



Article

Multi-Class Machine Learning to Quantify the Impact of Nitrogen Management Practices on Grassland Biomass

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Abstract

Grassland biomass yield reflects a complex interaction of management intensity and environmental factors, yet quantifying the relative role of practices such as mowing and fertilization remains challenging. In this study, we introduce a multi-class machine learning framework to predict above-ground biomass on 150 permanent grassland plots across eight years (2009–2016) in Germany's Biodiversity Exploratories and to evaluate the influence of key management variables. Following rigorous data cleaning, imputation of missing nitrogen values, feature standardization, and encoding of categorical practices, we trained CatBoost classifiers optimized via Bayesian hyperparameter search and mitigated class imbalance with ADASYN oversampling. We assessed model performance under binary, three-class, four-class, and five-class quantile-based categorizations, achieving test accuracies of 0.76, 0.57, 0.42, and 0.38, respectively. Across all schemes, mowing frequency and mineral nitrogen input emerged as the dominant predictors, while secondary variables such as drainage and conditioner use contributed as well. These results demonstrate that broad biomass categories can be forecast reliably from standardized management records, whereas finer distinctions necessitate additional environmental information or automated sensing to capture nonlinear effects and reduce reporting bias. This work shows both the potential and the limits of machine learning for informing sustainable grassland management and explainability thereof. Frequent mowing and higher mineral nitrogen inputs explained most of the predictable variation, enabling a 76% accurate separation of low and high biomass categories. Predictive accuracy fell below 60% for finer class resolutions, indicating that management records alone are insufficient for detailed yield forecasts without complementary environmental data.

Keywords: biomass prediction; grassland yields; fertilizer data; mowing practices; CatBoost; Bayesian optimization; ADASYN; feature importance analysis



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1. Introduction

Grasslands play a crucial role in global ecosystems, serving as a primary source of forage for livestock, supporting biodiversity, and contributing to carbon sequestration [1,2]. Understanding the factors that influence grassland productivity is essential for optimizing land management practices, ensuring sustainable agricultural yields, and minimizing environmental impacts [3]. Nitrogen input and mowing frequency are widely recognized as

major drivers of grassland biomass production, influencing both productivity and species composition [4,5]. The global rise in fertilizer use is largely driven by the need to sustain healthy biomass under increased mowing frequency, with improved yields further amplified by advancements in machinery and more efficient fertilization practices [6]. Nitrogen availability is a key limiting factor for primary productivity, directly influencing vegetative growth rates and biomass accumulation, but can lead to shifts in plant community composition, often promoting fast-growing, competitive species [7]. Mowing regimes, in turn, regulate regrowth dynamics and total biomass yield by periodically resetting plant developmental stages, reducing vertical structural complexity within the sward, which is, however, dependent on the plant species [8].

Machine learning (ML) offers tools to model complex, nonlinear relationships in agricultural data. ML and deep learning methods have been applied to forecasts in a diverse range of applications, e.g., in population studies, seizure prediction, and financial markets [9]. Within agriculture, ML models estimate crop yields and infer soil nitrogen status from field measurements [10]. Other examples of AI applications in agriculture can be found for supervised machine learning techniques in [11], for reinforcement learning in [12], and for unsupervised machine learning in [13,14].

In this study, we implement a multi-class ML pipeline to predict grassland biomass and to quantify the relative importance of management practices. Biomass is first grouped into two, three, four, and five classes using quantile-based thresholds. For each granularity, we train a CatBoost classifier—tuned via Bayesian optimization—and apply ADASYN oversampling to address class imbalance. We then evaluate model performance (accuracy, precision, recall, F1-score) on test and training sets, and extract feature importance scores to rank the influence of mineral and organic nitrogen inputs, mowing frequency, and other land use variables. This framework allows us to assess how predictive power varies with classification detail and which practices most strongly drive biomass yield.

1.1. Research Gap

Despite extensive use of machine learning techniques for biomass prediction—ranging from random forests to deep neural networks trained on remote sensing data—no study has combined a multi-class classification framework with a detailed feature importance analysis of management practices, as discussed in detail in Section 2. Our approach fills this gap by applying CatBoost across two to five biomass categories and quantifying the relative influence of mowing, mineral and organic nitrogen inputs, and other agronomic variables. Moreover, by evaluating model performance as class granularity increases, we clarify the limits of predicting yield outcomes from management records alone and identify which combinations of practices most reliably distinguish low, medium, and high biomass regimes.

1.2. Research Questions

Building on this gap, we address three research questions:

1. How accurately can ML models predict distinct biomass regimes, and which factors most strongly drive these predictions?
2. What is the relative influence of organic and mineral nitrogen inputs on biomass outcomes?
3. How do nitrogen inputs compare with mowing frequency and other management practices in determining biomass yield?

The remainder of the paper is organized as follows. Section 2 reviews related work. Section 3 describes the data, preprocessing steps, and ML methods. Section 4 presents classification performance and feature importance results. Section 5 summarizes conclusions and outlines future research directions.

2. Related Work

In the following section, we discuss two aspects of our approach: machine learning methods in agriculture, particularly to predict grassland biomass, and relevant publications from the Biodiversity Exploratories, which serve as the primary data source for this study.

Machine learning methods have been extensively applied to estimate biomass in various ecosystems, including grasslands and forests. Xu et al. [15] investigated the estimation of aboveground biomass (AGB) in degraded grasslands using terrestrial laser scanning (TLS). They evaluated several regression models—simple regression (SR), stepwise multiple regression (SMR), random forest (RF), and artificial neural networks (ANNs)—and found that SMR achieved the highest prediction accuracy, significantly influenced by minimum grass height and canopy coverage. Similarly, Wang et al. [16] analyzed 11 years of AGB data from the Three-River Headwaters Region, demonstrating that machine learning, particularly RF optimized through stepwise regression, effectively predicted grassland biomass across temporal and spatial scales. Their study highlighted the importance of variable selection for improving model accuracy. Peng and Karimi Sadaghiani [17] further extended the application of machine learning to forest biomass, illustrating its potential to enhance both quality and quantity through predictive modeling and decision support tools for forestry management.

Hyperspectral and remote sensing methods have become an important component in biomass estimation, offering scalable and efficient solutions for ecological monitoring. Huang et al. [18] combined hyperspectral remote sensing with various machine learning techniques to estimate grassland AGB in alpine meadows, identifying Gaussian process regression as the most accurate predictive model. Their work emphasized the improved predictive power achieved by combining spectral characteristics with temporal growth data. Complementing this, Morais et al. [19] reviewed the use of machine learning in combination with remote and proximal sensing data for grassland biomass estimation. They observed that prediction accuracy generally increased with sensor proximity and the number of field samples, although no single machine learning algorithm consistently outperformed the others. Finally, Shafizadeh et al. [20] applied machine learning to optimize hydrothermal liquefaction processes for biomass conversion, showing that Gaussian process regression could accurately predict optimal processing conditions. This body of research demonstrates the versatility and efficacy of machine learning in ecological biomass monitoring and optimization.

The Biodiversity Exploratories project, established in 2006, provides a comprehensive research platform to study interactions between land use, biodiversity, and ecosystem processes in forests and grasslands across Germany. With standardized data collection covering vegetation, soil, climate, and biodiversity, a wide range of research topics is addressed. Biomass estimation has been a central focus. Muro et al. [21] applied deep neural networks and remote sensing data, including Sentinel-1 and Sentinel-2, to predict grassland biomass and species richness, achieving improved prediction performance and robustness compared to conventional RF models.

Beyond biomass estimation, the Biodiversity Exploratories address broader ecological processes influenced by land use intensity. Künast et al. [22] examined the effects of mowing on arthropod populations, finding that some taxa are negatively affected while others benefit. Hartlieb et al. [23] developed an index to quantify mowing intensity, providing a tool for evaluating the relationship between grassland management and biodiversity. This tool can be integrated into the Land-Use Intensity (LUI) index by Blüthgen et al. [24], which combines mowing, grazing, and fertilization intensities. The LUI has shown that intensified land use reduces species and functional diversity across trophic levels, leading to ecological homogenization [25]. Collectively, these works illustrate the broad research

scope of the Biodiversity Exploratories, contributing to the understanding of land use impacts on biodiversity and ecosystem functionality.

Despite extensive use of machine learning for biomass prediction—ranging from random forests to deep neural networks trained on remote sensing data—no study has combined a multi-class classification framework with a detailed feature importance analysis of management practices. Our approach fills this gap by applying CatBoost across two to five biomass categories and quantifying the relative influence of mowing, mineral and organic nitrogen inputs, and other agronomic variables. Moreover, by evaluating model performance as class granularity increases, we clarify the limits of predicting yield outcomes from management records alone and identify which combinations of practices most reliably distinguish low, medium, and high biomass regimes.

