

# Rapid and Accurate Varieties Identification of Different Crop Seeds Under Sample-Limited Condition Based on Hyperspectral Imaging and Deep Transfer Learning

**Na Wu**

Zhejiang University

**Fei Liu**

Zhejiang University

**Yidan Bao**

Zhejiang University

**Mu Li**

Jilin Academy of Agricultural Sciences

**Wei Huang**

Jilin Academy of Agricultural Sciences

**Fanjia Meng**

China Agricultural University

**Chu Zhang**

Zhejiang University

**Yong He** (✉ [yhe@zju.edu.cn](mailto:yhe@zju.edu.cn))

Zhejiang University <https://orcid.org/0000-0001-6752-1757>

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## Research

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1 **Rapid and accurate varieties identification of different crop seeds under sample-lim-**  
2 **ited condition based on hyperspectral imaging and deep transfer learning**

3 Na Wu<sup>a</sup>, Fei Liu<sup>a</sup>, Yidan Bao<sup>a</sup>, Mu Li<sup>c</sup>, Wei Huang<sup>c</sup>, Fanjia Meng<sup>d</sup>, Chu Zhang<sup>a</sup>, Yong He<sup>a,b,\*</sup>

4 <sup>a</sup> College of Biosystems Engineering and Food Science, Zhejiang University, Hangzhou 310058, China

5 <sup>b</sup> State Key Laboratory of Modern Optical Instrumentation, College of Optical Science and Engineering,  
6 Zhejiang University, Hangzhou 310058, China

7 <sup>c</sup> Maize Research Institute, Jilin Academy of Agricultural Sciences, Gongzhuling 136100, China

8 <sup>d</sup> College of Information and Electrical Engineering, China Agricultural University, Beijing 100083, China

9 \* Corresponding Author at: College of Biosystems Engineering and Food Science, Zhejiang University,  
10 Hangzhou 310058, China.

11 E-mail: yhe@zju.edu.cn

12

13 **Abstract**

14 **Background:** Varieties identification of crop seeds is significant for breeders to screen out seeds with spe-  
15 cific traits and for market regulators to detect seeds purity. Hyperspectral imaging technology provides a fast  
16 and non-destructive means for varieties identification. And deep learning algorithm is suitable for effective  
17 analysis of redundant spectral data. However, deep learning algorithms have serious big data dependency,  
18 while collecting high-quality large-scale samples was high-cost in many cases. This made it difficult to build  
19 an accurate identification model. This study aimed to explore a rapid and accurate method for varieties iden-  
20 tification of different crop seeds under sample-limited condition based on hyperspectral imaging and deep  
21 transfer learning.

22 **Results:** Three deep neural networks with typical structures were designed based on a samples-rich Pea da-  
23 taset. Obtained the highest accuracy of 99.57 %, VGG-MODEL was transferred to classify four target da-  
24 taset (Rice, Oat, Wheat, Cotton) with limited samples. The accuracies of deep transferred model achieved  
25 95 %, 99 %, 80.8 %, and 83.86 % on the four datasets, respectively. Using training sets with different sizes,  
26 deep transferred model could always obtain higher performance than other traditional methods. Visualization  
27 of training process and classification results confirmed the portability of common features of seed spectra  
28 and provided an interpreted method for rapid and accurate varieties identification of crop seeds.

29 **Conclusions:** This study combined hyperspectral imaging and deep transfer learning to identify varieties of  
30 different crop seeds, which was proved to be efficient under sample-limited condition. This facilitated crop  
31 variety screening process under the scenario of sample scarcity. It also provided a new idea for the detection  
32 of other qualities of crop seeds based on hyperspectral imaging under sample-limited condition.

33 **Key words:** Hyperspectral imaging, Crop seeds, Deep learning, Transfer learning

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## 35 **Background**

36 High-quality seeds are conducive to continue excellent species and guarantee crop yield and quality.  
37 Due to the large differences of climate, soil, water resources in different regions, breeders have pointedly  
38 developed many crop varieties to adapt to the local planting environment. Growth rules, stress resistance and  
39 bio-chemical characteristics of different varieties crops vary greatly. For varieties that are still in breeding  
40 stage, screening a variety with specific traits often need to observe the phenotypic traits of the offspring  
41 plants, which is time-consuming and labor-intensive. As a seed carries all the genetic genes that develop into  
42 a plant, seed identification can be an alternative for screening variety with specific traits. For varieties that  
43 are already promoted widely, different varieties of seeds tend to be easily mixed with frequent circulation in  
44 the market. This makes the seed purity unable to be guaranteed. Conventionally, manual vision inspection  
45 method based on the external phenotypic traits of seeds, like color, texture and shape, is subjective and boring.  
46 The more accurate methods based on the internal biochemical properties of seeds, such as DNA molecular  
47 markers [1] and protein electrophoresis techniques [2], rely on chemical agents and complex operation. Ac-  
48 cordingly, it is necessary to develop a fast and accurate method for varieties identification of crop seeds.

49 As hyperspectral imaging (HSI) can obtain spectral and spatial location information simultaneously  
50 during one scan, it has the capability of probing the internal and external phenotypic traits of samples rapidly.  
51 HSI has gained great and continuous attention in breed screening [3], plant phenotyping [4] and environment  
52 monitoring [5]. In seed-related tasks like determination of seed quality [6], diagnosis of seed diseases [7] and  
53 detection of seed component [8], HSI has been utilized as a fast and accurate alternative. Since hyperspectral  
54 image contains a large amount of redundant collinear information, diverse linear and nonlinear machine  
55 learning approaches like partial least squares discriminant analysis (PLS-DA), extreme learning ma-  
56 chine(ELM), least square support vector machines (LSSVM), and partial least squares regression (PLSR)  
57 were introduced to couple the relationship between seed spectra and category label or component content [8-  
58 10].

59 In recent years, with the attention from academia and industry increasing, deep learning as the new state  
60 of art machine learning approach has also been applied in spectral analysis filed gradually [11-13]. Compared  
61 with traditional approaches, deep learning can extract various low-level and high-level features automatically  
62 through a multi-layered stack network structure [14]. This can reduce the requirement of prior knowledge

63 from specific tasks and human effort in feature engineering, which is very beneficial for the analysis of re-  
64 dundant and high-dimensional spectral data.

65 However, deep learning models have serious big data dependencies. A high-performance deep model  
66 requires enough samples to adequately learn the feature patterns hidden in the massive and redundant spectral  
67 data. Unfortunately, in some tasks like seeds screening with specific traits during breeding or quality detec-  
68 tion of precious agricultural products, it is very difficult to establish a large-scale high-quality dataset because  
69 of the high cost of obtaining and labeling samples [4,15-16]. In addition, the precious data acquired at great  
70 expense is very easy to be outdated and difficult to be reused in new tasks. This greatly limits the rapid  
71 application of well-performing methods like deep learning in spectral analysis. Another problem is that deep  
72 models developed for different tasks are generally based on a common assumption, that is, training and test-  
73 ing data lie in same feature space and have same distribution [17]. Therefore, even for similar tasks, the tiny  
74 differences in the distribution of different datasets caused by the variation in sample state and spectral acqui-  
75 sition parameters will make the model not reusable.

76 The emergence of transfer learning brings hope for solving the above two problems. Allowing the train-  
77 ing and testing data lie in different feature spaces, transfer learning mainly investigates methods how to  
78 transfer useful knowledge learnt from the relevant source domain into the target domain [18]. This not only  
79 relieve the demand for a large number of samples in target task, but also make reusing the useful knowledge  
80 like model structure and feature representation in the source domain possible. The target task can be expected  
81 completed using limited samples and computation overhead. Deep transfer learning is the product of the  
82 combination of deep learning and transfer learning. It aims to study how to make use of deep neural network  
83 to transfer knowledge and has been widely used in computer vision field [19-21].

84 However, deep transfer learning technique has not received much attention in the field of spectral anal-  
85 ysis. Most studies perform task analysis at pixel level based on remote sensing images, such as, poverty  
86 mapping [22], image superresolution processing [23] and crop yield prediction [24]. For ground spectral  
87 image, [25] showed the effectiveness of deep transfer learning in predicting soil clay content in different soils.  
88 For seeds of different crops, although many differences were existed, there are also certain similarities, for  
89 example the seeds structure. Most seeds contain seed coat, embryo and endosperm. These structures contain  
90 some conventional chemical components like starch, fat and enzymes which are necessary for seed to develop

91 into seedling [26-27]. This may lead to the similarities among the spectral characteristics of different crop  
92 seeds. Therefore, when constructing a deep model for seed varieties classification of a certain crop based on  
93 HSI, the knowledge in the model has the possibility to be transferred into the classification tasks of other  
94 crop seeds. In this study, we aimed to investigate the feasibility of deep transfer learning technique for vari-  
95 eties identification of different crop seeds based on HSI.

96 The specific objectives were: (1) to develop a deep network model with excellent performance based on  
97 a sample-rich dataset; (2) to transfer common knowledge to the varieties classification of other crop seeds  
98 with sample-limited datasets through the deep network; (3) to evaluate the impact of training set size on the  
99 performance of transfer learning; (4) to visualize the training and transferring process of deep network and  
100 the classification results. We hope to provide a common framework for accurate varieties identification of  
101 crop seeds under sample-limited condition through this study.

