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A Novel Ensemble Method for Predicting Wheat Yield Using Feature Selection-based Deep Learning and Hyperspectral Vegetation Indices

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Abstract

Background: Wheat is an important food crop globally, and timely prediction of wheat yield in breeding efforts can improve the efficiency of selection. Traditional plant breeding based on grain yield selection is time-consuming, costly, and destructive. There is a great need for innovative methods to enhance efficiency and accelerate genetic gains in the breeding cycle.

Results: In this study, a new ensemble learning method was developed to predict wheat yield by combining hyperspectral data and deep learning-based regression technology. For this, 207 wheat cultivars and breeding lines were grown under full and limited irrigation treatments, and their canopy hyperspectral reflectance was measured at the flowering, early grain fill (EGF), mid grain fill (MGF), and late grain fill (LGF). Firstly 115 vegetation indices (VIs) were extracted from the hyperspectral

reflectance and combined with four feature selection methods i.e., mean decrease impurity (MDI), Boruta, FeaLect, and Relief to train deep neural network (DNN) models for yield prediction. Then, a novel ensemble learning framework was developed by combining the predicted values of selected and the full features using multiple linear regression (MLR). The results show that feature selection methods achieved higher yield prediction accuracy than the full features, where MDI method performed best across growth stages, with the mean R^2 ranging from 0.634-0.666 (mean RMSE = 0.926-0.967 t ha⁻¹). The proposed ensemble method outperformed all the FS methods across growth stages, with the mean R^2 ranging from 0.648-0.679 (mean RMSE = 0.911-0.950 t ha⁻¹).

Conclusions: By integrating multiple FS methods and DNN, more prediction potential of hyperspectral data can be exploited, and this ensemble method is also applicable to trait estimation of other crops.

Keywords: wheat yield; hyperspectral; vegetation index; deep neural network; feature selection

Background

Declining crop yields due to climate change and global population growth are putting the global food supply at risk [1, 2]. The development of a large number of superior resistant varieties through plant breeding efforts is an immediate solution. In most cases, improving yields is the primary goal of crop breeding programs [3]. However, yield is influenced by both quantitative and qualitative traits, and measuring yield in large breeding populations consisting of thousands of genotypes can be time-consuming and laborious [3-5]. Secondary traits can help breeders predict grain yield at early stages to reduce the time and cost [6], while the traditional manual-based trait survey methods are still inefficient. In

55 recent years, developments in remote sensing and spectroscopy sensor
56 technologies have helped to establish low-cost, high-throughput
57 phenotyping platforms (HTPP) that can collect large amounts of data
58 related to yield at different stages under various growth environments in
59 breeding efforts [4, 6-8].

60 The spectroscopy science of agriculture is based on the ability to
61 measure different wavelengths of electromagnetic energy interacting with
62 different parts of a growing plant [8]. The goal of spectral science is to
63 quantify phenotypes through interactions between light and plants, such
64 as reflected, absorbed, transmitted, and/or emitted photons [8].
65 Commonly used sensors in precision agriculture are hyperspectral, RGB,
66 multispectral, and thermal [9-12]. Compared to other sensors,
67 hyperspectral sensors with a large number of continuous bands have been
68 successfully applied to estimate crop parameters including yield, biomass,
69 leaf area index (LAI), and chlorophyll content [13-15]. In addition to the
70 raw bands, hyperspectral data can also be derived from integer and
71 fractional order derivatives to reveal more hidden information related to
72 crop growth [15, 16]. The reflectance of electromagnetic energy at
73 different wavelengths is usually summarized as the vegetation index [8],
74 which is further used to predict physiological problems or agronomic
75 traits of plants. Related studies combined a large number of vegetation
76 indices in various wavelength regions to assess crop parameters [15,17],
77 and different VIs can complement each other to provide more information
78 related to plant growth.

