Nonlinear system identification in Sobolev spaces

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Abstract

We consider the problem of deriving from experimental data an approximation of an unknown function, whose derivatives also approximate the unknown function derivatives. Solving this problem is useful, for instance, in the context of nonlinear system identification for obtaining models that are more accurate and reliable than the traditional ones, based on plain function approximation. Indeed, models identified by accounting for the derivatives can provide a better performance in several tasks, such as multi-step prediction, simulation, Nonlinear Model Predictive Control, and control design in general. In this paper, we propose a novel approach based on convex optimization, allowing us to solve the aforementioned identification problem. We develop an optimality analysis, showing that models derived using this approach enjoy suitable optimality properties in Sobolev spaces. The optimality analysis also leads to the derivation of tight uncertainty bounds on the unknown function and its derivatives. We demonstrate the effectiveness of the approach with two numerical examples. The first one is concerned with approximation of an univariate function, the second one with multi-step prediction of the Chua chaotic circuit.

1 Introduction

Consider a nonlinear discrete-time system, represented in the following input-output regression form:

\[ y_{t+1} = f_o (x_t) + \xi_{t+1} \]

\[ x_t = (y_t, \ldots, y_{t-m_o+1}, u_t, \ldots, u_{t-m_u+1}) \]

where \( u_t \in U \subset \mathbb{R}^{n_u} \) is the input, \( y_t \in \mathbb{R}^{n_y} \) is the output, \( \xi_t \in \Xi \subset \mathbb{R}^{n_x} \) is a disturbance and \( t \in \mathbb{Z} \) is the discrete time index. The sets \( U \) and \( \Xi \) are compact with non-empty interior. The regression function \( f_o \) is supposed to be unknown: the objective of this paper is to obtain from a batch of experimental data an estimate \( \hat{f} \) of \( f_o \), such that (i) \( \hat{f} \) approximates \( f_o \), and (ii) the first derivatives of \( \hat{f} \) approximate the first derivatives of \( f_o \). Some relevant motivations for considering this problem are given next.

Multi-step prediction and simulation. A standard approach to the identification of system (2) is to adopt a parametrized NARX (Nonlinear Auto Regressive with eXogenous inputs) model structure and to estimate the involved parameters by minimizing the model prediction error; see, e.g., [32,13]. A relevant issue is that a model identified using this approach may be accurate when used for one-step ahead prediction but poor when used for multi-step prediction or simulation. This may happen, for example, when the model sampling time is too short; [9]. In this case, the identified model tends to become a so-called persistent model, where the prediction is close to the current value: \( \hat{y}_{t+1} \approx y_t \). Clearly, a persistent model cannot provide a decent performance when used for multi-step prediction or simulation. In general, the main reason behind these kind of issues is that the model just aims to minimize the one-step prediction error, without really trying to capture the relation between the output and the individual components of \( x_t \) and \( y_{t+1} \). An approach that may help overcoming these issues consists in adopting a NOE (Nonlinear Output Error) model structure, in which the involved parameters are estimated by minimizing the model simulation error, see, e.g., [32,13]. NOE models are often more accurate than NARX models in multi-step prediction and simulation but require a higher computational burden, since minimization of the simulation error is in general a hard nonlinear and non-convex problem. In any case, also for NOE models there are no guarantees that the relation between the components of \( x_t \) and \( y_{t+1} \) is correctly captured. The function derivatives express up to first order precisely these relations, hence approximating them, together with the system function \( f_o \), is crucial in determining an accurate model for control purposes.

Nonlinear Model Predictive Control (NMPC). NMPC is a widely used technique for controlling complex nonlinear plants, see, e.g., [6,14,11]. Data-driven versions of this technique can be found in [27,30,16,24,25]. NMPC is based on two main operations: (i) multi-step prediction of the plant behavior, and (ii) synthesis of a control law via on-line optimization, based on the predicted behavior. Clearly, the availability of an accurate multi-step prediction model is of paramount importance in NMPC. In particular, at every time \( t \), given the input and output regressors \((u_{t-1}, \ldots, u_{t-m_u+1})\) and \((y_{t}, \ldots, y_{t-m_o+1})\), the model should correctly describe the variations of the predicted output \( \hat{y}_{t+\tau} \), \( \tau \geq 1 \), due to variations of the command input sequence \((u_{t}, \ldots, u_{t+\tau-1})\). As discussed in the previous paragraph, the function derivatives de-
scribe these variations to first order, and this, again, motivates the need in a control context of approximating the system function \( f_o \) together with its derivatives.

Control sensitivity. The above considerations are not limited to NMPC. In general, when estimating a regression model that is to be used for control, e.g., of the type \( y_{t+1} = f(y_t, \ldots, y_{t-m+1}, u_t, \ldots, u_{t-m+1}) \), it is of paramount importance to capture the sensitivities of the output with respect to the commands \( u_t, \ldots, u_{t-m+1} \), and these are given, to first order approximation, by the derivatives of \( f \) w.r.t. these variables. Failing to get these sensitivities with sufficient precision may result in a model that responds to commands in a poor way.

Remark 1 Although the following one is an elementary fact, it is perhaps important to remark that a good uniform error bound on a function’s values need not imply a good error bound on the sensitivities (derivatives). Indeed, suppose that we have \( \hat{f}(x) = f(x) + e(x) \), where \( f \) is the true function, \( \hat{f} \) is the identified approximation, and \( e \) is the error term. If \( \hat{f} \) is approximated in a standard way, we may have that, over a given domain \( \mathcal{X} \), \( |e(x)| \leq \epsilon, \forall x \in \mathcal{X} \), that is, a uniform bound \( \epsilon \) on the absolute approximation error \( |\hat{f}(x) - f(x)| \). The point, however, is that even if \( \epsilon \) is small, the error on the sensitivity can be arbitrarily large. We have that \( \frac{\partial \hat{f}}{\partial x} = \frac{\partial f}{\partial x} + \frac{\partial e}{\partial x} \), whence \( |\frac{\partial \hat{f}}{\partial x} - \frac{\partial f}{\partial x}| = \frac{\partial |e|}{\partial x} \), and indeed it suffices to consider an example with \( e(x) = \epsilon \sin(\omega x) \), to see that \( |e(x)| \leq \epsilon \) for all \( x \), but \( \frac{\partial |e|}{\partial x} = \epsilon \omega |\cos(\omega x)| \), thus the error on the sensitivity can be arbitrarily large, for arbitrarily large \( \omega \).

Related literature. The literature appears to be quite scarce on the topic of approximating from data a function and its derivatives. The existing methods are based on different classes of approximators, including radial basis functions [15], neural networks [37,28,1], and deep neural networks [4]. The numerical results presented in these papers clearly show that using the information about the function derivatives leads to significant improvements of the model accuracy and generalization capabilities. This literature is interesting and effective in showing the potential of techniques relying on derivative identification. However, only a limited number of works carry out a theoretical analysis about the approximation properties of these techniques [12,37,4], and the provided results are often non-constructive, in the sense that they just prove existence of the required approximating function. Moreover, the works we found typically assume that the function derivative samples are available but this may not be true in practical applications. Also, we observe that the existing techniques allow for the identification of a model, but they do not provide a description of the uncertainty associated with this model and its predictions.

Main Contributions. In this paper, we propose a novel identification approach addressing all the mentioned issues. The approach allows the identification of a function together with its derivatives, and it is completely based on convex optimization. We develop a theoretical optimality analysis, showing that models obtained using the proposed approach enjoy certain optimality properties in Sobolev spaces. The optimality analysis also leads to the derivation of tight uncertainty bounds on the unknown function and its derivatives, quantifying the modeling error and the prediction uncertainty. The approach uses samples of the regressor \( x_t \), of the function output \( y_t \) and of the function derivative outputs. As already mentioned, these latter samples may be not available in a real-world application. Thus, we further propose a technique for estimating derivative samples from the function input-output data. We finally present two numerical examples. These examples show that the approach may provide significantly more accurate and reliable models than the traditional ones based on plain function approximation (i.e., identified without considering the derivatives).