## 102 **Materials and methods**

### 103 **Sample collection and dataset description**

104 This study investigated five kinds of crop seeds, including pea, rice, oat, wheat and cotton. The seeds  
105 were performed hyperspectral imaging immediately after collected. All images were obtained by a same line-  
106 scanning near-infrared hyperspectral imaging system covering a spectral range from 874.41 nm to 1733.91  
107 nm with a resolution of 5 nm [28]. A hyperspectral image containing 256 spectral channels could be obtained  
108 through each scan by this system and then calibrated using the following formula to reduce the negative  
109 impact of dark current.

$$110 \quad I_c = \frac{I_r - I_d}{I_w - I_d} \quad (1)$$

111 where  $I_r$  and  $I_c$  represented the raw hyperspectral image and the corrected image,  $I_w$  and  $I_d$  represented the  
112 white and dark reference image. Each seed in hyperspectral image was regarded as a region of interest (ROI).  
113 To get the mask of all the ROIs, the channel with strongest contrast between background and seeds was  
114 conducted a simple threshold segmentation and morphological operation. Then the spectral vectors of all  
115 pixels within each ROI were extracted and the bands in head and end range were removed to avoid noise  
116 introduced by instability of the system. The reserved spectra with a range of 975~1646 nm were further

117 processed by wavelet transform (WT). The spectrum vector representing a seed sample was finally obtained  
 118 by averaging all the transformed pixel spectra in one ROI.

119 Five spectra datasets with similar but different distributions were established in this study. Their detailed  
 120 collection parameters and description information were summarized in Table 1. It should be noted that dif-  
 121 ferent parameters were set for imaging different crop seeds clearly since different seeds have different exter-  
 122 nal phenotypes such as size, height and color. The most abundant dataset, Pea dataset, contained a total of  
 123 10420 samples from four varieties named Baiyan (2697), Heiyan (2848), Changshouren (2849) and Zhewan  
 124 1 (2026) which were widely cultivated in southern China. Peas of the first two varieties generally need to be  
 125 roasted before eating, while the latter two can be directly eaten due to the high water and sugar content. All  
 126 the seeds were purchased from Lv Feng seed company in Hangzhou, Zhejiang, China in 2018. The sub dataset  
 127 corresponding to each variety was randomly divided into a training set, a validation set and a testing set at a  
 128 ratio of 3:1:1. Then the sub datasets with same class were merged and shuffled. Because of its large volume  
 129 of data, Pea dataset was selected as source dataset.

130 **Table 1 Description of the datasets**

Datasets		Par.	#Variety	#Total	#Training	#Validation	#Testing
Source	Pea	(15.5, 3, 12)	4	10420	6252	2084	2084
	Rice	(9, 3, 11)	3	750	150	300	300
Target	Oat	(15.2, 3, 11.5)	4	1000	200	400	400
	Wheat	(15, 3, 13)	5	1250	250	500	500
	Cotton	(14, 3, 11.5)	7	1750	350	700	700

131 Note: Par. represents parameters of hyperspectral imaging system including the distance between camera and seed plate  
 132 (cm), the exposure time of the camera (ms), and the speed along the X-axis of seeds movement (mm.s<sup>-1</sup>).

133 The other four sample-limited datasets were used as target datasets which involved several common  
 134 staple crops. These datasets were designed to contain different numbers of seed varieties for investigating its  
 135 impact on the transferring effect. Each variety in these datasets contains 250 samples and was further divided  
 136 into three subsets at a ratio of 1:2:2 to reflect sample-limited condition.

137 The first target dataset only consisted 750 spectral samples of three varieties of rice seeds including  
 138 Yongyou 9, Nuoyou 6211 and Zhongbaiyouhuazhan. These varieties are all hybrid rice with indica property

139 and belong to hybrid indica-japonica, hybrid indica-glutinous and hybrid indica rice, respectively. All seeds  
140 were collected by College of Agriculture and Biotechnology, Zhejiang University in 2019.

141 The second dataset was Oat dataset with the same number of varieties as the source dataset. It contained  
142 1000 samples from four varieties named Bayan 6, Dingyan 2, Muwang and Jizhangyan 4 which were widely  
143 planted in the grasslands of northern China. The seeds harvested in 2017 were kindly provided by Academy  
144 of Agricultural and Animal Sciences, Inner Mongolia, China.

145 A total of 1250 samples from five varieties of wheat seeds, including Zhenmai 9, Annong 1124, Long-  
146 pingmian 6, Shannong 102 and Weilong 169, formed Wheat dataset. These five varieties were extensively  
147 cultivated in the winter wheat regions of southern China. The seed samples were friendly provided by Anhui  
148 longping high-tech seed industry co., LTD. in Hefei, Anhui, China in 2018.

149 The fourth dataset, Cotton dataset, was consisted by 1750 samples of seven varieties of cotton seeds.  
150 They were Jinxin 5, Jinxin 7, Shennongmian 1, Xinjiangzaomian 1, Xinluzaoimian 29, Xinluzhong 52 and  
151 Xinluzhong 42. These varieties were mainly grown in Xinjiang Uyghur Autonomous Region, the largest  
152 cotton-producing region in China. And the cotton seeds were collected by Shihezi University in 2016.

153 In this study, multiple deep neural networks with different structures were firstly developed using the  
154 source dataset. Then the optimal deep model was selected as the model to be transferred through comparing  
155 the classification accuracies. Transfer learning technique was investigated to transfer useful knowledge from  
156 the optimal deep model to the analysis of four target datasets. The training set of each target dataset were  
157 further transformed into 10 datasets to analyze the impact of sample size on transfer learning by randomly  
158 selected 10 %~100 % samples from original training set. Four commonly-used multivariate analysis methods,  
159 including two linear methods: linear discriminant analysis (LDA), PLS-DA, and two nonlinear methods:  
160 multi-layer perceptron (MLP) and support vector machines (SVM) were introduced as the benchmarks.

### 161 **Deep classification models development**

162 In computer vision field, the huge image library, ImageNet, has spawned many excellent deep learning  
163 models like VggNet, InceptionNet and ResNet [29]. The specialness of VggNet is using small convolution  
164 kernels. The designers believed that using multiple convolution layers equipped with a 3×3 kernel to replace  
165 a convolution layer with a 5×5 kernel could not only reduce the network parameters, but also increase non-  
166 linear mapping, thereby increasing the representation capability [30]. ResNet is also an outstanding network

167 with many variations. What makes it special is the introduction of residual learning idea. The residual module  
168 directly bypasses the input of a certain layer to the output, which makes ResNet only need to learn the residual  
169 between the input and output [31]. This manner solves the problem of performance degradation when the  
170 network depth increases. InceptionNet was born in the ILSVRC2014 competition. The biggest innovation of  
171 this network is introducing a module called Inception to replace the common structure of convolution layer  
172 cascading pooling layer [32]. This Inception module contains four branches with different receptive fields to  
173 perceive the input patterns. By utilizing this module, InceptionNet can increase its width and learn more local  
174 features of different scales.

175 Inspired by these network structures, three one-dimensional deep neural networks were developed for  
176 the source dataset in this study, as shown in Fig. 1.

177 The first one was VGG-MODEL. Two V blocks containing two convolution layers equipped with a  $1 \times 3$   
178 kernel were designed to extract the feature patterns hidden in the spectral vectors. A Batch Normalization  
179 (BN) and an activation function exponential linear unit (ELU) were inserted after each convolution for the  
180 purpose of reducing the overfitting risk and speeding up the convergence process. The number of convolution  
181 filters was set to 16 for the first V block, and 32 for the second V block. A max pooling layer was placed  
182 behind each V block to reduce feature dimension. The last max pooling layer was followed by a Flatten layer  
183 to convert its output features into a one-dimensional vector form. Layer Fc1 and Fc2, consisting of 64 and 4  
184 neurons respectively, were used to perform classification task like traditional neural networks. BN and ELU  
185 were also used behind Fc1. VGG-MODEL finally output the probability of the input spectral vector belong-  
186 ing to each category through a softmax function.

187 The second one was RES-MODEL. The first part of this network was similar to half of V block, which  
188 contained a convolutional layer followed by BN, ELU and a max pooling layer. The difference was that the  
189 convolutional layer used 32 kernels with a size of  $1 \times 7$ . The second part consisted of four cascaded residual  
190 modules, R block. This module was similar to the V block but added a transmission channel from input to  
191 output. The number of convolutional filters in the first R block was 32, and was doubled when the blocks  
192 going deeper. An average pooling layer was placed after the last R block to average the features in the spectral  
193 dimension. This layer could decrease the parameters in fully connected layers, thereby reducing over-fitting

194 risk. The last part of RES-MODELDE was similar to that of VGG-MODEL, but just equipped with one fully  
195 connected layer Fc1 with 4 neurons.

196 The third one was INCEPTION-MODEL. Having the same structure as that of RES-MODEL, the first  
197 part of this network utilized 16 convolution filters with a size of  $1 \times 3$ . It was followed by four I blocks, each  
198 of which cascaded a max pooling layer except the last one. The number of filters in the first I block was 16,  
199 and was also doubled when the blocks going deeper. As shown in Fig. 2, the I block transmitted its input to  
200 four parallel branches. Three of them were convolution layers with  $1 \times 1$ ,  $1 \times 3$ ,  $1 \times 5$  kernels, respectively. They  
201 were employed to extract local spectral features at different scales. A  $1 \times 1$  convolution was placed before  $1 \times 3$   
202 and  $1 \times 5$  convolution to reduce the number of input channels. The last branch performed the max pooling  
203 operation. The introduction of I block allowed INCEPTION-MODEL to increase its width and obtain richer  
204 representation information without slowing down running speed. The end of the INCEPTION-MODEL was  
205 similar to that of RES-MODELDE.

