Vol. 1(1), pp. 1-5, September 2022
DOI: xx.0001/AJPC2021.0207
ISSN xxxx-xxxx

ASEAN Journal of Process Control

Research Article

Locally weighted kernel partial least square model for nonlinear processes: A case study

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Academic Editor: Jobrun Nandong
Received: 30 November 2021; Accepted: 15 March 2022; Published: 01 September 2022

Abstract: A soft sensor, namely locally weighted partial least squares (LW-PLS) cannot cope with the nonlinearity of process data. To address this limitation, Kernel functions are integrated into LW-PLS to form locally weighted Kernel partial least squares (LW-KPLS). In this study, the different Kernel functions including Linear Kernel, Polynomial Kernel, Exponential Kernel, Gaussian Kernel and Multiquadric Kernel were used in the LW-KPLS model. Then, the predictive performance of these Kernel functions in LW-KPLS was accessed by employing a nonlinear case study and the analysis of the obtained results was then compared. In this study, it was found that the predictive performance of using Exponential Kernel in LW-KPLS is better than other Kernel functions. The values of root-mean-square errors (RMSE) for the training and testing dataset by utilizing this Kernel function are the lowest in the case study, which is 44.54% lower RMSE values as compared to other Kernel functions.

Keywords: Soft sensors, Locally weighted kernel partial least square, Nonlinearity, Kernel functions.

1. Introduction

Chemical processes are facing difficult challenges such as profitability targets to be achieved and tight control that are required specifically by the government on real time of product quality. Controlling and modelling action played as significant role in the production plants for many years in industrial processes. In the industrial processing plant, hardware sensors are adapted especially on control systems. However, several limitations of the implementation of hardware sensors exist from the prospect of technical and economic such as insufficient space, complicated environmental conditions, and utmost operational conditions. Thus, soft sensors are introduced to overcome the issue of hardware sensors limitation. Soft sensors are assorted as inferential models which require easily estimated variables to predict process variables that are difficult to estimate due to the limitations of technology, tremendous measurement delays or expensive investment costs.

On the other hand, the benefit of applying Kernel functions in soft sensors had brought convenience to nonlinear processes as there is no requirement on nonlinear optimization procedure [1]. To deal with the industrial processes more effectively, locally weighted partial least squares (LW-PLS) are further developed with the Kernel function to build locally weighted kernel partial least squares (LW-KPLS). By using the chosen Kernel function in the LW-PLS model, the work done of the drafting of primitive inconstant to be transformed into the high dimensional void is completed. After that, the LW-KPLS can then be derived successfully as the high dimensional conditions assumed were fulfilled.

Later, Yeo, Saptoro and Kumar [2] showed a demonstration of development regarding the LW-KPLS model designated for adaptive soft sensors. The differences between LW-PLS and LW-KPLS were established which is in accordance with the estimated performance and computational loads. The outcomes concluded that the predictive capability of LW-KPLS is more advance than LW-PLS. However, LW-PLS possesses a lower computational load. To counter this issue, Yeo, Saptoro and Kumar [2] came out with an ensemble solution where the variables required were assessed and a comparison of that was made with LW-PLS. The outcomes acquired proved that ensemble locally weighted Kernel partial least squares (E-LW-KPLS) possesses better quality as compared to LW-PLS.

The recommended method of LW-KPLS developed Yeo, Saptoro and Kumar [2] possesses the capability to sort out alternations that occurred in process characteristics. The efficiency and reliability of this method were evaluated via three different case studies which consist of a penicillin fermentation process, nonlinear numerical example, and a cleaning process that exists within the pharmaceutical industry. The results applied illustrated on recommending LW-KPLS produces superior estimation capability than that of PLS, KPLS, LW-PLS as well as E-LW-KPLS.

Moreover, Zhang, Kano and Li [3] suggested a novel LW-KPLS according to sparse nonlinear features subjected to virtual exhibits by nonlinear time-varying processes. As observed differently in the common LW-PLS, the recommended LW-KPLS composes the non-linear trait into the locally weighted framework enhancing its efficiency in handling strong nonlinearity. In addition, sparse Kernel feature characterization terms which depict not linear dependency within the training samples, as well as query, are taken for constructing LW-KPLS models.

According to one of the studies on LW-KPLS previously done by Zhang, Kano and Li [3], the limitation of LW-KPLS in holding a strong nonlinear connection of process variables subjected to soft sensors development is confirmed. Nevertheless, data involving the application of Kernel functions are general in processing industries of the chemical field. Hence, due to the limitation study of employing different Kernel functions in LW-KPLS, different Kernel functions involving Linear Kernel, Polynomial Kernel, Exponential Kernel, Gaussian Kernel and Multiquadric Kernel was carried out in this study [4].

2. Materials and Methods

By applying a Kernel function, the LW-KPLS model was built under the LW-PLS procedures. The procedures of the LW-KPLS model can be found and studied in Yeo, Saptoro and Kumar [2]. Besides, the description of case study used in this study is explained in the following sub-section.

