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# Toward Tractable Global Solutions to Bayesian Point Estimation Problems via Sparse Sum-of-Squares Relaxations* 

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#### Abstract

Bayesian point estimation is commonly used for system identification owing to its good properties for small sample sizes. Although this type of estimator is usually nonparametric, Bayes estimates can also be obtained for rational parametric models, which is often of interest. However, as in maximum-likelihood methods, the Bayes estimate is typically computed via local numerical optimization that requires good initialization and cannot guarantee global optimality. In this contribution, we propose a computationally tractable method that computes the Bayesian parameter estimates with posterior certification of global optimality via sum-of-squares polynomials and sparse semidefinite relaxations. It is shown that the method is applicable to certain discrete-time linear models, which takes advantage of the rational structure of these models and the sparsity in the Bayesian parameter estimation problem. The method is illustrated on a simulation model of a resonant system that is difficult to handle when the sample size is small.


## I. INTRODUCTION

Bayesian point estimation is widely used for system identification and other contexts in parameter estimation, mostly owing to its good properties for small sample sizes [1]-[3]. The connection between Bayesian point estimation and regularization in the context of system identification of nonparametric models is known and allows observing that Bayesian point estimation is useful since it deals effectively with biasvariance tradeoff so as to minimize the mean squared error of the estimator [4]. However, its computational implementation for common parametric models is complicated by the fact that it results in nonconvex optimization problems and it is difficult to verify that the Bayes estimator is unique [5]. The performance of the prevalent local optimization algorithms is greatly dependent on the choice of the initial estimate and one cannot guarantee convergence to the global solution.

Alternatively, one could solve the Bayesian parameter estimation problem via appropriate global optimization methods. Several approaches for global optimization have been reported in the literature, for example the popular branch-and-bound approach. In this method, the space of decision variables is divided into several subsets and the global optimum is sought by estimating upper and lower bounds of the cost and constraints for each subset. Then, the subsets where an optimum cannot be located are excluded from the

[^0]search and the remaining subsets are subdivided until the global optimum is found [6]. However, its computationally cost can be high due to being a tree-based method that relies on discretization. The worst-case computational complexity grows exponentially with the problem size [7].

This paper uses another approach, namely, the reformulation as a convex problem via the concept of sum-of-squares polynomials, which has been extensively studied in algebraic geometry [8], [9] and applied to a wide variety of problems, including applications in control theory, experimental design, parameter initialization, and set-membership estimation [10]-[17]. In particular, it is shown that the rational structure of certain models, such as the models of discrete-time linear systems, leads to sparsity patterns in the Bayesian parameter estimation problems. One can then exploit this fact for tractable computation of global solutions via the concept of sum-of-squares polynomials and sparse semidefinite relaxations. Interestingly, the methodology is similar to the one used recently by the same authors for tractable computation of maximum-likelihood parameter estimates with posterior certification of global optimality [18].

## II. PRELIMINARIES

## A. Parameter estimation for linear models

Consider the estimation of the parameters of a discretetime, linear time-invariant (LTI), single-input single-output (SISO) model with output $y(t)$ and input $u(t)$. A strictly causal model of order $n_{x}$ is described by the transfer function

$$
\begin{equation*}
P_{d}(z)=\frac{\sum_{k=1}^{n_{x}} b_{k} z^{-k}}{\sum_{k=0}^{n_{x}} a_{k} z^{-k}}, \quad a_{0}=1 \tag{1}
\end{equation*}
$$

Assume that the output $y(t)$ is corrupted by additive noise $e(t)$, such that it is given by the output-error (OE) model

$$
\begin{equation*}
y(t)=P_{d}(z) u(t)+e(t) . \tag{2}
\end{equation*}
$$

Then, the inputs and outputs satisfy the relation
$\sum_{k=0}^{n_{x}} a_{k}(y(t-k)-e(t-k))=\sum_{k=1}^{n_{x}} b_{k} u(t-k), t=1, \ldots, N$,
with $e\left(1-n_{x}\right)=\ldots=e(0)=y\left(1-n_{x}\right)=\ldots=y(0)=u(1-$ $\left.n_{x}\right)=\ldots=u(-1)=0$, the system response $g(t)$ to the unit impulse $\delta$ satisfies the relation

$$
\begin{equation*}
\sum_{k=0}^{n_{x}} a_{k} g(t-k)=\sum_{k=1}^{n_{x}} b_{k} \delta(t-k), t=1, \ldots, N \tag{4}
\end{equation*}
$$

with $g\left(1-n_{x}\right)=\ldots=g(0)=0$, and the goal is the estimation of the OE model (3) specified by the parameters
$\boldsymbol{\theta}:=\left(a_{1}, \ldots, a_{n_{x}}, b_{1}, \ldots, b_{n_{x}}\right)$ based on the observations $\mathbf{y}:=$ $(y(1), \ldots, y(N))$ and the knowledge of the inputs, where $N$ is the sample size. In this paper, $e(t)$ denote the output errors that satisfy the equations (3) for the true values of $\boldsymbol{\theta}$.

An alternative and compact way to write (3) and (4) is

$$
\begin{align*}
\mathbf{A}(\boldsymbol{\theta})(\mathbf{y}-\mathbf{e}) & =\mathbf{H b}(\boldsymbol{\theta}),  \tag{5}\\
\mathbf{A}(\boldsymbol{\theta}) \mathbf{g} & =\mathbf{b}(\boldsymbol{\theta}), \tag{6}
\end{align*}
$$

where $\mathbf{e}:=(e(1), \ldots, e(N)), \mathbf{g}:=(g(1), \ldots, g(N))$, and

$$
\begin{align*}
\mathbf{A}(\boldsymbol{\theta}) & :=\mathscr{T}\left(\left[\begin{array}{llll}
a_{0} & \cdots & a_{n_{x}} & \mathbf{0}_{N-n_{x}-1}^{\mathrm{T}}
\end{array}\right]^{\mathrm{T}}\right),  \tag{7}\\
\mathbf{H} & :=\mathscr{T}\left(\left[\begin{array}{llll}
u(0) & \cdots & u(N-1)
\end{array}\right]^{\mathrm{T}}\right)  \tag{8}\\
\mathbf{b}(\boldsymbol{\theta}) & :=\left[\begin{array}{llll}
b_{1} & \cdots & b_{n_{x}} & \mathbf{0}_{N-n_{x}}^{\mathrm{T}}
\end{array}\right]^{\mathrm{T}} \tag{9}
\end{align*}
$$

with the operator

$$
\mathscr{T}\left(\left[\begin{array}{lll}
v_{1} & \cdots & v_{N}
\end{array}\right]^{\mathrm{T}}\right):=\left[\begin{array}{cccc}
v_{1} & 0 & \cdots & 0  \tag{10}\\
v_{2} & v_{1} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
v_{N} & v_{N-1} & \cdots & v_{1}
\end{array}\right]
$$

that forms a lower triangular Toeplitz matrix from a vector.
The equalities (5) and (6) have two known implications:

1) The impulse response coefficients $\mathbf{g}$ can be written as an explicit function $\mathbf{g}_{\boldsymbol{\theta}}$ of the parameters $\boldsymbol{\theta}$, that is,

$$
\begin{equation*}
\mathbf{g}=\mathbf{g}_{\boldsymbol{\theta}}(\boldsymbol{\theta})=\mathbf{A}(\boldsymbol{\theta})^{-1} \mathbf{b}(\boldsymbol{\theta}) . \tag{11}
\end{equation*}
$$

2) The outputs $\mathbf{y}$ can be written as an explicit function of the parameters $\boldsymbol{\theta}$ and output errors $\mathbf{e}$, that is,

$$
\begin{equation*}
\mathbf{y}=\mathbf{A}(\boldsymbol{\theta})^{-1} \mathbf{H} \mathbf{b}(\boldsymbol{\theta})+\mathbf{e}=\mathbf{H g}+\mathbf{e} \tag{12}
\end{equation*}
$$

since $\mathbf{A}(\boldsymbol{\theta}) \mathbf{H}=\mathbf{H A}(\boldsymbol{\theta})$, which follows from the fact that $\mathbf{A}(\boldsymbol{\theta})$ and $\mathbf{H}$ are lower triangular Toeplitz matrices.