Paper organization. In Section 2, the notation used in the paper and some basic notions about functional norms and spaces are introduced. In Section 3, the identification problem of interest is formalized. In Section 4, two methods are derived for the joint function and derivative identification problem. The optimality properties of these methods are analyzed in Section 5. Based on this analysis, tight uncertainty bounds are provided in Section 6. In Section 7, an algorithm is proposed for estimating the derivative values, starting from the function input-output values. Section 8 presents the numerical examples. The conclusions are given in Section 9. All the theorem proofs can be found in the Appendix.

2 Notation and preliminaries

A column vector \( x \in \mathbb{R}^{n \times 1} \) is denoted by \( x = (x_1, \ldots, x_m) \). A row vector \( x \in \mathbb{R}^{1 \times n} \) is denoted by \( x = \begin{bmatrix} x_1, \ldots, x_n \end{bmatrix}^\top \). As a convention, the \( \ell_n \)-norm of a vector \( x = (x_1, \ldots, x_m) \) is defined as usual. The 2-norm (maximum singular value norm) of a matrix \( \Phi \in \mathbb{R}^{m \times n} \) is denoted by \( \|\Phi\|_2 \), and the infinity is denoted by \( \|\Phi\|_\infty = \max_{i=1, \ldots, m} \sum_{j=1}^n |\Phi_{ij}| \). The \( \ell_p \) norm of a function with domain \( X \subseteq \mathbb{R}^n \) and codomain in \( \mathbb{R} \), is defined as \( \|f\|_p \equiv \left( \int_X |f(x)|^p dx \right)^{\frac{1}{p}} \), for \( p \in (1, \infty) \), and as \( \sup_{x \in X} |f(x)|_\infty \) for \( p = \infty \). These norms give rise to the well-known \( \ell_p \) and \( \ell_p \equiv \ell_p(X) \) Banach spaces. The \( S_{tp} \) Sobolev norm of a differentiable function with domain \( X \subseteq \mathbb{R}^n \) and codomain in \( \mathbb{R} \), is defined as \( \|f\|_{S_p} \equiv \sum_{i=0}^n \|f^{(i)}\|_p \), where \( f^{(i)} \) is the \( i \)-th order derivative. The Sobolev norm gives rise to the \( S_{tp} \equiv S_{tp}(X) \) Sobolev space, also denoted in the literature with \( W_{1,p} \) or \( W_{1,p} \).

Definition 1 The Sobolev space \( S_{tp}(X) \) is the set of all functions \( f \in \mathbb{L}_p(X) \) such that, for every \( i > 0 \), the derivative \( f^{(i)} \) exists and \( f^{(i)} \in \mathbb{L}_p(X) \); \( S_{tp}(X) \equiv \{ f : f^{(i)} \in \mathbb{L}_p(X), i = 0, \ldots, n_p \} \). Sobolev norms (and related spaces) involving higher order derivatives can also be found in the literature. The concept of weak derivative, which is a generalization of
the standard derivative, is often used. In this paper, the interest is for the case of first order standard derivatives.

3 Problem formulation

Consider a function $f_o \in S_1 p(X)$, taking values $z = f_o(x)$, where $x \in X \subset \mathbb{R}^{n_x}$. $X$ is a compact set, and $z \in \mathbb{R}$. Suppose that $f_o$ is not known, but a set of noise-corrupted input-output data from the unknown function is available:

$$D = \{ \tilde{x}_k, \{ \tilde{z}^i_k \}_{i=0}^{n_z} \}_{k=1}^L \quad (2)$$

where $\tilde{x}_k \in X$ are the measurements of the function argument, $\tilde{z}^i_k = \tilde{z}_k$ are the measurements of the function output and $\tilde{z}^i_k, i > 0$, are the measurements of the $i$-th partial derivative output. The data (2) can be described by

$$\tilde{z}^i_k = f^{(i)}_o(\tilde{x}_k) + d^i_k, \; i = 0, \ldots, n_z, \; k = 1, \ldots, L, \quad (3)$$

where $d^i_k$ are noises and $d^o_k \equiv d_k$. If the data are generated by the system (2), we have that $\tilde{z}^i_k \equiv \tilde{z}_k = y_k + 1$, and the noise terms account for the disturbance $\xi_k$ and possible measurement errors.

We remark that in real-world applications, only the output of the function is usually measured, while the outputs of the derivatives may not be available. This more realistic situation is dealt with in Section 7, where an algorithm is presented for estimating the derivative output samples $\tilde{z}^i_k, i > 0$, from the input-output function samples $\tilde{x}_k$ and $\tilde{z}_k$.

Now, assume that the noise sequences $d^i = (d^i_1, \ldots, d^i_L)$ are unknown but bounded: $\|d^i\|_q \leq \mu^i$, where $\| \cdot \|_q$ is a vector $\ell_q$ norm and $0 \leq \mu^i < \infty$. In the case $q = 2$, it can be convenient to write $\mu^i$ as $\mu^i = \sqrt{\lambda^i}$, with $0 \leq \mu^i < \infty$. In some situations, the noise bounds $\mu^i$ are known from the physical knowledge about the system of interest and the involved sensors. In other situations, these bounds are not known and have to be estimated from the available data. An algorithm will be provided in Section 6 for performing this estimation.

In this paper, we consider the problem of identifying from the data (2) an “accurate” approximation $\hat{f}$ of the unknown function $f_o$, such that also the derivatives $\hat{f}^{(i)}$, $i > 0$, of $\hat{f}$ are “accurate” approximations of the derivatives $f^{(i)}_o$, $i > 0$, of $f_o$. The accuracy is measured by means of the following identification error $e(\hat{f}) = \|f_o - \hat{f}\|_{S_p}$, where $\| \cdot \|_{S_p}$ is a Sobolev norm. In other words, we are looking for an approximation of the unknown function $f_o$ in the $S_1 p$ Sobolev space. Besides the goal of obtaining such an approximation, we also aim at evaluating guaranteed estimate bounds for $f_o$.

A parametrized structure is adopted for the approximating function:

$$\hat{f}_j(x) = \sum_{j=1}^N a_j \phi_j(x) \quad (4)$$

where $\phi_j \in S_1 p(X)$ are given basis functions and $a_j \in \mathbb{R}$ are coefficients to be identified. The choice of the basis functions is clearly an important step of the identification process, see, e.g., [32,26]. In several cases, the basis functions are known from the physical knowledge of the system of interest. In other cases the basis functions are known a priori to belong to some “large” set of functions, see, e.g., the examples presented in Section 8.2 and in [22]. In yet other cases, the basis functions are not known a priori and their choice can be carried out by considering the numerous options available in the literature (e.g., Gaussian, sigmoidal, wavelet, polynomial, trigonometric, etc.); see [32] for a discussion on the main features of the most used basis functions and guidelines for their choice.

The problem considered in this paper is stated as follows.

**Problem 1** From the data set $D$ in (2), identify an estimate $\hat{f}$ of the form (4), such that:

(i) the Sobolev identification error $e(\hat{f})$ is small;

(ii) the estimate is equipped with guaranteed uncertainty bounds on the unknown function $f_o$ and its derivatives.

In the reminder of the paper, for numerical conditioning reasons, we assume that the components of $x$ in $z = f_o(x)$ have similar ranges of variation. This assumption can always be met through a suitable rescaling of the components.

4 Identification methods

In this section we propose two methods for solving Problem 1, both based on convex optimization. In Section 5 it will be shown that functions identified by means of these methods enjoy suitable optimality properties. In this section, we suppose that the derivative output samples $\tilde{z}^i_k, i > 0$ are available. In Section 7, we will show how these derivative samples can be estimated from the input-output function samples $\tilde{x}_k$ and $\tilde{z}_k$.

A simple yet fundamental observation is that the approximating function (4) and its derivatives are given by

$$\hat{f}^{(i)}(x) = \sum_{j=1}^N a_j \phi_j^{(i)}(x), \; i = 0, \ldots, n_x. \quad (5)$$

On the basis of this observation we can present the first identification method.

