npj | science of food

Article

Published in partnership with Beijing Technology and Business University

https://doi.org/10.1038/s41538-024-00310-w

Prediction of deoxynivalenol contamination in spring oats in Sweden using explainable artificial intelligence

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Weather conditions and agronomical factors are known to affect Fusarium spp. growth and ultimately deoxynivalenol (DON) contamination in oat. This study aimed to develop predictive models for the contamination of spring oat at harvest with DON on a regional basis in Sweden using machine-learning algorithms. Three models were developed as regional risk-assessment tools for farmers, crop collectors, and food safety inspectors, respectively. Data included: weather data from different oat growing periods, agronomical data, site-specific data, and DON contamination data from the previous year. Results showed that: (1) RF models were able to predict DON contamination at harvest with a total classification accuracy of minimal 0.72; (2) good predictions could already be made in June; (3) rainfall, relative humidity, and wind speed in different oat growing stages, followed by crop variety and elevation were the most important features for predicting DON contamination in spring oats at harvest.

Oats can be susceptible to fungal infection of Fusarium spp. and subsequent deoxynivalenol (DON) contamination during the cultivation season[1,2]. The presence of DON in oats-derived feed and food can affect human and animal health[3]. In Europe, the European Commission has set maximum legal limits (1750 µg/kg) for the presence of DON in unprocessed durum wheat and oats[4], and has defined maximum recommendation thresholds (8000 µg/kg) for the presence of DON for cereals and cereal products (with the exception of maize by-products) used for feed (Commission, 2006b). In Sweden, DON concentrations were too high to be fit for human consumption in half of all oats in 2011 and, since then, DON contamination of oats has gained significant attention (Hartman et al., 2021). After 2011, almost all oat products are monitored for DON contamination, which generates a high cost to stakeholders such as farmers, crop collectors, and food safety authorities. Early forecasting of the high-contamination regions of DON in oats at the regional (grid) level could provide timely advice on the need for crop protection and for risk-based monitoring to reduce the chance of contaminated oats entering the food chain and reduce the monitoring costs.

Weather conditions, such as temperature, relative humidity, and precipitation, have a significant effect on the presence of DON contamination in oats[5]. This is because weather conditions affect the life cycle of toxigenic fungi, influence the interaction between the pathogen and host, and the pathogen's ability to produce DON[6,7]. Apart from weather conditions, agronomical factors could directly or indirectly promote the infection of Fusarium spp. in grains. These factors may include crop variety, crop rotation (pre-crop and pre-pre-crop), soil type, elevation, and geolocation of the fields[8–11].

Previous studies aimed at developing prediction models for DON in oats have used weather data[5,12–14]. Only considering weather data may limit the model's application in different regions or farms with different oat agronomic practices. One study concluded that DON prediction in oats could be improved using agronomic factors with weather-based risk index outputs[5]. To date, only a few studies have used weather variables combined with agronomic and site-specific variables for early forecasting of DON contamination in oats. Also, for the prediction of DON in wheat, it has been reported that not considering agronomic and site-specific factors may restrict the model's application across different regions with varying wheat cultivation methods[15].

Apart from the data available for model development, the model algorithm used also affects the model performance. A study from Lindblad, et al.[16] who aimed to predict DON in oats, stated that very little of the variation in DON could be explained by weather conditions using a statistical model. In addition to statistical models, machine learning has been proven to be of added value in the prediction of mycotoxins in grains[17–20]. One of these cited studies has applied a deep neural network to predict mycotoxin contamination in maize and concluded that the machine learning approach has added value to classical statistical approaches (i.e., simple or multiple linear regression models)[20]. One study applied the random forest algorithm to predict multi-mycotoxin occurrence in wheat in Europe with >90% accuracy[17]. Another study applied gradient boosting and

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Bayesian network modeling to predict mycotoxin contamination in maize in the USA with an overall accuracy of 94%[18]. These studies showed high prediction accuracy using machine learning, however, these studies mainly focused on the prediction of the presence of different mycotoxins in maize and wheat, not in oats. In addition, only a few studies provided explanations of model prediction results (i.e. the impact of input variables on the different mycotoxin contamination levels). Machine learning approaches are often seen as black boxes that provide recommendations without sufficient explanation of "which and how input variables generated the result"[21]. This is not a functional practice when the model results are to be used as support for decision-making. Furthermore, effects of single management practices (such as cultivar, tillage, and longitude and latitude) on DON contamination in wheat have been investigated for mycotoxin prevention and control[22], but collective effects of multi-management practices (such as a combination of regional characteristics) on DON contamination have not been explored yet. Such a collective effect is essential to provide advises for reducing DON contamination in oats.

The aim of this study was to (1) develop predictive models for the contamination of DON in spring oats on a regional basis in Sweden using machine-learning algorithms, (2) explore the impacts of weather features, agronomical features, and site-specific features on the DON contamination levels, (3) explore the collective effect of multi management practices (combination of cultivar, crop rotation, and regional characteristics) on DON contamination and provide advice to reduce DON contamination in oats.

Results

Describe analysis of data

Figure 1 shows the grids with oats used in the investigation in 2012–2019, which were drawn using geo-referenced grid points using QGIS. Large variations in DON contamination levels can be seen in Table 1. The changes in weather variables from year 2012 to 2019 were displayed in Supplementary Fig. S1. It shows the variation of monthly and weekly rainfall and temperature. From year 2012 to 2019, the summer of 2012 was colder and wetter than normal whereas 2014 was warm but extremely wet in August in the Southwest part of Sweden. In 2018, the summer was exceptionally dry and warm with large negative effects on crop yields. Also, 2019 was a warm year, especially in the very south of Sweden, with normal amounts of rain.

Model result on Dataset 1

Following the model development procedure, the predictive model for DON contamination level (low, medium, high) in spring oats in Sweden was trained using training data from dataset 1 (80% of 2012–2019, except for 2016). The five-fold cross-validation result (mean prediction accuracies) for the SS model, MS model, and the FS model were 0.73, 0.72, and 0.72, respectively, i.e., five-fold cross-validation results for the SS-model were 0.72, 0.70, 0.72, 0.72, 0.72 with a mean of 0.72; for the MS-model, values were 0.72, 0.71, 0.74, 0.72, 0.72 with a mean of 0.72; for the FS-model, values were 0.71, 0.70, 0.73, 0.72, 0.73 with a mean of 0.72.

Then, models were tested on the "new" data (20% of all records of 2012 – 2019 except for the year 2016). The model results showed consistent performance with cross-validation results. The total prediction accuracies for the SS models, MS models, and FS models were 0.73, 0.72, and 0.73, respectively. Figure 2 displays the prediction results for each DON contamination levels (low, medium, high) of the internal validation (20% of 2012–2019 except 2016) in detail. The confusion matrix (upper figures in Fig. 2) visualized the internal model validation results by comparing the actual and predicted DON contamination levels. It shows the counts of actual versus predicted classifications. The normalized matrix (lower figures in Fig. 2) scales these counts to reflect proportions and shows the prediction accuracies for the high, medium, and low contamination levels[1].

The result of using weather data only (remove crop variety from dataset 1) for model training and validation refers to Supplementary Fig. S3. The external validation result for the prediction of DON contamination levels (low, medium, high) in oats in Sweden in 2016 using the model trained on weather data and crop variety from 2012 to 2019 except 2016 refer to Supplementary Fig. S5).

