

Article

Identifying maize yield drivers using statistical analysis and multilayer perceptron modelling

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Abstract: Maize yield formation is jointly determined by crop-year conditions, water availability, nutrient management, and their interactions, which may include complex nonlinear relationships. This study aimed to identify the principal agronomic and physiological variables associated with maize yield using classical statistical analyses complemented by multilayer perceptron modelling. Field data collected in Debrecen, Hungary, during 2024–2025 included crop year, irrigation, fertilizer treatment, phenological stage, SPAD chlorophyll readings, and grain yield. Pearson correlation and linear regression quantified individual relationships, while four MLP scenarios evaluated combined predictive effects. Fertilizer was positively associated with yield in both years and irrigation regimes, with the strongest relationship under irrigation in 2025 ($r = 0.770$; $R^2 = 0.594$). The SPAD–yield relationship generally strengthened during crop development, reaching its maximum at R3 under irrigation in 2025 ($r = 0.916$; $R^2 = 0.839$). The best-performing MLP scenario included year, fertilizer, and irrigation, confirming their central role in yield prediction and formation.

Keywords: maize; grain yield; SPAD; fertilizer; irrigation; phenological stage; multilayer perceptron; machine learning; yield prediction; precision agriculture

1. Introduction

Maize (*Zea mays* L.) is one of the world's most widely cultivated cereal crops and plays a central role in food security, animal nutrition, industrial processing, and bioenergy production. Owing to its high yield potential and broad range of uses, maize contributes substantially to meeting the food and feed demands of a continuously growing global population [1–7]. However, maintaining stable maize production is becoming increasingly difficult because crop performance is strongly affected by climate variability, particularly changes in temperature and precipitation patterns [5,6,8].

Among the environmental factors influencing maize production, water availability and temperature are of primary importance [8]. Drought and heat stress can substantially reduce plant growth and grain formation, whereas irrigation may alleviate water stress and limit yield losses under unfavourable conditions [9]. Nevertheless, the response to irrigation is not uniform across years, because the magnitude of its effect depends on the timing and severity of water deficits, seasonal temperature conditions, soil properties, and crop development stage. Consequently, crop-year effects may sometimes exert a stronger

Academic Editor: Adrienn Széles

Received: 2026.02.22.

Revised: 2026.03.15.

Accepted: 2026.05.03.

Published: 2026.08.19.

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influence on yield than individual agronomic interventions. Hybrid selection is also important, as genotypes differ in their productivity, stress tolerance, and grain-quality characteristics [10,11].

Nutrient management, particularly nitrogen fertilization, is another major determinant of maize yield and quality. Nitrogen is essential for leaf development, photosynthetic activity, biomass accumulation, and grain formation; however, both insufficient and excessive nitrogen supply may reduce production efficiency. The agronomic response to fertilizer depends strongly on environmental conditions and water availability, which highlights the importance of coordinating nutrient and irrigation management [12]. Determining the optimal fertilizer rate and application timing is therefore essential not only for maximizing yield but also for improving nitrogen-use efficiency and reducing environmental losses [13–15]. Long-term field experiments conducted under Central European conditions have demonstrated that the effect of fertilization on maize yield is closely related to crop year, water supply, and the interaction between these factors [9,13–15].

Rapid and nondestructive assessment of crop nitrogen status can improve the timing and precision of nutrient management. SPAD chlorophyll-meter readings are widely used as indirect indicators of leaf chlorophyll content and plant nitrogen status. Their relationship with final grain yield may, however, vary according to phenological stage, environmental conditions, and management treatment. Measurements conducted at later vegetative or reproductive stages may provide more direct information on the physiological status of the crop during critical periods of yield formation than measurements performed early in development. Evaluating the temporal development of the SPAD–yield relationship can therefore help identify the phenological stages that are most informative for yield assessment and crop-management decisions.

Traditional statistical methods, including analysis of variance, correlation, and linear regression, are valuable for quantifying individual effects and linear relationships among agronomic variables. However, maize yield is determined by multiple, interacting factors whose effects may be nonlinear. The increasing availability of field, sensor, spatial, and temporal data has therefore encouraged the application of machine-learning methods in crop research and precision agriculture [16]. Artificial neural networks can model complex relationships among environmental, physiological, and management variables without requiring these relationships to follow a predetermined functional form. Previous studies have shown that integrating spatial and temporal information with machine-learning methods can improve site-specific maize-yield prediction and support more precise management decisions [12,17]. Data-mining and machine-learning approaches have also shown potential for optimizing maize-yield forecasting under Central European production conditions [18].

Despite these advances, machine-learning predictions are most informative when interpreted together with classical statistical results. Statistical analyses can identify the direction, strength, and significance of individual relationships, while multilayer perceptron models can evaluate the joint predictive value of several variables and account for nonlinear interactions. Their combined application may therefore provide a more comprehensive understanding of maize yield formation than either approach alone.

Accordingly, the objective of this study was to identify and quantify the agronomic and physiological factors associated with maize grain yield under contrasting crop-year and irrigation conditions. Specifically, the study evaluated the effects of fertilizer supply, irrigation, crop year, phenological stage, and SPAD chlorophyll readings using classical statistical analyses and complementary multilayer perceptron modelling. In addition, alternative MLP scenarios were compared to determine which combinations of input variables provided the most accurate yield predictions and the greatest explanatory value for yield variability.

2. Materials and Methods

The field experiment was conducted in 2024 and 2025 at the Látókép Crop Production Experimental Station of the University of Debrecen, Hungary (47°33' N, 21°26' E; 111 m a.s.l.). The site is located on the Hajdúság loess plateau and is characterized by a lowland calcareous chernozem soil with favourable water-holding capacity. The long-term experiment was established as a two-replicate split-split-plot trial covering a total area of 1.5 ha and comprising 180 plots, each 1.5 m wide and 9 m long. In the original design, maize hybrids were assigned to the main plots, irrigation treatments (irrigated and rainfed) to the subplots, and fertilizer treatments to the sub-subplots. The present analysis was restricted to the Merida hybrid (FAO 370), which was evaluated in both crop years. Nitrogen was supplied as granular $\text{NH}_4\text{NO}_3 + \text{CaMg}(\text{CO}_3)_2$ fertilizer containing 27% N, 7% CaO, and 5% MgO. The treatments included an unfertilized control (A_0) and basal applications of 60 (A_{60}) or 120 kg N ha⁻¹ (A_{120}). The basal treatments were supplemented by 30 kg N ha⁻¹ at the V6 stage, producing cumulative rates of 90 (V6_90) and 150 kg N ha⁻¹ (V6_150), respectively. A further 30 kg N ha⁻¹ was applied at V12, resulting in final cumulative rates of 120 (V12_120) and 180 kg N ha⁻¹ (V12_180). Irrigation was supplied using a Valley 8120 linear irrigation system; the irrigated treatment received 60 mm of additional water in 2024 and 25 mm in 2025. Relative chlorophyll content was measured using a MINOLTA SPAD-502 chlorophyll meter. SPAD readings were recorded at V6, V8, V10, V12, R1, and R3, and grain yield was determined at harvest. Measurements were taken on the 6th, 7th, and 8th plants in the second row from the left of each plot. The graphs were prepared using Microsoft Excel 2016. Statistical analyses were performed using IBM SPSS Statistics for Windows, version 31.0.0.0. Harvested grain yield was adjusted to a moisture content of 14%. Harvesting was carried out using a Sampo plot combine harvester. Following harvest, grain composition parameters were determined using a Perten DA 7250 NIR Analyzer.

