Parameter Estimation of Linear Dynamical Systems with Gaussian Noise

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Abstract—We present a novel optimization-based method for parameter estimation of a time-varying dynamic linear system. This method optimizes the likelihood of the parameters given measured data using an optimization algorithm tailored to the structure of this maximum likelihood estimation problem. Some parameters of the covariance process and measurement noise can also be estimated. This is particularly useful when offset-free Model Predictive Control with a linear disturbance model is performed. To reduce the complexity of the maximum likelihood estimation problem we also propose an approximate formulation and show how it is related to the actual problem. We present the advantages of the proposed approach over commonly used methods in the framework of Moving Horizon Estimation. We also present how to use Sequential Quadratic Programming efficiently for the optimization of our formulations. Finally, we show the performance of the proposed methods through numerical simulations. First, on a minimal example with only one parameter to be estimated, and second, on a system with heat and mass transfer. Both methods can successfully estimate the model parameters in these examples.

I. INTRODUCTION

Identifying a model from measurements is an important task, especially before Model Predictive Control (MPC) can be used to control a plant [1]. Indeed, to successfully implement MPC, an accurate model and reliable online state estimation are required. As for the first requirement, subspace methods for identifying linear systems are widely used [2]–[4]. However, these methods cannot enforce any particular structure, which is often given by the laws of physics. Parametric system identification overcomes this limitation [4]. For online state estimation of nonlinear systems, there are several methods such as the Extended Kalman Filter (EKF) or Moving Horizon Estimation [5], [6]. For linear systems, the Kalman filter is optimal and computationally favorable due to its closed form [7]. To apply one of these state estimation methods, it is often necessary to tune the covariances in the noise model using the available data. Several methods exist for this task, e.g., covariance matching [8], maximum likelihood approaches [9], [10], or correlation techniques [11]–[13]. The joint task of system identification and covariance estimation for the same operating data was studied in [14].

In this paper, we present a novel approach to parameter estimation for linear state-space systems. We first show the versatility of our problem formulation. Indeed, it can consider any differentiable parameterization of a linear system and prior knowledge in the form of convex inequality constraints. In addition, it can jointly estimate the parameters of the process, the state noise covariances, and the measurement noise covariances. In particular, we show that our framework can be used to identify linear disturbance models that are typically used for offset-free MPC [15]. We formulate the Maximum Likelihood (ML) estimation problem for this task and an approximate formulation. For input-to-output models, similar methods are discussed in [4] section 7.2. Similar methods for general nonlinear dynamics have also been presented in [16].

We prove a statistical result regarding our approach. Moreover, we show why our formulations provide better estimates than Trajectory Optimization (TO) methods for parameter estimation, which are widely used methods in Moving Horizon Estimation (MHE) settings [17]–[19]. We also discuss how to implement a suitable Sequential Quadratic Programming (SQP) algorithm to efficiently solve the resulting optimization problems. Finally, we show how this method can be used on two examples: a minimal example for illustration purposes, and a realistic example to show a typical use case of our algorithm. These examples also serve to assess the performance of the proposed methods in terms of prediction accuracy.

Outline: In Section III we define the estimation problem we are interested in and provide examples of what this class of problem can be used for. Section IV describes our methods. In Section V we compare the two methods with another common method in Subsection V-A and provide a statistical result about them. In Section VI we describe an optimization algorithm for the formulations presented in Section III. Section VII presents numerical results of the proposed method for two simple examples of systems.

Notation: We denote by $\mathcal{N}(\mu, \Sigma)$ the Gaussian distribution with mean $\mu \in \mathbb{R}^n$ and covariance matrix $\Sigma \in \mathbb{R}^{n \times n}$, and with $\mathcal{f}_{\text{gauss}}(x; \mu, \Sigma)$ its density function at the value $x$. We use $\mathcal{U}(a, b)$ for the uniform probability distribution on the interval $[a, b]$. We denote by $S_{n+} \subset \mathbb{R}^{n \times n}$ the set of symmetric Positive Definite (PD) matrices, and $S_{n}^{+} \subset \mathbb{R}^{n \times n}$ the set of symmetric Positive Semi-Definite (PSD) matrices. For a vector $e \in \mathbb{R}^n$ and a PD matrix $W \in S_{n+}^{+}$, we define the weighted norm $\|e\|_W := e^TW e$. For the unweighted $L_2$ norm, we omit the index: $\|e\|^2 := e^T e$. We write $|M|$ for the determinant of a square matrix $M \in \mathbb{R}^{n \times n}$. The symbol $I_n$ stands for the identity matrix. Throughout the paper, we use plain symbols for measured data (e.g. $y_k$) and hat symbols for estimates (e.g. $\hat{y}_k$).