79 Parsing large data sets acquired by high-throughput phenotyping
80 platforms requires intensive computational and statistical analysis, which
81 remains a challenge in plant breeding programs [18]. Nowadays, many

82 statistical and machine learning-based regression techniques, such as
83 support vector regression (SVR), random forest regression (RFR) and
84 extreme learning machines (ELM), have been applied to build predictive
85 models for plant traits and achieve accurate predictions [15,19-21]. As a
86 subfield of machine learning, deep learning can automatically learn
87 representations from data using multi-layer architecture [22]. The
88 architecture supports complex nonlinear functions, which are learned
89 from the hierarchical output of the previous layers [22]. Deep learning
90 methods such as convolutional neural network (CNN), deep neural
91 network (DNN), and residual neural network (ResNet) have yielded
92 higher accuracy in various regression and classification tasks in the field
93 of precision agriculture [23-25].

94 To obtain accurate yield predictions and avoid model overfitting,
95 machine learning algorithms benefit from using feature selection (FS)
96 methods to reduce the redundancy of the data [26]. FS methods such as
97 recursive feature elimination (RFE), Pearson correlation coefficient
98 (PCC), random forest-based mean decrease impurity (MDI) and Partial
99 least squares based variable importance in the projection (VIP) methods
100 have been used in estimating crop parameters ranging from alfalfa and
101 soybean yield prediction to sorghum leaf chlorophyll concentration
102 estimation [3, 16, 17]. Each FS method has its unique focus, and most
103 studies have utilized only an individual FS method for modeling, which
104 inspired us to combine the characteristics of multiple FS methods.
105 Ensemble learning such as stacking regression is gaining a lot of attention
106 in the machine learning community. Ensemble models usually achieve
107 better prediction results than individual models [17, 27, 28]. During the
108 process of ensemble learning, a set of basic individual learners is first

used for training, and then the predictions of all learners are combined to make the final prediction. In general, heterogeneity among basic learners motivates the accuracy-improving effect of ensemble models [29]. Similarly, there are differences in the features selected by various FS methods, resulting in heterogeneity among the output predictions, and combining multiple FS methods in a stacking pattern has the potential to obtain higher prediction accuracy than individual FS methods and full features.

Based on the above descriptions, the main objectives of this study are: (1) to explore the potential application of hyperspectral data and DNN in predicting wheat yield, (2) to compare the yield prediction accuracy of individual feature selection methods and proposed ensemble method, and (3) to identify the optimal stage for acquiring hyperspectral data at late wheat growth.

Materials and Methods

Experimental design

Fig. 1 Test site location.

This study adopted a diverse panel of 207 varieties. During growing season 2018-2019, all accessions were cultivated at the research station of

Chinese Academy of Agricultural Sciences (CAAS) at Xinxiang (35°18'N, 113°51'E; Henan Province, China) (Fig. 1) under two water irrigation levels, full and limited irrigation. The field experiments were set up in randomized complete blocks with two replications. Each plot was 4.2 m² in size, with dimensions of 3 m×1.4 m and six rows with 0.2 m spacing. At the tillering stage, both the full and limited irrigation treatments received 250 mm of water, with irrigation continuing for the full irrigation treatment at the early jointing, heading, and early grain filling stages. The application of fertilizer was optimized based on the soil conditions in the area. All plants were harvested at physiological maturity using the combined harvester. Grain yield was measured at a 12.5% grain moisture level. The overall flow of this study is shown in Fig. 2.

Fig. 2 Overall workflow conducted in this study.

MDI, mean decrease impurity; EGF, early grain fill; MGF, min grain fill; LGF, late grain fill; *P*, model predictions.

Hyperspectral data acquisition and processing

A high-spectral-resolution spectrometer (Fieldspec 3, Analytical Spectral Devices ASD, Boulder, CO, USA) connected with a 25° field of view fiber optic was used to collect the canopy reflectance parameters of each plot from 400 to 2500 nm. The visible-to-near-infrared range (350-1000nm) had a spectral resolution of 3 nm, while the shortwave infrared region had a spectral resolution of 10 nm (1000-2500 nm). The sensor was placed 100 cm above the canopy in a nadir position and operated vertically. Canopy reflectance was measured at four separate

