

RESEARCH ARTICLE

Accuracy Evaluation of the Crop-Weather Yield Predictive Models of Italian Ryegrass and Forage Rye Using Cross-Validation

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Abstract

The objective of this study was to evaluate the accuracy of the yield predictive models of Italian ryegrass (IRG, *Lolium multiflorum* Lam.) and forage rye (FR, *Secale cereale* L.) reported in previous studies through K-fold cross-validation method. In previous studies, statistical models were constructed for dry matter yield prediction of IRG and FR using general linear model based on climatic data by locations in the Republic of Korea. The yield predictive model for IRG cultivated in the southern region of the Korean Peninsula and Jeju Island were $DMY = 78.178AGD - 254.622MTJ + 64.156SGD - 76.954PAT150 + 4.711SAP + 1028.295 + \text{Location}$ and $DMY = -8.044AAT + 18.640SDS - 7.542SAT + 9.610SAP + 17282.191$, respectively. The yield predictive model for FR was as follows: $DMY = 20.999AGD + 163.705LTJ + 113.716SGD + 64.379PAT100 - 4964.728 + \text{Location}$. However, accuracy evaluation was not performed in the previous research. In this study, the reported models and the data set used for model construction were investigated. Subsequently, K-fold cross-validation was performed to assess the accuracy of the models. The results showed that the yield predictive models fit to the data sets well, while the accuracy of these models was in the common level since the data sources might keep major variances in cultivars, climatic conditions, and cultivated locations. Therefore, models with better fitness and accuracy might be constructed based on a data set with smaller variance. Hence, the standardization of the crop cultivation experiments is very necessary to decrease the variance in the historical data used for future crop yield modeling.

Key words : Cross-validation, yield predictive model, Italian ryegrass, forage rye

Introduction

Research on yield predictive modeling is actively being carried out nowadays since it is important for measuring the effects of environmental factors such as climate and soil conditions on the growth of field crops (Kim et al. 2015; Kim and Yoo 2015; Ko et al. 2014; Ko and Ahuja 2013). Meanwhile, it could also be helpful to forecast the impacts of climate change on crop yield production and the land use suitability for agricultural crops (Salvacion and Martin 2016). Yield prediction based on soil or climatic data to construct a

statistical model has been widely applied in many studies (Lobell et al. 2009). In Korea, Italian ryegrass (IRG, *Lolium multiflorum* Lam.) and forage rye (FR, *Secale cereale* L.) are representative forage crops (Kim et al. 2014; Seo 2016). In previous research, yield predictive models for IRG and FR were reported (Peng et al. 2016a, 2016b). Statistical methods such as correlation analysis, stepwise approach of multiple regression analysis, and general linear model method were performed in the previous studies to construct the yield predictive models. Meanwhile, since the models were constructed through regression analysis, residual diagnostics

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were also performed to check the fitness of the models. However, the accuracy which means the fitness of the models when applying them to the new data set was not evaluated. As Kozak and Kozak (2003) mentioned, the main objective of regression modeling is to construct a model which could best predict the dependent variable. Residual diagnostics and cross-validation were the two necessary steps to be performed to evaluate the constructed models.

Cross-validation is a popular method to evaluate the accuracy of the yield predictive models (Osten 1988; Picard and Cook 1984; Schaffer 1993; Shao 1993; Zhang and Yang 2015). After the predictive model was constructed, the accuracy of the model, which means the accurate predictive ability of the model when applied the model to a new data set not used in the model construction, should be assessed (Hawkins et al. 2003). There are several cross-validation methods used to evaluating the accuracy of models such as: Hold-Out method, K-fold cross-validation method, and Leave-P-Out cross-validation method. Compared to Hold-Out method, K-fold cross-validation satisfies the requirement that the training and test sets should cross-over in successive rounds to ensure each data point gets a chance to be validated against. Meanwhile, K-fold cross-validation method is much more succinct than Leave-P-Out cross-validation method which should repeat the validation process many times since it uses p observations as the test set and the rest of the observations as the training set. Therefore, K-fold cross-validation is the basic method and commonly used to evaluate the predictive ability of models, especially for statistical models (Kuhn and Johnson 2013; Refaeilzadeh et al. 2009). Gennadi et al. (2015) reported a model for quantification of essential oil components directly