206 To fairly compare the performance of these three deep models, all networks employed cross-entropy as  
207 objective function and used stochastic gradient descent (SGD) optimization algorithm. The learning rate and  
208 momentum of these networks were all set to 0.001 and 0.9, respectively. After debugging for many times,  
209 the number of samples input into the network at one time, *batch\_size*, was set to 128, and the number of  
210 training iterations, *epoch*, was set to 400. All networks were trained using the training set of the source da-  
211 taset, and the best models with the highest accuracy on the validation set were saved to evaluate the effec-  
212 tiveness of the corresponding network on the testing set. The detailed parameters of these three networks  
213 were shown in Additional file 1: Table S1.

#### 214 **Transfer learning strategy**

215 As an emerging tool in machine learning, transfer learning was proposed to remit the requirement of  
216 models for sufficient training data by transferring available knowledge from relevant source domain to target  
217 domain [18]. The common process of transfer learning was shown in Fig. 3a. We defined a domain  $\mathcal{D} =$   
218  $\{\mathcal{X}, P(\mathcal{X})\}$  where  $\mathcal{X}$  represented a feature space and  $P(\mathcal{X})$  represented its probability distribution, and a task  
219  $\mathcal{T} = \{\mathcal{Y}, f(\cdot)\}$  where  $\mathcal{Y}$  represented a label space and  $f$  represented a transformed function. When the task  
220  $\mathcal{T}$  was performed in the domain  $\mathcal{D}$ ,  $f$  modeled  $P(y|x)$ , where  $y \in \mathcal{Y}, x \in \mathcal{X}$ . In transfer learning field, there

221 are two domains: source domain  $\mathcal{D}_S$  with task  $\mathcal{T}_S$  and target domain  $\mathcal{D}_T$  with task  $\mathcal{T}_T$ . The main goal of trans-  
222 fer learning is to improve the performance of transformed function in target domain  $f_T(\cdot)$  using the  
223 knowledge learned in  $\mathcal{D}_S$  and  $\mathcal{T}_S$ , where  $\mathcal{D}_S$  (or  $\mathcal{T}_S$ ) and  $\mathcal{D}_T$  (or  $\mathcal{T}_T$ ) are different but relevant, that is,  $\mathcal{D}_S \neq \mathcal{D}_T$   
224 or  $\mathcal{T}_S \neq \mathcal{T}_T$ .

225 For deep transfer learning,  $f(\cdot)$  is various deep models designed for specific tasks. These deep models  
226 that take a large amount of data and time to train contain rich knowledge. Some knowledge is closely related  
227 to the specific task, while other is some common knowledge which can be shared between different tasks or  
228 objects. Deep transfer learning aims to transfer the common knowledge into current target task to avoid  
229 collecting a large number of samples to learn this knowledge repeatedly, and thus can achieve rapid modeling.  
230 The model's structure and the network's weight are two important kinds of knowledge contained in the deep  
231 model. In this study, the optimal deep model structure based on the source dataset was reused to simplify and  
232 shorten the modeling process as much as possible. Since the number of seed varieties of different crops was  
233 different, the number of neurons in the output layer of the model was modified correspondingly. As the initial  
234 weights have a great influence on the convergence speed and the final performance of the network, this study  
235 transferred the weights of the optimal deep model based on the source dataset to the models based on the  
236 target datasets according to the network structure. It should be noted that the weights of the last fully con-  
237 nected layer in deep models based on the Rice, Wheat and Cotton dataset needed to be randomly initialized  
238 because the number of output neurons in these models were different from that in models based on source  
239 Pea dataset. During the transferring process, the weights of the layers before the flatten layer were frozen,  
240 and the target dataset were used to fine tune the subsequent full connected layers (Fig. 3b). The first reason  
241 was that the target dataset was too small to retrain the entire network. The second reason was that the convo-  
242 lutional layers before the flatten layer had extracted important feature patterns of the seed spectra, which  
243 could be reused in the target tasks. According to the size of the target datasets, the *batch\_size* of the trans-  
244 ferred network was set to 3, and the learning rate was set to 0.0001. The other configurations were the same  
245 as those of the deep network based on the source dataset.

## 246 **Comparison methods**

247 In this study, the deep neural networks based on the source dataset and four target datasets were com-  
248 pared with conventional linear and nonlinear multivariate analysis methods to confirm their validities in  
249 spectra analysis from both data-rich and data-poor sides.

250 LDA aims to find an optimal projected direction for raw variables. In the projected feature space, sam-  
251 ples between classes hold maximal dispersion degree, while samples within classes hold minimal dispersion  
252 degree [33]. This projection manner facilitates transforming the samples into a linear separable state. The  
253 number of variables in the projected space,  $n\_lda$ , is the only parameter which needs to be adjusted. We set  
254  $n\_lda$  to 1~20, and selected the optimal  $n\_lda$  according to the classification performance of LDA.

255 The core principle of PLS-DA is also to conduct a linear transformation. Unlike LDA, the transformed  
256 latent variables (LVs) can not only carry the main information hidden in the raw variables, but also maximize  
257 the correlation between the independent and the dependent variables [34]. In spectral analysis, the number of  
258 LVs,  $n\_pls-da$ , that minimize the sum of prediction residual error was usually selected. The range of  $n\_pls-$   
259  $da$  was also set to 1~20 in this study.

260 SVM can enable raw linear unseparable variables to transform into a linear separable space through a  
261 nonlinear kernel function [33]. Because of the ability to cluster samples with same categories closely and  
262 make them tend to be linear separable, radial basis function (RBF) kernel was often used with SVM in many  
263 spectral analysis tasks. In this study, SVM equipped with RBF kernel was introduced as a nonlinear bench-  
264 mark. Two parameters, penalty coefficient  $c$  and kernel parameter  $g$  were set to {10, 100, 1000, 10000} and  
265 {0.1, 0.01, 0.001, 0.0001}, respectively.

266 MLP is a fully connected artificial neural network with one or more hidden layers [35]. To obtain opti-  
267 mal performance, a total of 32 structures were attempted to process the source dataset, which contained 1~4  
268 hidden layers, and each was equipped with 8 configurations for nodes in hidden layers. The number of nodes  
269 in hidden layers of the structure with 4 hidden layers was set to {(200-100-50-25), (180-90-45-23), (160-80-  
270 40-20), (140-70-35-18), (120-60-30-15), (100-50-25-13), (80-40-20-10), (60-30-15-8)}, and was simplified  
271 as the number of hidden layer decreases. For the target datasets, 24 same structures with 1~3 hidden layers  
272 were tried to get the optimal classifier.

273 Parameters of all models in this study were adjusted toward optimal states using corresponding valida-  
274 tion set. All models were coded using python language in Spyder 3.2.6 environment (Anaconda, Austin, TX,

275 USA). The famous machine learning library, Sklearn (<https://scikit-learn.org/stable/>), was introduced to im-  
276 plement the conventional models, and the popular deep learning framework, Keras, was employed to program  
277 deep models. A Win10 64-bit operating system with Inter (R) Core(TM) i5-8500 CPU and 8GB RAM con-  
278 stituted the basic platform.

### 279 **Model Visualization**

280 Model visualization is significant for intuitively understanding the decision-making mechanism and  
281 clearly showing the computational result. In this study, visualization techniques were investigated from the  
282 perspective of training process of the deep model and classification results of the crop seeds. The accuracy  
283 and loss of the optimal deep model were exhibited to examine the convergence state. In addition, the raw  
284 seed spectra in different datasets and the feature representation of different layers in optimal deep model were  
285 extracted and their distributions were then expressed by t-distribution stochastic neighbor embedding (t-  
286 SNE). As an effective method for high-dimensional data visualization, t-SNE converts the similarity between  
287 sample points in high-dimensional space into Gaussian joint probability form, and constructs a similar prob-  
288 ability distribution in low-dimensional space [36]. The ability of maintaining local structure of data is con-  
289 ducive for observing data patterns in low-dimensional space. Moreover, the advantage of hyperspectral im-  
290 aging to obtain both spatial and spectral information was fully exploited. The sample's label predicted by the  
291 deep model was projected into the corresponding spatial position and represented by different colors to es-  
292 tablish classification maps of crop seeds.

## 293 **Results and discussion**

### 294 **Spectroscopic analysis**

295 The average spectra with standard deviation of different varieties of seeds in five datasets was shown in  
296 Fig. 4. It could be obviously observed that these spectral curves possessed similar fluctuation patterns and  
297 locations of peaks and valleys. The absorption bands at approximately 1119.45 and 1206.92 nm were caused  
298 by the second overtone of carbohydrates (C–H stretch) [37]. The peak near 1307.97 nm (in the range of 1254  
299 ~1348 nm) was reported to be associated with the combinations of the first overtone of amide B (N–H stretch)  
300 and the fundamental vibrations of amide II and III (C–N stretch and N–H in-plane bend) [38]. The band at  
301 1469.95 nm (in the region of 1410~1502 nm) could be attributed to the first overtone of Amide A (N–H

302 stretch), which might be the key band for protein detection [38-39]. The similar chemical components con-  
303 tained in the crop seeds led to the similarities between the spectral curves. This also meant that certain  
304 common features were hidden in the spectral information of different crop seeds, which laid a foundation for  
305 effective transfer learning.

