Estimation of Free Fatty Acids in Stored Paddy Rice Using Multiple-Kernel Support Vector Regression

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Abstract: Grain quality changes during the storage period, and an important grain quality indicator is the free fatty acid (FFA) content. Understanding real-time change of FFA content in stored grain is significant for grain storage safety. However, the FFA content requires manual detection with time-consuming and complex procedures. Thus, this paper is dedicated to developing a method to estimate FFA content in stored grain accurately. We proposed a machine learning approach—multiple-kernel support vector regression—to complete this goal, which improved the accuracy and robustness of the FFA estimation. The effectiveness of the proposed approach was validated by the grain storage data collected from northeast China. To show the merits of the proposed method, several prevailing prediction methods, such as single-kernel support vector regression, multiple linear regression, and back propagation neural network, were introduced for comparative purposes, and several quantitative statistical indexes were adopted to evaluate the performance of different models. The results showed that the proposed approach can achieve a high accuracy with mean absolute error of 0.341 mg KOH/100 g, root mean square error of 0.442 mg KOH/100 g, and mean absolute percentage error of 2.026%. Among the four models tested, the multiple-kernel support vector regression model performed best and made the most robust forecasts of FFA content in stored grain.

Keywords: food security; free fatty acid; grain storage; support vector regression; multiple-kernel learning

1. Introduction

Food security has been a research hotspot all over the world due to its impact on the environment, economy, and society [1,2]. Approximately a third of food produced in the world is wasted every year [3]. As a result of poor grain storage management, the grain’s quality and nutritional value deteriorate rapidly during storage [4]. Ensuring that the process of grain storage is of high quality is particularly important. The free fatty acid (FFA) content, a sensitivity indicator of the quality changes, is often employed as a measure of deterioration of stored grain [5,6]. In the process of grain storage, an increase of FFA content in stored grain has been observed during storage, which is attributed to the role of lipase hydrolysis [5,7,8]. This can impact the physical properties of rice in terms of its textural, flavor, composition, and eating quality [9–11]. Generally, FFA increases with storage period and the quality of stored grain reduces concomitantly [4,12,13]. Grain will deteriorate and become inedible when its FFA content reaches a certain standard value [7,14]. It is reasonable to use the fatty acid value as a quality index during wheat flour storage. Thus, it is of significance to study the changes in FFA accumulation, as they are directly related to the quality loss of stored grain.
In order to detect FFAs in food, researchers have developed a variety of accurate and reliable methods, such as classic titration with Fourier transform infrared spectroscopy [15] and gas chromatography [16]. In addition, a new method based on a homemade olfactory visualization sensor has been proposed to realize the quantitative determination of FFAs during rice storage [7]. The detectability of FFAs allows us to analyze changes of food quality. There have been many studies involving various grains, such as rice [6,17] and wheat [18], that have investigated the changing regularity of FFA during storage. Some mathematical equations [19,20] were developed to predict the FFA content during storage. These models estimate the FFA content of grain by establishing the relationship between FFA values and the storage period. Therefore, it is necessary to develop an efficient and rapid method to achieve an accurate prediction of FFA during storage.

In fact, the FFA content during grain storage is affected by many factors. Therefore, it is not possible to use the relationship between storage period and FFA content to predict the FFA value. Machine learning (ML) methods can help solve problems involving multiple independent variables, whether responses are linear or not. So far, the development of ML has provided a new idea for grain storage security, and has been used in many applications, such as FFA determination [21], grain storage loss analysis [22], and stored grain insect detection [23]. The successful application of ML in grain storage is of great significance to grain storage safety.

In ML, artificial neural networks (ANN) have been widely used for a variety of tasks [24,25]. However, ANN suffers from its weak generalization ability and over-fitting. On the contrary, support vector regression (SVR) has a better generalization ability and exhibits better prediction accuracy due to its implementation of the structural risk minimization principle which considers both the training error and the capacity of the regression model [26]. However, the kernel function and hyperparameters of SVR have profound impacts on the results, and it is time-consuming to determine the kernel and its hyperparameters [27]. Several researchers have proposed multiple kernel learning (MKL) to deal with these problems [28,29]. In this paper, we propose a model by means of multiple kernel support vector regression to predict the FFA content in stored grain during storage.

2. Materials and Methods

2.1. Study Area

Northeast China accounted for about 16–20% of China’s total paddy rice output. The study sites were located in the Heilongjiang, Jilin, and Liaoning provinces of northeast China. The experimental data were collected from 7 grain reserve depots, including 3 in Heilongjiang province, 3 in Jilin province, and 1 in Liaoning province (Figure 1).

2.2. Determination of FFA and Moisture

The FFA content of stored grain was measured by the national standard GB/T 20569-2006 (Guidelines for evaluation of paddy storage character). The fatty acids in paddy rice were extracted with anhydrous ethanol at room temperature, and then titrated with potassium hydroxide standard solution, after which the fatty acid value was calculated. The standard stipulated that each sample should be determined twice by the same inspector and the average value was taken as the result, and the difference between the two measured values should not be more than 2 mg KOH/100 g.

The moisture content of stored grain was measured by the national standard GB 5009.3-2016 (National Food Safety Standard—Determination of Moisture Content in Foods). Based on the physical properties of water in paddy rice, the weight lost during drying was determined by volatilization at 101.3 kPa and temperature 101–105 °C; then, the moisture content was calculated by weighing values before and after drying. The standard stipulated that each sample should be tested twice by the same inspector and the average value was taken as the result, and the absolute difference between the two measured values must not exceed 10% of the arithmetic mean.
2.3. Temperature Measurement System

The temperature was measured by a digital wireless monitoring system. A temperature monitoring system is shown in Figure 2. This system generally includes temperature sensors, temperature measuring cables, and a computer monitoring terminal. A set of temperature sensors were deployed in the granary. These sensors were encapsulated in cables and the cables were inserted into the grain pile at certain places. In addition, one digital temperature and humidity sensor was arranged at the central position over the grain surface in the granary to detect the temperature of the granary. The wire bus communication protocol was used between the computer monitoring terminal and the sensors to transmit the control command and report sensory data, and finally, the collected data were stored in the remote-control computer. Generally, the detection time of the grain temperature was from 09:00 a.m. to 10:00 a.m. every day, when the temperature was close to the daily mean temperature. As the temperature in the granary fluctuated little throughout the day, all data were sampled once a day.

