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APPLICATION OF LINEAR AND DECISION TREE METHODS IN ASSESSING THE INFLUENCE OF METEOROLOGICAL FACTORS AND CROP ON THE LEVEL OF AIRBORNE CLADOSPORIUM SPORES

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The article analyses the influence of environmental factors on the concentration of spores of the Cladosporium fungi in the atmospheric air of Zaporizhzhia in 2016-2020. The seasonal characteristics of fungi spores were analysed: total number of spores; the beginning, duration, and end of the season; maximum value in spores/m^3 and the day it was recorded; average day; the number of days that was equal to or exceeded the clinical value (3000 spores/m^3). The total number of Cladosporium spores in the period from 2016 to 2020 was 552,470 spores/m^3. The highest level of spores – 157904 spores/m^3 and the highest daily concentration – 5928 spores/m^3 were recorded in 2019. In the same year, the number of days that exceeded the clinical threshold was 13. This is the highest number in all 5 years of monitoring. In contrast, the lowest number of spores was counted in 2020. The total number was 30986 spores/m^3, and the daily concentration was 1470 spores/m^3. The earliest season started in 2020 and lasted the longest – 166 days. The shortest season lasted 145 days in 2016. Forty five parameters were studied, including 42 meteorological parameters (temperature, pressure, temperature and dew point difference, 16 wind directions, 5 meteorological phenomena in 4 different time intervals of 6 hours (00-05, 05-11, 11-17, 17-23), and 3 types of clouds. The other 3 are crop parameters: daily harvested areas of barley, wheat, and sunflower. Linear regression with two regularisation methods (Ridge regression and The lasso) and decision tree methods (Bagging, Random forests, Boosting, BART) were used to investigate the relationship between Cladosporium spore levels and weather conditions and agricultural activity. The cross-validation mean squared error (CV MSE) was determined to determine the best model and assess the importance of the parameters. The best linear model includes 8 parameters (temperature, pressure, westerny wind, humidity, low-level clouds, fog, the area of daily barley and sunflower harvest). The best decision tree is Bagging. The most meaningful parameters are: dew point, temperature, area of daily harvest of barley and sunflower, pressure, west wind). *Key words:* taxonomic groups, micromycetes, fungi, moulds, fungal spores, Cladosporium, meteorological conditions, sunflower, barley, wheat, yield, human health, correlation, regression.

Застосування лінійних методів та методів на основі дерев рішень у оцінці впливу метеорологічних факторів та врожаю на рівень повітряних спор Cladosporium. Гавриленко К. В.

У статті проаналізовано вплив факторів навколишнього середовища на концентрацію спор грибів роду Cladosporium в атмосферному повітрі м. Запоріжжя у 2016-2020 роках. Проаналізовано сезонні характеристики спор грибів: загальна кількість спор; дата початку та кінця сезону; тривалість сезону, максимальна добова кількість спор та день, коли реєструвалась максимальна кількість спор; середній день; кількість днів, коли концентрація спор дорівнювала чи перевищувала порогове значення (3000 спор/м^3). Загальна кількість спор за 2016-2020 роки склала 552470 спор\м^3. Найбільша кількість спор – 157904 спор/м^3 та найвища добова концентрація – 5928 спор/м^3 реєструвалась у 2019 році. В цьому ж році, кількість днів, яка перевищувала клінічне порогове значення склала 13 днів. Це найбільша кількість за усі 5 років моніторингу. Натомість, у 2020 році було підраховано найнижчу кількість спор. Загальна кількість склала – 30986 спор/м^3, а добова концентрація – 1470 спор/м^3. Найраніше, сезон розпочався у 2020 році та тривав найдовше – 166 днів. Найкоротший сезон тривав 145 днів у 2016 році. Було досліджено 45 параметрів, серед яких 42 – метеорологічні параметри (температуру, тиск, різницю температури і точки роси, 16 напрямів вітру, 5 метеофеноменів у 4 різні проміжки часу по 6 годин (00-05, 05-11, 11-17, 17-23), та 3 види хмар. Інші 3 – параметри врожаю: добові площі збору ячменю, пшениці та соняшника. Для дослідження зв’язку рівню спор Cladosporium з погодними умовами та сільськогосподарською активністю було використано лінійну регресію з двома методами регуляризації (Ridge regression and The lasso), а також методи дерев рішень (Bagging, Random forests, Boosting, BART). Було визначено середню квадратичну похибку, отриману шляхом кросвалідації (CV MSE) для визначення кращої моделі і для оцінки важливості параметрів. Найкраща лінійна модель включає в себе 8 параметрів (температура, тиск, західний вітер, вологість, хмари низького рівня, туман, площа добового збору ячменю та соняшнику) Найкраще дерево рішень – Bagging. Найбільш значущі параметри: точка роси, температура, площа добового збору ячменю і соняшника, тиск, західний вітер). *Ключові слова:* таксономічні групи, мікроміцети, гриби, плісняві гриби, спори грибів, Cladosporium, метеорологічні умови, соняшник, ячмінь, пшениця, урожайність, здоров’я людини, кореляція, регресія