on dried intact leaves of sage through the attenuated total reflectance-Fourier transform infrared spectroscopy method and confirmed the model was a reliable calibration one through 10-fold cross-validation. Shokri et al. (2016) performed 5-fold cross-validation to check the accuracy of the model developed in their research. Peng et al. (2017) used 10-fold cross-validation to evaluate a statistical yield predictive model of IRG, and confirmed the accuracy of the model was in the good level.

Therefore, validation of the models was necessary and K-fold cross-validation method was considered as the proper way to perform the accuracy evaluation of the yield predictive models of IRG and FR. Therefore, this research was conducted to evaluate the accuracy of the yield predictive models of IRG and FR reported in the previous research through K-fold cross-validation.

Materials and Methods

Performance of the yield predictive models of Italian ryegrass and forage rye

In previous research, yield predictive models of IRG (Peng et al. 2016b) and FR (Peng et al. 2016a) were reported. As reported, for the IRG yield predictive model, based on all the variables in the data sets of the two regions, the southern region of the Korean Peninsula (22 cultivated locations) and Jeju Island (Fig. 1), had significant differences ($P < 0.05$), the models were developed separately according to cultivated locations. The yield predictive model for IRG cultivated in the southern region of the Korean Peninsula (Model I) was

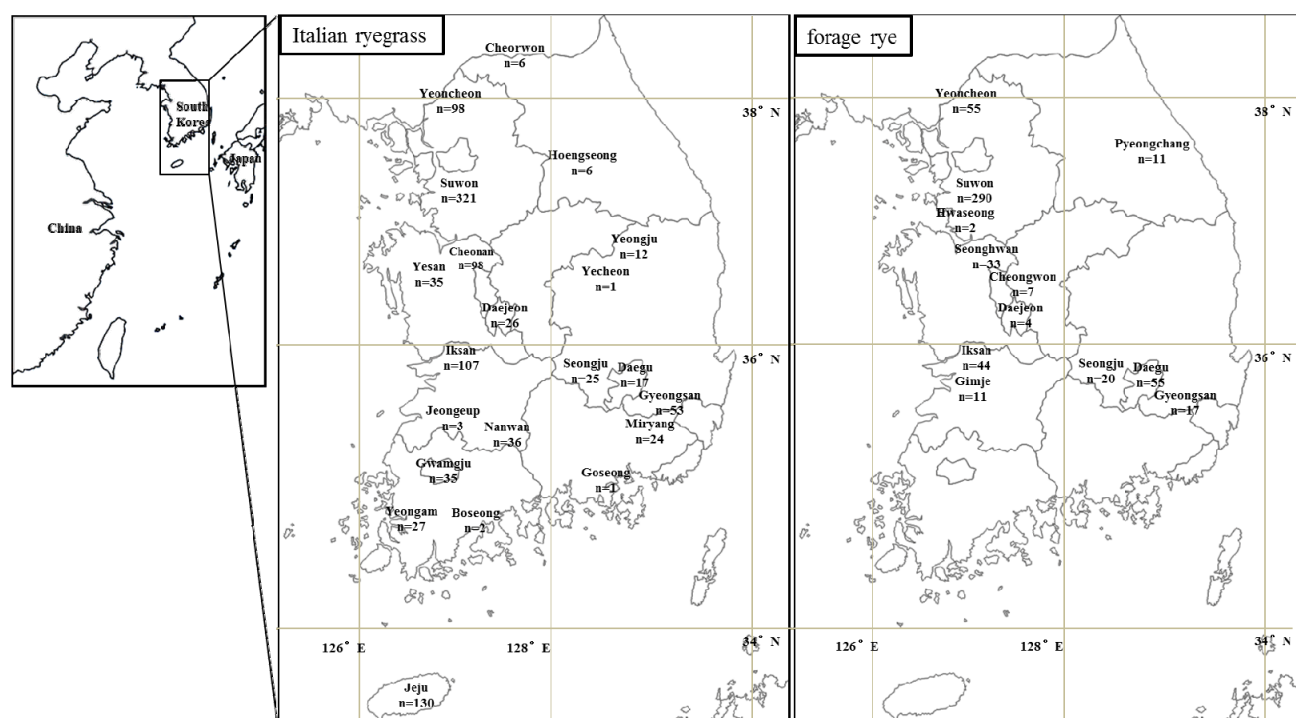


Fig. 1. Map with sample size of the cultivated locations in the Italian ryegrass and forage rye data sets.

Table 1. The reported yield predictive models for Italian ryegrass and forage rye.

Forage crop	Yield predictive model	Coefficients of cultivated locations	R ²
Italian ryegrass	DMY = 78.178AGD – 254.622MTJ + 64.156SGD – 76.954PAT150 + 4.711SAP + 1028.295 + Location	Gyeongsan: –1898.667, Goseong: 2499.449, Gwangju: –3098.979, Namwon: –1070.803, Daegu: –322.419, Daejeon: –1305.577, Miryang: –1778.048, Boseong: –2887.403, Seongju: –1222.198, Seonghwan: –3254.752, Suwon: –1077.516, Yeoncheon: 147.703, Yeongam: –4618.791, Yeongju: 1344.523, Yesan: –683.427, Yecheon: –2448.484, Iri: –1854.719, Iksan: –445.436, Jeongeup: 16.648, Cheonan: 942.728, Cheorwon: –2929.780, Hoengseong: 0.	37.7%