2.4. Preliminary Analysis

During the storage process, the granary was a large time lag system, and the grain pile can form a “cold core” (Figure 3); this phenomenon was caused by the cycle of convection currents when the ambient air outside the granary was warm and the grain was cold. The grain pile can form a “warm core” in winter when the grain core was warm, and the outside edges was colder. To research the effects of temperature distribution on FFA, we selected a tall granary with a paddy rice pile that was 59 m in length, 19 m wide, and 6 m high (No. 6 Warehouse at Grain Reserve Depot of Shenyang, Liaoning, China). We took samples every three months from the end of warehousing (October 2017). An electric suction sampler was used to carry out sampling at four heights of 0, 1.9, 3.8, 5.7 m from the grain surface. Eighteen locations distributed evenly were sampled in each layer. Approximately 5 kg stored grain was sampled in each location, and each sample was poured from the sampler and individually bagged. The average moisture of the upper layer (UL), second layer (SL), third layer (TL), and lower layer (LL) of the stored grain was then be obtained, as shown in Figure 4.
Figure 2. The structure of a digital wireless grain condition monitoring system. The width of the granary was generally 18–36 m and the length was 36–60 m. The headspace above the grain surface was not less than 1.8 m. The wall material was a reinforced concrete structure and the roof was made of a heat preserving material. In the granary, the temperature sensors layout was as follows: The distance between the rows and columns of the horizontal temperature measuring cables should be no more than 5 m; the distance between the vertical sensors should be no more than 2 m; and the distance from the cables to the grain surface, granary bottom, and granary wall should be within 0.3 m to 0.5 m.

Figure 3. Schematic diagram of “cold core” in granary.
Table 1 shows the average temperature of four layers at each three-month interval. As the depth of the grain layer increased, the average temperature reduced. Figure 4 and Table 1 show that during the storage period, the FFA in stored grain at the UL, SL, and TL increased at a rate significantly higher than that of the LL. In particular, the FFA in stored grain of the UL increased by 20.4%, while that of the LL increased by 11.3%. Furthermore, the greater the distance from the grain surface, the slower the increase of FFA in stored grain. This indicates that the storage conditions are better in the lower layers of the grain pile, that is, the lower the storage temperature, the better the conditions for long-term storage of grain.

Table 1. The average temperature (°C) of four layers at each three-month interval.

| Period of Time | Average Temperature of UL | Average Temperature of SL | Average Temperature of TL | Average Temperature of LL |
|---------------|---------------------------|---------------------------|---------------------------|---------------------------|
| 0–3           | 0.32                      | 0.66                      | −2.63                     | −3.41                     |
| 3–6           | −1.12                     | −3.39                     | −9.11                     | −12.53                    |
| 6–9           | 17.65                     | 8.59                      | −2.78                     | −6.37                     |
| 9–12          | 20.28                     | 17.45                     | 5.79                      | −1.12                     |
| 12–15         | 3.03                      | 3.72                      | 0.01                      | −3.59                     |
| 15–18         | −0.79                     | −4.41                     | −7.30                     | −8.12                     |
| 18–21         | 17.56                     | 8.58                      | −2.76                     | −4.35                     |

* The temperature of the UL refers to the temperature of ambient air in the headspace of granary of the day. The temperature of SL, TL, and LL refer to the average temperature of stored grain in the layer of the day. UL: Upper layer; SL: Second layer; TL: Third layer; LL: Lower layer.

Figure 5 shows the change in average moisture of the grain in each layer during storage. The reason for the sudden drop of moisture of stored grain in the third month was that aeration was carried out in the second month after the end of warehousing. On the whole, the moisture content in all layers decreased during storage, while the moisture in the UL and LL decreased faster than that in the SL and TL, because the UL was in direct contact with the ambient air in the headspace of the granary, and the LL was closest to the ventilation equipment. Table 1 and Figure 5 show that the LL is the region with low temperature and low moisture, while the UL is the region with high temperature and low moisture. This results in significant differences of fatty acid changes in each layer. Therefore, moisture content is related to FFA accumulation.
while the extensive activities of the fungi can produce heat and moisture, which in turn accelerates fungal growth and may lead to the emergence of other biological entities [33,34]. To calculate the effective accumulated temperature (EAT) of grain storage which can be calculated by

\[ S_{EAT} = \begin{cases} 
\sum_{d=0}^{H} (T_d - T_0), & \text{if } T_d < T_0, \\
0, & \text{for } T_d \leq T_0 
\end{cases} \]  

(1)

where \( S_{EAT} \) is the EAT of grain storage (°C), \( d \) is the \( d^{th} \) day, \( H \) is the total days (\( d \)), \( T_0 \) is the threshold temperature (°C), and \( T_d \) is the actual mean temperature of the day above threshold temperature (°C). Suitable storage temperature and moisture levels promote the germination and development of fungi, while the extensive activities of the fungi can produce heat and moisture, which in turn accelerates fungal growth and may lead to the emergence of other biological entities [33,34]. To calculate the accumulated temperature, we considered the minimum activity temperature of fungi in stored grain as the threshold temperature, which might be more favorable to the predicted results. Research shows that molds can still be detected when the stored temperature is −8 °C [35], so −8 °C was set as the threshold temperature in this paper. In addition, the stored grain temperature changes little over two consecutive days, so we consider the temperature measured by the sensor as \( T_d \) of the day.