II. PROBLEM STATEMENT

In this section, we define the class of parameter estimation problems we are interested in. We consider the following parametric linear discrete-time system with state and output
noise

\[ x_{k+1} = A_k(\alpha)x_k + b_k(\alpha) + w_k, \quad k = 0, \ldots, N - 1, \]
\[ y_k = C_k(\alpha)x_k + v_k, \quad k = 0, \ldots, N, \quad (1) \]
\[ w_k \sim \mathcal{N}(0, Q_k(\alpha)), \quad k = 0, \ldots, N - 1, \]
\[ v_k \sim \mathcal{N}(0, R_k(\alpha)), \quad k = 0, \ldots, N, \]

where \( x_k \in \mathbb{R}^{n_x} \), \( y_k \in \mathbb{R}^{n_y} \) are the states and the measurements while \( \alpha \in \mathbb{R}^{n_\alpha} \) stacks the unknown parameters of the dynamical model and of the noise covariance model. The functions \( A_k(\cdot), B_k(\cdot), C_k(\cdot), Q_k(\cdot), R_k(\cdot) \) are of appropriate dimensions and are assumed to be known. We assume that the random variables \( w_0, \ldots, w_{N-1} \) and \( v_0, \ldots, v_N \) are drawn independently. Additionally, we consider that the initial state comes from the following distribution

\[ x_0 \sim \mathcal{N}(\hat{x}_0, P_0), \quad (2) \]

with \( \hat{x}_0 \in \mathbb{R}^n \) and \( P_0 \in S_n^+ \) assumed to be known. Note that this assumption does not lead to any loss of generality, because choosing \( A_0(\alpha) \) and \( b_0(\alpha) \) is equivalent to choosing the Gaussian distribution of the state \( x_0 \).

The set of possible parameters \( \alpha \) is denoted by \( A \) and is assumed to be convex with the following form

\[ A := \{ \alpha \in \mathbb{R}^{n_\alpha} \mid h(\alpha) \leq 0 \}, \quad (3) \]

where all components of the function \( h : \mathbb{R}^{n_\alpha} \rightarrow \mathbb{R}^{n_h} \) are convex. This function might express prior knowledge about the parameters. For instance, it can specify the ranges in which the parameters can take value. It is also necessary to ensure that for any \( \alpha \in A \), the matrices \( Q_k(\alpha) \) and \( R_k(\alpha) \) are PD.

We assume that measurements are available, i.e., we know the sequence \( y_0, \ldots, y_N \). We denote by \( \mathcal{Y}_k \) the information set up to time \( k \) as \( \mathcal{Y}_k := \{ y_0, \ldots, y_k \} \). The task is to find the parameter \( \alpha \) which makes measurements as likely as possible.

A. Applications

\textit{a) Controlled data:} The equations (1) notably model the case where the dynamical equations contain inputs \( u_k \) which have already been chosen and are assumed to be known. Hence, these equations easily extend to the following case

\[ x_{k+1} = A(u_k, \alpha)x_k + b(u_k, \alpha) + w_k, \quad k = 0, \ldots, N - 1, \]
\[ y_k = C(u_k, \alpha)x_k + v_k, \quad k = 0, \ldots, N. \quad (4) \]

\textit{b) Scaling linear disturbance model:} One important application of this setting is the estimation of a disturbance model which can be used to achieve offset-free MPC [15]. The model is modified as follows

\[ x_{k+1} = A_k(\alpha)x_k + b_k(\alpha) + w^e_k, \quad k = 0, \ldots, N - 1, \]
\[ d_{k+1} = d_k + w^d_k, \quad k = 0, \ldots, N - 1, \]
\[ y_k = C_k(\alpha)x_k + d_k + v_k, \quad k = 0, \ldots, N. \quad (5) \]

The noise \( w_k := [w^e_k, w^d_k]^{T} \) now contains two terms with different meaning. Scaling them in general not obvious. This is why we propose the following parameterization, which falls into the class of systems that is considered

\[ \begin{bmatrix} w^e_k \\ w^d_k \end{bmatrix} \sim \mathcal{N}\left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \alpha_1 Q_x & 0 \\ 0 & \alpha_2 Q_d \end{bmatrix} \right), \quad k = 0, \ldots, N - 1, \]
\[ v_k \sim \mathcal{N}(0, \alpha_3 R), \quad k = 0, \ldots, N. \quad (6) \]