Weather conditions during the maize growing season differed between the two experimental years (Figure 1). In 2024, April was 2.4 °C warmer and received 14.7 mm less precipitation than the 1981–2010 mean. May precipitation exceeded the long-term mean by 12.2 mm, while June precipitation was equal to the long-term mean (66.0 mm). In contrast, rainfall in July (28.6 mm) and August (33.3 mm) was 37.4 and 15.7 mm below the corresponding long-term means, respectively. From May onward, monthly mean air temperature exceeded the long-term mean by 0.9–3.4 °C. Thus, the 2024 season was characterized by pronounced heat and rainfall deficits during July and August, coinciding with critical reproductive and grain-filling periods.

The 2025 growing season was also warm and dry, although the temporal distribution of precipitation differed from that in 2024 (Figure 1). April was warm (12.9 °C) and dry (23.0 mm), while May remained relatively cool (14.2 °C) and precipitation-deficient (44.0 mm). June was exceptionally dry, receiving only 18.0 mm of precipitation, 48.0 mm below the long-term mean, together with a mean temperature of 22.2 °C. Conditions improved in July, when 81.5 mm of rainfall and a mean temperature of 22.0 °C provided more favourable conditions for flowering. August remained warm (21.6 °C) and moderately dry (27.0 mm), whereas September was both warm (18.4 °C) and comparatively wet (65.5 mm).

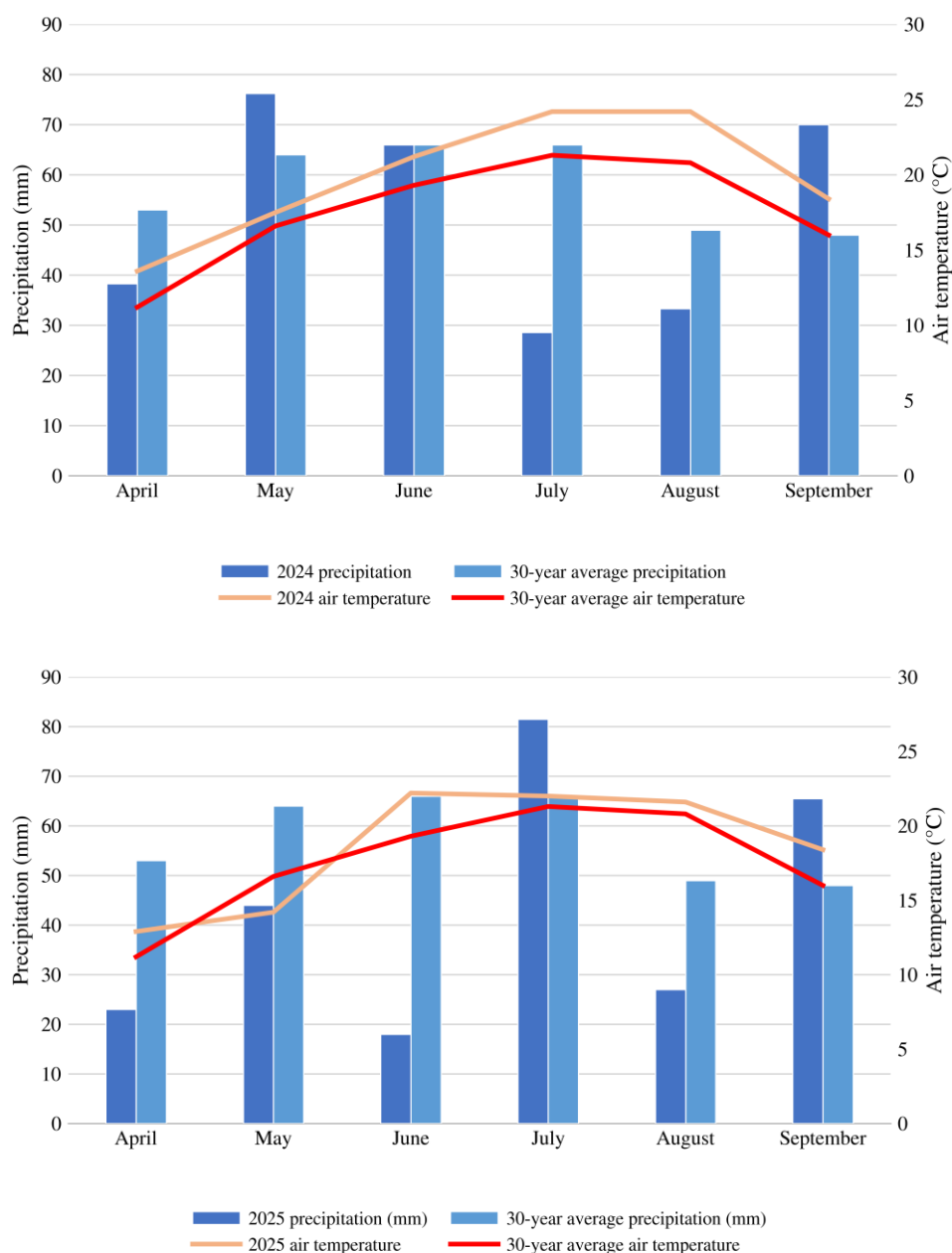


Figure 1 Monthly precipitation and mean air temperature during the 2024 and 2025 maize growing seasons at the Látókép experimental site compared with the 30-year average

In the scope of the analyses, relationships between maize grain yield and the investigated agronomic and physiological variables were evaluated: Pearson's correlation coefficient (r) and simple linear regression were used to examine the association between fertilizer rate and grain yield separately for each crop year and irrigation regime. The relationship between SPAD value and grain yield was also evaluated separately for each phenological stage (V6, V8, V10, V12, R1, and R3), crop year, and irrigation treatment. The coefficient of determination (R^2) was used to quantify the proportion of yield variation explained by each linear relationship, while significance was evaluated at the 0.1%, 1%, and 5% probability levels. These analyses provided a basis for interpreting the individual relationships before evaluating the combined and potentially nonlinear predictive effects using the MLP models.