The spores of microscopic fungi, micromycetes, are the predominant component of atmospheric air. They arouse great interest among scientists and doctors due to their impact on human health, namely to their ability to contribute to the development and aggravation of allergic diseases [1, 2]. The leading taxonomic group of fungi in many European countries [3] and in Ukraine [4] in particular are fungi of the genus Cladosporium. Sensitisation to Cladosporium is often associated with severe asthma, allergic rhinitis and less frequently with chronic urticaria and atopic eczema [5]. It has been reported that high airborne spore concentrations can lead to exacerbation of allergic symptoms and increased incidence of hospitalisations associated with asthma exacerbation [6, 7]. Therefore, the research of the dynamics of fungal spores and the impact of meteorological factors and agricultural activity on their level is quite relevant today.

The aim of the study is to investigate the influence of meteorological conditions and agricultural activity on the concentration of spores of the Cladosporium fungi using linear and decision tree methods.

Connection of the author's research with important scientific and practical tasks. The study was conducted at the Aerobiology Laboratory based at the Department of Medical Biology, Parasitology and Genetics of Zaporizhzhia State Medical and Pharmaceutical University as a part of the topic «Aerobiological studies of the formation of the dangerous aeropalynological situation in the city of Zaporizhzhia» (state registration number 0115U003878). Up-to-date information on aeroallergenic pollution and forecasts are displayed on the website of the European Aerobiology Society (https://ean.polleninfo.eu/) and used by specialists for the treatment and prevention of allergic diseases.

Analysis of recent researches and publications. The influence of meteorological factors on the level of fungal spores in the air is widely studied. According to the literature, the most important environmental factors are temperature, humidity, precipitation, atmospheric pressure, ultraviolet radiation, wind direction, and insolation. Sind at al. consider average temperature and precipitation to be the most significant factors affecting the level of spores in the air. In contrast, relative humidity, duration of sunlight, wind speed and direction, in their studies, showed no correlation, except for one monitoring station where the annual amount of sunlight had a positive effect on the level of Cladosporium spores [8]. The average temperature was the most important meteorological parameter that positively influenced the concentration of Cladosporium spores in the air in the study by Kasprzyk et al. The authors also reported that the maximum air temperature had the least influence. Humidity and wind speed had a minor impact on the level of spores [9]. The average temperature had the largest contribution to the spore load in the studies by Grinn-Gofron & Bosiacka [10] and Grinn-Gofroń & Rapiejko [11]. The negative effect of precipitation was noted in the study by Recio et al. and the positive correlation was observed with the temperature and insolation [12].

The literature also reports the role of summer storms and ozone concentrations in the air. This gas occurs in the lower atmosphere during thunderstorms and is formed in the polluted air of large cities. It is noted that the concentration of Cladosporium spores increases before a thunderstorm, and during and after it, a decrease in their concentration is observed. This means that the increase in spore levels is caused by an increase in temperature and ozone concentration before the storm, and the decrease in spore levels is caused by a decrease in these parameters during and after the storm [13].

The effect of wind on spore concentration is studied somewhat less. Different contributions of regional and local winds to the spore load was reported [14, 15]. However, this parameter requires further study.

