A Comparative Study of Different Kernel Functions Applied to LW-KPLS Model for Nonlinear Processes

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Abstract: Soft sensors are inferential estimators when the employment of hardware sensors is inapplicable, expensive, or difficult in industrial plant processes. Currently, a simple soft sensor, namely locally weighted partial least squares (LW-PLS), which can cope with the nonlinearity of the process, has been developed. However, LW-PLS exhibits the disadvantages of handling strong nonlinear process data. To address this problem, Kernel functions are integrated into LW-PLS to form locally weighted Kernel partial least squares (LW-KPLS). Notice that a minimal study was carried out on the impact of different kernel functions that have not been integrated with the LW-KPLS, in which this model has the potential to be applied to different chemical-related nonlinear processes. Thus, this study investigates the predictive performance of LW-KPLS with several different Kernel functions using three nonlinear case studies. As the results, the predictive performances of LW-KPLS with Polynomial Kernel are better than other Kernel functions. The values of root-mean-square errors (RMSE) and error of approximation (Ea) for the training and testing dataset by utilizing this Kernel function are the lowest in their respective case studies, which are 34.60% to 95.39% lower for RMSEs values and 68.20% to 95.49% smaller for Ea values.

Keywords: soft sensors; locally weighted kernel partial least squares; kernel functions; linear kernel; polynomial kernel; nonlinear chemical processes.

Abbreviations: CPU: Central Processing Unit; CSTR: Continuous Stirred Tank Reactor; ITHS: Intelligent Tuned Harmony Search; GK: Gaussian Kernel; JIT: Just-In-Time; KPLS: Kernel Partial Least Squares; LW-KPLS: Locally Weighted Kernel Partial Least Squares; LW-PLS: Locally Weighted Partial Least Squares; MK: Multiquadric Kernel; MLR: Multiple Regression; PCR: Principle Component Regression; PLS: Partial Least Squares; RMSE: Root-Mean-Square Error; STHE: Shell and tube heat exchangers; x: Input variables; y: Output variables; n: Number of samples; L: Number of output variables; M: Number of input variables; T: Transpose matrix; X: Matrix of input; Y: Matrix of output; Ỹ: Predicted output; Xq: Queried matrix of input; 1n: Vector with length n; 1nT: Vector with length nT; B: Dual representation of the scaling of the projection direction; S: Latent variables number; Ω: Similarity matrix; ωn: Index of similarity; ϕ: Localization parameter; σn: Standard deviation of d_n; t_s: s^th latent variable of X_s; w_s: Eigenvector of X_sΩY_sY_sTΩX_s that correlates to maximal eigenvalue; p_s: s^th loading vector of X_s; q_s: s^th regression coefficient vector; t_q,s: s^th latent variable of X_q; N_s: Total samples number; N_1: Number of training samples; N_2: Number of testing samples; Y: Actual values of output; Ỹ: Predicted values of output; Ỹ: Actual output mean value: RMSE: Root-Mean-Square Error of Training Data; RMSE: Root-Mean-Square Error of Testing Data; b: Kernel Parameter; E_a: Error of Approximation; σ: Sigma.

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1. Introduction

Hardware sensors are generally adapted in chemical plants for process sensing and control systems [1]. However, there are several existing drawbacks for the hardware sensors from the prospect of technical and economic. For instance, shortages of technology, the time delay from measurement, and many online variables contribute to costly devices [2]. Meanwhile, these sensors allow better process control and monitoring for optimization, which can lead to business profit targets and minimize costs while meeting the desired product quality [3]. Moreover, they also allow chemical plants to be in a more sustainable and profitable situation by achieving operational excellence goals.

Soft sensors, therefore, are being introduced to overcome the limitations of the hardware sensors. Soft sensors, which are inferential estimators, are preferable when the employment of hard sensors is inapplicable, expensive, or difficult in the industrial plant processes. Generally, soft sensors are assorted as inferential models, which require only a simple step on variables estimation. Moreover, soft sensors can easily predict hard-to-measure process variables and provide beneficial information from the view of fault detection using easy-to-measured variables from the hardware sensors [4]. In other words, soft sensors are ordinarily adopted for online predictions according to the analysis of measurement signals from hardware sensors with software executed mathematical models [5,6]. In industry, it is commonly used in industrial processes for providing predictions to the control system in achieving their operational excellence, which ultimately leads to more sustainable and profitable operations [7,8]. Besides, soft sensors with better measurements can generate better product quality and improve the system's performance through enhanced operation, fault detection, and process management [9,10]. Thus, they are commonly used in the industrial process to settle issues that correspond to cost, availability, quality, and reliability of measurements [11].