306 However, for seeds of different varieties of the same crop, there were also some heterogeneities between  
307 their spectral curves due to the content difference of chemical components. For example, the spectral curves  
308 of four varieties of pea seeds in the source dataset were naturally divided into two groups: Baiyan and Heiyan  
309 formed one group while Changshouren and Zhewan 1 formed the other one. This was consistent with the  
310 classification results according to edible manner which results from the difference of sugar and water content.  
311 In addition, for the Rice target dataset, it was because of the introduction of japonica characteristic that the  
312 reflectance of variety Yongyou 9 was quite different from the other two varieties. [40] also confirmed spectra  
313 differences were existed between different varieties of rice seeds. [41] found the optical characteristics of  
314 different varieties of hybrid okra and luffa seeds were very different and the metabolic analysis results  
315 showed that the components content of different seeds varied greatly. The heterogeneity of the spectral fea-  
316 tures between different varieties could be utilized as the basis of using hyperspectral imaging to identify  
317 different varieties of crop seeds.

### 318 **Identification results analysis on source dataset**

319 The accuracies and the optimal parameters of all models on training set and testing set of the source  
320 dataset were summarized in Table 2. The over-fitting phenomenon for all models was not serious due to the  
321 large-scale training set which might contain the spectral patterns in the testing set.

322 The accuracies of three deep models on the testing set were all above 99 % which was higher than most  
323 conventional methods. Owing to the convolution operation, the deep models were able to extract much dis-  
324 criminative information hidden in the raw redundant spectral data. Their performance superiorities were pre-  
325 dictable. VGG-MODEL with accuracy of 99.57 % on the testing set was slightly conspicuous than the other  
326 two models. It was reported in computer vision field that the difficulty of improving performance increases  
327 with the model performance being better. For example, in 2014 ILSVRC competition, a 22-layers Inception-  
328 Net won the championship with a top-5 error rate of 6.7 % which was only 0.6 % lower than the runner-up,

329 VGGNet with 19-layers structure [32]. In addition, the high version of Inception, Inception-v4, achieved a  
 330 top-5 error rate of 3.08 % which was only 0.42 % lower than the previous version, Inception V3 [42].

331 **Table 2 Identification accuracies and optimal parameters of all models on source dataset**

<b>Methods</b>	<b>Par.</b>	<b>Training (%)</b>	<b>Testing (%)</b>
<b>VGG-MODEL</b>	(16, 32, 128, 201)	99.98	99.57
<b>RES-MODEL</b>	(32, 32, 64, 64, 128, 194)	99.76	99.14
<b>INCEPTION-MODEL</b>	(16, 32, 64, 128, 256, 349)	100	99.09
<b>LDA</b>	(1)	99.39	98.90
<b>PLS-DA</b>	(20)	87.14	86.90
<b>SVM</b>	(104, 10-3)	99.70	99.28
<b>MLP</b>	(200, 100, 50, 25)	93.81	93.52

332 Note: Par. represents (number of major convolution filters, best *epoch*) for deep models, (*n\_lda*) for LDA, (*n\_pls-da*) for  
 333 PLS-DA, (*c, g*) for SVM, (number of nodes in hidden layers) for MLP.

334 Since the structures of the three deep models were continuously adjusted to the optimal states according  
 335 to the source dataset, they possessed different depths. In this study, INCEPTION-MODEL and RES-MODEL  
 336 had a deeper structure than VGG-MODEL. In general, the deeper the model is, the richer the extracted fea-  
 337 tures are. But this was based on a very large dataset like ImageNet and it should be guaranteed that the  
 338 gradient would not disappear during model training. [43] developed a network with inception structure named  
 339 Deepspectra which showed better performance than a comparison network, Model3, similar structure to  
 340 VGG-MODEL. However, the authors also pointed out that the superiority of deep model was not in pro-  
 341 cessing small dataset. Model 3 in [43] couldn't learn enough effective patterns from very little information.  
 342 They also indicated that the performance of Model 3 improved significantly when the size of sample set  
 343 increased slightly. The source dataset in this study was much larger than all the datasets in [43] and was  
 344 enough for VGG-MODEL training. For structure like ResNet, [44] compared the classification accuracy of  
 345 a developed ResNet with a general deep convolutional neural network on cotton datasets, and also found that  
 346 ResNet was not as effective as the latter one.

347 The structure of the optimal model for a specific dataset was the result of constant tradeoff and adjust-  
348 ment, which was closely related to the size and distribution of the sample set. A complex deep network  
349 couldn't always obtain higher performance than a simple one. In this study, for the source dataset, VGG-  
350 MODEL with the simplest structure and the shallowest depth got a small victory when faced the relatively  
351 complex INCEPTION-MODEL and RES-MODEL. For conventional models, SVM performed best and its  
352 accuracy on the testing set was second only to VGG-MODEL. But different from our common sense that  
353 nonlinear models generally performed better than linear models, nonlinear model MLP achieved lower ac-  
354 curacy than linear model LDA in this study [41, 45-46]. Thus, many models need to be tried to determine  
355 which is the optimal one if we use traditional multivariate analysis methods [45-48]. Conversely, deep models  
356 will generally achieve satisfactory results if the training data is sufficient and the structure is properly de-  
357 signed. In the field of spectral analysis, deep learning is a very competitive and potential tool.

#### 358 **Identification results analysis on target datasets**

359 Although deep learning might not work well on small dataset, its advantages would carry forward again  
360 after combining with transfer learning. To verify the effect of deep transfer learning, the slightly better-per-  
361 forming VGG-MODEL was used as the source model to be transferred in this study. 10 training sets with  
362 different sizes were built based on the original training sets to investigate the influence of training set size on  
363 the transferring effect. The identification results of the deep transferred model and the comparison methods  
364 were showed in Fig. 5.

365 It could be seen that the deep transferred model was the only model that always performed well on the  
366 four datasets. For the 100 % training set which was still very small compared with the training set of the  
367 source dataset, the deep model achieved accuracies of 95 %, 99 %, 80.8 %, and 83.86 % on the testing set of  
368 Rice, Oat, Wheat and Cotton dataset, respectively. Such good results could not be obtained if these small  
369 datasets were used to build deep models directly. It was because of combination with transfer learning that  
370 deep learning model could also obtain satisfactory results on small datasets. Transfer learning enabled deep  
371 learning to take advantage of itself, and also avoided the requirement for a large number of samples [19]. As  
372 similar patterns were existed among the spectra vectors of different crop seeds, varieties identification of  
373 different crop seeds belonged to different but similar tasks in the same domain. Thus, transfer learning was  
374 very suitable for the spectral analysis in this study.

375         Although other models could also achieve good performance on some datasets, they could not always  
376 perform well on all. For example, for the 100 % training set, LDA model achieved an accuracy of 87.71 %  
377 on the Cotton dataset which was even higher than that achieved by the deep transferred model. However, it  
378 just obtained accuracies of 93.33 %, 94.5 %, and 71.2 % on the Rice, Oat and Wheat datasets. SVM per-  
379 formed relatively stable on the four datasets like performed in [40-41, 46], and achieved accuracies of 90 %,  
380 96.75 %, 76.6 % and 75.86 % when using the 100 % training sets. As expected, as a shallow neural network,  
381 MLP performed much worse than the deep neural network, especially on the Wheat dataset. It only got an  
382 accuracy of 32.4 % on the testing set which was just a little better than random guessing. Shallow neural  
383 network could not extract valuable discriminative information from redundant spectral data, which led to  
384 unsatisfactory results [49]. PLS-DA commonly used in spectral analysis was also very unstable. Although it  
385 could obtain an accuracy of 92.25 % on the Oat dataset, it performed rather badly on the Wheat and Cotton  
386 datasets which contained more varieties. This was consistent with the results in [41]. With the increasing of  
387 the number of seed varieties, the possibility of samples being linearly separable became smaller, and the  
388 difficulty of distinguishing different varieties became greater. In a word, for traditional multivariate analysis  
389 methods, different datasets might correspond to different optimal models. Conversely, deep transferred mod-  
390 els could generally achieve satisfactory results.

391         In addition, it was worth mentioning that deep transferred model could also achieve good results when  
392 fine-tuned using very small datasets. For example, using 10 % training set which only contained 5 samples  
393 for each variety, it could achieve accuracies of 86.67 %, 88.74 % and 70.14 % on the Rice, Oat and Cotton  
394 dataset. And the accuracy rose rapidly with the increasing of training set size. Even on the Wheat dataset  
395 where all models failed, deep transferred model outperformed all the conventional methods. Deep transfer  
396 learning brings hope for scenarios with very limited samples. On the contrary, the accuracies of most con-  
397 ventional methods were very low when trained using such a small dataset, and the increased speed were  
398 relatively slowly. The result that LDA got a high classification accuracy of 93 % on the Oat dataset was  
399 unexpected. This could be because this little training set just fitted the classification rule of LDA, since its  
400 accuracy dropped to 80 % soon for 30 % training set, and then slowly increased.

401 Moreover, it could be observed that almost models showed high accuracies on the Rice and Oat dataset  
402 but performed badly on the Wheat and Cotton dataset. The samples distribution of a dataset with few cate-  
403 gories was generally simple. Contrarily, the distribution of a dataset with more categories was relatively  
404 complicated, which was not conducive to discrimination. Thus, dataset was an important factor affecting the  
405 performance of models [43, 50]. In addition, it could be seen that deep transferred model got the best per-  
406 formance in Oat dataset. Using just 20 % training set, it obtained an accuracy of 97.25 % on the testing set.  
407 Since the Oat dataset had the same number of varieties as the source dataset, all the weight parameters in the  
408 source deep model including the weights in fully connected layers could be transferred. This allowed maxi-  
409 mum transferring of features in the source model.