Model result on dataset 2

To analyze the feature impact on DON contamination levels taking into account the weather, agronomical, and site-specific features, a predictive model was developed using dataset 2 (2016 and 2017) following the same

Fig. 1 | Maps of grids with oats in Sweden. The maps show the grids used for oats investigation in the period of 2012 to 2019. Scale: 1:17936700 (1 cm on the map equals 17,936,700 cm). Source: OpenStreetMap.

Table 1 | The number of grid cells categorized by monitored DON (deoxynivalenol) contamination levels—low (<500 μg/kg), medium (≥500 μg/kg and <1000 μg/kg), and high (≥1000 μg/kg) — recorded over various years

Contamination levels	Year							
	2012	2013	2014	2015	2016	2017	2018	2019
Low	292	374	663	571	535	449	519	755
Medium	139	163	86	9	39	5	19	3
High	154	123	68	12	55	5	12	3

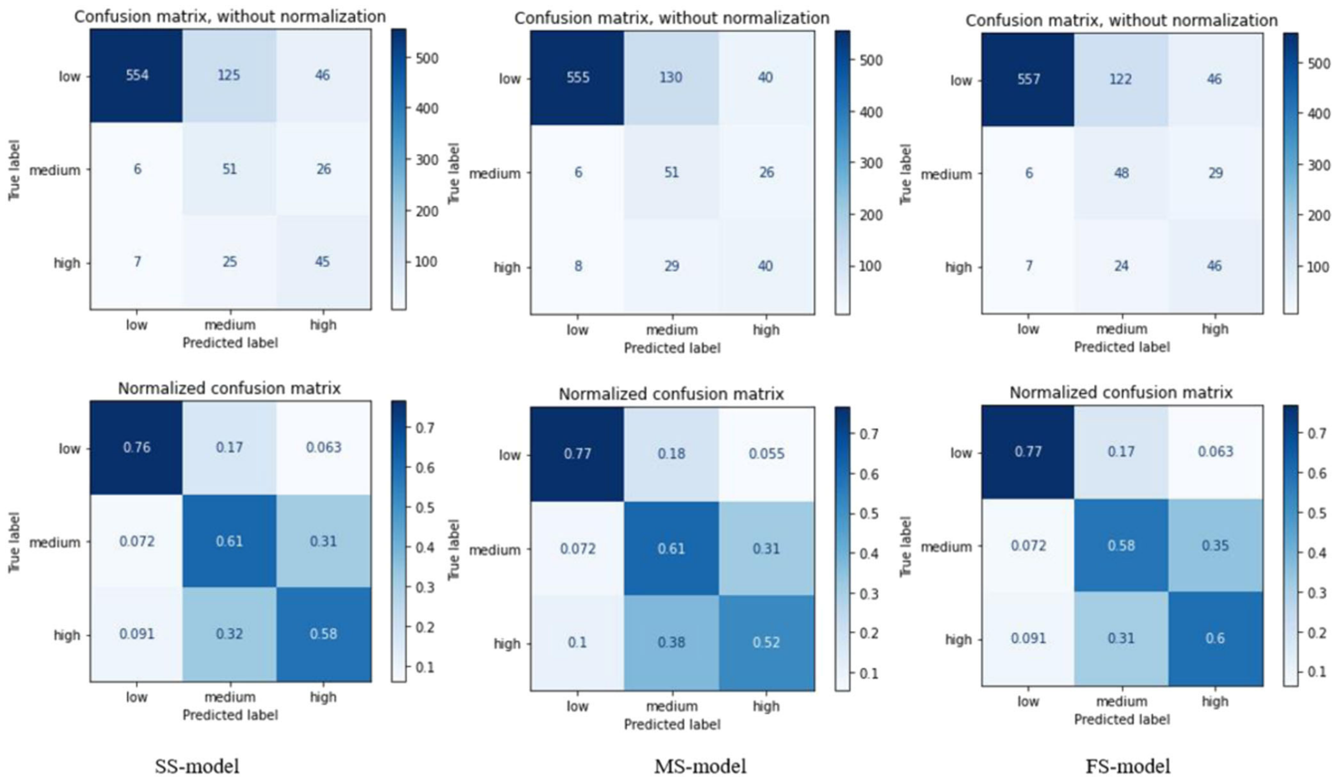

Fig. 2 | Prediction results using weather data and crop variety. The confusion matrix (upper) presents internal model validation results using the internal validation dataset 1 (20% of 2012–2019 except 2016) to predict the contamination levels (low contamination, medium contamination, and high contamination) of DON in oats in Sweden between 2012 and 2019 except 2016.

model development procedure as described in section 3.1. Note that agronomical and site-specific features (except crop variety) were only available in the years 2016 and 2017, which is the reason a separate model has been developed using data from those two years. The total accuracy for the SS-model, MS-model, and FS-model was 0.94, 0.95, and 0.96, respectively (Fig. 3). If using weather data only, the total accuracy for each model was, 0.82, 0.81, and 0.88, respectively (Supplementary Fig. S4). The result shows that (1) weather features are the most important variables for DON contamination model development, (2) adding crop variety, and agronomical variables could improve the overall DON contamination classification accuracy, as well as the accuracy of each class.

Feature impact analysis

SHAP (SHapley Additive exPlanations) values were used to explain how much each independent variable contributes to the final prediction on DON in oats in Sweden. Features were ranked based on their importance in predicting DON contamination levels.

Figure 4a shows the overall average impact and variables are ordered by importance (in terms of the absolute value of their contribution). Variables used for SHAP analysis in supplementary (Table S1). The key predictors for forecasting DON contamination levels in oats encompassed rainfall, relative humidity, and wind speed across various growth stages, alongside crop variety and elevation. For example, from Fig. 4a it can be seen that the most important variable in determining DON contamination levels was the average rainfall in December ("NED_MAVE,12"). Figure 4b–d show the directionality of the impact on the low contamination level (4b), the medium contamination level (4c), and the high contamination level (4d), respectively. Positive SHAP values represent the positive impact on the contamination level, negative SHAP values represent the negative impact on the contamination level. For example, the results in Fig. 4b indicate that lower average rainfall in December ("NED_MAVE,12") contributes to low levels of DON contamination. Conversely, the results in Fig. 4c and d indicate that higher average rainfall in December contributes to both medium and high levels of DON contamination.

Feature impact analysis on weather features

Figure 5 presents in detail the feature impact on the model outcomes for several weather features based on feature dependency analysis. The two variables average rainfall in December ("NED_MAVE,12") and weekly average maximum temperature in the beginning of August ('HTEMP_AVE', 32) were selected since these were the input weather features that had the highest impact on the model output. For example, in Fig. 5, the three figures on the top show that a low precipitation in December contributed to a low DON contamination level (positive contribution). This was the other way around for medium and high levels of DON contamination (negative contribution). The three figures at the bottom show that the lower average maximum temperature in the beginning of August contributed to a high frequency of medium and high levels of DON contamination (positive contribution), whereas this was the other way around for low levels of DON contamination (negative contribution).

Feature impact analysis on agronomical features

Figure 6 presents a detailed explanation of agronomical features for feature impact on the model outputs using feature dependency analysis. The three variables of crop varieties BELINDA, GALANT, and KERSTIN, were selected because they were the non-weather feature that gave the highest impact on the model output. Low levels of DON contamination were seen for the crop variety GALANT and BELINDA (1.0 in X-axis), and medium and high levels of Con contamination were seen for the crop variety KERSTIN. Crop rotation did not explain much of the variations in DON contamination levels and were therefore not displayed here (see Supplementary Fig. S6).