Soft sensors have been broadly developed to measure hard-to-measure variables such as product quality or other significant online or offline indexes, which cannot be estimated by hardware sensors in real-time [12]. The term soft measurement is advocated and acts as a parameter forecast tool subjected to online process measurement [13]. In an extremely impressive view, soft sensors are classified into two distinct classes: model-driven and data-driven based soft sensors. The model-driven or first principal models depict the process physically and chemically. However, they are sometime difficult to use since they require the structure's complexity and insufficient professional knowledge of the chemical processes [12]. Therefore, data-driven soft sensors are preferable in this situation.

The data-driven-based soft sensors predict the connection between the primary and secondary variables extracted from the processes in the circumstance of real conditions [14]. They acquire a great amount of interest [12]. Data-driven modeling is superior for mapping out the model if the development of the modeling sample is enough to train the model [13]. Besides, multivariate regression models are usually used for data-driven soft sensors development. They include multiple regression (MLR), principal component regression (PCR), and partial least squares (PLS) regression [15]. However, the predictive performance of the MLR is disappointing and imprecise when it comes to handling a huge amount of collinear data and noise estimation [16,17]. Hence, PCR, and PLS are adopted to overcome these drawbacks.

PCR and PLS can overcome the constraints or regression when they set up a MLR model with the low capability to create a nonlinear connection between dependent and
independent variables [18,19]. PLS also generates the components in terms of modeling the relationship between input and output variables and retaining most of the information in input variables simultaneously, which is dissimilar from PCR which uses input variables in modeling [20]. Due to better predictive performance, the PLS model is proved to be more used as a dominant multivariate statistical tool when applied in the real world than PCR [21]. However, both PCR and PLS, which are latent-variable-based methods, cannot handle nonlinear process data [22].

Nonlinear models are postulated to generate better accuracy estimation in processing high nonlinearity data [23]. Nonlinear soft sensors usually employ artificial neural or Kernel-based methods such as Kernel-PLS (KPLS), support vector regression, and artificial neural network [15]. The assembling of Kernel functions in PLS supports KPLS to become better efficiency algorithms in conquering nonlinearity data since KPLS maps the data into a higher-dimensional space. Nonetheless, the accuracy of the non-adaptive and nonlinear soft sensors degrades due to the alternation in the process conditions.

To adapt the alternation in process characteristics and nonlinearity, Just-In-Time (JIT) modeling can be resorted to developing adaptive soft-sensors or virtual sensors. Locally weighted partial least squares (LW-PLS), a JIT model, has been studied and prosperity applied in various industries due to its simplicity and capability [24]. Nevertheless, LW-PLS fails to accomplish a successful estimation for nonlinear processes. Hence, the locally weighted Kernel partial least squares (LW-KPLS) model is established by assembling Kernel functions with LW-PLS to handle the highly nonlinear issue [25]. Due to the good predictive performance, the LW-KPLS was also studied by Yeo, Saptoro, and Kumar [25], Yeo and Lau [26], and Yeo, et al. [27]. However, the impact of other different Kernel functions on the predictive performance of LWKPLS has not been detailly carried out. This study investigates the effect of these different Kernel functions that have not been accomplished yet in the LW-KPLS model. Then, the performance of LW-KPLS, which was subjected to different Kernel functions, was evaluated and compared.

2. Materials and Methods

In this section, the description of LW-KPLS is expressed. Then, it is followed by optimizing parameters, data splitting and setting of parameters, measurement of quality prediction, kernel functions, and specifications of computer configuration.

2.1. Locally weighted Kernel partial least squares.

By applying a Kernel function, the LW-KPLS model was built under the LW-PLS procedures. As shown in (1) and (2), the input variables and output variables, x, and y, are expressed [25].

\[
x_n = [x_{n1}, x_{n2}, \ldots, x_{nM}]^T
\]

\[
y_n = [y_{n1}, y_{n2}, \ldots, y_{nL}]^T
\]

The symbols n, M, L, and T represent the number of samples, number of input variables, number of output variables, and a transpose of a matrix, respectively. The input matrix is symbolized by \( X \in \mathbb{R}^{n \times M} \), while the output matrix is symbolized by \( Y \in \mathbb{R}^{n \times L} \). These input and output matrices are the databases saved x and y in MATLAB. To obtain the predicted output,
\[ \hat{y}_q \text{ for a query, } x_q \text{ for a nonlinear process, and LW-KPLS algorithm was developed by Yeo, Saptoro, and Kumar [25], and it is shown as follows:} \]

**Step 1:** To obtain the Kernel matrices for input variables, \( V \), and query, \( V_q \), they are mapped into a high dimensional feature space by applying a Kernel function.

