Letters

Support Vector Machines for Nonlinear Kernel ARMA System Identification

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Abstract—Nonlinear system identification based on support vector machines (SVM) has been usually addressed by means of the standard SVM regression (SVR), which can be seen as an implicit nonlinear autoregressive and moving average (ARMA) model in some reproducing kernel Hilbert space (RKHS). The proposal of this letter is twofold. First, the explicit consideration of an ARMA model in an RKHS (SVM-ARMA2K) is proposed. We show that stating the ARMA equations in an RKHS leads to solving the regularized normal equations in that RKHS, in terms of the autocorrelation and cross correlation of the (nonlinearly) transformed input and output discrete time processes. Second, a general class of SVM-based system identification nonlinear models is presented, based on the use of composite Mercer's kernels. This general class can improve model flexibility by emphasizing the input-output cross information (SVM-ARMA $_{4K}$), which leads to straightforward and natural combinations of implicit and explicit ARMA models (SVR-ARMA_{2K} and SVR-ARMA $_{4K}$). Capabilities of these different SVM-based system identification schemes are illustrated with two benchmark problems.

I. INTRODUCTION

A common problem in digital signal processing is to model a functional relationship between two simultaneously recorded discrete-time processes (DTP) [1]. When this relationship is linear and time-invariant, it is usually addressed with autoregressive and moving average (ARMA) modeling, but if linearity cannot be assumed, nonlinear system identification techniques are required. General nonlinear models, such as artificial neural networks, wavelet, and fuzzy models, are common and effective choices [1], [2], but the temporal structure of these nonlinear models cannot be easily analyzed, because it remains inside a black-box model.

Support vector machines (SVM) were originally conceived for pattern recognition and classification tasks [3], and support vector regression (SVR) was subsequently proposed as the SVM implementation for regression and function approximation [4]. SVMs have been successfully used in a huge variety of problems in signal processing, bioengineering or image processing [5], among others. Main advantage of SVM current algorithms is their capability for giving nonlinear algorithms by the statement of a well-known linear data model (classification or regression) in a nonlinearly transformed domain, known as reproducing kernel Hilbert space (RKHS). In [6]–[10], SVR algorithm was used for nonlinear system identification, but the time-series

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structure of the data was not scrutinized. In [11], SVM was explicitly formulated for modeling linear time-invariant ARMA systems (linear SVM-ARMA), and this kind of formulation has been recently extended to a general framework for linear signal processing problems [12].

This paper introduces an explicit formulation of the ARMA data structure in an RKHS by using the well-known *kernel trick*. The so-called SVM-ARMA $_{2K}$ allows us to study the time-series structure on a straightforward and natural way. Additionally, we introduce a general and still simple class of SVM-based system identification algorithms, by using *composite kernels*. In this context, a second algorithm is presented to take into account the input–output cross information (SVM-ARMA $_{4K}$). A full family of natural combinations of implicit and explicit ARMA models (SVR-ARMA $_{2K}$ and SVR-ARMA $_{4K}$ algorithms) is finally proposed.

The scheme of this work is as follows. Section II summarizes the SVR algorithm for nonlinear system identification. Section III presents the novel formulation of an explicit ARMA models in the RKHS. Section IV introduces the use of composite kernels for further model flexibility. Section V shows the advantages of the proposed methods in some benchmark examples. Section VI gives conclusions and outlines future work. Appendices I and II show the relationships between SVM system identification and the classical system identification families described in [1]: prediction error models (PEM) and correlation models (CM).

II. IMPLICIT ARMA SYSTEM IDENTIFICATION WITH SVR

Previous SVM-based approaches to nonlinear system identification have taken advantage of both the kernel trick and the well-developed SVR algorithmic implementations [6]–[10]. The nonlinear SVR-based system identification is briefly presented in this section, with the aims of reviewing the kernel trick, highlighting the implicit ARMA nature of this problem statement, and introducing the ε -Huber cost function in this setting.

A. Mercer's Kernels and Nonlinearity

Let us consider two DTPs, $\{u_n\}$ and $\{y_n\}$, which are the input and the output, respectively, of a nonlinear system. Let $\boldsymbol{y}_{n-1} = [y_{n-1}, y_{n-2}, \ldots, y_{n-P}]^T$ and $\boldsymbol{u}_n = [u_n, u_{n-1}, \ldots, u_{n-Q+1}]^T$ denote the states of input and output DTP at time instant n, so that $\boldsymbol{z}_n = [\boldsymbol{y}_{n-1}^T, \boldsymbol{u}_n^T]^T$ is just the vector concatenation of input and output states at that instant. We assume that P and Q are large enough so that the predictable part of the process is completely captured. The SVR-based system identification uses a nonlinear transformation $\boldsymbol{\phi}_z(\boldsymbol{z}_n): \mathbb{R}^P \times \mathbb{R}^Q \to \mathcal{H}_z$, which maps the concatenation vector to an RKHS \mathcal{H}_z , or *feature space*. For a properly chosen transformation $\boldsymbol{\phi}_z$, a linear regression model can be built in \mathcal{H}_z , and it is given by

$$y_n = \langle \boldsymbol{v}, \boldsymbol{\phi}_z(\boldsymbol{z}_n) \rangle + e_n \tag{1}$$

where $v \in \mathcal{H}_z$, $\langle \cdot, \cdot \rangle$ denotes the dot product, and $\{e_n\}$ is a DTP standing for the effect of measurement errors.

