CROP PRODUCTION

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USING MULTILOMIAL LOGISTIC REGRESSION TO PREDICT NITRATE NITROGEN CONTENT IN SOIL

Research article

Abstract

This paper presents a multinomial logistic regression model that allows predicting and thereby quickly determining the content of nitrate nitrogen in the 0-40 cm soil layer before sowing. To build and train the model the data of a long-term multifactorial stationary field experiment of the Siberian Research Institute of Husbandry and Chemicalization of Agriculture (SRIHCA) of the Siberian Federal Scientific Centre of AgroBioTechnologies (SFSCA) of the Russian Academy of Sciences (RAS) of the time period of 2009 -2018 were used. During the analysis of the data sample (observations), the main predictors of the model that affect the content of nitrate nitrogen in the soil (target indicator) were identified. The predictors are represented by qualitative and quantitative parameters of the working area: predecessor, tillage, weather conditions, productive moisture content in the soil before sowing, nitrate nitrogen content by appropriate gradations. The quality of the developed multinomial logistic regression model was assessed using the coefficient of determination, which was 78% according to the Nagelkerke measure, and 72% according to the Cox - Snell measure. The predictive capabilities of the trained model were evaluated. The overall proportion of correct predictions for the multinomial logistic regression is 80.6%.

Keywords: machine learning, multinomial logistic regression, nitrate nitrogen, soil.

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ИСПОЛЬЗОВАНИЕ МУЛЬТИНОМИАЛЬНОЙ ЛОГИСТИЧЕСКОЙ РЕГРЕССИИ ДЛЯ ПРОГНОЗИРОВАНИЯ СОДЕРЖАНИЯ НИТРАТНОГО АЗОТА В ПОЧВЕ

Научная статья

Аннотация

В данной работе представлена модель мультиномиальной логистической регрессии, которая позволяет прогнозировать и тем самым быстро определять содержание нитратного азота в слое почвы 0-40 см перед посевом. Для построения и обучения модели использовались данные долгосрочного многофакторного стационарного полевого опыта СибНИИЗиХ СФНЦА РАН за временной период 2009-2018 гг. В ходе анализа выборки данных (наблюдений) были выявлены основные предикторы модели, влияющие на содержание нитратного азота в почве (целевой показатель). Предикторы представлены качественными и количественными параметрами рабочего участка: предшественник, обработка почвы, погодные условия, содержание продуктивной влаги в почве перед посевом, содержание нитратного азота в соответствующих градациях. Качество разработанной модели мультиномиальной логистической регрессии оценивалось с использованием коэффициента детерминации, который составил 78% по мере Нэйджелкерка и 72% по мере Кокса - Снелла. Были оценены прогностические возможности обученной модели. Общая доля правильных прогнозов для мультиномиальной логистической регрессии составляет 80,6%.

Ключевые слова: машинное обучение, мультиномиальная логистическая регрессия, нитратный азот, почва.

1. Introduction

The size and quality of the grain crop yield depends on a complex of natural and agrotechnical factors, the leading place among which is the provision of plants with nutrients, and above all nitrogen. The yield of grain crops decreases both with a lack of nitrogen and with its excess. Therefore, determining the optimal dose of fertilizers becomes important. However, the optimal dose of nitrogen fertilizers varies greatly, since the nitrogen content is not a constant value and varies greatly depending on many factors: soil properties, predecessor, time and type of main tillage, weather conditions, etc. [1], [2], [4], [5]. In Russia, the main and more accurate method of soil diagnostics of nitrogen nutrition of field crops is the traditional method. It is carried out on the basis of soil sampling in the field and laboratory analyzes of their elemental composition. At the same time, this method has disadvantages, such as the high laboriousness of taking soil samples for analysis, especially in subsurface horizons, and the insufficient knowledge of the amount of mineral nitrogen used by plants from the lower soil layers limits the application of this approach [6], [7]. Also, chemical analyzes require a lot of time, money and are difficult to operate. Therefore, the creation of alternative methods for the rapid determination of the nitrogen content in the soil before sowing is important for agricultural land [8].