**Step 2:** Using (3) and (4), mean centering is done on the mapped \( V \) and \( V_q \).

\[
\begin{align*}
\bar{V} &= \left( I - \frac{1}{n} 1_n 1_n^T \right) V \left( I - \frac{1}{n} 1_n 1_n^T \right) \\
\bar{V}_q &= \left( V_q - \frac{1}{n} 1_n 1_n^T V \right) \left( I - \frac{1}{n} 1_n 1_n^T \right)
\end{align*}
\]

(3) (4)

where the length vector with \( n \) and the length vector with \( n_t \) are symbolized by \( 1_n \) and \( 1_{nt} \), respectively.

**Step 3:** Dual KPLS discrimination is conducted by applying (5) to produce \( B \).

\[
B = YY^T V \beta \text{ with normalization, } \beta = \frac{\beta}{\|\beta\|}
\]

(5)

where \( B \) represented the dual representation of the scaling in the projection direction.

**Step 4:** The computation on re-scaled queried and input, \( V_q \), and \( V \) variables are conducted using (6) and (7).

\[
\begin{align*}
X_q &= V_q B \\
X &= VB
\end{align*}
\]

(6) (7)

More details about the LW-KPLS model can be found in Yeo, Saptoro, and Kumar [25].

### 2.2. Optimisation of parameters.

By carrying the optimization of parameters in a model, the model can be presumed as a well-performing model. In the LW-KPLS algorithm, the parameters used are \( N_t \), \( S \), \( \emptyset \) and \( b \). \( N_t \) symbolizes the total number of samples; \( S \) symbolizes the amount of latent variable while the localization parameter is symbolized by \( \emptyset \) , and \( b \) is a kernel parameter. \( N_t \) is the total number of samples used for the LW-KPLS model, and it is an insensitive parameter to the LW-KPLS algorithm. Moreover, according to the study carried out by Yeo, Saptoro, and Kumar [25], the first few latent variables of PLS-based models can indicate the predominant data feature; hence \( S \) is set at 1. LW-KPLS model uses \( \emptyset \) to cope with the nonlinearity of the process data. The nonlinearity of the process can be handled by the model when the \( \emptyset \) is small, thus \( \emptyset \) is set as 0.1 [25]. In addition, the Kernel parameter, \( b \) is the most ingenious parameter of the LW-KPLS algorithm; hence it must be fine-tuned properly for each case study.

### 2.3. Data splitting and setting of parameters.

A total of 5,000 data sets is achieved and separated into training and testing sets. Hence, a dataset ratio of 90% to 10% is used for training and testing purposes, respectively. Then, \( N_t \) is 5,000 while \( N_1 \) and \( N_2 \) represent the number of training and testing data are 4,500 and 500, respectively. As mentioned earlier, \( S \) is allocated as 1, and an optimal value of 0.1 is allocated \( \emptyset \). By referring to Table 1, the parameter values involved in each case study are summarized.

| Parameters | \( N_t \) | \( N_1 \) | \( N_2 \) | \( S \) | \( \emptyset \) |
|------------|----------|----------|----------|-------|-------|
| Values     | 5,000    | 4,500    | 500      | 1     | 0.1   |

Table 1. Values of parameters in the algorithm.
2.4. Measurement of quality prediction.

The implementation of indexes which are root-mean-square error (RMSE) and error of approximation (E_a), are carried out to evaluate the prediction performance of LW-KPLS quantitatively. The formula of RMSE is demonstrated in (8), while E_a is calculated using (9) [28-30].

\[
RMSE = \sqrt{\frac{1}{N_1} \sum_{i=1}^{N_1} (\hat{y}_i - y_i)^2}
\]

(8)

\[
E_a = \left( \frac{N_I}{N_T} \right) RMSE_I + \left( \frac{N_2}{N_T} \right) RMSE_2 + |RMSE_I - RMSE_2|
\]

(9)

where \( \hat{y}_i \) and \( y_i \) are the predicted and actual values of the output variable, respectively, while \( \bar{y} \) is the mean of the actual output. RMSE_1 and RMSE_2 are the RMSE of training and testing data, respectively. Sometimes, the overall predictive performance of the LW-KPLS model is difficult to be determined when two RMSE values (RMSE_1 and RMSE_2) for each case study are varied. For instance, there could be a case where the error of training data is the smallest, the testing set error could be high. To solve this issue, E_a is applied. The lower the E_a, the better the predictive performance of the model [25].