3. Methodology

This section details the experimental framework and machine learning techniques used to predict grassland biomass yield from fertilizer and mowing practice data. The methodology is implemented in Python, to automate data preprocessing, categorization, model training, evaluation, and logging of outputs. The full code is available in a corresponding GitHub repository: https://github.com/Raubkatz/Nitrogen_Classification (accessed on 1 April 2025).

The Biodiversity Exploratories

Our data is obtained from the Biodiversity Exploratories, which are a long-term research platform, established in 2006, designed to explore the relationship between land use, biodiversity, and ecosystem processes within forest and grassland ecosystems [26]. The project involves standardized data collection on 300 plots, recording vegetation, soil parameters, climatic conditions, and various fauna and microbial communities. The studies are conducted across three distinct regions of Germany: the Schwäbische Alb (located in Baden-Württemberg, southwest Germany), the Hainich (in central Thüringen), and the Schorfheide-Chorin (in Brandenburg, northeast Germany). Our research focused on the 150 grassland plots—50 in each region—each spanning 50 m by 50 m. These plots encompass a wide range of land use intensities, from intense to minimally managed areas, and are situated within larger management units where land use practices are consistent. Approximately 35% of the plots are meadows, 35% grazed pastures, 27% mown pastures (which experience both grazing and mowing within the same year), and 3% left fallow. Fertilization was applied to about two-thirds of the meadows and mown pastures, but only 15% of the grazed pastures received fertilization [27].

3.1. The Dataset

Our analysis draws on two openly available data sets. The first is the biomass series, which reports annual dry-matter yield for all 150 permanent grassland plots from 2009 onward [28]. The second is the grassland management file released with [27]; it lists mowing, grazing and fertilizer inputs for the same plots from 2006 to 2016. Because the management file ends in 2016 and biomass sampling starts in 2009, the merged working table is limited to 2009–2016. The reason to choose these particular files is that they are openly available and thus accessible to us and other researchers who want to expand or reproduce this study.

3.1.1. Biomass Sampling

Each spring, eight 0.25 m² sub-plots per plot were clipped to a 4 cm stubble before any land management activity between mid-May and mid-June. The harvested material was

oven-dried at 80°C for 48 h and weighed to 0.01 g accuracy. The response variable is the mean dry mass per square meter [28,29].

3.1.2. Management Variables

Annual questionnaires completed by farmers record the number and timing of cuts, grazing pressure, machine type, conditioner use, and separate mineral and organic fertilizer amounts. Dung from grazing livestock is excluded from fertilizer totals. Nitrogen figures come from producer certificates or standard conversion factors. Overall, 116 variables are available for every plot-year between 2006 and 2016, from which we use a subset, as detailed in Table 1.

Table 1. Features used as model inputs after cleaning.

Variable	Description	Unit	Scale
Mowing	Cuts per year	1 yr ⁻¹	Qty.
minNitrogen_kgNha	Mineral-N input	kg ha ⁻¹	Ratio
orgNitrogen_kgNha	Organic-N input	kg ha ⁻¹	Ratio
MowingConditioner	Conditioner on mowing machine	—	Bool
NbFertilization	Fertilizer applications per year	—	Qty.
totalNitrogen_kgNha	Total N (min. + org.)	kg ha ⁻¹	Ratio
Drainage	Drainage applied (yes/no)	—	Spec.
Leveling	Levelling/matting break-up	—	Qty.
Manure_tha	Solid manure applied	t ha ⁻¹	Ratio
Slurry_m3ha	Slurry applied	m ³ ha ⁻¹	Ratio
Maintenance	Other maintenance present	—	Bool
MowingMachine	Machine type (rotary, knife, mulcher)	—	Spec.
minPhosphorus_kgPha	Mineral P input	kg ha ⁻¹	Ratio
Fertilization	Any fertilizer added	—	Bool
WaterLogging	Water-storage action	—	Spec.
Sulphur_kgSha	Sulfur input	kg ha ⁻¹	Ratio
minPotassium_kgKha	Mineral K input	kg ha ⁻¹	Ratio

3.1.3. Data Preprocessing and Cleaning

Both datasets include a unique identifier for each plot and the corresponding survey year. Biomass measurements were matched with features describing mowing and other management practices, forming a dataset where biomass serves as the target variable. Table 1 provides an overview of these features and the target variable.

Raw data is imported from a merged biomass and management practices file. The processing begins by removing non-informative features and discarding rows with missing target values. The remaining features are divided into numeric and categorical groups. Numeric features are standardized using a `StandardScaler`, which subtracts the mean

and scales the data to unit variance. Missing values are kept as missing values except for nitrogen, which is discussed below.

Furthermore, biomass values are segmented into discrete categories using quantile-based thresholds. The script supports various classification schemes:

- **Binary Classification:** The mean value is used to distinguish between “low” and “high” biomass.
- **Three-Class Classification:** The 33rd and 66th percentiles define thresholds for “low”, “medium”, and “high” biomass.
- **Four-Class Classification:** The 25th, 50th, and 75th percentiles are used to assign four classes, typically labeled as “low”, “medium-low”, “medium-high”, and “high” biomass.
- **Five-Class Classification:** Quintiles (20%, 40%, 60%, 80%) are computed to assign labels “very_low”, “low”, “medium”, “high”, and “very_high” biomass.

In Table 1 we give a listing and brief description of the used variables to predict biomass quantiles from. Note that “org” and “min” refer to fertilizers of organic or mineral origin, respectively. Further details can be found in [27].

3.1.4. Fertilization Preprocessing

Accurate quantification of fertilizer-derived nutrients is essential for assessing grassland fertility; however, direct measurements are often incomplete or confounded by placeholder zeros. To avoid bias, we applied a uniform preprocessing rule to every fertilizer-related variable in the dataset:

```
NbFertilization, Manure_tha, Slurry_m3ha, orgNitrogen_kgNha, minNitrogen_kgNha,
totalNitrogen_kgNha, minPhosphorus_kgPha, minPotassium_kgKha, Sulphur_kgSha
```

- **Step 1: Remove non-positive entries.** For each variable, values ≤ 0 (including special codes such as -1) were set to missing.
- **Step 2: Distinguish fertilized from non-fertilized samples.** If the categorical field Fertilization was “no,” every fertilizer variable for that sample was left as missing. This prevents artificial zeros from compressing distribution ranges.

By removing spurious zeros, it preserves the natural spread of the fertilizer distributions and prevents downward bias in subsequent analyses.

3.2. Machine Learning

In this work, we used CatBoost, a widely utilized boosting algorithm [30,31]. Decision trees, which underlie boosting methods, are non-parametric supervised learning models that can handle both classification and regression tasks [32].

Boosting classifiers build on the principle of iteratively training multiple weak learners, typically shallow decision trees, and combining their predictions to form a robust ensemble. In contrast to bagging techniques, which train models independently and in parallel, boosting methods focus on errors identified at each iteration. Notable boosting frameworks include Random Forest [33], XGBoost [34], and LightGBM [35].

CatBoost implements gradient boosting with a permutation-based approach to handle categorical variables, minimizing the need for data transformation. It often achieves reliable accuracy across diverse applications with only minor hyperparameter adjustments [36,37]. CatBoost has also shown consistent results when utilizing complexity metrics and engineered features in domains such as software testing and particularly agriculture [11,38]. Its built-in GPU support further helps manage large-scale datasets.

To fine-tune parameters such as learning rate, tree depth, and regularization terms, we employed Bayesian optimization [39], a model-based method that seeks high-performance

configurations while balancing exploration and exploitation. We automated this procedure using the scikit-opt Python package [40].

Feature Importance Analysis

We conducted a feature importance analysis to determine how each feature influenced model predictions. This was carried out using CatBoost's built-in functionality, which evaluates a feature's impact on the model output [41].

Specifically, we applied the PredictionValuesChange method, which calculates the average variation in the predicted value when a particular feature is altered. This approach quantifies how the model's output changes as feature values vary and is the default setting for non-ranking metrics. It helped us pinpoint the most significant features and offered insights into the relationships captured by the model.

Train/Test Split and Scaling

The dataset is partitioned into training (90%) and validation (10%) sets using stratified sampling to maintain the class distribution. Numeric features in both sets are scaled with a StandardScaler fitted on the training data.

Data Augmentation with ADASYN

To address class imbalance, the Adaptive Synthetic Sampling (ADASYN) algorithm is applied to the training set. The oversampling strategy is defined such that each class is upsampled to a target count determined by multiplying the majority class count by a specified OVERSAMPLE_FACTOR. ADASYN generates synthetic samples for classes based on the local feature space density, effectively balancing the dataset.

Hyperparameter Tuning

A CatBoost classifier is utilized for all prediction tasks. To optimize its performance, Bayesian Optimization is performed using BayesSearchCV from the scikit-optimize library. The optimization is configured to run for 20 iterations with 3-fold cross-validation, targeting the maximization of accuracy. The best hyperparameter set identified during the search is then used to train the final model and tested against the out-of-the-box implementation of CatBoost. We do this because it is known that CatBoost's out-of-the-box implementation already yields strong performances across various problems [37]. We then kept the optimized or out-of-the-box implementation based on their performance.