Today, global agriculture has moved to a new stage of technological development (Agriculture 4.0), which consists in the integrated introduction of digital technologies: the internet of things, geographic information systems (GIS), unmanned aerial vehicles, robotic devices, mobile applications, platform technologies for collecting, processing data and computer learning [9], [10], [11], [12].

The application of machine learning in agriculture is currently accompanied by massive interest from the global scientific community. Machine learning uses various models: linear, logistic, polynomial regression, Bayesian and neural networks, support vector machines, decision trees, random forest, k-nearest neighbors, etc., performing tasks of predictive analytics. The central essence of predictive analytics is the task of determining a predictor or several predictors (parameters or entities that affect the predicted event). Without predicting the transformation of conditions, objects and processes occurring in agriculture, it is difficult or almost impossible to make the right decision on its management. Abroad, these methods are actively used to solve the problems of agriculture, in particular, to predict the nitrogen content in the soil [13], [14], [17], [18].

Therefore, in our opinion, for a more rapid determination of the nitrogen content in the soil before sowing, as an alternative to the traditional method, it is quite possible to use various artificial intelligence methods with elements of machine learning.

The purpose of the research is to build, using machine learning methods, models capable of predicting the content of nitrate nitrogen in the soil, to evaluate the accuracy of predictive models.

2. Methods

When constructing the model, we used the data of a long-term multifactorial stationary field experiment of the SRIHCA of the SFSCA of the RAS (founded in 1981), located on the territory of the “Elitnaya” ES (experimental station), a branch of the SFSCA of the RAS of the Novosibirsk Region (central forest-steppe subzone). The data include the results of studies of a four-field grain fallow crop rotation (fallow-wheat-wheat-wheat) with different options for the main tillage from 2004 to 2018: plowing (for 1 and 3 crops by 20-22 cm, for 2 by 25-27 cm); non-moldboard tillage (non-moldboard loosening with Siberian Institute of Mechanization and Electrification (SibIME) tines for crops 1 and 3 to a depth of 20-22 cm and for crops 2 to a depth of 25-27 cm); zero processing (without autumn processing). The soil cover on which the studies were carried out is represented by medium-thick leached chernozem of medium loam granulometric composition. For modeling, we used data on the content of nitrate nitrogen in the 0-40 cm soil layer before sowing.

The construction of multinomial regression was carried out using the software package of modules SPSS version "26". When modeling, 80% of the data from the original sample were used to train the models, 20% as testing. The dimensionality of the level of nitrate nitrogen in the soil was set in accordance with the scale of A.E. Kochergi

3. Results

The construction of the multinomial logistic regression (MLR).

To predict the target indicator - the content of nitrate nitrogen (N-NO3 in kg/ha of soil), we studied the relationship of this indicator (dependent variable) from independent variables (factors). At the same time, both qualitative factors were taken into account: the predecessor, the method of tillage, and quantitative ones, which characterize the weather conditions and the reserves of productive soil moisture before sowing.

Qualitative (categorical) factors have the following gradations (categories):

1. Tillage with three gradations - plowing, non-moldboard, no-tillage;
2. Predecessor with four gradations - fallow, first fallow wheat, second fallow wheat, third fallow wheat

Quantitative factors include weather conditions, namely the sum of active air temperatures > 0° (greater than zero degrees) and precipitation for the periods: September-November, March-April, the content of productive moisture in a meter layer of soil before sowing agricultural crops.

The dependent variable can be classified as a categorical one, with nitrate nitrogen values of 0-40 cm described by three gradations: very low from 0-25 kg/ha, low 25-50 kg/ha, higher than 50 kg/ha.

Since the dependent variable N-NO3 is categorical and takes on the values of the listed 3 categories, the required dependence cannot be obtained using conventional regression approaches. In this case, the required dependence can be obtained using the multinomial logistic regression (MLR) model [19], [20].