2.6. Support Vector Regression

Support vector machine (SVM) is an ML algorithm which is a discriminative classifier proposed for binary classification problems and is based on statistical learning theory [26,36]. Given the training set \( S = \{(x_1, y_1), \ldots, (x_m, y_m)\} \) of points \( x_i \in \mathbb{R}^d \) with the corresponding labels \( y_i \in \{-1, +1\} \), SVM classifiers attempt to find a classification hyperplane induced from the maximum margin principle and predicted to belong to a category based on the side of the gap on which they fall. Similar to SVM classification, the basic concept of SVM regression is to nonlinearly map the original data \( x \) into a high-dimensional feature space, and to solve a linear regression problem in this feature space. In a regression problem, each \( y_i \) is the desired target, or output, value for the input vector \( x_i \).

![Figure 5. Moisture content changes of grain during storage. The value of each point is the average of the 18 positions in the layer.](image-url)
For SVR, a margin of tolerance (epsilon) is set in approximation to the SVM which would have already requested from the problem [37,38]. The regression function is expressed as:

\[ f(x) = \langle w, \phi(x) \rangle + b \]  

(2)

where \( \langle \cdot, \cdot \rangle \) indicates the inner product of the involved arguments, \( w \) is the weight vector, \( \phi(x) \) is the nonlinear mapping function, and \( b \) is the threshold.

Based on the principle of minimizing the regularized risk, the objective function and constraints for SVR can be defined as follows:

\[
\min_{w, b, \xi, \xi^*} \frac{1}{2} \langle w, w \rangle + C \sum_{i=1}^{l} (\xi_i + \xi_i^*) \\
\text{s.t.} \begin{cases} 
\langle w, \phi(x_i) \rangle + b - y_i \leq \epsilon + \xi_i \\
y_i - \langle w, \phi(x_i) \rangle - b \leq \epsilon + \xi_i^* \\
\xi_i, \xi_i^* \geq 0, i = 1, \ldots, l 
\end{cases}
\]

(3)

where \( C \) is a parameter which adjusts the tradeoff between the regression error and the regularization on \( f \), \( l \) is the number of training patterns, \( \xi_i, \xi_i^* \) is slack variables allowing for errors around the regression function, and \( \epsilon \geq 0 \) is the parameter in the \( \epsilon \)-insensitive loss function and controls the accuracy of the regressor.

By adding Lagrangian multipliers \( \alpha, \hat{\alpha} \), the quadratic programming problem can be optimized as a dual problem. Then, the dual problem of Equation (3) can be written as

\[
\max_{\alpha, \hat{\alpha}} \sum_{i=1}^{l} y_i (\hat{\alpha}_i - \alpha_i) - \frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} (\hat{\alpha}_i - \alpha_i) (\hat{\alpha}_j - \alpha_j) K(x_i, x_j) \\
\text{s.t.} \begin{cases} 
\sum_{i=1}^{l} (\hat{\alpha}_i - \alpha_i) = 0 \\
C \geq \alpha_i, \hat{\alpha}_i \geq 0, i = 1, \ldots, l 
\end{cases}
\]

(4)

where \( \alpha = \{\alpha_1, \ldots, \alpha_l\} \) and \( \hat{\alpha} = \{\hat{\alpha}_1, \ldots, \hat{\alpha}_l\} \) are the dual variables, and \( K(x_i, x_j) \) is a kernel function which represents the inner product \( \langle \phi(x_i), \phi(x_j) \rangle \). The sequential minimal optimization (SMO) [39] algorithm can be used to solve Equation (4). By solving \( \alpha, \hat{\alpha} \) and \( b \) in Equation (4) using the KKT (Kurash–Kuhn–Tucker) condition, the regression function of Equation (1) becomes:

\[
f(x) = \sum_{i=1}^{l} (\hat{\alpha}_i - \alpha_i) K(x_i, x) + b.
\]

(5)

Several kernel functions have been used successfully [37,40], and the most common of which are listed as follows:

Linear kernel:

\[ K(x_i, x_j) = \langle x_i, x_j \rangle; \]

(6)

Polynomial kernel:

\[ K(x_i, x_j) = \left( \langle x_i, x_j \rangle + 1 \right)^s; \]

(7)

Sigmoid kernel:

\[ K(x_i, x_j) = \tanh \left( x \langle x_i, x_j \rangle + 1 \right); \]

(8)
\[ K(x_i, x_j) = e^{-\frac{|x_i - x_j|^2}{\sigma^2}}. \]  

\[ K(x, x') = \sum_{m=1}^{M} \mu_m K_m(x, x') \text{ with } \mu_m \in [0, 1], \sum_{m=1}^{M} \mu_m = 1, \]  

where \( M \) denotes the total number of kernels, and \( d_m \) is a weight of the kernel. These weights are considered a vector of weights \( \mu = [\mu_1, \mu_2, \ldots, \mu_M]^T \). To avoid over-fitting, we require the sum of weights to reach unity to restrict the range of the search space [47]. By referring to Equation (1), the objective function and constraints for MKSVR become:

\[
\begin{align*}
\min_{\mu} \max_{w, b} & \quad \frac{1}{2} \langle w, w \rangle + C \sum_{i=1}^{l} (\xi_i + \hat{\xi}_i) \\
\text{s.t.} & \quad (\langle w, \Phi(x_i) \rangle + b) - y_i \leq \varepsilon + \xi_i \\
& \quad y_i - (\langle w, \Phi(x_i) \rangle + b) \leq \varepsilon + \hat{\xi}_i \\
& \quad \xi_i, \hat{\xi}_i \geq 0, i = 1, \ldots, l \\
& \quad \mu_m \geq 0, m = 1, \ldots, M \\
& \quad \sum_{m=1}^{M} \mu_m = 1 
\end{align*}
\]  

where \( \Phi \) is the vector of function mappings.