B. Kalman filter

For a given parameter \( \alpha \) and past measurements \( \mathcal{Y}_{k-1} \), the Kalman Filter (KF) yields a Gaussian probability density of the state \( x_k \) at time \( k \), which is defined by its mean \( \hat{x}_k \) and its covariance \( P_k \). Taken from [7], these are defined with the initial conditions \( \hat{x}_0, P_0 \) and the following recursive equations for \( k = 0, \ldots, N - 1 \)

\[ K_k = P_k C_k^{T} \left( C_k P_k C_k^{T} + R_k \right)^{-1}, \]
\[ \hat{x}_{k+1} = (A_k - K_k C_k) \hat{x}_k + K_k y_k + b_k, \]
\[ P_{k+1} = A_k (P_k - K_k C_k) A_k^{T} + Q_k, \quad (7) \]

where the matrix \( K_k \in \mathbb{R}^{n_x \times n_y} \) is called the Kalman gain. Note that we omitted the dependencies on \( \alpha \) for simplicity. We remark that \( P_k \) is independent of the initial state estimate \( \hat{x}_0 \) and measurements \( \mathcal{Y}_{k-1} \). This is due to the linearity of the model (1). The function that maps past data and parameters to the prediction of the next measurement and its covariance is given by

\[ \hat{y}_k(\alpha, \mathcal{Y}_{k-1}) := C_k \hat{x}_k, \]
\[ S_k(\alpha) := C_k P_k C_k^{T} + R_k. \quad (8) \]

Note that \( S_k(\alpha) \in S_{n_y}^{++} \) for any \( \alpha \in A \). It is proven in [7] that these estimates are exact in the case of a linear model. More precisely, the probability density function of \( y_k \) given the probabilistic model (1) for some \( \alpha \), and the measurements \( \mathcal{Y}_{k-1} \) is the following

\[ p(y_k \mid \mathcal{Y}_{k-1}, \alpha) = f_{\text{Gauss}}(y_k, \hat{y}_k(\alpha, \mathcal{Y}_{k-1}), S_k(\alpha)). \quad (9) \]

III. PROPOSED MAXIMUM LIKELIHOOD FORMULATIONS

Here we formulate two optimization problems that allow us to identify \( \alpha \) from the data \( \mathcal{Y}_N = \{ y_0, \ldots, y_N \} \). The first one is the Maximum Likelihood (ML) problem for identifying \( \alpha \) in the probabilistic model (1). The second one is simpler but only approximates the ML problem. Though similar formulations have been derived to estimate the matrices \( Q \) and \( R \) in [9], in this work we allow the joint estimation of parameters in the matrices \( Q \) and \( R \) and in the linear system.

A. Maximum Likelihood formulation

The ML estimation problem here consists in solving the following problem

\[ \maximize_{\alpha \in A} p(\mathcal{Y}_N \mid \alpha) \quad (10) \]

where \( p(\mathcal{Y}_N \mid \alpha) \) stands for the value of the probability density function of the measurements \( y_0, \ldots, y_N \) given the probabilistic model (1). We can write this problem explicitly, with the following proposition. The same formulation has been presented for a more general nonlinear system in [16]. Note,
however, that this formulation is the exact ML formulation only when the model is linear.

**Proposition 1.** The ML formulation \([10]\) is equivalent to the following optimization problem

\[
\text{minimize } \sum_{k=0}^{N} \| y_k - \hat{y}_k(\alpha, \mathbf{y}_{k-1}) \|^2_{S_k(\alpha)^{-1}} + \log |S_k(\alpha)|
\]

(11)

where \( \hat{y}_k(\alpha, \mathbf{y}_{k-1}) \) and \( S_k(\alpha) \) are defined in \([8]\).

**Proof.** Using basic probability rules, it is easy to derive the following formula

\[
p(Y_N | \alpha) = \prod_{k=0}^{N} p(y_k | Y_{k-1}, \alpha),
\]

where \( p(y_k | Y_{k-1}, \alpha) \) is defined in the previous section. Combining equations \((12)\) and \((9)\), the likelihood in \((10)\) can be written explicitly

\[
p(Y_N | \alpha) = \prod_{k=0}^{N} f_{\text{gauss}}(y_k, \hat{y}_k(\alpha, \mathbf{y}_{k-1}), S_k(\alpha)),
\]

\[
= \prod_{k=0}^{N} ((2\pi S_k(\alpha)))^{-\frac{1}{2}} e^{-\frac{1}{2} \| y_k - \hat{y}_k(\alpha, \mathbf{y}_{k-1}) \|^2_{S_k(\alpha)^{-1}}}
\]

Furthermore, maximizing the likelihood is equivalent to minimizing the following doubled negative log-likelihood

\[
-2 \log(p(Y_N | \alpha)) = \sum_{k=0}^{N} \| y_k - \hat{y}_k(\alpha, \mathbf{y}_{k-1}) \|^2_{S_k(\alpha)^{-1}} + \log |S_k(\alpha)| + n_y \log (2\pi)
\]

Finally, the additive constant \( n_y \log (2\pi) \) does not play any role in the optimization algorithm, hence it can be disregarded.