2.5. Kernel functions.

Kernel functions map the nonlinear data to a high dimension space [31]. In this study, several different Kernel functions are integrated into the LW-KPLS model; then, their results were accessed and compared. Table 2 shows the equations for Kernel functions employed in this study, where the majority of them have not been tested in the LW-KPLS model yet.

| Type of Kernel function            | Kernel function                                      |
|------------------------------------|------------------------------------------------------|
| Linear Kernel (1)                  | \( k(x, y) = x^T y + \sigma \)                      |
| Linear Kernel (2)                  | \( k(x, y) = bx^T y + \sigma \)                     |
| Polynomial Kernel (1)              | \( k(x, y) = (x^T y + 1)^b \)                       |
| Polynomial Kernel (2)              | \( k(x, y) = (bx^T y + b)^b \)                      |
| Gaussian Kernel                    | \( k(x, y) = \exp \left( -\frac{||x - y||^2}{2\sigma^2} \right) \) |
| Laplacian Kernel                   | \( k(x, y) = \exp \left( -\frac{||x - y||}{\sigma} \right) \) |
| Hyperbolic Tangent (Sigmoid) Kernel| \( k(x, y) = \tanh (bx^T y + 1) \)                   |
| Multiquadric Kernel                | \( k(x, y) = \sqrt{||x - y||^2 + b^2} \)            |
| Inverse Multiquadric Kernel        | \( k(x, y) = \frac{1}{\sqrt{||x - y||^2 + b^2}} \) } |
2.6. Specifications of computer configuration.

In this section, the computer configuration used to execute the LW-KPLS model is specified. The operating system (OS) is Windows 10 (64-bit). Besides, Intel(R) Core (TM) i7-4500U j(1.80 GHz) 2.40 GHz is the central processing unit or the main processor. Furthermore, the random-access memory installed is 4.00 GB, while the MATLAB version R2019b is used.

3. Results and Discussion

3.1. Case Studies.

The LW-KPLS model with different Kernel functions was applied to three different case studies. The first case study is a predictive control of a wastewater treatment process [32]. The second case study is re-scaled the Rosenbrock function, which was studied by Turgut et al. [33]. Lastly, the third case study is the process of polymerization of methyl methacrylate, which was adopted from Shafiee et al. [34].

3.1.1. Case study 1: Predictive control of a wastewater treatment process.

Case study 1 demonstrates the wastewater treatment process studied by Caraman, Sbarciog and Barbu [32]. One of the most significant environmental conservation processes in the industry is the wastewater treatment process. It is usually complicated, nonlinear, and multivariable as it has multiple inputs and outputs. In this wastewater treatment process, an aeration tank, a biological reactor, consists of a mixture of liquid and suspended solids. A microorganism population is raised to eliminate the organic substrate from the mixture. A settler acts as a clarifier tank to split the sludge and the clear effluent using gravity. An amount of sludge is recycled back to the aeration tank while the other amount is eliminated. The details of this case study, including the mass balance equations and their notations, can be found in Caraman, Sbarciog, and Barbu [32].

3.1.2. Case study 2: Rescaled Rosenbrock function.

This case study was carried out by Turgut, Turgut, and Coban [33] and Picheny, et al. [35], in which a nonlinear test function expressed in (10) is, the Rosenbrock function, is employed. This function is re-scaling to keep a mean of zero and one variance [35].

\[
y(x) = \frac{1}{3.755 \times 10^5} \sum_{j=1}^{3} \left[ 100 (x_{j+1} - x_j)^2 + (1 - x_j)^2 \right] - 3.827 \times 10^3
\]

where \( \bar{x} = 15x - 5 \) and \(-2.048 \leq x_i \leq 2.048 \).
3.1.3. Case study 3: Polymerization of methyl methacrylate.

In this case study, a continuous stirred tank reactor (CSTR) with a cooling jacket is employed to polymerize Methyl Methacrylate. Surplus heat is delivered throughout the exothermic polymerization. Hence, the cooling jacket of CSTR plays an important role in removing the heat. There are three feed streams for CSTR, which include the feed streams for solvent, monomer, and initiator. At the outlet stream of CSTR, the unreacted polymer, initiator, solvent, and polymer product are transmitted downstream to undergo the separation process. Table 3 tabulates the input variables for this case study. On the other hand, zeroth, first, and second molecular weight distribution moments are the output variables. More details of this case study can be obtained in [34].

| Input variable | x₁ | x₂ | x₃ |
|----------------|----|----|----|
| Variable description | Initiator concentration (gmol/L) | Monomer concentration (gmol/L) | Reactor temperature (K) |

3.2. Results and discussion.

3.2.1. Case study 1: Predictive control of a wastewater treatment process.

As shown in Table 4, the values of RMSE for training and testing datasets and $E_a$ with the Kernel functions after tuning the $b$ in Case study 1 were tabulated in ascending order. The $b$ must be tuned with care to prevent overestimation and underestimation [36]. A lower RMSE indicates the closeness of the regression line to the data points and gives a better fit to the data. In this case study, Linear Kernel (1) and Linear Kernel (2), as well as Polynomial Kernel (1) and Polynomial Kernel (2), gave the same results, and they have the lowest RMSEs. From Table 2 above, it can be seen that Linear Kernel and Polynomial functions have slightly different characteristics in which Linear Kernel is equivalent to a Polynomial Kernel of degree one [37]; hence the result of RMSEs as well as $E_a$ by using Linear Kernel (1) and Linear Kernel (2) were equivalent. However, Linear Kernel (1), Linear Kernel (2), Polynomial Kernel (1), and Polynomial Kernel (2) were chosen as the best Kernel functions since they gave the lowest RMSEs, comparable central processing unit (CPU) running time, and more accurate as compared to other Kernel functions in this case study.