Model Evaluation and Visualization

The best trained CatBoost model is evaluated on the validation set, the training set and the ADASYN-synthesized training set. Performance is quantified using accuracy metrics, a detailed classification report, and a confusion matrix. All feature importances are calculated from the CatBoost model and visualized as a bar plot, providing insights into the relative contributions of each feature to the biomass prediction.

Overview Experimental Setup

The key points of our experimental design are depicted in Figure 1 and detailed in the following:

1. **Data Loading and Cleaning:** Load the raw dataset, remove irrelevant columns, and handle missing values.
2. **Feature Engineering:** Separate features into numeric and categorical sets, standardize numeric variables, and encode categorical variables.
3. **Biomass Categorization:** Compute quantile-based thresholds and assign biomass observations to binary, three, four, or five classes.

4. **Data Splitting and Scaling:** Split the data into training and validation sets; fit a `StandardScaler` on the training set and apply it to both sets.
5. **Oversampling:** Use ADASYN to generate synthetic samples for minority classes and balance the training set.
6. **Hyperparameter Optimization and Training:** Perform Bayesian Optimization with `BayesSearchCV` to tune CatBoost hyperparameters on the ADASYN training data, then train the final model.
7. **Validation and Analysis:** Evaluate each model's accuracy and other metrics on the original training set, the ADASYN-augmented training set, and the validation set. Generate confusion matrices, classification reports, distribution plots for nitrogen-related features, and extract feature importance scores.

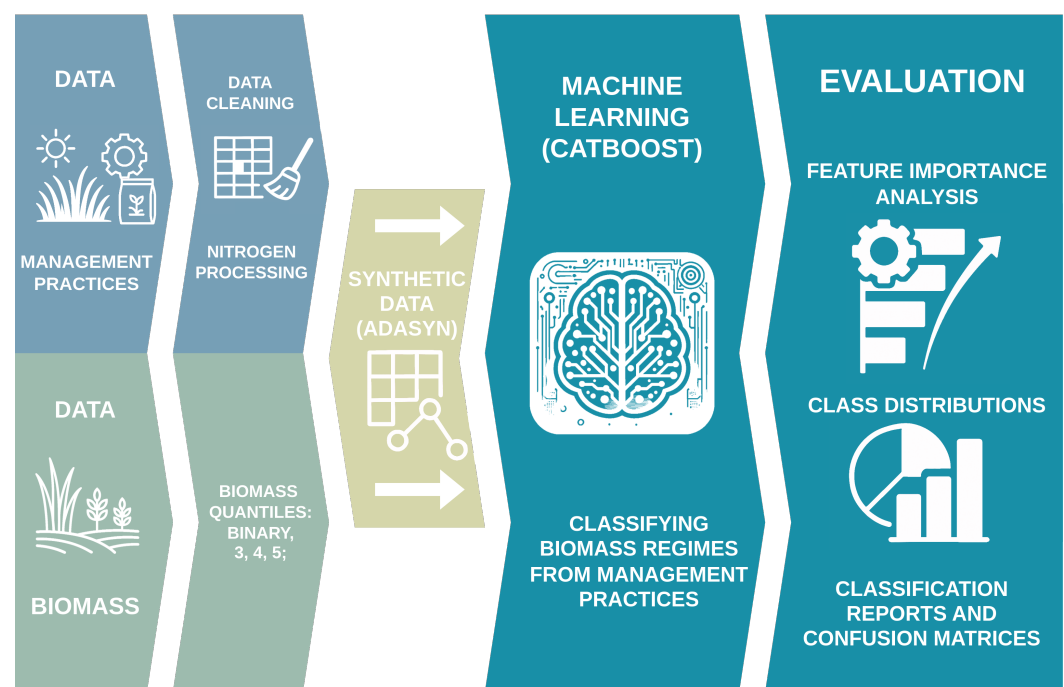


Figure 1. Overview of the experimental pipeline. Starting from raw grassland management and biomass data, we perform cleaning and quantile-based categorization into two to five classes. The training set is then upsampled using ADASYN, and a CatBoost classifier is trained to predict biomass categories. Finally, we evaluate model performance on test, original, and augmented training sets using classification reports, confusion matrices, feature importance rankings, and distribution plots of key predictors.

4. Results and Discussion

This section presents the outcomes of our classification experiments, comparing performance across four quantile-based schemes (binary, three-class, four-class, and five-class). For each scheme, we report accuracy, precision, recall, and F1-scores on test, augmented, and original training sets. We then examine how predictive performance changes as class granularity increases, and identify the best-performing models under default and Bayesian-optimized hyperparameters.

Feature importance results are presented to highlight the relative influence of mowing frequency, mineral and organic nitrogen inputs, and other management variables. Finally, we interpret these findings in light of similar studies, discuss potential sources of bias—such as imputation effects—and outline limitations and directions for future improvement.

4.1. Preliminary Evaluation

To examine relationships between management practices and biomass yield, we perform an initial exploratory analysis using quantile-based class definitions. For each of the four classification schemes (binary, three-class, four-class, and five-class), biomass values were divided according to the relevant quantile thresholds. We generated box-plots of mowing frequency, mineral nitrogen input (`minNitrogen_kgNha`), total nitrogen input (`totalNitrogen_kgNha`), and organic nitrogen input (`orgNitrogen_kgNha`) for each biomass class (Figures 2–5).

These visualizations facilitated a clear comparison of feature distributions across increasing biomass levels.

Overall, the preliminary analysis reveals that mowing frequency and nitrogen inputs generally increase with higher biomass classes under coarse segmentation (binary and three-class schemes). As class granularity increases, the spreads broaden almost monotonically up to four classes, indicating consistent positive relationships between inputs and yield. In the five-class scheme, however, the interquartile ranges for mineral and total nitrogen inputs in the *High* class narrow relative to the *Medium* class, suggesting that at finer resolution the relationship between nitrogen application and biomass yield becomes more complex and non-linear.

With a binary split the *High* class shows wider full ranges for all four variables than the *Low* class. The boxes for `orgNitrogen_kgNha` and the lower end of `totalNitrogen_kgNha` nearly collapse at the median, meaning that when organic nitrogen was applied as a fertilizer, farmers used mostly the same amount, with some rare events of drastically high amounts of fertilizer and many plots not applying any organic nitrogen (i.e., zero).

Using three quantiles, both *High* and *Medium* retain broader inter-quartile ranges for all variables, while the *Low* class remains compact for all features. Here we further see decreased ranges and interquartile ranges for low yields, supporting the previous findings for the binary biomass categories; increased amounts of mowing and nitrogen fertilization accompany increased biomass.

With four quantiles the spread increases almost monotonically from *Very Low* through *Very High*; only the *Low* group deviates slightly. Further, for mineral nitrogen we see a deviation in the interquartile ranges for the high biomass class, i.e., the high biomass class has a slightly lower interquartile range than the low biomass class.

At five quantiles the pattern becomes non-monotonic; for `minNitrogen_kgNha` and `totalNitrogen_kgNha` the inter-quartile range of the *High* class is narrower than that of the *Medium* class. This indicates a more complex, non-linear relationship in which additional nitrogen does not always lead to higher biomass once the classes are defined more finely.

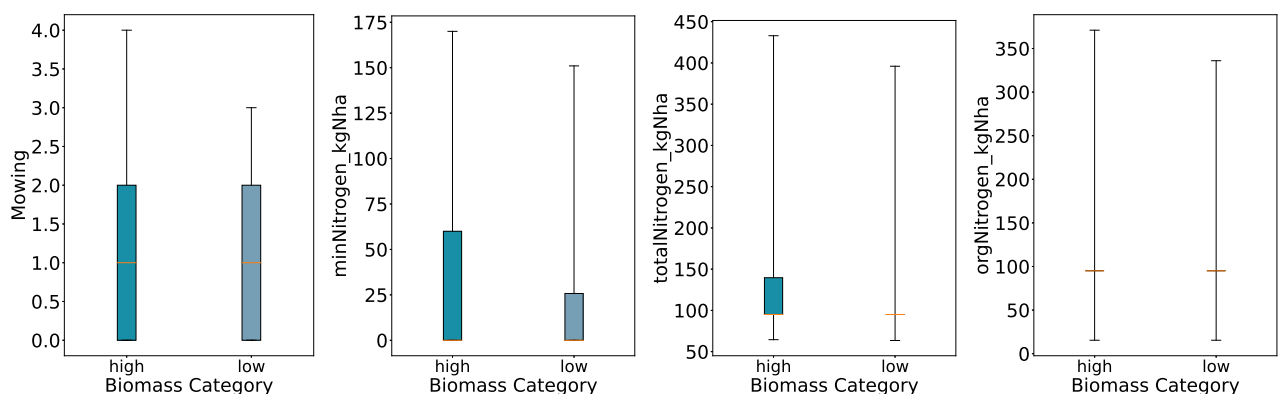


Figure 2. Distributions of key features for predicted categories (two quantiles, full whisker range).