The concentration of Cladosporium spores also depends on the geographical location, vegetation, and the level of urbanisation. The level of spores was studied in urban, rural and mountain environments. The highest concentration was found in the urban region [16, 17]. Olsen et al. noted the role of agricultural activity on the spore levels. Harvesting of grain crops was a possible cause of the peak concentrations of Cladosporium [18].

Since, despite the large number of studies, the meteorological factors that affect the level of Cladosporium spores are not precisely defined and ambiguous, it is quite relevant to study this issue in the area of our region with its inherent weather conditions and other predictors.

The specification of previously unresolved parts of the general problem, the article is devoted to. This article is devoted to the study of the influence of meteorological conditions and agricultural activity on the level of spores of the Cladosporium fungi in the air of Zaporizhzhia city.

Novelty. It is the first time, when the analysis of seasonal dynamics of spores of the Cladosporium fungi in the atmospheric air of Zaporizhzhia city was carried out on the basis of five-year aeromonitoring.

Methodological and scientific significance. The results of the study can be used to improve the effectiveness of fungal allergy and bronchial asthma prevention measures by studying the causes that lead to changes in the concentration of fungal spores and developing modern methods for predicting the aeroallergenic situation for timely warning of the population.

Materials and methods. The study was conducted in the aerobiology laboratory at ZSMPhU from 1 March to 31 October over a five-year period. The data were obtained using a 7-day Hearst-type volumetric sampler calibrated to take air samples at a rate of 10 l/min. The device was installed on the roof of the educational building No. 3 of ZSMPhU at a height of approximately 30 m above ground level. The sampler drum was changed weekly. The adhesive tape on which the samples were taken was cut into 7 fragments after exposure, each of which corresponded to one day of observation. Before analysis, the slides were coated with a glycerol-fuchsin mixture. The samples were analysed under a light microscope at a magnification of x400. Spore identification and counting were limited to genus levels. The final number of spores was expressed as the concentration of spores per cubic metre of air.

To identify the peculiarities of seasonal distribution of spores, the following characteristics were analysed:

– total number of spores, calculated as the sum of daily spore concentrations during the observation period;

– the beginning, duration, and end of the season, determined by the 90% method (Nilsson and Persson 1981);

– maximum value in spores/m^3 and the day it was recorded;

– average day – 50th percentile;

– the number of days that was equal to or exceeded the clinical value (3000 spores/m^3).

The meteorological data were obtained from the weather station located at Zaporizhzhia airport. Agricultural activity was analysed using open data from the Department of Agricultural Development and the State Statistics Service of Ukraine. The analysis was carried out using the R programming language environment.

A total of 45 parameters were analysed, including 42 meteorological parameters:

– average daily temperature, pressure, temperature difference and dew point (an indicator of air humidity);

– average daily wind speed in 16 directions;

– the presence of meteorological phenomena (fog, rain, downpour, thunderstorm, precipitation) in 4 different time periods (00-05, 05-11, 11-17, 17-23);

– the presence of different types of clouds (high, medium and low – CH, CM, CL);

And 3 crop parameters: daily harvested areas of barley, wheat and sunflower.

Linear regression with two regularisation methods (Ridge regression and The lasso) and Decision Trees-based methods (Bagging, Random forests, Boosting, BART) were used to investigate the relationship between Cladosporium spore levels and environmental factors. 10 Fold Cross-validated mean squared error was used in order to evaluate the performance of different statistical methods and to select the appropriate level of flexibility.

Due to increases and decreases of variation during the year, the Cladosopium distribution shows positive skewness. To stabilise its variation and reduce the impact of outliers, the logarithmic transformation was amplified. Presentation of the main material.

Results. The total number of Cladosporium spores in the period from 2016 to 2020 was 552,470 spores/m^3.

The Cladosporium season in 2016 started on 12 May, lasted 145 days and ended on 4 October. The maximum number of spores was recorded on 24 July with a value of 4212 spores/m^3. The annual number of spores was 124,611 spores/m^3. The number of days when the spore concentration exceeded the clinical threshold was 8.

In 2017, the season started on 14 May, lasted 155 days and ended on 16 October. On 14 June, the maximum value of Cladosporium was recorded, which was 5145 spores/m^3. In total, 12,286 spores/m^3 were counted during the year. The number of days when the spore concentration exceeded the clinical threshold was 8.