## III. PARAMETER ESTIMATION PROBLEM

## A. Bayesian parameter estimation for linear models

Below, we review some concepts of Bayesian point estimation, in the context of estimation of the impulse response coefficients $\mathbf{g}$ in the set $\mathscr{G}$ that are compatible with parametric models specified by $\boldsymbol{\theta}$ from the data $\mathbf{y}$ in the set $\mathscr{Y}$. The estimation uses decision rules $\boldsymbol{\delta}$ in the set $\mathscr{D}$, which maps the data $\mathbf{y}$ to actions $\hat{\mathbf{g}}$ in the set $\mathscr{A} \subseteq \mathscr{G}$, that is, $\mathscr{D}=(\mathscr{Y} \rightarrow \mathscr{A})$.

Furthermore, $L(\mathbf{g}, \hat{\mathbf{g}})$ denotes a loss function, while a probability density function (p.d.f.) of a distribution related to probability of occurrence and degree of belief is denoted by $f$ and $\pi$, respectively. In particular, $\pi(\mathbf{g})$ and $f(\mathbf{y} \mid \mathbf{g})$ denote a prior p.d.f. and a likelihood function that will be defined later, which result in a marginal likelihood $f(\mathbf{y}):=$ $\int_{\mathscr{G}} f(\mathbf{y} \mid \mathbf{g}) \pi(\mathbf{g}) \mathrm{d} \mathbf{g}$ and a posterior p.d.f. $\pi(\mathbf{g} \mid \mathbf{y}):=\frac{f(\mathbf{y} \mid \mathbf{g}) \pi(\mathbf{g})}{f(\mathbf{y})}$.

The risk function is defined as

$$
\begin{equation*}
R(\mathbf{g}, \boldsymbol{\delta}):=\int_{\mathscr{Y}} L(\mathbf{g}, \boldsymbol{\delta}(\mathbf{y})) f(\mathbf{y} \mid \mathbf{g}) \mathrm{d} \mathbf{y} \tag{13}
\end{equation*}
$$

while the posterior expected loss is defined as

$$
\begin{equation*}
\rho(\mathbf{y}, \hat{\mathbf{g}}):=\int_{\mathscr{G}} L(\mathbf{g}, \hat{\mathbf{g}}) \pi(\mathbf{g} \mid \mathbf{y}) \mathrm{d} \mathbf{g}, \tag{14}
\end{equation*}
$$

which means that the average risk is

$$
\begin{aligned}
& r(\boldsymbol{\delta}):=\int_{\mathscr{G}} R(\mathbf{g}, \boldsymbol{\delta}) \pi(\mathbf{g}) \mathrm{d} \mathbf{g}=\int_{\mathscr{G}} \int_{\mathscr{\mathscr { O }}} L(\mathbf{g}, \boldsymbol{\delta}(\mathbf{y})) f(\mathbf{y} \mid \mathbf{g}) \mathrm{d} \mathbf{y} \pi(\mathbf{g}) \mathrm{d} \mathbf{g} \\
& =\int_{\mathscr{Y}} \int_{\mathscr{G}} L(\mathbf{g}, \boldsymbol{\delta}(\mathbf{y})) \pi(\mathbf{g} \mid \mathbf{y}) \mathrm{d} \mathbf{g} f(\mathbf{y}) \mathrm{d} \mathbf{y}=\int_{\mathscr{Y}} \rho(\mathbf{y}, \boldsymbol{\delta}(\mathbf{y})) f(\mathbf{y}) \mathrm{d} \mathbf{y} .(15)
\end{aligned}
$$

Since the Bayes estimator is defined as [1]

$$
\begin{equation*}
\boldsymbol{\delta}_{B E}^{*}:=\arg \min _{\boldsymbol{\delta}} r(\boldsymbol{\delta}) \text { s.t. } \boldsymbol{\delta} \in \mathscr{D} \tag{16}
\end{equation*}
$$

and $\boldsymbol{\delta}_{B E}^{*}$ can be chosen individually for each $\mathbf{y}$ so as to minimize (15), the Bayes estimate is

$$
\begin{equation*}
\boldsymbol{\delta}_{B E}^{*}(\mathbf{y})=\arg \min _{\hat{\mathbf{g}}} \rho(\mathbf{y}, \hat{\mathbf{g}}) \text { s.t. } \hat{\mathbf{g}} \in \mathscr{A} \tag{17}
\end{equation*}
$$

The use of $q(\boldsymbol{\delta}):=-\int_{\mathscr{Y}} \pi(\boldsymbol{\delta}(\mathbf{y}) \mid \mathbf{y}) f(\mathbf{y}) \mathrm{d} \mathbf{y}$ in lieu of $r(\boldsymbol{\delta})$ allows defining the maximum a posteriori (MAP) estimator

$$
\begin{equation*}
\boldsymbol{\delta}_{M A P}^{*}:=\arg \max _{\boldsymbol{\delta}}-q(\boldsymbol{\delta}) \text { s.t. } \boldsymbol{\delta} \in \mathscr{D} \tag{18}
\end{equation*}
$$

which, by using similar arguments, yields the MAP estimate

$$
\begin{equation*}
\boldsymbol{\delta}_{M A P}^{*}(\mathbf{y})=\arg \max _{\hat{\mathbf{g}}} \pi(\hat{\mathbf{g}} \mid \mathbf{y}) \text { s.t. } \hat{\mathbf{g}} \in \mathscr{A} \tag{19}
\end{equation*}
$$

Since we are interested in impulse response coefficients $\mathbf{g}$ that are compatible with parametric models specified by $\boldsymbol{\theta}$, we restrict the previous estimates to actions in the set

$$
\begin{equation*}
\mathscr{A}=\left\{\hat{\mathbf{g}} \in \mathscr{G}: \exists \boldsymbol{\theta} \hat{\mathbf{g}}=\mathbf{g}_{\boldsymbol{\theta}}(\boldsymbol{\theta})\right\} \tag{20}
\end{equation*}
$$

Since $\mathbf{y}=\mathbf{H g}+\mathbf{e}$ according to (12), the p.d.f. $f(\mathbf{y} \mid \mathbf{g})$ is determined by the distributions of the random variables with the realizations $e(1), \ldots, e(N)$. If we assume that (i) these random variables are independent and identically distributed (i.i.d.), which implies that $e(1), \ldots, e(N)$ can be seen as realizations of the same random variable $E$, and (ii) $E$ is normally distributed with zero mean and variance $\sigma^{2}$, then

$$
\begin{equation*}
f(\mathbf{y} \mid \mathbf{g})=p\left(\mathbf{y} \mid \mathbf{H g}, \sigma^{2} \mathbf{I}_{N}\right) \tag{21}
\end{equation*}
$$

where $p\left(\mathbf{x} \mid \overline{\mathbf{x}}, \boldsymbol{\Sigma}_{\mathbf{x}}\right)$ is the p.d.f. of the multivariate normal distribution with mean $\overline{\mathbf{x}}$ and covariance $\boldsymbol{\Sigma}_{\mathbf{x}}$ [3].

Furthermore, we assume here that the prior p.d.f. also corresponds to a normal distribution and is given by

$$
\begin{equation*}
\pi(\mathbf{g})=p\left(\mathbf{g} \mid \mathbf{0}_{N}, \mathbf{K}\right) \tag{22}
\end{equation*}
$$

with symmetric $\mathbf{K}$. One can show that this implies that [3]

$$
\begin{align*}
& f(\mathbf{y})=p\left(\mathbf{y} \mid \mathbf{0}_{N}, \boldsymbol{\Sigma}_{\mathbf{y}}\right),  \tag{23}\\
& \pi(\mathbf{g} \mid \mathbf{y})=p\left(\mathbf{g} \mid \overline{\mathbf{g}}, \boldsymbol{\Sigma}_{\mathbf{g}}\right) \tag{24}
\end{align*}
$$

with

$$
\begin{align*}
\boldsymbol{\Sigma}_{\mathbf{y}} & =\sigma^{2} \mathbf{I}_{N}+\mathbf{H K} \mathbf{H}^{\mathrm{T}}  \tag{25}\\
\overline{\mathbf{g}} & =\left(\mathbf{H}^{\mathrm{T}} \mathbf{H}+\sigma^{2} \mathbf{K}^{-1}\right)^{-1} \mathbf{H}^{\mathrm{T}} \mathbf{y}  \tag{26}\\
\boldsymbol{\Sigma}_{\mathbf{g}} & =\sigma^{2}\left(\mathbf{H}^{\mathrm{T}} \mathbf{H}+\sigma^{2} \mathbf{K}^{-1}\right)^{-1} \tag{27}
\end{align*}
$$

We also assume that the loss function corresponds to the mean squared error (MSE) weighted by some matrix $\mathbf{W}$

$$
\begin{equation*}
L(\mathbf{g}, \hat{\mathbf{g}})=\frac{1}{N}\|\mathbf{g}-\hat{\mathbf{g}}\|_{\mathbf{W}}^{2} \tag{28}
\end{equation*}
$$

with the notation $\|\mathbf{g}\|_{\mathbf{w}}=\sqrt{\mathbf{g}^{\mathbf{T}} \mathbf{W g}}$ used in the paper. Then, for the constrained case $\hat{\mathbf{g}} \in \mathscr{A}$, we can show the following result, which is well known in the unconstrained case $\hat{\mathbf{g}} \in \mathscr{G}$.