**Method 1**

1. Define

$$z^i \doteq \begin{bmatrix} \tilde{z}^i_1 \\ \vdots \\ \tilde{z}^i_L \end{bmatrix}, \quad \Phi^i \doteq \begin{bmatrix} \phi_1^{(i)}(\tilde{x}_1) & \cdots & \phi_N^{(i)}(\tilde{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_1^{(i)}(\tilde{x}_L) & \cdots & \phi_N^{(i)}(\tilde{x}_L) \end{bmatrix} \quad (6)$$

2. Estimate the vector $a = (a_1, \ldots, a_N)$ of model coefficients in (5) by solving the following convex op-
timization problem:
\[
a = \arg \min_{\alpha \in \mathbb{R}^N} \| \alpha \|_r \quad (7)
\]
s.t. \( \| \tilde{z}^i - \Phi^i \alpha \|_q \leq \mu^i, \ i = 0, \ldots, n_x \), \( (8) \)

where integers \( r, q \) indicate suitable vector norms.

The rationale behind this method can be explained as follows: the constraints (8) ensure that the resulting model (5) is consistent with the available information on the noises corrupting the data. If the optimization problem is not feasible, it means that either the chosen basis function set is not sufficiently rich or the noise bounds \( \| d^i \|_q \leq \mu^i \) are too small. The minimization of the coefficient vector \( \ell_1 \) norm in (7) is carried out for regularization reasons, allowing also to limit the issue of overfitting. Typical norms that can be used are the \( \ell_2 \) and \( \ell_1 \) norms. In particular, the \( \ell_1 \) norm allows one to obtain a sparse coefficient vector \( \alpha \) (see, e.g., [8,34,36,5]), resulting in a low-complexity model. This is an important property, especially in view of the model implementation on real-time processors.

We now present the second identification method.

**Method 2**

1. Define \( \tilde{z}^i \) and \( \Phi^i \) as in (6).

2. Estimate the vector \( a = (a_1, \ldots, a_N) \) of model coefficients in (5) by solving the following convex optimization problem:
\[
a = \arg \min_{\alpha \in \mathbb{R}^N} \sum_{i=0}^{n_x} \lambda^i \| \tilde{z}^i - \Phi^i \alpha \|^2 + \Lambda \| \alpha \|_r \quad (9)
\]

where where integers \( r, q \) indicate suitable vector norms, and \( \lambda^i \geq 0, \Lambda \geq 0 \) are given weights.

Problem (9) is aimed at minimizing a tradeoff between the model fitting error on the identification data and a regularization term. For \( r = 1 \), (9) is a Lasso problem, see, e.g., [34]; for \( r = 2 \), it becomes a classical Ridge regression problem, see, e.g., [10]. Note that, for suitable values of the parameters \( \mu^i, \lambda^i \) and \( \Lambda \), the optimization problems (7) and (9) are equivalent to each other.

**Remark 2** It is worth to stress the fact that Method 1 and Method 2 are here considered in terms of the guarantees they provide for the ensuing models, and that this paper’s contribution lies in the specific models that lead to Sobolev space identification through Method 1 and Method 2, and in their analysis, and not in the actual numerical solution of problems in (8) or (9). These problems indeed have a well-known regularized regression structure, and a plethora of efficient numerical methods already exist for their solution.

5 Optimality analysis

In Section 4, two identification methods have been presented, allowing us to derive parameterized approximations of the unknown function \( f_o \). In this section, following a Set Membership approach [21], [17], [31], [2], [20], [33], we show that such approximations enjoy suitable optimality properties in Sobolev spaces. Two cases are covered: in the first one, we suppose that the true function \( f_o \) belongs to a Sobolev space \( S_{1,p} \); in the second one, we make an additional assumption, regarding the Lipschitz continuity of the derivatives of the function \( f_o - \tilde{f} \), which allows us to prove stronger optimality properties of the approximations with respect to the first case. The analysis and results developed here are extensions to Sobolev spaces of those regarding approximation in \( L_q \) spaces presented in [18,20].

5.1 Optimality analysis in Sobolev spaces

Consider that the function \( f_o \) and its derivatives are unknown, while instead we have the experimental information given by (2) and (3), and the prior information given by the inclusion \( f_o \in S_{1,p}(X) \) and the noise bounds \( \| d^i \|_q \leq \mu^i \). It follows that \( f_o \in \text{FFS}_S \), where \( \text{FFS}_S \) is the so-called Feasible Function Set, defined below.

**Definition 2** The Feasible Function Set \( \text{FFS}_S \) is defined as \( \text{FFS}_S = \{ f \in S_{1,p}(X) : \| \tilde{z}^i - f^{(i)}(\tilde{x}) \|_q \leq \mu^i, \ i = 0, \ldots, n_x \} \), where \( f^{(i)}(\tilde{x}) = (f^{(1)}(\tilde{x}_1), \ldots, f^{(i)}(\tilde{x}_L)) \).

In words, the Feasible Function Set is the set of all functions consistent with the prior assumptions and with the available data. The Feasible Function Set thus summarizes all the experimental and a-priori information that can be used for identification. If at least a function exists that is consistent with the assumptions and the data (i.e., if \( \text{FFS}_S \neq \emptyset \)), we say that the assumptions are validated. Otherwise (i.e., if \( \text{FFS}_S = \emptyset \)), we say that the assumptions are falsified; see [17,2].

**Definition 3** The prior assumptions are considered validated if \( \text{FFS}_S \neq \emptyset \).

The following theorem gives a sufficient conditions for prior assumption validation.

**Theorem 1** \( \text{FFS}_S \neq \emptyset \) if the optimization problem (7)-(8) is feasible.

**Proof.** See the Appendix.

If the optimization problem (7)-(8) is not feasible, it means that either the chosen basis function set is not sufficiently rich or the noise bounds \( \| d^i \|_q \leq \mu^i \) are too small. In the case where reliable noise bounds are available, a sufficiently rich basis function set has to be found, considering the numerous options available in the literature (e.g., Gaussian, sigmoidal, wavelet, polynomial, trigonometric). If no basis functions are found for which the optimization problem is feasible, a relaxation of the noise bounds is needed.

In the reminder of the paper, it is assumed that the prior assumptions are true and, consequently, \( f_o \in \text{FFS}_S \). Under this assumption, for a given approximation \( \hat{g} \) of \( f_o \), a tight bound on the identification error \( e(\hat{g}) \) is given by the following worst-case error.

**Definition 4** We define the worst-case identification error as \( WE(\hat{g}, \text{FFS}_S) = \sup_{f \in \text{FFS}_S} \| f - \hat{g} \|_{S_p} \), where \( \| \cdot \|_{S_p} \) is the Sobolev norm.
An optimal approximation is defined as a function \( f_{op} \) which minimizes the worst-case approximation error.

**Definition 5** An approximation \( f_{op} \) is FFS\(_S\)-optimal if \( WE(f_{op}, FFS_S) = \inf_j WE(\hat{f}, FFS_S) \leq \mathcal{R}(FFS_S) \), where \( \mathcal{R}(FFS_S) \) is called the radius of information and is the minimum worst-case error that can be achieved on the basis of the available prior and experimental information.

In other words, an optimal approximation is the best approximation that can be found on the basis of the available prior and experimental information (this information is summarized by the Feasible Function Set). Finding optimal approximations is in general hard and sub-optimal solutions can be looked for. In particular, approximations called almost-optimal are often considered in the literature, see, e.g., [35], [17].

**Definition 6** An approximation \( f_{ao} \) is FFS\(_S\)-almost-optimal if \( WE(f_{ao}, FFS_S) \leq 2 \inf_j WE(\hat{f}, FFS_S) = 2 \mathcal{R}(FFS_S) \).

The following result gives sufficient conditions under which an approximation (possibly obtained by the methods of Section 4) is almost-optimal.

**Theorem 2** Assume that:

i) the optimization problem (7)-(8) is feasible.

ii) the approximation \( \hat{f} \) given in (4)-(5) has coefficients \( a_j \) satisfying inequalities (8).

Then, the approximation \( \hat{f} \) is FFS\(_S\)-almost-optimal.

**Proof.** See the Appendix.

This theorem shows that an approximation obtained by Method 1 is always almost-optimal. Instead, an approximation obtained by Method 2 is almost-optimal if its coefficients satisfy inequalities (8).

### 5.2 Optimality analysis with Lipschitz information

As discussed in Section 5.1, the function \( f_o \) and its derivatives are unknown, while instead we have available the experimental information given by (2) and (3), and the prior information given by the inclusion \( f_o \in \mathcal{S}_{ip}(X) \) and the noise bounds. In this section, we make an additional assumption on the Lipschitz continuity of the derivatives of the so-called residue function \( f_o - \hat{f} \). This allows us to prove stronger optimality properties with respect to those discussed in Section 5.1.