In 2018, the season started on 29 May, the latest in the entire observation period, and ended on 28 October. The season lasted 152 days. On 28 June, the peak value was 5117 spores/m^3. In total, 117683 spores/m^3 were counted during the year. Only 5 days a year the spore concentration exceeded the clinical threshold.

In 2019, the season for Cladosporium began on 9 May. It lasted 149 days and ended on 5 October. Over the whole period of observation, it was in 2019 that the highest daily number of spores was recorded, which was 5928 spores/m^3 on 27 July, and the highest number of days (13) when the spore level was equal to or above the clinical threshold. The total number of spores was 157904 spores/m^3, which was also the highest value for the entire monitoring period.

In 2020, the season started the earliest – on 27 April – but lasted the longest – 166 days. The season ended on 10 October. In total, 30986 spores/m^3 were counted this year, the lowest value in the five-year monitoring period. The peak value of Cladosporium spores this year was also the lowest, at 1470 spores/m^3 on 14 June. There were no days when the number of spores exceeded the thresholds.

According to open data from the Department of Agricultural Development and the State Statistics Service of Ukraine, the main crops planted in Zaporizhzhia region are barley, wheat and sunflower. The total area under these crops is approximately 1,400 thousand hectares (Zaporizhzhia region covers 2,700 thousand hectares), which suggests that this biomass is important as the main source of the spore spread. In the period from 2016 to 2020, the sown area of barley remained almost unchanged (fig.1), but there was the decrease in the sown area of sunflower (from 602 thousand hectares in 2016 to 526 thousand hectares in 2020). On the other hand, the area under wheat increased every year (from 536 thou hectares in 2016 to 664 thou hectares in 2020).

The fig. 2 shows the daily harvest in different years. Harvesting of winter crops generally begins in mid-June. Spring crops are harvested in early September. Harvesting dynamics are usually uneven due to the influence of weather factors, which can shift the harvesting periods in different parts of the region.

The linear model, which included all 45 parameters, has R2 = 0.38, F-statistics = 9.8, which indicates the presence of important parameters. The cross-validated error was 1.171.

For computational reasons, best subset selection cannot be applied with 45 parameters (The number of possible models that must be considered is 2 in the 45 degree). Thus, we applied the stepwise selection method available in R environment, which explore a far more restricted set of models and uses Bayesian information criterion (BIC) to indirectly estimate their performance (fig. 3, fig. 4).

Each row of the plot 1 contains a black square for each variable selected according to the optimal model. We can see that several models share a BIC close to

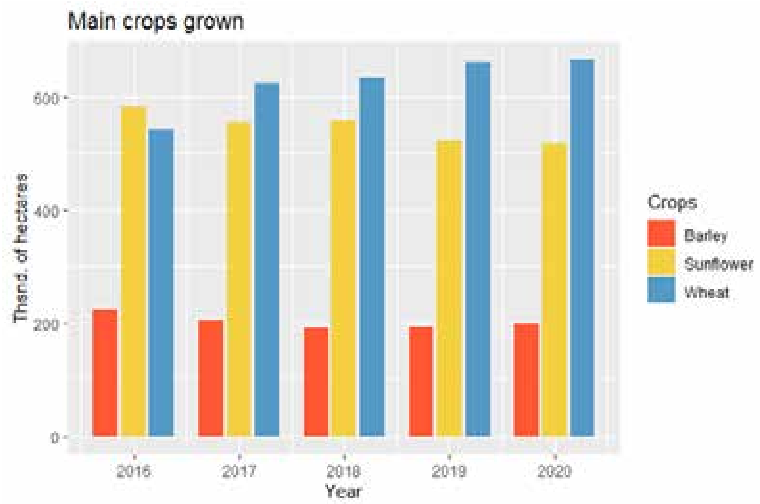


Fig. 1. Total harvested area of the main crops planted in Zaporizhzhia region

Fig. 2. Seasonal harvest area by agricultural crops

–260. However, the model with the lowest BIC is the eight-variable model that contains only Temperature, Pressure, Dew point, West wind, Fog at 00-06 AM and Wheat harvested area with positive coefficients as well as Sunflower area and CL (low level) clouds with negative coefficients (fig. 5). The cross-validated error was 1.1, which is a slight improvement over the full linear.

