, a given function $\boldsymbol{f}$ and the consistent initial condition [5]

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0. \tag{2}$$

The output equations

$$\boldsymbol{y} - \boldsymbol{C}\boldsymbol{x} = \boldsymbol{0} \tag{3}$$

describe which states can be measured. Here $\boldsymbol{C}$ is a time independent matrix, typically an identity matrix extended by zero columns. The number of output functions n_y are typically far less than the number of involved states n_x. We require that the system is observable [6, 7, 10], i.e. the map $\mathcal{F} : \boldsymbol{x}_0 \longmapsto \boldsymbol{y}$ given by (1)– (3) is injective for any given $\boldsymbol{u}$ and $\boldsymbol{p}$. Hence given an output $\boldsymbol{y} \in Im(\mathcal{F})$ we can reconstruct uniquely $\boldsymbol{x}$ using (1) and (3).

To include possible model errors into the model equations the DAE's are extended linearly by unknown error functions $\boldsymbol{w}$ and $\boldsymbol{v}$, which results into the equations

$$\boldsymbol{G}\dot{\boldsymbol{x}} - \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) - \boldsymbol{W}\boldsymbol{w} = \boldsymbol{0} \tag{4}$$
$$\boldsymbol{y} - \boldsymbol{C}\boldsymbol{x} - \boldsymbol{V}\boldsymbol{v} = \boldsymbol{0}. \tag{5}$$

The matrices $\boldsymbol{W}$ and $\boldsymbol{V}$ are typically identity matrices enlarged by zero rows. They reflect which equations are trusted. The above model eqns (4), (5) and (2) describe the process on a given interval (time horizon on $[t_0, t_0 + T]$) which is assumed to be projected onto $[0, 1]$. For convenience we omit the interval $[0, 1]$ in the following. Moreover, we only assume that the equations are fulfilled in the weak sense, i.e.: let L_2 be space of the square integrable functions and H^1 the space of weakly differentiable functions (Sobolev space), denote by $\langle ., . \rangle$ the L_2 scalar product $\langle f, \nu \rangle = \int_0^1 f(t)\nu(t)\,dt$ then an equation $f(t) = g(t)$ is weakly fulfilled if $\langle f, \nu \rangle = \langle g, \nu \rangle$ for all $\nu \in L_2$, respectively H^1 or its dual space $(H^1)'$. For simplicity if the dimension $n = n_x$ etc. is obvious in the context, we omit the exponent n and write L_2 and H^1 instead of the precise notation $(H^1)^n$.

Inequality constraints reflect, for example, safety restrictions and control limits and can be written as

$$\boldsymbol{c}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) \le \boldsymbol{0}. \tag{6}$$

For state estimation they are typically of the form $\boldsymbol{c}_i(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) = x_i - \bar{c}_i$ and $\boldsymbol{c}_{i+n_x}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) = -x_i + \bar{c}_{i+n_x}$ for $i = 1, \ldots, n_x$.

2.2. The Inverse Problem and Regularization

Given $\boldsymbol{x}_0, \boldsymbol{w}$ and $\boldsymbol{v}$ the solution $\boldsymbol{y}$ is uniquely determined by (4) and (5). This defines an operator (in case of $\boldsymbol{G} = \boldsymbol{I}$)

$$\boldsymbol{T}\begin{pmatrix} \boldsymbol{x}_0 \\ \boldsymbol{w} \\ \boldsymbol{v} \end{pmatrix} := \boldsymbol{y} \quad \text{with} \quad \boldsymbol{T} : \mathbb{R}^{n_x} \times (L_2)^{n_w} \times \left(H^1\right)^{n_v} \longrightarrow \left(H^1\right)^{n_y}. \tag{7}$$

For state estimation one wants to determine $\boldsymbol{x}_0, \boldsymbol{w}$ and $\boldsymbol{v}$ and, hence, $\boldsymbol{x}$ from given data. If the data are clean they shall coincide with $\boldsymbol{y}$. However, in general only noisy measurements are available. Assuming that the measurements taken at discrete times can be processed to signal functions $\boldsymbol{z}$, these functions are typically not in H^1 but in L_2. Hence, the output functions $\boldsymbol{y}$ cannot match the measurements $\boldsymbol{z}$ exactly. The estimation solution is given as a least squares solution, i.e. $\boldsymbol{T}^\dagger \boldsymbol{z} := \left(\boldsymbol{x}_0^T, \boldsymbol{w}^T, \boldsymbol{v}^T\right)^T$ where $\|\boldsymbol{T}\left(\boldsymbol{x}_0^T, \boldsymbol{w}^T, \boldsymbol{v}^T\right)^T - \boldsymbol{z}\|_{(L_2)^{n_y}}$ is minimal. Taking into account that each output function can be weighted separately the optimization problem is formulated as

$$\min_{\boldsymbol{x}_0,\boldsymbol{w},\boldsymbol{v}} 1/2 \int_0^1 (\boldsymbol{y} - \boldsymbol{z})^T \boldsymbol{R}_y (\boldsymbol{y} - \boldsymbol{z})\, dt \qquad \text{with} \qquad \boldsymbol{T}\left(\boldsymbol{x}_0^T, \boldsymbol{w}^T, \boldsymbol{v}^T\right) = \boldsymbol{y} \tag{8}$$

with some time independent, positive definite matrix $\boldsymbol{R}_y$.