The residue function is defined as \( \Delta(x) = f_o(x) - \hat{f}(x) \). We assume that this function and its derivatives are Lipschitz continuous. That is, for given Lipschitz constants \( \gamma_i < \infty, i = 0, \ldots, n_x \), \( \Delta^{(i)} \in \mathcal{L}(\gamma_i, X) \), where \( \mathcal{L}(\eta, X) = \{ f \in \mathcal{S}_{ip}(X) : |f(x) - f(w)| \leq \eta \|x - w\|_\infty, \forall x, w \in X \} \). This assumption is reasonable, since we already know that \( \Delta \in \mathcal{S}_{ip}(X) \), which implies that \( \Delta \) is Lipschitz continuous and its derivatives are continuous (a slightly weaker condition with respect to Lipschitz continuity). The constants \( \gamma_i \) can be estimated from the available data by means of the procedure presented at the end of this section.

Under the Lipschitz condition, we have that \( f_o \in FFS_L \), where \( FFS_L \) is the following Feasible Function Set.

**Definition 7** We let \( FFS_L := \{ f \in \mathcal{S}_{ip}(X) : f^{(i)}(\tilde{x}) \in \mathcal{L}(\gamma_i, X), \| \tilde{z}^i - f^{(i)}(\tilde{x}) \|_q \leq \mu_i, i = 0, \ldots, n_x \} \), where \( f^{(i)}(\tilde{x}) = (f^{(i)}(\tilde{x}_{L}), \ldots, f^{(i)}(\tilde{x}_{L})) \).

\( FFS_L \) is the set of all functions consistent with the prior assumptions and the available data. Recalling Definition 3, a result is now presented, giving sufficient conditions for assumption validation.

**Theorem 3** \( FFS_L \neq \emptyset \) if the optimization problem (7)-(8) is feasible.

**Proof.** See the Appendix.

To see how the assumption about the Lipschitz continuity of the function derivatives helps to obtain stronger optimality properties, consider Definitions 2 and 7. These definitions imply that \( FFS_L \subseteq FFS_S \) and, consequently, \( \mathcal{R}(FFS_L) \subseteq \mathcal{R}(FFS_S) \). This inequality shows that the Lipschitz continuity assumption yields a reduction of the worst-case identification error.

The following result gives sufficient conditions, under which an approximation is almost-optimal, when the Feasible System Set is \( FFS_L \).

**Theorem 4** Let the assumptions of Theorem 2 hold and the functions \( \Delta^{(i)}, i = 1, \ldots, n_x \), be Lipschitz continuous. Then, the approximation \( \hat{f} \) is FFS\(_L\)-almost-optimal.

**Proof.** See the Appendix.

This section is concluded with a procedure for estimating the constants \( \gamma_i \) from the available data. The procedure is the following:

1. Let \( \Delta_i \hat{z}_k = \tilde{z}_k - \hat{f}^{(i)}(\tilde{x}_k) \). The values \( \tilde{z}_k, k = 1, \ldots, L \), are either known/measured or estimated from the data \( \{ \tilde{x}_k, \tilde{z}_k \}_{k=L}^{L} \) using Algorithm 1 presented next in Section 7.

2. Let \( \Delta_{ij} \hat{z}_k \) be the samples of the \( j \)th derivative of \( \Delta^{(i)} \). The values \( \Delta_{ij} \hat{z}_k, k = 1, \ldots, L, i, j = 1, \ldots, n_x \), are estimated from the data \( \{ \tilde{x}_k, \tilde{z}_k - \hat{f}^{(j)}(\tilde{x}_k) \}_{k=1}^{L} \) using Algorithm 1. Note that the estimation of the \( \Delta_{ij} \hat{z}_k \)'s requires the function \( f_o \) to be locally twice differentiable at the points \( \tilde{x}_k, k = 1, \ldots, L \).

3. Estimate the Lipschitz constants \( \gamma_i, i = 0, \ldots, n_x \), as

\[
\gamma_0 = \nu \max_{k=1, \ldots, L} \| (\Delta_{11} \hat{z}_k, \ldots, \Delta_{n_1 n_2} \hat{z}_k) \|_\infty \\
\gamma_l = \nu \max_{k=1, \ldots, L} \| (\Delta_{11} \hat{z}_k, \ldots, \Delta_{n_1 n_2} \hat{z}_k) \|_\infty
\]

where \( \nu \geq 1 \) is a coefficient introduced to guarantee a desired safety level.

This procedure is based on the observation that the Lipschitz constant of a differentiable function is an upper bound of the function’s gradient norm, which gives the
motivation for (10).

6 Uncertainty bounds

In this section, we derive tight uncertainty bounds for the unknown function $f_o$ and its derivatives $f_o^{(i)}$, $i = 1, \ldots, n_x$. These bounds allow us to quantify the modeling error and the prediction uncertainty. They can be useful in real-world applications for several purposes, such as robust control design [7], [29], prediction interval evaluation [19], and fault detection [23]. Based on the uncertainty bounds, we present an algorithm allowing us to estimate the noise bounds $\mu^i$. The result presented here regarding the uncertainty bound derivation is an extension of the one in [18,20,23] to the case where the bounds are derived not only for a function but also for its first-order derivatives.

Under the Lipschitz assumption $\Delta^{(i)} \in \mathcal{L}(\gamma^i, X)$, we can define the following functions:

$$
\overline{\Delta}^i(x) = \min_{k=1, \ldots, L} \left( \bar{h}_k^i + \gamma^i \|x - \bar{x}_k^i\|_{\infty} \right)
$$

$$
\underline{\Delta}^i(x) = \max_{k=1, \ldots, L} \left( \underline{h}_k^i - \gamma^i \|x - \bar{x}_k^i\|_{\infty} \right)
$$

(11)

where $\bar{h}_k^i = \bar{z}_k^i - \hat{f}^{(i)}(\bar{x}_k^i)$, $\underline{h}_k^i = \underline{z}_k^i - \hat{f}^{(i)}(\bar{x}_k^i) - \mu^i$, and $i = 0, \ldots, n_x$.

A result is now presented, providing tight uncertainty bounds in closed form for the unknown function $f_o$ and its derivatives $f_o^{(i)}$. The result holds in the case where the noise is bounded in $\ell_\infty$ norm. The case where the noise is bounded in $\ell_2$ norm is discussed afterwards.

Theorem 5 Let the assumptions of Theorem 2 hold and $q = \infty$ in the noise bounds $\|d^i\|_q \leq \mu^i$. Then, $\tilde{f}^i(x) \leq f_o^{(i)}(x) \leq \overline{f}^i(x)$, where

$$
\overline{f}^i(x) = \hat{f}^{(i)}(x) + \min \left( \gamma^i, \overline{\Delta}^i(x) \right)
$$

$$
\underline{f}^i(x) = \hat{f}^{(i)}(x) + \max \left( -\gamma^i, +\underline{\Delta}^i(x) \right)
$$

(12)

and $\gamma^i \equiv 0$ if $i = 0$ or $\gamma^i \equiv \gamma^0$ otherwise. Moreover,

$$
\overline{f}^i(x) = \sup_{f \in \mathcal{F}} f(x)
$$

$$
\underline{f}^i(x) = \inf_{f \in \mathcal{F}} f(x)
$$

(13)

where $\mathcal{F}^i = \{ f : f - \hat{f}^{(i)} \in \mathcal{L}(\gamma^i, X), \| \hat{z}^i - f(\bar{x}) \|_{\infty} \leq \mu^i \}$.

Proof. See the Appendix.

This theorem shows that, for a given $i \in \{0, \ldots, n_x\}$, $\overline{f}^i$ and $\underline{f}^i$ are the tightest upper and lower bounds of $f_o^{(i)}$ that can be defined on the basis of the information available about $f_o^{(i)}$, summarized by the function set $\mathcal{F}^i$. This result is important since it shows that the bounds $\overline{f}^i$ and $\underline{f}^i$ are tight. Examples of these bounds are reported in Figures 2 and 3 below. Note that improved bounds on $f_o^{(i)}$ could be formally defined under the assumption $f \in \mathcal{F}$, instead of $f \in \mathcal{F}^i$. However, the evaluation of such bounds would be hard from a computational point of view. On the contrary, the bounds (12) are written in closed form and are simple to evaluate.