**Remark 1.** This ML formulation can be underdetermined depending on the choice of the uncertain parameters \( \alpha \). Indeed, it is possible that some parameters are impossible to estimate from the data. This might even happen when the linear state-space system \((1)\) is observable, as one can see in the example below. In this paper, we simply assume that the parameterization and the measured data are such that there is a unique parameter that maximizes the likelihood in \((10)\). We do not discuss the conditions for the problem \((10)\) to have a unique solution.

**Example 1.** Let us consider the following probabilistic model, which falls into the class of equations \((1)\)

\[
x_{k+1} = x_k + w_k, \quad k = 0, \ldots, N - 1
\]

\[
y_k = \alpha_1 x_k + v_k, \quad k = 0, \ldots, N
\]

\[
\begin{bmatrix}
\hat{w}_k \\
\hat{v}_k
\end{bmatrix}
\sim N
\begin{bmatrix}
0 \\
\alpha_2 0
\end{bmatrix}, \quad k = 0, \ldots, N.
\]

(13)

In this example, it is impossible to estimate the parameters \( \alpha_1, \alpha_2 \) from measurements. One can prove it for example by rewriting equations \((13)\) after the transformation \( \hat{x}_k = \frac{1}{\sqrt{\alpha_2}} x_k \), \( \hat{w}_k = \frac{1}{\sqrt{\alpha_2}} w_k \) as follows

\[
\hat{x}_{k+1} = \hat{x}_k + \hat{w}_k, \quad k = 0, \ldots, N - 1
\]

\[
y_k = \frac{\alpha_1}{\sqrt{\alpha_2}} \hat{x}_k + v_k, \quad k = 0, \ldots, N
\]

(14)

This system now only depends on \( \frac{\alpha_1}{\sqrt{\alpha_2}} \), hence, the couple \( (\alpha_1, \alpha_2) \) cannot be estimated.

**B. Approximate Maximum Likelihood formulation**

For large datasets, optimization problems of the form \((11)\) can be difficult to solve. One possibility is to approximate it by ignoring the innovation covariance \( S_k(\alpha) \) and replacing it by the identity matrix. This corresponds to minimizing the \( L_2 \) norm of the prediction error, as it is suggested in \([4, \text{equation (7.15)}]\) or in \([20]\). The Approximate Maximum Likelihood (AML) formulation is then stated as follows

\[
\text{minimize } \sum_{k=0}^{N} \| y_k - \hat{y}_k(\alpha, \mathbf{y}_{k-1}) \|^2_{S_k(\alpha)^{-1}}
\]

(15)

Note that in this formulation, when the chosen parameterization does not fix the scaling of the matrices \( Q \) and \( R \), the optimization problem \((15)\) always has infinitely many solutions. Indeed, we remark that the gain \( K_k \) in equations \((7)\) is invariant with respect to the scale of the triplet of matrices \((P_0, Q, R)\), hence the prediction \( \hat{y}_k(\alpha, \mathbf{y}_{k-1}) \) is also invariant with respect to this scale. To remove this undesired degree of freedom, one could restrict the feasible set \( \mathcal{A} \) with an equality constraint of the form \( g(\alpha) = 0 \).

Also note, however, that the system can still be underdetermined depending on the parameterization of the problem, as pointed out in Remark \(1\).

**C. Unifying formulation**

In this part we unify problems \((11)\) and \((15)\) under the same general problem. Note that we remove the dependency of \( \alpha \) in \( C_k(\alpha) \) for the sake of compactness, but the problem can easily be extended to the general case. Using equations \((7)\) and \((8)\), the problem is stated as follows

\[
\text{minimize } \sum_{k=0}^{N} L(e_k, S_k)
\]

subject to

\[
S_k = C_k P_k C_k^T + R_k(\alpha),
\]

\[
e_k = y_k - C_k \hat{x}_k,
\]

\[
\hat{x}_{k+1} = A_k(\alpha) \hat{x}_k + P_k C_k S_k^{-1} e_k + b_k(\alpha),
\]

\[
P_{k+1} = A_k(\alpha) (P - P C_k^T S_k^{-1} C_k P) A_k(\alpha)^T + Q_k(\alpha)
\]

where \( \alpha \in \mathcal{A} \) are the parameters, \( e := (e_0, \ldots, e_N) \) are the prediction errors, \( S := (S_0, \ldots, S_N) \) are the covariance matrices of the innovation, \( \hat{x} := (\hat{x}_1, \ldots, \hat{x}_N) \) are the state
predictions, and \( P := (P_1, \ldots, P_N) \) are the state prediction covariances. Note that the two first constraints of the optimization problem (16) are for \( k = 0, \ldots, N \) and the two last are for \( k = 0, \ldots, N - 1 \). Finally, \( L : \mathbb{R}^n_y \times S^+_1 \rightarrow \mathbb{R} \) is one of the following functions, depending on the chosen formulation

\[
L_{\text{ML}}(e, S) = e^\top S^{-1} e + \log |S|, \\
L_{\text{A--ML}}(e, S) = |e|^2.
\]  

While one can easily see the convexity of \( L_{\text{A--ML}}(\cdot, \cdot) \), function \( L_{\text{ML}}(\cdot, \cdot) \) is nonconvex. A possible way to handle this non-convexity is described in Section V.