The generalized inverse $\boldsymbol{T}^\dagger : (L_2)^{n_y} \longrightarrow \mathbb{R}^{n_x} \times (L_2)^{n_w} \times \left(H^1\right)^{n_v}$ is an unbounded operator, since highly oscillatory functions $\boldsymbol{z} \in \left(H^1\right)^{n_y}$ with uniformly bounded L_2- or L_∞-norms can lead to unbounded L_2-, respectively, L_∞-norms of $\boldsymbol{w}$ due to the involved differential operator (for example $z(t) = \varepsilon \sin(t/\varepsilon^2)$). Additionally the problem of non-uniqueness in $\boldsymbol{w}$ and $\boldsymbol{v}$ can occur.

One possible regularization technique to overcome the ill-posedness is Tikhonov-type regularization [8, 13]. This leads to the following ansatz for the cost functional:

$$1/2 \int_0^1 (\boldsymbol{y}-\boldsymbol{z})^T \boldsymbol{R}_y (\boldsymbol{y}-\boldsymbol{z}) + \boldsymbol{v}^T \boldsymbol{R}_v \boldsymbol{v} + \boldsymbol{w}^T \boldsymbol{R}_w \boldsymbol{w}\, dt \tag{9}$$

with some time independent, positive definite matrices $\boldsymbol{R}_v$, $\boldsymbol{R}_w$. The resulting optimization problem for state estimation on a fixed horizon projected onto $[0,1]$ is then given by minimizing (9) with the model eqns (4), (5) and the initial condition (2) as equality constraints and the inequality constraints (6). We would like to mention that typically the initial values $\boldsymbol{x}_0$ are regularized too (for e.g. [12, 16, 19]) with estimated reference values $\boldsymbol{x}_0^{ref}$. The additional regularization of the initial values origins from the classical way of Tikhonov-regularization, which regularizes all unknowns. Moreover, in a receding horizon estimator it is used to reflect the measurements of a past time horizon into the current horizon [19], where then the regularization matrices can be adjusted according to linear filter theory. In the context of nonlinear state estimation this is not reasonable any longer [16, 19]. In addition, for the first time horizon appropriate reference values may be missing. In all cases precise values are not given. Bias may occur as the simple one-dimensional linear example $\dot{x} - \alpha x = 0, y = x, z \equiv 0$ with the solution $x(t) = x_0 \exp(\alpha t)$ shows: while omitting regularization of x_0 leads to $x \equiv 0$, which corresponds to z, regularization of x_0 with a reference value $x_0^{ref} \neq 0$ yields $x_0 = x_0^{ref} \frac{2\alpha}{\exp(2\alpha)-1+2\alpha}$ and hence $x \not\equiv z$. Therefore, as mentioned in the beginning, we omit the regularization of the initial values on purpose to avoid unnecessary bias.

3. REDUCTION OF THE PROBLEM FORMULATION

Since $\boldsymbol{x}_0$ is unknown we observe that the initial condition (2) has in case of an estimation problem no information and need for the optimization problem. Hence, the eqn. (2) can be omitted in the problem formulation. Moreover, we do not have to distinguish between $\boldsymbol{u}$ and $\boldsymbol{p}$ for analytical reasons, since both are given. In the following we include $\boldsymbol{p}$ into $\boldsymbol{u}$.

In the next step we exploit the relations to the Lagrange multipliers corresponding to the equality constraints. Therefore, we consider in detail the first order necessary optimality conditions leading to the Euler–Lagrange equations, which are obtained by the Pontryagin's maximum principle [9, 11, 17]. Since no inequality constraints on $\boldsymbol{y}$ and $\boldsymbol{v}$ are present, we obtain —using the Lagrange multiplier with respect to (5)— the equations

$$\boldsymbol{v} = {\boldsymbol{R}_v}^{-1} \boldsymbol{V}^T \boldsymbol{R}_y (\boldsymbol{z} - \boldsymbol{y}). \tag{10}$$

and

$$\boldsymbol{y} = \left(\boldsymbol{I} + \boldsymbol{V} {\boldsymbol{R}_v}^{-1} \boldsymbol{V}^T \boldsymbol{R}_y\right)^{-1} (\boldsymbol{C}\boldsymbol{x} - \boldsymbol{z}) + \boldsymbol{z}. \tag{11}$$

Let us define now $\boldsymbol{Q} := \left({\boldsymbol{R}_y}^{-1} + \boldsymbol{V} {\boldsymbol{R}_v}^{-1} \boldsymbol{V}^T\right)^{-1}$ then the problem formulation (4)–(6), (9) is equivalent to the following minimization.