In general, the RKHS dimension (H_z) will be greater than the input space dimension (P+Q), and for some choices of the transformation it can be even infinite. However, the SVM methodology allows to still work in that high-dimensional RKHS by using Mercer's kernels [13]. If a bivariate function $K_z(z_i, z_j)$ fulfills Mercer's condition,

i.e., $\int K_z(z_i,z_j)f(z_i)f(z_j) \geq 0$ for any square integrable functions f(z), then there exist a Hilbert space \mathcal{H}_z and a mapping ϕ_z such that $K_z(z_i,z_j) = \langle \phi_z(z_i),\phi_z(z_j) \rangle$. Therefore, the kernel trick in SVM consists of stating the problem at hand (such as classification, regression, and many others) in terms of dot products in the RKHS, and then substituting these products by Mercer's kernels. The kernel expression is actually used in a given SVM algorithm, but neither the mapping function ϕ_z , nor the RKHS, need to be explicitly known.

The widely used Gaussian Mercer's kernel is given by $K_z(z_i,z_j)=\exp(-(\|z_i-z_j\|^2/2\sigma^2))$, where σ is the kernel width and can be seen as a parameter that controls the distortion in the input space to provide with an RKHS in which linear regression (1) is an appropriate model. For the Gaussian kernel, the explicit expression of nonlinear transformation $\phi_z(z)$ is unknown, and the corresponding RKHS dimension is infinite [13].

B. The ε -Huber Residual Cost

SVM algorithms minimize a cost function of the residuals (CFR) that is regularized with the L_2 norm of the model coefficients in an RKHS. Two CFRs have been used in previous SVM-based system identification research: 1) the ε -insensitive CFR [6], [7], which yields sparse solutions, is essentially a L_1 cost, and hence appropriate for dealing with outliers, and 2) the quadratic CFR used in least-squares (LS) SVM approaches [8]–[10], which is optimal when Gaussian noise is present, but it is sensitive to outliers, and more, it does not produce sparse solutions. The ε -Huber cost [11] contains the preceding ones as particular cases, and it is expressed as

$$\ell_P(e_n) = \begin{cases} 0, & |e_n| \le \varepsilon \\ \frac{1}{2\gamma} (|e_n| - \varepsilon)^2, & \varepsilon < |e_n| \le e_C \\ C(|e_n| - \varepsilon) - \frac{1}{2} \gamma C^2, & |e_n| > e_C \end{cases}$$
 (2)

where $e_c = \varepsilon + \gamma C$. Parameter γ controls the width of the L_2 interval between ε and e_c , so that the function is continuous and derivable, and the L_1 interval has slope C. The ε -insensitivity zone provides with sparse solutions in SVM formulation, which is a very desirable characteristic in nonlinear formulations. The quadratic cost is optimal, in a maximum likelihood (ML) sense, when the noise is Gaussian, whereas the linear cost is optimal for exponential noise. Here, we propose to use the ε -Huber CFR because it has the ability to deal simultaneously with different kinds of noise [11]. The use of ε -insensitive CFR is not appropriate when Gaussian noise is present in the data, whereas a quadratic CFR (according to LS-SVM) does not produce sparse solutions.

C. Algorithm Statement for SVR System Identification

The algorithm for SVR system identification using the proposed ε -Huber cost reduces to the minimization of

$$L_P^{\text{SVR}}\left(v_j, \xi_n^{(*)}\right) = \frac{1}{2} \sum_{j=1}^{H_z} v_j^2 + \frac{1}{2\gamma} \sum_{n \in I_1} \left(\xi_n^2 + \xi_n^{*2}\right) + C \sum_{n \in I_2} \left(\xi_n + \xi_n^{*}\right) - \sum_{n \in I_2} \frac{\gamma C^2}{2}$$
(3)

where ξ_n , ξ_n^* , are the slack variables or losses, I_1 is the set of samples for which $\varepsilon \leq \xi_n^{(*)} \leq e_c$, I_2 is the set of samples for which $\xi_n^{(*)} > e_c$, and constrained to

$$y_n - \mathbf{v}^T \boldsymbol{\phi}_z(\mathbf{z}_n) \le \varepsilon + \xi_n \qquad \forall n = n_0, \dots, N$$
 (4)

$$-y_n + \mathbf{v}^T \boldsymbol{\phi}(\mathbf{z}_n) < \varepsilon + \xi_n^* \qquad \forall n = n_0, \dots, N$$
 (5)

where $\xi_n^{(*)} \geq 0$, n_0 is given by the required initial conditions (without loss of generality, $n_0 = 1$ and null initial conditions), N is the number of available samples, and $\xi_n^{(*)}$ denotes both ξ_n and ξ_n^* .

The Lagrangian for this problem is obtained by introducing a coefficient (Lagrange multiplier) for each constraint [14]. In particular, α_n and α_n^* are the (nonnegative) Lagrange multipliers corresponding to (4) and (5), respectively. By making zero the gradient of the Lagrangian with respect to v_j and $\xi_n^{(*)}$, we obtain

$$\boldsymbol{v} = \sum_{n=1}^{N} (\alpha_n - \alpha_n^*) \, \boldsymbol{\phi}_z(\boldsymbol{z}_n) = \sum_{n=1}^{N} \beta_n \boldsymbol{\phi}_z(\boldsymbol{z}_n)$$
 (6)

and $0 \le \alpha_n^{(*)} \le C$, where $\beta_n = \alpha_n - \alpha_n^*$. After introducing these conditions into the Lagrangian, the primal variables are removed, and a term-grouping can be done by writing down the Gram matrix of dot products in the RKHS, or kernel matrix