To evaluate the predictive contribution of agronomic and physiological variables, four multilayer perceptron scenarios were developed using different combinations of crop year, fertilization, irrigation, phenological stage, and SPAD value. The scenarios were designed to compare management-based models with those incorporating physiological and phenological information. The input-variable structure of each scenario is summarized in Table 1 and illustrated in Figure 2.

Table 1. Composition of the applied scenarios

Scenario	Input variables
SC1	crop year, fertilization, irrigation
SC2	fertilization, phenological stage, SPAD value
SC3	crop year, fertilization, irrigation, phenological stage, SPAD value
SC4	crop year, fertilization, irrigation, SPAD value

The allocation of input variables across the four MLP scenarios is illustrated in the alluvial diagram (Figure 2). The figure provides a visual overview of how crop year, fertilization, irrigation, phenological stage, and SPAD value were combined in the different model structures. SC1 represents the agronomic management variables, whereas SC2 emphasizes fertilization together with phenological and physiological information. SC3 includes the complete set of agronomic, phenological, and physiological predictors, while SC4 combines crop year, fertilization, irrigation, and SPAD value without explicitly including phenological stage. The connections indicate whether a variable was included in a given scenario; ribbon width does not represent variable importance or effect magnitude.

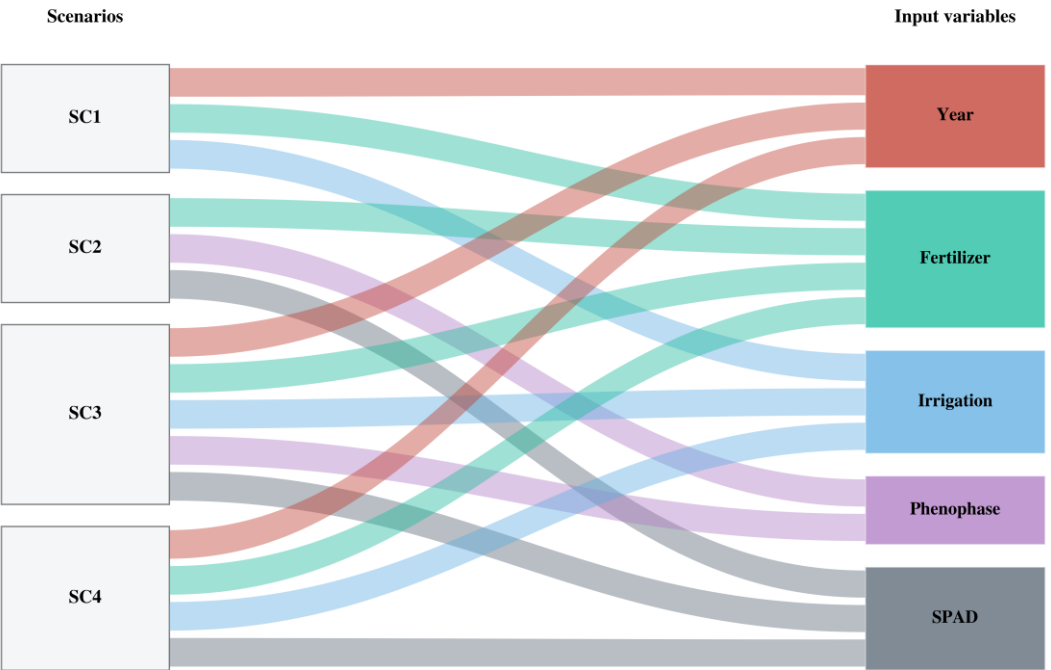


Figure 2 Alluvial diagram of the distribution of input variables within the different scenarios

The four MLP scenarios were implemented in Python 3.13.5 using the MLPRegressor class of the scikit-learn library (1.8.0). Maize grain yield was defined as the continuous target variable. Crop year, irrigation status, and phenological stage were treated as nominal categorical predictors and transformed using one-hot encoding. Fertilizer rate and SPAD

value were treated as continuous numerical predictors and standardized before model fitting. The dataset was divided using a fixed 70:30 training-testing partition with a random seed of 42, ensuring that SC1–SC4 were trained and evaluated using identical subsets. Each network contained one hidden layer with six neurons, used the hyperbolic tangent activation function, and was optimized with the limited-memory BFGS algorithm. Training was allowed to proceed for a maximum of 5000 iterations. Model performance was evaluated on the testing dataset. Pearson's correlation coefficient (R), the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE) were used as the principal performance indicators. Additional evaluation measures included Nash–Sutcliffe efficiency (NSE), mean absolute percentage error (MAPE), the RMSE–standard deviation ratio (RSR), Kendall's rank correlation coefficient (τ), Spearman's rank correlation coefficient (ρ), Willmott's index of agreement (d), and the concordance correlation coefficient (CCC). Scatter plots were used to examine agreement with the 1:1 line, Bland–Altman plots to assess bias and limits of agreement, and raincloud and ridgeline plots to compare the distributions of measured and predicted yield values. Normalized permutation importance was calculated to assess the relative predictive contribution of the input variables within each scenario.

3. Results

3.1 Fertilizer–yield relationships

Fertilizer rate was positively associated with maize grain yield in both crop years and under both irrigation regimes. In 2024, the relationship was weaker under rainfed conditions ($r = 0.557$, $R^2 = 0.310$) than under irrigation ($r = 0.731$, $R^2 = 0.535$). A similar pattern was observed in 2025, when the correlation increased from $r=0.662$ ($R^2 = 0.438$) in the rainfed treatment to $r=0.770$ ($R^2 = 0.594$) under irrigation (Figure 3).

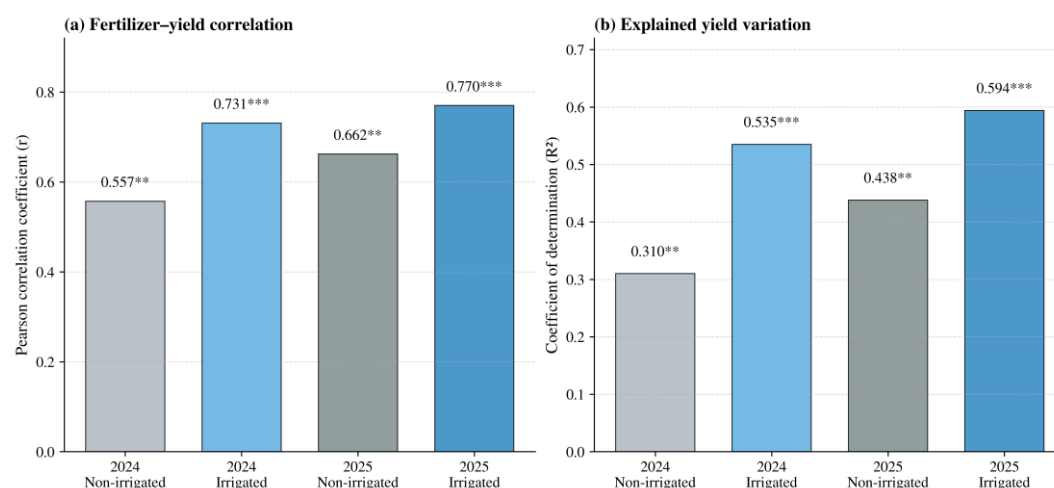


Figure 3 Pearson correlation coefficients and coefficients of determination describing the relationship between fertilizer rate and maize grain yield under irrigated and rainfed conditions in 2024 and 2025. ***, ** indicate significance at the 0.1% and 1% probability levels, respectively.