sites in each plot between 11:00 a.m. and 1:00 p.m. local time on a clear day. For each site, ten readings were taken, and the average of these 40 readings was used to calculate the canopy reflectance of the plot. Before measuring canopy reflectance, a BaSO₄ calibration panel was used to estimate incoming radiation and reflectance. This process was done every ten plots. Spectral measurements were carried out at flowering, early grain fill (EGF), mid grain fill (MGF), and late grain fill (LGF). View Spec software (ASD Inc, Boulder, CO, USA) was used to eliminate noise from spectral curves, calculate the average of numerous spectral curves, and generate a reflectance file. To overcome the noise probability during the spectrum collecting process, the adaptive degree polynomial filter (ADPF) was used. ADPF adds a statistical heuristic to the Savitzky-Golay method to improve signal fidelity while reducing statistical noise. Following filtering, a database of 115 vegetation indices (Table S1) was created as input features to the yield prediction model.

Deep neural network

The deep neural network (DNN) has been increasingly applied to solve regression problems in various fields of research [23, 30-31]. The schematic diagram of DNN is shown in Fig. 3. DNN generally consists of an input layer, several hidden layers, and an output layer [32]. The number of features corresponds to the neurons (units) in the input layer. The hidden layer neurons perform nonlinear transformations of the original input attributes. The number of output neurons depends on the number of response variables that are predicted for continuous response variables (grain yield in this study), and it receives the output of the hidden neurons as input and produces the associated predicted values as output.

Fig. 3 A schematic diagram of the deep neural work.

w , weight; h , hidden layer.

Screening for appropriate hyperparameters is a key step in the successful implementation of deep learning models. The grid search method was applied to tune the hyperparameters. Through the literature [32], we set the following parameters: The units values used for the grid search were 50 to 150 in increments of 10, and for the hidden layers we used 3, 4, 5 and 6. The regularization method "dropout" was used to randomly remove a subgroup of hidden neurons and their connections. The activation function applied was the rectified linear activation unit (RELU) function. All DNN models were built in R software with the "h2o" package.

Feature selection method

Mean Decrease Impurity (MDI)

MDI is a random forest-based FS method. The random forest utilizes randomized decision trees and impurity measurements to calculate the

importance of various features [33]. When the random forest employs the Gini index as its impurity measurement, one such technique is known as mean decrease impurity (MDI). Breiman (2001) presented to estimate the importance of a variable k for predicting y (i.e., grain yield) by cumulate the weighted impurity decreases ($p(t) \Delta i(s_t, t)$) for all nodes t where k is used and averaged over all N_T trees in the forest as in the following equation:

$$MDI_k = \frac{1}{N_T} \sum_T \sum_{t \in T: v(s_t)=k} p(t) \Delta i(s_t, t) \quad (1)$$

where $p(t)$ represents the proportion Nt/N of sample reaching t , and $v(s_t)$ represents the variable used in split s_t .

Boruta

Boruta is a wrapper method developed based on the random forest algorithm. The principle of Boruta is different with MDI method. The Boruta algorithm is an extension of the idea proposed by [34]. The significant input parameters are defined by comparing the correlation between the real features and the random probes. Boruta calculates the Z-scores for each input predictor concerning the shading attribute [35]. The significant factors of the predictors are determined by the distribution of the Z-score indicators. Based on the significant factors determined by Boruta, a minimum optimal FS strategy was used, by ranking and residuals, followed by stepwise modeling. The outlined Boruta algorithm is as follows [11]: (a) The eigenvalues of each feature matrix consisting of the independent and dependent variables are shuffled to obtain shadow features, and then the true and shadow features are combined to form a new feature matrix for training. (b) Inputting the newly constructed feature matrix to obtain the trained feature importance model. (c)

Calculate the scores of the real and shadow features and determine the maximum Z-score of the shadow features. (d) The real features with scores greater than the maximum Z-score were classified as important factors, while the real features with scores significantly less than the maximum Z-score were classified as unimportant factors. Repeat steps (a)-(d) until the importance of all feature attributes is marked as "important" or "not important". In this study, the importance ranking was based on the average Z-score score of each feature.