$$G_{ij} = \langle \phi_z(z_i), \phi_z(z_j) \rangle = K_z(z_i, z_j). \tag{7}$$

The dual problem consists in maximizing with constraints

$$L_{D}^{\text{SVR}}\left(\alpha_{n}^{(*)}\right) = -\frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{*})^{T}[\boldsymbol{G} + \gamma \boldsymbol{I}](\boldsymbol{\alpha} - \boldsymbol{\alpha}^{*}) + (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{*})^{T}\boldsymbol{y} - \varepsilon \boldsymbol{1}^{T}(\boldsymbol{\alpha} + \boldsymbol{\alpha}^{*})$$
(8)

where $\boldsymbol{\alpha}^{(*)} = \left[\alpha_1^{(*)}, \ldots, \alpha_N^{(*)}\right]^T$ and $\boldsymbol{y} = [y_1, \ldots, y_N]^T$. This is a constrained quadratic programming (QP) problem that has a single minimum. It can be shown that the predicted output for a new observed sample y_r , given \boldsymbol{z}_r , is

$$\hat{y}_r = \sum_{n=1}^N \beta_n K_z(\boldsymbol{z}_n, \boldsymbol{z}_r). \tag{9}$$

This solution is expressed in terms of the observation vectors, and hence, if sparsity is allowed in the ε -Huber CFR by making $\varepsilon>0$, only some of the Lagrange multipliers are nonzero. Those samples with a nonzero coefficient are called *support vectors*, and they contain all the information that is relevant for building the model.

Property 1: The following nonlinear relationship between the residuals and the model coefficients holds:

$$\beta_n = g_{nl}(e_n) = \begin{cases} \operatorname{sign}(e_n)C, & |e_n| \ge e_c \\ \frac{\operatorname{sign}(e_n)}{\gamma} (|e_n| - \varepsilon), & \varepsilon \le |e_n| \le e_c \\ 0, & |e_n| < \varepsilon. \end{cases}$$
(10)

Proof: When using the ε -Huber CFR in SVM regression-like problems, a straightforward relationship between the residuals and the Lagrange multipliers can be derived from the Karush–Khun–Tucker (KKT) conditions [11], [12]. We have that $\alpha_n = C$ for $e_n \geq e_c$, that $\alpha_n = (1/\gamma)(e_n - \varepsilon)$ for $\varepsilon \leq e_n \leq e_c$, and that $\alpha_n = 0$ for $e_n < \varepsilon$. Also, we have that $\alpha_n^* = C$ for $e_n \leq -e_c$, that $\alpha_n^* = (1/\gamma)(-e_n - \varepsilon)$ for $-\varepsilon \geq e_n \geq -e_c$, and that $\alpha_n^* = 0$ for $e_n > -\varepsilon$. Given that $\beta_n = \alpha_n - \alpha_n^*$, then (10) holds.

According to (9), nonlinear relationship (10) can be conveniently used to control the impact of an outlier on the final solution by choosing appropriate values of the cost function parameters [12], i.e., an outlier will have, at most, a weight $|\beta_n| = C$. However, β_n for $\varepsilon < |e_n| < e_C$ can be more flexibly valuated than in ε -insensitive CFR. Free parameters of both the CFR and Mercer's kernel are usually determined in SVM algorithms by using cross-validation search.

III. EXPLICIT ARMA MODELS IN RKHS

The formulation presented in Section II uses a time-series model given by a nonlinear regression in an RKHS, whose input space is given by the concatenated vector z_n . Therefore, that model can be considered as an ARMA model only in a wide and implicit sense, given that both the AR and the MA component of the observed DTP are stacked and jointly transformed into that RKHS. Although this can be a valid and powerful approach, no useful insight about the temporal statistical properties of the data can be gained. This is a similar situation to the neural network (NN)-based analysis of time series, where the temporal structure remains inside a black-box equation [2]. Alternatively, we propose here to build an explicit ARMA model in some given RKHS, by taking advantage of Mercer's kernels, which will allow us to study the time-series structure of the data, even it being a nonlinear model.

Assume that both the input and the output DTP state vectors can be separately mapped to \mathcal{H}_u and \mathcal{H}_y , by using two possibly different nonlinear mappings $\boldsymbol{\phi}_u(\boldsymbol{u}_n):\mathbb{R}^Q \to \mathcal{H}_u$ and $\boldsymbol{\phi}_y(\boldsymbol{y}_n):\mathbb{R}^P \to \mathcal{H}_y$, respectively. A linear MA (AR) model component can be built in \mathcal{H}_u (\mathcal{H}_y) , and now, the ARMA difference equation is

$$y_n = \boldsymbol{a}^T \boldsymbol{\phi}_n(\boldsymbol{y}_{n-1}) + \boldsymbol{b}^T \boldsymbol{\phi}_n(\boldsymbol{u}_n) + e_n$$
 (11)

where $\boldsymbol{b} = [b_1, \dots, b_{H_u}]^T$ and $\boldsymbol{a} = [a_1, \dots, a_{H_y}]^T$ are vectors determining the MA and the AR coefficients of the system, respectively, in the RKHS; and H_u and H_y are the RKHS dimensions.