Similar to Equation (4), by introducing the Lagrangian, Equation (11) can be converted to the following Wolfe dual form:

\[
\begin{align*}
\min_{\mu} \max_{\alpha, \hat{\alpha}} & \quad -\frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} (\hat{\alpha}_i - \alpha_i) (\hat{\alpha}_j - \alpha_j) \tilde{K}_m(x_i, x_j) \\
& \quad -\varepsilon \sum_{i=1}^{l} (\hat{\alpha}_i + \alpha_i) + \sum_{i=1}^{l} y_i (\hat{\alpha}_i - \alpha_i) \\
\text{s.t.} & \quad \sum_{i=1}^{l} (\hat{\alpha}_i - \alpha_i) = 0 \\
& \quad C \geq \alpha_i, \hat{\alpha}_i \geq 0, i = 1, \ldots, l \\
& \quad \mu_m \geq 0, m = 1, \ldots, M \\
& \quad \sum_{m=1}^{M} \mu_m = 1 
\end{align*}
\]  

where \( \tilde{K}_m(x_i, x_j) = \sum_{m=1}^{M} \mu_m K_m(x_i, x_j) \).
The final regression estimation function is:

$$f(x) = \sum_{i=1}^{l} (\hat{\alpha}_i^* - \alpha_i^*) \tilde{K}(x_i, x) + b', \quad (13)$$

where $b^* = y_k + \varepsilon - \sum_{i=1}^{l} (\hat{\alpha}_i^* - \alpha_i^*) \tilde{K}(x_i, x_k)$ with $k \in \{i \in [1, \ldots, l] | 0 < \alpha_i^*, \hat{\alpha}_i^* < C \}$.

### 2.8. SimpleMKL for SVR

The SimpleMKL [48] algorithm was introduced to solve the optimization problem and has been used in many applications [27,49]. In this method, function $J(d)$ is defined as the optimal objective value of problem of MKSVR. Due to the strong duality, $J(\mu)$ is also the objective value of the dual problem:

$$J(\mu) = \frac{1}{2} \sum_{i,j=1}^{l} (\hat{\alpha}_i - \alpha_i)(\hat{\alpha}_j - \alpha_j) \sum_{m=1}^{M} \mu_m K_m(x_i, x_j)$$

$$-\varepsilon \sum_{i=1}^{l} (\hat{\alpha}_i + \alpha_i) + \sum_{i=1}^{l} y_i(\hat{\alpha}_i - \alpha_i) \quad (14)$$

First, by simple differentiation of the dual function (11) with respect to $\mu_m$, we have:

$$\frac{\partial J}{\partial \mu_m} = -\frac{1}{2} \sum_{i,j=1}^{l} (\hat{\alpha}_i - \alpha_i)(\hat{\alpha}_j - \alpha_j) K_m(x_i, x_j) \forall m. \quad (15)$$

Let $q$ be the index of the largest element of vector $\mu$; the differentiation of $J(\mu)$ with respect to $\mu_q$ is:

$$\frac{\partial J}{\partial \mu_q} = -\frac{1}{2} \sum_{i,j=1}^{l} (\hat{\alpha}_i - \alpha_i)(\hat{\alpha}_j - \alpha_j) K_q(x_i, x_j) \forall q. \quad (16)$$

The descent direction $D$ of gradients is computed by the following formula:

$$D_m = \begin{cases} 0 & \text{if } \mu_m = 0 \text{ and } \frac{\partial J}{\partial \mu_m} - \frac{\partial J}{\partial \mu_q} > 0 \\ -\frac{\partial J}{\partial \mu_m} + \frac{\partial J}{\partial \mu_q} & \text{if } \mu_m > 0 \text{ and } m \neq q \\ \sum_{p \neq q, p > 0} \left( \frac{\partial J}{\partial \mu_p} - \frac{\partial J}{\partial \mu_m} \right) & \text{for } m = q \end{cases}, \quad (17)$$

where $p$ is the index of an element of vector $\mu$, which satisfies the condition that $\mu_p > 0$ and $p$ is not the index of the largest component of $\mu$. Then, we find the descent direction $D$ of gradients and update $\mu$ as:

$$\mu = \mu + \tau D, \quad (18)$$

where $\tau$ is the step size. Note that the stopping criterions can be performed according to the duality gap, KKT conditions, and the variation of $\mu$ between two consecutive steps or, even more simply, on a maximal number of iterations.
2.9. Performance Metrics

The performance of the model was evaluated by the measures of deviation between actual and theoretical values. The measures we used were the mean absolute error (MAE), mean absolute percentage error (MAPE), and root mean square error (RMSE). They can be computed as:

\[
MAE = \frac{1}{N} \sum_{t=1}^{N} |y_p(t) - y(t)|, \quad (19)
\]

\[
MAPE = \frac{1}{N} \sum_{t=1}^{N} \left| \frac{y_p(t) - y(t)}{y(t)} \right| \times 100\%, \quad (20)
\]

\[
RMSE = \sqrt{\frac{1}{N} \sum_{t=1}^{N} (y_p(t) - y(t))^2}, \quad (21)
\]

where \( N \) represents the total number of FFA data which are needed to be estimated, \( y_p(t) \) and \( y(t) \) are the estimated and true value of the \( t \)th sample.

3. Results

In this section, we perform an experiment on the prediction of FFA in stored grain to evaluate the efficacy of the proposed MKSVR approach and compare it with several ML methods, including SKSVR, multiple linear regression (MLR), and back propagation neural network (BPNN). The criteria MAE, MAPE, and RMSE were employed to evaluate model performance. All experiments were run on a Windows 10 computer with Intel 2.50 GHz, 8 GB RAM, and MATLAB R2016a environment. The experiments were repeated 20 times to evaluate the robustness of the algorithms.