IV. ANALYSIS OF THE FORMULATIONS

In this section, we derive some properties of the proposed methods. The first part compares our formulations with another one, namely, trajectory optimization for parameter estimation. The second provides part a statistical result concerning both formulations which justifies their use for estimation.

A. Comparison with trajectory optimization

The formulations stated so far fall into the class of prediction error estimation methods [20]. Another class of methods widely used for parameter estimation is Trajectory Optimization (TO) [17]-[19]. These methods are typically used in Moving Horizon Estimation (MHE) settings for jointly estimating the state and the parameters of a model. In this section, we show that these methods are in general sub-optimal compared to the presented ones and can fail to estimate some parameters.

In TO methods, when the matrices \( Q_k \) and \( R_k \) are fixed, the parameters are found by solving the following problem

\[
\begin{align*}
\text{minimize} & \quad \sum_{k=0}^{N-1} \| x_{k+1} - A_k(\alpha)x_k - b_k(\alpha) \|^2_{Q_k} \\
& + \sum_{k=0}^N \| C_k(\alpha)x_k - y_k \|^2_{R_k} \\
& + \| x_0 - \hat{x}_0 \|^2_{P_0^{-1}}
\end{align*}
\]  

which is proportional to the exponential of half the negative objective in (18), when the covariance matrices \( Q_k \) and \( R_k \) are independent of \( \alpha \).

Furthermore, note that the likelihood used in (10) can also be written as follows, using the law of total probability

\[
p(Y_N | \alpha) \propto \int_{\mathbb{R}^N_y} p(X_N, Y_N | \alpha) \, dX_N.
\]  

This formula gives a new perspective on TO for parameter estimation: it relies on the following approximation

\[
\begin{align*}
\max_{\alpha \in \mathcal{A}} & \quad \int_{\mathbb{R}^N_y} \phi_{\text{TO}}(\alpha, X_N) \, dX_N \\
\approx & \quad \max_{\alpha \in \mathcal{A}} \left( \max_{X_N \in \mathbb{R}^N_y} \phi_{\text{TO}}(\alpha, X_N) \right).
\end{align*}
\]  

While the latter approximation can sometimes give decent results, it fails in general to give an unbiased estimation of \( \alpha \) as we see in the example below.

Example 2. Let us consider the following probabilistic model, where only one parameter \( \alpha \) needs to be estimated

\[
\begin{align*}
x_{k+1} &= x_k + w_k, & k = 0, \ldots, N - 1, \\
y_k &= \alpha x_k + v_k, & k = 0, \ldots, N, \\
w_k &\sim \mathcal{N}(0, 1), & v_k &\sim \mathcal{N}(0, 1), & k = 0, \ldots, N, \\
x_0 &= 0.
\end{align*}
\]  

The task is to estimate \( \alpha \geq 0 \) from measurements \( y_0, \ldots, y_N \).

The TO formulation for the problem (22) reads

\[
\begin{align*}
\text{minimize} & \quad \sum_{k=0}^{N-1} (x_{k+1} - x_k)^2 + \sum_{k=0}^N (\alpha x_k - y_k)^2 \\
\text{subject to} & \quad \alpha \geq 0,
\end{align*}
\]  

For any number \( N \), and any sequence \( y_1, \ldots, y_N \), the solution of problem (24) can only be \( \alpha = +\infty \). Indeed, for \( x_k = \varepsilon y_k \) and \( \alpha = 1/\varepsilon \) with some \( \varepsilon > 0 \), the objective value of (24) is \( \varepsilon^2 \sum_{k=0}^{N-1} (y_{k+1} - y_k)^2 \) which is arbitrarily small when \( \varepsilon \) is close to zero. Hence, the TO method is totally incapable to estimate \( \alpha \) in this example. Meanwhile, formulations (10) and (15) provide a good estimation of \( \alpha \) as we show in Section VI-A. Figure 1 illustrates the objective functions corresponding to the problem (18), (10) and (15) for Example 2.