It is worth noting that these parameters are often present in models of different sizes, which further indicates their influence on the concentration of fungal spores.

We also used alternative methods of variable selection, such as Ridge regression and The Lasso. As with least squares, Ridge regression minimize the residuals sum but also adds the shrinkage penalty to the equation. This penalty is small only when regression coefficients are close to 0. The tuning parameter λ serves to control the relative impact of new term on the coefficient estimates. When λ =0, the penalty term has no effect, and ridge regression will produce the least squares estimates. However, as λ grows, the impact of the shrinkage penalty grows as well, and the ridge regression coefficient estimates will approach zero. In the case of the Lasso, some of the coefficient's estimates will be exactly equal to zero when the tuning parameter λ is sufficiently large.

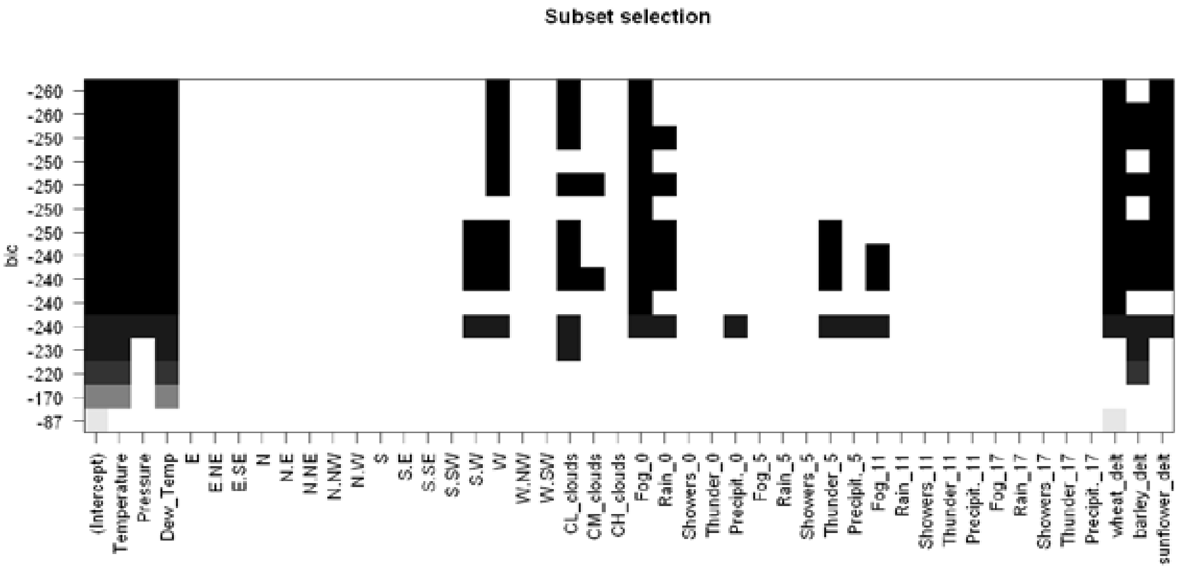


Fig. 3. Stepwise regression results

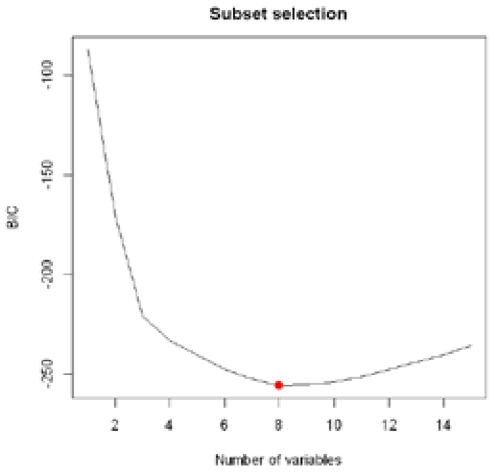
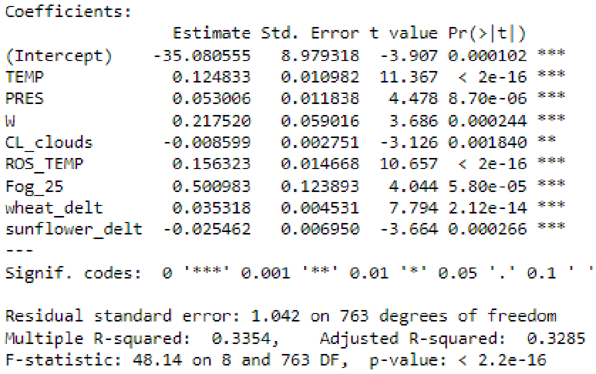