3.1. Data Description and Preprocessing

Details of storage factors are shown in the Table 2. We used the first 12 storage factors as the input characteristic parameters, and the output parameter “detected FFA” is also the stored grain quality parameter to be predicted in this paper. It should be noted that all experimental data are from paddy rice during the storage in this paper.

| Abbreviation | Description | Units |
|--------------|-------------|-------|
| LOT          | Longitude of grain reserve depot. | °    |
| LAT          | Latitude of grain reserve depot. | °    |
| IM           | Initial moisture of grain when warehousing. | %    |
| DM           | Detected moisture when sampling. | %    |
| WMON         | The month when warehousing. | -    |
| SMON         | The month when sampling. | -    |
| SGT          | Average temperature of stored grain in the layer for the 10 days prior to sampling. | °C   |
| GT           | Average temperature of ambient air in the headspace of granary for the 10 days prior to sampling. | °C   |
| DWS          | Days from warehousing to sampling. | day  |
| SGEAT        | EAT of stored grain from warehousing to sampling. | °C day |
| GEAT         | EAT of granary from warehousing to sampling. | °C day |
| IFFA         | Initial FFA when warehousing. | mg KOH/100 g |
| DFFA         | Detected FFA when sampling. | mg KOH/100 g |

* Calculation method of average temperature: the temperatures for the ten days (include the day of sampling) prior to sampling were extracted, and then calculated the average temperature for these ten days.

As the temperature was collected by the digital wireless monitoring system, which comes from different grain reserve depots where equipment faults, weather and human factors that cause a lack or abnormality of the collected data often occur, we used the linear interpolation method [50] to
complete the missing data and the Pauta criterion [51] to eliminate abnormal data. Finally, a total of 258 experimental data were obtained.

We used the “mapminmax” algorithm in MATLAB to scale inputs and targets so that they fell in the range 0–1. To avoid systematic differences between the training set and the test set, which leads to sample representativeness issues [52], we randomly selected 80% of the data as the training set, and the remaining 20% of the data as the test set.

3.2. Parameter Settings and Steps of Experiments

The results for the experiments depended on properly setting the types of the basis kernels and their parameters [53]. For SKSVR, we chose Gaussian kernel and performed the particle swarm optimization (PSO) [54] algorithm and ten-fold cross-validation procedure to find the optimal parameters for the data sets. The parameter \( \varepsilon \) was set to 0.001, the acceleration coefficients were \( c_1 = c_2 = 2 \), the population size was 30, the inertia weight was 0.9, the maximum number of iterations was 100, and parameters \( C \) and \( \sigma \) were forced to lie in the following intervals: \( C \in [10^0, 10^3] \), \( \sigma \in [10^{-2}, 10^2] \). For the BPNN, the structural parameter was 10-15-1, where the number of the input layer neurons was 10, the number of hidden layer neurons was 15, the number of output layer neurons was 1, the learning rate was 0.01, and it iterated 5000 times. For MKSVR, we used the SimpleMKL Toolbox (http://asi.insa-rouen.fr/enseignants/~arakoto/code/mklindex.html) to implement algorithms, and the multiple kernel function was composed of 32 different basis kernels including 28 Gaussian kernels with parameter \( \sigma \in \{0.01, 0.02, \ldots, 0.09, 0.1, 0.2, \ldots, 0.9, 1, 2, \ldots, 9, 10\} \) and 4 polynomial kernels with parameter \( s \in \{1, 2, 3, 4\} \).

The detailed steps of the procedure we followed are listed as follows:

**Step 1**: Import the pre-prepared dataset of grain storage parameters.

**Step 2**: Divide the whole dataset into the training (80%) and test (20%) sets randomly.

**Step 3**: Train the MLR model, ANN model, SKSVR model (by PSO algorithm), and MKSVR model (by SimpleMKL algorithm) with the training set.

**Step 4**: Use the test set to test the performances of the MLR model, ANN model, SKSVR model, and MKSVR model.

**Step 5**: Repeat steps 2–5 until the number of experiment repetitions is reached (20 times).

3.3. Comparison Results

Our experimental results from 20 experiments are shown in Table 3. The average values of MAE, MAPE, and RMSE for each algorithm were computed and are shown with the form of average ± standard deviation (SD). For each criterion, the algorithm with the minimum average and SD is considered to be the best on this criterion.

| Algorithm | MAE      | MAPE (%) | RMSE     |
|-----------|----------|----------|----------|
| MLR       | 1.359 ± 0.172 | 7.595 ± 0.953 | 1.702 ± 0.173 |
| BPNN      | 0.431 ± 0.093  | 2.531 ± 0.552  | 0.574 ± 0.132  |
| SKSVR     | 0.475 ± 0.053  | 2.804 ± 0.310  | 0.600 ± 0.055  |
| MKSVR     | 0.341 ± 0.038  | 2.026 ± 0.237  | 0.442 ± 0.037  |

As can be seen in Table 3, the MKSVR model proposed in this paper achieves the best results. Compared with the MLR, BPNN, and SKSVR, the average predicting errors of MKSVR were improved. Compared with the MLR model, MAE dropped by 1.018, MAPE dropped by 5.569%, and RMSE dropped by 1.260. Compared with the BPNN model, MAE decreased by 0.090, MAPE decreased by 0.505%, and RMSE decreased by 0.132. Compared with the SKSVR model, MAE decreased by 0.134, MAPE decreased by 0.778%, and RMSE decreased by 0.132. Although the average values of each
criterion of BPNN were slightly smaller than SVR, the SD of each criterion of BPNN was higher than that of SVR. By considering both the average and the SD of each criterion, the performance of SKSVR and BPNN are very similar, and are at an acceptable level. However, the MLR model shows extremely poor performance for each criterion.

By analyzing Table 2, we find that the MKSVR prediction model is superior to the SKSVR and BPNN models, as well as the MLR models, and it can better predict the FFA content of grain during storage. As can be seen from the SD, the prediction model also has better accuracy and robustness.