B. A statistical result concerning the method

The theorem below shows a statistical result concerning the ML and the A-ML formulations, which underscores the motivation for using them for parameter estimation. For this purpose, we first define the function \( \varphi(\cdot, \cdot) \) as the objective function of the problems (10) and (15)

\[
\varphi(\alpha, Y_N) := \sum_{k=0}^{N} \| y_k - \hat{y}_k(\alpha, Y_{k-1}) \|_{M_k(\alpha)}^2 - \log \left| M_k(\alpha) \right|,
\]  

where \( M_k(\alpha) = Q_k + \alpha R_k \) and \( \hat{y}_k(\alpha, Y_{k-1}) \) is the output estimate given by the ML. Theorem 1 shows that for any number \( N \), the covariance matrices \( Q_k \) and \( R_k \) are independent of \( \alpha \).
true parameter

Now note that both these inequalities are equalities when \( \alpha^* \) is independent of \( \alpha \). For the ML formulation, it uses the fact that for any PD matrix \( S \in S_{++}^n \), the convex function \( M \to \Tr(MS) - \log |M| \) reaches its minimum for \( M = S^{-1} \) and that \( \tilde{M}_k(\alpha^*) = S_k(\alpha^*)^{-1} \).

Remark that strong convergence theorems for this class of estimators are derived in [4, eq. (8.29)]. More precisely, the asymptotic behavior of the solution of prediction error methods when \( N \to \infty \) is described. Furthermore, let us remark that these results always concern the convergence to the set of minimizer of the expected value of the objective function

\[
\mathbb{E}_{Y_\infty} \left[ \lim_{N \to +\infty} [\varphi(\alpha, Y_N) | \alpha^*] \right].
\]

With the result of Theorem 1, we show that in our problem formulations the actual parameter \( \alpha^* \) belongs to this set.

V. OPTIMIZATION METHOD

To solve efficiently the problem [16], standard Nonlinear Programming (NLP) techniques can be used [21]. The problem being not convex, classical algorithms only yield local minima of the problem. However, we assume that a local minimum of the problem [16] already gives a correct estimate. A hand-tailored method benefits from the ability to compute derivatives of the constraints and objective functions in a more efficient way. In particular, the inverse matrices \( \tilde{S}_k^{-1} \) are computed only once, while they are used a few times, for example, in the constraints of (16), or in the derivatives of the term \( \log |\tilde{S}_k| \) in the objective. Due to the nonlinear constraints and the possibly nonconvex objective, we face a nonconvex optimization problem. Regarding the objective function, a convex Hessian approximation is usually required when Sequential Quadratic Programming (SQP) methods are used. Concerning the nonlinear constraints, these are simply linearized at each iteration of the algorithm. Finally, we choose to use single-shooting method here.

This sequential algorithm solves a Quadratic Program (QP) at each iteration, which results from a linearization of the constraints in (16) and a quadratic approximation of the function \( L(\cdot, \cdot) \) defined in (17). Note that \( L_{A-ML}(\cdot, \cdot) \) is already quadratic. For the function \( L_{ML}(\cdot, \cdot) \), we use the following convex quadratic approximation

\[
L_{ML}(e + \delta e, S + \delta S) \approx f_{quad}(\delta e, \delta S; e, S) + \log |S| + \Tr(\delta S S^{-1}),
\]

where \( f_{quad}(\delta e, \delta S; e, S) \) is the quadratic approximation of the convex function \( f(e, S) = e^\top S^{-1} e \) around the points \( (e, S) \), in the direction \( \delta e, \delta S \). This is defined in (29) in the Appendix, where also the convexity of \( f(\cdot, \cdot) \) and the derivation of its first and second derivatives needed for \( f_{quad} \) are shown in Proposition 2. Note that this quadratic approximation leads to an upper approximation of the Hessian of the concave function \( \log |\cdot| \) [22, Appendix A4].

The variable \( \alpha^* \) is updated in the direction found by the QP, using a globalization technique [21], typically a line-search.

![Figure 1. Objective functions for problems (15), (10) and (15) applied to the Example 2. The data \( Y_N \) is generated from the probabilistic model (22) with \( \alpha^* = 1 \) and \( N = 1000 \). Each objective function is transformed affinely such that its values are between 0 and 1 on the interval [0, 1].](image-url)
Eventually, the other optimization variables in (10) are updated by simulation of the system described by the constraints.

The resulting method is equivalent to the constrained Gauss-Newton (GN) method for the A-ML formulation [23]. For the ML formulation, this method is called the Generalized Gauss-Newton (GGN) method [24].

VI. NUMERICAL EXAMPLES

In this section we apply our method to two examples of parameter estimation problems. The first one is the minimal example from Example 2. The second is a larger problem where five parameters need to be estimated, including the noise covariance parameters. The purpose of this example is to investigate the performance of our methods on a more complex estimation task.

A. Simple example

In this part, we apply our method to the simple example from Example 2. This allows us to show that our methods succeed where the methods from TO fail. We also use this example to compare the performance and asymptotic behavior of the ML and A-ML formulations. It should be noted that in this example there is only one parameter to estimate and therefore the optimization problem has only one optimization variable. This allows the optimization algorithm described in Section V to be replaced by a simple line search.