The strongest fertilizer–yield relationship was therefore detected in the irrigated treatment in 2025, while the weakest occurred in the rainfed treatment in 2024. These results indicate that the yield response to fertilization was more pronounced when water availability was improved.

3.2 Development of the SPAD–yield relationship across phenophases

The strength of the relationship between SPAD values and grain yield varied markedly across phenological stages. During the early vegetative stages, particularly at V6 and V8, correlations were generally weak or non-significant. As crop development progressed, the relationship became stronger, especially from V10 onward. In 2025, relatively strong associations were detected at V12, R1, and R3 in both irrigation treatments. The strongest relationship was observed in the irrigated treatment at R3 in 2025 ($r = 0.916$, $R^2 = 0.839$). Under rainfed conditions in the same year, R3 SPAD values also showed a strong relationship with yield ($r = 0.784$, $R^2 = 0.615$). Overall, the results indicate that SPAD measurements obtained during late vegetative and reproductive development were more informative for final yield assessment than measurements taken during early crop growth (Figure 4).

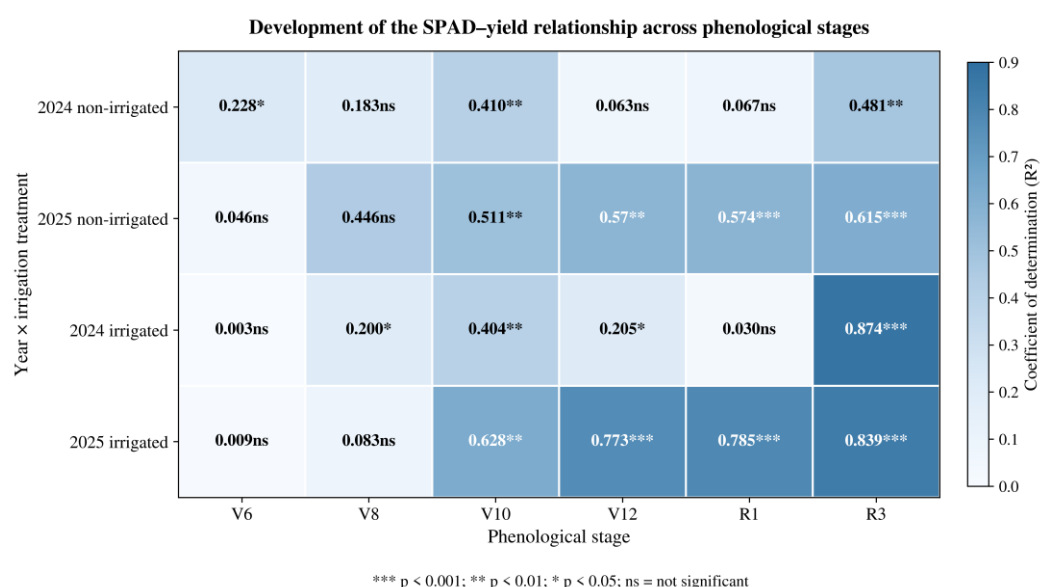


Figure 4 Phenophase-specific coefficients of determination (R^2) for the relationship between SPAD values and maize grain yield under irrigated and rainfed conditions in 2024 and 2025. Significance levels are shown within the cells.

3.3. Performance and interpretation of the MLP scenarios

3.3.1. Predictive performance of the four scenarios

The predictive performance of the MLP models differed according to the combination of input variables included in each scenario. SC1, which incorporated crop year, fertilization, and irrigation, achieved the best performance on the testing dataset, with an R^2 of 0.803, an RMSE of 1.135 t ha⁻¹, and an MAE of 0.805 t ha⁻¹. This indicates that the model explained approximately 80.3% of the observed variation in grain yield while maintaining the lowest prediction error among the four scenarios.

SC2, based on fertilization, phenological stage, and SPAD value, showed the weakest testing performance, with an R^2 of 0.554 and an RMSE of 1.707 t ha⁻¹. Its lower accuracy indicates that physiological and phenological information alone did not capture the full extent of the year- and management-related variability in yield. SC3, which included all five predictors, achieved an intermediate testing performance ($R^2 = 0.735$; RMSE = 1.315 t

ha⁻¹), while SC4, comprising crop year, fertilization, irrigation, and SPAD, produced a similar but slightly weaker result ($R^2 = 0.726$; RMSE = 1.337 t ha⁻¹).

The superior performance of SC1 demonstrates that a relatively compact set of agronomic variables provided the most informative combination for yield prediction. The addition of SPAD and phenological stage in SC3 and SC4 did not improve predictive accuracy beyond that obtained with crop year, fertilization, and irrigation alone.

The results are summarized in Table 2.

Table 2 Testing performance of the four MLP scenarios

Scenario	R	R ²	RMSE	MAE
SC1	0.897	0.803	1.135	0.805
SC2	0.754	0.554	1.707	1.284
SC3	0.860	0.735	1.315	0.935
SC4	0.855	0.726	1.337	0.913

3.3.2. Scatter plot analysis of MLP model performance

Scatter plots were generated to visually assess the correspondence between measured and predicted maize yield across the four MLP scenarios (Figure 5). They show the alignment of predictions with the 1:1 reference line, the dispersion of individual predictions, clustering patterns, and possible compression of the predicted yield range. Clear differences were observed among the scenarios. SC1 showed the strongest predictive agreement, with the highest correlation coefficient ($R=0.897$) and the closest overall alignment of predicted values with the 1:1 line. Although the predictions formed distinct clusters, this pattern reflected the discrete structure of the agronomic input variables rather than poor model performance. SC3 and SC4 also demonstrated strong relationships between measured and predicted yield ($R=0.860$ and $R=0.855$, respectively), but their point distributions were more dispersed than those of SC1. SC2 showed the weakest predictive agreement ($R=0.754$), with greater deviation from the 1:1 line and a tendency to compress predictions toward the central yield range, resulting in underestimation of the highest yields. Overall, the scatter plots confirmed the ranking obtained from R^2 , RMSE, and MAE, with SC1 providing the most accurate and consistent out-of-sample predictions.