4. Discussion

In China, grains are usually stored for 3–5 years after harvest. During the period of storage, the quality of the grains will decline over time. Grain quality is affected by many physical and biological factors during storage [33,55]. An increase of FFA content in stored grain has been observed during storage, which is related to the temperature distribution—the higher the storage temperature, the faster the fatty acid value increases [5,56]. Figure 6 shows the temperature distribution of a cross section of the stored grain on 26 July 2018 in Section 2.4. It can be clearly seen that a “cold core” similar to that in Figure 3 is formed inside the stored grain pile, which leads to significant differences in FFA content. In view of the effect of temperature on FFA accumulation, we included the effective accumulated temperature of grain storage as the input feature of ML, for the reason that the effect of temperature on FFA accumulation can be considered as reducing the error of the prediction results. The theory of accumulated temperature has been widely used in many fields [57–59]. The value of threshold temperature has a crucial significance [58,60], so we take the developmental zero temperature of the biological entities including insects and molds inside the stored grain as the threshold temperature in this paper.

![Figure 6](image-url) Temperature distribution of stored grain as a cross section on 26 July 2018. The upper left corner is the schematic diagram of the selected cross section.

In fact, we obtained little data of the FFA content in stored grain because of the sparsity of sample locations, which are not representative of all stored grain in a granary. In such cases, temperature sensors arranged inside the grain pile are invaluable assets for the estimation of grain quality. Generally, the number of temperature sensors is much larger than that of sample locations. For example, a total of 417 sensors were arranged (one temperature and humidity sensor, and 416 temperature sensors); however, there were only 72 locations when sampling. Therefore, a wider range of grain quality monitoring can be achieved through the temperature sensors, and continuous monitoring can be conducted. Sampling consumes labor, and the subsequent quality determination still requires a lot of manpower and material resources.
Prior to this, researchers have established mathematical regression models between FFA and storage time for FFA estimation during grain storage [19,20], but these models are not very applicable once storage conditions change. To solve the problem associated with traditional mathematical methods not being able to fully reveal the essential characteristics of the grain during storage, our aim was to train the storage data set using ML to predict the FFA in stored grain. This work, of course, depends on the data set collected, that is, if the data set is larger, we typically obtain a better model in the case of selecting input features appropriately; then, we can obtain a good prediction effect on any given storage factors. The results from this paper demonstrate the applicability of the MKSVR model in realizing the real-time monitoring of grain quality changes, which can reduce any economic losses caused by grain quality reductions.

5. Conclusions

Here, we proposed an MKSVR approach for FFA estimation during grain storage. To validate the performance of MKSVR, ANN, MLR, and SKSVR were also applied to the FFA estimation. The performance of models was assessed by MAE, RMSE, and MAPE. All of the experiments were conducted using real data. The experimental results showed that the proposed MKSVR model outperformed the other models when estimating FFA content in stored grain. The smallest mean value of MAE was 0.341 mg KOH/100 g, the smallest RMSE was 0.442 mg KOH/100 g, and the smallest MAPE was 2.026%. The proposed MKSVR method integrates linear and nonlinear relations between FFA content and storage factors, effectively improving the predictive power and robustness of the model. Specifically, it provides technical support for the precise control of the stored grain quality and also plays a certain role in the management of grain storage.

In further study, there is a need to formulate a model that is more practical to suit the full range of grain types and qualities. This requires a larger number of samples and a greater number of independent variables in the analysis. We will collect more grain storage data, such as weather conditions, aeration, and humidity, and increase the number of input feature parameters of the model to improve its accuracy. We will analyze the influence of the collected characteristic parameters on fatty acid accumulation, then select characteristic parameters with a significant influence to retrain the model to try to improve the models.

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References

1. Alexander, P.; Brown, C.; Arneth, A.; Finnigan, J.; Moran, D.; Rounsevell, M.D. Losses, inefficiencies and waste in the global food system. Agric. Syst. 2017, 153, 190–200. [CrossRef] [PubMed]
2. Sasson, A. Food security for Africa: An urgent global challenge. Agric. Food Secur. 2012, 1, 2. [CrossRef]
3. FAO. Food Waste Footprint Full-Cost Accounting; FAO: Rome, Italy, 2014.
4. Tipples, K.H. Quality and nutritional changes in stored grain. In Stored Grain Ecosystems; Marcel Dekker: New York, NY, USA, 1995; pp. 325–351.
5. Yasumatsu, K.; Moritaka, S. Fatty Acid Compositions of Rice Lipid and their Changes during Storage. Agric. Biol. Chem. 1964, 28, 257–264. [CrossRef]
6. Genkawa, T.; Uchino, T.; Inoue, A.; Tanaka, F.; Hamanaka, D. Development of a low-moisture-content storage system for brown rice: Storability at decreased moisture contents. Biosyst. Eng. 2008, 99, 515–522. [CrossRef]
7. Jiang, H.; Liu, T.; He, P.; Chen, Q. Quantitative analysis of fatty acid content during rice storage based on olfactory visualization sensor technology. *Sens. Actuators B Chem.* 2020, 309, 127816. [CrossRef]

8. Srikaeo, K.; Panya, U. Efficiencies of Chemical Techniques for Rice Grain Freshness Analysis. *Rice Sci.* 2013, 20, 292–297. [CrossRef]

9. Teo, C. On the roles of protein and starch in the aging of non-waxy rice flour. *Food Chem.* 2000, 69, 229–236. [CrossRef]

10. Zhou, Z.; Robards, K.; Hellwell, S.; Blanchard, C.; Baxterb, G. Rice Ageing. I. Effect of Changes in Protein on Starch Behaviour. *Starch-Stärke* 2003, 55, 162–169. [CrossRef]

11. Liu, L.; Waters, D.L.E.; Rose, T.J.; Bao, J.; King, G.J. Phospholipids in rice: Significance in grain quality and health benefits: A review. *Food Chem.* 2013, 139, 1133–1145. [CrossRef]