For a first experiment, we generate measurement time series \(Y_{N,1}, \ldots, Y_{N,m}\) by simulating the system (22) with different parameters \(\alpha_{1}, \ldots, \alpha_{m} \in [0, 2]\). Then we compute the corresponding estimates \(\hat{\alpha}_{ML,i}\) and \(\hat{\alpha}_{A-ML,i}\) that solve the problems (10) and (15). Figure 2 shows the value of these estimates against the value of the true parameter \(\alpha^{*}\) for \(N = 50, 1000\) and \(m = 200\).

From this experiment, we observe that both the ML and the A-ML formulations provide good estimates, and a slightly better performance is observed for the ML formulation. Furthermore, as expected, the performance increases with the quantity of measurements \(N\).

To observe the asymptotic behavior of these estimates when \(N\) goes to infinity, we repeat the same experiment for many values of \(N\). For each of these, we compute the Mean Squared Error (MSE) as follows

\[
E_{\text{MSE}} = \frac{1}{m} \sum_{i=1}^{m} (\hat{\alpha}_i - \alpha_i)^2.
\]

The profile of the MSE as a function of \(N\) is depicted in Figure 3.

This profile seems to imply convergence the following result

\[
\mathbb{E}_{Y_N} \left[ ||\hat{\alpha}(Y_N) - \alpha^{*}||^2 \right] \sim C \frac{1}{N},
\]

with some constant \(C > 0\) different for each method.

B. Temperature control through conduction, mass transport and convective heat-transfer

We consider the problem of controlling the temperature of a fluid through conduction, mass transport, and convective heat transfer from an external temperature. We consider a “1-D” model where the fluid moves with velocity \(q_k\) along an axis. Convective heat transfer with an external temperature \(\theta_{ext}(t)\) is considered, the fluctuations of which are considered a disturbance. The temperature profile of the fluid is spatially discretized into 5 values. The first of them \(\theta_k^0\) is an input, while the rest together with the external temperature define the state of the system

\[
x_k := [\theta_k^1, \theta_k^2, \theta_k^3, \theta_k^4, \theta_k^{ext}]^T \in \mathbb{R}^5.
\]

We measure only the temperatures \(\theta_k^2\) and \(\theta_k^3\) with some additive measurement noise assumed to be independent and normally distributed with variance one. The system is depicted in Figure 4. The unknown parameters of the model equations are the coefficients \(a, b, \) and \(c\), which correspond to heat conduction, mass transfer, and convective heat transfer from
the external temperature, respectively. In addition, we consider normally distributed process noise with unknown variance. We denote $s_{\text{ext}}$ as the noise corresponding to the variations of the external temperature, and $s_Q$ as the noise applied to the remaining state components. Finally, all parameters are combined in the following vector

$$\alpha := [a \ b \ c \ s_Q \ s_{\text{ext}}]^{\top} \in \mathbb{R}^5. \quad (31)$$

The equations are translated into standard form (11) with the following, for $k = 0, \ldots, N - 1$

$$A_k(\alpha) := 0.05 \begin{bmatrix} \gamma_k - a & a & 0 & 0 & c \\ \tilde{a}_k & \gamma_k - a & a & 0 & c \\ 0 & \tilde{a}_k & \gamma_k - a & a & c \\ 0 & 0 & \tilde{a}_k & \gamma_k & c \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$b_k(\alpha) := 0.05 \begin{bmatrix} \tilde{a}_k \theta^Q_k \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}^{\top},$$

$$C_k(\alpha) := \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix},$$

$$Q_k(\alpha) := \text{diag}(0.1 s_Q, 0.1 s_Q, 0.1 s_Q, 0.1 s_Q, 4.0 s_{\text{ext}}).$$

$$R_k(\alpha) := I_2$$

with $\tilde{a}_k := a + bq_k$ and $\gamma_k := 1 - \tilde{a}_k - c$. Note that the numerical values in the above definitions are for scaling. We also choose a random profile for the inputs $\theta^Q_k$ and $q_k$, which are generated as piecewise constant functions. These are constantly equal to a value randomly chosen during 50 time steps. These values are drawn from the uniform distributions $\mathcal{U}(0, 200)$ for $\theta^Q_k$ and $\mathcal{U}(0, 20)$ for $q_k$. Finally, to sample the true parameters $\alpha^* := [a^* \ b^* \ c^* \ s_Q^* \ s_{\text{ext}}^*]$, we use independent uniform probability distributions $\mathcal{U}(0, 1)$ for each of the parameters. An example of a time series generated using this process is shown in Figure 5.

We sample data series by simulating the probabilistic model described for $m = 5$ different values of the true parameter $\alpha^*$. Then we apply the optimization algorithms described in Section V to the ML (11) and A-ML (15) formulations for each of the sampled data series.

Concerning the initial point, we choose $\alpha^0 = E[\alpha^*] = [0.5 \ 0.5 \ 0.5 \ 0.5 \ 0.5]$. Regarding the inequality constraints imposed, we choose $\mathcal{A} = [0, 1]^5$.