	DMY = –8.044AAT + 18.640SDS – 7.542SAT + 9.610SAP + 17282.191	Jeju	51.0%
Forage rye	DMY = 20.999AGD + 163.705LTJ + 113.716SGD + 64.379PAT100 – 4964.728 + Location	Gyeongsan: 696.999, Gimje: –2248.628, Daegu: –896.506, Daejeon: –1282.072, Seongju: –167.449, Seonghwan: 2021.597, Suwon: 405.696, Yeoncheon: 14.913, Iksan: –402.635, Cheongwon: –74.431, Pyeongchang: –7576.968, Hwaseong: 0.	24.4%

as follows: DMY = 78.178AGD – 254.622MTJ + 64.156SGD – 76.954PAT150 + 4.711SAP + 1028.295 + Location. The yield prediction model for IRG cultivated in Jeju Island (Model II) was as follows: DMY = –8.044AAT + 18.640SDS – 7.542SAT + 9.610SAP + 17282.191. The yield predictive model for WCR based on climatic data by locations in South Korea (Model III) was as follows: DMY = 20.999AGD + 163.705LTJ + 113.716SGD + 64.379PAT100 – 4964.728 + Location. The coefficients of the Location in each model were shown in Table 1. The coefficients of determination of the models were 37.7% (Model I), 51.0% (Model II), and 24.4% (Model III). The results of residual diagnostics of the models showed that the homoscedasticity and the assumption that the mean of the residuals are equal to zero were satisfied. Meanwhile, the fitness of the models was visually evaluated as in the good level based on most scatters of predicted DMY values fell in the 95% confidence interval. However, precise assessment of the accurate predictive ability of the models was not performed.

Data sets used for validating the yield predictive models of Italian ryegrass and forage rye

The data used for validate the yield predictive models for IRG and FR included yield-related data and climatic data. Both the IRG and FR yields related data were collected from five data sources including the adaptability test of imported varieties of grasses and forage crops operated by National Agricultural Cooperative Federation, the reports on joint research projects for new plant variety development operated by Rural Development Administration, research papers in Journal of the Korean Society of Grassland and Forage Science, research reports about livestock experiments operated by Korean National Livestock Research Institute, and Korean crop (farm) survey reports.