12. Manjula, J.; Singaravadivel, K.; Sureshkumar, K. Quality changes of Paddy stored in three types of godown (Grain Care Project). *J. Chem. Biol. Phys. Sci.* 2019, 9. [CrossRef]

13. Gras, P.W.; Bason, M.L.; Esteves, L.A.; Sabio, G.C.; Annis, P.C.; Graver, J.E.v.S. Quality changes in maize stored in sealed bag stacks. *J. Stored Prod. Res.* 1990, 26, 199–206. [CrossRef]

14. Nikolić, N.; Radulović, N.; Momcilović, B.; Nikolić, G.; Lazić, M.; Todorovic, Z. Fatty acids composition and rheology properties of wheat and wheat or white or brown rice flour mixture. *Eur. Food Res. Technol.* 2008, 227, 1543–1548. [CrossRef]

15. Koczor, P.; Lipińska, E.; Czerniawska-Piłatowska, E.; Mikula, M.; Bartyzel, B.J. The change of fatty acids composition of Polish biscuits during storage. *Food Chem.* 2016, 202, 341–348. [CrossRef] [PubMed]

16. Mazurek, B.; Chmiel, M.; Górecka, B. Fatty Acids Analysis Using Gas Chromatography-Mass Spectrometer Detector (GC/MSD) Method Validation Based on Berry Seed Extract Samples. *Food Anal. Methods* 2017, 10, 2868–2880. [CrossRef]

17. Park, C.E.; Kim, Y.S.; Park, K.J.; Kim, B.K. Changes in physicochemical characteristics of rice during storage at different temperatures. *J. Stored Prod. Res.* 2012, 48, 25–29. [CrossRef]

18. Kechkin, I.A.; Ermolaev, V.A.; Ivanov, M.V.; Romanenko, A.I.; Gurkovskaya, E.A. Dependence of fat acidity value on wheat grain storage conditions. *BIO Web Conf.* 2020, 17, 00107. [CrossRef]

19. Alencar, E.R.d.; Faroni, L.R.D.; Peternelli, L.A.; Silva, M.T.C.d.; Costa, A.R. Influence of soybean storage conditions on crude oil quality. *Revista Brasileira de Engenharia Agrícola e Ambiental* 2010, 14, 303–308. [CrossRef]

20. Junka, N.; Rattanamechaikul, C.; Wongs-Aree, C. Free Fatty Acid Deformation of Treated Black Glutinous Rice During Storage by Fluidization Drying. *J. Food Process Eng.* 2016, 40, e12427. [CrossRef]

21. Igne, B.; Rippke, G.R.; Hurburgh, C.R. Measurement of Whole Soybean Fatty Acids by Near Infrared Spectroscopy. *J. Am. Oil Chem. Soc.* 2008, 85, 1105–1113. [CrossRef]

22. Liu, X.; Li, B.; Shen, D.; Cao, J.; Mao, B. Analysis of Grain Storage Loss Based on Decision Tree Algorithm. *Procedia Comput. Sci.* 2017, 122, 130–137. [CrossRef]

23. Shen, Y.; Zhou, H.; Li, J.; Jian, F.; Jayas, D.S. Detection of stored-grain insects using deep learning. *Comput. Electron. Agric.* 2018, 145, 319–325. [CrossRef]

24. Escamilla-García, A.; Soto-Zarazúa, G.M.; Toledano-Ayala, M.; Rivas-Araiza, E.; Castelúm-Barrios, A. Applications of Artificial Neural Networks in Greenhouse Technology and Overview for Smart Agriculture Development. *Appl. Sci.* 2020, 10, 3835. [CrossRef]

25. Dimilola, S. A Review of Unsupervised Artificial Neural Networks with Applications. *Int. J. Comput. Appl.* 2019, 181, 22–26. [CrossRef]

26. Vapnik, V.N. *The Nature of Statistical Learning Theory*; Springer: New York, NY, USA, 1995. [CrossRef]

27. Xiao, J.; Wei, C.; Liu, Y. Speed estimation of traffic flow using multiple kernel support vector regression. *Phys. A Stat. Mech. Appl.* 2018, 509, 989–997. [CrossRef]

28. Gönen, M.; Alpaydın, E. Multiple Kernel Learning Algorithms. *J. Mach. Learn. Res.* 2011, 12, 2211–2268.

29. Wang, H.-Q.; Sun, F.-C.; Cai, Y.-N.; Chen, N.; Ding, L.-G. On Multiple Kernel Learning Methods. *Acta Autom. Sin.* 2010, 36, 1037–1050. [CrossRef]

30. Pomeranz, Y.; Zeleny, L. Biochemical and functional changes in stored cereal grains. *Crit. Rev. Food Technol.* 1971, 2, 45–80. [CrossRef]
31. Fourar-Belaifa, R.; Fleurat-Lessard, F.; Bouznad, Z. A systemic approach to qualitative changes in the stored-wheat ecosystem: Prediction of deterioration risks in unsafe storage conditions in relation to relative humidity level, infestation by *Sitophilus oryzae* (L.), and wheat variety. *J. Stored Prod. Res.* 2011, 47, 48–61. [CrossRef]

32. Nagel, C.M.; Semeniuk, G. Some Mold-Induced Changes in Shelled Corn. *Plant Physiol.* 1947, 22, 20–33. [CrossRef]

33. Wu, Z.D.; Zhang, Q.; Yin, J.; Wang, X.M.; Zhang, Z.J.; Wu, W.F.; Li, F.J. Interactions of Multiple Biological Fields in Stored Grain Ecosystems. *Sci. Rep.* 2020, 10, 9302. [CrossRef]

34. Serna-Saldivar, S.O. Storage of Cereal Grains and Detrimental Effects of Pests. In *Cereal Grains*; CRC Press: Boca Raton, FL, USA, 2012; pp. 133–150. [CrossRef]

35. Christensen, C.M. Storage of Cereal Grains and Their Products; American Association of Cereal Chemists: Saint Paul, MN, USA, 1974. [CrossRef]

36. Boser, B.E.; Guyon, I.M.; Vapnik, V.N. A training algorithm for optimal margin classifiers. In *Proceedings of the Fifth Annual Workshop on Computational Learning Theory-COLT’92*, Pittsburgh, PA, USA, 27–29 July 1992.