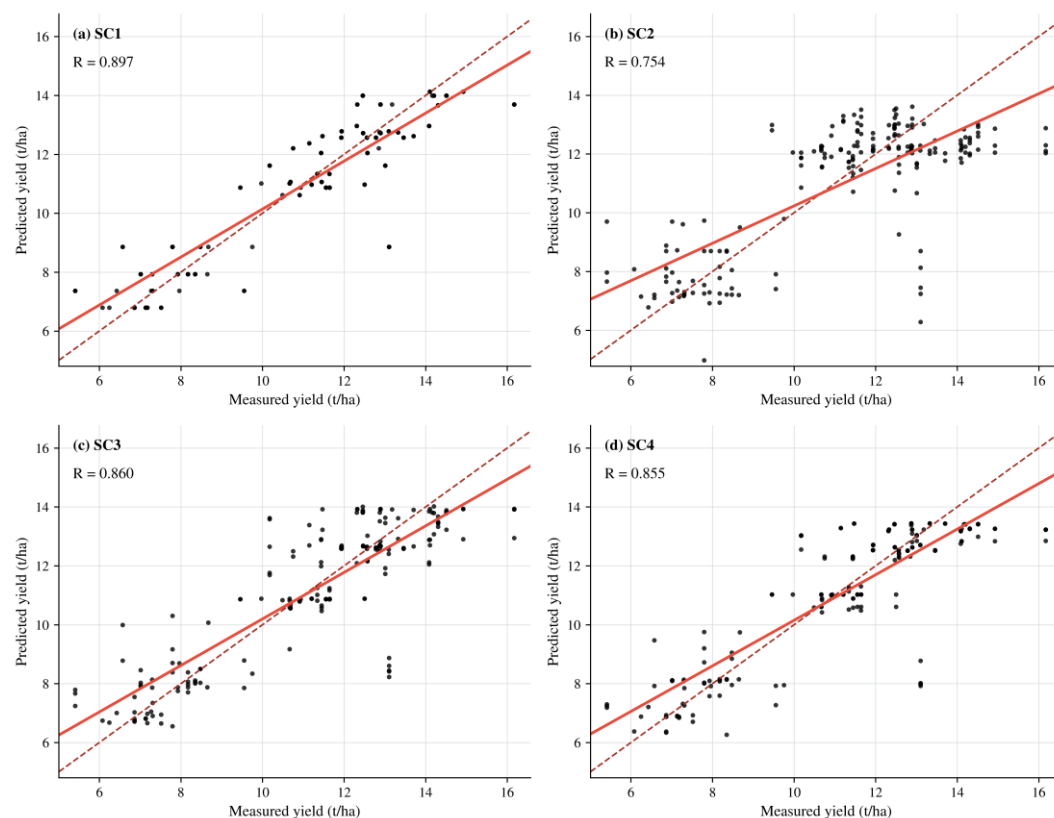


Figure 5 Measured versus predicted maize grain yield for the four MLP scenarios, visualized as scatter plots

3.3.3. Bland–Altman plots

Bland–Altman plots complemented the scatter plots by displaying the differences between predicted and measured yield against their mean. Whereas scatter plots illustrate association and alignment with the 1:1 line, Bland–Altman plots quantify mean prediction bias, the 95% limits of agreement, and whether the magnitude or variability of prediction errors changes across the yield range. SC1 showed the most favourable agreement, with comparatively small bias and narrower error dispersion, whereas SC2 displayed the widest spread of differences. SC3 and SC4 showed intermediate agreement, confirming the performance ranking obtained from the scatter plots and numerical error metrics (Figure 6).

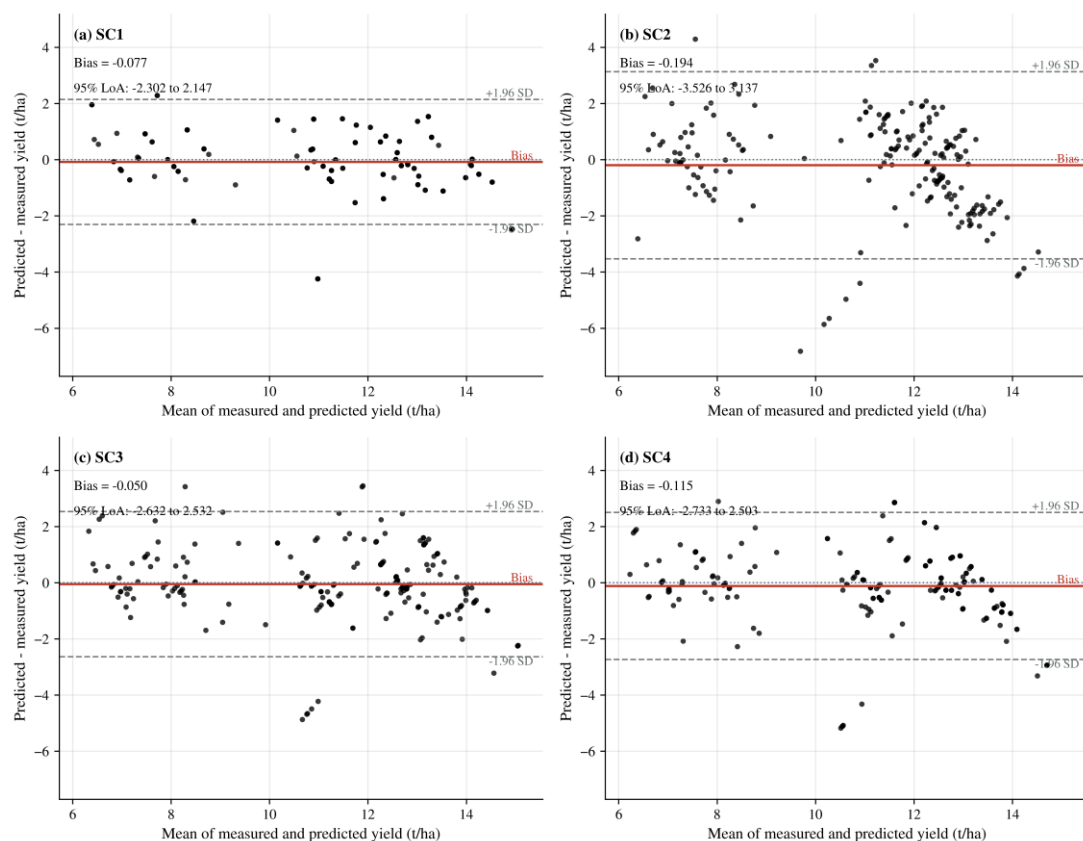


Figure 6 Bland–Altman plots showing agreement between measured and predicted maize grain yield for the four MLP scenarios. The solid line indicates mean bias, while the dashed lines represent the 95% limits of agreement.