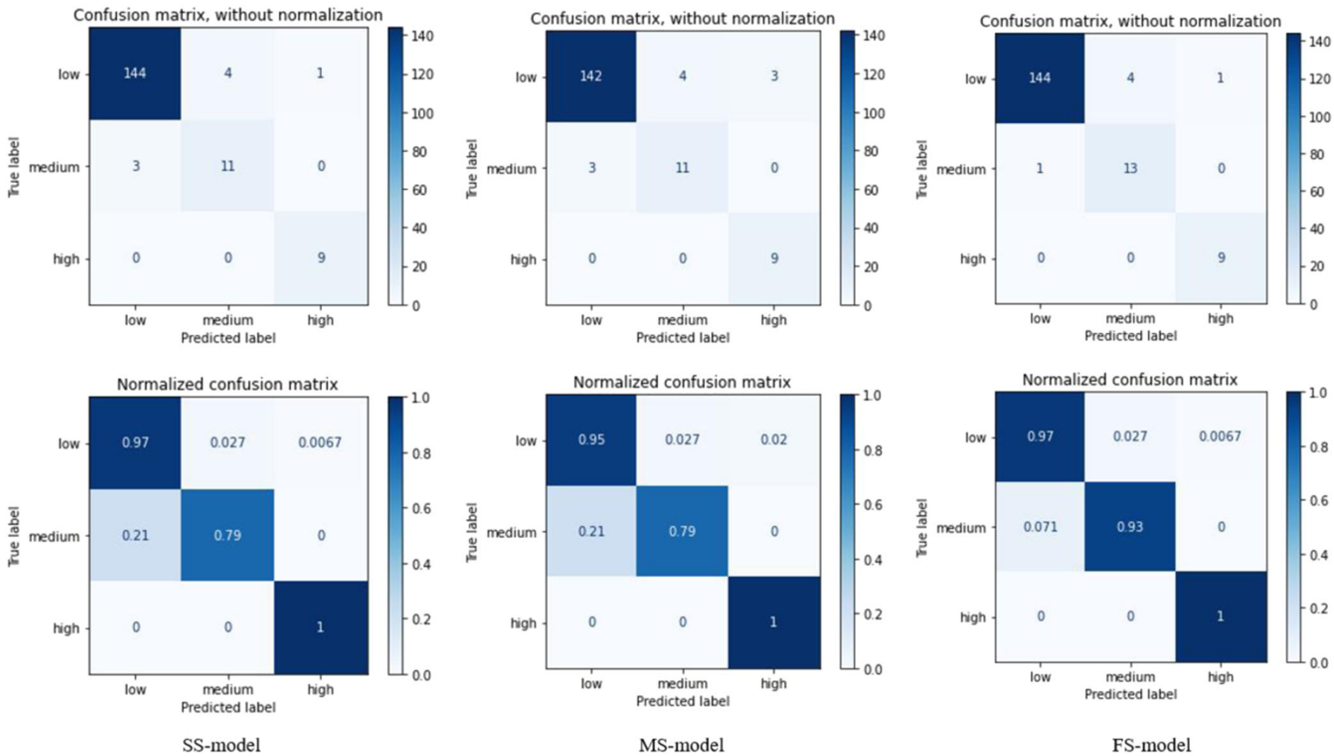

Fig. 3 | Prediction results using the combined data of weather, crop variety, agronomical, and site-specific features. The confusion matrix (upper) presents internal model validation results using the test dataset (2016–2017) to predict the contamination levels (low contamination, medium contamination, high contamination) of DON in oats in Sweden during 2016 and 2017.

Feature impact analysis on site-specific features

Figure 7 shows the feature dependency analysis of mean value and range value of elevation and mean value of soil type (percentage of sand or lay) variables on DON contamination levels. These variables were site-specific features that gave the highest impact on the model output. For example, larger variations in elevation within fields contributed to higher DON levels (elevation range <25 m negative contribution, and elevation range >25 m positive contribution to high DON levels). On high-elevation fields (>60 m) soils with high sand content and low clay content contributed to high DON levels, and the reason could be stress (due to draught in the high-elevation field) makes the crop more vulnerable to fungi infection.

Discussion

In the current study, three different predictive models (SS, MS, and FS model) for DON contamination levels at the regional scale in oats in Sweden were developed. Model classification accuracy showed to be high, ranging from 0.7 to 0.9 depending on different years and models. The developed models can provide valuable information to three different stakeholder groups in the oat supply chain; farmers, crop collectors, and food safety authorities, as a tool that can help in the management of mycotoxins in the oats supply chain and risk-based testing. Results showed that (1) weather variables are the most important for predicting DON contamination in oats, (2) adding relevant agronomical and site-specific factors, such as crop variety, crop rotation, soil type and DON contamination condition in the previous year could improve the performance of the models, (3) good predictions could be made already in June by using the SS-model, as based on internal validation, and 4) rainfall, relative humidity, and wind speed in different growing stages as well as crop variety and elevation were the most important features for predicting DON contamination levels in oats. However, predicting individual years not included in the training of the models proved to be difficult.

To date, few studies have incorporated weather, agronomical, and site-specific data to predict the regional DON contamination in oats using machine learning. However many studies have paved the way for using these data for DON contamination prediction. One study modeling the effects of weather features on DON contamination in oats indicated that the model accuracy could be improved if more factors (such as field tillage and the soil type) were included, in addition to the weather data[12]. One study investigated the association of several agronomic factors (including harvest date, crop season, county, farming system, moisture, test weight, oats variety, and previous crop) to the occurrence of Fusarium mycotoxins in Irish oats[23]. This study concluded that the level of DON was modeled best by the variables of the previous crop and oat variety, and indicated the importance of exploring crop rotation in future studies. Another study investigated the prevention and control of mycotoxins in grains, and emphasized the importance of matching crop varieties to a specific agro-ecological zone with specific weather conditions[24], indicating the necessity of linking weather data to the crop variety for model development. In our study, we used weather factors and relevant agronomical and site-specific factors as model inputs. Similarly to the previous studies, oat variety was the non-weather feature that had the highest impact on the model output. The comparison of model performance using weather data, with and without agronomical and site-specific factors confirmed that, in improving the performance of the DON predictive models, weather variables are the most important factors, and adding agronomical and site-specific factors could further improve the overall classification accuracy (from 0.72 to 0.73 using dataset 1, from 0.81 to 0.95 using dataset 2). This was in line with the expectation of a previous study which suggested that DON prediction in oats could potentially be improved by combining weather-based risk index outputs with agronomic factors[5].