37. Smola, A.J.; Schölkopf, B. A tutorial on support vector regression. *Stat. Comput.* 2004, 14, 199–222. [CrossRef]

38. Awad, M.; Khanna, R. Support Vector Regression. In *Efficient Learning Machines: Theories, Concepts, and Applications for Engineers and System Designers*; Apress: Berkeley, CA, USA, 2015; pp. 67–80. [CrossRef]

39. Platt, J. Sequential Minimal Optimization: A Fast Algorithm for Training Support Vector Machines. 1998. Available online: https://www.microsoft.com/en-us/research/publication/sequential-minimal-optimization-a-fast-algorithm-for-training-support-vector-machines/ (accessed on 19 September 2020).

40. Brereton, R.G.; Lloyd, G.R. Support Vector Machines for classification and regression. *Analyst* 2010, 135, 230–267. [CrossRef] [PubMed]

41. Yu, H.; Chen, Y.; Hassan, S.; Li, D. Dissolved oxygen content prediction in crab culture using a hybrid intelligent method. *Sci. Rep.* 2016, 6. [CrossRef] [PubMed]

42. Bansal, S.; Roy, S.; Larachi, F. Support vector regression models for trickle bed reactors. *Chem. Eng. J.* 2012, 207–208, 822–831. [CrossRef]

43. Damoulas, T.; Girolami, M.A. Probabilistic multi-class multi-kernel learning: On protein fold recognition and remote homology detection. *Bioinformatics* 2008, 24, 1264–1270. [CrossRef]

44. Yu, C.; Lam, K.C. Applying multiple kernel learning and support vector machine for solving the multicriteria and nonlinearity problems of traffic flow prediction. *J. Adv. Transp.* 2012, 48, 250–271. [CrossRef]

45. Lanckriet, G.R.G.; Cristianini, N.; Bartlett, P.; Ghahoui, L.E.; Jordan, M.I. Learning the Kernel Matrix with Semidefinite Programming. *J. Mach. Learn. Res.* 2004, 5, 27–72.

46. Lee, W.-J.; Verzakov, S.; Duin, R.P.W. Kernel Combination Versus Classifier Combination. In *Multiple Classifier Systems*; Springer: Berlin/Heidelberg, Germany, 2007; pp. 22–31. [CrossRef]

47. Yeh, C.-Y.; Huang, C.-W.; Lee, S.-J. A multiple-kernel support vector regression approach for stock market price forecasting. *Expert Syst. Appl.* 2011, 38, 2177–2186. [CrossRef]

48. Rakotomamonjy, A.; Bach, F.; Canu, S.; Grandvalet, Y. SimpleMKL. *J. Mach. Learn. Res.* 2008, 9, 2491–2521.

49. Liu, X.; Wang, L.; Yin, J.; Liu, L. Incorporation of radius-info can be simple with SimpleMKL. *Neurocomputing* 2012, 89, 30–38. [CrossRef]

50. Salomon, D. Linear Interpolation. In *The Computer Graphics Manual*; Salomon, D., Ed.; Springer: London, UK, 2011; pp. 483–503. [CrossRef]

51. Duan, S.; Yang, W.; Wang, X.; Mao, S.; Zhang, Y. Forecasting of grain pile temperature from meteorological factors using machine learning. *IEEE Access* 2019, 7, 130721–130733. [CrossRef]

52. Liu, H.; Cocea, M. Semi-random partitioning of data into training and test sets in granular computing context. *Granul. Comput.* 2017, 2, 357–386. [CrossRef]

53. Cherkassky, V.; Ma, Y. Practical selection of SVM parameters and noise estimation for SVM regression. *Neural Netw.* 2004, 17, 113–126. [CrossRef]

54. Kennedy, J.; Eberhart, R. Particle swarm optimization. In *Proceedings of the ICNN’95-International Conference on Neural Networks*, Perth, Australia, 27 November–1 December 1995; pp. 1942–1948.

55. Manandhar, A.; Milindi, P.; Shah, A. An Overview of the Post-Harvest Grain Storage Practices of Smallholder Farmers in Developing Countries. *Agriculture* 2018, 8, 57. [CrossRef]

56. Liu, K.; Li, Y.; Chen, F.; Yong, F. Lipid oxidation of brown rice stored at different temperatures. *Int. J. Food Sci. Technol.* 2016, 52, 188–195. [CrossRef]
57. Mei, J.; Wei, D.; Li, Q.; Li, J.; Qian, W. Effective accumulated temperature is associated with the efficiency of hybrid ovary culture between *Brassica napus* and *B. oleracea*. *Acta Physiol. Plant.* 2015, 37, 18. [CrossRef]

58. Ma, L.-Q.; Gao, S.-J.; Wen, J.-B.; Zong, S.-X.; Xu, Z.-C. Effective accumulated temperature and developmental threshold temperature for *Semanotus bifasciatus* (Motschulsky) in Beijing. *For. Stud. China* 2008, 10, 125–129. [CrossRef]

59. Xu, M.; Li, Z. Accumulated temperature changes in desert region and surrounding area during 1960–2013: A case study in the Alxa Plateau, Northwest China. *Environ. Earth Sci.* 2016, 75, 1276. [CrossRef]

60. Damos, P.; Savopoulou-Soultani, M. Temperature-Driven Models for Insect Development and Vital Thermal Requirements. *Psyche A J. Entomol.* 2012, 2012, 123405. [CrossRef]

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