The primal problem can be here formulated as the minimization of

$$L_P^{2k}\left(a_i, b_j, \xi_n^{(*)}\right) = \frac{1}{2} \sum_{i=1}^{H_y} a_i^2 + \sum_{j=1}^{H_u} b_j^2 + \frac{1}{2\gamma} \sum_{n \in I_1} \left(\xi_n^2 + \xi_n^{*2}\right) + C \sum_{n \in I_2} \left(\xi_n + \xi_n^*\right) - \sum_{n \in I_2} \frac{\gamma C^2}{2}$$
(12)

constrained to

$$y_n - \boldsymbol{a}^T \boldsymbol{\phi}_y(\boldsymbol{y}_{n-1}) - \boldsymbol{b}^T \boldsymbol{\phi}_u(\boldsymbol{u}_n) \le \varepsilon + \xi_n$$
 (13)

$$-y_n + \boldsymbol{a}^T \boldsymbol{\phi}_n(\boldsymbol{y}_{n-1}) + \boldsymbol{b}^T \boldsymbol{\phi}_n(\boldsymbol{u}_n) \le \varepsilon + \xi_n^*$$
 (14)

and $\xi_n^{(*)} \geq 0$, for $n = 1, \dots, N$. By stating the Lagrangian and making its gradient zero, the AR and MA vector coefficients are given by

$$\boldsymbol{a} = \sum_{n=1}^{N} \beta_n \boldsymbol{\phi}_y(\boldsymbol{y}_{n-1}) \quad \boldsymbol{b} = \sum_{n=1}^{N} \beta_n \boldsymbol{\phi}_u(\boldsymbol{u}_n)$$
 (15)

which is a different expression for the model coefficients in (6), because AR and MA coefficients are now uncoupled in the RKHS.

After introducing (15) into the Lagrangian, we can identify two different Gram matrices, one for the input and other for the output DTP, denoted as

$$\boldsymbol{R}_{y,ij} = \left\langle \boldsymbol{\phi}_{y}(\boldsymbol{y}_{i-1}), \boldsymbol{\phi}_{y}(\boldsymbol{y}_{j-1}) \right\rangle = K_{y}(\boldsymbol{y}_{i-1}, \boldsymbol{y}_{j-1}) \tag{16}$$

$$\mathbf{R}_{u,ij} = \langle \boldsymbol{\phi}_{u}(\boldsymbol{u}_{i}), \boldsymbol{\phi}_{u}(\boldsymbol{u}_{i}) \rangle = K_{u}(\boldsymbol{u}_{i}, \boldsymbol{u}_{i}). \tag{17}$$

Equations (16) and (17) can be seen as uncoupled Gram matrices that also account for the sample estimators of input and output DTP autocorrelation functions [15], respectively, in the RKHS. The dual problem consists now in the constrained maximization of

$$L_D^{2k}\left(\alpha_n^{(*)}\right) = -\frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T [\boldsymbol{R}_u + \boldsymbol{R}_y + \gamma \boldsymbol{I}](\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) + (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T \boldsymbol{y} - \varepsilon \boldsymbol{1}^T (\boldsymbol{\alpha} + \boldsymbol{\alpha}^*). \quad (18)$$

The output for a new observation vector is obtained as

$$\hat{y}_r = \sum_{n=1}^N \beta_n \left(K_y(\boldsymbol{y}_{n-1}, \boldsymbol{y}_{r-1}) + K_u(\boldsymbol{u}_n, \boldsymbol{u}_r) \right). \tag{19}$$

Note that the model complexity, in terms of number of coefficients, is, as in (9), equal to the number of training samples N. We will denote this algorithm as SVM-ARMA $_{2K}$.

To gain further insight about the structure that SVM-ARMA $_{2K}$ has, we can analyze the temporal structure of the proposed model. According to [1], there are two main general classes of system identification algorithms: prediction error methods (PEM), which are based on the minimization of a function of the residual variance for a given model (e.g., least-squares and/or maximum a posteriori estimators); and correlation methods (CM), which minimize the cross correlation between a (possibly nonlinear) function of the residuals and some transformation of the data. In [11], a comparison of linear SVM-ARMA system identification with PEM and CM was presented. The SVM-ARMA2K nonlinear system identification model solves the regularized normal equations in some RKHS while minimizing the cross correlation between the data and a nonlinear function of the residuals, as shown in Appendices I and II. This nonlinear relationship is determined by the free parameters of the ε -Huber CFR.

IV. SVM SYSTEM IDENTIFICATION WITH COMPOSITE KERNELS

In Sections II and III, we have described the SVR-based and the SVM-ARMA $_{2K}$ system identification algorithms. Two questions can be raised at this moment. First, note that (19) in SVM-ARMA $_{2K}$ shows an apparent uncoupling between the input and the output DTP in the final solution, with no explicit consideration of the (maybe relevant) cross information between them. Although we are solving the normal equations in the RKHS, and the cross correlation is indeed implicitly considered therein, the SVM-ARMA_{2K} model could be somewhat limited in the cases when strong cross information was present. Therefore, we will look for an SVM-ARMA system identification model capable of considering a cross comparison between input and output DTP states, when this becomes necessary in the problem at hand. This new algorithm will be called SVM-ARMA_{4K}. Second, if we observe prediction equations (9) and (19), we can think of the possibility of combining them into a joint model for improving performance and flexibility simultaneously. These two additional algorithms are called SVR-ARMA $_{2K}$ and SVR-ARMA $_{4K}$.

In this section, we first describe the elements of a generic nonlinear mapping into an RKHS in an SVM system identification problem. Then, we use composite kernels as direct sum of different RKHS (a well-known result of functional analysis theory, see e.g., [16]), which allows us both to represent the previously described SVM models, and to formulate the aforementioned new system identification algorithms.