3.1. Case study

In industrial, one of the most significant environmental conservation processes is wastewater treatment process. The process is said to be complicated, non-linear, and multivariable as it has multiple inputs and outputs. **Figure 1** demonstrates the wastewater treatment process studied by Caraman, Sbarciog and Barbu [5]. In this wastewater treatment process, an aeration tank which is a biological reactor that consists of a mixture of liquid and suspended solid is used. To eliminate the organic substrate from the mixture, a microorganism population is raised. A settler is acted as a clarifier tank to split the sludge and the clear effluent by using gravity. An amount of sludge is recycled back to the aeration tank while the other amount is eliminated [5]. The mass balance equations are shown in **Equations (1)** to **(5)**. The notations of these equations and the details of the study can be found in the study carried by Caraman, Sbarciog and Barbu [5]. MATLAB Simulink was used to generate the data based on these equations.

$$\frac{dX}{dt} = \mu(t)X(t) - D(t)(1+r)X(t) + rD(t)X_r(t) \tag{1}$$

$$\frac{dS}{dt} = -\frac{\mu(t)}{Y}X(t) - D(t)(1+r)X(t) + D(t)S_{in} \tag{2}$$

$$\frac{dDO}{dt} = -K_0\frac{\mu(t)}{Y}X(t) - D(t)(1+r)DO(t) + \alpha W(DO_{max} - DO(t)) + D(t)DO_{in} \tag{3}$$

$$\frac{dX_r}{dt} = D(t)(1+r)X(t) - D(t)(\beta + r)X_r(t) \tag{4}$$

$$\mu(t) = \mu_{max} \frac{S(t)}{k_S + S(t)} \frac{DO(t)}{K_{DO} + DO(t)} \tag{5}$$

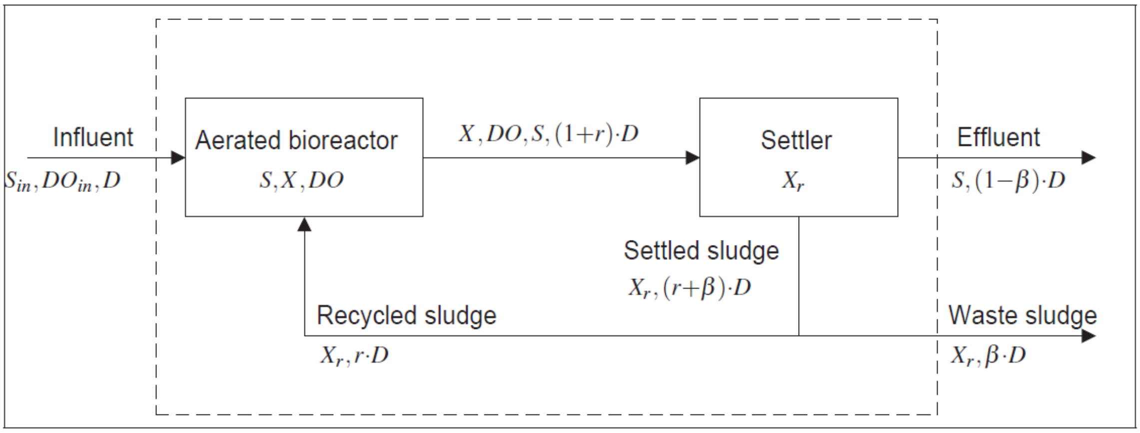

Figure 1. Demonstration of the wastewater treatment process [5]

3. Results and Discussion

The tabulation of root-mean-square errors (RMSE) values for training and testing datasets with the different Kernel functions in LW-KPLS model after tuning of the Kernel parameter, b in the case study is shown in **Table 1**. In Table 1, the $RMSE_1$ and $RMSE_2$ are the RMSE of training data and testing data, respectively. Meanwhile, CPU_1 and CPU_2 are the central processing unit (CPU) running time of training data and testing data, respectively. In order to avoid overestimation and underestimation, the tuning of b must be conducted with care [6]. The proximity of the regression line to the data points can be expressed by a lower RMSE as it provides a better fit to the data. In this case study, Exponential Kernel has the lowest RMSEs where their RMSE values for training and testing data are 0.66 and 0.50, respectively. The Exponential Kernel is tightly concerned with the Gaussian Kernel by squaring out the norm which also can be referred to as the radial basis function Kernel [6]. Moreover, the CPU running time for the training and testing data set, CPU_1 and CPU_2 of Exponential Kernel were 250.73s and 27.31s, respectively, which are the lowest CPUs as can be seen in **Table 1**.