Reduced optimization problem:

$$\min 1/2 \int_0^1 (\boldsymbol{C}\boldsymbol{x} - \boldsymbol{z})^T \boldsymbol{Q} (\boldsymbol{C}\boldsymbol{x} - \boldsymbol{z}) + \boldsymbol{w}^T \boldsymbol{R}_w \boldsymbol{w}\, dt \tag{12}$$

s.t.

$$\boldsymbol{G}\dot{\boldsymbol{x}} - \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}) - \boldsymbol{W}\boldsymbol{w} = \boldsymbol{0} \tag{13}$$

$$\boldsymbol{c}(\boldsymbol{x}, \boldsymbol{u}) \leq \boldsymbol{0}. \tag{14}$$

Considering the obtained optimization problem we can deduce:

Remark 1. *The inclusion of $\boldsymbol{v}$ as a model error function into the problem formulation is not necessary for the solution of the optimization problem. We can view $\boldsymbol{C}\boldsymbol{x}$ as in (3) as outputs and, after obtaining the estimates, distinguish as in (5) which amount $\boldsymbol{y}$ of the outputs $\boldsymbol{C}\boldsymbol{x}$ is trustful and which amount is considered as error $\boldsymbol{v}$. Consequently, we can also avoid the problem of finding an appropriate regularization matrix $\boldsymbol{R}_v$.*

Exploiting the Lagrange multiplier $\boldsymbol{\lambda}$ with respect to (13) we obtain the relation

$$\boldsymbol{w} = \boldsymbol{R}_w{}^{-1}\boldsymbol{W}^T\boldsymbol{\lambda}. \tag{15}$$

Defining $\boldsymbol{R} := \boldsymbol{W}\boldsymbol{R}_w{}^{-1}\boldsymbol{W}^T$ we can make the substitutions $\boldsymbol{W}\boldsymbol{w} = \boldsymbol{R}\boldsymbol{\lambda}$ and $\boldsymbol{w}^T\boldsymbol{R}_w\boldsymbol{w} = \boldsymbol{\lambda}^T\boldsymbol{R}\boldsymbol{\lambda}$ and eliminate the model error function $\boldsymbol{w}$ in the optimization process.
Necessary first order conditions: The remaining first order necessary optimality conditions for the solution of the estimation problem are the equations

$$\begin{aligned} \boldsymbol{G}\dot{\boldsymbol{x}} - \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u}) - \boldsymbol{R}\boldsymbol{\lambda} &= \boldsymbol{0} && (16)\\ -\frac{d}{dt}\left(\boldsymbol{G}^T\boldsymbol{\lambda}\right) - \left(\frac{\partial}{\partial \boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x},\boldsymbol{u})\right)^T\boldsymbol{\lambda} + \boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\boldsymbol{x} + \left(\frac{\partial}{\partial \boldsymbol{x}}\boldsymbol{c}(\boldsymbol{x},\boldsymbol{u})\right)^T\boldsymbol{\nu} &= \boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{z} && (17)\\ \left(\boldsymbol{G}^T\boldsymbol{\lambda}\right)(0) = \boldsymbol{0} \quad \text{and} \quad \left(\boldsymbol{G}^T\boldsymbol{\lambda}\right)(1) &= \boldsymbol{0} && (18)\\ \boldsymbol{\nu}^T\boldsymbol{c}(\boldsymbol{x},\boldsymbol{u}) = 0, \quad \boldsymbol{c}(\boldsymbol{x},\boldsymbol{u}) \le \boldsymbol{0}, \quad \boldsymbol{\nu} &\ge \boldsymbol{0} && (19) \end{aligned}$$

with unknown Lagrange multipliers $\boldsymbol{\lambda}$, $\boldsymbol{\nu}$ and unknown states $\boldsymbol{x}$.

The output function $\boldsymbol{y}$ is given by (11), the model error functions $\boldsymbol{v}$ by (10) and $\boldsymbol{w}$ by (15). Equations (18) reflect the fact that no boundary conditions and no regularization of the boundary values of the states $\boldsymbol{x}$ are given.

If no inequality constraints are present, (16)–(18) is a DAE system of order one, where for at most half of the variables boundary conditions are given, while for the others the boundary values are unknown. In case that the state equations are given by ODE's only, we obtain with (15)

Remark 2. *If $\boldsymbol{G} = \boldsymbol{I}$ then the model error functions $\boldsymbol{w}$ are in H^1 and vanish at the boundary $t = 0$ and $t = 1$. The boundary values are enforced by the described Tikhonov–regularization.*

It is questionable whether one would like to have possible model errors also at the boundary. Regularization by discretization may offer this possibility. In case of regularization of the initial values of the states $\boldsymbol{x}$ with some reference guesses $\bar{\boldsymbol{x}}_0$, which is seen mostly in the literature, the model errors are free at the boundary too. However, as mentioned, for wrong reference data undesired bias may appear in the states.