#### 410 **Model Visualization**

411 In order to inspect the convergence status, the accuracy and the loss curves of the training and validation  
412 set of five datasets (for the target datasets, the 100 % training set was used) were shown in Fig. 6. For the  
413 source Pea dataset, it could be seen that these two measurements on the training set and the validation set  
414 were basically the same and soon entered stable state with little fluctuation. According to the program design,  
415 the VGG-MODEL at epoch = 201 where the accuracy on the validation set reached maximized was saved  
416 and used for subsequent analysis. For target datasets, the accuracy and the loss curves changed into stable  
417 states with large fluctuations. Different from the source dataset, these two measurements on the validation  
418 set of the target datasets performed better than that on the training set. We guessed that it might be because  
419 of the small sample size of the training set. Similar to the source dataset, the deep models at epoch = 327, 93,  
420 262, and 184 were saved for the Rice, Oat, Wheat and Cotton datasets.

421 Visualizing the feature distribution at each layer of deep network was another important channel to  
422 understand the training process of deep model [51-53]. In this study, t-SNE technique was used to visualize  
423 the original high-dimensional spectra and the features output by the Flatten, Fc1 and Fc2 layer in deep model  
424 in a two-dimensional space, as shown in Fig. 7 and Fig. S1~S4 in Additional file 2~5. For the Pea dataset,  
425 the original spectral samples were aggregated into two categories, which was consistent with the average  
426 spectral analysis. After passed the Flatten layer, the samples with easily confused categories like Baiyan and  
427 Heiyan, or Changshouren and Zhewan 1, were gradually became distinguishable. As the layers of the network  
428 deepened, the samples within a category were clustered closely, while those between different categories

429 became discrete. The samples were clearly gathered into four categories after output by the Fc2 layer. It could  
430 be seen that the deep model gradually transformed the samples from a cluttered state to a distinguishable  
431 state. This was why the deep model could obtain better performance than the traditional methods which used  
432 the original spectral vectors directly.

433 For the four target datasets, the raw spectra in Rice and Oat dataset, especially in Rice dataset, were  
434 slightly more regular than those in Wheat and Cotton dataset. The variety Yongyou9 was strongly distin-  
435 guishable from the other two varieties. This was also consistent with previous spectral analysis. Thus, most  
436 traditional methods performed better on the Rice and Oat dataset than on the other two datasets. Since all the  
437 weights before the Flatten layer were transferred from the source deep model directly, the features output by  
438 the Flatten layer in the deep transferred model contained the spectral patterns learnt from the source dataset.  
439 From Fig. S1~S4 in Additional file 2~5, it could be seen that for the Rice, Oat and Cotton dataset, the features  
440 output by the Flatten layer presented a more aggregated distribution pattern than the raw spectral samples.  
441 This intuitively verified the effectiveness of transfer learning. Through transferring, the spectral features  
442 learnt from the source dataset was reused, which facilitates the identification of small target datasets. The  
443 Wheat dataset might be too cluttered so that the output of the Flatten layer didn't show distinguishability.  
444 The target datasets began to work from Fc1 layer. The samples gradually showed strong separability with the  
445 layers deepened. After output by the final Fc2 layer, the Rice and the Oat samples had been divided into 3  
446 and 4 categories, respectively. Thus, the deep transferred model achieved two high accuracies of 95 % and  
447 99 %. However, the Wheat and the Cotton samples had still some overlapping phenomenon, which led to  
448 relatively low accuracies of deep transferred model.

449 The classification visualization of crop seeds was helpful for breeders to select varieties that meet re-  
450 quirements and for market supervision authorities to check seed purity. In this study, the advantage of hyper-  
451 spectral imaging to obtain spectral and spatial information simultaneously was fully exploited. The categories  
452 of pea seeds predicted by the optimal model, VGG-MODEL, were visualized in a map, as shown in the Fig.  
453 8. In the original hyperspectral images, variety Baiyan and Heiyan showed similar smooth texture features,  
454 while variety Changshouren and Zhewan 1 showed rough texture due to water loss during drying process.  
455 According to human vision, these four varieties were naturally divided into two categories, which was con-  
456 sistent with the visualization analysis of the samples' distribution. Among the predicted 180 seeds, only 2

457 seeds with variety Heiyan were misclassified into similar Baiyan category. This accuracy was sufficient for  
458 variety selection during breeding process or purity detection in actual production.

## 459 **Conclusion**

460 In this study, we attempted to use hyperspectral imaging and deep transfer learning to achieve accurate  
461 and rapid varieties identification of crop seeds under sample-limited condition. The VGG-MODEL based on  
462 the sample-rich dataset stood out from three deep neural networks with typical structures and was utilized as  
463 the deep source model to be transferred. The transfer results on four small target datasets showed that deep  
464 transferred model could make full use of the common spectral features of crop seeds extracted by the source  
465 deep model and could still achieve better performance than traditional multivariate analysis methods under  
466 sample-limited condition, especially under the condition of very few samples. Giving a glimpse into the  
467 process of deep transfer learning, the visualization of the feature distribution at each layer of deep network  
468 further confirmed the portability of common spectral features, and revealed the reason why the deep network  
469 achieved high accuracy. The visualization of classification results provided an intuitive and convenient man-  
470 ner for varieties identification of crop seeds. In conclusion, hyperspectral imaging combined with deep trans-  
471 fer learning was a great potential tool to be applied in the identification of seed varieties with limited samples,  
472 which will greatly accelerate seed screening process in the fields with scarce samples, for example in breed-  
473 ing field. This study also provided a new idea for the detection of other qualities of crop seeds based on  
474 hyperspectral imaging under sample-limited condition.

## 475 **Additional files**

476 [Additional file 1: Table S1](#). The detailed parameters of three deep neural networks.

477 [Additional file 2: Fig. S1](#). Feature visualization of VGG-MODEL on Rice dataset using t-SNE.

478 [Additional file 3: Fig. S2](#). Feature visualization of VGG-MODEL on Oat dataset using t-SNE.

479 [Additional file 4: Fig. S3](#). Feature visualization of VGG-MODEL on Wheat dataset using t-SNE.

480 [Additional file 5: Fig. S4](#). Feature visualization of VGG-MODEL on Cotton dataset using t-SNE.

## 481 **Abbreviations**

482 BN: Batch Normalization; ELM: extreme learning machine; ELU: exponential linear unit; HSI: hyper-  
483 spectral imaging; LDA: linear discriminant analysis; LSSVM: least square support vector machines; LV:  
484 latent variables; MLP: multi-layer perceptron; PLS-DA: partial least squares discriminant analysis; PLSR:  
485 partial least squares regression; RBF: radial basis function; SVM: support vector machines; t-SNE: t-distribution  
486 stochastic neighbor embedding.

#### 487 **Declarations**

#### 488 **Authors' contributions**

489 All authors have made significant contributions to this study. NW, FL and YH conceived and designed the  
490 experiments. NW, ML and CZ performed the experiment and conducted data analysis. NW, FL interpreted  
491 data analysis. FL, YB, WH, FM and YH provided suggestions on the experiment design. YB and YH provided  
492 financial support. NW drafted the manuscript. All authors read and approved the final manuscript.

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#### 495 **Competing interests**

496 The authors declare that they have no competing interests.

#### 497 **Ethics approval and consent to participate**

498 Not applicable.

#### 499 **Consent for publication**

500 Not applicable.

#### 501 **Availability of data and materials**

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505

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626

627

628 **Figure captions**

629 **Fig. 1.** The structures of three developed deep neural networks

630 **Fig. 2.** The inner structures of three typical blocks

631 **Fig. 3.** Transfer learning strategy. **a** The common process of transfer learning. **b** The deep transfer learning  
632 strategy in this study

633 **Fig. 4.** The average spectra with standard deviation of five crop seeds

634 **Fig. 5.** Classification accuracies of all models on the four target datasets

635 **Fig. 6.** The accuracies and losses of VGG-MODEL on the training and validation set