Fig. 4. MSE changes with the number of parameters



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Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)   -35.080555   8.979318  -3.907 0.000102 ***
TEMP            0.124833   0.010982  11.367  < 2e-16 ***
PRES            0.053006   0.011838   4.478 8.70e-06 ***
W               0.217520   0.059016   3.686 0.000244 ***
CL_clouds      -0.008599   0.002751  -3.126 0.001840 **
ROS_TEMP        0.156323   0.014668  10.657  < 2e-16 ***
Fog_25          0.500983   0.123893   4.044 5.80e-05 ***
wheat_delt      0.035318   0.004531   7.794 2.12e-14 ***
sunflower_delt -0.025462   0.006950  -3.664 0.000266 ***
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Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.042 on 763 degrees of freedom
Multiple R-squared:  0.3354,    Adjusted R-squared:  0.3285
F-statistic: 48.14 on 8 and 763 DF,  p-value: < 2.2e-16
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Fig. 5. The best line model with 8 parameters, selected by stepwise regression

Unlike least squares, which generates only one set of coefficients estimates, ridge regression produce a different set of coefficients estimates for each value of λ. We used 10-fold cross-validation to select best λ for both methods.

Figure 6 shows cross-validated error that result from applying Ridge regression and the Lasso with various values of λ. Top axis shows how many coefficients left after the shrinkage.

We can see that the Ridge regression does not give a significant result and the residual is the lowest when no shrinkage occurs. Instead, The Lasso reaches a minimum at $\lambda = 0.001$ (or $\log(\lambda) = -3.5$), when only 28 coefficients are not equal to 0. Among them are all 8 variables selected by the stepwise method, as well as the coefficients for meteorological phenomena, mostly with negative values.

The error of the Ridge regression was 1.198, the Lasso regression was 1.133, which is a slight improvement over the full model, but worse than the 8-variable model obtained by stepwise regression.

Using the results of the 8-variable linear regression as a starting point, we moved on to applying methods based on Decision Trees. Such models are more flexible and able to detect nonlinear relationships among the parameters, and unlike more complex non-parametric methods, they retain a wide range of possibilities for interpreting the results. Building the Regression Tree involves stratifying the predictor space into a number of simple regions. Each region uses the mean response value for the training observations in the region to which it belongs.

The usual Regression tree is shown in figure 7. The optimal size of the tree was determined by cross-vali-