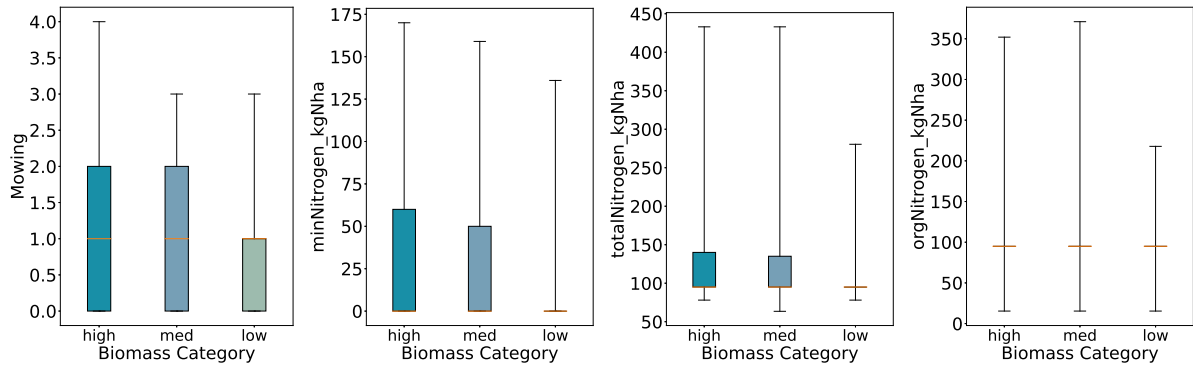


Figure 3. Distributions of key features for predicted categories (three quantiles, full whisker range).

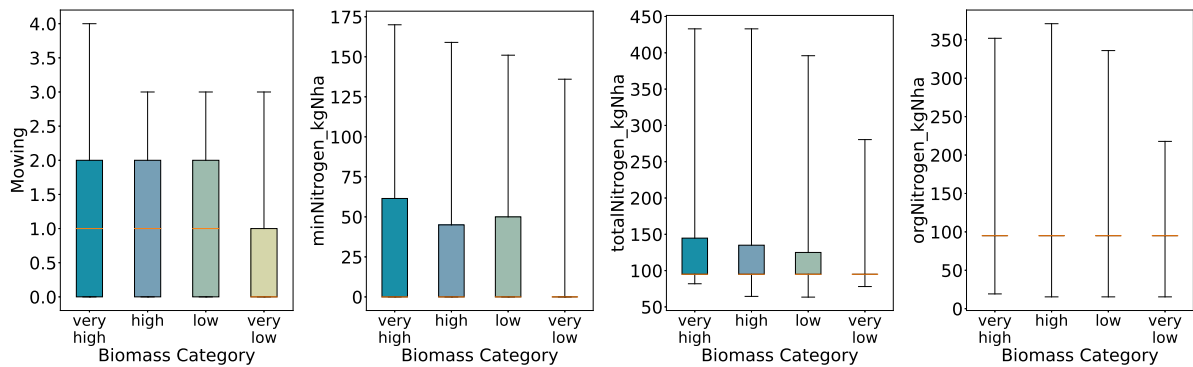


Figure 4. Distributions of key features for predicted categories (four quantiles, full whisker range).

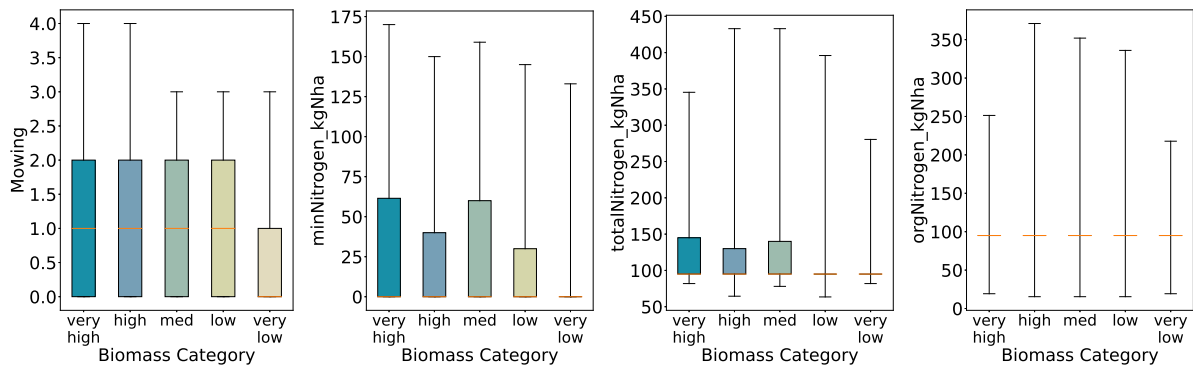


Figure 5. Distributions of key features for predicted categories (five quantiles, full whisker range).

4.2. Results of Binary Quantile Classification

Dividing biomass into *Low* and *High* classes at the median yields robust discrimination. On the test set (Table 2), overall accuracy reaches 0.7667. Precision for the *High* class is 0.72, with a recall of 0.69 (34 of 49 correctly identified), while the *Low* class attains precision 0.79 and recall 0.82 (58 of 71 correctly identified). The macro-averaged F1-score of 0.76 indicates balanced performance across classes. Confusion matrices (Figure 6) reveal that most errors consist of *High* samples misclassified as *Low* (15 of 49) rather than the reverse, a pattern consistent across original and ADASYN-augmented training sets, where accuracy remains near 0.76–0.77. This suggests the model is slightly conservative in assigning the *High* label but maintains overall stability after oversampling.

For the distribution of the predicted classes of mowing and nitrogen (Figure 7), we see similar behavior as for the initial evaluation, shown in Figure 2; however, for the predicted classes the differences in the distribution for Mowing and minNitrogen_kgNha are much

more pronounced. This indicates that the behavior the model learned from the data is that increased mowing intensity and increased mineral nitrogen applied lead to increased yields. Both distributions for organic nitrogen and total nitrogen look very similar to the initial evaluation; however, particularly for total nitrogen we see an increased median in the boxplots of the distribution, which accords with the previous findings of a more pronounced increase in mineral nitrogen for the high-yield regime, as total nitrogen is just the sum of organic and mineral nitrogen.

Feature importance analysis (Figure 8) highlights mowing frequency as the strongest predictor (13.1%), followed by mineral nitrogen input (`minNitrogen_kgNha`, 11.7%) and total nitrogen input (`totalNitrogen_kgNha`, 10.7%). Drainage application (8.5%) and the use of a mowing conditioner (8.3%) also contribute substantially. Lower importance scores for secondary variables—such as phosphorus input (2.0%) and a generic fertilization indicator (2.2%)—indicate that precise nitrogen measures and specific management practices drive model decisions. Overall, the prominence of mowing and nitrogen features confirms that both mechanical and nutrient inputs are key determinants of end-of-season biomass under a coarse, two-class framework.

Table 2. Binary quantile classification report.

Test Data				
Class	Precision	Recall	F1-Score	Support
high	0.72	0.69	0.71	49
low	0.79	0.82	0.81	71
Accuracy			0.77	120
Macro Avg	0.76	0.76	0.76	120
Weighted Avg	0.77	0.77	0.77	120
Synthetic Training Data (ADASYN)				
high	0.84	0.64	0.73	1530
low	0.73	0.89	0.80	1650
Accuracy			0.77	3180
Macro Avg	0.78	0.76	0.76	3180
Weighted Avg	0.78	0.77	0.76	3180
Original Training Data (No ADASYN)				
high	0.83	0.66	0.73	546
low	0.71	0.86	0.78	525
Accuracy			0.76	1071
Macro Avg	0.77	0.76	0.76	1071
Weighted Avg	0.77	0.76	0.75	1071

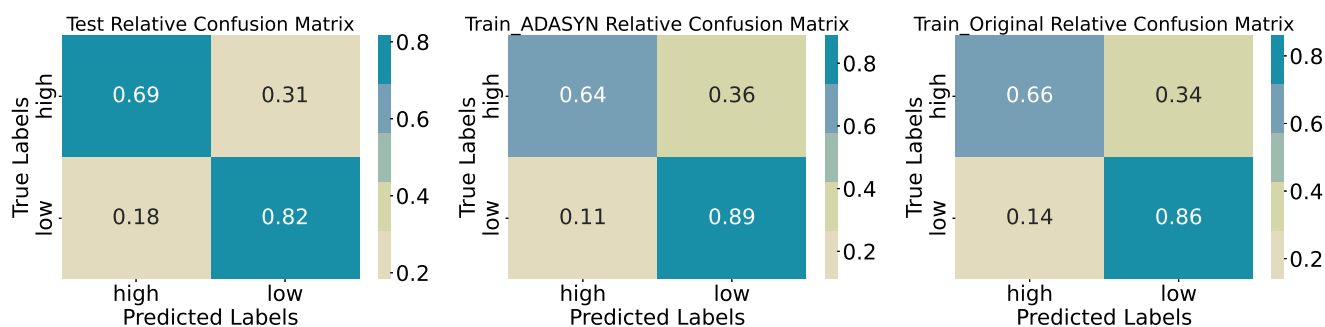


Figure 6. Confusion matrices for training, synthetic training, and test sets (binary quantiles).