The feature impact analysis indicated that rainfall, relative humidity, and wind speed in different oat growing stages as well as oat variety and elevation were the most important features for predicting DON contamination levels in oats. In general, weather variables (e.g., temperature, rainfall) in December of the previous year, weather variables (e.g., relative humidity, wind speed) around end of June (close to flowering season), and

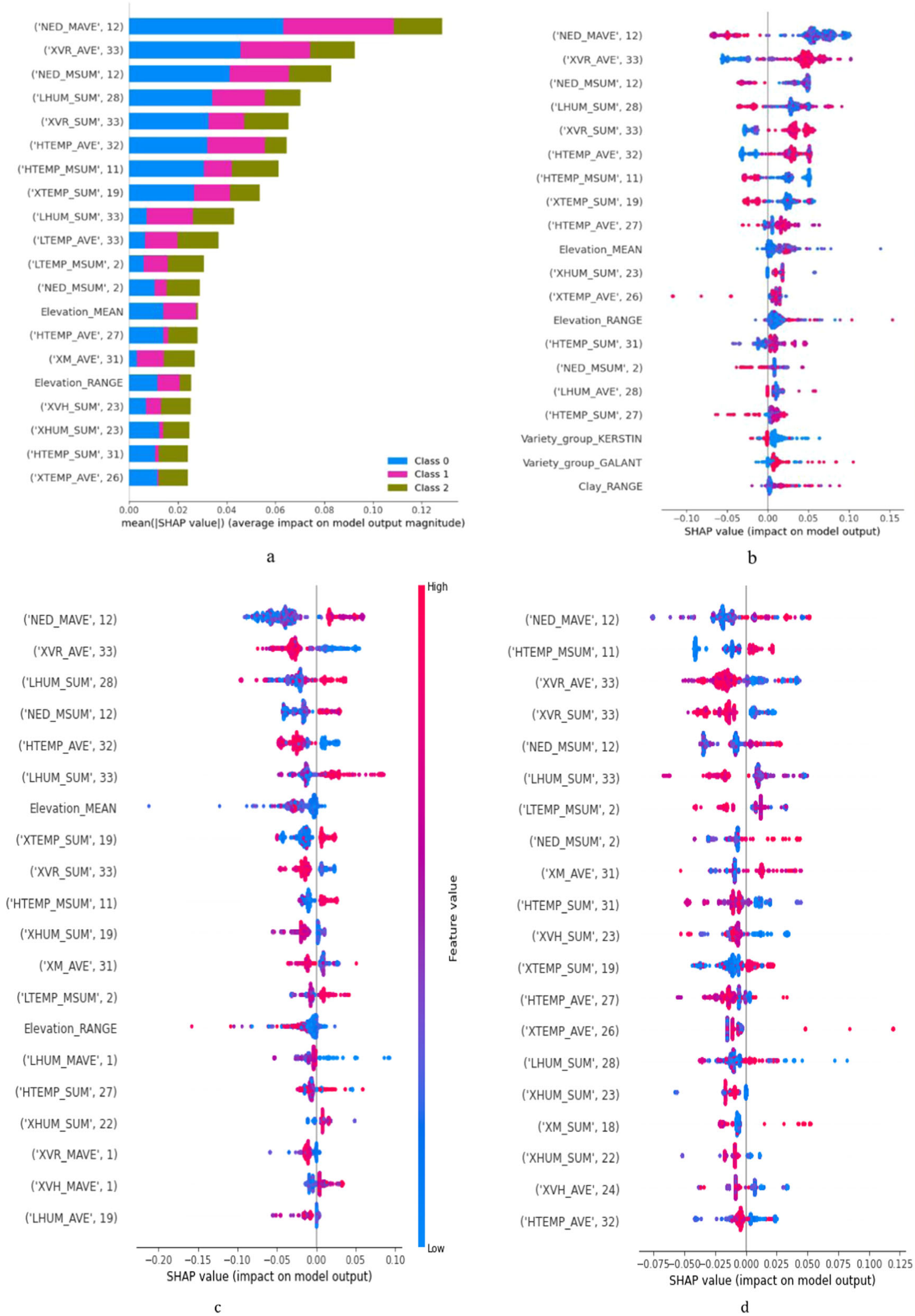

Fig. 4 | Feature average impact ranking (top 20) using the dataset 2 for FS-model. Figure shows the overall average impact (**a**), the directionality (positive or negative) of impact on the low contamination level (**b**), the directionality of impact on the medium contamination level (**c**), and the directionality of impact on the high contamination level (**d**). The feature is indicated on the y-axis and the SHAP value of it is shown on the x-axis. Positive SHAP values represent the positive impact on the contamination level, negative SHAP values represent the negative impact on the contamination level.

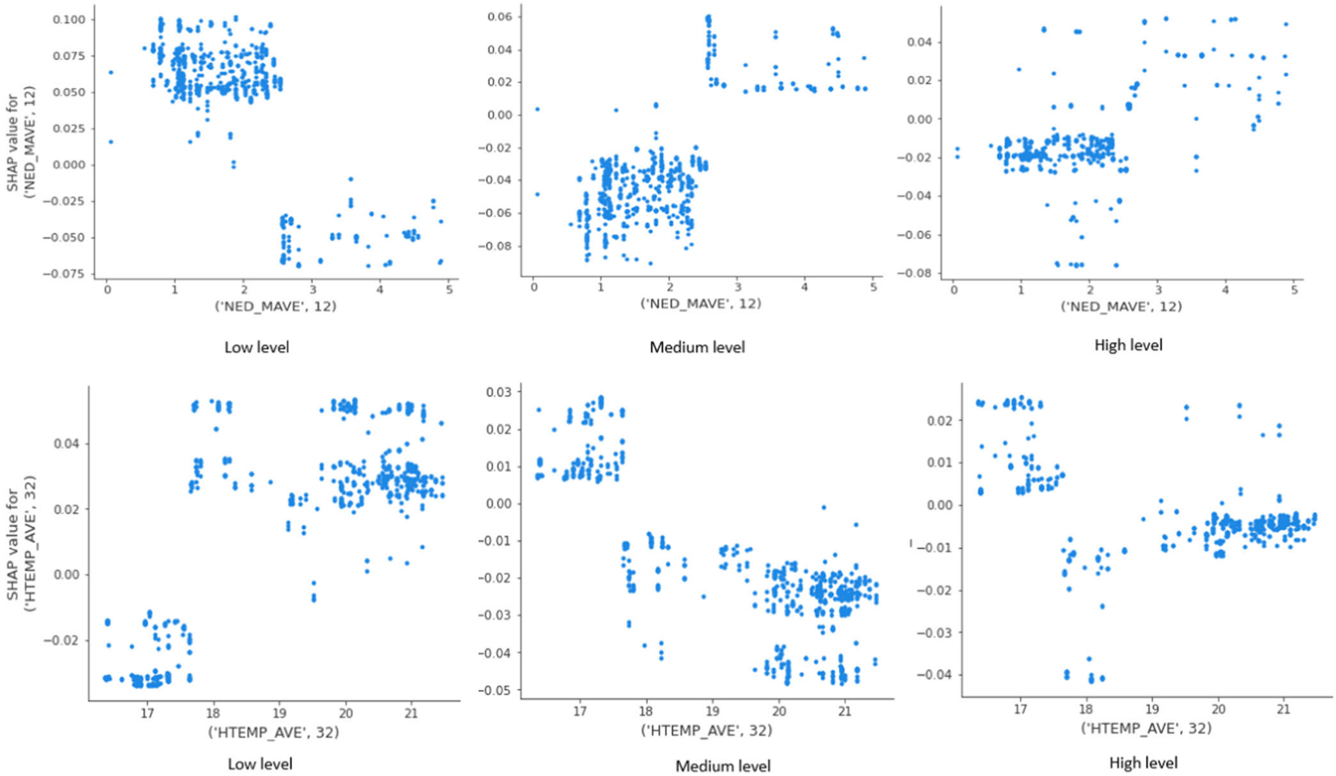

Fig. 5 | Feature dependency analysis for weather features (dataset 2) for the FS-model. Feature dependency of average rainfall in December ("NED_MAVE", 12) and average maximum temperature in the beginning of August ("HTEMP_AVE", 32) on the impact of the low, medium, and high contamination levels. The value of the feature is shown on the x-axis and the SHAP value is shown on the y-axis. Positive SHAP values represent the positive impact on the contamination level, negative SHAP values represent the negative impact on the contamination level.

weather variables (e.g., relative humidity, temperature) around August (week 31, 32 and 33 close to harvest season) were the most important features (Fig. 3). These results are in line with Hjelkrem et al.,[1] who showed that dry periods during germination (March to April) contribute to high DON contamination of oats, and warm, rainy and humid weather around flowering contributed to high DON accumulation in oat. Marzec-Schmidt, et al.[12] also confirmed that high relative humidity and precipitation around flowering correlated with high DON contamination levels in oat. Interestingly, the site-specific characteristics associated with high DON contamination levels in our study, high elevation and sandy soils, is related to dry conditions which may indicate that draught stress might have been important in the data set from 2016–2017.