3.1. Linear Case

To gain more insight in the properties of the chosen problem formulation and, in particular, to study its well-posedness and its behaviour for noisy measurements we consider as a start in the next section the case of linear ODE's, i.e. $\boldsymbol{G}\dot{\boldsymbol{x}} - \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u}) = \dot{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{x} - \boldsymbol{u}$ with time independent coefficients where we additionally summarize all given parameters, controls and their perhaps nonlinear influence to a given function $\boldsymbol{u}$. Furthermore, let model error functions $\boldsymbol{w}$ be present in all state equations. This implies that $\boldsymbol{W}$, and consequently $\boldsymbol{R}$ are invertible. Moreover we drop the inequality constraints, which may be for state estimation not of major interest. This case enhances already some of the main features we face for state estimation if the initial data are not regularized in the problem formulation. Under this assumption the problem formulation simplifies to the unconstraint minimization problem

$$min_{\boldsymbol{x}\in H^1}\left\{\|\boldsymbol{Q}^{1/2}\left(\boldsymbol{C}\boldsymbol{x}-\boldsymbol{z}\right)\|_{L_2}^2 + \|\boldsymbol{R}^{-1/2}\left(\dot{\boldsymbol{x}}-\boldsymbol{A}\boldsymbol{x}-\boldsymbol{u}\right)\|_{L_2}^2\right\}. \tag{20}$$

As necessary first order conditions we obtain the second order differential equation

$$\begin{aligned} -\boldsymbol{R}^{-1}\ddot{\boldsymbol{x}} + \left(\boldsymbol{R}^{-1}\boldsymbol{A} - \boldsymbol{A}^T\boldsymbol{R}^{-1}\right)\dot{\boldsymbol{x}} + \left(\boldsymbol{A}^T\boldsymbol{R}^{-1}\boldsymbol{A} + \boldsymbol{R}^{-1}\dot{\boldsymbol{A}} + \boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\right)\boldsymbol{x}&\\ = \boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{z} - \boldsymbol{R}^{-1}\dot{\boldsymbol{u}} - \boldsymbol{A}^T\boldsymbol{R}^{-1}\boldsymbol{u}& \end{aligned} \tag{21}$$

with the boundary conditions $\dot{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{x} = \boldsymbol{u}$ at $t = 0$ and $t = 1$.

While the strong formulation does not look symmetric, the weak formulation reflects the symmetry given by the formulation (20).

$$\langle\dot{\boldsymbol{\zeta}} - \boldsymbol{A}\boldsymbol{\zeta}, \boldsymbol{R}^{-1}\left(\dot{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{x}\right)\rangle + \langle\boldsymbol{C}\boldsymbol{\zeta}, \boldsymbol{Q}\boldsymbol{C}\boldsymbol{x}\rangle = \langle\boldsymbol{C}\boldsymbol{\zeta}, \boldsymbol{Q}\boldsymbol{z}\rangle + \langle\dot{\boldsymbol{\zeta}} - \boldsymbol{A}\boldsymbol{\zeta}, \boldsymbol{R}^{-1}\boldsymbol{u}\rangle \qquad \text{for all } \boldsymbol{\zeta} \in H^1. \tag{22}$$

4. PROPERTIES OF THE INVOLVED OPERATORS

As motivated in Section 3.1 we consider as a start the linear case, with time independent coefficients and without inequality constraints in more detail. We first consider a model with one state only. In this case we can determine the solution explicitly and analyse its dependency on perturbation in the signal $\boldsymbol{z}$. For the numerical approach however, eqn. (22) or equivalent formulations are used. Hence, the properties of the operator corresponding to (22) are analysed in more detail. In the second subsection we then extend most ideas to systems with several states taking into account the issue of observability.

4.1. Linear Model with one State Function

With $n_x = 1$, $\boldsymbol{A} = \alpha$, $\boldsymbol{C} = \delta$, $\boldsymbol{W} = 1$, $\boldsymbol{R}_w = r$ and $\boldsymbol{Q} = q$ above differential equations reduce to

$$\begin{aligned} -r\ddot{x} + \left(r\alpha^2 + q\delta^2\right)x &= q\delta z - r\dot{u} - r\alpha u \\ \text{s.t.} \quad \dot{x}(1) - \alpha x(1) = u(1) \quad \text{and} \quad & \dot{x}(0) - \alpha x(0) = u(0). \end{aligned} \tag{23}$$