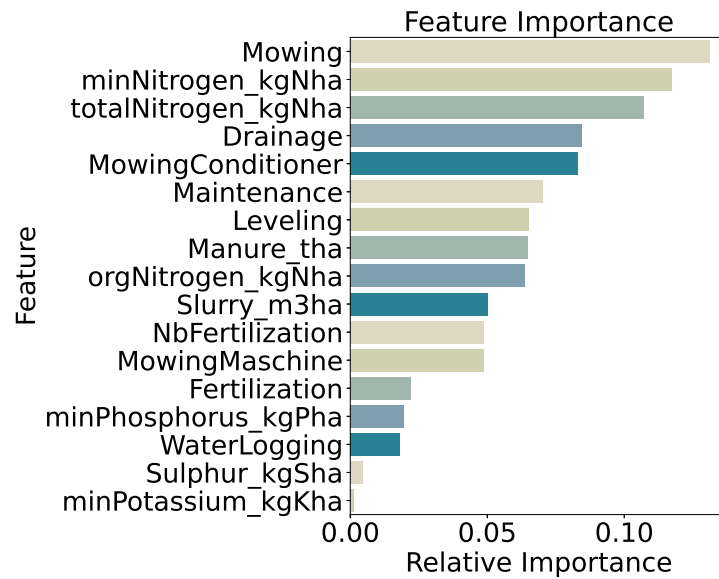


Figure 7. Feature importance for binary quantile classification.

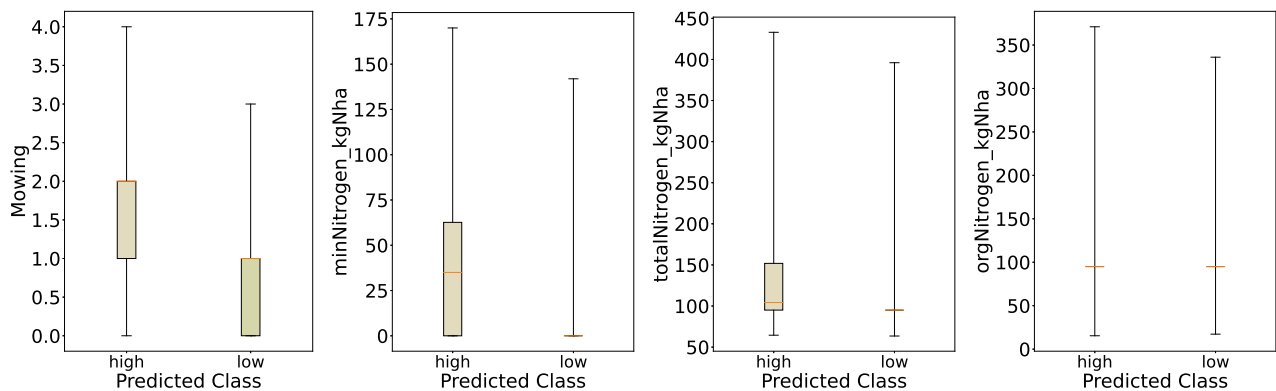


Figure 8. Distributions of key features for predicted categories (binary quantiles).

4.3. Results of Three-Quantile Classification

The three-class model attains an accuracy of 0.5833 on the test set (Table 3). Precision and recall vary substantially across classes; the *High* class achieves 0.66 precision and 0.64 recall (25 of 39 correctly identified), the *Low* class reaches 0.55 precision and 0.88 recall (36 of 41), while the *Medium* class lags with 0.56 precision and 0.23 recall (9 of 40). The confusion matrix (Figure 9) shows that 22 of 40 true *Medium* samples are misclassified as *Low*, and 9 as *High*, indicating substantial overlap in feature distributions at intermediate biomass levels. On the original training data, accuracy is 0.6788 with medium recall 0.48, and ADASYN oversampling raises training accuracy to 0.7129 and medium recall to 0.53, though the medium class remains the most error-prone. This difference in training and testing accuracies and performance shows that the model is overfitted on the training data and the model does not generalize well for predicting three quantiles of biomass regimes.

For the distribution of the predicted classes of mowing and nitrogen (Figure 10), we see similar behavior to the initial evaluation, shown in Figure 3; however, for the predicted classes the differences in the distributions of Mowing and minNitrogen_kgNha are changed. First, the medians are shifted for the medium biomass class, i.e., we see increased medians for mowing, mineral, and organic nitrogen in the medium class. Further, the medium biomass class shows a decreased interquartile range for mowing, pointing toward reduced variation in biomass for regimes with, on average, more cuts per year. We see similar behavior for mineral nitrogen: an increased median for the medium class and an increased

interquartile range, indicating that the highest biomass is not necessarily linked to the highest amount of mineral nitrogen applied to the fields.

Feature importance for the three-class model (Figure 11) is led by use of a mowing conditioner (14.6%), mowing frequency (13.7%), and drainage application (11.9%). Mineral nitrogen input (minNitrogen_kgNha, 11.7%) and total nitrogen input (totalNitrogen_kgNha, 10.8%) are also highly ranked, with general maintenance practices (10.2%) following. The prominence of these management-related features confirms that mechanical disturbance and precise nutrient inputs drive differentiation among low, medium, and high biomass classes, while lower-ranked variables contribute marginally to model decisions.

Table 3. Three-quantile classification report.

Test Data				
Class	Precision	Recall	F1-Score	Support
high	0.66	0.64	0.65	39
medium	0.56	0.23	0.32	40
low	0.55	0.88	0.67	41
Accuracy			0.58	120
Macro Avg	0.59	0.58	0.55	120
Weighted Avg	0.59	0.58	0.55	120
Synthetic Training Data (ADASYN)				
high	0.79	0.72	0.75	743
medium	0.79	0.53	0.63	710
low	0.63	0.88	0.74	776
Accuracy			0.71	2229
Macro Avg	0.74	0.71	0.71	2229
Weighted Avg	0.73	0.71	0.71	2229
Original Training Data (No ADASYN)				
high	0.75	0.70	0.73	366
medium	0.74	0.48	0.58	353
low	0.60	0.85	0.70	352
Accuracy			0.68	1071
Macro Avg	0.70	0.68	0.67	1071
Weighted Avg	0.70	0.68	0.67	1071

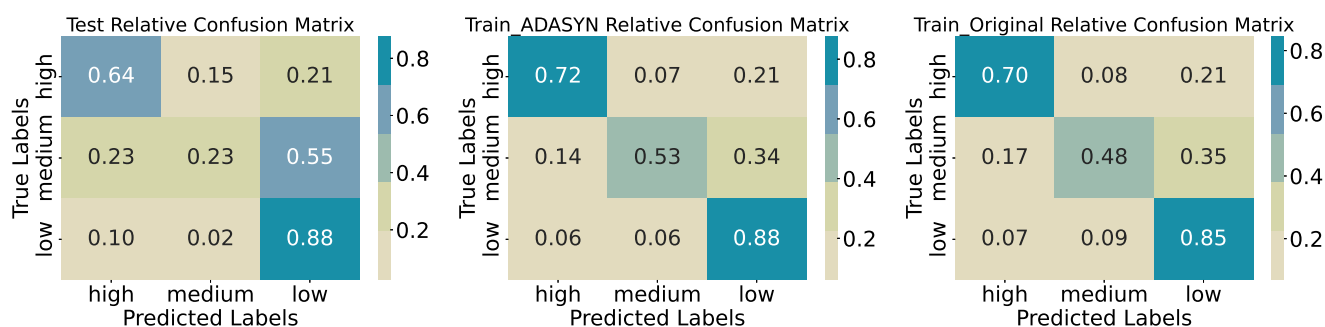


Figure 9. Confusion matrices for training, synthetic training, and test sets (three quantiles).

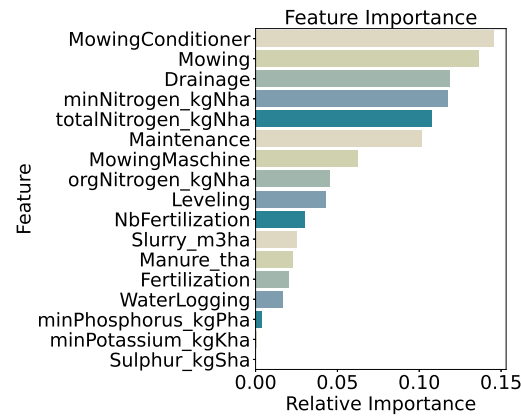


Figure 10. Feature importance for three-quantile classification.