Moreover, from Table 4, the range of central processing unit (CPU) running time for the training and testing data set, $\text{CPU}_1$ and $\text{CPU}_2$ of Linear Kernel (1), Linear Kernel (2), Polynomial Kernel (1), and Polynomial Kernel (2) were between 252s and 263s as well as 29s and 33s, respectively which are comparable to other Kernel functions. Moreover, they have similar results that gave the values of 0.6703, 0.6728, and 0.6731 for the RMSE of training and testing data and the $E_a$, respectively. Since the values of the output variable in this case study were small, between -1.9536 to 23.9143, thus the RMSE and $E_a$ values were also small. In other words, the higher the values of the output variables, the bigger the values for RMSE and $E_a$. Besides, as the testing data set utilized training data to develop the model, hence it is observed that the $\text{RMSE}_1$ is smaller than $\text{RMSE}_2$ [38]. Other than that, among the Kernel functions, Multiquadric Kernel (MK) gave the largest value of RMSEs and $E_a$ at 1.1922, 2.5505, and 2.6863, respectively, when its Kernel parameter, $b$ was tuned at 2. These results indicate that MK, which transforms the scattered data into a very precise, appropriate model of a graph or surface [39], does not fit the data in this case study. By comparing the results from
MK, the Linear Kernel (1), Linear Kernel (2), Polynomial Kernel (1), and Polynomial Kernel (2) improved the results by 43.78% for RMSE\(_1\), 73.62% for RMSE\(_2\), and 74.94% for Ea.

Hence, it can be concluded that the predicted data from the LW-KPLS model with the Linear Kernel (1), Linear Kernel (2), Polynomial Kernel (1), and Polynomial Kernel (2) are said to be closer to the real nature of the data set as the Ea is lower as compared to the rest of the kernel functions. The training and testing data graphs on their actual output values against the predicted outputs from the LW-KPLS model with the Linear Kernel (1) were plotted and shown in Figures 1 and 2. Since these Kernel functions gave the best results, Linear Kernel (1) was chosen to plot Figures 1 and 2. From these figures, the predicted output of training and testing data is allocated more concentrated along with the actual output of training and testing data. These results indicate that the LW-KPLS model with Linear Kernel (1), Linear Kernel (2), Polynomial Kernel (1), and Polynomial Kernel (2) can fit the data in Case study 1 well.

![Figure 1](image1.png)

**Figure 1.** Graph of a training dataset of output variable of actual and predicted output values for output 1 from LW-KPLS model with Linear Kernel (1) in Case Study 1.

![Figure 2](image2.png)

**Figure 2.** Graph of testing dataset of output variable of actual query and predicted query output values for output 1 from LW-KPLS model with Linear Kernel (1) in Case Study 1.

### 3.2.2. Case study 2: Rescaled Rosenbrock function.

The RMSE values for training and testing data and the value of Ea with Kernel functions for Case study 2 were organized in ascending order, as shown in Table 5. By comparing the results obtained from the Kernel functions, Polynomial Kernel (1) gave the lowest RMSEs and Ea. When b was tuned at a value of 4, the RMSE values for training and testing data sets and Ea obtained from Polynomial Kernel (1) were 55.6670, 59.5754, and 59.9662, respectively. From Table 2, the results indicate the Polynomial Kernel (1) had mapped the dataset in this case study to a high dimensional space, enabling the LW-KPLS model to predict better results than the rest of the kernel functions.

From Table 5, it can be found that the Polynomial Kernel (2) and Gaussian Kernel (GK) obtained the nearest values when their b were tuned at 10. Polynomial Kernel (2) gave the values of RMSEs and Ea as 57.3369, 61.4174, and 61.8255, respectively, while GK gave the
values of RMSEs and $E_a$ 61.3635, 61.9157, and 61.9710, respectively. The Polynomial Kernel (2) can adapt to problems of normalized training data, while GK can estimate the anticipated value [40]. Thence, both Kernel functions can be considered to obtain the nearest values of RMSEs and $E_a$. Additionally, the results obtained using MK are the highest among the Kernel functions. This result indicates that the MK with a non-positive definite Kernel [41] does not work well with the data in this case study. MK gave the values of RMSEs and $E_a$ which are 85.1186, 224.8771, and 238.8530, respectively. As compared to MK, Polynomial Kernel (1) performed an improvement of 34.60%, 73.51%, and 74.89% for RMSE_1, RMSE_2, and $E_a$, respectively.