A previous study applied different models, including statistical analysis and machine learning techniques, for DON prediction in oats, resulting in different model performances[16]. Their results showed that very little of the variation in DON levels could be explained by agronomical or weather factors, and it was not possible to predict DON levels based on these variables. This low model performance could have been caused by the unbalanced data related to DON contamination, meaning only a few records were related to high DON values, and most of the records were related to low DON values. Poor model performance for predicting high mycotoxin contamination levels due to unbalanced datasets has also been encountered in other studies[19,25]. Their results showed that the developed models have higher performance for predicting the samples with low-level contamination than for the samples with high-level contamination. Our study applied a machine learning technique (the random forest algorithm) to handle unbalanced data, resulting in a relatively balanced classification accuracy in each DON contamination level (high, medium, low). Detailed model performance discussion refer to supplementary: Model performance discussion.

Our study had several limitations as we were not able to include all biologically relevant factors for predicting deoxynivalenol (DON) due to insufficient data on those factors. These factors include crop management practices, such as fertilization, irrigation, and pest control[2], the use of fungicides against Fusarium spp. around flowering[25–27] and the harvest conditions (such as timely harvest). Future studies could explore data collection on these factors, followed by including these variables to enhance model performance, along with leveraging open-source data like satellite imagery[28]. Additionally, our study focused solely on DON contamination in oats, omitting consideration of other mycotoxins; future research could expand to predict multi-mycotoxin contamination if more data on the presence of other mycotoxins in oats becomes available.

It can be concluded that the use of machine learning algorithms for DON prediction in oats, using contamination levels at the regional level in Sweden provides good prediction results when considering several years. Unfortunately, the models were not general enough to manage to predict DON-levels from individual years not included in the training of the model, i.e., model performance did not as high as internal validation when do external validation using leave one year out approach. One reason for this discrepancy could be the variability in DON contamination levels observed across the years studied. Given these fluctuations, it might be advantageous to adopt a simplified approach using two risk levels—above or below a specified threshold.. Moreover, the diverse fungi within the Fusaria complex underscores the complexity of predicting mycotoxin levels in oats. Such models could be used as regional risk-assessment tools for farmers, crop collectors, and food safety inspectors for logistics in the oats supply chain, improved mycotoxin control, and risk-based testing. Given EC regulation 2017/625, food safety authorities need to apply risk-based control. Predictive models can assist in this process by guiding authorities to allocate more intensive sampling and testing efforts to regions with medium to high levels of DON contamination. This targeted approach ensures that resources are effectively prioritized where contamination risks are higher. Collectors and food safety authorities of oats can also use the model

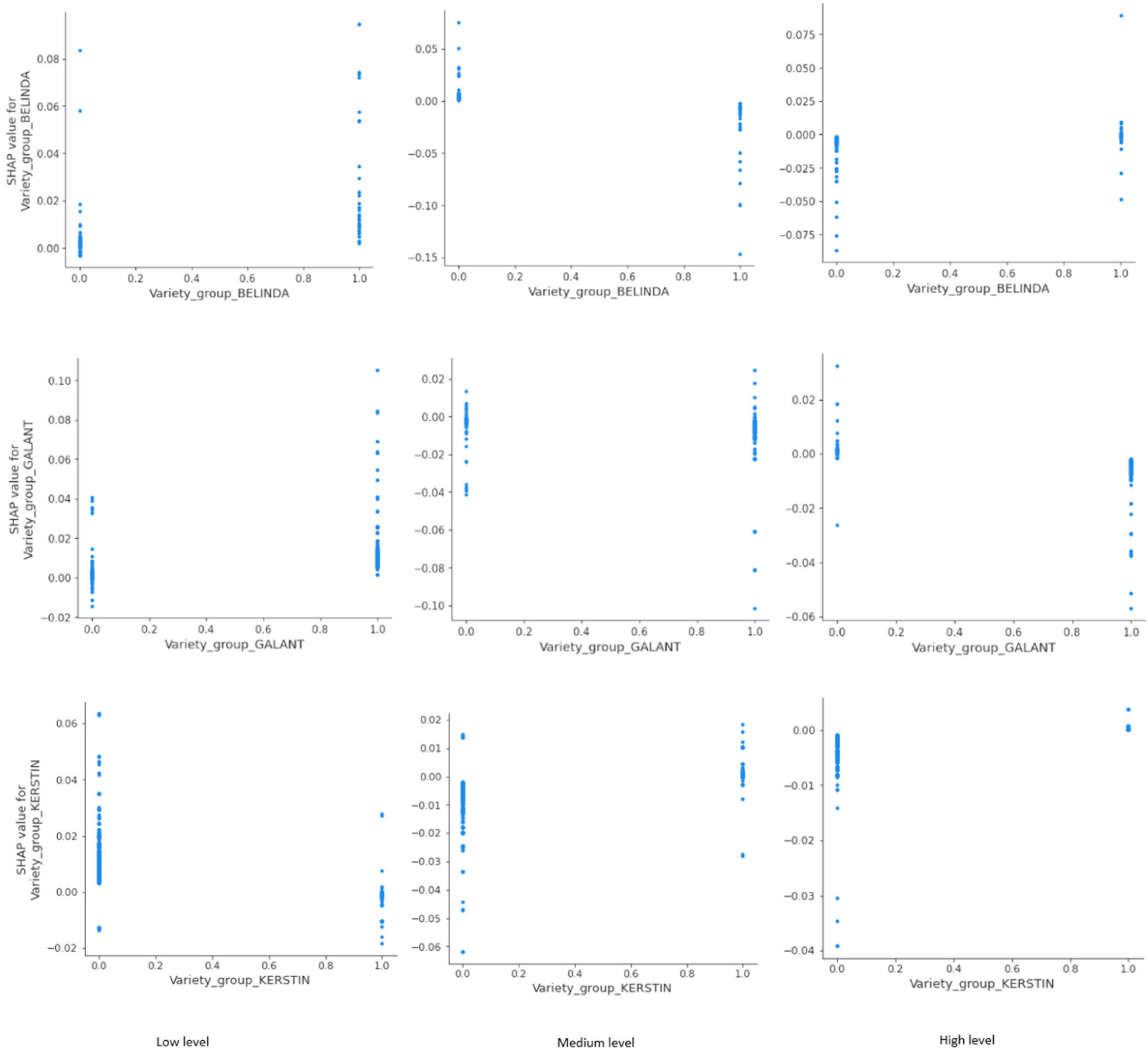

Fig. 6 | Feature dependency analysis for agronomic features (dataset 2) for the FS-model. The feature dependency of the oats variety BELINDA, GALANT, and KERSTIN on the impact of the low, medium, and high DON contamination levels.

predictions for deciding on testing frequencies, and they can use the predictions for routing and logistics in their oats supply chain.