In this case study, the values of the output variable were small, which were between -1.9536 to 23.9143, thus all the RMSE values from all models were small. The lower the values of the output variables, the lesser the values for RMSE. Also, the $RMSE_1$ is usually smaller than $RMSE_2$ since the testing data set utilized training data to develop the model [7]. Other than that, Multiquadric Kernel gave the largest value of RMSEs for training and testing datasets which are at 1.19 and 2.55, respectively when its Kernel parameter, b was tuned at 2. Multiquadric Kernel performed the transformation of the scattered data into a very precise appropriate model of a graph or surface [8], but it is proven by Multiquadric Kernel does not fit the data in this case study. By contrasting the results from Multiquadric Kernel, Exponential Kernel improved the results by 44.54% for $RMSE_1$ and 80.00% for $RMSE_2$.

To conclude, the predicted data from the LW-KPLS model with the Exponential Kernel is said to be closer to the real nature of the data set as it gave the lowest RMSE among the applied kernel functions. From **Figures 2** and **3**, the graphs of the training and testing data on their actual output values against the predicted outputs from the LW-KPLS model with the Exponential Kernel were plotted. The predicted output of training and testing data can be observed are allocated more concentrated along with the actual output of training and testing data. These results indicate the LW-KPLS model with Exponential Kernel function can fit the data in this case study well.

Table 1. $RMSE_1$ and $RMSE_2$ using LW-KPLS model with different Kernel functions for the case study.

Kernel	**Exponential Kernel**	Linear Kernel	Polynomial Kernel	Gaussian Kernel	Multiquadric Kernel
b	**10**	3	1	1	2
$RMSE_1$	**0.66**	0.67	0.67	1.24	1.19
CPU_1 (s)	**250.73**	251.22	256.49	251.67	268.36
$RMSE_2$	**0.50**	0.67	0.67	1.12	2.55
CPU_2 (s)	**27.31**	30.41	32.44	27.78	48.88

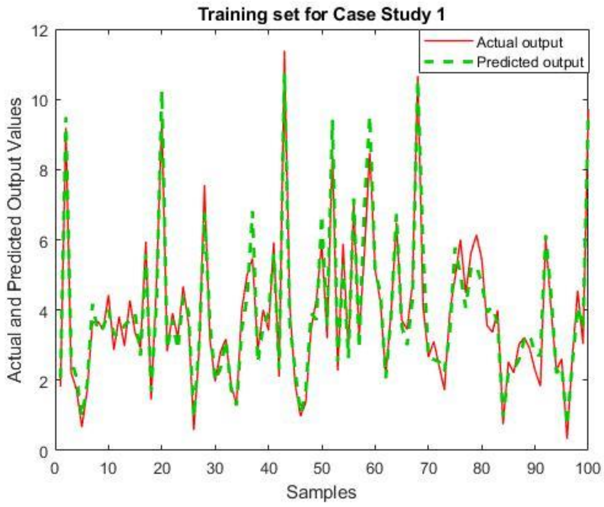

Figure 2. Graph of training dataset of output variable of actual and predicted output values from LW-KPLS model with Exponential Kernel in the case study

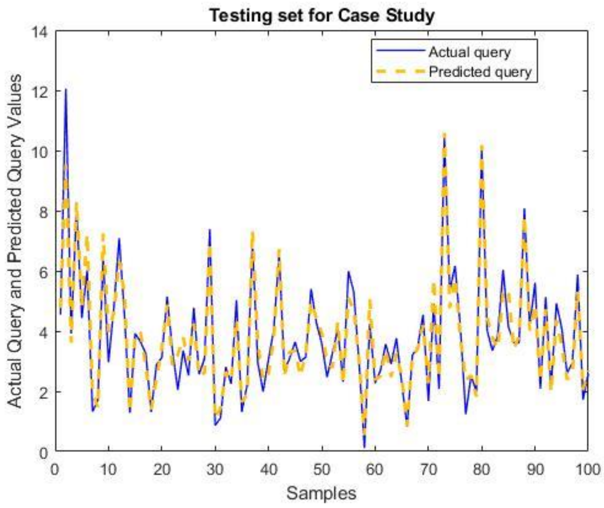

Figure 3. Graph of testing dataset of output variable of actual query and predicted query output values from LW-KPLS model with Exponential Kernel in the case study

5. Conclusions

In a nutshell, Kernel functions possess the ability to cope with the nonlinearity of the data and to map the data to the different high dimensions of space. In this study, a comparative study on the predictive performance of different Kernel functions in the LW-KPLS model has been done via a case study, which is the predictive control of a wastewater treatment process. It was found that Exponential Kernel has provided the best results among Kernel functions including Linear Kernel, Polynomial Kernel, Gaussian Kernel and Multiquadric Kernel. The values of RMSE for the training and testing dataset by utilizing this Exponential Kernel function are the lowest in the case study, which is 44.54% lower for RMSE values, especially the comparison made with the Multiquadric Kernel which gave the highest values of RMSEs. Future studies can be carried out to examine the performance of LW-KPLS model in widely range of applications such as colour, agriculture and aquaculture related research areas.

Acknowledgments: To the best of my knowledge and belief, this manuscript contains no material previously published by any other person except where due acknowledgment has been made. This manuscript contains no material which has been accepted for the award of any other degree or diploma in any university.

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