On the other hand, the average CPU running time for the training and testing data set, CPU_1 and CPU_2 of Polynomial Kernel (1), were 265.08s and 32.41s, respectively, which are not the lowest. However, it is still the best model since it gave the lowest RMSEs and $E_a$ compared to other Kernel functions. In Figures 3 and 4, the comparison of the actual output values against the predicted outputs from the LW-KPLS model with Polynomial Kernel (1) for training and testing data were plotted and shown. Both predicted values of the training and testing data sets are to be seen within the data range of actual output. These results express the integration of nonlinear features in LW-KPLS with the Polynomial Kernel (1) function and have proved the effectiveness of LW-KPLS when dealing with the high nonlinearity of data [42].

Figure 3. Graph of a training dataset of output variable of actual and predicted output values for output 1 from LW-KPLS model with polynomial Kernel (1) in Case Study 2.

Figure 4. Graph of testing dataset of output variable of actual query and predicted query output values for output 1 from LW-KPLS model with polynomial Kernel (1) in Case Study 2.
3.2.3. Case study 3: Polymerization of methyl methacrylate.

This case study is a multi-input and multi-output case study with three outputs; hence three sets of RMSE values for the training and testing data sets and \( E_a \) in Kernel functions are being studied. Tables 6 and 7 show the values of RMSE for training and testing data, and \( E_a \) with the Kernel functions after tuning the Kernel parameter in this case study were demonstrated in ascending order. By carrying out the comparison, it can be concluded that the lowest RMSEs and \( E_a \) have been achieved by adopting Linear Kernel (1) and (2) as well as Polynomial Kernel (1) and (2). Hence, they are selected as the best models in this case study.

For output 1, Linear Kernel (1) and Linear Kernel (2), as well as Polynomial Kernel (1) and Polynomial Kernel (2), provided the values of \( 1.0117 \times 10^{-5} \), \( 5.9672 \times 10^{-5} \), and \( 6.2180 \) for the RMSE for training and testing data sets and \( E_a \), respectively. For output 2, Linear Kernel (1) and Linear Kernel (2), as well as Polynomial Kernel (1) and Polynomial Kernel (2) gave the values of the RMSE for training and testing data sets and \( E_a \) which are \( 3.2955 \times 10^{-5} \), 0.0197, and 21.3119, respectively. Moreover, output 3 gave the RMSEs for training and testing data and \( E_a \) of \( 3.5239 \times 10^{-5} \), 0.0211, and 22.8213, respectively. Furthermore, in Table 6, \( \text{CPU}_1 \) and \( \text{CPU}_2 \) of Linear Kernel (1) and Linear Kernel (2), as well as Polynomial Kernel (1) and Polynomial Kernel (2), were ranged from 252s to 260s for training data, and 26s to 32s for testing data. It can be said that they gave lower CPUs running times than the majority of other Kernel functions.

Referring to Table 6, MK provided the highest values of RMSEs and \( E_a \) for the three outputs. It gave values of \( 3.2006 \times 10^{-5} \), 0.0191, 20.0034 for RMSE1 of outputs 1, 2 and 3, respectively, \( 4.7745 \times 10^{-4} \), 0.3383, 462.2747 for RMSE2 of outputs 1, 2 and 3, respectively, \( 5.2200 \times 10^{-4} \), 0.3702, 506.5018 for \( E_a \) of outputs 1, 2 and 3, respectively. According to Drewnik and Pasternak-Winiarski [43], MK is a non-positive and definite Kernel function. However, MK does not cope well with the data in this case study. As a result, Linear Kernel (1) and Linear Kernel (2), as well as Polynomial Kernel (1) and Polynomial Kernel (2), are greater than MK as they can enhance the performance better by 68.39% to 68.92% for RMSE1, 93.10% to 95.39% for RMSE2, and 93.25% to 95.49% for \( E_a \), respectively.

![Figure 5](https://biointerfaceresearch.com/)

**Figure 5.** Graph of a training dataset of output variable of actual and predicted output values for output 1 from LW-KPLS model with Linear Kernel (1) in Case Study 3.