A. Generic SVM Algorithm for System Identification

Property 2: Let $\phi(z_n)$ be a composite nonlinear transformation (into an RKHS \mathcal{H}) given by the concatenation of M single nonlinear transformations to their RKHS, i.e.,

$$\boldsymbol{\phi}(\boldsymbol{z}_n) = \left[\boldsymbol{\phi}_1(\boldsymbol{z}_n)^T, \boldsymbol{\phi}_2(\boldsymbol{z}_n)^T, \dots, \boldsymbol{\phi}_M(\boldsymbol{z}_n)^T\right]^T. \tag{20}$$

The corresponding SVM system identification model is given by $y_n = \langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{z}_n) \rangle + e_n$, where $\boldsymbol{w} \in \mathcal{H}$. The kernel matrix is $+(\boldsymbol{\alpha}-\boldsymbol{\alpha}^*)^T\boldsymbol{y}-\varepsilon\mathbf{1}^T(\boldsymbol{\alpha}+\boldsymbol{\alpha}^*).$ (18) $\boldsymbol{K}_{ij}=\langle \boldsymbol{\phi}(\boldsymbol{z}_i),\boldsymbol{\phi}(\boldsymbol{z}_j)\rangle$, and it allows to state a dual QP problem that yields the model coefficients. The dual problem consists of maximizing with constraints

$$L_{D}\left(\alpha_{n}^{(*)}\right) = -\frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{*})^{T}[\boldsymbol{K} + \gamma \boldsymbol{I}](\boldsymbol{\alpha} - \boldsymbol{\alpha}^{*}) + (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{*})^{T}\boldsymbol{y} - \varepsilon \boldsymbol{1}^{T}(\boldsymbol{\alpha} + \boldsymbol{\alpha}^{*})$$
(21)

and the prediction model is $\hat{y}_r = \sum_{n=1}^N \beta_n K(\boldsymbol{z}_n, \boldsymbol{z}_r)$. *Proof:* The derivation is similar to those presented in Sections II and III.

Property 3: VR From Composite Kernels: It is straightforward to see that the SVR system identification model is obtained for $\phi(z_n) =$ $\phi_z(z_n)$. In this case, the kernel matrix is (7). Given that prediction model is (9), where a single kernel is used, the explicit consideration of input and output DTP is lost, and the normal equations are generated in an RKHS where the input and output effects are coupled.

Property 4: SVM-ARMA_{2K} From Composite Kernels: The proposed SVM-ARMA2K algorithm can be obtained from a composite kernel formulation by using $\phi(z_n) = [\phi_y(y_{n-1})^T, \phi_u(\mathbf{u}_n)^T]^T$. It is straightforward to see that the model kernel is

$$K(\boldsymbol{z}_{i}, \boldsymbol{z}_{j}) = \left\langle \left[\boldsymbol{\phi}_{y}(\boldsymbol{y}_{i-1})^{T}, \boldsymbol{\phi}_{u}(\boldsymbol{u}_{i})^{T} \right]^{T}, \left[\boldsymbol{\phi}_{y}(\boldsymbol{y}_{j-1})^{T}, \boldsymbol{\phi}_{u}(\boldsymbol{u}_{j})^{T} \right]^{T} \right\rangle$$
$$= K_{y}(\boldsymbol{y}_{i-1}, \boldsymbol{y}_{i-1}) + K_{u}(\boldsymbol{u}_{i}, \boldsymbol{u}_{j})$$
(22)

where the kernel (being the sum of two kernels) accounts for the input and output DTP.

B. Composite Kernels for Input-Output Cross Information

Composite kernels can be used to emphasize, if necessary, the cross information between input and output DTP. Assume a nonlinear mapping $\varphi(\cdot)$ into an RKHS \mathcal{H}_{φ} and three linear transformations A_i from \mathcal{H}_{φ} to \mathcal{H}_i , i = 1,2,3. Note, however, that in this case, \boldsymbol{u}_n and \boldsymbol{y}_n need to have the same dimension for the formulation to be valid. For simplicity, we force $P' = Q' = \max(P, Q)$, which yields input and output vectors u'_n and y'_{n-1} that are ensured to contain all the relevant time-series information (plus some amount of redundant information).

For the following composite transformation:

$$\phi(z') = \left[\mathbf{A}_1 \varphi(\mathbf{u}')^T, \mathbf{A}_2 \varphi(\mathbf{y}')^T, \mathbf{A}_3 \left(\varphi(\mathbf{u}') + \varphi(\mathbf{y}') \right)^T \right]^T$$
 (23)

the obtained kernel is

$$K\left(\mathbf{z}_{i}^{\prime}, \mathbf{z}_{j}^{\prime}\right) = \boldsymbol{\varphi}^{T}\left(\mathbf{y}_{i}^{\prime}\right) \boldsymbol{R}_{1} \boldsymbol{\varphi}\left(\mathbf{y}_{j}^{\prime}\right) + \boldsymbol{\varphi}^{T}\left(\mathbf{u}_{i}^{\prime}\right) \boldsymbol{R}_{2} \boldsymbol{\varphi}\left(\mathbf{u}_{j}^{\prime}\right) + \boldsymbol{\varphi}^{T}\left(\mathbf{y}_{i-1}^{\prime}\right) \boldsymbol{R}_{3} \boldsymbol{\varphi}\left(\mathbf{u}_{i}^{\prime}\right) + \boldsymbol{\varphi}^{T}\left(\mathbf{u}_{i}^{\prime}\right) \boldsymbol{R}_{3} \boldsymbol{\varphi}\left(\mathbf{y}_{i-1}^{\prime}\right)$$
(24)

where $\mathbf{R}_1 = \mathbf{A}_1^T \mathbf{A}_1 + \mathbf{A}_3^T \mathbf{A}_3$, $\mathbf{R}_2 = \mathbf{A}_2^T \mathbf{A}_2 + \mathbf{A}_3^T \mathbf{A}_3$, and $\mathbf{R}_3 =$ $\boldsymbol{A}_{3}^{T}\boldsymbol{A}_{3}$ are three (independent) definite-positive matrices. The last two terms can be grouped into a Mercer's kernel K_{uy} accounting for cross information