The climatic data was collected from the database of the Korea Meteorological Administration. According to the reported models, the collected raw climatic data in both the IRG and FR data sets were converted into climatic variables including Dry Matter Yield (DMY, kg ha⁻¹), Autumnal Growing Days (AGD, d), Autumnal Accumulated Temperature (AAT, °C), the Highest Temperature in January (HTJ, °C), Mean Temperature in January (MTJ), the Lowest Temperature in

January (LTJ), Period to Accumulated Temperature 150°C (PAT150, d), Period to Accumulated Temperature 100°C (PAT100, d), Spring Growing Days (SGD, d), Spring Accumulated Temperature (SAT, °C), Spring Amount of Precipitation (SAP, mm), Spring Days with Precipitation (SDP, d), and Spring Duration of Sunshine (SDS, h).

Then the yield related data and the climatic variable data were combined into one data set at each forage crop and then used for further analysis. The sample sizes of the IRG data set in the southern region of the Korean Peninsula (22 cultivated locations) and Jeju Island (Fig. 1) were 933 and 130, respectively. For the FR data set, the data set (n=549) with yield values, 12 cultivated locations (Fig. 1), and climatic variables was used in the following analyses.

Cross-validation for evaluation of the model fit of the yield predictive models

The K-fold cross-validation was performed to evaluate the expected level of fit of the model generated in this research to the data set used (Picard and Cook 1984). As shown in Fig. 2, the data in the final data set was randomly split into K subsamples. The cross-validation process was repeated K times, with each of the K subsamples used once as the test set. In each time of the validation, a single subsample was retained as the test set, and the remaining K-1 subsamples were utilized as a training set to generate a model containing the variables same as the existed yield predictive models of IRG and FR. The predicted values of both the training and test sets were calculated based on the newly constructed model and the regression scatter plot were generated between the predicted values and observed values for both the training and test sets at each validation. The R² and the normalized root-mean-square error (NRMSE) were calculated for each regression. The average R² and average NRMSE of the training sets (R² fit and NRMSE fit) and test sets (R² val and NRMSE val) were calculated to measure the accurate predictive ability of the model. The higher the R² is the better the accuracy of the model is. NRMSE could be used to measure the goodness-of-fit of the model (Akhtar et al. 2009; Behdani et al. 2016; Chatterjee and Bandopadhyay 2012; Uno et al. 2005). The calculation equation of NRMSE was as follows:

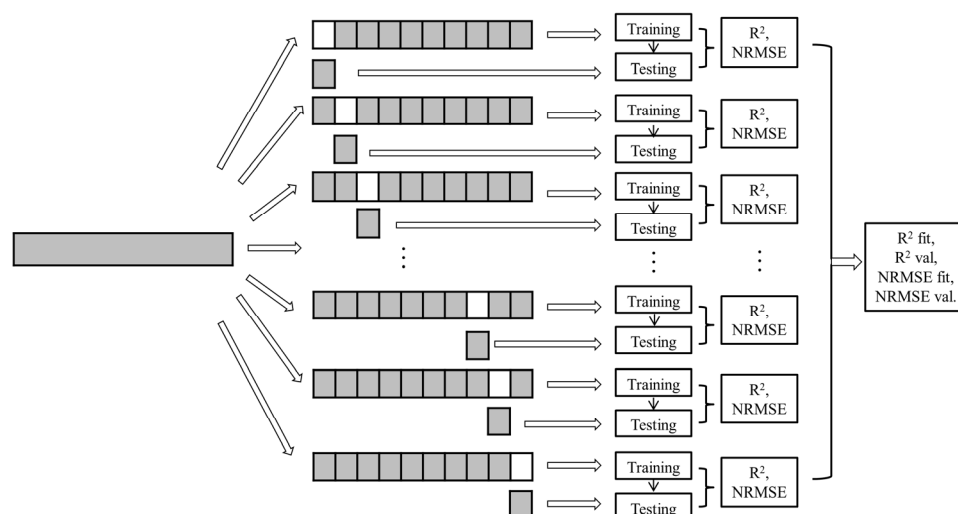


Fig. 2. Flowchart of K-fold cross-validation used for evaluating the accuracy of yield predictive models.