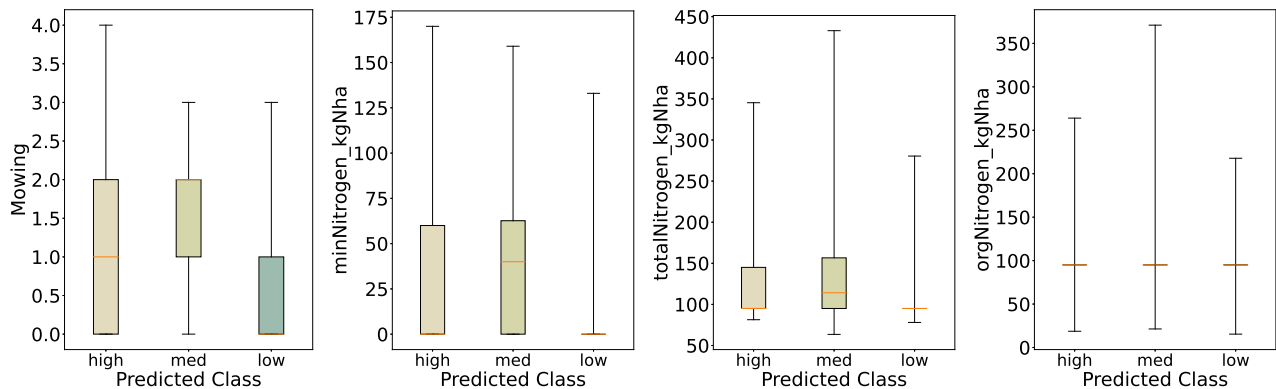


Figure 11. Distributions of key features for predicted categories (three quantiles).

4.4. Results of Four-Quantile Classification

Dividing biomass into four classes (*very_low*, *low*, *high*, *very_high*) yields a test accuracy of 0.4250 (Table 4). Performance varies markedly by class; *very_high* achieves precision 0.57 and recall 0.47, while *very_low* reaches precision 0.45 and recall 0.59. The middle classes fare worse—*high* records precision 0.21 and recall 0.33; *low* has precision 0.42 and recall 0.28—resulting in a macro-averaged F1-score of 0.41.

The confusion matrices (Figure 12) show frequent misclassification between adjacent classes. Only 33% of true *high* samples are correctly identified, with 27% mislabelled as *very_high* and 27% as *very_low*. Similarly, 44% of true *low* samples are predicted as *very_low*, indicating limited separation in the feature space at intermediate biomass levels. On the original training set, accuracy rises to 0.6153, with recall 0.70 for *very_high* and 0.78 for *very_low*. ADASYN oversampling further increases training accuracy to 0.6692 and recall across classes (*very_high*: 0.73; *high*: 0.54; *low*: 0.56; *very_low*: 0.84), though the *high* class remains challenging. Again, as for the three-quantile classification, this shows that the model does not generalize well, as the performance drops sharply for the test data set, meaning that the model overfits the training data.

Again, the distributions of the predicted four-class results (Figure 13) are similar to the initial distributions (Figure 4); however, we observe narrower interquartile ranges for the *high* and *low* classes in terms of mowing intensity per year, and an increased median—particularly for the *high* class—compared with the initial evaluation. A further difference is that the *low*-biomass class shows a very low median for mineral nitrogen input. Mineral nitrogen also lost feature importance relative to the binary classification, which means the class differences are less distinct for this variable within the model. We see slightly similar behavior for total nitrogen, as it is linked to mineral nitrogen, while organic nitrogen remains mostly unchanged. Moreover, the model does not generalize well

and appears overfitted; we therefore conclude that these deviations for the non-extreme classes mark areas where the model fails to account for variation.

Feature importance (Figure 14) is led by mowing frequency (15.5%) and use of a mowing conditioner (13.4%), followed by drainage (11.5%), mineral nitrogen input (minNitrogen_kgNha, 11.1%), general maintenance practices (9.7%), and total nitrogen input (9.1%). Distributions of these features across classes (Figure 14) show generally increasing medians and interquartile ranges from very_low to very_high, confirming that both mechanical disturbance and nutrient inputs remain the primary drivers of biomass even under finer class segmentation.

Table 4. Four-quantile classification report.

Test Data				
Class	Precision	Recall	F1-Score	Support
very_high	0.57	0.47	0.52	34
high	0.21	0.33	0.26	15
low	0.42	0.28	0.34	39
very_low	0.45	0.59	0.51	32
Accuracy			0.42	120
Macro Avg	0.41	0.42	0.41	120
Weighted Avg	0.45	0.42	0.43	120
Synthetic Training Data (ADASYN)				
very_high	0.78	0.73	0.76	1274
high	0.76	0.54	0.63	1218
low	0.68	0.56	0.62	1208
very_low	0.55	0.84	0.67	1225
Accuracy			0.67	4925
Macro Avg	0.69	0.67	0.67	4925
Weighted Avg	0.69	0.67	0.67	4925
Original Training Data (No ADASYN)				
very_high	0.70	0.70	0.70	264
high	0.68	0.49	0.57	282
low	0.60	0.49	0.54	259
very_low	0.53	0.78	0.63	266
Accuracy			0.62	1071
Macro Avg	0.63	0.62	0.61	1071
Weighted Avg	0.63	0.62	0.61	1071

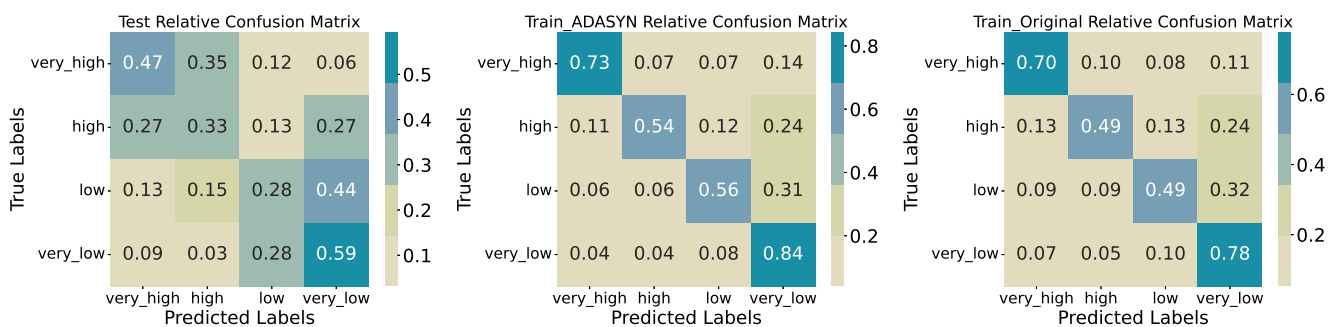


Figure 12. Confusion matrices for training, synthetic training, and test sets (four quantiles).

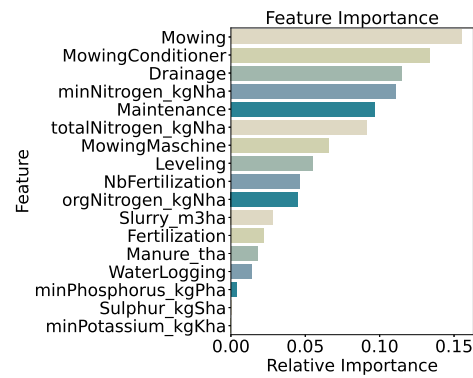


Figure 13. Feature importance for four-quantile classification.

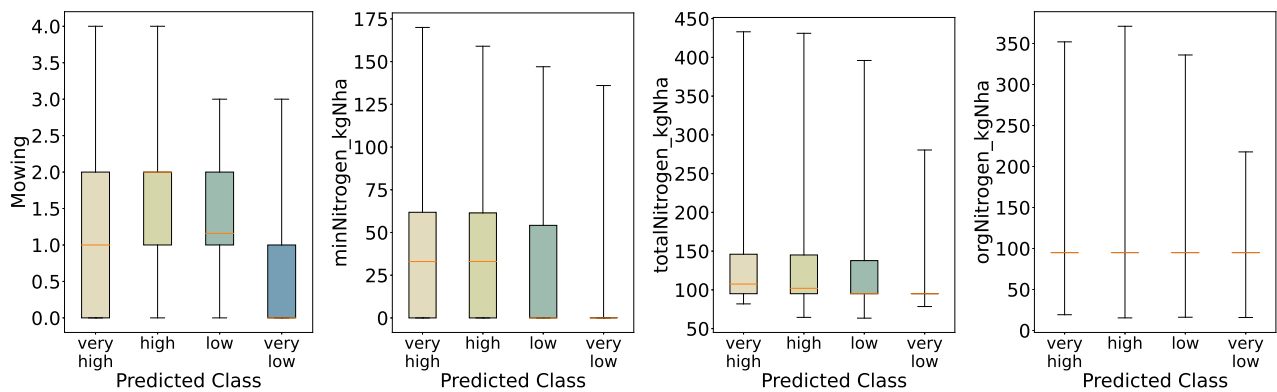


Figure 14. Distributions of key features for predicted categories (four quantiles).