$$K_{uy}\left(\boldsymbol{u}_{i}^{\prime},\boldsymbol{y}_{j-1}^{\prime}\right)=K_{3}\left(\boldsymbol{y}_{i-1}^{\prime},\boldsymbol{u}_{j}^{\prime}\right)+K_{3}\left(\boldsymbol{u}_{i}^{\prime},\boldsymbol{y}_{j-1}^{\prime}\right) \tag{25}$$

which is warranted to be a valid Mercer kernel if K_3 is a valid Mercer kernel. Then, the final kernel expression is

$$K\left(\boldsymbol{z}_{i}^{\prime},\boldsymbol{z}_{j}^{\prime}\right)=K_{y}(\boldsymbol{y}_{i-1},\boldsymbol{y}_{j-1})+K_{u}(\boldsymbol{u}_{i},\boldsymbol{u}_{j})+K_{uy}\left(\boldsymbol{u}_{i}^{\prime},\boldsymbol{y}_{j-1}^{\prime}\right)\ (26)$$

TABLE I SYSTEM IDENTIFICATION SIMULATION RESULTS. BOLD AND ITALICS INDICATE THE TWO BEST MODELS FOR EACH MERIT FIGURE

	Eq.	ME	MSE	MAE	r	nMSE
SVR	(9)	0.29	3.08	1.08	0.991	-0.82
SVM-ARMA _{2K}	(19)	0.14	2.08	0.88	0.992	-0.92
SVR-ARMA _{2K}	(26)	0.13	2.13	0.90	0.991	-0.88
SVM-ARMA _{4K}	(26)	0.16	2.50	0.95	0.991	-0.85
SVR-ARMA _{4K}	(30)	0.03	3.76	1.11	0.976	-0.77

and using this kernel in the generic SVM system identification algorithm gives us the so-called SVM-ARMA4K algorithm. It can be seen that we are now using four different kernels to build the composite kernel. A cross information analysis of this algorithm can be made, according to the corresponding normal equations in the RKHS for this case (not included here and left as further work).

C. Composite Kernels for Improved Versatility

Instead of using separately the proposed algorithms for SVM system identification, one can think of using in a collaborative way the different kernel structures that have been presented here.

Property 5: The first possibility is using three concatenated transformations into RKHS, one for input u_n , one for output y_{n-1} , and one for their concatenation z_n . The result is a combination between the SVM-ARMA and the SVR structures described in the preceding sections. The transforming concatenation is

$$\boldsymbol{\phi}(\boldsymbol{z}_n) = \left[\boldsymbol{\phi}_y(\boldsymbol{y}_{n-1})^T, \boldsymbol{\phi}_u(\boldsymbol{u}_n)^T, \boldsymbol{\phi}_z(\boldsymbol{z}_n)^T\right]^T. \tag{27}$$

It is straightforward to see that the corresponding kernel is

$$K(z_i, z_j) = K_y(y_{i-1}, y_{i-1}) + K_u(u_i, u_j) + K_z(z_i, z_j)$$
 (28)

and its introduction in the generic SVM system identification model yields the so-called SVR-ARMA $_{2K}$ algorithm.

Property 6: A composite transformation given by

$$\phi(z') = \left[\mathbf{A}_1 \varphi(\mathbf{u}')^T, \mathbf{A}_2 \varphi(\mathbf{y}')^T, \mathbf{A}_3 \left(\varphi(\mathbf{u}') + \varphi(\mathbf{y}') \right)^T, \phi_z(z)^T \right]^T$$
(29)

gives the following composite kernel:

$$K\left(\boldsymbol{z}_{i}^{\prime},\boldsymbol{z}_{j}^{\prime}\right) = K_{y}(\boldsymbol{y}_{i-1},\boldsymbol{y}_{j-1}) + K_{u}(\boldsymbol{u}_{i},\boldsymbol{u}_{j}) + K_{uy}\left(\boldsymbol{u}_{i}^{\prime},\boldsymbol{y}_{j-1}^{\prime}\right) + K_{z}(\boldsymbol{z}_{i},\boldsymbol{z}_{j}) \quad (30)$$

which produces the SVR-ARMA $_{4K}$ algorithm.

Note that SVR-ARMA_{2K} and SVR-ARMA_{4K} have not a straightforward interpretation in terms of normal equations in the RKHS, but rather they can contain all the relevant model information that can be extracted from the data by each component kernel. Therefore, despite that SVM-ARMA and SVR nonlinear system identification are different problem statements, both underlying models can be combined and embedded into a more general SVM signal processing framework for nonlinear system identification.

In conclusion, we can say that composite kernels can be used to provide us with model flexibility in terms of: 1) emphasized consideration, if necessary, of the input-output cross information; and 2) straightforward and natural combinations of implicit and explicit ARMA models.

	Poly	Rat	$\begin{array}{c} \textbf{Loc} \\ d = 1 \end{array}$	Loc $d=2$	RBF	MLP	SVR	SVM -ARMA _{2K}	SVR -ARMA _{2K}	SVM -ARMA _{4K}	SVR -ARMA _{4K}
MG17	-1.95	-1.14	-1.48	-1.89	-1.97	-2.00	-2.36	-2.83	-2.87	-2.88	-2.86
MG30	-1.40	-1.33	-1.24	-1.42	-1.60	-1.5	-1.87	-1.73	-1.76	-1.73	-1.76

TABLE II
NMSE IN VALIDATION SET FOR THE SVM MODELS AND METHODS IN [19]

V. EXPERIMENTAL RESULTS

In this section, we compare the performance of the SVR and the SVM-ARMA formulations in the previous sections. In all kernel computations, we used the Gaussian kernel, which provides universal nonlinear mapping capabilities and computational convenience [17], [18]. Different types of kernels (linear, polynomial, etc.) could be considered for the input, output or cross-information kernels, according to *a priori* knowledge of the system.