Remark 3 It can be proven that the function $f_c$ defined as $f_c(x) = \frac{1}{2} \left( \overline{f}^i(x) + \underline{f}^i(x) \right)$ is an optimal approximation of $f_o$ in any $\mathcal{L}_p$ space [18]. However, $f_c$ is not an optimal approximation of $f_o$ in a Sobolev space. Indeed, the derivatives of $f_c$ are discontinuous and thus are not appropriate for approximating the derivatives of $f_o$, which instead are continuous.

In the case where the noise is bounded in $\ell_2$ norm (i.e., $q = 2$ in the noise bounds $\|d^i\|_q \leq \mu^i$), Theorem 5 cannot be applied as is, since the $\ell_2$ norm bound on the sequence gives no information on how the individual elements $d_k^i$ are bounded. In order to overcome this issue, some additional assumption has to be made on the element-wise boundedness of the noise sequence $d^i$. Suppose that the estimates $\hat{f}^{(i)}$ obtained from some of the two identification methods in Section 4 are sufficiently accurate approximations of the functions $f_o^{(i)}$: $\hat{f}^{(i)}(\bar{x}_k) \equiv f_o^{(i)}(\bar{x}_k)$. It follows that $d_k^i = \bar{z}_k^i - f_o^{(i)}(\bar{x}_k) \equiv \bar{z}_k^i - \hat{f}^{(i)}(\bar{x}_k) \equiv \delta_k^i$. It is then natural to consider the following relative-plus-absolute error bound:

$$
|d_k^i| \leq \zeta_k^i \equiv \zeta_k^i \| \delta_k^i \| + \zeta_k^i, \quad k = 1, \ldots, L
$$

(14)

where the term $\zeta_k^i \| \delta_k^i \|$ accounts for the fact that $d_k^i \equiv \delta_k^i$ and $\zeta_k^i$ accounts for the fact that $d_k^i$ and $\delta_k^i$ are not exactly equal. The parameters $\zeta_k^i, \zeta_A^i$ have to be taken such that $\zeta_k^i \mu^i + \zeta_A^i \sqrt{L} \leq \mu^i$. Indeed, if this inequality is satisfied, (14) is consistent with $\|d^i\|_q \leq \mu^i$, since $\|d^i\|_2 \leq \zeta_k^i \mu^i + \zeta_A^i \sqrt{L} \leq \mu^i$. Following this indication, $\zeta_k^i$ and $\zeta_A^i$ can be chosen by means of the procedure presented at the end of this section. Assuming the bound (14), Theorem 5 holds, where the functions $\overline{\Delta}$ and $\underline{\Delta}$ in (12) are defined as in (11), with $\mu^i \to \zeta_k^i$.

Now, a procedure for estimating the noise bounds $\mu^i$ in is proposed, based on the optimal function bounds given in Theorem 5. For a given $i$, consider the case where $\hat{f}^{(i)}(x) = 0, \forall x \in X$. Suppose that the Lipschitz constant $\gamma^i$ of the function $\Delta^{(i)} \equiv f_o^{(i)} - \hat{f}^{(i)}$ has been estimated by means of Algorithm 1 in Section 7. According to Theorem 5, for some suitable $\mu^i \geq 0$, the functions $\overline{f}^i$ and $\underline{f}^i$ (in (12) are upper and lower bounds of the unknown function $f_o^{(i)}$. Clearly, it must hold that $\overline{f}^i(x) > \underline{f}^i(x), \forall x \in X$. The following procedure provides an estimate of $\mu^i$ such that this inequality is met on the measured data.

1. Let $\hat{f}^{(i)}(x) = 0, \forall x \in X$.

2. Solve the following optimization problem:

$$
\mu^i = \min_{\mu^i \geq 0} \mu^i
$$

s.t.

$$
\overline{f}^i(\bar{x}_k) > \underline{f}^i(\bar{x}_k), \quad k = 1, \ldots, L.
$$

(15)
(3) Estimate the noise bound as $\tilde{p}^i = \nu \mu^i$, where $\nu \geq 1$ is a coefficient introduced to guarantee a desired safety level.

The optimization problem (15) can be easily solved since the decision variable $p^i$ is scalar and the number of constraints is finite. Notice that this procedure uses data only to estimate the noise bounds, and no preliminary approximations of the unknown function are required.

7 Estimation of the derivative values

In practical situations, only the output of the function that describes the system of interest is usually measured, while the outputs of its derivatives are not. In this section, we propose an algorithm for estimating the derivative output samples $\tilde{x}_k$ and $\tilde{z}_k$.

Suppose that the data $D^0 = (\tilde{x}_k, \tilde{z}_k)_{k=1}^L$ is available. The algorithm for estimating the derivative output samples $\tilde{x}_k^i$, $i > 0$, is the following.

**Algorithm 1** For $k = 1, \ldots, L$:

1. Define the set of indexes $\Upsilon_{pk} \doteq \{j \in \{1, \ldots, L\} : \|\tilde{x}_j - \tilde{x}_k\|_2 \leq \rho\}$
   where $\rho > 0$ is a user-defined radius.

2. Define the following quantities:
   
   $\tilde{z}_{pk} = \begin{bmatrix} \tilde{z}_{j_1} - \tilde{z}_k \\ \vdots \\ \tilde{z}_{j_M} - \tilde{z}_k \end{bmatrix}, \quad \Phi_{pk} = \begin{bmatrix} \tilde{x}_{j_1}^\top - \tilde{x}_k^\top \\ \vdots \\ \tilde{x}_{j_M}^\top - \tilde{x}_k^\top \end{bmatrix}$
   
   where $\{j_1, \ldots, j_M\} = \Upsilon_{pk}$ and $M = \text{card}\Upsilon_{pk}$.

3. Compute
   
   $g_k = \arg\min_{g \in \mathbb{R}^d} \frac{1}{M} \|\tilde{z}_{pk} - \Phi_{pk}g\|^2_2$.  \hspace{1cm} (16)

4. Estimate the derivative output samples as $\tilde{x}_k^i = g_{k_{i+1}}, k = 1, \ldots, L, i = 1, \ldots, n_x$, where $g_{k_{i+1}}$ are the components of $g_k$.

5. In the case where the data are affected by a relevant noise and/or the data set is not sufficiently large, the estimated gradient sequence $\{g_k\}_{k=1}^L$ can be smoothed by means of a suitable anti-causal discrete-time filter.

The idea behind the algorithm is to identify a local linear model at each point $\tilde{x}_k$ (steps 1-3). The gradient of $f_o$ is then estimated by taking the gradient of this local model, whose coefficients are indeed the gradient components (step 4). The following result provides a bound on the gradient estimation error.

**Theorem 6** Assume that:

(i) The derivatives $f_o^{(i)}, i = 1, \ldots, n_x$, are Lipschitz continuous on $X$.

(ii) For any $\rho > 0$, a $M_0 > 0$ exists such that $\frac{1}{M}\Phi_{pk}^\top \Phi_{pk} > 0, \forall M \geq M_0$.

Then, for any $\epsilon > 0$, some $M_0 > 0$ and $\rho > 0$ exist such that the gradient estimation error is bounded as

\[ \|\nabla f_o(\tilde{x}_k) - g_k\|_q \leq 2\|\Phi_{pk}\|_q \mu + \epsilon, \quad \forall M \geq M_0 \]  \hspace{1cm} (17)

where $\Phi_{pk}^\dagger = (\Phi_{pk}^\top \Phi_{pk})^{-1}\Phi_{pk}^\top$ is the pseudo-inverse matrix of $\Phi_{pk}$ and $q \in [2, \infty]$.

**Proof.** See the Appendix. \hfill $\Box$

This theorem can be interpreted as follows. Two main conditions are sufficient for obtaining a bound on the gradient estimation error. The first one (assumption (i) in the theorem) is Lipschitz continuity of the derivatives $f_o^{(i)}, i = 1, \ldots, n_x$. This assumption is reasonable, since we already know that $f_o \in \mathcal{S}_p(X)$, which implies that $f_o^{(i)}, i = 1, \ldots, n_x$, are continuous (a slightly weaker condition with respect to Lipschitz continuity). The second one (assumption (ii)) is a standard persistence of excitation condition $[13, 26]$. The next result shows that, under these two assumptions and some further technical conditions, the gradient estimate converges to its true value as $\rho \to 0$ and $M \to \infty$.