Theorem 1: Suppose that the loss function is given by (28) with $\mathbf{W}=\sigma^{2} \boldsymbol{\Sigma}_{\mathbf{g}}^{-1}$. Then, the estimates (17) and (19) satisfy

$$
\begin{equation*}
\boldsymbol{\delta}_{B E}^{*}(\mathbf{y})=\boldsymbol{\delta}_{M A P}^{*}(\mathbf{y})=\arg \min _{\hat{\mathbf{g}}} \frac{\sigma^{2}}{N}\|\overline{\mathbf{g}}-\hat{\mathbf{g}}\|_{\mathbf{\Sigma}_{\mathbf{g}}^{-1}}^{2} \text { s.t. } \hat{\mathbf{g}} \in \mathscr{A} . \tag{29}
\end{equation*}
$$

Proof: One can consider (17) and (19) and observe that

$$
\begin{align*}
& \rho(\mathbf{y}, \hat{\mathbf{g}})= \int_{\mathscr{G}} \frac{1}{N}\|\mathbf{g}-\overline{\mathbf{g}}\|_{\mathbf{W}}^{2} p\left(\mathbf{g} \mid \overline{\mathbf{g}}, \boldsymbol{\Sigma}_{\mathbf{g}}\right) \mathrm{d} \mathbf{g} \\
&+\int_{\mathscr{G}} \frac{1}{N}\|\overline{\mathbf{g}}-\hat{\mathbf{g}}\|_{\mathbf{W}}^{2} p\left(\mathbf{g} \mid \overline{\mathbf{g}}, \boldsymbol{\Sigma}_{\mathbf{g}}\right) \mathrm{d} \mathbf{g} \\
&+\int_{\mathscr{G}} \frac{2}{N}(\mathbf{g}-\overline{\mathbf{g}})^{\mathrm{T}} \mathbf{W}(\overline{\mathbf{g}}-\hat{\mathbf{g}}) p\left(\mathbf{g} \mid \overline{\mathbf{g}}, \boldsymbol{\Sigma}_{\mathbf{g}}\right) \mathrm{d} \mathbf{g} \\
&= \frac{1}{N} \operatorname{tr}\left(\mathbf{W} \boldsymbol{\Sigma}_{\mathbf{g}}\right)+\frac{1}{N}\|\overline{\mathbf{g}}-\hat{\mathbf{g}}\|_{\mathbf{W}}^{2}  \tag{30}\\
& \frac{2 \sigma^{2}}{N} \log \pi(\hat{\mathbf{g}} \mid \mathbf{y})=-\frac{\sigma^{2}}{N}\|\hat{\mathbf{g}}-\overline{\mathbf{g}}\|_{\boldsymbol{\Sigma}_{\mathbf{g}}^{-1}}^{2}-\frac{\sigma^{2}}{N} \log \frac{\operatorname{det}\left(\boldsymbol{\Sigma}_{\mathbf{g}}\right)}{(2 \pi)^{-N}} \tag{31}
\end{align*}
$$

which implies that (29) holds as claimed.
Hence, we denote these estimates as $\boldsymbol{\delta}^{*}(\mathbf{y})$ and note that

$$
\begin{align*}
\boldsymbol{\delta}^{*}(\mathbf{y}) & =\arg \min _{\hat{\mathbf{g}}} \frac{\sigma^{2}}{N}\|\hat{\mathbf{g}}\|_{\mathbf{\Sigma}_{\mathbf{g}}^{-1}}^{2}-\frac{2 \sigma^{2}}{N} \hat{\mathbf{g}}^{\mathrm{T}} \boldsymbol{\Sigma}_{\mathbf{g}}^{-1} \overline{\mathbf{g}} \text { s.t. } \hat{\mathbf{g}} \in \mathscr{A} \\
& =\arg \min _{\hat{\mathbf{g}}} \frac{1}{N}\|\hat{\mathbf{g}}\|_{\mathbf{H}^{\mathrm{T}} \mathbf{H}+\sigma^{2} \mathbf{K}^{-1}}^{2}-\frac{2}{N} \hat{\mathbf{g}}^{\mathrm{T}} \mathbf{H}^{\mathrm{T}} \mathbf{y} \text { s.t. } \hat{\mathbf{g}} \in \mathscr{A} \\
& =\arg \min _{\hat{\mathbf{g}}} \frac{1}{N}\|\hat{\mathbf{g}}\|_{\mathbf{D}}^{2}+\frac{1}{N} \| \mathbf{y}-\mathbf{H} \hat{\mathbf{I}_{N}} \mathbf{I}^{2} \text { s.t. } \hat{\mathbf{g}} \in \mathscr{A}, \tag{32}
\end{align*}
$$

that is, $\boldsymbol{\delta}^{*}(\mathbf{y})$ is the solution to a nonlinearly constrained, regularized least-squares problem with a regularization matrix $\mathbf{D}=\sigma^{2} \mathbf{K}^{-1}$. The fact that $\boldsymbol{\delta}^{*}(\mathbf{y}) \in \mathscr{A}$ allows defining properly (i) the estimate of $\boldsymbol{\theta}$ given by $\left\{\boldsymbol{\theta}: \mathbf{A}(\boldsymbol{\theta}) \boldsymbol{\delta}^{*}(\mathbf{y})=\mathbf{b}(\boldsymbol{\theta})\right\}$ and (ii) the cost that $\boldsymbol{\delta}^{*}(\mathbf{y})$ minimizes as the function of $\boldsymbol{\theta}$

$$
\begin{equation*}
\hat{J}(\boldsymbol{\theta}):=\frac{\sigma^{2}}{N}\|\overline{\mathbf{g}}-\hat{\mathbf{g}}\|_{\boldsymbol{\Sigma}_{\mathbf{g}}^{-1}}^{2} . \tag{33}
\end{equation*}
$$

One can also write $\hat{J}(\boldsymbol{\theta})$ in terms of prediction errors as

$$
\begin{align*}
\hat{J}(\boldsymbol{\theta}) & =\frac{1}{N}\|\overline{\mathbf{g}}-\hat{\mathbf{g}}\|_{\mathbf{W}}^{2} \\
& =\frac{1}{N}\|\overline{\mathbf{y}}-\hat{\mathbf{y}}\|_{\mathbf{I}_{N}}^{2}+\frac{1}{N}\|\overline{\mathbf{g}}-\hat{\mathbf{g}}\|_{\mathbf{D}}^{2} \\
& =\frac{1}{N}\|\hat{\mathbf{e}}\|_{\mathbf{I}_{N}}^{2}+\frac{1}{N}\|\hat{\mathbf{d}}\|_{\mathbf{D}}^{2} \tag{34}
\end{align*}
$$

with $\mathbf{W}=\mathbf{H}^{\mathrm{T}} \mathbf{H}+\mathbf{D}, \overline{\mathbf{g}}=\left(\mathbf{H}^{\mathrm{T}} \mathbf{H}+\mathbf{D}\right)^{-1} \mathbf{H}^{\mathrm{T}} \mathbf{y}, \hat{\mathbf{y}}:=\mathbf{H} \hat{\mathbf{g}}$, and $\overline{\mathbf{y}}:=\mathbf{H} \overline{\mathbf{g}}$, and the prediction errors $\hat{\mathbf{d}}:=\overline{\mathbf{g}}-\hat{\mathbf{g}}$ and $\hat{\mathbf{e}}:=\overline{\mathbf{y}}-\hat{\mathbf{y}}$.

Note that the estimate $\boldsymbol{\delta}^{*}(\mathbf{y})$ is the vector-valued counterpart of the one in Proposition 4 by [2] that is also valid when $\mathbf{W}$ is not diagonal, and it is similar to an estimate that was recently suggested [5]. However, this section motivates it as a straightforward and unambiguous consequence of the use of concepts of Bayesian point estimation that bridges the gap between nonparametric and parametric models.