Example 1. Nonlinear Feedback System: We first consider the following system. Input DTP is generated with Lorenz equations, given by $du/dt = -\rho u + \rho y$, dy/dt = -uz + ru - y, and dz/dt = uy - bz, and using $\rho = 10$, r = 28, and b = 8/3. Only component u is used as the input signal to the system, and it enters through an eighth-order low-pass FIR filter H(z) with cutoff frequency $\omega_n = 0.5$ and normalized gain 6 dB at ω_n . The output signal goes through a feedback loop consisting of a high-pass minimum-phase channel $G(z) = (1.00 + 2.01z^{-1} + 1.46z^{-2} + 0.39z^{-3})^{-1}$ and then distorted with nonlinearity $f(\cdot) = \log(\cdot)$.

This system was used to generate 10 000 input–output DTP samples that were split into a training set (first 50 samples) and a test set (following 500 samples). The experiment was repeated 100 times with randomly selected starting points in the DTP. Free parameters were selected through eight-fold cross-validation using the training set, and average results for the test set are shown in Table I for mean error (ME), mean-squared error (MSE), mean-absolute error (MAE), correlation coefficient (r), and normalized MSE (nMSE = $\log_{10}(\sqrt{\text{MSE/var}(y)})$ of models in the test set. It is worth noting that SVM-ARMA_{2K} is the best model for this example, and that also SVR-ARMA_{2K} and SVM-ARMA_{4K} outperform the SVR. However, the composite SVR-ARMA_{4K} turns to be here the worst model specification. SVR-ARMA_{4K} is a more complex model, which can be appropriate for much more complex dynamics; otherwise, the complexity of the model may degrade the generalization performance.

Example 2. The Mackey–Glass Time Series: We also compared the performance of SVM models in the standard Mackey–Glass time-series prediction problem following the same approach as in [20], where the use of the standard SVR was originally presented for time-series prediction. This classical high-dimensional chaotic system is generated by the following delay differential equation:

$$\frac{dx(t)}{dt} = -0.1x(t) + \frac{0.2x(t - t_{\Delta})}{1 + x(t - t_{\Delta})^{10}}$$
(31)

with delays $t_{\Delta}=17$ and 30, yielding time series MG17 and MG30, respectively. For comparison with [20], we considered 500 training samples and used next 1000 for free parameter selection (validation set). This procedure also allows us a direct comparison with previous results in the literature [19], [21], [22], in terms of nonlinear MSE (nMSE).

Results are shown in Table II. The SVR algorithm outperformed the preceding methods for both time series. The methods proposed here widely outperform SVR in MG17; note that a difference of 0.5 between SVR and SVM-ARMA $_{4K}$ in nMSE is equivalent to almost one order of magnitude in MSE. Nevertheless, they did not outperform SVR in MG30; this could be due to differences in the kernel choice (RBF instead of trigonometric kernel [20]) or the considered embedding.

VI. CONCLUSION

This paper presents the explicit formulation of nonlinear SVM-ARMA models in RKHS, which makes possible to scrutinize the statistical properties and the time-series structure in system identification problems. In addition, a full family of methods for nonlinear system identification have been proposed, by taking advantage of composite kernels, in which dedicated mappings are used for input, output, and cross terms. Simulation results reveal the potential capabilities of this approach, as recently demonstrated in the field of image processing [23]. This framework also allows a successful integration and combination of nonlinear SVR and SVM-ARMA models.

APPENDIX I

NONLINEAR SVM-ARMA AND PREDICTION ERROR METHODS

Property 7: Let us denote quadratic cost conditions (QCC) as $\varepsilon=0$ and $C=\infty$ in (12). Then, for QCC we have that model weights in (19) are proportional to the residuals, that is $\beta_n=(1/\gamma)e_n$. The proof is immediate by making $\varepsilon=0$ and $C=\infty$ in (10).

Property 8: For QCC, the linear SVM-ARMA model can be viewed as a regularization of the normal equations of the Wiener filter for system identification. See [11] for proof.

Theorem 1: For QCC, nonlinear SVM-ARMA $_{2K}$ algorithm solves the regularized normal equations in the RKHS.

Proof: Let $\phi_u(\boldsymbol{x}_i) \in \mathcal{H}_u$ and $\phi_y(\boldsymbol{y}_i) \in \mathcal{H}_y$, vectors of size $(H_u \times 1)$ and $(H_y \times 1)$, respectively, for $i = 1, \ldots, N$. Let the data matrix in each RKHS be given by $\boldsymbol{\Phi}_u = [\phi_u(\boldsymbol{u}_1), \ldots, \phi_u(\boldsymbol{u}_N)]$ and $\boldsymbol{\Phi}_y = [\phi_y(\boldsymbol{y}_1), \ldots, \phi_y(\boldsymbol{y}_N)]$. Then, the matrix-form equation of the model for the observed data is $\boldsymbol{y} = \boldsymbol{\Phi}_u^T \boldsymbol{b} + \boldsymbol{\Phi}_y^T \boldsymbol{a} + \boldsymbol{e}$. Dual problem (18) can now be expressed (in matrix form) as the maximization of

$$L_{\text{QCC}}^{2k}(\boldsymbol{e}) = \frac{1}{2\gamma^2} \boldsymbol{e}^T \left(\boldsymbol{\Phi}_y^T \boldsymbol{\Phi}_y + \boldsymbol{\Phi}_u^T \boldsymbol{\Phi}_u \right) \boldsymbol{e} - \frac{1}{\gamma} \boldsymbol{y}^T \boldsymbol{e} + \frac{1}{2\gamma} \boldsymbol{e}^T \boldsymbol{e}. \quad (32)$$