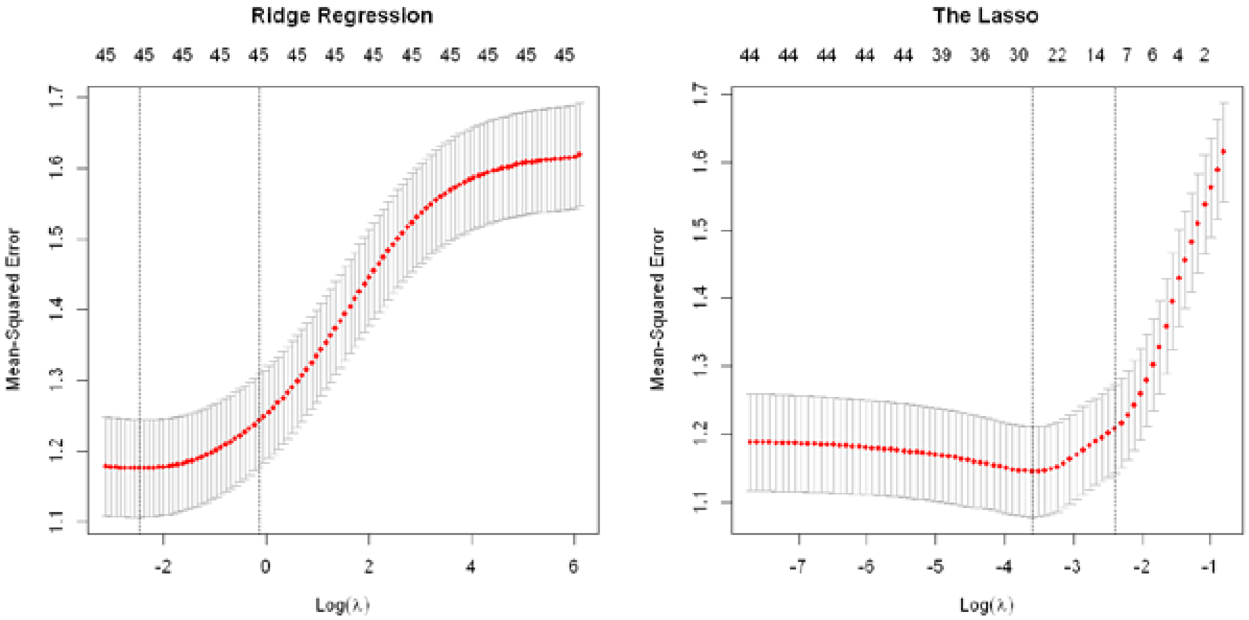

Fig. 6. Penalty impact on MSE in Ridge Regression and The Lasso

dation and amounted to 11 internal nodes. The most important parameters are those that form the top of the tree. The increase in pollen concentration was always observed during the barley and wheat harvesting periods, and partially during the sunflower harvesting periods, when favorable weather conditions were present – south wind, high pressure, high temperature and humidity, and morning fog. The cross-validation error was 1.176

Decision Trees generally do not have the same level of predictive accuracy as some other regression approaches. Additionally, trees can be very non-robust, in a sense that a small change in the data can cause a large change in the estimated tree. By aggregating many decision trees, using methods like Bagging, Random Forests, Boosting, and Bayesian Additive Regression Trees (BART), the

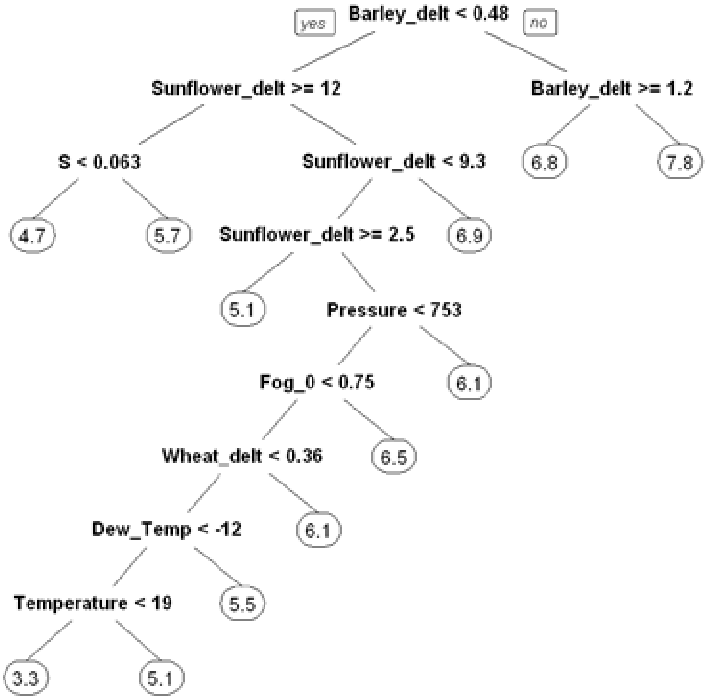

Fig. 7. Simple (pruned) regression decision tree

predictive performance of trees can be substantially improved.

Each of these approaches involves producing multiple trees which are then combined to yield a single consensus prediction.

Using the 500-tree bagging method, we achieved a reduction in cross-validation error to 0.898 (46.34% Variance explained), which is a significant improvement over the 8-variable linear model. Although the bagged trees is much more difficult to interpret than a single tree, we can obtain an overall summary of the importance of each predictor using the residuals sum. The left measurement on figure 8 shows the total amount that the RSS is decreased due to splits over a given predictor, averaged over all 500 trees. The right is a measure of the total decrease in node impurity (node is considered to be of high purity if the observations are split equally) that results from splits over that variable.