Hence, the Bayesian point estimation of $\boldsymbol{\theta}$ in the case of i.i.d. Gaussian noise and normal prior distribution is formulated as the following constrained optimization problem:

$$
\begin{align*}
& \min _{\boldsymbol{\theta}, \hat{\mathbf{d}}, \hat{\mathbf{e}}} \frac{1}{N} \hat{\mathbf{e}}^{\mathrm{T}} \hat{\mathbf{e}}+\frac{1}{N} \hat{\mathbf{d}}^{\mathrm{T}} \mathbf{D} \hat{\mathbf{d}}  \tag{35a}\\
& \text { s.t. } \mathbf{A}(\boldsymbol{\theta})(\hat{\mathbf{d}}-\overline{\mathbf{g}})+\mathbf{b}(\boldsymbol{\theta})=\mathbf{0}_{N},  \tag{35b}\\
& \mathbf{A}(\boldsymbol{\theta})(\hat{\mathbf{e}}-\overline{\mathbf{y}})+\mathbf{H b}(\boldsymbol{\theta})=\mathbf{0}_{N} . \tag{35c}
\end{align*}
$$

Note that (i) the first $N$ equality constraints can be expressed linearly in the $N$ variables $\hat{\mathbf{d}}$, and (ii) the last $N$ equality constraints can be expressed linearly in the $N$ variables $\hat{\mathbf{e}}$. Also, we assume in the remainder that $\mathbf{D}$ is a tridiagonal matrix (only the main diagonal, the first diagonal above the main one, and the first diagonal under the main one are nonzero) since this yields a sparse estimation problem.

It is then possible to formulate (35) explicitly using $\hat{\mathbf{d}}=$ $(\hat{d}(1), \ldots, \hat{d}(N)), \hat{\mathbf{e}}=(\hat{e}(1), \ldots, \hat{e}(N))$ as decision variables:

$$
\begin{align*}
& \min _{\boldsymbol{\theta}, \hat{\mathbf{d}}, \hat{\mathbf{e}}} \sum_{t=1}^{N} \frac{\hat{e}(t)^{2}+D_{t, t} \hat{d}(t)^{2}}{N}+\sum_{t=2}^{N} \frac{2 D_{t, t-1} \hat{d}(t) \hat{d}(t-1)}{N},  \tag{36a}\\
& \text { s.t. } \hat{d}(t)-\bar{g}(t)+\sum_{k=1}^{n_{x}} a_{k}(\hat{d}(t-k)-\bar{g}(t-k))+b_{k} \delta(t-k)=0, \\
& t=1, \ldots, N,  \tag{36b}\\
& \hat{e}(t)-\bar{y}(t)+\sum_{k=1}^{n_{x}} a_{k}(\hat{e}(t-k)-\bar{y}(t-k))+b_{k} u(t-k)=0, \\
& t=1, \ldots, N . \tag{36c}
\end{align*}
$$

Alternatively, one can solve the $2 N$ equality constraints in the constrained problem (35) for the $2 N$ decision variables $\hat{\mathbf{d}}, \hat{\mathbf{e}}$ and formulate an equivalent unconstrained problem:

$$
\begin{equation*}
\min _{\boldsymbol{\theta}} \frac{1}{N}\left(\overline{\mathbf{g}}-\mathbf{A}(\boldsymbol{\theta})^{-1} \mathbf{b}(\boldsymbol{\theta})\right)^{\mathrm{T}} \mathbf{W}\left(\overline{\mathbf{g}}-\mathbf{A}(\boldsymbol{\theta})^{-1} \mathbf{b}(\boldsymbol{\theta})\right) \tag{37}
\end{equation*}
$$

Although $\mathbf{A}(\boldsymbol{\theta})$ is a lower triangular Toeplitz matrix with $\operatorname{det}(\mathbf{A}(\boldsymbol{\theta}))=1$, which simplifies its inversion, the cost function of this unconstrained optimization problem is typically a polynomial of high degree (up to $2 N$ ) in $\boldsymbol{\theta}$.

Unfortunately, both (36) and (37) are nonconvex problems, which means that local optimization algorithms are prone to attain local optima and cannot guarantee global optimality. Hence, it would be useful to find a method that is able to converge to the global optimum and certify this convergence. The concept of sum-of-squares polynomials that is used for global optimization in the paper is introduced in Appendix A.

## B. Choice of regularization matrix

Regarding the matrix $\mathbf{K}$ that results in the regularization matrix $\mathbf{D}$, it can be chosen by making $\mathbf{K}$ depend on some hyperparameters $\boldsymbol{\eta}$ according to a predefined structure, that is, $\mathbf{K}(\boldsymbol{\eta})$ and $\mathbf{D}(\boldsymbol{\eta})=\sigma^{2} \mathbf{K}(\boldsymbol{\eta})^{-1}$. As mentioned, in this paper we restrict the analysis to matrices $\mathbf{K}(\boldsymbol{\eta})$ that result in tridiagonal matrices $\mathbf{D}(\boldsymbol{\eta})$, which is sufficient to handle the typical diagonal, diagonal/correlated, and tuned/correlated structures of $\mathbf{K}(\boldsymbol{\eta})$ [3], [4]. For example, one can use a diagonal/correlated structure $K(\boldsymbol{\eta})_{i, j}=c \lambda^{(i+j) / 2} \alpha^{|i-j|}$, with $\boldsymbol{\eta}=(c, \lambda, \alpha), c \geq 0,0 \leq \lambda \leq 1,|\alpha| \leq 1$, or a diagonal structure that is obtained by fixing $\alpha=0$. To estimate the hyperparameters $\boldsymbol{\eta}$ from the data $\mathbf{y}$, one can maximize the marginal likelihood $f(\mathbf{y})$, which corresponds to the problem

$$
\begin{equation*}
\hat{\boldsymbol{\eta}}=\arg \max _{\boldsymbol{\eta}} f(\mathbf{y}) \tag{38}
\end{equation*}
$$

where

$$
\begin{equation*}
\frac{2 \sigma^{2}}{N} \log f(\mathbf{y})=-\frac{\sigma^{2}}{N}\|\mathbf{y}\|_{\Sigma_{\mathbf{y}}(\boldsymbol{\eta})^{-1}}^{2}-\frac{\sigma^{2}}{N} \log \frac{\operatorname{det}\left(\boldsymbol{\Sigma}_{\mathbf{y}}(\boldsymbol{\eta})\right)}{(2 \pi)^{-N}} \tag{39}
\end{equation*}
$$

which implies that, since $\boldsymbol{\Sigma}_{\mathbf{y}}(\boldsymbol{\eta})=\sigma^{2}\left(\mathbf{I}_{N}+\mathbf{H D}(\boldsymbol{\eta})^{-1} \mathbf{H}^{\mathrm{T}}\right)$,

$$
\begin{equation*}
\hat{\boldsymbol{\eta}}=\arg \min _{\boldsymbol{\eta}} \frac{1}{N}\|\mathbf{y}\|_{\mathbf{V}(\boldsymbol{\eta})}^{2}+\frac{\sigma^{2}}{N} \log \frac{\operatorname{det}\left(\mathbf{V}(\boldsymbol{\eta})^{-1}\right)}{\left(2 \pi \sigma^{2}\right)^{-N}} \tag{40}
\end{equation*}
$$

with $\mathbf{V}(\boldsymbol{\eta}):=\left(\mathbf{I}_{N}+\mathbf{H D}(\boldsymbol{\eta})^{-1} \mathbf{H}^{\mathrm{T}}\right)^{-1}$. This problem is nonconvex but involves only a few hyperparameters. The chosen regularization matrix $\mathbf{D}(\boldsymbol{\eta})$ affects the estimation of $\boldsymbol{\theta}$.

## IV. GLOBAL SOLUTIONS TO BAYESIAN POINT ESTIMATION PROBLEMS FOR LINEAR MODELS

This section contains a main contribution of this paper since it shows how to apply the concept of SOS polynomials presented in Appendix A to obtain tractable global solutions to the Bayesian point estimation problems in Section III-A, which is not obvious without the following results.

It has been shown in Section III-A that the Bayesian point estimation problem for the model in (3) can be formulated as the constrained problem (36) or the unconstrained problem (37). Using the notation in Appendix A, the problem (36) involves $n=2 N+2 n_{x}$ decision variables, and each polynomial in the cost function and the constraints is at most of degree 2 , which means that $v=1$, whereas the problem (37) involves $n=2 n_{x}$ decision variables, and the cost function is of degree $2 N$, which means that $v=N$. Since each relaxation order $d$ in the hierarchy of nonsparse semidefinite relaxations requires solving one LMI of size $\binom{n+d}{n}$, with $d \geq v$, both problem formulations become intractable for large $N$.