The solution x and the model error function w are given with $\zeta := \sqrt{\alpha^2 + \frac{q\delta^2}{r}}$ by:

$$x_0 = \frac{-1}{\sinh(\zeta)} \int_0^1 \left\{ \sinh(\zeta - \zeta s)u(s) + \frac{1}{\delta}\left[\alpha \sinh(\zeta - \zeta s) - \zeta \cosh(\zeta - \zeta s)\right] z(s) \right\} ds \tag{24}$$

$$\begin{aligned} x(t) &= \frac{1}{\zeta}\left(\zeta \cosh(\zeta t) + \alpha \sinh(\zeta t)\right) x_0 \\ &\quad + \frac{1}{\zeta} \int_0^t \left\{ \left(\zeta \cosh(\zeta(t-s)) + \alpha \sinh\left(\zeta(t-s)\right)\right) u(s) - \frac{q\delta}{r} \sinh\left(\zeta(t-s)\right) z(s) \right\} ds \end{aligned} \tag{25}$$

$$\begin{aligned} w(t) &= \frac{q\delta^2}{\zeta r} \sinh(\zeta t) x_0 \\ &\quad + \frac{q\delta^2}{\zeta r} \int_0^t \left\{ \sinh\left(\zeta(t-s)\right) u(s) + \frac{1}{\delta}\left(\alpha \sinh\left(\zeta(t-s)\right) - \zeta \cosh(\zeta(t-s))\right) z(s) \right\} ds. \end{aligned} \tag{26}$$

One typically has $\delta = 1$ meaning the state x corresponds to the measurements z in the output eqn. (5). The parameters influencing the solution are the regularization parameters r, q and the coefficient α of the ODE.

Analysing the above functions (see [4]) we obtain

Theorem 1. *Assuming a linear model with one state function and time independent coefficients and omitting inequality constraints we obtain with above notation:*

1. *The regularized problem formulation (13)–(14) of state estimation, i.e. given z determining x_0 and w, is well-posed.*
2. *Small perturbation of z in the L_2–norm can lead to arbitrarily large error propagation in the initial data x_0 independently of r and q if $\alpha \longrightarrow -\infty$.*
3. *For perturbations of z in the L_∞–norm we have bounds independently of α:*

$$|x_0^\varepsilon| \le \frac{2}{|\delta|}\|z^\varepsilon\|_{L_\infty} \quad \text{and} \quad |w^\varepsilon(t)| \le \frac{2\sqrt{q/r}}{1 - e^{-2\delta\sqrt{q/r}}}\|z^\varepsilon\|_{L_\infty}$$

where we used the abbreviation $z^\varepsilon = z - \tilde{z}$ etc. for the perturbation.

For the numerical approach not only the map $z \longmapsto (x_0, w)$ is of interest but also the properties of the discretization matrix corresponding to the eqn. (22), respectively to (23). Let us define the symmetric bilinear form $a : H^1 \times H^1 \to \mathbb{R}$

$$a(\xi, x) \quad = \quad r\langle\dot{\xi} - \alpha\xi, \dot{x} - \alpha x\rangle + q\delta^2\langle\xi, x\rangle. \tag{27}$$

Obviously, a is positive definite if $r, q\delta^2 > 0$. Given the operator $\boldsymbol{\mathcal{S}} : H^1 \longrightarrow (H^1)'$ defined as $(\xi, \boldsymbol{\mathcal{S}}x) := a(\xi, x)$, the equation (22) is equivalent to $(\xi, \boldsymbol{\mathcal{S}}x) = q\delta\langle\xi, z\rangle + r\langle\dot{\xi}, u\rangle - r\alpha\langle\xi, u\rangle$. For any function $g \in \left(H^1\right)'$ we set $u = 0$ and $z = 1/(q\delta)g$. Then $x = \boldsymbol{\mathcal{S}}^{-1}g$ is given by (24) and (25). Furthermore, we obtain the following estimates for the norm of $\boldsymbol{\mathcal{S}}$ and its inverse. Here we employ the H^1–norm $\|x\|_{H^1}^2 = \|x\|_{L_2}^2 + \|\dot{x}\|_{L_2}^2$.

Theorem 2. *The operator $\boldsymbol{\mathcal{S}}$ is a linear isomorphism and we have:*

$$\begin{aligned} \min(4r, q\delta^2) \leq \quad & \|\boldsymbol{\mathcal{S}}\|_{H^1 \to (H^1)'} & \leq 2r\max(1,\alpha^2) + q\delta^2, \qquad (28) \\ \frac{c(\alpha)}{q\delta^2} \leq \quad & \|\boldsymbol{\mathcal{S}}^{-1}\|_{(H^1)' \to H^1} & \leq \max\left\{\frac{2}{r}, \frac{2\alpha^2+1}{q\delta^2}\right\}, \qquad (29) \end{aligned}$$

with $c(\alpha) \approx 0.38 \cdot |\alpha|^{3/2}$ for large $|\alpha|$.