Materials and Methods

Three models were developed as regional risk-assessment tools to be used by, farmers, crop collectors, and food safety inspectors, respectively. To provide a timely forecast of DON contamination for the different user groups, the three models aimed to provide the regional DON predictions at three different times during the oats vegetation period: i) SS-model: Start of Season model Nov 1 to June 1), which would allow for recommendations on crop protection activities, such as using fungicides[29], for farmers, ii) MS-model: Mid-Season model (Nov 1 to July 1), which would allow for recommendations on sampling strategies and as an early warning concerning regional differences for crop collectors and food safety inspectors, and iii) FS-model: Full Season model (Nov 1 to Aug 15), as compared to MS-model, the FS-model includes full season data to allow for a more reliable indication on how to plan for sampling strategies. In each of the three models, the predictions of DON contamination levels were provided into one out of three levels of: low (<500 μg/kg), medium (≥500 μg/kg, and <1000 μg/kg), and high (≥1000 μg/kg). The thresholds was set lower than the EU regulation (1750 μg/kg) to provide a more conservative and cautious approach to managing DON contamination.

Weather factors and relevant agronomical and site-specific factors were used as model inputs. The weather features were selected as the monthly average from November to April and the weekly average from May to August. The reason for using more detailed information from May to August is that this is the period from oats stem elongation to harvest, when oats are known to be more sensitive to fungal infection[1,2]. The other input factors were selected since they are known to be relevant to the DON contamination of crops, including the oats variety, crop rotation, and other agronomical features[30–32]; and site-specific factors such as soil type and elevation[16,27]. For example, crop variety influences the susceptibility of crops to abiotic factors, such as drought stress, that favor fungal growth and ultimately mycotoxin contamination[23]. Crop rotation has an impact on DON contamination in grain due to the fact that Fusarium spp. contaminated debris from the earlier crop can

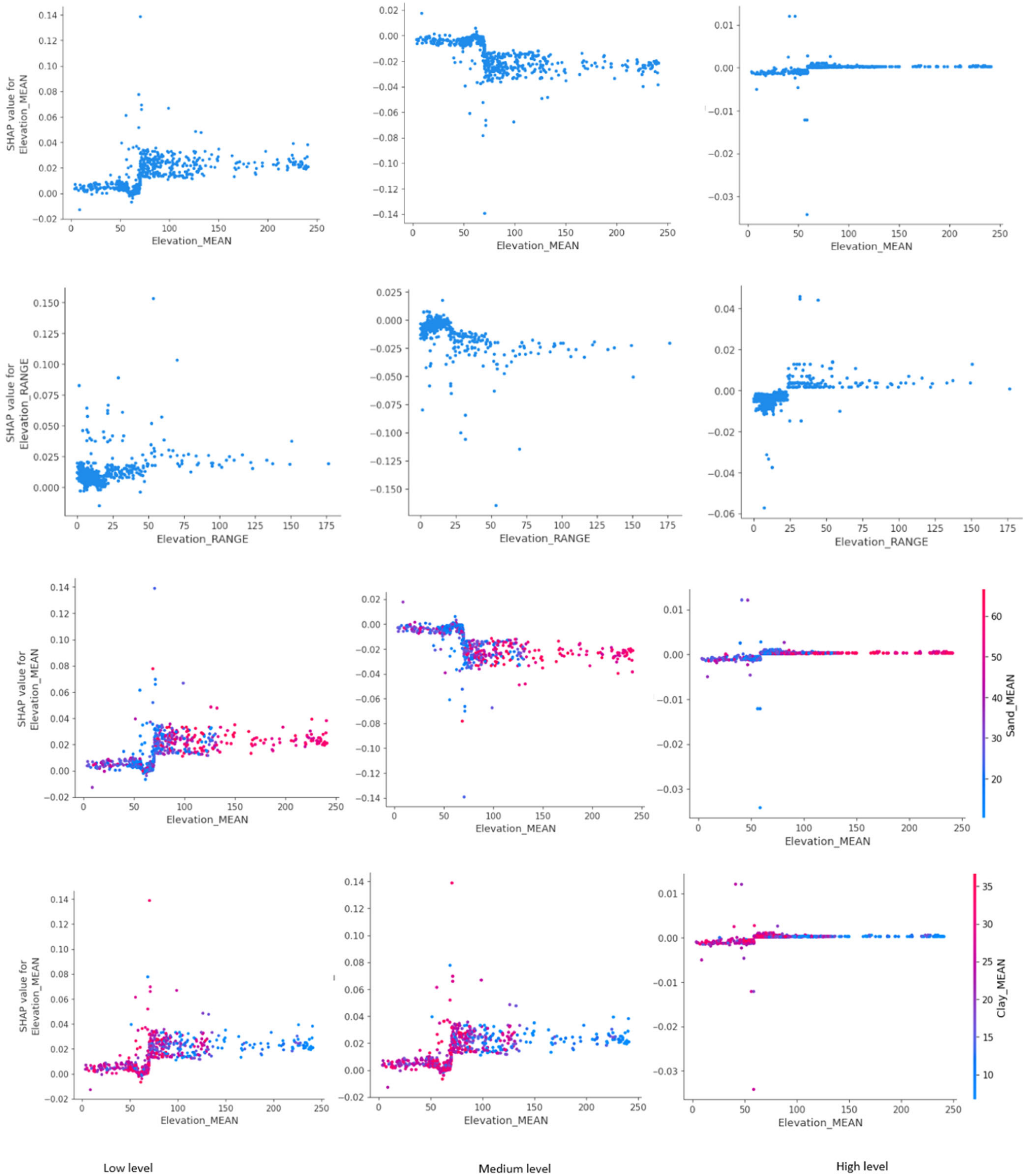

Fig. 7 | Feature dependency analysis for site-specific features (dataset 2) for the FS-model. Figure shows examples of the feature dependency of the elevation and soil type on the impact of the low, medium, and high DON contamination levels.

survive on the soil surface for a long period and act as a reservoir for contamination[30–33].

Data

This study used DON contamination data, weather data, agronomical data and site-specific data, in Sweden. These data were selected for the period Nov 1 of the previous year to August 15 of the current oat growing year, to include all relevant stages of fungal infection and DON contamination of spring oat. Data were firstly pre-processed (see section related to each dataset below) and then linked together into one dataset based on the grid (11 × 11 km), year, and crop variety (Fig. 8). Data from the period Nov 1 to June 1 were used for developing the Start of Season (SS) model; the period Nov 1 to July 1 for developing the Mid-Season (MS) model; and data from the period Nov 1 to Aug 15 for the Full Season (FS) model. Then, two types