Finally, we perform the same experiment as in the previous example: we calculate the MSE of the two proposed estimates for different values of $N$. To better understand where the leading term of the error in this example comes from, we split the MSE for the parameters of the model and the parameters of the noise covariances. This is described by the following formula

$$E_{\text{MSE}}^{\text{model}} = \frac{1}{m} \sum_{i=1}^m (\hat{a}_i - a_i)^2 + (\hat{b}_i - b_i)^2 + (\hat{c}_i - c_i)^2,$$

$$E_{\text{MSE}}^{\text{noise}} = \frac{1}{m} \sum_{i=1}^m (s_{Q,i}^* - s_{Q,i})^2 + (s_{\text{ext},i}^* - s_{\text{ext},i})^2.$$  (33)

The MSE is plotted against the number of available data points in Figure 6. The results show that the parameters are correctly estimated on average, and it seems easier to fit model parameters than covariance parameters. With the parameters of the model fitting better than the parameters of the noise covariances, which seem more difficult to be estimated. We also note that the parameters of the noise covariances are better estimated with the ML formulation than with the A-ML. However, both methods give similar results in terms of the parameters of the model. Since neither the number of iterations required for convergence nor the stopping criterion of the SQP algorithm are discussed in this paper, we simply apply a fixed number of SQP iterations for each problem. This number of iterations is chosen to be sufficiently large; in this example it is fixed at 30 iterations. The efficiency and performance of the optimization algorithms is not part of this paper at hand, but is reserved for future research.

VII. CONCLUSION AND OUTLOOK

This paper presented a systematic method for formulating the maximum likelihood problem for estimating parameters of a linear model that might comprise disturbance models, together with a less complex approximate formulation. The theoretical properties shown for these formulations provide good reasons to use them as estimation methods. The optimization algorithms presented here show that these formulations are not only good in theory, but can also be used in practice. The ability of this method to estimate a model along with its associated perturbation parameters has been demonstrated in a realistic numerical example. However, the asymptotic behavior of the resulting estimator has not been proven, and
the efficiency of the algorithm has not been studied. A more
detailed description and analysis of this optimization method is
planned for a future publication, together with an open-source
fast implementation of the algorithm.

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APPENDIX

Proposition 2. The function $f : \mathbb{R}^n_v \times S^n_{++} \to \mathbb{R}$, $(e, S) \mapsto e^T S^{-1} e$ is convex. Its derivative in the direction $(\delta_e, \delta_S)$ and
evaluated for $(e, S)$ is the following quantity, after defining $M := S^{-1}$.

$$f'(e, S)[\delta_e, \delta_S] := 2\delta^T e M e - e^T (M \delta_S M) e.$$  \hfill (34)

Furthermore, its second derivative is the following positive quantity

$$f''(e, S)[\delta_e, \delta_S] := 2(\delta_e - \delta_S M e)^T M (\delta_e - \delta_S M e).$$  \hfill (35)

Proof. We fix some directions $(\delta_e, \delta_S) \in \mathbb{R}^n_v \times \mathbb{R}^{n_v \times n_v}$ for some symmetric matrix $\delta_S$, and evaluation point $(e, S) \in \mathbb{R}^n_v \times S^n_{++}$. We also define $M := S^{-1}$. For the derivation of the first derivative, the following holds

$$\frac{d}{dt} [f(e + t\delta_e, S + t\delta_S)]_{t=0} = \frac{d}{dt} \left[(e + t\delta_e)^T (S + t\delta_S)^{-1} (e + t\delta_e)\right]_{t=0} = 2\delta^T e M e - e^T (M \delta_S M e).$$

Concerning the second derivative, the following holds

$$\frac{d^2}{dt^2} [f(e + t\delta_e, S + t\delta_S)]_{t=0} = \frac{d^2}{dt^2} \left[(e + t\delta_e)^T (S + t\delta_S)^{-1} (e + t\delta_e)\right]_{t=0} + e^T \frac{d^2}{dt^2} \left[(S + t\delta_S)^{-1}\right]_{t=0} e$$

$$= 2\delta^T e M e - 4\delta^T e M \delta_S M e + 2e^T M \delta_S M \delta_S M e$$

$$= 2(\delta_e - \delta_S M e)^T M (\delta_e - \delta_S M e),$$

which is non-negative. This shows, in addition to the derivation of second derivatives, the convexity of $f(\cdot, \cdot)$.

We define the quadratic approximation of $f$ around the point $(e, S)$ by its second-order Taylor series as follows

$$f_{\text{quad}}(\delta_e, \delta_S; e, S) := f(e, S) + f'(e, S)[\delta_e, \delta_S]$$

$$+ \frac{1}{2} f''(e, S)[\delta_e, \delta_S].$$  \hfill (36)