3.3.4. Distributional agreement between measured and predicted yield (raincloud plots)

The raincloud plots provided a distribution-based comparison of measured and predicted maize yield across the four MLP scenarios (Figure 7). SC1 showed the closest agreement between the two distributions, with similar medians, interquartile ranges, and overall spread. This supports the superior testing performance of SC1 and indicates that the model reproduced not only the average yield level but also much of the observed variability. SC3 and SC4 showed moderate agreement, although their predicted distributions differed somewhat from the measured data in shape and dispersion. SC2 displayed the greatest mismatch, with a narrower predicted distribution and reduced representation of the highest and lowest observed yields, indicating compression toward the central yield range. Overall, the raincloud plots were consistent with the scatter plots and error metrics, confirming that SC1 provided the most accurate distributional reproduction of measured yield, while SC2 showed the weakest performance.

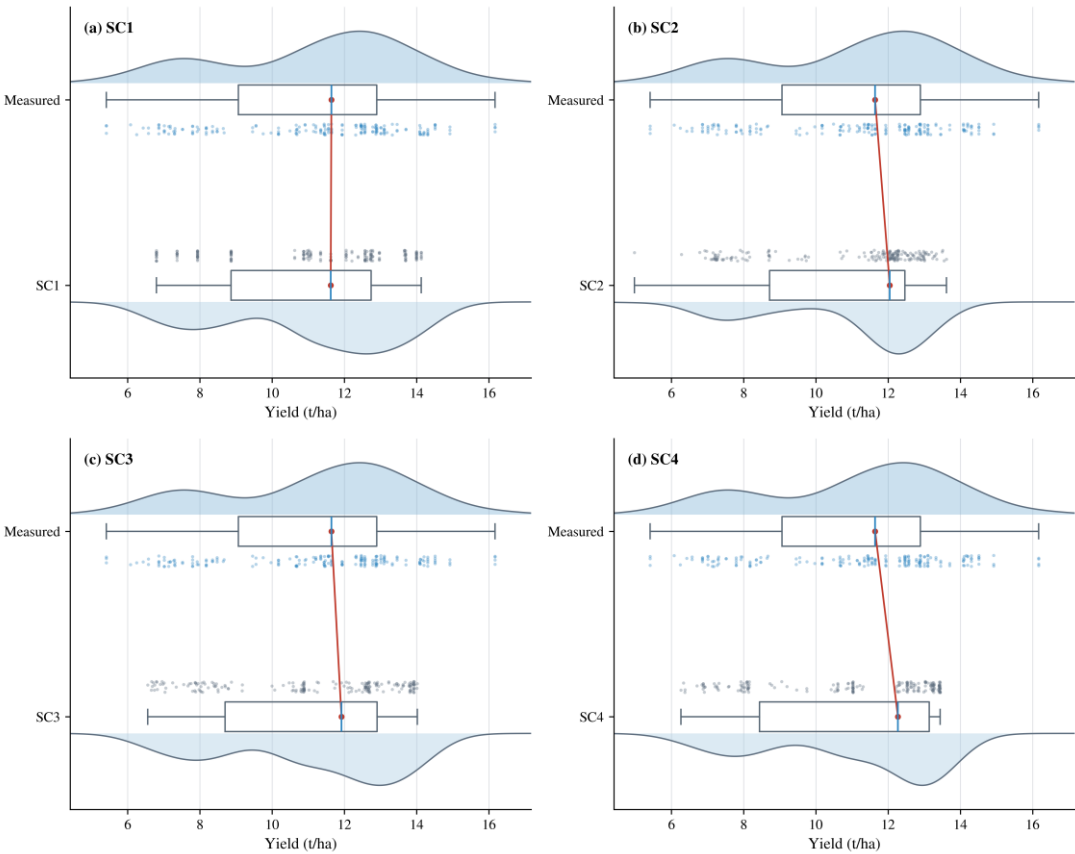


Figure 7 Raincloud plots comparing the distributions of measured and predicted maize grain yield for the four MLP scenarios. Density curves, boxplots, and individual observations illustrate differences in median, spread, and distribution shape.

3.3.5. Statistical evaluation of predictive accuracy using performance indices

To complement the performance indicators reported earlier in Table 2, the four MLP scenarios were further evaluated using Nash–Sutcliffe efficiency (NSE), mean absolute percentage error (MAPE), the RMSE–standard deviation ratio (RSR), Kendall’s rank correlation coefficient (τ), Spearman’s rank correlation coefficient (ρ), Willmott’s index of agreement (d), and the concordance correlation coefficient (CCC). These indicators provide additional information on predictive efficiency, relative error, rank agreement, and agreement between measured and predicted yield values (Table 3).

Table 3 Additional performance indicators for the four MLP scenarios on the testing dataset.

Scenario	Performance indicators						
	NSE	MAPE (%)	RSR	Kendall’s τ	Spearman’s ρ	Willmott’s (d)	CCC
SC1	0.803	7.57	0.444	0.686	0.850	0.944	0.892
SC2	0.554	11.83	0.668	0.402	0.577	0.859	0.741
SC3	0.735	8.78	0.514	0.622	0.800	0.925	0.857
SC4	0.726	8.46	0.523	0.606	0.782	0.922	0.850

SC1 showed the strongest performance across all additional indicators. It achieved the highest NSE, Kendall’s τ , Spearman’s ρ , Willmott’s d, and CCC, together with the lowest MAPE and RSR. These results indicate that SC1 reproduced both the magnitude and rank order of measured yield values most accurately. SC3 and SC4 exhibited broadly comparable intermediate performance. SC3 showed slightly stronger efficiency, rank agreement, and concordance, whereas SC4 produced a marginally lower MAPE. SC2 performed least effectively, with the lowest agreement coefficients

and the highest relative error. These additional indicators therefore confirmed the model ranking reported in Table 2 and supported the results obtained from the scatter, Bland–Altman, and rain-cloud analyses.

3.3.6. Ridgeline plot analysis of predicted and measured yields

Figure 8 compares the distributions of measured and predicted maize yields across the four MLP scenarios. SC1 reproduced the location and overall shape of the measured yield distribution most closely, although its predictions were more concentrated around the main yield ranges. SC3 and SC4 also captured the central part of the measured distribution but showed some smoothing and reduced representation of the extreme values. SC2 produced the narrowest predicted distribution and showed the greatest deviation from the measured yield pattern, consistent with its weaker performance indicators. Overall, the figure demonstrates that the models differed not only in prediction error but also in their ability to reproduce the observed variability and distributional structure of maize yield.