FeaLect

FeaLect is a FS method proposed by [36] based on combinatorial analysis of LASSO. Set B be a random sample of size m , generated by selecting without replacement from the given training data D , where $n = |D|$ and $\gamma \in (0,1)$ represents a parameter that controls the size of sample set. The Lars algorithm is applied to efficiently recover the entire regularization path using training set B . Let F_k^B be the set of selected features by the Lasso when λ allowing the selection of k features. The number of selected features is decreasing in λ and we get the formula:

$$\emptyset = F_0^B \subset \dots F_k^B \subset F_{k+1}^B \subset \dots \subset F_d^B = F \quad (2)$$

For each feature f , a scoring mechanism was defined based on whether or not it is selected in F_k^B :

$$S_k^B(f) := \begin{cases} \frac{1}{k} & \text{if } f \in F_k^B \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

The above randomized process is randomly cycled several times for various random subsets B to compute the average score of f when k features are selected. The sum of average scores is then used to calculate the total score for each feature:

$$S(f) := \sum_k \mathbb{E}_B[S_k^B(f)] \quad (4)$$

Relief

The Relief algorithm's central principle is to evaluate the quality of attributes with weights greater than the thresholds by comparing the value of an attribute between a given instance and the two nearest instances [37]. For the regression problem, a detailed procedure has been given [38]. The Relief algorithm is given by the following equation:

$$\Delta W(f) = -\frac{\text{diff}(f, R, H)}{m} + \frac{\text{diff}(f, R, M)}{m} \quad (5)$$

Where f and W represent the feature and weight, respectively. m and R represent the number of training data and target data, respectively. H and M represent the nearest neighbor of the target with same and opposite class, respectively.

Framework of ensemble feature selection

The proposed ensemble method based on DNN in this study draws on the verification pattern of the stacking ensemble method (Fig. 4). According to the importance ranking of each FS method, each feature is input to the DNN in turn until the training accuracy reaches the maximum, at which time the input features are considered the optimal combination of features, together with the full features, five deep neural network models are generated. The main steps for ensemble models applied in this study are as follows [39]:

(a) The original datasets of each FS method and full features are divided into a training dataset and test dataset in the ratio of 4:1;

(b) For each DNN model at level-1, the 5 fold cross-validation is used to train and output the val_pre dataset for the validation dataset and test_pre set for the test dataset in each fold. The val_pre sets are combined as the new training dataset and the test_pre sets are averaged as the new testset;

(c) The new training set is employed to train the ensemble feature selection by multiple linear regression (MLR) at level-2 through 5 fold cross-validation and to output the final prediction of new test dataset for each fold, and then averaged over them to obtain final predictions.

To avoid interference by chance, the above process was repeated 20 times, the average accuracy parameters of 100 tests generated in the cross-validation process are used to evaluate model performance.

Fig. 4 Structure of the ensemble learning model.

DNN, deep neural network; M, mean decrease impurity; B, Boruta; F, FeaLect; R, Relief; FF, full features; CV, cross-validation; MLR, multiple linear regression.

Model accuracy assessment parameters

Coefficient of determination (R^2) and root mean square error (RMSE) were used to evaluate the accuracy of the yield prediction model. The equations are as follow:

$$R^2 = 1 - \frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (6)$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{n}} \quad (7)$$

where y_i and $\hat{y}_i$ are the measured and the predicted grain yield, respectively. $\bar{y}$ is the mean of measured grain yield, and n is the total number of testing samples. A larger R^2 and a smaller RMSE indicates a stronger predictive capability of the model.

Statistical analysis

A mixed linear model was adopted to test the significance of variation between genotypes, irrigation treatments, and their interactions for measured and predicted grain yield. The equation of the model is as follows [40]:

$$Y = X\beta + Z\mu + \varepsilon \quad (8)$$

where Y is the response demonstrated by fixed effect (β) and random effect (μ) with random error (ε). X and Z denote fixed and random effects, respectively. Broad-sense heritability refers to the percentage of genetic variation to the total variation in the phenotype, with a value between 0 and 1. Heritabilities of 0 and 1 indicate that phenotypic variation is entirely influenced by environmental and genetic factors, respectively. Heritability was calculated by the following formula:

$$H^2 = \sigma_g^2 / (\sigma_g^2 + \sigma_\varepsilon^2 / r) \quad (9)$$

where r represents the number of replications per treatment; σ_g^2 and σ_ε^2 are the genotypic and error variances, respectively.