The importance of barley, wheat and sunflower harvested area, as well as temperature, dew point and pressure, is significantly higher than the other variables, which is consistent with the results of other approaches.

As in bagging, we build a number of decision trees on bootstrapped samples. Each time a split is considered, a random sample of predictors is chosen as split candidates, allowing decorrelate the trees. In this study, 15 parameters were used and the error was 0.931.

Boosting works in a similar way to bagging, except that the trees are grown sequentially: each tree is grown using residuals from previously grown trees. Thus, each new tree attempts to capture signal that is not yet accounted for by the current set of trees. Using this method, the error was 1.03.

Another ensemble method, BART, based on Bayesian statistics and related to random forests and boosting, was also used. When using this method, the error was 1.04.

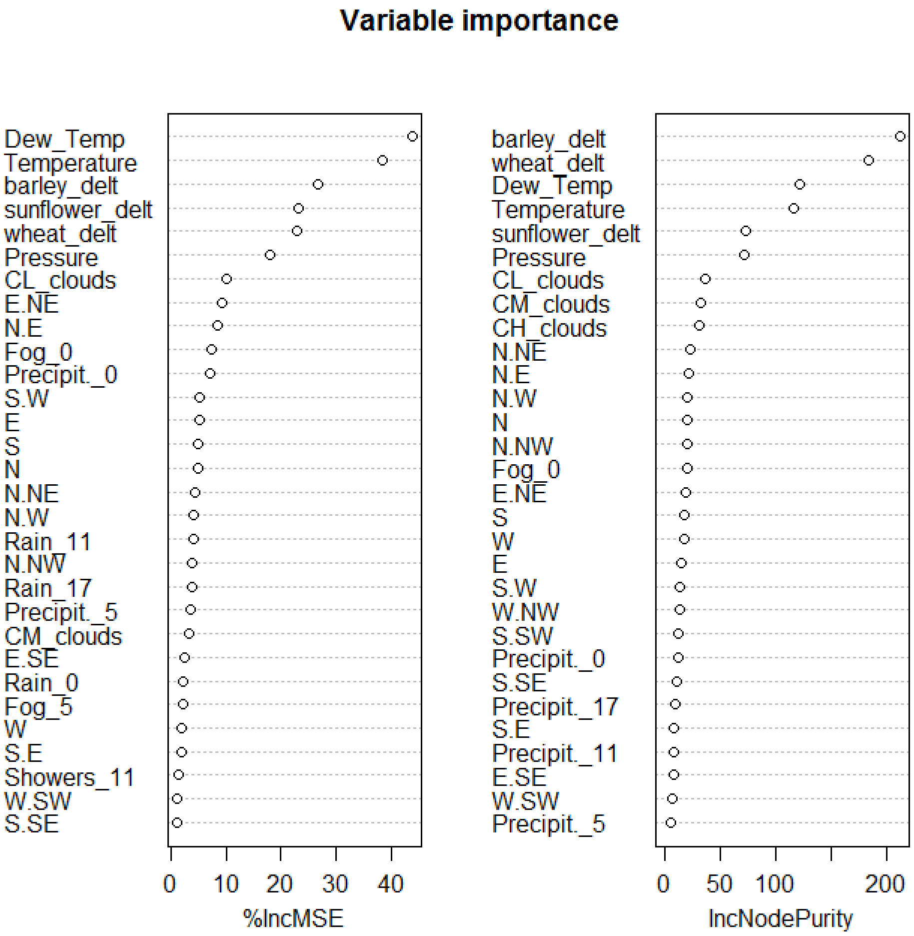

Fig. 8. Variable importance measurement in a bagged Disicion Tree model

Conclusions.

1.The most meaningful parameters according to the results of stepwise regression were: temperature, pressure, westerly wind, humidity, low-level clouds, fog, area of daily harvest of barley and sunflower.

2. The most meaningful parameters according to the results of Bagging. decision tree were: dew point, temperature, area of daily harvest of barley and sunflower, pressure, westerly wind.

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