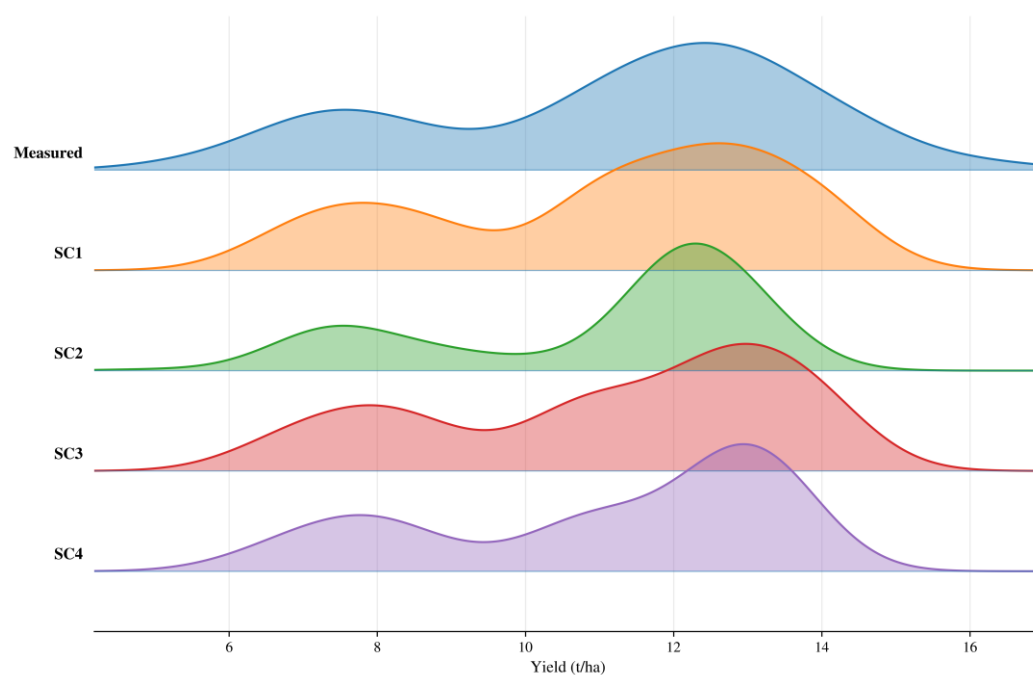


Figure 8 Ridgeline distributions of measured and predicted maize yields for the four MLP scenarios. The curves illustrate differences between the observed yield distribution and the distributions reproduced by each model configuration

3.4 Normalized importance of the input variables

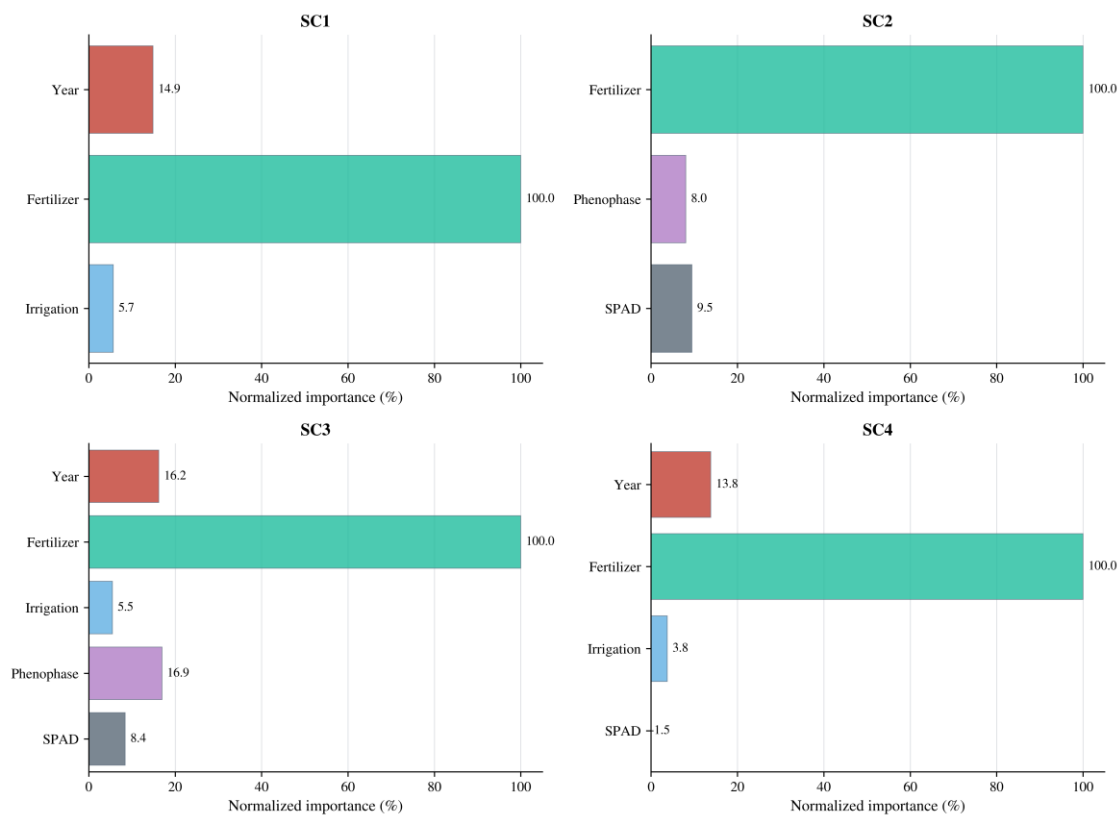


Figure 9 Relative importance of the input variables within the MLP scenarios

The relative predictive contribution of the input variables differed among the four MLP scenarios, although fertilization was consistently the dominant predictor (Figure 9). In SC1, fertilization reached a normalized importance of 100%, whereas crop year and irrigation contributed 14.9% and 5.7%, respectively. In SC2, fertilization again showed the maximum importance, while SPAD and phenophase had substantially lower values of 9.5% and 8.0%. In the most comprehensive model, SC3, fertilization remained the leading predictor, followed by phenophase (16.9%) and crop year (16.2%), while SPAD and irrigation contributed 8.4% and 5.5%, respectively. In SC4, crop year accounted for 13.8% of normalized importance and irrigation for 3.8%, whereas SPAD showed a slightly negative permutation importance (−1.5%), indicating that it provided no additional predictive benefit within that particular variable combination. Overall, Figure 9 demonstrates that fertilization supplied the strongest predictive information across all model structures, while the relative contribution of crop year, phenophase, irrigation, and SPAD depended on the composition of the individual scenario.

4. Discussion

The results consistently showed that fertilization, crop-year conditions, and water availability were the main factors structuring yield variability, whereas the contribution of SPAD and phenological stage depended on the developmental period and on the other predictors included in the model.