**Theorem 7** Let the assumptions of Theorem 6 be true. Let also the following limits hold:

\[
\lim_{\rho \to 0} \lim_{M \to \infty} \frac{1}{M} \sum_{k=1}^{M} f_o(\tilde{x}_k) = \sigma_D^2 \quad (18)
\]

\[
\lim_{\rho \to 0} \lim_{M \to \infty} \frac{1}{M} \sum_{k=1}^{M} \frac{1}{M} \sum_{j=1}^{M} (f_o(\tilde{x}_k) - f_o(\tilde{x}_j))^2 = 0 \quad (19)
\]

where $D_k \doteq (d_{1k}, \ldots, d_{Mk} - d_k)$ and $0 \leq \sigma_D^2 < \infty$. Then, $\lim_{\rho \to 0} \lim_{M \to \infty} \frac{1}{M} \|\nabla f_o(\tilde{x}_k) - g_k\|_q = 0$.

**Proof.** See the Appendix. \hfill $\Box$

This theorem shows that, in order to ensure convergence of the estimate to the true gradient, the limits (18) and (19) must hold (besides the basic assumptions of Theorem 6). The limit (18) means convergence of the sample noise variance. The limit (19) implies sample uncorrelation between the noise and the regressor. Both these limits (in their statistical version) represent standard assumptions in the literature on system identification, see, e.g., [13].

8 Numerical examples

Two numerical examples are presented in this section. The first one is a very simple example concerning a scalar function of a scalar variable. The second one discusses a more complex application to multi-step prediction of the Chua chaotic circuit. These examples show that the proposed approach may provide significantly more accurate and reliable models than traditional approaches based on plain function approximation.
8.1 Example: univariate function approximation

The following univariate function is considered in this example:

\[ f_o(x) = \sin(1.1x) \]

where \( x \in \mathbb{R} \) and \( f_o : \mathbb{R} \rightarrow \mathbb{R} \).

The function and its derivative were evaluated in \( L = 100 \) linearly equally spaced points in the domain \( X = [-2, 3] \). A normally distributed noise with zero mean and standard deviation 0.05 was added to both the function values and its derivative values, computed analytically. Hence, a noise-corrupted identification dataset of the form (2) was obtained. A validation dataset of length \( L = 1000 \) was also obtained in the same domain \( X \). This set consists of noise-free data, in order to compare the output of the models that will be identified with the true function values.

A model function of the form (4) was considered, with a basis function set composed of univariate monomials up to degree \( d = 5 \). Two models were identified from the identification dataset:

- **Model 1.** Function values used for model identification, function derivative values not used. The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 0, \) and \( \Lambda = 1 \).

- **Model 2.** Both function and derivative values used for model identification. The derivative values were computed analytically. The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 2, \) and \( \Lambda = 1 \).

The results obtained by the two models on the validation dataset are summarized in Table 1, where the obtained Root Mean Square Errors are reported. RMSE is the error between the true function \( f_o \) and the model \( \hat{f} \); \( \text{RMSE}^{(1)} \) is the error between the true function derivative \( f_o^{(1)} \) and the model derivative \( \hat{f}^{(1)} \). The upper plot in Figure 1 shows the comparison between the true function values and the outputs of the identified models. The lower plot in Figure 1 shows the comparison between the true derivative values and the outputs of the model derivatives. In Figure 2, the Model 2 uncertainty bounds, computed according to (12), are reported.

From these results, we can conclude that the model identified using the derivative values (Model 2) provides a more accurate approximation of the true function derivative with respect to the model identified not using the derivative values (Model 1). What is quite surprising is that Model 2 provides also a better approximation of the true function itself.

### Table 1

| Estimations | RMSE  | RMSE\(^{(1)}\) |
|-------------|-------|----------------|
| Model 1     | 2.54e-02 | 5.86e-02       |
| Model 2     | 1.19e-02 | 2.57e-02       |

8.2 Example: multi-step prediction for the Chua chaotic circuit

The Chua circuit is a simple electronic circuit showing a chaotic behavior, see [3]. It is composed of two capacitors, an inductor, a locally active resistor and a nonlinear resistor. The circuit continuous-time state equations are the following:

\[
\begin{align*}
\dot{x}_1 &= \alpha(x_2 - x_1 - \rho(x_1)) \\
\dot{x}_2 &= x_1 - x_2 + x_3 + u + \xi \\
\dot{x}_3 &= -\beta x_2 - R x_3 \\
y &= x_1
\end{align*}
\]

where the states \( x_1 \in \mathbb{R} \) and \( x_2 \in \mathbb{R} \) represent the voltages across the capacitors, \( x_3 \in \mathbb{R} \) the current through the inductor, \( u \in \mathbb{R} \) is an external input, \( y \in \mathbb{R} \) is the system output, \( \xi \in \mathbb{R} \) is a disturbance, and \( \alpha \in \mathbb{R}, \beta \in \mathbb{R} \) and \( R \in \mathbb{R} \) are parameters. In this example, the following nonlinear resistor characteristic and parameter values are assumed: \( \rho(x_1) = -1.16 x_1 + 0.041 x_1^3, R = 0.1, \alpha = 10.4, \beta = 16.5 \). With this parameter values and nonlinearity, the system exhibits a chaotic behavior and thus prediction is an extremely hard task.
The system (20), discretized via the forward Euler method, can be written in the following input-output regression form:

\[
y_t = b_1 y_{t-1} + b_2 y_{t-2} + b_3 y_{t-3} + b_4 \rho(y_{t-1}) + b_5 \rho(y_{t-2}) + b_6 \rho(y_{t-3}) + b_7 u_{t-2} + b_8 u_{t-3} + \xi_t
\]  

where \( \xi_t \) is a noise accounting for the disturbance \( \xi^c \) in (2) and \( b_i \) are suitable parameters. Equivalently, it can be written in the form (2), with \( x_t = (y_t, y_{t-1}, y_{t-2}, u_{t-1}, u_{t-2}) \).

The system (20) has been implemented in Simulink. The input \( u \) was simulated as a normally distributed random signal with zero mean and standard deviation (std) 1. The disturbance \( \xi^c \) was simulated as a normally distributed random signal with zero mean. Two std values were considered for this disturbance: 0.01 and 0.05. For each of these std values, two simulations of duration 60 s were carried out and, correspondingly, two sets of data of the form (2) were collected with a sampling time \( T_s = 0.01 \) s, corresponding to an experiment length \( L = 6000 \) for every dataset. The first dataset was used for model identification, the second one for model validation.

For each std value of the disturbance \( \xi^c \), the following prediction models were identified from the identification dataset.

- **One-step predictor identified not using any derivative information (P1_NOD).** The predictor P1_NOD is given by

\[
y_{t+1} = \hat{f}(x_t) \quad x_t = (y_t, y_{t-1}, y_{t-2}, u_{t-1}, u_{t-2})
\]  

where \( \hat{f} \) is of the form (4). A basis function set composed of multivariate monomials has been used, defined as

\[
\{ \phi_j \}_{j=1}^N = \prod_{i=1}^{n_x} x_{i,t}^{a_{i,t}-1}; \alpha_i = 1, 2; i = 1, \ldots, n_x \}
\]  

where \( x_{i,t} \) is the \( i \)th component of \( x_t \) and \( n_x = 5 \). This set consists of \( N = 2^{3n_x} \) basis functions. The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 200, i > 0, \) and \( \Lambda = 50 \).

- **One-step predictor identified using the true derivative values (P1_D).** The predictor P1_D is of the form (21). The basis functions are the same as those used in (22). The true derivative values computed from (21) were used to construct the vector \( \hat{z}^i, i > 0 \), in (6). The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 200, i > 0, \) and \( \Lambda = 50 \).