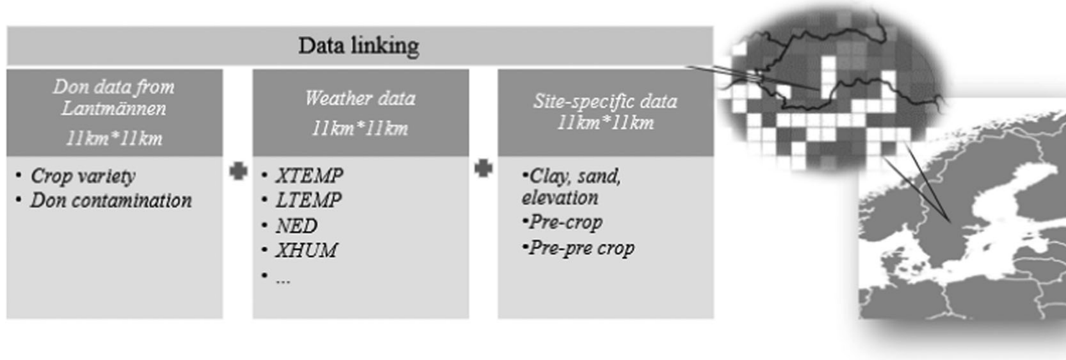

Fig. 8 | Data linking from three datasets. Three datasets, related to DON contamination, agronomical and site-specific features, and weather features in three different periods (SS-model (Nov 1–June 1), MS-model (Nov 1–July 1), and FS-model (Nov 1–Aug 15)) were linked per grid cell in Sweden (11 km × 11 km grid) for each year and each crop variety. Note that the site-specific data are not collected grid-wise, but field-wise.

of datasets were composed using different input variables separately for modeling. Dataset 1: weather and crop variety variables from the years 2012–2019. Dataset 2: weather, crop variety, agronomical and site-specific variables from the years 2016–2017. Agronomical and site-specific variables were only available for the years 2016–2017.

DON contamination data

Data related to DON concentration in spring oats include 8 years (2012-2019) of monitoring results from oats grown in Sweden (54350 records in total) at the grid level (11 km × 11 km). These data were derived from analyses of oats delivered to Lantmännen elevators in Sweden. Three contamination levels were set: low (82% records) (<500 μg/kg), medium (9% records) (≥500 μg/kg and <1000 μg/kg), and high (8% records) (≥1000 μg/kg). These settings were chosen from a practical farming point of view; with a DON concentration below 500 un/kg, there is no need for farmers to take any actions, whereas with DON concentrations above 1000 ug/kg, farmers are recommended to always consider spraying or to check the level by taking out a reference sample. The variety was known for most of the samples, and the following varieties were occurring and used as input group variables: Belinda, Ingeborg, Galant, Guld, Symphony, Fatima, Kerstin and Matilda. Furthermore, one group called Feed oats (that could be different varieties) was also recorded as well as one group for which the variety had not been specified. Whether the oats was grown for feed or food use; if it was organically cultivated (EKO) or not; and mean DON value of the previous year in the same grid were used as model input variables. Mean DON values represented the average values of DON concentrations of each oats variety group in the particular grid in each year, provided the number of oat deliveries of that variety group was more than 10 in that particular grid in that year. DON contamination levels were used as a model output variable and were defined based on the mean values of DON concentration per region per year. 31% of the records referred to DON concentrations that were below limits of quantification (LOQ = 100 μg/kg) of analytical methods used (Ridascreen ELISA or Charm Later Flow Devices had been used for analyzing DON contents); 4% of the records referred to DON concentrations that were above maximum legal limits in foodstuffs (1750 μg/kg), and; 0.2% of the records were above maximum legal limits in feed (8000 μg/kg).

Weather data

Weather data include 8 years (2012–2019) of weather features in Sweden at grid level (11 km × 11 km). These data were derived from the Swedish Meteorological and Hydrological Institute (SMHI). Selected variables included the maximum air temperature (°C) (HTEMP), minimum air temperature (°C) (LTEMP), mean air temperature (°C) (XTEMP), rainfall (mm) (NED), mean relative humidity (%) (XHUM), minimum relative humidity (%) (LHUM), maximum relative humidity (%) (HHUM), wind speed (km/h) (XVH), wind direction (XVR), and global radiation (kWh/m^2) (XM). Weekly mean values and weekly sum values per grid of the above-mentioned weather features were calculated in different oat growing periods for the development of three prediction models: SS-model (week 18–21), MS-model (week 18–26), and FS-model (week 18–33). In addition, monthly mean values and monthly sum values per grid of the above-mentioned weather features from Nov 1 of the previous year to April 30 of the current year were calculated and added to the three models.

Agronomical and site-specific data

Agronomical and site-specific data include 2 years (2016–2017) of agronomical features in Sweden at oat field level aggregated to the grid level (11 km × 11 km). These data were derived by linking the oats deliveries from one producer to the fields at which oats had been grown by that producer that year, and that geographical information. Data were extracted from several sources, and then linked with DON contamination levels per grid per year (11 km × 11 km). The derived variables included: oats variety; year; the value range and mean value of clay, sand, and elevation; the percentage of oat, ley, other cereals except for oat; and other crops grown in the fields in the previous year (pre-crop); and two years before (pre-pre crop). Information on pre-crops was extracted from the Land Parcel Identification System Maps provided by the Swedish Board of Agriculture. Elevation data were extracted from a 2 × 2 m digital elevation model in raster format provided by Lantmäteriet (Swedish National Survey, Gävle, Sweden) and soil texture information was extracted from a digital soil mapping of arable land in Sweden[34].

Data split for model training and validation

Figure 9 shows the model development steps using dataset 1 and dataset 2.

For dataset 1, records from the years 2012–2019 (except 2016) were split randomly into a training set (80%) for model learning, and a test set (20%) for internal model validation. Data from the year 2016 were used for external model validation only. The reason is that the distribution of DON contamination levels in the year 2016 was close to the average of the year 2012–2019. The predicted model results for the test set were graphically compared with the measured (observed) mycotoxin data to visualize the model prediction ability.

For dataset 2, records were split randomly into a training set (80%) for model learning, and a testing set (20%) for internal model validation. Because agronomical and site-specific data were only available in the year 2016 and 2017, no external validation was conducted here.

In addition, to test the importance of adding other features to weather data in promoting the model's predictive accuracy, for each dataset, the model performance was compared when using weather features only and when using weather with agronomical and site-specific features (the result of this comparison is added in the supplementary).