Results

Descriptive statistics of measured wheat yields

The descriptive statistics and distribution of measured yields from both irrigation treatments are shown in Fig. 5. The resulting mean yield values for the full and limited irrigation treatments were 9.64 and 7.79 t ha⁻¹, respectively. The yield under full irrigation treatment had a wider range of distribution with a higher standard deviation (1.43 t ha⁻¹) compared to limited irrigation treatment (1.11 t ha⁻¹). The results of the Shapiro-Wilk test ($P<0.05$) indicated that the yields under both irrigation treatments were normally distributed.

Fig. 5 Distribution of wheat yield in full and limited irrigation treatments.

Feature selection results

The 115 VIs were ranked using the MDI, Boruta, FeaLect, and Relief strategies, respectively. The detailed ranking of VIs is shown in Table S2-S5. The results show that there are differences in the ranking of VIs among the four FS methods. Meanwhile, the performance of some VIs was stable and excellent. For example, the Datt8, PWI, Datt7, DPI,

PRI, PRI_norm, mREIP, and REP_Li were ranked in the top 30 for all four FS methods at flowering (Table S2-S5). These better-performing indices form the basis for the model's outperformance.

Fig. 6 Deep neural network model training accuracy as a function of the number of features.

MDI, mean decrease impurity; EGF, early grain fill; MGF, min grain fill; LGF, late grain fill.

Vegetation indices were iteratively added into the DNN model according to the ranking and updated the model training performance (R^2 and RMSE) until all 115 indices were included to further investigate the features with superior performance. With the input of more features, the training accuracy of DNN model first rose to the best and then slightly decreased (Fig. 6). The training accuracy of the MDI method was the highest at all measured stages. Furthermore, the MDI method can achieve the best prediction accuracy with the minimum number of features at early, mid, and late grain filling stages. The performances of the remaining FS methods were variable across the stages. For each FS method, the number of features that achieve the best training accuracy

was selected for the ensemble FS model development. The Venn diagrams (Fig. 7) are used to represent the number of features that are common and unique to multiple FS methods.

Fig. 7 The Venn diagram of selected features for each feature selection method. (a) flowering, (b) early grain fill, (c) mid grain fill, and (d) late grain fill.

Performance of yield prediction model

To validate the model adaptability, the DNN prediction accuracy of selected features, all features and ensemble method on the test set was analyzed, the accuracy statistics are shown in Fig. 8. For the FS methods of flowering, the MDI method yielded the highest mean R^2 of 0.636 (mean RMSE = 0.964 t ha⁻¹), followed by Boruta method (mean R^2 = 0.627, mean RMSE = 0.977 t ha⁻¹) and FeaLect method (mean R^2 = 0.617, mean RMSE = 0.990 t ha⁻¹). Compared to full features (mean R^2 = 0.604, mean RMSE = 1.006 t ha⁻¹), prediction accuracy of Relief was slightly

lower (mean $R^2 = 0.589$, mean RMSE = 1.030 t ha⁻¹). The best predictive performance of EGF was achieved by the MDI method with the mean R^2 value of 0.634 and a RMSE value of 0.967 t ha⁻¹, followed by the Boruta method (mean $R^2 = 0.612$, mean RMSE = 0.995 t ha⁻¹). It was also noted that the FeaLect method (mean $R^2 = 0.608$, mean RMSE = 1.001 t ha⁻¹) had a similar predictive result to the Relief method (mean $R^2 = 0.607$, mean RMSE = 1.003 t ha⁻¹). Full features yielded the lowest mean R^2 of 0.570 (mean RMSE = 1.046 t ha⁻¹). The best FS method of MGF was also achieved by MDI (mean $R^2 = 0.666$, mean RMSE = 0.926 t ha⁻¹), followed by Boruta (mean $R^2 = 0.658$, mean RMSE = 0.938 t ha⁻¹), Relief (mean $R^2 = 0.643$, mean RMSE = 0.958 t ha⁻¹), FeaLect (mean $R^2 = 0.639$, mean RMSE = 0.963 t ha⁻¹), and full features (mean $R^2 = 0.616$, mean RMSE = 0.992 t ha⁻¹). Differ from the first three stages, the FS method with the highest prediction accuracy at LGF was Boruta (mean $R^2 = 0.643$, mean RMSE = 0.957 t ha⁻¹), followed by MDI (mean $R^2 = 0.639$, mean RMSE = 0.962 t ha⁻¹). The prediction performance of methods FeaLect (mean $R^2 = 0.624$, mean RMSE = 0.982 t ha⁻¹), Relief (mean $R^2 = 0.627$, mean RMSE = 0.979 t ha⁻¹) and full features (mean $R^2 = 0.622$, mean RMSE = 0.985 t ha⁻¹) was similar. Compared to the individual FS method with the highest prediction accuracy, the ensemble method improved the mean R^2 value to 0.648, 0.650, 0.679 and 0.652 for flowering, EGF, MGF and LGF, respectively, also the values of RMSE had decreased (Fig. 8). In the process of the ensemble method, MDI contributed more and the regression coefficients assigned within MLR were higher in all periods (Fig. 9).