By making zero the gradient of L^{2k}_{QCC} and after some manipulations, the following is obtained:

$$\boldsymbol{\Phi}_{y}^{T}\boldsymbol{\Phi}_{y}\boldsymbol{y} - \boldsymbol{\Phi}_{y}^{T}\boldsymbol{\Phi}_{y}\boldsymbol{\Phi}_{u}^{T}\boldsymbol{b} - \boldsymbol{\Phi}_{y}^{T}\boldsymbol{\Phi}_{y}\boldsymbol{\Phi}_{y}^{T}\boldsymbol{a} + \boldsymbol{\Phi}_{u}\boldsymbol{\Phi}_{u}^{T}\boldsymbol{y} - \boldsymbol{\Phi}_{u}^{T}\boldsymbol{\Phi}_{u}\boldsymbol{\Phi}_{u}^{T}\boldsymbol{b} - \boldsymbol{\Phi}_{u}^{T}\boldsymbol{\Phi}_{u}\boldsymbol{\Phi}_{u}^{T}\boldsymbol{b} - \boldsymbol{\Phi}_{u}^{T}\boldsymbol{a} - \gamma\boldsymbol{\Phi}_{u}^{T}\boldsymbol{b} - \gamma\boldsymbol{\Phi}_{u}^{T}\boldsymbol{a} = 0.$$
 (33)

By denoting $\Phi_y \Phi_y^T = R_{yy}$, $\Phi_u \Phi_u^T = R_{uu}$, $\Phi_u \Phi_y^T = R_{uy}$, $\Phi_y \Phi_u^T = R_{yu}$, and

$$\mathbf{r}_{zy}^{2k} = \begin{bmatrix} \mathbf{\Phi}_{y} \mathbf{y} \\ \mathbf{\Phi}_{n} \mathbf{y} \end{bmatrix} \quad \mathbf{R}^{2k} = \begin{bmatrix} \mathbf{R}_{yy} & \mathbf{R}_{yu} \\ \mathbf{R}_{nn} & \mathbf{R}_{nn} \end{bmatrix}$$
(34)

the following term grouping can be done:

$$\left[\boldsymbol{\Phi}_{y}^{T}, \boldsymbol{\Phi}_{u}^{T}\right] \boldsymbol{r}_{zy}^{2k} = \left[\boldsymbol{\Phi}_{y}^{T}, \boldsymbol{\Phi}_{u}^{T}\right] (\boldsymbol{R}^{2k} + \gamma \boldsymbol{I}) [\boldsymbol{a}^{T}, \boldsymbol{b}^{T}]^{T}$$
(35)

which holds if and only if $\boldsymbol{r}_{zy}^{2k} = (\boldsymbol{R}^{2k} + \gamma \boldsymbol{I})[\boldsymbol{a}^T, \boldsymbol{b}^T]^T$, that are the regularized Wiener equations in RKHS.

Therefore, the SVM-ARMA $_{2K}$ formulation for nonlinear kernels and QCC leads naturally to the statement of the equations in the joint RKHS. Note that for some Mercer's kernels, the dimension of these equations can be infinite; however, as far as we are not solving them explicitly, but rather implicitly in (18) and by means of the kernel trick, we will still be able to scrutinize the statistical properties of the time-series problem, specially if these properties can be conveniently expressed with dot products in the RKHS and subsequently analyzed using Mercer's kernels.

APPENDIX II NONLINEAR SVM-ARMA AND CORRELATION METHODS

CM for system identification are based on the assumption that a good model produces residuals that are uncorrelated with past data, and, consequently, these methods minimize the cross correlation between a function of the residuals and a transformation of the data, both of them being possibly nonlinear. Different approaches in the literature [1] are based on different methods for determining suitable residual functions and data transformations.

Property 9: For QCC, the nonlinear SVM-ARMA $_{2K}$ system identification model minimizes the cross correlation between the data transformed to the RKHS and the residuals.

Proof: Taking into account (15) and Property 2, we have $a = \Phi_y e$ and $b = \Phi_u e$, and according to the primal problem statement (12), we are minimizing the L_2 norm of the coefficients, even though they are in the RKHS and they cannot be explicitly known (see [11] for details on the equivalent property for linear SVM-ARMA).

Property 10: Under the set of nonzero and finite possible values for the free parameters of the ε -Huber cost function ($0 < \varepsilon, C, \gamma < \infty$), the nonlinear SVM-ARMA_{2K} system identification algorithm minimizes the correlation between the data and a nonlinear transformation of the residuals.

Proof: For each given fixed subset of the free parameters $0 < \varepsilon$, C, $\gamma < \infty$, the nonlinear relationship between the model coefficients and the residuals is given by (10). According to (15) and (10), we have $a = \Phi_y g_{nl}(e)$ and $b = \Phi_u g_{nl}(e)$, which stand for the model coefficients being the (uncoupled) cross correlation between the nonlinearly transformed residuals and the data in the RKHS. Furthermore, we are minimizing the norm of these coefficients in (12).

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