However, one can note that, in the problem (36), each equality constraint corresponds to a quadratic polynomial that involves only the $2 n_{x}$ variables $\boldsymbol{\theta}$ and $n_{x}+1$ variables from $\hat{\mathbf{d}}$ or $\hat{\mathbf{e}}$, and the cost function can be written as a sum of quadratic polynomials that involve only a few variables. This allows the use of sparse semidefinite relaxations if each equality constraint is transformed into a pair of inequality constraints to obtain a basic semi-algebraic set.

Hence, we introduce the following definitions:

$$
\begin{align*}
& f(\mathbf{x}):=J(\mathbf{x})-\tau,  \tag{41a}\\
& g_{j}(\mathbf{x}):=\left\{\begin{array}{l}
-h_{j}^{d}(\mathbf{x}), j=1, \ldots, N, \\
-h_{j-N}^{e}(\mathbf{x}), j=N+1, \ldots, 2 N, \\
h_{j-2 N}^{d}(\mathbf{x}), j=2 N+1, \ldots, 3 N, \\
h_{j-3 N}^{e}(\mathbf{x}), j=3 N+1, \ldots, 4 N,
\end{array}\right. \tag{41b}
\end{align*}
$$

with $\mathbf{x}:=(\boldsymbol{\theta}, \hat{\mathbf{d}}, \hat{\mathbf{e}})=\left(a_{1}, \ldots, a_{n_{x}}, b_{1}, \ldots, b_{n_{x}}, \hat{d}(1), \ldots, \hat{d}(N)\right.$, $\hat{e}(1), \ldots, \hat{e}(N))$ and

$$
\begin{array}{r}
J(\mathbf{x}):=\sum_{t=1}^{N} \frac{\hat{e}(t)^{2}+D_{t, t} \hat{d}(t)^{2}}{N}+\sum_{t=2}^{N} \frac{2 D_{t, t-1} \hat{d}(t) \hat{d}(t-1)}{N}, \\
h_{t}^{d}(\mathbf{x}):=\hat{d}(t)-\bar{g}(t)+\sum_{k=1}^{n_{x}} a_{k}(\hat{d}(t-k)-\bar{g}(t-k))+b_{k} \delta(t-k), \\
t=1, \ldots, N \\
h_{t}^{e}(\mathbf{x}):=\hat{e}(t)-\bar{y}(t)+\sum_{k=1}^{n_{x}} a_{k}(\hat{e}(t-k)-\bar{y}(t-k))+b_{k} u(t-k), \\
t=1, \ldots, N . \tag{41e}
\end{array}
$$

Then, the problem (36) is equivalent to that of computing the maximum $\tau$ such that $f(\mathbf{x})$ is strictly positive $\forall \mathbf{x} \in \mathbb{K}=\left\{\mathbf{x}: g_{j}(\mathbf{x}) \geq 0, \forall j=1, \ldots, 4 N\right\}$. The previous definitions seem to suggest the choice of $n_{k}=3 n_{x}+1$ variables $\mathbf{x}\left(I_{k}\right)=\left(a_{1}, \ldots, a_{n_{x}}, b_{1}, \ldots, b_{n_{x}}, \hat{d}(k), \ldots, \hat{d}\left(k+n_{x}\right)\right)$ and corresponding index subsets $I_{k}=\left\{1, \ldots, 2 n_{x}, k+2 n_{x}, \ldots, k+3 n_{x}\right\}$, for $k=1, \ldots, N-n_{x}$, and $n_{k}=3 n_{x}+1$ variables $\mathbf{x}\left(I_{k}\right)=$ $\left(a_{1}, \ldots, a_{n_{x}}, b_{1}, \ldots, b_{n_{x}}, \hat{e}(k), \ldots, \hat{e}\left(k+n_{x}\right)\right)$ and corresponding index subsets $I_{k}=\left\{1, \ldots, 2 n_{x}, k+3 n_{x}, \ldots, k+4 n_{x}\right\}$, for $k=$ $N-n_{x}+1, \ldots, p$, with $p:=2 N-2 n_{x}$. We now show that the conditions in Theorem 2 are satisfied for these index subsets.

Condition 1 is satisfied by using $f_{k}\left(\mathbf{x}\left(I_{k}\right)\right)=D_{1,1} \hat{d}(1)^{2} / N$ $+2 D_{2,1} \hat{d}(2) \hat{d}(1) / N+D_{2,2} \hat{d}(2)^{2} / N+\ldots+D_{n_{x}, n_{x}} \hat{d}\left(n_{x}\right)^{2} / N$ $+2 D_{n_{x}+1, n_{x}} \hat{d}\left(n_{x}+1\right) \hat{d}\left(n_{x}\right) / N+D_{n_{x}+1, n_{x}+1} \hat{d}\left(n_{x}+1\right)^{2} / N$ for $k=1, f_{k}\left(\mathbf{x}\left(I_{k}\right)\right)=2 D_{n_{x}+k, n_{x}+k-1} \hat{d}\left(n_{x}+k\right) \hat{d}\left(n_{x}+k-1\right) / N+$ $D_{n_{x}+k, n_{x}+k} \hat{d}\left(n_{x}+k\right)^{2} / N$ for all $k=2, \ldots, N-n_{x}, f_{k}\left(\mathbf{x}\left(I_{k}\right)\right)=$ $\hat{e}(1)^{2} / N+\ldots+\hat{e}\left(n_{x}+1\right)^{2} / N-\tau$ for $k=N-n_{x}+1$, and $f_{k}\left(\mathbf{x}\left(I_{k}\right)\right)=\hat{e}\left(k-N+2 n_{x}\right)^{2} / N$ for all $k=N-n_{x}+2, \ldots, p$. The running intersection property mentioned in Condition 2 is also satisfied since, for all $k=1, \ldots, N-n_{x}-1$, $I_{k+1} \cap\left(\cup_{j=1}^{k} I_{j}\right)=\left\{1, \ldots, 2 n_{x}, k+1+2 n_{x}, \ldots, k+3 n_{x}\right\} \subseteq I_{k}$, for $k=N-n_{x}, I_{k+1} \cap\left(\cup_{j=1}^{k} I_{j}\right)=\left\{1, \ldots, 2 n_{x}\right\} \subseteq I_{k}$, and, for all $k=N-n_{x}+1, \ldots, p-1, I_{k+1} \cap\left(\cup_{j=1}^{k} I_{j}\right)=\left\{1, \ldots, 2 n_{x}\right.$, $\left.k+1+3 n_{x}, \ldots, k+4 n_{x}\right\} \subseteq I_{k}$. Condition 3 is satisfied by construction since, for all $j=1, \ldots, N, g_{j}(\mathbf{x})$ involves only the variables $\mathbf{x}\left(I_{K_{j}}\right)$, with $K_{j}=\max \left(1, j-n_{x}\right)$, for all $j=N+$ $1, \ldots, 2 N, g_{j}(\mathbf{x})$ involves only the variables $\mathbf{x}\left(I_{K_{j}}\right)$, with $K_{j}=$ $\max \left(N-n_{x}+1, j-2 n_{x}\right)$, for all $j=2 N+1, \ldots, 3 N, g_{j}(\mathbf{x})$ involves only the variables $\mathbf{x}\left(I_{K_{j}}\right)$, with $K_{j}=\max (1, j-2 N-$ $n_{x}$ ), and, for all $j=3 N+1, \ldots, 4 N, g_{j}(\mathbf{x})$ involves only the variables $\mathbf{x}\left(I_{K_{j}}\right)$, with $K_{j}=\max \left(N-n_{x}+1, j-2 N-2 n_{x}\right)$.