Fertilizer rate was positively associated with grain yield in both years and under both irrigation regimes, confirming nutrient supply as a major yield-related factor. This interpretation was also supported by the normalized importance analysis, in which fertilization was the dominant predictor in every scenario. However, the strength of the fertilizer–yield relationship differed among crop-year and irrigation combinations. The relationship

was weakest under rainfed conditions in 2024 and strongest under irrigation in 2025. This indicates that the response to fertilization depended on the production environment. Improved water availability likely enhanced nutrient dissolution, root uptake, canopy development, and photosynthetic activity, allowing the crop to convert additional nutrient supply into grain yield more effectively.

Increasing fertilizer input alone does not necessarily result in a proportional yield increase if water availability limits nutrient uptake or crop growth. The results therefore support integrated nutrient and water management [14]. Due to the above, drought deficit can be reduced [19]. Approaching crop formation in both the rainfed and the irrigated versions, the correlation coefficient value increases. This indicates that the correlation between the two variables is becoming stronger.

Crop year represented the combined effects of precipitation, temperature, evaporative demand, soil-water availability, and the timing of stress relative to sensitive growth stages. Its importance also explains the weaker performance of SC2, which excluded crop year and irrigation. Fertilization, SPAD, and phenological stage described crop management and physiological status but did not fully represent the environmental conditions under which those responses developed. Similar SPAD values may therefore have different implications for final yield in different years. Crop year should consequently be interpreted as a proxy for several unmeasured environmental factors rather than simply as a calendar variable. Future models could improve biological interpretation by replacing or complementing the year category with direct meteorological and soil-water variables, including precipitation distribution, temperature, soil moisture, heat accumulation, and drought indices.

The relationship between SPAD and yield generally became stronger during later developmental stages. The correlation between SPAD value and yield became more and more pronounced as the crop approached maturity [20]. Early measurements probably reflected crop nitrogen and chlorophyll status before the full effects of treatments and environmental stress had emerged, whereas measurements during reproductive development were more closely associated with kernel formation, grain filling, and canopy persistence. Later SPAD measurements were therefore more informative for yield estimation, whereas earlier measurements, despite their weaker relationship with final yield, may be more useful for in-season management. The strongest relationship was observed for R3 SPAD under irrigated conditions ($r = 0.916$; $R^2 = 0.839$), supporting previous reports of significant associations between reproductive-stage SPAD values and maize grain yield [21–24].

Although several phenophase-specific SPAD–yield relationships were strong, adding SPAD to the main agronomic predictors did not improve MLP performance. SC1 achieved the highest R and R^2 and the lowest RMSE and MAE, while SC3 and SC4 showed intermediate performance and SC2 performed least effectively. This suggests that crop year, fertilization, and irrigation captured most of the predictable yield variation. SPAD probably provided partly redundant information because chlorophyll status is itself influenced by nutrient supply, water availability, and seasonal conditions. Accordingly, the slightly negative permutation importance of SPAD in SC4 should not be interpreted as a negative biological effect, but as a lack of additional predictive value within that predictor combination. The results demonstrate that adding more variables does not necessarily improve prediction when they introduce overlapping information or noise.

The clustered SC1 predictions reflected the discrete experimental combinations of crop year, fertilizer treatment, and irrigation rather than necessarily indicating poor model performance. The modelling helps interpret the interrelated effects of key parameters and supports previous findings that machine learning methods can complement traditional agronomic analyses by capturing complex relationships that are difficult to describe using purely linear methods [23–24].

Overall, maize yield was primarily associated with nutrient supply and its interaction with seasonal and water conditions. SPAD provided useful physiological information, particularly during reproductive development, but contributed limited additional predictive information when the main agronomic variables were already included. Variable-importance values should be interpreted as scenario-specific predictive contributions rather than causal effects. Because the study covered only two years, one location, and one hybrid, the observed relationships and model ranking require validation across additional environments, soil conditions, and genotypes. Future studies should also compare alternative machine-learning methods and apply model-interpretation techniques using identical validation procedures.

5. Conclusions

This study investigated the agronomic, environmental, phenological, and physiological factors associated with maize grain yield and evaluated their combined predictive value using four multilayer perceptron scenarios. The findings demonstrate that yield formation in the examined field experiment was primarily associated with fertilization, crop-year conditions, and water availability. Fertilizer rate was positively related to yield in both years and under both irrigation regimes. However, the relationship was stronger under irrigated conditions, demonstrating that nutrient response depended on water availability. Fertilization should therefore not be interpreted as an isolated production factor; its yield effect is closely connected to seasonal conditions and the crop's capacity to use the supplied nutrients.

The SPAD–yield relationship strengthened as crop development progressed. Early vegetative measurements were generally weak predictors of final yield, whereas late vegetative and reproductive-stage measurements showed substantially stronger associations. This indicates that late-season leaf chlorophyll status reflects physiological processes directly connected with grain formation and grain filling. Nevertheless, SPAD provided limited additional predictive information when crop year, fertilization, and irrigation were already included, probably because it partially reflected the effects of these variables.

Among the four MLP configurations, SC1, containing crop year, fertilization, and irrigation, achieved the strongest testing performance. SC3 and SC4 showed intermediate accuracy, while SC2, which excluded crop year and irrigation, performed least effectively. The results demonstrate that adding physiological and phenological predictors did not automatically improve prediction and that a compact set of agronomically meaningful variables may provide more robust performance than a larger but partly redundant input set.

Overall, the combined statistical and MLP analyses identify fertilization as the dominant yield-related predictor while also emphasizing the modifying roles of crop year and irrigation. SPAD measurements are valuable indicators of crop status, particularly during later phenological stages, but they should be interpreted within the broader environmental and management context. These findings support integrated nutrient and water management and demonstrate the value of combining classical relationship analysis with non-linear modelling to improve understanding of maize yield variability. Since the study was limited to two years, one location, and one hybrid, the results should be validated under broader environmental and production conditions. Future research should replace crop-year categories with direct meteorological and soil-water variables, apply grouped or external validation, and investigate nonlinear interactions among nutrient supply, water availability, crop development, and physiological status.

Author Contributions: Conceptualization, P.F. and É.H.; methodology, P.F.; software, P.F.; validation, A.Sz.; formal analysis, P.F.; investigation, P.Z.; resources, É.H.; data curation, P.Z.; writing—

original draft preparation, P.F. and É.H.; writing—review and editing, A.Sz.; visualization, P.F. and É.H.; supervision, A.Sz. and P.Z.; project administration, A.Sz.; funding acquisition, A.Sz. All authors have read and agreed to the published version of the manuscript.

Funding: The research behind the study was supported by the «EKÖP-25-4-II ; EKÖP-25-4-I» University Research Scholarship Program Of The Ministry For Culture And Innovation From The Source Of The National Research, Development And Innovation Fund. The paper was also supported by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences

Conflicts of Interest: The authors declare no conflicts of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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