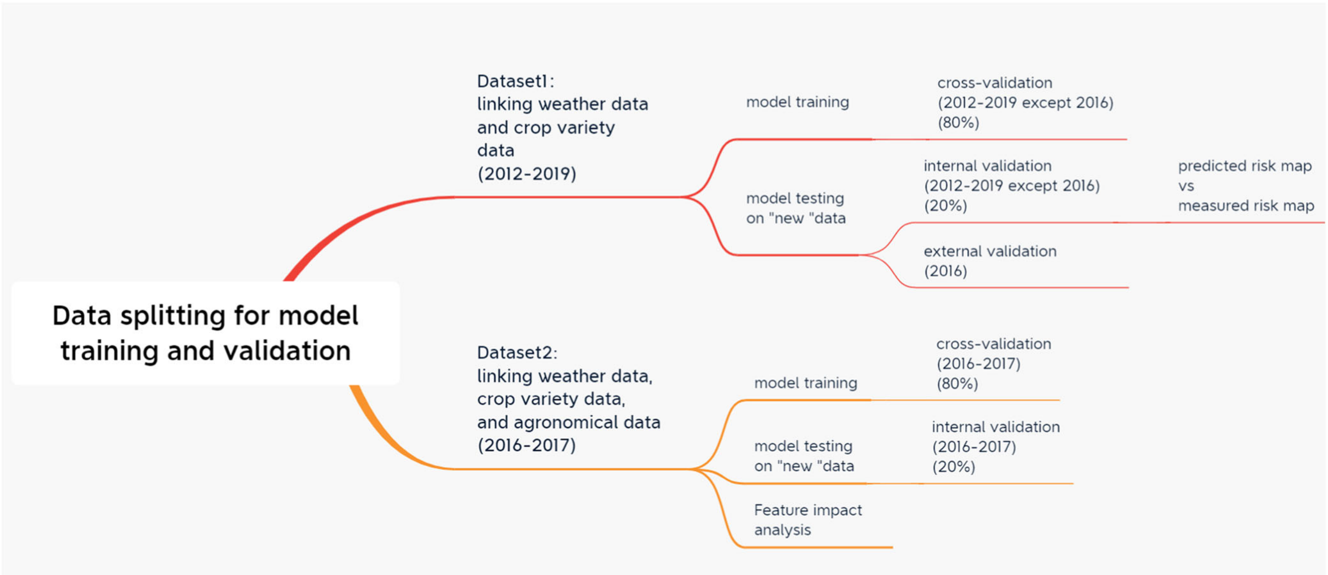

Fig. 9 | Data splitting for model training and validation. Dataset 1 contains records from the years 2012-2019 linking weather data and crop variety data. Dataset 2 contains records from the years 2016–2017 because agronomical and site-specific data were only available in the year 2016 and 2017.

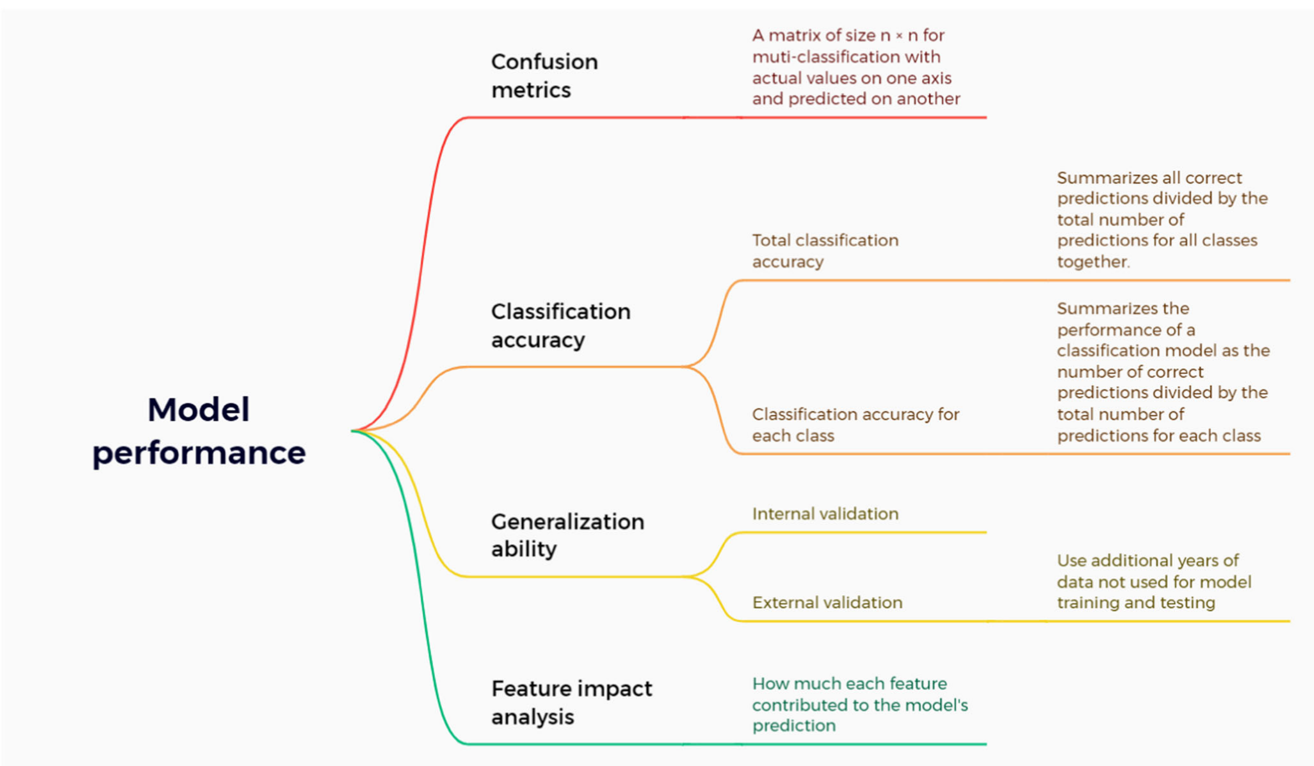

Fig. 10 | Model performance evaluation. Confusion metrics, classification accuracy, and generalization ability were used to assess the predictive model's performance.

Predictive model

A machine learning module was developed to predict the contamination of DON in oats at the grid level in Sweden, in three levels for the likelihood of contamination (low, medium, high) using above-mentioned variables as input. A random forest (RF) algorithm was applied because RF can automatically handle missing values, can efficiently handle non-linear parameters, is comparatively little impacted by noise, is robust to outliers and new data, avoids overfitting, is able to deal with unbalanced data, and is widely used to deal with spatial data[35]. Python (version 3.9) programming language and data analysis library Scikit-learn (version 1.0) were used. Confusion metrics, classification accuracy, and generalization ability were used as evaluation criteria to evaluate the performance of the predictive model[36] (Fig. 10). Confusion metrics reflected actual values on one axis and predicted values on another. Classification accuracy for each level and total classification accuracy reflected the model performance on each level and all levels. Generalization ability reflects the model's capability to adapt and react properly to previously unseen, new data. In this study, we performed five-fold cross-validation for model training (hyperparameter tuning)[37].

A predictive model was first trained on dataset 1, and model performances were evaluated based on the above-mentioned aspects. Then, following the same model development procedure, we trained the predictive model on dataset 2 to analyze the importance of weather features, agronomical features and site-specific features.

The feature impact of the input variables of the developed models was analyzed and sorted. Tree SHAP (SHapley Additive exPlanations) algorithm was used to perform the feature impact analysis[38]. Tree SHAP allows interpreting predictions made by often complex black box machine learning algorithms. Feature impact provides (often desirable) interpretation of the model input variables' contribution towards the model prediction and highlights the positive and negative impact of such variables for identifying different contamination levels of DON contamination.

Data availability
The data presented in this study are not available due to DON contamination data are highly sensitive for the individual farmers.

Code availability
The code used in this study is available upon request.

Received: 22 February 2024; Accepted: 15 September 2024;
Published online: 04 October 2024

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Acknowledgements
The authors acknowledge the contribution of the private partners and all growers who participated in this project. This study is funded by the European Commission on the EIP-agri grant 2017-1345 Infofusion Fusarium administrated by the Swedish Board of Agriculture. The FORMAS project Baby Grain Passport, Grant 2019-02280 has co-funded this study.

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X.W.: Conceptualization, Methodology, Formal Analysis, Investigation, Writing—Original Draft Preparation, Writing—Review and Editing, Visualization. I.F.: Conceptualization, Supervision, Project Administration, Funding Acquisition, Writing—Review and Editing; T.B.: Conceptualization, Resources, Data Curation, Writing—Review and Editing, Funding Acquisition; J.W.: Conceptualization, Resources, Data Curation, Writing—Review and Editing; All authors have read and agreed to the published version of the manuscript.

Competing interests
The authors declare no competing interests.

Additional information
Supplementary information The online version contains supplementary material available at https://doi.org/10.1038/s41538-024-00310-w.

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