Unfortunately, Condition 4 is not satisfied initially, but it is possible to add additional constraints to ensure that it is satisfied. For this, we redefine $\mathbb{K}=\left\{\mathbf{x}: g_{j}(\mathbf{x}) \geq 0, \forall j=1, \ldots, m\right\}$, with $m:=6 N-2 n_{x}$, by adding the quadratic polynomials
$g_{j}(\mathbf{x}):=\left\{\begin{array}{l}-\bar{h}_{j-4 N+n_{x}}^{d}(\mathbf{x}), j=4 N+1, \ldots, 5 N-n_{x}, \\ -\bar{h}_{j-5 N+2 n_{x}}^{e}(\mathbf{x}), j=5 N-n_{x}+1, \ldots, m,\end{array}\right.$
with

$$
\begin{array}{r}
\bar{h}_{t}^{d}(\mathbf{x}):=-r^{2}+\hat{d}(t)^{2}+\sum_{k=1}^{n_{x}}\left(a_{k}^{2}+b_{k}^{2}+\hat{d}(t-k)^{2}\right) \\
t=n_{x}+1, \ldots, N \\
\bar{h}_{t}^{e}(\mathbf{x}):=-r^{2}+\hat{e}(t)^{2}+\sum_{k=1}^{n_{x}}\left(a_{k}^{2}+b_{k}^{2}+\hat{e}(t-k)^{2}\right) \\
t=n_{x}+1, \ldots, N \tag{41h}
\end{array}
$$

where $r$ is some finite constant. It is important to observe that, if $r$ is chosen large enough to ensure that the minimizers $\mathbf{x}^{*}$ of problem (36) are such that $\left\|\mathbf{x}\left(I_{k}\right)^{*}\right\| \leq r$, for $k=$ $1, \ldots, p$, then the new constraints are redundant because adding them does not change the minimizers. Moreover, the polynomials (41g), (41h) are chosen to be quadratic since the polynomials with compact superlevel sets are at least of degree 2 and the polynomials that specify the other constraints
are also of degree $2 v_{j}=2$. Then, Condition 3 is still satisfied with the new constraints since, for all $j=4 N+1, \ldots, m$, $g_{j}(\mathbf{x})$ involves only the variables $\mathbf{x}\left(I_{K_{j}}\right)$, with $K_{j}=j-4 N$. In addition, now Condition 4 is also satisfied since, for all $k=1, \ldots, p$, the superlevel set $\left\{\mathbf{x}\left(I_{k}\right): g_{k, q_{k}}\left(\mathbf{x}\left(I_{k}\right)\right) \geq 0\right\}=$ $\left\{\mathbf{x}\left(I_{k}\right):\left\|\mathbf{x}\left(I_{k}\right)\right\| \leq r\right\}$ is compact for $q_{k}=k+4 N$.

Some comments about the boundedness of $\left\|\mathbf{x}\left(I_{k}\right)^{*}\right\|$, for $k=1, \ldots, p$, are necessary at this point. Since $\mathbf{x}\left(I_{k}\right)=$ $\left(a_{1}, \ldots, a_{n_{x}}, b_{1}, \ldots, b_{n_{x}}, \hat{d}(k), \ldots, \hat{d}\left(k+n_{x}\right)\right)$, for $k=1, \ldots, N-$ $n_{x}$, and $\mathbf{x}\left(I_{k}\right)=\left(a_{1}, \ldots, a_{n_{x}}, b_{1}, \ldots, b_{n_{x}}, \hat{e}(k), \ldots, \hat{e}\left(k+n_{x}\right)\right)$, for $k=N-n_{x}+1, \ldots, p$, this boundedness implies that the parameters $\boldsymbol{\theta}$ and $n_{x}+1$ prediction errors from $\hat{\mathbf{d}}$ or $\hat{\mathbf{e}}$ are bounded. At least in the case of bounded-input boundedoutput (BIBO) stable systems, it seems reasonable to assume that the parameters $\boldsymbol{\theta}$ are bounded. Regarding the prediction errors, they are expected to have the same magnitude as the output errors, which are assumed to be realizations of a normally distributed random variable with zero mean and variance $\sigma^{2}$ in this paper. Although in theory the support of this random variable is unbounded, in practice it can be bounded with a very high confidence level. To be more precise, one can observe that $(41 \mathrm{~g}),(41 \mathrm{~h})$ include the sums of squares of $n_{x}+1$ predicted errors $\hat{v}(t)^{2}:=\sum_{k=0}^{n_{x}} \hat{d}(t-k)^{2}$, $\hat{w}(t)^{2}:=\sum_{k=0}^{n_{x}} \hat{e}(t-k)^{2}$. Hence, we propose the bound $r^{2}=$ $r_{\|\boldsymbol{\theta}\|}^{2}+\max \left(r_{\hat{v}}^{2}, r_{\hat{w}}^{2}\right)$ for $(41 \mathrm{~g}),(41 \mathrm{~h})$, where $r_{\|\boldsymbol{\theta}\|}^{2}$ is an upper bound on $\|\boldsymbol{\theta}\|^{2}$ and $r_{\hat{v}}^{2}, r_{\hat{w}}^{2}$ are upper bounds on $\hat{v}(t)^{2}$ and $\hat{w}(t)^{2}$ that are chosen according to the desired robustness.

Since all the conditions in Theorem 2 are satisfied, the problem that consists in computing the global minimum of $J(\mathbf{x})$ subject to $g_{j}(\mathbf{x}) \geq 0$, for $j=1, \ldots, m$, can be formulated as the SDP (45) for some integer relaxation order $d \geq$ $v_{j}=1$ as described in Appendix A. A certificate of the representation in terms of SOS polynomials for some order $d$ can be obtained upon convergence of the SDP as shown in Theorem 3, which is a certificate of global optimality of the solution $\mathbf{x}^{*}:=\left(\boldsymbol{\theta}^{*}, \hat{\mathbf{d}}^{*}, \hat{\mathbf{e}}^{*}\right)$ and the MSE $\tau^{*}=J^{*}$.

Suppose that a global optimum is computed and certified for the relaxation order $d=2$ (in fact, this is always the case in the example of Section V). This implies that the SDP (45) has been solved for $d=2$, which is an SDP with $p\binom{n_{k}+2 d}{n_{k}}-\sum_{k=1}^{p-1}\binom{\left|I_{k} \cap I_{k+1}\right|+2 d}{\left|I_{k} \cap I_{k+1}\right|} \leq \frac{\left(4 N-n_{x}+1\right)\left(3 n_{x}+2\right)\left(3 n_{x}+3\right)\left(3 n_{x}+4\right)}{12}$ equality constraints, $p=2 N-2 n_{x}$ LMIs of size $\binom{n_{k}+d}{n_{k}}=$ $\frac{\left(3 n_{x}+2\right)\left(3 n_{x}+3\right)}{2}$, and $m=6 N-2 n_{x}$ LMIs of size $\binom{n_{k}+d-v_{j}}{n_{k}}=$ $3 n_{x}+2$. Note that, thanks to the sparse representation, the input size of this SDP is linear in the sample size $N$, which would not be possible with the nonsparse representation. Since the complexity of SDPs is polynomial in their input size, that is, the number of constraints and the size of the LMIs, it means that it has been possible to compute and certify a global solution $\mathbf{x}^{*}$ in polynomial time.

## V. SIMULATION EXAMPLE

In this section, we consider a third order LTI system adapted from [5]. The implementation was performed on MATLAB R2018a running on an Intel Core i5 1.8 GHz processor. MOSEK 8.1 was used as SDP solver.


Fig. 1. Bode diagram for the 100 repetitions with the sample size $N=15$. The blue line corresponds to the true model, the yellow lines correspond to the models estimated via the proposed approach (BPE), and the red lines correspond to the models estimated via oe (PEM). The dashed lines represent the mean $\pm$ standard deviation for the 100 repetitions.

The discrete-time transfer function of the system is

$$
\begin{equation*}
P_{d}(z)=\frac{0.4100 z^{-1}}{1-1.3000 z^{-1}+1.1025 z^{-2}-0.5620 z^{-3}} \tag{42}
\end{equation*}
$$

A pseudo-random binary signal (PRBS) of size $N$ in a range from -1 to 1 is applied as the input of this system of order $n_{x}=3$ for system identification. The output is corrupted by additive i.i.d. Gaussian noise with the standard deviation $\sigma=0.1$. The problem (38) is solved to obtain $\mathbf{D}$ according to a diagonal structure of $\mathbf{K}$. Then, the SDP (45) is formulated using the input and output data, where $f(\mathbf{x})$ and $g_{j}(\mathbf{x})$, for $j=1, \ldots, m$, are given in (41). For each $N \in\{15,31\}, 100$ repetitions of this procedure are performed, with different realizations of the noise for each repetition.

In all the repetitions, it is possible to extract the unique solution $\boldsymbol{\theta}^{*}=\left(a_{1}^{*}, a_{2}^{*}, a_{3}^{*}, b_{1}^{*}, b_{2}^{*}, b_{3}^{*}\right)$ from the solution to the SDP for the relaxation order $d=2$ and the global optimality of the solution $\boldsymbol{\theta}^{*}$ that corresponds to the cost $J^{*}$ is certified. Hence, the proposed approach avoids local minima and certifies the global optimality of the solution.