$$RMSE = \sqrt{\sum_{i=1}^n (OBS_i - PRE_i)^2 / n}$$

$$NRMSE = RMSE / \overline{OBS}$$

where PRE_i is the i th predicted yield value, OBS_i is the i th observed yield value, \overline{OBS} is the mean of observed yield values, and n is the sample size.

According to the research results of the previous studies (Feng 2010; Rinaldi et al. 2003), if the value of NRMSE was less than 10%, the degree of the fitness was considered as in the excellent level; if $10\% \leq NRMSE < 20\%$, the degree of the fitness was considered as in the good level; when $20\% \leq NRMSE < 30\%$, the degree of the fitness was considered as in the common level; and if the value NRMSE was larger than 30%, the degree of the fitness was considered as in the poor level.

Since sufficient sample sizes were required for general linear modeling (Maxwell 2000), depending on their sample sizes, 10-fold cross-validation was performed for IRG yield predictive model (southern region of the Korean Peninsula, $n=933$) and FR yield predictive model ($n=549$). While limited

to the sample size ($n=130$) of IRG data from Jeju Island, the validation of the IRG yield predictive model (Jeju Island) was performed through 3-fold cross-validation.

Analysis software

Microsoft Excel 2010 (Microsoft Corp, Redmond, USA) and Stata 12.0 (StataCorp, College Station, USA) were used to perform the cross-validation processes and generate the statistical analysis figures.

Results and Discussion

For Model I, Fig. 3 shows the relationship between predicted and observed yield values for each partition of the 10-fold cross-validation. The results in each subfigure were segregated into training and test sets. The black bold lines are the fitting lines of the predicted and observed yield values in the training set, while the red dash lines are the fitting lines of the predicted and observed yield values in the test set. The coefficients of determination (R^2) and the NRMSE of the training sets and test sets were shown in Table 2. As shown in Table 2

Table 2. Results of 10-fold cross-validation of the yield predictive model of Italian ryegrass cultivated in the southern region of the Korean Peninsula.

Iterations of cross validation	R ² of the fitting lines of the training and test sets in each validation										average
	I ¹⁾ -1	I-2	I-3	I-4	I-5	I-6	I-7	I-8	I-9	I-10	
Training Set	43.0%	44.4%	43.6%	42.6%	42.3%	42.3%	42.9%	43.0%	42.5%	41.9%	42.85%
Test Set	39.0%	32.7%	30.9%	43.3%	48.4%	44.1%	40.1%	39.3%	42.8%	50.6%	41.12%
Iterations of cross validation	NRMSE ²⁾ values of the training and test sets in each validation										average
	I-1	I-2	I-3	I-4	I-5	I-6	I-7	I-8	I-9	I-10	
Training Set	0.275	0.280	0.290	0.290	0.292	0.291	0.295	0.292	0.291	0.294	0.289
Test Set	0.293	0.367	0.303	0.304	0.278	0.297	0.270	0.286	0.298	0.274	0.297

¹⁾I: Iteration,

²⁾NRMSE, the normalized root-mean-square error.