4.5. Results of Five-Quantile Classification

Splitting biomass into five quantile-based classes yields a test accuracy of 0.3250 (Table 5). Precision and recall vary substantially across classes; *very_high* achieves precision 0.59 and recall 0.36, while *very_low* attains precision 0.39 and recall 0.64. The intermediate classes perform poorly—*high* has precision 0.15, recall 0.18; *medium* and *low* register recalls of 0.21 and 0.19, respectively—resulting in a macro-averaged F1-score of 0.31. Confusion matrices (Figure 15) reveal that many true *high* and *medium* instances are misclassified into adjacent categories (e.g., 29% of *high* as *medium*, 24% as *very_high*; 33% of *medium* as *very_low*), indicating limited separability at finer granularity. Training accuracy improves to 0.5621 on the original data and to 0.6237 with ADASYN oversampling, yet misclassification patterns persist, particularly among the middle three classes.

Feature importance for the five-class model (Figure 16) remains dominated by management variables; mowing frequency (15.9%) and use of a mowing conditioner (13.8%) together account for nearly 30% of total importance. Drainage (12.4%) and mineral nitrogen input (*minNitrogen_kgNha*, 12.2%) follow, with general maintenance (9.4%) and total nitrogen input (*totalNitrogen_kgNha*, 8.8%) also contributing. The relative decline in importance of nitrogen features compared to the two- and three-class models suggests that at very fine biomass resolution, mechanical management practices drive most of the predictive signal. Distributions of these top features across quantile classes (Figure 17) show progressively increasing medians and interquartile ranges from *very_low* to *very_high*, confirming their central role even under challenging classification conditions.

Once more, the distributions obtained from the five-class predictions (Figure 17) resemble those from the initial analysis (Figure 5) and the four-quantile scheme; nevertheless, the *medium* and *low* groups exhibit tighter interquartile ranges for annual mowing intensity and a higher median—most pronounced in the *medium* class—than in the initial evaluation. Another notable change is that the *very_high* biomass class displays a low

median for mineral nitrogen input. This suggests that the model inferred a link between reduced mineral nitrogen and increased biomass. Again, consistent with this, mineral nitrogen has lost feature importance relative to the binary classification, so class contrasts for this variable are less sharp. Total nitrogen follows a broadly similar pattern, as it depends on mineral nitrogen, whereas organic nitrogen remains largely unchanged. Finally, because the model does not generalize well and appears overfitted, we interpret these shifts in the non-extreme classes as signs of where the model fails to capture underlying variability.

Table 5. Five-Quantile classification report.

Test Data				
Class	Precision	Recall	F1-Score	Support
very_high	0.59	0.36	0.44	28
high	0.15	0.18	0.16	17
medium	0.24	0.21	0.22	24
low	0.24	0.19	0.21	26
very_low	0.39	0.64	0.48	25
Accuracy			0.33	120
Macro Avg	0.32	0.31	0.31	120
Weighted Avg	0.34	0.33	0.32	120
Synthetic Training Data (ADASYN)				
very_high	0.77	0.70	0.73	1548
high	0.71	0.54	0.61	1552
medium	0.69	0.61	0.65	1558
low	0.58	0.53	0.56	1577
very_low	0.48	0.75	0.58	1477
Accuracy			0.62	7712
Macro Avg	0.65	0.63	0.63	7712
Weighted Avg	0.65	0.62	0.63	7712
Original Training Data (No ADASYN)				
very_high	0.69	0.62	0.66	210
high	0.59	0.45	0.51	221
medium	0.60	0.54	0.57	214
low	0.52	0.49	0.50	212
very_low	0.47	0.71	0.57	214
Accuracy			0.56	1071
Macro Avg	0.58	0.56	0.56	1071
Weighted Avg	0.58	0.56	0.56	1071

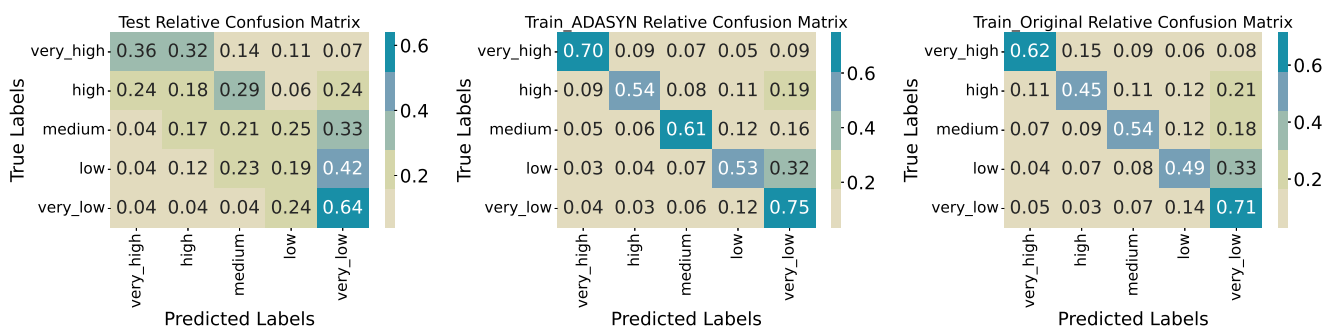


Figure 15. Confusion matrices for training, synthetic training, and test sets (five quantiles).

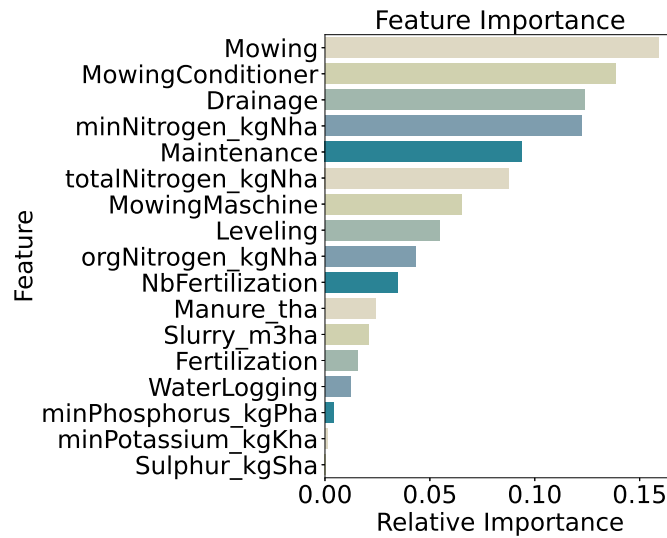


Figure 16. Feature importance for five-quantile classification.

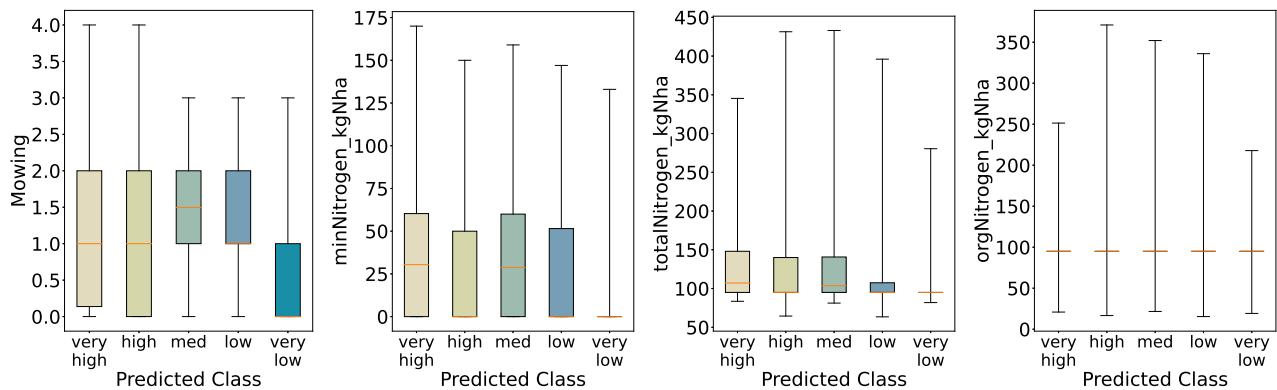


Figure 17. Distributions of key features for predicted categories (five quantiles).