Hence cond($\boldsymbol{\mathcal{S}}$) $= \|\boldsymbol{\mathcal{S}}\|_{H^1 \to (H^1)'} \|\boldsymbol{\mathcal{S}}^{-1}\|_{(H^1)' \to H^1}$ is bounded but tends to infinity with $|\alpha| \to \infty$ for fixed regularization parameters r and q.

Proof: The bilinear form a is continuous and coercive since

$$a(\xi, x) \leq r\|\dot{\xi} - \alpha\xi\|_{L_2}\|\dot{x} - \alpha x\|_{L_2} + q\delta^2\|\xi\|_{L_2}\|x\|_{L_2} \leq C_0\|\xi\|_{H^1}\|x\|_{H^1}$$

with $C_0 = 2r\max(1,\alpha^2) + q\delta^2$ and the parallelogram identity yields

$$c_0\|x\|^2_{H^1} \quad = \quad c_0\|\dot{x} - \alpha x + \alpha x\|^2_{L_2} + c_0\|x\|^2_{L_2} \leq 2c_0\|\dot{x} - \alpha x\|^2_{L_2} + c_0(2\alpha^2+1)\|x\|^2_{L_2} \leq a(x,x)$$

with $c_0 = \min\left\{\frac{r}{2}, \frac{q\delta^2}{2\alpha^2+1}\right\}$. Hence, due to the theorem of Lax Milgram the operator $\boldsymbol{\mathcal{S}} : H^1 \longrightarrow (H^1)'$ is a linear isomorphism and we have the upper bounds of (28) and (29).

For the lower bound in (28) we set $\tilde{x} = \exp(-\alpha t)$. Then

$$\begin{aligned} \|\boldsymbol{\mathcal{S}}\|_{H^1 \to (H^1)'} \quad & \geq \quad \|\boldsymbol{\mathcal{S}}\tilde{x}\|_{(H^1)'}/\|\tilde{x}\|_{H^1} \geq a(\tilde{x},\tilde{x})/\|\tilde{x}\|^2_{H^1} = \\ & = \quad (4r\|\dot{\tilde{x}}\|^2_{L_2} + q\delta^2\|\tilde{x}\|^2_{L_2})/\|\tilde{x}\|^2_{H^1} \geq \min(4r, q\delta^2). \end{aligned}$$

For the lower bound in (29) we consider the function $\tilde{x} = \exp(\alpha t)$. Obviously it holds $\boldsymbol{\mathcal{S}}\tilde{x} = q\delta^2\tilde{x}$ and hence $\|\boldsymbol{\mathcal{S}}^{-1}\|_{(H^1)' \to H^1} \geq \frac{c(\alpha)}{q\delta^2}$ with $c(\alpha) := \|\tilde{x}\|_{H^1}/\|\tilde{x}\|_{(H^1)'}$. Determining these norms (see [4]) we conclude $c(\alpha) \approx |\alpha|^{3/2}\sqrt{\frac{e^2-1}{2(e^2+1)}}$ for large $|\alpha|$. q.e.d.

This indicates clearly that regularization with r is sufficient to obtain a bounded inverse $\boldsymbol{\mathcal{S}}^{-1}$. However, for large $|\alpha|$ the norm is still very large independently of r and q.

4.2. Linear Model with Several State Functions

In case of a linear model with constant coefficients with several state functions we define correspondingly to (22) and (27) the symmetric bilinear form

$$a(\boldsymbol{\zeta}, \boldsymbol{x}) \quad = \quad \langle \dot{\boldsymbol{\zeta}} - \boldsymbol{A}\boldsymbol{\zeta}, \boldsymbol{R}^{-1}(\dot{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{x})\rangle + \langle \boldsymbol{C}\boldsymbol{\zeta}, \boldsymbol{Q}\boldsymbol{C}\boldsymbol{x}\rangle \qquad (30)$$

and the operator $\boldsymbol{\mathcal{S}}$ given by $(\boldsymbol{\zeta}, \boldsymbol{\mathcal{S}}\boldsymbol{x}) := a(\boldsymbol{\zeta}, \boldsymbol{x})$. Taking into account the observability of the system we can extend most ideas of the previous subsection to obtain bounds on the operator and then to conclude well-posedness of the regularized problem formulation.

Theorem 3. *For any $\boldsymbol{z}, \boldsymbol{u} \in L_2$ the solution $\boldsymbol{x}$ of (22) determines the unique solution of the minimization problem (20).*

Proof: For the complete proof we refer to [4]. Here we illuminate only the importance of observability, which provides positive definiteness of a: given $a(\boldsymbol{x}, \boldsymbol{x}) = 0$ then $\boldsymbol{x}$ is the solution of the system $\dot{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{x} \equiv \boldsymbol{0}$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$ and $(\boldsymbol{y} \equiv)\boldsymbol{C}\boldsymbol{x} \equiv \boldsymbol{0}$. Since the system is observable $\boldsymbol{y} \equiv \boldsymbol{0}$ yields $\boldsymbol{x}_0 = \boldsymbol{0}$ and consequently $\boldsymbol{x} \equiv \boldsymbol{0}$. Hence, $a(\boldsymbol{x}, \boldsymbol{x}) > 0$ for $\boldsymbol{x} \not\equiv 0$. Then showing $a(\boldsymbol{\zeta}, \boldsymbol{x})$ is continuous and coercive we can conclude the assertion. q.e.d.