The graphs of training and testing data of the three output variables, which show the actual and predicted output values from LW-KPLS with Linear Kernel were also plotted, as illustrated in Figures 5 to 10. Similar to Case study 1, since these Kernel functions gave the best results, Linear Kernel (1) was chosen to plot Figures 5 to 10. Figures 5, 7, and 9 show that the predicted output values of training data sets for outputs 1, 2, and 3 are also close to their
actual output values. In contrast, the predicted query outputs of testing data for the 3 outputs are also close to their actual query output values by observing Figures 6, 8, and 10. To conclude, LW-KPLS with Linear Kernel (1) and Linear Kernel (2) as well as Polynomial Kernel (1) and Polynomial Kernel (2) can fit the data in this study very well and accomplish superior performance when compared to other Kernel functions.

![Figure 6. Graph of testing dataset of output variable of actual query and predicted query output values for output 1 from LW-KPLS model with Linear Kernel (1) in Case study 3.](image1)

![Figure 7. Graph of training dataset of output variable of actual and predicted output values for output 2 from LW-KPLS model with Linear Kernel (1) in Case study 3.](image2)

![Figure 8. Graph of testing dataset of output variable of actual query and predicted query output values for output 2 from LW-KPLS model with Linear Kernel (1) in Case study 3.](image3)
4. 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, the predictive performance of Kernel functions in the LW-KPLS model has been evaluated via 3 case studies, which are the predictive control of a wastewater treatment process denoted as Case study 1, rescaled Rosenbrock function designated as Case study 2; thus the process of polymerization of methyl methacrylate denoted as Case study 3. It was found that Linear Kernel (1), Linear Kernel (2), Polynomial Kernel (1), and Polynomial Kernel (2) have provided the best results among Kernel functions in Case studies 1 and 3 while Polynomial Kernel (1) is the best model in Case study 2. Since Polynomial Kernel (1) performed well in these nonlinear case studies, it can conclude that it is the more suitable Kernel function for the LW-KPLS model. From the results in these case studies, it was found that Polynomial Kernel (1) gave 34.60% to 95.39% lower for RMSEs values and 68.20% to 95.49% smaller for $E_a$ values, especially the comparison made with the MK, which gave the highest values of RMSEs and $E_a$ values.
Table 4. RMSE1, RMSE2 and E using LW-KPLS model with different Kernel functions for Case Study 1.

| Kernel | LNK (1) | LNK (2) | PK(1) | PK(2) | GK | PK | HTK | LK | CK | IMK | LPK | MK |
|--------|---------|---------|-------|-------|----|----|-----|----|----|-----|-----|----|
| b      | 3       | 3       | 1     | 1     | 7  | 7  | 7   | 10 | 1  | 2   | 2   |    |
| RMSE1  | 0.6703  | 0.6703  | 0.6703 | 0.6703 | 1.2412 | 1.5566 | 1.3468 | 1.3468 | 1.3571 | 1.3057 | 1.1201 | 1.1922 |
| CPU1 (s) | 251.22  | 262.81  | 256.49 | 259.12 | 251.67 | 286.39 | 258.20 | 291.57 | 263.51 | 263.20 | 253.62 | 268.36 |
| RMSE2  | 0.6728  | 0.6728  | 0.6728 | 0.6728 | 1.1214 | 2.2697 | 2.4264 | 2.4264 | 2.4432 | 2.4672 | 2.4910 | 2.5505 |
| CPU2 (s) | 30.41   | 32.42   | 32.44  | 28.62  | 27.78  | 68.95  | 32.66  | 67.39  | 47.18  | 46.90  | 40.20  | 48.88  |
| Ea     | 0.6731  | 0.6731  | 0.6731 | 0.6731 | 1.3489 | 2.3410 | 2.5344 | 2.5344 | 2.5518 | 2.5833 | 2.6281 | 2.6863 |

Legends: LNK(1) – Linear Kernel (1); LNK(2) – Linear Kernel (2); PK(1) – Polynomial Kernel (1); PK(2): Polynomial Kernel (2); GK - Gaussian Kernel; PK - Power Kernel; HTK - Hyperbolic Tangent (Sigmoid) Kernel; LK - Log Kernel; CK - Cauchy Kernel; IMK - Inverse Multiquadric Kernel; LPK – Laplacian Kernel; MK - Multiquadric Kernel.

Table 5. RMSE1, RMSE2 and E using LW-KPLS model with different Kernel functions for Case Study 2.