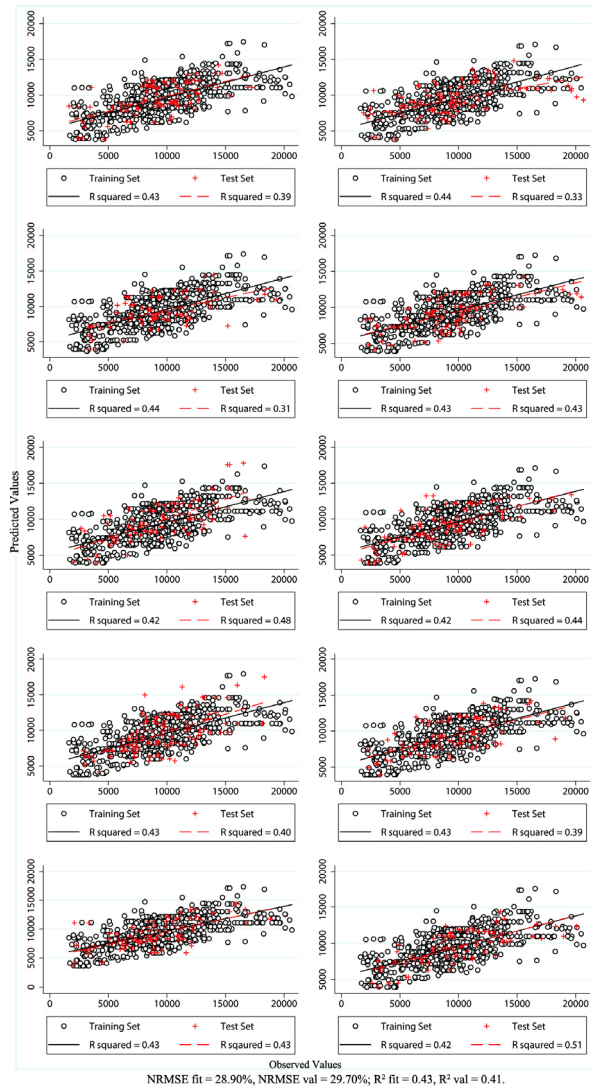


Fig. 3. Results of 10-fold cross-validation for Italian ryegrass yield prediction model used in the southern region of the Korean Peninsula, showing fit of predicted yield values for both training and test sets in relation to observed yield values (o refers to the training set, + refers to the test set).

and Fig. 3, the average coefficient of determination (R^2 fit) and the average NRMSE (NRMSE fit) for the training sets were 0.43 and 28.90%, respectively; while for the test sets, the average coefficient of determination (R^2 val) and the average NRMSE (NRMSE val) were 0.41 and 29.70%, respectively. These results indicated that the yield prediction model fit to the data set well and the accuracy of this model was in the common level.

For Model II, Fig. 4 shows the relationship between predicted and observed yield values for each partition of the 3-fold cross-validation. The results in each subfigure were segregated into training and test sets. The black bold lines are the fitting lines of the predicted and observed yield values in the training set, while the red dash lines are the fitting lines of the predicted and observed yield values in the test set. The R^2 and the NRMSE of the training sets and test sets were shown in Table 3. The