Fig. 8 The statistical distributions of the prediction accuracy of various FS and ensemble methods.

EGF, early grain fill; MGF, min grain fill; LGF, late grain fill.

Fig. 9 Mean value of regression coefficients assigned to each feature selection method.

EGF, early grain fill; MGF, min grain fill; LGF, late grain fill.

Analysis of yield prediction value

Predicted wheat yield was output using the ensemble method for both irrigation treatments. Wheat yield under full irrigation treatment was higher than that under limited irrigation treatment for all measured stages (Fig. 10). ANOVA (Table 1) revealed that genotypes, treatments, and genotype×treatment interactions had significant effects on predicted yield for all measured stages, which was consistent with the measured yield. Similar to measured yield ($H^2 = 0.63$), the H^2 of predicted yield was high, with the value of 0.73, 0.71, 0.77, and 0.62 for flowering, EGF, MGF, and LGF across two irrigation treatments, respectively, suggesting that most of the phenotypic variation was determined by genetic factors.

Fig. 10 Distribution of yield prediction values output by proposed ensemble method.

EGF, early grain fill; MGF, min grain fill; LGF, late grain fill.

Table 1 Analysis of variance for predicted grain yield output by ensemble feature selection method and measured grain yield.

Grain yield	F-value			H^2
	Genotype (G)	Treatment (T)	G×T interaction	
Flowering	5.27***	1789.08***	1.59***	0.73
EGF	5.43***	1487.70***	1.80***	0.71
MGF	6.60***	2334.92***	1.68***	0.77
LGF	4.64***	2050.94***	2.23***	0.62
Measured	3.43***	781.97***	1.44***	0.63

EGF, early grain fill; MGF, min grain fill; LGF, late grain fill.

Discussion

The application of canopy hyperspectral data to predict crop yields in precision agriculture management is not new [3, 14, 17]. The similarity of traits among a large number of breeding lines will lead to a heavy workload and make it difficult to perform accurate monitoring efforts [41]. The traditional method of collecting phenotypes reduces the efficiency of selecting superior breeding varieties [11]. Hyperspectral remote sensing method with high spectral resolution can obtain

continuous and fine spectral profiles of terrestrial objects at wide range wavelengths [42]. In contrast to RGB and multispectral data, hyperspectral data contains a wealth of information related to plant growth and can help detect minor differences between various breeding varieties [11].

Previous studies have shown that the full bands of hyperspectral reflectance achieved higher yield prediction accuracy than the VIs set [8, 14], but the ultra-high dimensionality of the full bands makes the program run much longer. Strong collinearity and information overlap among a large number of VIs composed of hyperspectral data, thus choosing the appropriate input features thus play an important role in reducing the dimensionality and improving the prediction accuracy. For this reason, four FS methods, and a newly proposed ensemble method were applied. The results showed that the MDI method performed better among four FS methods at all growth stages, which is consistent with previous study [16]. MDI score is computed based on node impurity, which is a measure of homogeneity of the variable [16]. Our selected vegetation indices used a wide band interval, which makes a lot of vegetation indices vary widely from each other. In addition, since MDI is a tree-based scoring measure, the problem of multicollinearity was avoided, the features selected are simple and efficient [16]. Compared to MDI, only a few have investigated the effectiveness of Boruta in estimating crop parameters [11, 43]. The Boruta method in this study showed a predictive performance second only to MDI (Flowering, EGF and MGF) or comparable to MDI (LGF). The excellent performance of MDI and Boruta methods proved the usefulness of random forest algorithms in selecting features. The Fealect method has only been used in the diagnosis of lymphoma and has