636 **Fig. 7.** Feature visualization of VGG-MODEL on Pea dataset using t-SNE

637 **Fig. 8.** Classification maps of pea seeds

638

# Figures

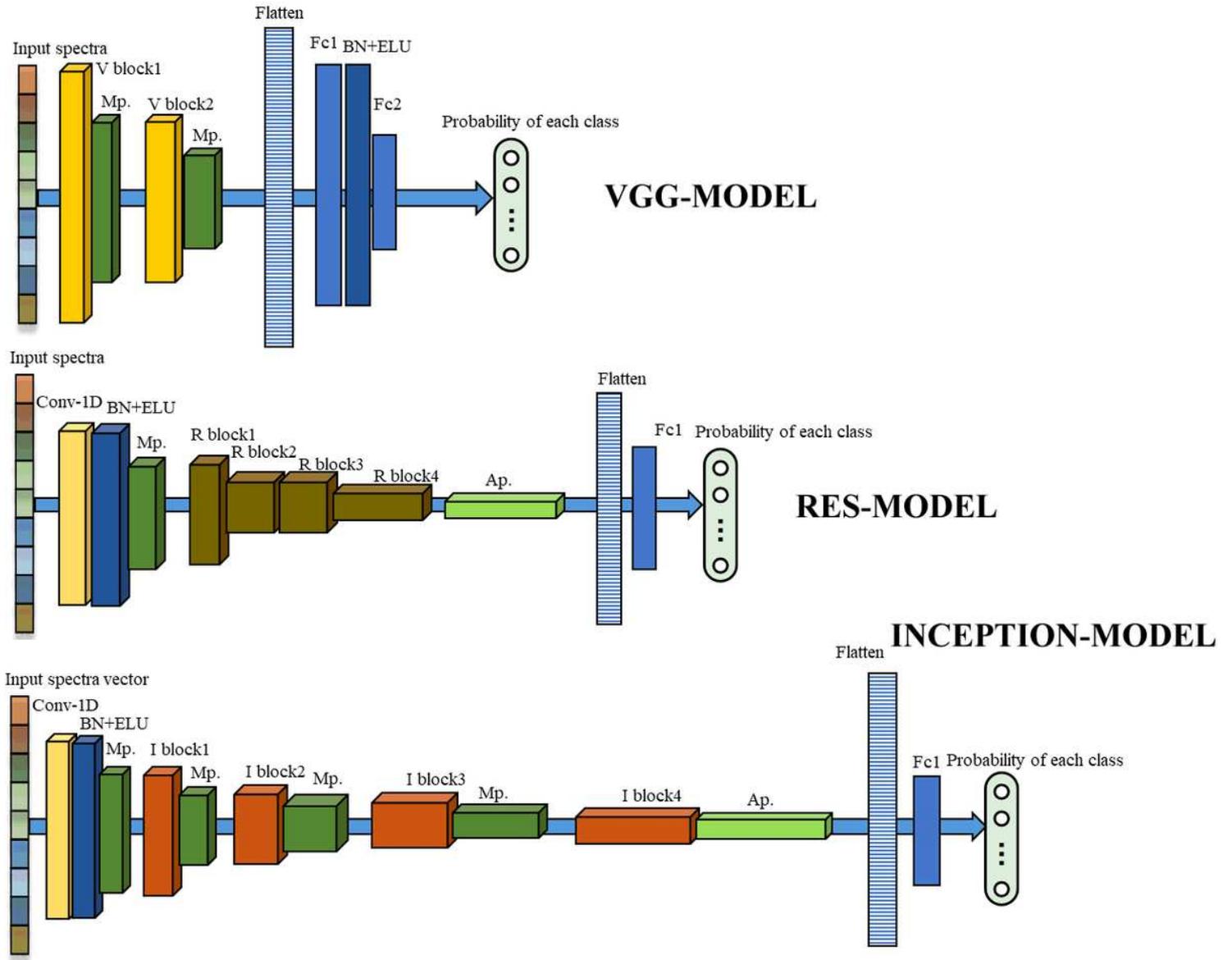


Figure 1

The structures of three developed deep neural networks

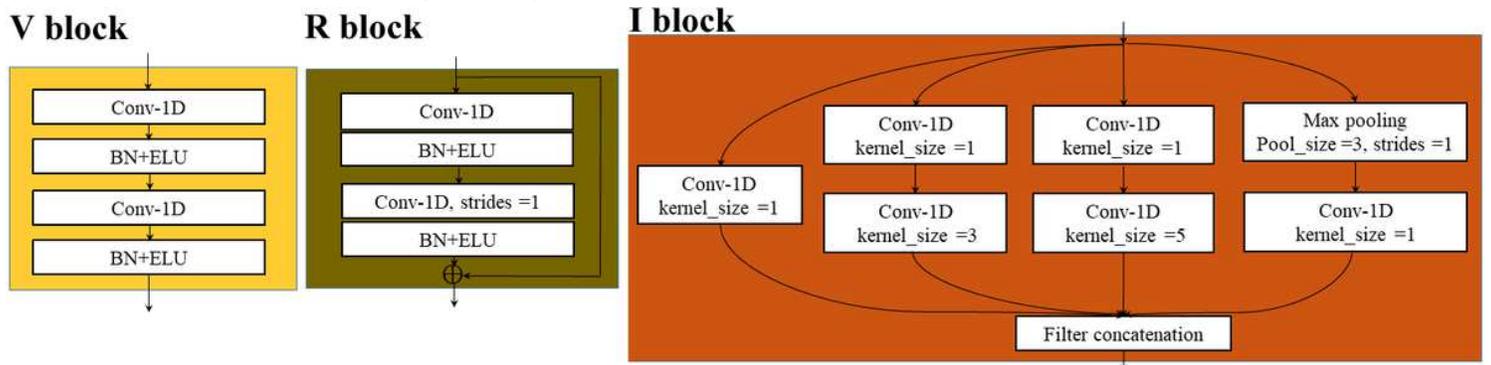
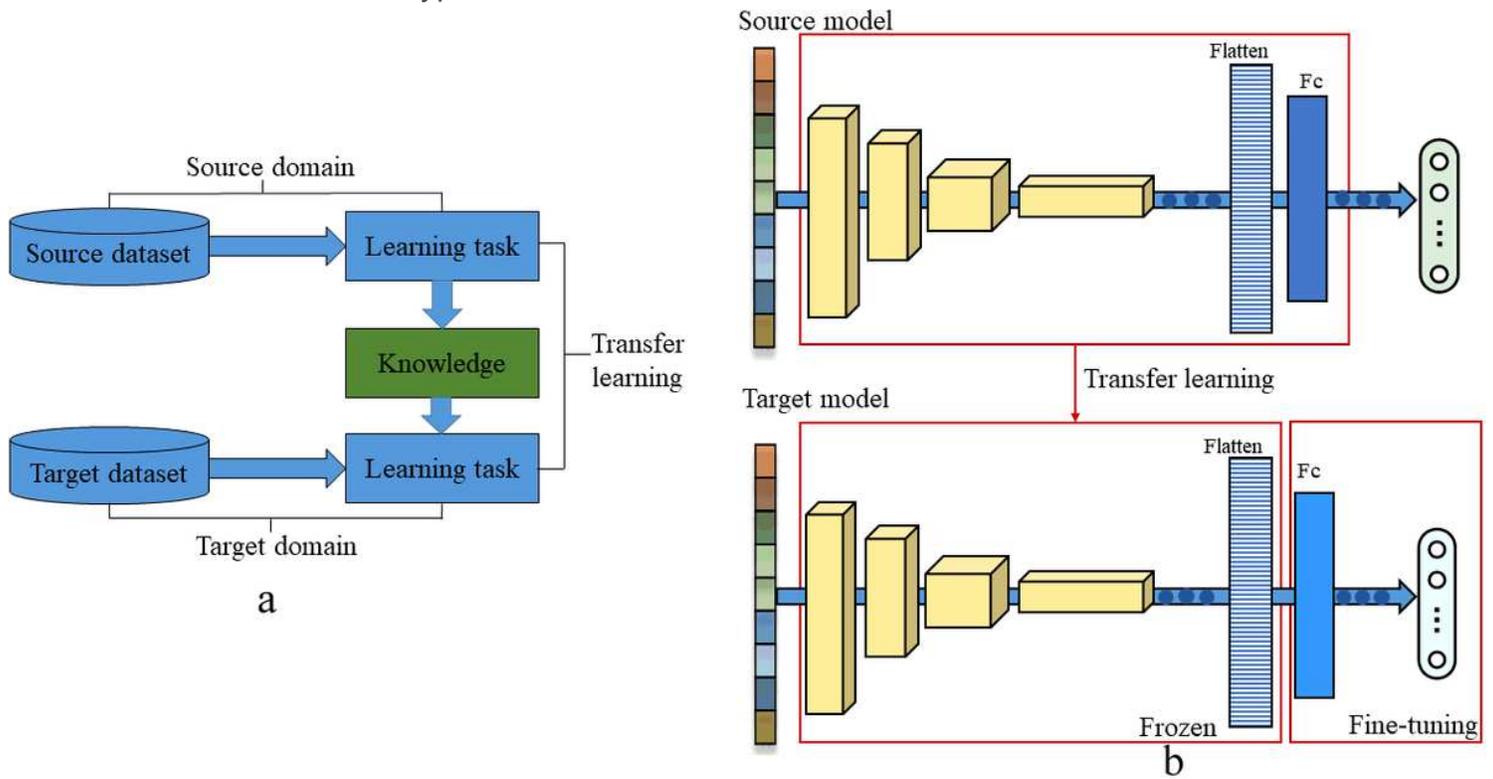