For the operator $\boldsymbol{\mathcal{S}}$ and its inverse we obtain the following specific estimates depending on the model matrices and the regularization matrices.

Theorem 4. *The operator $\boldsymbol{\mathcal{S}} : H^1 \to \left(H^1\right)'$ is a linear isomorphism and has a bounded inverse.*

Furthermore, we have

$$\|\boldsymbol{\mathcal{S}}\|_{H^1 \to (H^1)'} \leq 2\|R\|^{-1}\max(1, \|\boldsymbol{A}\|^2) + \|\boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\|, \qquad (31)$$

and

$$\max\{k_S(\boldsymbol{v})|\boldsymbol{v} \text{ eigenvector of } \boldsymbol{A} \text{ with } \|v\|_{l_2}=1\} \quad \leq \quad \|\boldsymbol{\mathcal{S}}\|_{H^1\to(H^1)'}, \tag{32}$$

$$\max\{c(\alpha)k_{S^{-1}}(\boldsymbol{v})|\alpha, \boldsymbol{v} \text{ with } \boldsymbol{A}\boldsymbol{v}=\alpha\boldsymbol{v} \text{ with } \|v\|_{l_2}=1\} \quad \leq \quad \|\boldsymbol{\mathcal{S}}^{-1}\|_{(H^1)'\to H^1}, \tag{33}$$

with

$$k_S(\boldsymbol{v}) \quad = \quad \min\{4(\bar{\boldsymbol{v}}^T\boldsymbol{R}^{-1}\boldsymbol{v}), (\bar{\boldsymbol{v}}^t\boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\boldsymbol{v})\} > 0, \tag{34}$$

$$\infty > k_{S^{-1}}(\boldsymbol{v}) \quad = \quad 1/\|\boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\boldsymbol{v}\|_{l_2} > 1/\|\boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\| > 0 \tag{35}$$

and $c(\alpha)$ given as in Theorem 2.
If the spectral radius $\rho(\boldsymbol{A})$ is larger than 1, we can choose $k_S(\boldsymbol{v}) = 2\bar{\boldsymbol{v}}^T\boldsymbol{R}^{-1}\boldsymbol{v} \geq 2/\|\boldsymbol{R}\|$.

Proof: sketched only, details can be found in [4].
Since $a(\boldsymbol{\zeta},\boldsymbol{x})$ is continuous and coercive the Riesz representation theorem yields that $\boldsymbol{\mathcal{S}}$ is an linear isomorphism with an bounded inverse. For the lower bounds let α be an eigenvalue of $\boldsymbol{A}$ and $\boldsymbol{v}$ a normalized corresponding eigenvector. Then, defining $\tilde{\boldsymbol{x}} = exp(-\alpha t)\boldsymbol{v}$, respectively $\tilde{\boldsymbol{x}} = exp(\alpha t)\boldsymbol{v}$ we can extend the ideas of Theorem 2 to obtain above estimates taking into account that the eigenvalues and eigenvectors can have the complex values. However, for $k_S(\boldsymbol{v}) > 0$ and $\infty > k_{S^{-1}}(\boldsymbol{v})$ we need the observability assumption: We consider the model equations $\dot{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$ and $\boldsymbol{y} = \boldsymbol{C}\boldsymbol{x}$, which is required to be observable. Hence $\boldsymbol{x}_0 \mapsto \boldsymbol{y}$ is injective. Therefore defining $\boldsymbol{x}_0 := \boldsymbol{v} \neq \boldsymbol{0}$ we follow $exp(\alpha t)\boldsymbol{C}\boldsymbol{v} = \boldsymbol{y} \not\equiv \boldsymbol{0}$ and thus $\boldsymbol{C}\boldsymbol{v} \neq 0$. Then $\bar{\boldsymbol{v}}^t\boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\boldsymbol{v} = \|\boldsymbol{Q}^{1/2}\boldsymbol{C}\boldsymbol{v}\|^2 \geq \|\boldsymbol{C}\boldsymbol{v}\|^2/\|\boldsymbol{Q}^{-1}\| > 0$ and $k_S(\boldsymbol{v}) > 0$. Since $\boldsymbol{C}^T\boldsymbol{Q}\boldsymbol{C}\boldsymbol{v} \neq 0$ we also have $\infty > k_{S^{-1}}(\boldsymbol{v})$. q.e.d.