In the multinomial logistic regression model, one of the categories of the dependent variable is declared the pivot (reference), and all other categories are compared with it. The independent variables can be categorical or quantitative. The multinomial logistic regression level predicts the probability that the dependent variable will belong to categories based on the values of the independent variables. The final choice of the predictive category for the dependent variable is made according to the rule of the greatest probability of membership.

To obtain the parameters (coefficients) of the multinomial logistic regression, a data sample was used, formed in the form of a table of 96 observations (rows) and 8 factors (columns), including the dependent variable. Moreover, according to the nitrate nitrogen content, the observations are distributed as follows: very low (code 0) - 30, low (code 1) - 47, higher kg/ha 50 (code 2) - 19. The category of the average content of nitrate nitrogen was chosen as the pivot category.

Let us briefly describe the multinomial logistic regression model. It is assumed that there is a series of N observations. Each observation consists of a set of m independent variables Xi, i=1, ... m (also called predictors) and the corresponding categorical value of the dependent variable Yj, j=1,…K, which can take one of K possible values (categories) . For each category of the dependent variable (with the exception of the pivot variable), a binary logistic regression equation is constructed, which determines the ratio p_j - the probability of referring the observation under consideration to this category to the probability for the pivot category - p1:

$$\ln\left(\frac{p_j}{p_1}\right) = \alpha_j + \sum_i \beta_j^i X_i, j = 2, \dots K \tag{1}$$

where αj – α is a constant, βji - the regression coefficient associated with the ith independent variable for category j

The unknown coefficients αj, βji, j=2…K , i=1, ... m are jointly estimated for the entire sample of observations by the maximum a posteriori estimate (MAP), which is an extension of the maximum likelihood using regularizing weights. Solution is found iteratively by Minimizing Revised Least Squares (IRLS) [20], [21], [22].

Using formula (1) and the fact that the sum of all K probabilities should be one, we obtain the desired probabilities of belonging to categories:

$$p_1\text{=}1/(1\text{+}\textstyle\sum_j \exp(\alpha_j + \sum_i \beta_j^i X_i)) \tag{2}$$

and

$$p_j = exp(\alpha_j + \sum_i \beta_j^i X_i)/(1 + \sum_j exp(\alpha_j + \sum_i \beta_j^i X_i)), \text{для } j = 2, \dots K \tag{3}$$

Table 1 shows the values of the multinomial regression coefficients, their exponential values and estimates of the significance of factors obtained using Wald statistics.

Table 1 – Estimation of parameters (coefficients) of logistic regression

N-NO3 by category[a]	Predictors	Coefficients of variables (B)	The significance of the coefficient (P)	Exp-exponent (B)
0	Total precipitation, mm (September-November)	0,270	0,157	1,310
	Total precipitation, mm (December-February)	-1,069	0,054	0,343
	Total precipitation, mm (March- April)	3,425	0,048	30,729
	Sum of temperatures >0° (September-November)	-0,017	0,067	0,983
	Sum of temperatures >0° (March-April)	0,176	0,000	1,192
	The content of productive moisture before sowing in the soil layer (0-100 cm), mm	-0,055	0,594	0,946
	Predecessor first fallow wheat	-14,819	0,029	3,7363E-07
	Predecesso second fallow wheat	-11,530	0,122	1,01301E-05
	Predecessor third fallow wheat	-13,818	0,017	1,01563E-06
	Predecessor fallow	-24,202	0,011	3,09082E-11
	Tillage non-moldboard	1,151	0,504	3,161
	Tillage plowing	-,455	0,051	0,634
	Tillage no-tillage	0[c]	-	-
1	Total precipitation, mm (September-November)	0,320	0,213	1,377
	Total precipitation, mm (December-February)	-1,027	0,047	0,358
	Total precipitation, mm (March- April)	3,173	0,033	23,889
	Sum of temperatures >0° (September-November)	-0,013	0,998	0,987
	Sum of temperatures >0° (March-April)	0,179	0,000	1,196