shown satisfactory classification results [36], and this study is the first to deal with the regression problem. FeaLect showed better prediction results than Relief and full features and could be widely used to investigate its potential in estimating crop parameters. The Relief method performs the worst, this is probably a result that Relief was initially designed to deal with binary classification problems and has been applied to select features in classification problems in most subsequent studies [44-46]. The advantage of the Relief method is that it does not require training, which helps to save program running time. As a deep learning method, DNN has shown high prediction accuracy in assessing crop yields and has advantages in handling large samples of complex nonlinear data [23]. Although DNNs are generally considered to be good at extracting information from raw features, this study suggests that feature engineering in deep learning is still beneficial. The feature selection in deep learning has also been performed by previous report when combining remote sensing data and DNN to predict crop yield [24].

Different FS methods may yield feature subsets that can be considered as local optima in the feature subset space, while ensemble FS can combine the local optima in each feature subset space to obtain a better model performance. The ensemble FS method proposed by [47] selected the top-ranked features of multiple FS methods but ignored the heterogeneity of each FS method and the diversity of features. A new ensemble FS method based on the stacking regression was proposed in this study. The results showed that the ensemble method improved prediction accuracy at all growth stages and gave good predictions of wheat yield, and the significant differences between treatments and varieties indicated the practical value of the proposed ensemble method in

screening target varieties (Table 1). Overall, the newly proposed ensemble method maximizes the potential of the huge VIs dataset for crop yield predicting, allowing the best yield trait-related information to be fully utilized. Meanwhile, the unsatisfactory performance of Relief inspires future research to try to combine more model training-based FS methods, such as Recursive Feature Elimination (RFE) and Variable Importance in Projection (VIP), to explore a more reasonable combination of multi-FS methods. To verify the adaptability of the proposed ensemble method, the experiments will be conducted on other crops for future analyses.

Winter wheat canopy display different structural properties during the growth cycle, which affects the optical signal at different growth stages [48]. Therefore, the difference in collection time may lead to some prediction errors of winter wheat yield. The middle and late stages of wheat growth were proven to have higher yield prediction accuracy compared to the early stages [9, 19]. Our results indicate that the MGF achieved the highest prediction accuracy, which can help to save the number of data collection and reduce the cost.

Conclusions

Pre-harvest insight to yield can help reduce breeding efforts and optimize field management practices. The use of remote sensing platforms to predict yield has been widely applied, which is not only a fast way to collect data but also reduces labor costs and problems associated with destructive sampling. In our study, an ensemble method that combines multiple FS methods based on deep neural network (DNN) and hyperspectral vegetation indices was developed. The results indicated that mean decrease impurity (MDI) performs best in grain yield

prediction among the four FS methods at most measured stages, followed by Boruta, FeaLect, and Relief. The ensemble method outperformed all individual FS methods, and the highest accuracy was achieved at the mid grain filling (MGF) stage. Our study demonstrated the efficacy of using hyperspectral VIs and the proposed ensemble method for predicting wheat yield. For future work, comprehensive studies in different environments are still needed to validate the transferability of this ensemble method and to identify the best combination of FS methods.

Ethics approval and consent to participate

Not applicable.

Consent for publication

All authors agreed to publish this manuscript.

Availability of data and materials

All the data used in this study is available upon the approval of Dr. Yonggui XIAO from the Institute of Crop Sciences, Chinese Academy of Agricultural Sciences, China.

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Authors' contributions

S.F. and L.L. collected the data, S.F. analyzed the data and wrote the paper, Z.C. and Y.X. managed and directed the trial, Y.X. and Z.H. gave comments and suggestions to improve the manuscript. All authors have

read and agreed to the published version of the manuscript.

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