While the boundedness of the inverse $\boldsymbol{\mathcal{S}}^{-1}$ is known, a specified upper bound is missing. However, in an analogous manner to the case of one state function we obtain:

Proposition 1. *For an invertible matrix $\boldsymbol{C}$ the inverse operator $\boldsymbol{\mathcal{S}}^{-1}$ is bounded by*

$$\|\boldsymbol{\mathcal{S}}^{-1}\|_{(H^1)'\to H^1} \leq \max\{2\|\boldsymbol{R}\|, (2\|\boldsymbol{A}\|^2+1)\|\boldsymbol{Q}^{-1}\|\|\boldsymbol{C}^{-1}\|^2\}.$$

As a direct consequence of Theorem 4 we have:

Corollary 1. *For any fixed regularization parameters $\boldsymbol{R}$ and $\boldsymbol{Q}$, $cond(\boldsymbol{\mathcal{S}}) \geq c(\alpha)k_S(\boldsymbol{v})k_{S^{-1}}(\boldsymbol{v})$ can be arbitrarily large,*

1. *if the spectral radius $\rho(\boldsymbol{A})$ is large or*
2. *if there is an eigenvector $\boldsymbol{v}$ of the model matrix $\boldsymbol{A}$ which is close to the null space of $\boldsymbol{C}$.*

Due to the boundedness of the inverse and the compact imbedding $H^1 \hookrightarrow C^0$ we have:

Corollary 2. *The regularized problem formulation (9) with time independent, linear ODE's as constraints and no inequality constraints is well-posed, i.e.* $\max\{|x_0|, \|\boldsymbol{w}\|_{L_2}\} \leq c\|\boldsymbol{z}\|_{L_2}$. *Furthermore we have $\|\boldsymbol{x}\|_{C^0} \leq c\|\boldsymbol{z}\|_{L_2} \leq c\|\boldsymbol{z}\|_{L_\infty}$ with a generic constant c.*

However, such strong assertions as they are given in Theorem 1 are currently not available.

Finally, we would like to bring to the readers attention the influence of a long time horizon. As mentioned in the beginning state estimation uses measurements of a past time horizon $[t_0, t_0+T]$, which is then projected onto $[0,1]$. Given a fixed model equation $\dot{\boldsymbol{x}}(t) - \boldsymbol{A}\boldsymbol{x}(t) - \boldsymbol{u}(t) = \boldsymbol{0}$ for $t \in [t_0, t_0+T]$ the projection onto $[0,1]$ leads to $\dot{\tilde{\boldsymbol{x}}}(s) - T\boldsymbol{A}\tilde{\boldsymbol{x}}(s) - \tilde{\boldsymbol{u}}(s) = \boldsymbol{0}$ for $s \in [0,1]$. Hence in the estimation for $cond(\boldsymbol{\mathcal{S}})$ and for the error propagation into $\boldsymbol{x}_0$ (see Theorem 1) the spectral radius $T\rho(\boldsymbol{A})$ is relevant.

Remark 3. *While long horizons may be favourable for stability reasons concerning the confidence into the obtained measurements, from the point of view of the resulting system and estimating the initial data long horizons should be avoided, since they increase the condition number respectively the error propagation.*

Some first approaches for the choice of an appropriate length of the time horizon are known under stochastical assumptions on the underlying measurement errors and for linear systems [14, 16, 18]. However, this is still a fairly open research problem, in particular if stochastical assumptions cannot be assured in the applications or nonlinearity occurs. The above remark ensures the importance of closing this gap and illuminates an additional issue which should to be considered for the choice of the horizon length.

5. CONCLUSIONS

The formulation of state estimation as an optimization problem including possible model error functions but without regularization of the initial data offers solutions without bias.

It turnes out that the inclusion of model error functions into the output equations is not necessary for the computation process. In this way the otherwise difficult task of choosing an appropriate regularization parameter for these model error function can be avoided. Moreover, one can reduce the resulting optimization problem without disadvantage to the unknown states and the model error functions in the state equations.

For linear ODE's with time independent coefficients and without inequality constraints it is shown that the regularized problem formulation is well-posed. However we see already in one-dimensional problems, that we can face large error propagation with respect to L_2 disturbances depending only on the model. For the, from the engineering side perhaps, more interesting case of L_∞ disturbances we have bounds independent of the model.

The evolving solution operators and their inverses are bounded. Nevertheless, a large spectral radius of the system matrix can lead to a large condition numbers. In addition the issue of observability comes into play, since also eigenvectors of the system matrix which are close to the null space of the output election matrix can cause arbitrary large norms. These condition numbers influence for example essentially the numerical solution process.

Finally, while long time horizons may be favourable for stability reasons concerning the confidence into the obtained measurements, from the point of view of the resulting system and estimating the initial data long horizons should be avoided, since they increase the condition number respectively the error propagation.

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