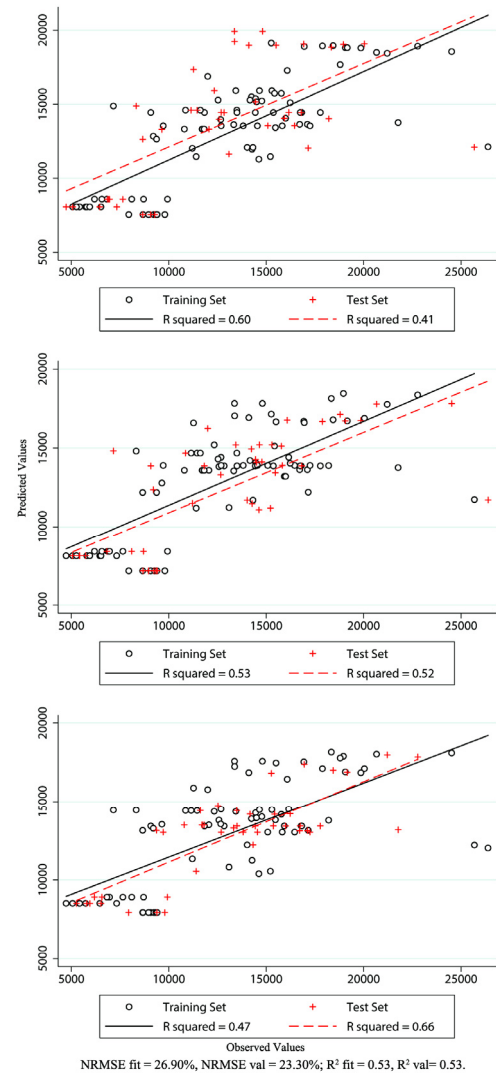


Fig. 4. Results of 3-fold cross-validation for the model for Italian ryegrass yield prediction in Jeju Island, showing fit of predicted yield values for both training and test sets in relation to observed yield values (o refers to the training set, + refers to the test set).

R^2 fit and NRMSE fit for the training sets were 0.53 and 26.90%, respectively; while for the test sets, the R^2 val and NRMSE val were 0.53 and 23.30%, respectively. These results indicated that the yield prediction model fit to the data set used well and the accuracy of this model was in the common level.

For Model III, Fig. 5 shows the relationship between predicted and observed yield values for each partition of the 10-fold cross-validation. The results in each subfigure were segregated into training and test sets. The black bold lines are the fitting lines of the predicted and observed yield values in the training set, while the red dash lines are the fitting lines of the predicted and observed yield values in the test set. The coefficients of determination (R^2) and the NRMSE of the training sets and test sets were shown in Table 4. The R^2 fit and NRMSE fit for the training sets were 0.29 and 27.06%, respectively; while for the test sets, the R^2 val and NRMSE

Table 3. Results of 3-fold cross-validation of the yield predictive model of Italian ryegrass cultivated in Jeju Island.

Iterations of cross validation	R ² of the fitting lines of the training and test sets in each validation			
	I ¹ -1	I-2	I-3	average
Training Set	59.7%	53.2%	47.4%	53.5%
Test Set	40.8%	51.5%	65.5%	52.6%

Iterations of cross validation	NRMSE ²⁾ values of the training and test sets in each validation			
	I-1	I-2	I-3	average
Training Set	0.301	0.236	0.270	0.270
Test Set	0.226	0.268	0.205	0.233

1) I: Iteration,
2) NRMSE, the normalized root-mean-square error.