Table I reports the execution time of the whole procedure for global Bayesian point estimation, the fit between the estimated impulse response $\hat{\mathbf{g}}$ and the true impulse response $\mathbf{g}^{*}$ given by $W=100\left(1-\frac{\left\|\hat{\mathbf{g}}-\mathbf{g}^{*}\right\|}{\left\|\hat{\mathbf{g}}-\mathbf{I}_{N}^{N} \mathbf{g}^{*} / N\right\|}\right)$, and the parameter estimates for the different sample sizes $N$. For each sample size, these results that are labeled as BPE (Bayesian point estimation) are compared to the ones provided by the oe function from the MATLAB System Identification Toolbox and labeled as PEM (prediction error method). The duration of the pre-processing steps (formulation of the SDP) and the post-processing steps (extraction and certification of the global solution) is much smaller than the execution time of the SDP solver. One can observe that the execution time seems to be approximately a linear function of $N$, the mean fit and the standard deviation of the fit and the parameter estimates provided by BPE are better than the ones provided

TABLE I
EXECUTION TIME IN SECONDS, FIT $W$, AND ESTIMATES $a_{1}^{*}, a_{2}^{*}, a_{3}^{*}, b_{1}^{*}, b_{2}^{*}, b_{3}^{*}$ (MEAN $\pm$ STANDARD DEVIATION FOR 100 REPETITIONS) OF GLOBAL
BAYESIAN PARAMETER ESTIMATION (BPE) AND PREDICTION ERROR METHOD (PEM) FOR DIFFERENT SAMPLE SIZES $N$.

|  | $N$ | Time (s) | $W$ | $a_{1}^{*}$ | $a_{2}^{*}$ | $a_{3}^{*}$ | $b_{1}^{*}$ | $b_{2}^{*}$ | $b_{3}^{*}$ |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| BPE | 15 | $28.2 \pm 3.6$ | $84.36 \pm 5.00$ | $-1.2542 \pm 0.0954$ | $0.9776 \pm 0.1101$ | $-0.4885 \pm 0.0562$ | $0.4055 \pm 0.0254$ | $0.0220 \pm 0.0659$ | $-0.0451 \pm 0.0469$ |
|  | 31 | $83.8 \pm 17.7$ | $89.36 \pm 3.53$ | $-1.2430 \pm 0.0468$ | $0.9905 \pm 0.0636$ | $-0.4912 \pm 0.0369$ | $0.4069 \pm 0.0196$ | $0.0420 \pm 0.0425$ | $-0.0407 \pm 0.0278$ |
| PEM | 15 | - | $83.01 \pm 7.41$ | $-1.2969 \pm 0.1058$ | $1.0825 \pm 0.1239$ | $-0.5515 \pm 0.0729$ | $0.4078 \pm 0.0280$ | $0.0032 \pm 0.0726$ | $-0.0112 \pm 0.0976$ |
|  | 31 | - | $92.58 \pm 2.22$ | $-1.2989 \pm 0.0427$ | $1.1012 \pm 0.0449$ | $-0.5600 \pm 0.0249$ | $0.4129 \pm 0.0211$ | $-0.0007 \pm 0.0392$ | $-0.0009 \pm 0.0379$ |

by PEM in the case $N=15$ but worse in the case $N=31$, and the parameter estimates converge to the true parameters for larger $N$ with both BPE and PEM, but PEM provides parameter estimates closer to the true parameters.

Fig. 1 compares the Bode diagram for the true model and the models estimated via the proposed approach (BPE) and via oe (PEM) for $N=15$. The diagram shows that the models estimated via the proposed approach are more biased with respect to the true model than the models estimated via oe, but also less variable, which provides additional insight into the better results achieved by BPE in the case $N=15$.

## VI. CONCLUSIONS

This paper has defined unambiguously a Bayes estimator that bridges the gap between nonparametric and parametric models and has shown that the hierarchy of sparse semidefinite relaxations that results from the concept of SOS polynomials can be used for tractable computation of Bayesian point estimates with posterior certification of global optimality. This computation and certification has been detailed for the case of discrete-time OE LTI SISO models. The use of sparse semidefinite relaxations for Bayesian parameter estimation takes advantage of the fact that this method results in a sparse structure of the optimization problem for certain rational model structures. These properties have been illustrated by a simulation example of a third-order LTI SISO system.

The efficiency of the method may be the focus of future work, for example by further increasing the sparsity of the estimation problem. Also, it would be interesting to extend this method to the Bayesian parameter estimation of other linear and nonlinear models. For example, the potential of the method could be investigated for stochastic WienerHammerstein models [19] and nonlinear model structures of biological systems described by Monod terms [20].

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## Appendix

## A. Sum-of-squares polynomials for global optimization

This appendix summarizes the discussion about the concept of sum-of-squares polynomials and its application to global optimization. For a more comprehensive discussion, the reader is referred to the authors' previous paper [18].

A polynomial $p(\mathbf{x})$ of degree $2 d$ in the $n$ variables $\mathbf{x}:=$ $\left(x_{1}, \ldots, x_{n}\right)$ is a sum-of-squares (SOS) polynomial if it can be written as a sum of squares of polynomials of degree up to $d$ in $\mathbf{x}$. The concept of SOS polynomials is useful for optimization because $p(\mathbf{x})$ is an SOS polynomial if and only if there exists a positive semidefinite matrix $\mathbf{Q}$ such that $p(\mathbf{x})=\mathbf{v}_{d}(\mathbf{x})^{\mathrm{T}} \mathbf{Q} \mathbf{v}_{d}(\mathbf{x})=\operatorname{tr}\left(\mathbf{v}_{d}(\mathbf{x}) \mathbf{v}_{d}(\mathbf{x})^{\mathrm{T}} \mathbf{Q}\right)$, where $\mathbf{v}_{d}(\mathbf{x})$ is the $s(n, d)$-dimensional vector of monomials of degree up to $d$ in the $n$ variables $\mathbf{x}$, with $s(n, d):=\binom{n+d}{n}$ [9]. Hence, constraining $p(\mathbf{x})$ to the set of SOS polynomials amounts to satisfying the linear matrix inequality (LMI) $\mathbf{Q} \succeq$ $\mathbf{0}_{s(n, d) \times s(n, d)}$, which can be done via a convex semidefinite program (SDP) [21]. However, it is not generally true that a nonnegative polynomial is an SOS polynomial [22].

On the other hand, if $f(\mathbf{x})$ of degree $2 v_{0}$ or $2 v_{0}-1$ is a strictly positive polynomial on a compact basic semialgebraic set $\mathbb{K}$ specified by some polynomials $g_{j}(\mathbf{x})$ of degree $2 v_{j}$ or $2 v_{j}-1$, that is, if $f(\mathbf{x})>0 \forall \mathbf{x} \in \mathbb{K}=$ $\left\{\mathbf{x}: g_{j}(\mathbf{x}) \geq 0, \forall j=1, \ldots, m\right\}$ and $\mathbb{K}$ satisfies some technical assumptions, then $f(\mathbf{x})$ can be represented as a combination of SOS polynomials up to some degree $2 d$, where $d \geq v:=$ $\max _{j=0,1, \ldots, m} v_{j}$ is the relaxation order [23].

A sparse representation can be obtained by taking advantage of the fact that each polynomial $g_{j}(\mathbf{x})$ may involve only a few variables, and $f(\mathbf{x})$ may be written as a sum of polynomials that also involve only a few variables [24]. For this, we define $p$ index subsets $I_{k}$ with the corresponding $n_{k}:=\left|I_{k}\right|$ variables $\mathbf{x}\left(I_{k}\right)=\left\{x_{i}: i \in I_{k}\right\}$, for $k=1, \ldots, p$, such that $\cup_{k=1}^{p} I_{k}=\{1, \ldots, n\}$. This important result about sparse representation is summarized in the following theorem [25].