4.6. Discussion

Our experiments demonstrate that machine learning can reliably distinguish broad biomass yield categories from standardized grassland management data, but that predictive power diminishes as class granularity increases. In the binary classification (Table 2), the CatBoost model achieved 77% accuracy on unseen data. Mowing frequency and mineral nitrogen input together accounted for just under 25% of feature importance (Figure 7), confirming that both mechanical disturbance and precise nutrient inputs are primary drivers of overall biomass. The high ranking of mowing conditioner and drainage variables further indicates that intensive management regimes—characterized by frequent cutting, use of conditioners, and effective water control—are strongly associated with higher yields.

When the task was extended to three classes, accuracy fell to 58% (Table 3). The confusion matrix (Figure 9) reveals that the *Medium* class overlaps substantially with both *Low* and *High*, resulting in only 23% recall for medium yields. This reflects the preliminary distribution analysis (Section 4.1), where interquartile ranges for key features in the medium class remained relatively broad and similar over all classes. Moving to four and five classes further reduced accuracy to 42% and 33%, respectively (Tables 4 and 5). In these finer schemes, misclassifications occur predominantly between adjacent categories, e.g., true high yields labeled as *very_high* or *low*, indicating that small differences in management inputs do not translate into clear class separations.

It is noteworthy that, for all schemes beyond the binary classification, accuracy drops substantially from training to test data. This suggests overfitting to the training samples

rather than capture of underlying relationships between management practices and biomass outcomes. Consequently, our binary classification results—and the associated feature importance rankings—are the most reliable. In that model, mowing frequency and mineral nitrogen input emerge as the dominant drivers of increased biomass. Total nitrogen (the sum of organic and mineral nitrogen) ranks third, but organic nitrogen alone never appears among the top five features, indicating that the mineral component drives its importance. Although existing studies highlight the role of soil/organic nitrogen in plant-based crop rotation planning and overall soil fertility (e.g., [12,42,43]), our findings cannot rule out its true influence; rather, they underscore the need for more complete data on organic nitrogen application.

Despite declining accuracy and generalizability, feature importance patterns remained stable across the three- to five-class schemes (Figures 10–16). Mowing frequency and conditioner use consistently ranked highest, followed by drainage, mineral nitrogen input, and general maintenance. This suggests that, even when precise class assignments are unreliable, these core practices dominate the available information on biomass regimes. However, given the low accuracy and limited generalizability, these importance scores most likely reflect strong patterns in the training data rather than true causal effects.

Secondary features—such as phosphorus input and binary fertilization flags—contributed minimally across all schemes, implying that precise, quantitative measures of nitrogen and exact mowing records carry more predictive value than simple categorical indicators.

Compared to regression or correlation analyses, our multi-class classification approach offers two key advantages. First, it quantifies classification limits; the stepwise decline in test accuracy with increasing class number (77% → 58% → 42% → 33%) defines how much yield detail can be inferred from management logs. Second, it provides direct measures of model confidence for each class—valuable for advisory purposes where broad categories (e.g., “low” vs. “high” yield) can be forecast reliably, while finer distinctions are gradually more difficult.

Data quality and completeness remain major constraints. Monotonic values in fertilization measurements compress distribution ranges (Section 3.1.4) and may bias importance estimates, particularly for organic nitrogen. Agricultural data acquisition is resource-intensive and methods evolve rapidly, making long-term consistency challenging. Beyond farmer questionnaires, valuable data sources now include (i) satellite imagery such as Sentinel-2 and Landsat-9 for annual to decadal coverage, (ii) UAV multispectral or hyperspectral surveys that capture sub-plot nitrogen status and canopy traits, (iii) LiDAR for three-dimensional biomass and surface roughness, (iv) on-board yield monitors on harvesters, and (v) ground-based IoT probes that stream soil moisture, temperature, and mineral nitrogen in real time [44–47]. UAV-derived red-edge and chlorophyll indices have already estimated leaf nitrogen concentration with a root-mean-square error (RMSE) below 1.5 mg g^{-1} for winter wheat [48]. Integrating these sources with local weather stations, and potentially other data sources, will enlarge spatial and temporal coverage, reduce reliance on self-reported inputs, and support site-specific fertilizer decisions. Thus, future work should integrate automated sensing (e.g., drone-based hyperspectral imaging, in-field robotic probes) to obtain continuous, objective measurements of nutrient status and soil moisture, reduce reliance on farmer-reported entries, and improve spatial and temporal coverage.

5. Conclusions

This study applied a multi-class machine learning pipeline to predict grassland biomass yield from detailed management records collected by the Biodiversity Explorato-

ries. Using CatBoost classifiers tuned via Bayesian optimization and balanced with ADASYN oversampling, we achieved robust separation of low versus high biomass (77 % accuracy) and progressively finer, though less reliable, classification into three (58 %), four (42 %), and five (33 %) quantile-based classes. Across all schemes, mowing frequency and precise nitrogen inputs—particularly mineral nitrogen and total nitrogen—emerged as the dominant drivers of biomass variability, together accounting for just under one quarter of the total feature importance in the binary model. Secondary management factors (e.g., conditioner use, drainage) contributed meaningfully, whereas broad nutrient indicators (e.g., binary fertilization flags, phosphorus input) offered limited additional predictive value.

Using the same pipeline, we again observed that, beyond the binary split, model accuracy dropped substantially from the training to the test set, indicating limited generalizability and a tendency to overfit the training data when class granularity increased. Across all schemes and particularly for the binary model, mowing frequency and nitrogen inputs—especially mineral nitrogen and total nitrogen—are dominant drivers of biomass variability, together accounting for nearly one quarter of the total feature importance. Secondary management factors (e.g., conditioner use, drainage) contributed meaningfully, whereas broad nutrient indicators (e.g., binary fertilization flags, phosphorus input) offered limited additional predictive value.

Our results quantify the practical limits of predicting fine-grain yield categories from farmer-reported management data alone. The decline in accuracy with increasing class number highlights nonlinear and threshold effects in the input–yield relationship, and indicates that subsampling errors and missing values introduce additional uncertainty at intermediate yield levels. To improve precision for three-class and finer schemes, future work should integrate complementary environmental covariates—such as soil moisture, weather data, or plant species composition—and employ automated sensing technologies (e.g., drone-mounted hyperspectral imagery, in-field soil probes) to capture key variables more objectively and at higher resolution.

These findings also have direct implications for grassland management. The clear dichotomy between high-intensity regimes (frequent mowing, high nitrogen input) and low-intensity regimes suggests distinct farmer strategies. Advisory services or incentive schemes could target mid-intensity practitioners to optimize yield without excessive inputs.

Research Questions Answered

Based on our results, we address the three research questions as follows:

1. *Prediction accuracy and key drivers:* Machine learning models can predict broad biomass regimes (binary split) with good accuracy (77%) and clearly identify key drivers, but their reliability declines with finer class granularity.
2. *Influence of nitrogen inputs:* Mineral nitrogen input consistently ranks among the top predictors; while organic nitrogen's role cannot be fully assessed due to data limitations, total nitrogen remains an important feature.
3. *Comparison of management factors:* Mowing frequency and mineral nitrogen inputs outweigh other management practices in determining biomass yield, with secondary factors (e.g., drainage, maintenance) providing additional, but smaller, predictive value.

To the best of our knowledge, this is the first study that (i) applies a *multi-class* CatBoost framework—tuned by Bayesian optimization and balanced with ADASYN—to grassland biomass prediction, (ii) couples those predictions with a systematic, model-intrinsic feature importance ranking of mowing and fertilizer variables, and (iii) quantifies how both accuracy and variable relevance decline step-wise as class granularity increases from two to five categories. By working only with farmer-reported management data and an eight-year, plot-level time series, we show the practical resolution limit of such records and provide a

workflow that can be transferred to other long-term ecological datasets or extended with remote sensing covariates in future work.

Consequently, this study highlights the value of long-term, standardized datasets like the Biodiversity Exploratories, while underscoring the need for improved data protocols and novel sensing technologies to capture soil variables more completely. By combining robust field experiments with advanced machine learning and automated sensing, future research can develop more precise and sustainable grassland management strategies.

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Data Availability Statement: All code used in this study is publicly available in the corresponding GitHub repository: https://github.com/Raubkatz/Nitrogen_Classification, accessed on 1 April 2025. Reproducibility is further ensured through the use of openly accessible datasets. Biomass data were sourced from [29] and can be downloaded via the BEXIS database at <https://www.bexis.uni-jena.de/ddm/data/Showdata/31448>, accessed on 1 April 2025. Grassland management data are from [27] and are available on the project's data portal: <https://bdj.pensoft.net/article/36387/element/4/5226558//>, accessed on 1 April 2025. Together, these resources provide a fully transparent foundation for replicating and extending our findings.

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Abbreviations

The following abbreviations are used in this manuscript:

ADASYN	Adaptive Synthetic Sampling Approach
CAT	CatBoost
BO	Bayesian Optimization
ML	Machine Learning

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