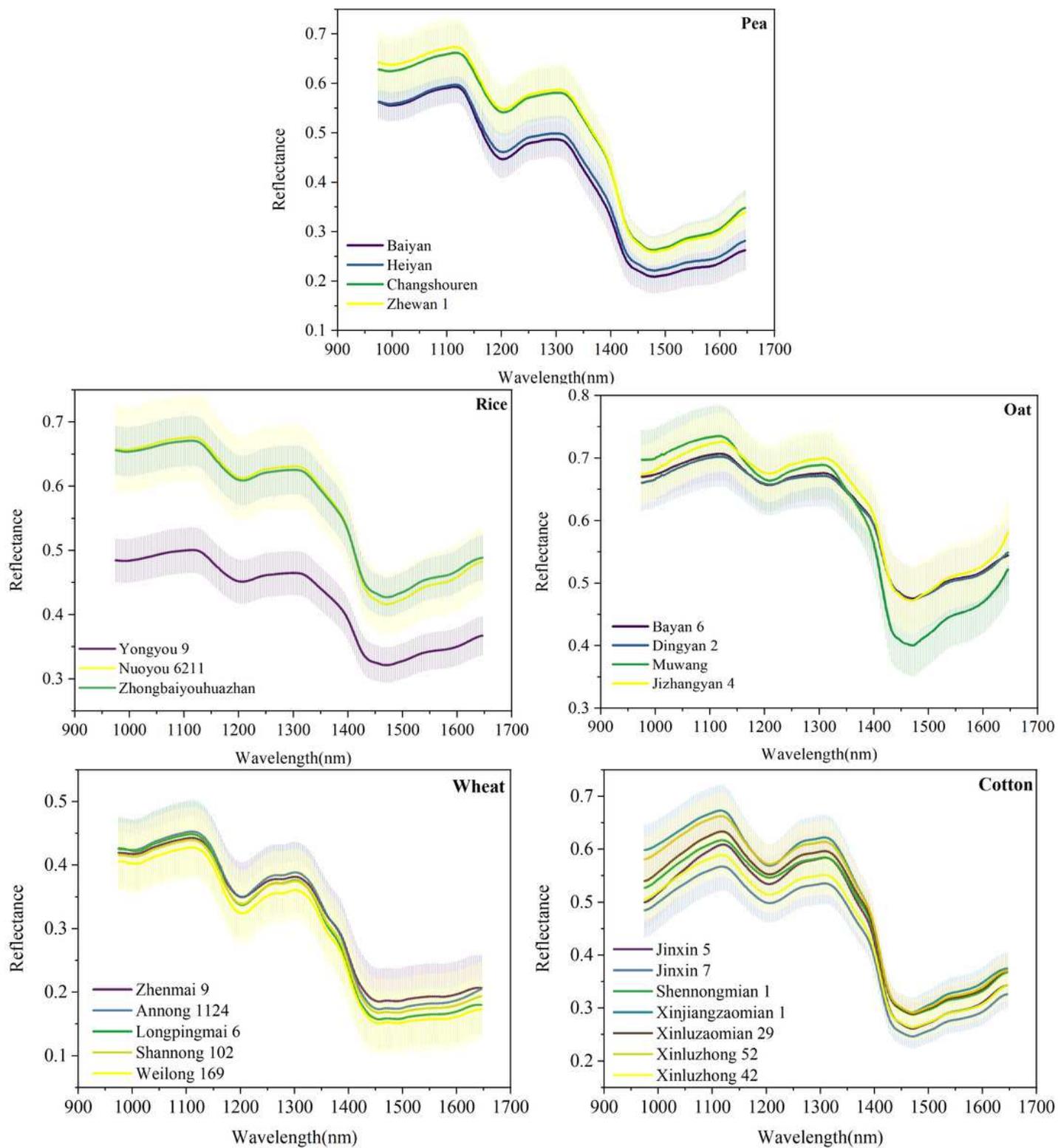
Figure 2

The inner structures of three typical blocks



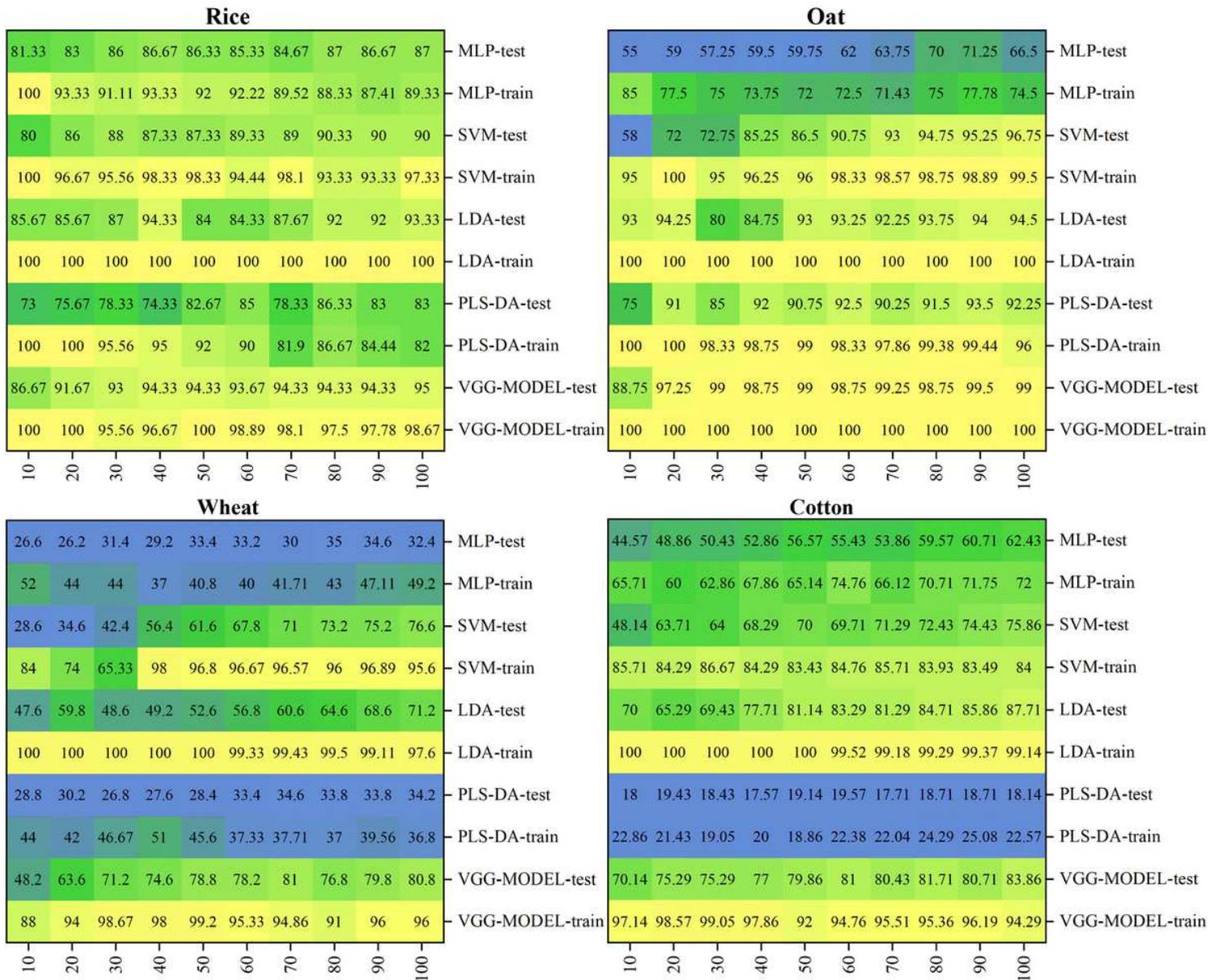
**Figure 3**

Transfer learning strategy. a The common process of transfer learning. b The deep transfer learning strategy in this study