End of table 1 – Estimation of parameters (coefficients) of logistic regression

N-NO3 by category[a]	Predictors	Coefficients of variables (B)	The significance of the coefficient (P)	Exp-exponent (B)
1	The content of productive moisture before sowing in the soil layer (0-100 cm), mm	-0,046	0,651	0,955
	Predecessor first fallow wheat	-14,548	0,0526	5,04348E-07
	Predecessor second fallow wheat	-12,049	0,046	6,14421E-06
	Predecessor third fallow wheat	-13,675	0,034	1,2405E-06
	Predecessor fallow	-21,652	0,051	4,1614E-10
	Tillage non-moldboard	0,130	0,933	1,139
	Tillage plowing	-1,013	0,019	0,363
	Tillage no-tillage	0[c]	-	-

Note: a – pivot category 2; c – this parameter is set to zero because it is redundant

From the formula (3) for assessing the probability of belonging to categories, it follows that predictors with significant negative coefficients reduce the probability of this category in relation to the pivot category, and predictors with positive coefficients, on the contrary, increase the probability of this category. The degree of influence of predictors on the calculated probabilities of belonging to the categories is indicated by the exponential values of the corresponding coefficients given in the last column of the table.

Large values of the absolute value of the coefficients of predictors indicate the significance of these factors. If the significance of the P coefficient <0.05, then the relationship is statistically significant. The result $P> 0.05$ indicates that the relationship between the variables is weak or not found. The table shows that the most significant are the following factors: the predecessor, the amount of precipitation and temperature (March-April), the amount of precipitation (December-February), tillage.

To assess the quality of a conventional linear regression model, the R-squared indicator is used, which describes the part of the variance that can be explained using regression. In the case of multinomial logistic regression, this role is played by the Pseudo R-squared indicator. The most common are the measures proposed by Nagelkerke, Cox - Snell. In our case, the explained part of the variance is 78% according to the Nagelkerke measure (usually the most used), and 72% according to the Cox - Snell measure, which indicates the high predictive capabilities of the method.

As a criterion for evaluating the predictive model, the value of the deviation (error) of the actual content of nitrate nitrogen from the predicted one was determined. Table 2 presents the comparative predictive abilities of this method, tested on the original sample.

Table 2 – Classification table of the multinomial logistic regression model

Number of observations	Predicted			% correct predictions
	very low 0-25 kg/ha	low 25-50 kg/ha	higher than 50 kg/ha	
very low 0-25 kg/ha (30)	21	9	0	69,7
low 25-50 kg/ha (47)	6	38	3	81,1
higher than 50 kg/ha (19)	0	1	18	95,5
Overal share	–	–	–	80,6

For a sample of observations with a very low content of nitrate nitrogen (0-25 kg/ha), the proportion of correct forecasts was 69.7%, of which 21 observations were correctly predicted, 9 forecasts were incorrect, which fell into the category of low content (25-50 kg/ha). For the low nitrate nitrogen category, 38 observations out of 47 were correctly predicted, with a percentage of correct predictions of 81.1%. The highest percentage (corresponds to 95.5) of correct forecasts is in the gradation higher than 50 kg/ha, out of 19 observations, 1 observation was incorrectly predicted belonging to the low content category. The total share of correct forecasts for all categories is 80.6%.

Thus, given the small size of the statistical sample and the small number of predictors, the predictive properties of the tested model can be considered satisfactory.

4. Conclusion

In the course of the study, using multinomial logistic regression, a model was built and trained that allows you to quickly determine (predict) the content of nitrate nitrogen before sowing in a 0-40 cm soil layer with acceptable reliability, using only data on weather, tillage, predecessor and stock productively moisture before sowing. Based on the forecast, it is possible to plan and develop recommendations on approximate rate of application of fertilizer application, depending on the predicted gradation, a possible increase in yield from fertilizers.

In the future, it is planned to improve the quality of the models by adding other predictors that affect the resultant trait, to search for machine learning methods that allow the analysis of small data.

Conflict of Interest

None declared.

Конфликт интересов

Не указан.

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