| Kernel | PK(1) | PK(2) | GK | EK | LNK (1) | LNK (2) | HTK | CK | IMK | PK | LK | MK |
|--------|-------|-------|----|----|---------|---------|-----|----|-----|----|----|----|
| b      | 4     | 10    | 10 | 10 | 1       | 1       | 1   | 1  | 1   | 1  | 9  | 1  |
| RMSE1  | 0.55670 | 57.3369 | 61.365 | 91.3526 | 124.9340 | 124.9340 | 131.2939 | 162.5037 | 157.9390 | 147.9563 | 140.5478 | 85.1186 |
| CPU1 (s) | 263.23  | 262.04  | 255.24 | 258.67 | 258.66  | 257.97  | 252.84  | 263.50  | 271.94  | 264.69  | 286.57  | 273.10  |
| RMSE2  | 0.59754 | 61.4174 | 61.9157 | 92.7694 | 126.9206 | 126.9206 | 131.9680 | 177.4952 | 179.9464 | 189.9410 | 193.9760 | 224.8771 |
| CPU2 (s) | 34.39   | 27.68   | 28.89  | 28.12  | 32.76   | 26.07   | 28.99   | 45.92   | 56.50   | 52.53   | 69.59   | 50.36   |
| Ea     | 0.59662 | 61.8255 | 61.9710 | 92.9111 | 127.1193 | 127.1193 | 132.0354 | 178.9943 | 182.1471 | 194.1395 | 199.3189 | 238.8530 |

Legends: LNK(1) – Linear Kernel (1); LNK(2) – Linear Kernel (2); PK(1) – Polynomial Kernel (1); PK(2) - Polynomial Kernel (2); GK - Gaussian Kernel; PK - Power Kernel; HTK - Hyperbolic Tangent (Sigmoid) Kernel; LK - Log Kernel; CK - Cauchy Kernel; IMK - Inverse Multiquadric Kernel; LPK – Laplacian Kernel; MK - Multiquadric Kernel.

Table 6. RMSE1, RMSE2 and E using LW-KPLS model with different Kernel functions for Case Study 3.

| Kernel | LNK (1) | LNK (2) | PK(1) | PK(2) | GK | HTK | CK | IMK | PK | MK |
|--------|---------|---------|-------|-------|----|-----|----|-----|----|----|
| b      | 5      | 10     | 1     | 1    | 3  | 1   | 1  | 1   | 1  |    |
| RMSE1  | 1.0117×10^5 | 1.0117×10^5 | 1.0117×10^5 | 1.0117×10^5 | 2.3970×10^5 | 2.2783×10^5 | 4.8152×10^5 | 4.6910×10^5 | 4.9723×10^5 | 4.7201×10^5 | 3.2006×10^5 |
| RMSE2  | 5.9672×10^3 | 5.9672×10^3 | 5.9672×10^3 | 5.9672×10^3 | 0.0168 | 0.0161 | 0.0303 | 0.0291 | 0.0303 | 0.0286 | 0.0191 |
| CPU1 (s) | 259.84  | 259.84  | 253.95 | 251.74 | 265.81 | 251.81 | 311.74 | 315.63 | 301.61 | 340.23 | 267.44 |
| RMSE1  | 3.2955×10^5 | 3.2955×10^5 | 3.2955×10^5 | 3.2955×10^5 | 4.8407×10^5 | 4.6463×10^4 | 4.6578×10^4 | 4.6979×10^4 | 4.7655×10^4 | 4.7754×10^4 | 4.7745×10^4 |
| RMSE2  | 0.0197  | 0.0197  | 0.0197 | 0.0197 | 0.0289 | 0.0327 | 0.0324 | 0.0321 | 0.0331 | 0.3383 | 0.3383 |
| CPU1 (s) | 31.00   | 29.28   | 29.33  | 25.15  | 32.00  | 42.98  | 93.18  | 94.46  | 75.38  | 117.59 | 47.11  |
| RMSE1  | 3.5239×10^5 | 3.5239×10^5 | 3.5239×10^5 | 3.5239×10^5 | 5.0851×10^5 | 5.0881×10^4 | 5.0755×10^4 | 5.1208×10^4 | 5.1923×10^4 | 5.2075×10^4 | 5.2200×10^4 |
| RMSE2  | 0.0211  | 0.0211  | 0.0211 | 0.0211 | 0.0301 | 0.3544 | 0.3544 | 0.3591 | 0.3678 | 0.3693 | 0.3702 |
| CPU1 (s) | 22.8213 | 22.8213 | 22.8213 | 22.8213 | 31.2935 | 468.2575 | 470.2402 | 480.1904 | 501.1385 | 505.6184 | 506.5018 |

Legends: LNK(1) – Linear Kernel (1); LNK(2) – Linear Kernel (2); PK(1) – Polynomial Kernel (1); PK(2) - Polynomial Kernel (2); GK - Gaussian Kernel; PK - Power Kernel; HTK - Hyperbolic Tangent (Sigmoid) Kernel; LK - Log Kernel; CK - Cauchy Kernel; IMK - Inverse Multiquadric Kernel; MK - Multiquadric Kernel;
Therefore, it can also be concluded that the MK is not the right Kernel function for the LW-KPLS model. Future studies can further improve the LW-KPLS model to cope with missing data.

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Conflicts of Interest

The authors declare no conflict of interest.

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