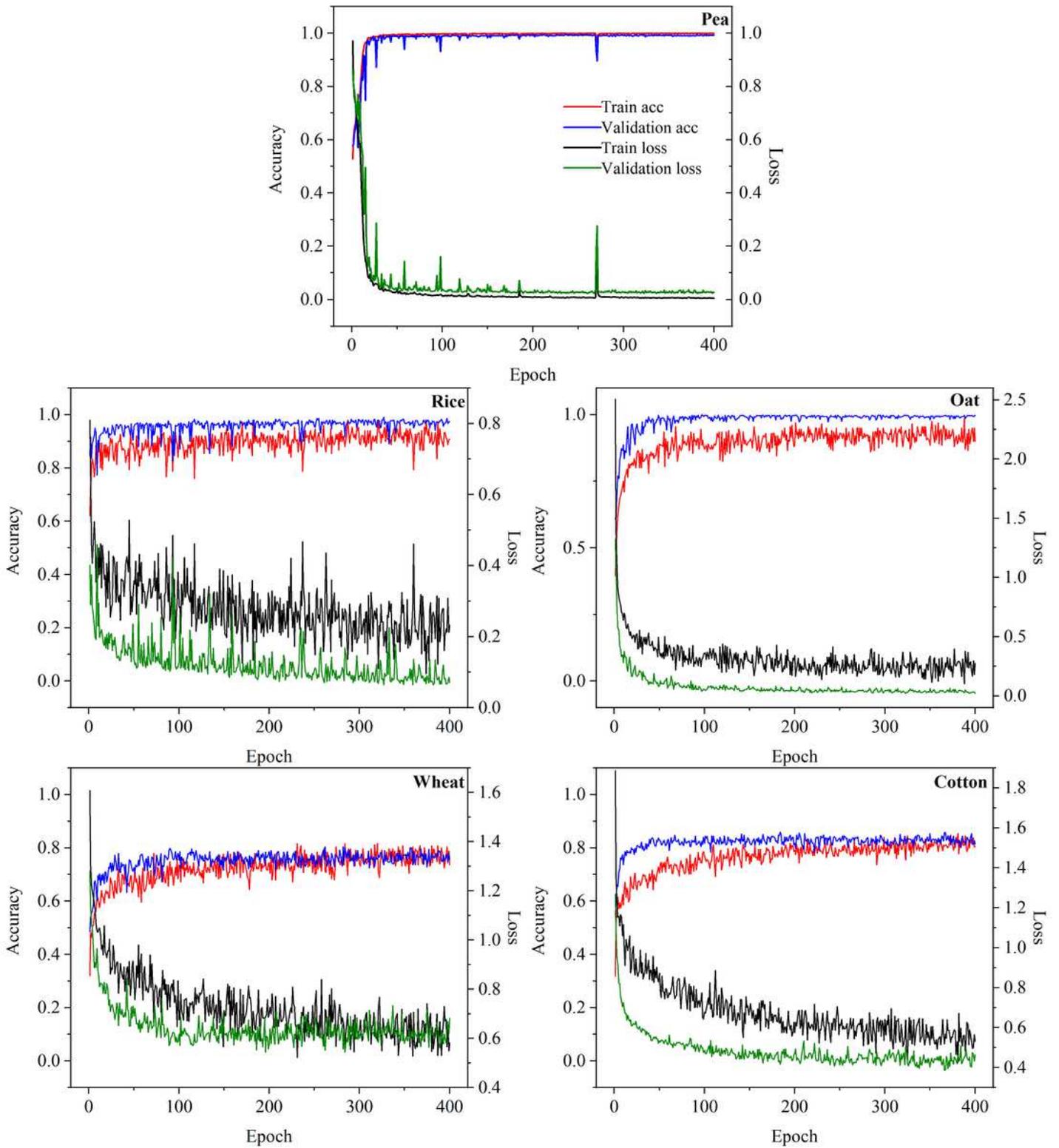
**Figure 4**

The average spectra with standard deviation of five crop seeds



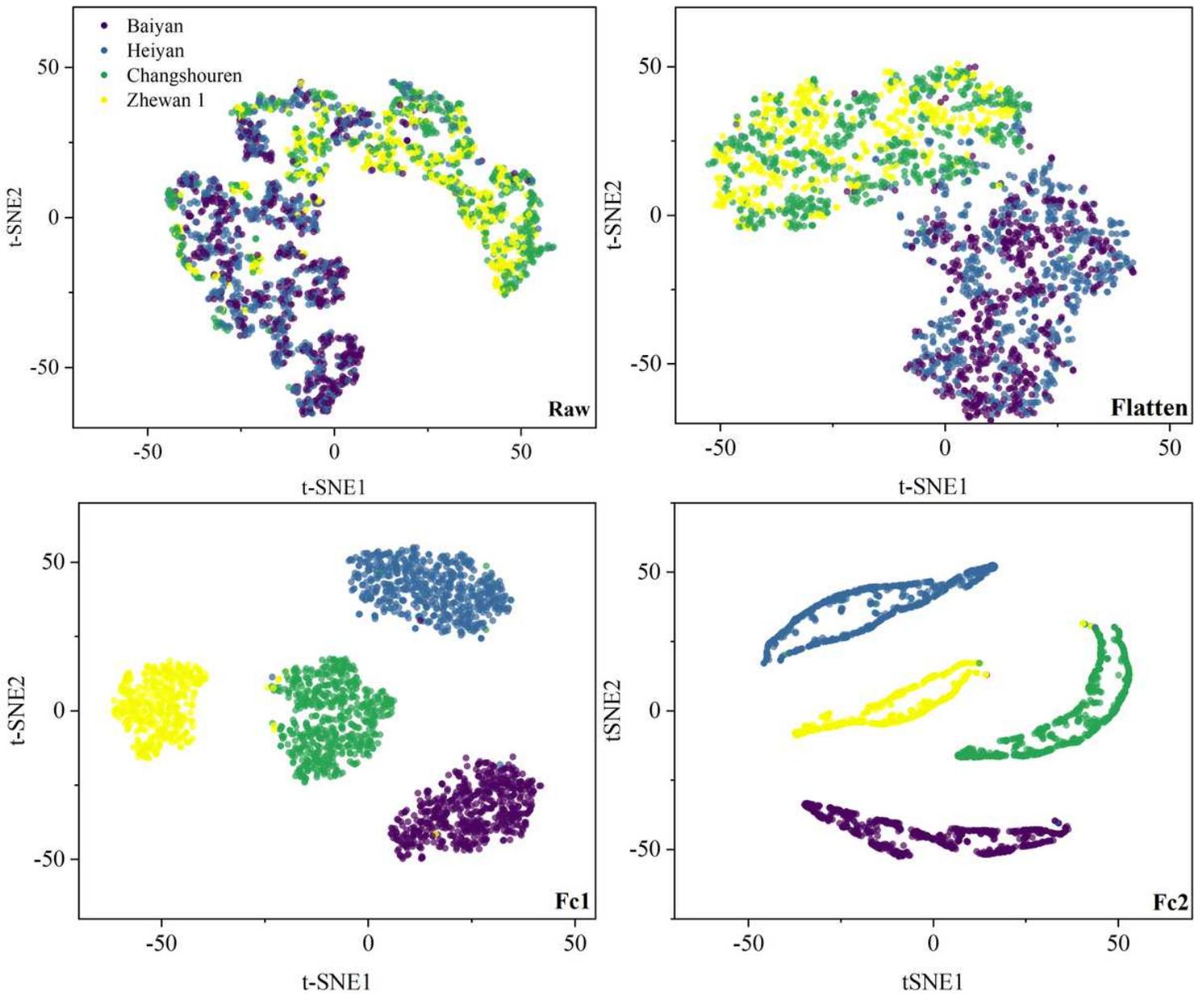
**Figure 5**

Classification accuracies of all models on the four target datasets



**Figure 6**

The accuracies and losses of VGG-MODEL on the training and validation set



**Figure 7**

Feature visualization of VGG-MODEL on Pea dataset using t-SNE

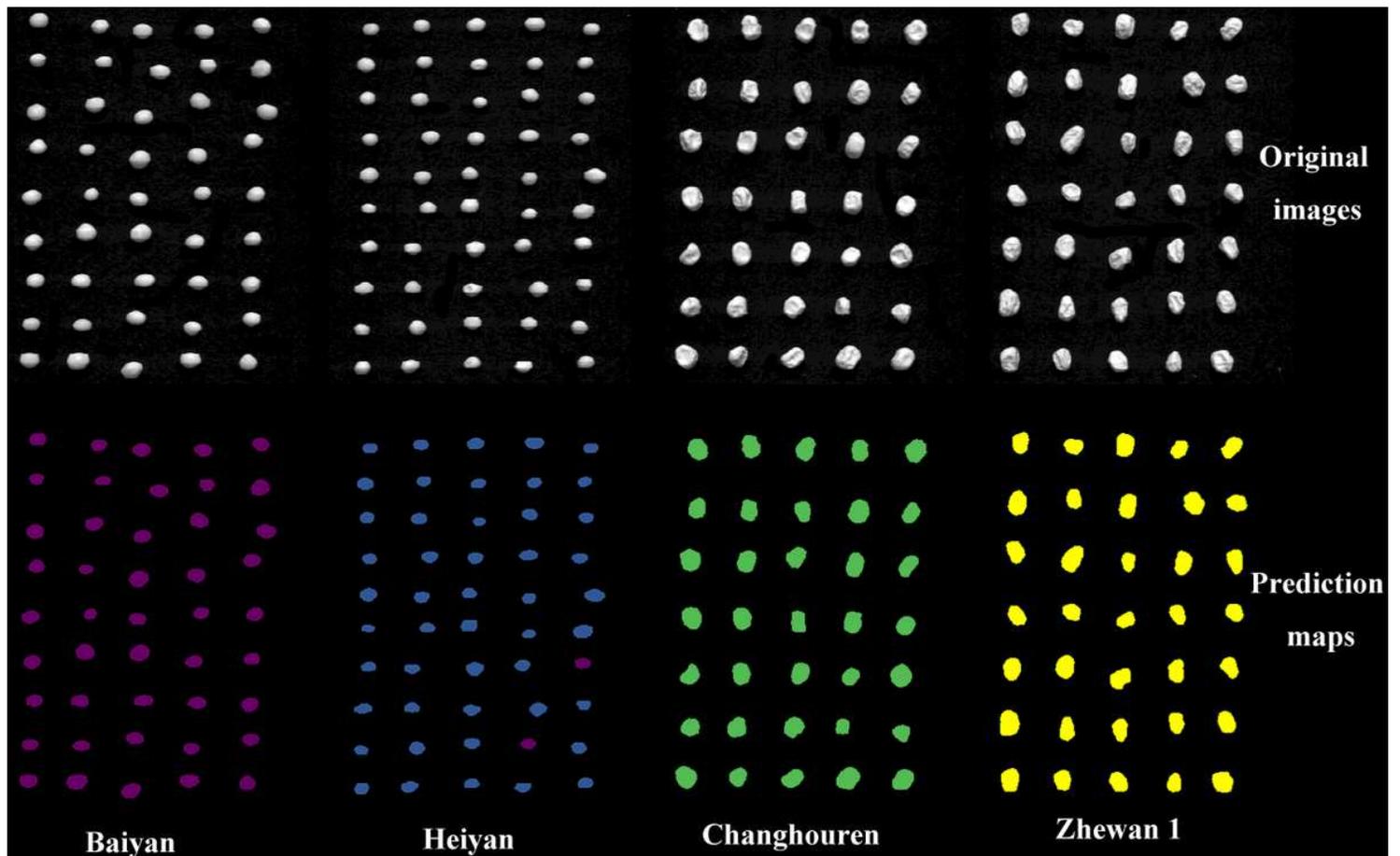


Figure 8

Classification maps of pea seeds

## Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- [Additionalfile1TableS1.docx](#)
- [Additionalfile2Fig.S1.tif](#)
- [Additionalfile3Fig.S2.tif](#)
- [Additionalfile4Fig.S3.tif](#)
- [Additionalfile5Fig.S4.tif](#)