Theorem 2: Consider the basic semi-algebraic set $\mathbb{K}:=$ $\left\{\mathbf{x}: g_{j}(\mathbf{x}) \geq 0, \forall j=1, \ldots, m\right\}$ and assume that the index subsets $I_{1}, \ldots, I_{p}$ satisfy the following conditions:

1) The polynomial $f(\mathbf{x})$ can be written as a sum of $p$ polynomials that involve only the variables $\mathbf{x}\left(I_{1}\right), \ldots, \mathbf{x}\left(I_{p}\right)$, that is, $f(\mathbf{x})=\sum_{k=1}^{p} f_{k}\left(\mathbf{x}\left(I_{k}\right)\right)$.
2) The running intersection property holds, that is, for all $k=1, \ldots, p-1, I_{k+1} \cap\left(\cup_{j=1}^{k} I_{j}\right) \subseteq I_{s}$ for some $s \leq k$.
3) For all $j=1, \ldots, m$, there exists some $K_{j} \in\{1, \ldots, p\}$ that indicates that $g_{j}(\mathbf{x})$ involves only the variables $\mathbf{x}\left(I_{K_{j}}\right)$, that is, $g_{j}(\mathbf{x})=g_{K_{j}, j}\left(\mathbf{x}\left(I_{K_{j}}\right)\right)$.
4) For all $k=1, \ldots, p$, there exists some $q_{k} \in\{1, \ldots, m\}$ such that the set $\left\{\mathbf{x}\left(I_{k}\right): g_{k, q_{k}}\left(\mathbf{x}\left(I_{k}\right)\right) \geq 0\right\}$ is compact.
If $f(\mathbf{x})$ is strictly positive $\forall \mathbf{x} \in \mathbb{K}$, then

$$
\begin{equation*}
f(\mathbf{x})=\sum_{k=1}^{p} p_{0, k}\left(\mathbf{x}\left(I_{k}\right)\right)+\sum_{j=1}^{m} g_{j}(\mathbf{x}) p_{j}\left(\mathbf{x}\left(I_{K_{j}}\right)\right) \tag{43}
\end{equation*}
$$

for some SOS polynomials $p_{0,1}\left(\mathbf{x}\left(I_{1}\right)\right), \ldots, p_{0, p}\left(\mathbf{x}\left(I_{p}\right)\right)$ and $p_{1}\left(\mathbf{x}\left(I_{K_{1}}\right)\right), \ldots, p_{m}\left(\mathbf{x}\left(I_{K_{m}}\right)\right)$.

Proof: The proofs of Theorems $2-3$ can be found in the references before each theorem and are not replicated.

Remark 1: This representation can be used to relax the verification of positivity of $f(\mathbf{x}) \forall \mathbf{x} \in \mathbb{K}$ as a hierarchy of sparse LMI feasibility problems of increasing order $d$ [25]. To introduce the sparse relaxations, note that the monomials $\mathbf{x}^{\boldsymbol{\alpha}}:=x_{1}^{\alpha_{1}} \ldots x_{n}^{\alpha_{n}}$ of degree up to $2 d$ in the variables $\mathbf{x}\left(I_{k}\right)$ involve powers $\boldsymbol{\alpha}:=\left(\alpha_{1}, \ldots, \alpha_{n}\right)$ in the set $\overline{\mathscr{X}}_{d, k}:=$ $\mathscr{X}_{d} \cap\left\{\left(\alpha_{1}, \ldots, \alpha_{n}\right) \in \mathbb{N}_{0}^{n}: \alpha_{i} \neq 0 \Rightarrow i \in I_{k}\right\}$, for $k=1, \ldots, p$, where $\mathscr{X}_{d}:=\left\{\left(\alpha_{1}, \ldots, \alpha_{n}\right) \in \mathbb{N}_{0}^{n}: 0 \leq \alpha_{1}+\ldots+\alpha_{n} \leq 2 d\right\}$. We define $\overline{\mathscr{X}}_{d}:=\cup_{k=1}^{p} \overline{\mathscr{X}}_{d, k}$ and use $f_{\boldsymbol{\alpha}}$ and $g_{j, \boldsymbol{\alpha}}$ to denote the coefficients of $f(\mathbf{x})$ and $g_{j}(\mathbf{x})$ such that $f(\mathbf{x})=\sum_{\boldsymbol{\alpha} \in \overline{\mathscr{X}}_{d}} f_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}}$ and $g_{j}(\mathbf{x})=\sum_{\boldsymbol{\alpha} \in \bar{X}_{v_{j}}} g_{j, \boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}}$, for $j=1, \ldots, m$. Moreover, the matrices $\mathbf{R}_{v, k, \boldsymbol{\alpha}}$ are defined such that $\sum_{\boldsymbol{\alpha} \in \overline{\mathscr{X}}_{d-v}} \mathbf{R}_{v, k, \boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}}=$ $\mathbf{v}_{d-v}\left(\mathbf{x}\left(I_{k}\right)\right) \mathbf{v}_{d-v}\left(\mathbf{x}\left(I_{k}\right)\right)^{\mathrm{T}}$, for $v=0, \ldots, d$ and $k=1, \ldots, p$. If Theorem 2 applies and $f(\mathbf{x})$ is strictly positive $\forall \mathbf{x} \in \mathbb{K}$, then there exists a positive integer $d$ such that $\forall \boldsymbol{\alpha} \in \overline{\mathscr{X}}_{d}$

$$
\begin{equation*}
f_{\boldsymbol{\alpha}}=\sum_{k=1}^{p} \operatorname{tr}\left(\mathbf{R}_{0, k, \boldsymbol{\alpha}} \mathbf{Q}_{0, k}\right)+\sum_{j=1}^{m} \sum_{\substack{\boldsymbol{\beta} \in \overline{\mathscr{X}}_{d-v_{j}} \\ \boldsymbol{\alpha}-\boldsymbol{\beta} \in \mathscr{X}_{v_{j}}}} g_{j, \boldsymbol{\alpha}-\boldsymbol{\beta}} \operatorname{tr}\left(\mathbf{R}_{v_{j}, K_{j}, \boldsymbol{\beta}} \mathbf{Q}_{j}\right) \tag{44a}
\end{equation*}
$$

and

$$
\begin{align*}
& \mathbf{Q}_{0, k} \succeq \mathbf{0}_{s\left(n_{k}, d\right) \times s\left(n_{k}, d\right)}, k=1, \ldots, p  \tag{44b}\\
& \mathbf{Q}_{j} \succeq \mathbf{0}_{s\left(n_{K_{j}}, d-v_{j}\right) \times s\left(n_{K_{j}}, d-v_{j}\right)}, j=1, \ldots, m . \tag{44c}
\end{align*}
$$

This result is very useful for the problem of computing $J^{*}$, an accurate approximation of the global minimum of $J(\mathbf{x})$ subject to the constraints $g_{j}(\mathbf{x}) \geq 0$, for $j=1, \ldots, m$, or equivalently, the maximum value $\tau$ such that $f(\mathbf{x})=J(\mathbf{x})-\tau$ is strictly positive $\forall \mathbf{x} \in \mathbb{K}=\left\{\mathbf{x}: g_{j}(\mathbf{x}) \geq 0, \forall j=1, \ldots, m\right\}$. Using (44), such a problem can be formulated as the SDP

$$
\begin{equation*}
\min _{\tau, \mathbf{Q}_{0,1}, \ldots, \mathbf{Q}_{0, p}, \mathbf{Q}_{1}, \ldots, \mathbf{Q}_{m}}-\tau, \quad \text { s.t. (44). } \tag{45}
\end{equation*}
$$

Hence, if $n_{k}$ and the maximum degree $v$ of the polynomials in the problem are relatively small, the SDP can be solved efficiently since the relaxation order $d$ that provides a sparse representation in terms of SOS polynomials is usually not much larger than $v$. If this representation exists for some order $d$, a certificate can be obtained upon convergence of the SDP. The result about the sparse representation for the order $d$ is stated as follows [26]:

Theorem 3: Denote the optimal values of the dual variables for the constraints (44a) as $\mu_{\boldsymbol{\alpha}}^{*} \forall \boldsymbol{\alpha} \in \bar{X}_{d}$ and of the dual variables for the LMIs (44b) as $\mathbf{L}_{0, k}^{*} \forall k=1, \ldots, p$. If $\exists G: G=\operatorname{rank}\left(\mathbf{L}_{0, k}^{*}\right)=\operatorname{rank}\left(\sum_{\boldsymbol{\alpha} \in \overline{\mathscr{X}}_{d-1}} \mathbf{R}_{1, k, \boldsymbol{\alpha}} \mu_{\boldsymbol{\alpha}}^{*}\right) \quad \forall k=$ $1, \ldots, p$, then $f(\mathbf{x})=J(\mathbf{x})-J^{*}$ can be represented as in (43) with $p_{0, k}\left(\mathbf{x}\left(I_{k}\right)\right)$ of degree $2 d$, for $k=1, \ldots, p$, and $p_{j}\left(\mathbf{x}\left(I_{K_{j}}\right)\right)$ of degree $2\left(d-v_{j}\right)$, for $j=1, \ldots, m$. In addition, the global minimum $J^{*}=\tau^{*}$ and $G$ global minimizers $\mathbf{x}^{*}$ can be computed using the fact that $\mathbf{v}_{d}\left(\mathbf{x}\left(I_{k}\right)^{*}\right)$ lie both in the null space of $\mathbf{Q}_{0, k}^{*}$ and in the row space of $\mathbf{L}_{0, k}^{*}, \forall k=1, \ldots, p$.


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