- **One-step predictor identified using the estimated derivative values (P1_ED).** The predictor P1_ED is of the form (22). The basis functions are the same as those used in (22). The derivative values estimated by Algorithm 1 were used to construct the vector \( \hat{z}^i, i > 0 \), in (6). The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 200, i > 0, \) and \( \Lambda = 50 \).

\[\hat{f}(x_t) = y_{t+1},  \quad \hat{f}(x_t) = \hat{f}(x_t) + \hat{f}(x_t) + \hat{f}(x_t) + \hat{f}(x_t) \]

For each std value of the disturbance \( \xi^c \) (std \( \in \{0.01, 0.05\})\), the identified models were tested on the validation set in the task of \( \kappa \)-step ahead prediction, with \( k \in \{3, 5, 7\} \). The \( \kappa \)-step prediction of models P1_NOD, P1_D and P1_ED was computed by iterating \( k \) times equation (22). The \( \kappa \)-step prediction of models PK_NOD and PK_ED was computed directly using equation (24).

\[\hat{z}^i, i > 0, \in (6)\]

The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 200, i > 0, \) and \( \Lambda = 50 \).

- **Direct multi-step predictor identified not using any derivative information (PK_NOD).** The predictor PK_NOD is given by

\[
y_{t+k} = \hat{f}(x_t) \quad x_t = (y_t, y_{t-1}, y_{t-2}, u_{t+k-2}, u_{t+k-3}, \ldots, u_{t-2})
\]  

where \( \hat{f} \) is of the form (4) and \( k \in \{3, 5, 7\} \). The basis function set is defined as in (23), with \( n_x = 4 + k \). This set consists of \( N = 2^{4+k} \) basis functions. The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 0, i > 0, \) and \( \Lambda = 50 \).

- **Direct multi-step predictor identified using the estimated derivative values (PK_ED).** The predictor PK_ED is of the form (24). The basis functions are the same as those used in (24). The derivative values estimated by Algorithm 1 were used to construct the vector \( \hat{z}^i, i > 0, \in (6) \). The coefficients \( a_j \) in (4) were identified by Method 2, with \( q = 2, r = 1, \lambda^0 = 1, \lambda^1 = 200, i > 0, \) and \( \Lambda = 50 \).

For each std value of the disturbance \( \xi^c \) (std \( \in \{0.01, 0.05\} \)), the identified models were tested on the validation set in the task of \( \kappa \)-step ahead prediction, with \( k \in \{3, 5, 7\} \). The \( \kappa \)-step prediction of models PK_NOD, PK_D and PK_ED was computed by iterating \( k \) times equation (22). The \( \kappa \)-step prediction of models PK_NOD and PK_ED was computed directly using equation (24).

The results of these tests are summarized in Tables 8.2 and 8.2, where the Root Mean Square prediction Errors RMSEk are reported, for \( k \in \{3, 5, 7\} \) and \( \text{std} \in \{0.01, 0.05\} \). Figure 3 shows the true system output, the 3-step prediction of the model PK_ED (in the case where std = 0.05) and the related uncertainty bounds, for a portion of the validation set. Note that these results were obtained using Method 2. Similar results can be obtained using Method 1 (they are not reported here for the sake of brevity).

The main observation arising from these results is that the models identified by the proposed method, using the information about the derivatives, are significantly more...
These inequalities are equivalent to the following ones: form (4) exists, such that inequalities (8) are satisfied.

lem (7)-(8) is feasible, then an approximation is that the direct the other two in the context considered in this paper) identified using the true derivative values. A third ob-
ervation is that the models identified using the estimated identified not using this information. A second obser-
accurate (about one order of magnitude) than those
errors.

In this example, the models identified using our meth-
has been developed, guaranteed uncertainty bounds
Within this approach, an optimality analysis
An approach for the identification of a function to-
9 Conclusions
An approach for the identification of a function to-
gether with its derivatives has been proposed in this
paper. Within this approach, an optimality analysis
has been developed, guaranteed uncertainty bounds
have been derived and a technique for estimating the
derivative values from the input-output data has been
presented. The approach has been tested in two sim-
ulated examples. One of these examples is concerned
with multi-step prediction of the Chua chaotic circuit.
In this example, the models identified using our meth-
ods resulted to be significantly more accurate than
other models obtained using a standard identification
technique, demonstrating the potential of the proposed
identification approach. Future research activities will
regard the derivation of prediction models suitable for
the data-driven NMPC techniques of [24,25] and the
application to problems of practical interest.

Appendix: Theorem proofs

Proof of Theorems 1 and 2. If the optimization problem (7)-(8) is feasible, then an approximation \( \hat{f} \) of the
form (4) exists, such that inequalities (8) are satisfied. These inequalities are equivalent to the following ones:
\[ \| \hat{f} - f^i(\tilde{x}) \|_2 \leq \mu_i, \quad i = 0, \ldots, n_x. \] Moreover, \( \hat{f} \in \mathcal{S}_{1\mu}(X) \) by definition. It follows that \( \hat{f} \in \text{FFS}_S \), which
implies \( \text{FFS}_S \neq \emptyset \). This proves Theorem 1.

As shown in [35], [17], if \( \hat{f} \in \text{FFS}_S \), then \( \hat{f} \) is \( \text{FFS}_S \)-almost-optimal. This proves Theorem 2.

Proof of Theorems 3 and 4. The proof of Theorem 1 shows that, if the optimization problem (7)-(8) is feasible,
then an approximation \( \hat{f} \) of the form (4) exists, and \( \hat{f} \in \text{FFS}_S \). Consider now the function \( f = \hat{f} + \Delta \),
with \( \Delta = 0 \). Obviously, \( f = \hat{f} \in \text{FFS}_S \) and \( f^{(i)} - \hat{f}^{(i)} = \Delta = 0 \in \mathcal{L}(\gamma^i, X) \), for any \( \gamma^i \geq 0 \). From Definitions 2 and 7,
it follows that \( f = \hat{f} \in \text{FFS}_\mathcal{L} \), which implies \( \text{FFS}_\mathcal{L} \neq \emptyset \). This proves Theorem 3.

As shown in [35], [17], if \( \hat{f} \in \text{FFS}_\mathcal{L} \), then \( \hat{f} \) is \( \text{FFS}_\mathcal{L} \)-almost-optimal. This proves Theorem 4.

Proof of Theorem 5. The proof for the case \( i = 0 \) comes from Theorem 3 in [23]. This theorem shows that the following bounds hold for every \( x \in X \):
\[
\begin{align*}
fo(x) & \leq \hat{f}^0(x) + 0 \leq \hat{f}(x) + 0 = f(x) \\
fo(x) & \geq \hat{f}^0(x) + 0 \geq \hat{f}(x) + 0 = f(x).
\end{align*}
\]
In the case \( i > 0 \), under the assumption (5.2), we can follow the same arguments of the proof of Theorem 3 in [23]. In this way, we obtain that the following bounds hold for every \( x \in X \):
\[
\begin{align*}
fo^{(i)}(x) & \leq \hat{f}^{(i)}(x) + \gamma^i(x) \\
fo^{(i)}(x) & \geq \hat{f}^{(i)}(x) + \gamma^i(x).
\end{align*}
\]

Moreover, we know that \( \gamma^0 \) is Lipschitz continuous with constant \( \gamma^0 \). This implies that
\[
\left| f_o^{(i)}(x) - \hat{f}^{(i)}(x) \right| \leq \gamma^0 \equiv \gamma, \quad i = 1, \ldots, n_x.
\]

The bounds (12) for \( i > 0 \) are obtained from (25) and (26). Equations (13) follow from Theorem 2 in [18].