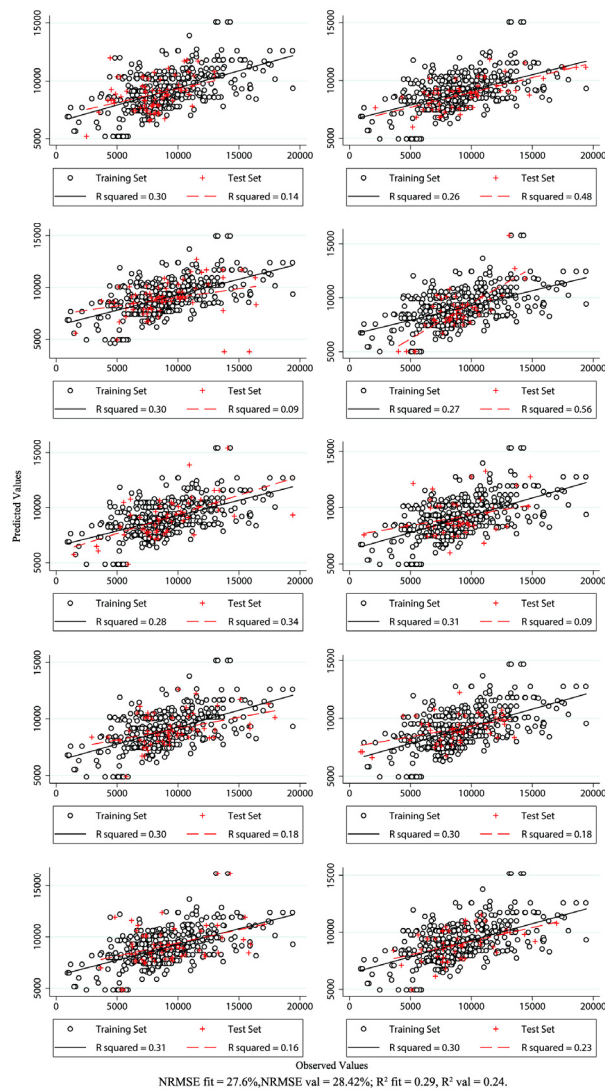


Fig. 5. Results of 10-fold cross-validation for forage rye yield prediction model, showing fit of predicted yield values for both training and test sets in relation to observed yield values (o refers to the training set, + refers to the test set).

val were 0.24 and 28.42%, respectively. These results indicated that the yield prediction model fit to the data set well and the accuracy of this model was in the common level.

Peng et al. (2017) reported a statistical yield predictive model of Italian ryegrass using a data set with smaller sample size and fewer data sources (two data sources: the results of an adaptability test of imported varieties of grasses and forage crops operated by the National Agricultural Cooperative Federation and reports on a joint research project for new plant variety development operated by Rural Development Administration), which means the variance in the data was lower than the data containing more data sources. The model’s adjusted R² was 73.6% and the results of residual diagnostics and 10-fold cross-validation of the models were in the good levels (the R² fit and NRMSE fit of the training sets: 0.75 and 15.50%; the R² val and NRMSE val of the test sets were 0.66 and 17.80%). These results showed that the fitness and accuracy of the model using low variance data were better than Model I, II, and III which used the data sets with higher variance. More data sources may lead to a larger variance in the data set and subsequently the worse fitness and accuracy of the generated models. Models with better fitness and accuracy might be constructed based on a data set with smaller variance on cultivars, data sources, cultivated locations, etc. Therefore, the standardization of the crop cultivation experiments is very necessary to decrease the variance in the data used for future yield prediction model construction for field crops.

Conclusion

In this research, the K-fold cross-validation was performed to evaluate the yield predictive models of Italian ryegrass and forage rye reported in previous studies. The results showed that the accuracy of the models were in the common level. Through comparing the results of the model with higher accuracy model, it could be concluded that models constructed based on data sets with smaller variance on cultivars, data sources, cultivated locations might have a higher coefficient of determination and better accuracy. Therefore, the standardization of the crop cultivation experiments and improvement of data accumulation is very necessary for improving modeling quality when using statistical methods.

Table 4. Results of 10-fold cross-validation of the yield predictive model of forage rye.

Iterations of cross validation	R2 of the fitting lines of the training and test sets in each validation										average
	I ¹ -1	I-2	I-3	I-4	I-5	I-6	I-7	I-8	I-9	I-10	
Training Set	26.3%	29.8%	27.4%	27.8%	30.9%	30.0%	29.6%	29.6%	30.5%	29.2%	29.1%
Test Set	48.0%	8.6%	56.3%	33.9%	8.1%	18.0%	13.5%	17.7%	15.7%	22.7%	24.3%
Iterations of cross validation	NRMSE ² values of the training and test sets in each validation										average
	I-1	I-2	I-3	I-4	I-5	I-6	I-7	I-8	I-9	I-10	
Training Set	0.270	0.269	0.280	0.273	0.271	0.269	0.272	0.270	0.268	0.263	0.270
Test Set	0.303	0.332	0.165	0.276	0.291	0.293	0.289	0.304	0.314	0.274	0.284

1) I: Iteration,

2) NRMSE, the normalized root-mean-square error.

Acknowledgments

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