Proof of Theorem 6. Let us consider the Taylor expansion of \( f_o \) around a point \( \tilde{x}_k \):
\[
f_o(x) = f_o(\tilde{x}_k) + (x - \tilde{x}_k)\nabla f_o(\tilde{x}_k) + R(x - \tilde{x}_k)
\]
where \( \nabla f_o = (f_o^{(1)}, \ldots, f_o^{(n_x)}) \) is the gradient of \( f_o \) and \( R(\cdot) \) is a reminder. This expression, evaluated at a point \( \tilde{x}_j \), with \( j \in \mathcal{T}_{pk} \), becomes
\[
f_o(\tilde{x}_j) = f_o(\tilde{x}_k) + (\tilde{x}_j - \tilde{x}_k)\nabla f_o(\tilde{x}_k) + R(\tilde{x}_j - \tilde{x}_k).
\]
From (3), this can be written as
\[
\tilde{z}_j - \tilde{z}_k = (\tilde{x}_j - \tilde{x}_k)\nabla f_o(\tilde{x}_k) + R(\tilde{x}_j - \tilde{x}_k) + d_j - d_k.
\]

For \( j = j_1, \ldots, j_M \), we obtain the following equation in matrix form:
\[
\tilde{z}_{pk} = \Phi_{pk}\nabla f_o(\tilde{x}_k) + \Xi_k + D_k
\]
where $\Xi_k = (R(\bar{x}_{j_1} - \bar{x}_k), \ldots, R(\bar{x}_{j_M} - \bar{x}_k))$ and $D_k = (d_{j_1} - d_k, \ldots, d_{j_M} - d_k)$. It follows that

$$\nabla f_o(\bar{x}_k) = \Phi_{pk}^\top \tilde{z}_{pk} - \Phi_{pk}^\top (\Xi_k + D_k)$$

where $\Phi_{pk}^\top = (\Phi_{pk}^\top \Phi_{pk})^{-1} \Phi_{pk}^\top$. The inverse $(\Phi_{pk}^\top \Phi_{pk})^{-1}$ exists and is finite since $\frac{1}{M} \Phi_{pk}^\top \Phi_{pk} > 0$, $\forall M \geq M_0$, by assumption. This matrix inequality also implies that the solution of the optimization problem (16) is given by $g_k = \Phi_{pk}^\top \tilde{z}_{pk}$. The vector $g_k$ is an estimate of the gradient $\nabla f_o(\bar{x}_k)$. The resulting estimation error $\nabla f_o(\bar{x}_k) - g_k$ is bounded as

$$\|\nabla f_o(\bar{x}_k) - g_k\|_q = |\Phi_{pk}^\top (\Xi_k + D_k)\|_q$$

$$\leq |\Phi_{pk}^\top|_q \|\Xi_k + D_k\|_q \leq |\Phi_{pk}^\top|_q (\|\Xi_k\|_q + 2\rho^0).$$

Being $f_o(i)$ Lipschitz continuous by assumption, each element of $\Xi_k$ is bounded as

$$|R(\bar{x}_j - \bar{x}_k)| \leq \gamma_R |R| \bar{x}_j - \bar{x}_k| \leq \rho \gamma_R, \forall \bar{x}_j \in X$$

for some $\gamma_R \geq 0$, $\gamma_R < \infty$. It follows that, for $\forall M \geq M_0$,

$$\|\Xi_k\|_q \leq \left\{ \begin{array}{ll} \rho \sqrt{M} \gamma_R, & q = 2 \\ \rho \gamma_R, & q = \infty. \end{array} \right. \quad (27)$$

Hence,

$$\|\nabla f_o(\bar{x}_k) - g_k\|_q \leq |\Phi_{pk}^\top|_q \|\Xi_k\|_q + |\Phi_{pk}^\top|_q + 2\rho^0$$

$$\leq |\Phi_{pk}^\top|_q \rho \sqrt{M} \gamma_R + |\Phi_{pk}^\top|_q + 2\rho^0 (q = 2)$$

or $\|\Phi_{pk}^\top|_q \rho \gamma_R + |\Phi_{pk}^\top|_q + 2\rho^0 (q = \infty)$.

The statement is proven choosing $\rho = \epsilon / (|\Phi_{pk}^\top|_q \sqrt{M} \gamma_R)$ ($q = 2$) or $\rho = \epsilon / (|\Phi_{pk}^\top|_q \gamma_R)$ ($q = \infty$).

Proof of Theorem 7. Let us denote the function gradient as $g_k = \nabla f_o(\bar{x}_k)$ and, for a certain gradient estimate $g$, the estimation error as $\delta g = g_o - g$. The objective function of the optimization problem (16) is

$$J(g) = \frac{1}{M} M \|	ilde{z}_{pk} - \Phi_{pk} g\|_2^2$$

This function can be written as

$$J(g) = \frac{1}{M} (\tilde{z}_{pk} - \Phi_{pk} g)^\top (\tilde{z}_{pk} - \Phi_{pk} g)$$

$$= \frac{1}{M} (\tilde{z}_{pk} - \Phi_{pk} g_o + \Phi_{pk} \delta g)^\top (\tilde{z}_{pk} - \Phi_{pk} g_o + \Phi_{pk} \delta g)$$

$$= \frac{1}{M} (\Xi_k + D_k + \Phi_{pk} \delta g)^\top (\Xi_k + D_k + \Phi_{pk} \delta g)$$

$$= \frac{1}{M} \Xi_k^\top \Xi_k + \frac{1}{M} D_k^\top D_k + \frac{1}{M} \delta g^\top \Phi_{pk}^\top \Phi_{pk} \delta g$$

$$+ \frac{2}{M} D_k^\top \Xi_k + \frac{2}{M} \Xi_k^\top \Phi_{pk} \delta g + \frac{2}{M} D_k^\top \Phi_{pk} \delta g.$$

From (27) and the noise bounds $\|d^\top\|_q \leq \rho^i$, a sufficiently large $M_0$ exists such that

$$\frac{1}{M} \Xi_k^\top \Xi_k \leq \gamma_R^2 \rho^0, \forall M \geq M_0$$

$$\frac{1}{M} (D_k^\top D_k)^{\gamma_R} \leq 2 \rho^0 \gamma_R, \forall M \geq M_0.$$

From (18) and (19), for every $\epsilon > 0$, a sufficiently large $M_0$ exists such that

$$\left| \frac{1}{M} D_k^\top D_k - \sigma^2 \right| \leq \epsilon, \forall M \geq M_0$$

$$\left| \frac{1}{M} M \Phi_{pk} \delta g \right| \leq \|\delta g\|_2 \epsilon, \forall M \geq M_0.$$

Moreover,

$$\frac{1}{M} \|\Xi_k^\top \Phi_{pk} \delta g\| \leq \frac{1}{\sqrt{M}} \|\Phi_{pk}\|_2 \|\delta g\| \|2\gamma_R\rho.$$

The quantity $\|\Phi_{pk}\|_2 / \sqrt{M}$ is bounded as

$$\frac{1}{\sqrt{M}} \|\Phi_{pk}\|_2 \leq \frac{\sqrt{M}}{M} \left( \sum_{i=1}^M \left( \frac{\phi_{pk,i}^2}{2} \right)^{1/2} \right)$$

$$\leq \sqrt{M} (n \Theta \max_{i,j} (\Phi_{pk})_{ji})^{1/2} = \sqrt{\theta} \max_{i,j} (\Phi_{pk})_{ji}$$

where the first inequality is a standard result in the literature and $(\Phi_{pk})_{ji}$ are the entries of $\Phi_{pk}$. Note that $\max_{i,j} (\Phi_{pk})_{ji}$ is bounded, since the measurements $\tilde{x}_j$ are assumed to be in a compact set. The quantity $\|\delta g\|_2$ is bounded on any compact set $G$ containing $g_0$; for all $g \in G$, $\|\delta g\|_2 \leq \tilde{G}$, for some $G \leq \tilde{G} < \infty$.

From all the above inequalities, we have that

$$|J(g) - J_o(g)| \leq \gamma_R^2 \rho^0 + 4 \rho^0 \delta g + 2 \rho^0 \delta g + 2 \sqrt{\rho} \max_{i,j} (\Phi_{pk})_{ji} \|\delta g\| \|G\| \|\delta g\| \|R\| \rho^0$$

where

$$J_o(g) = \frac{1}{M} \|\delta g\|_2 \Phi_{pk} \Phi_{pk}^\top \delta g + \sigma^2.$$ 

It follows that, as $\rho \to 0$ and $M \to \infty$, $J(g)$ converges to $J_o(g)$.

This convergence is uniform on any compact set $G$ containing $g_0$. It follows that the minimizers of $J(g)$ converge to the minimizers of $J_o(g)$, see [13]. The condition $\frac{1}{M} \Phi_{pk}^\top \Phi_{pk} \rho > 0$ ensures that $J_o(g)$ has a unique minimizer, given by $g_o = \nabla f_o(\bar{x}_k)$. The claim follows.

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