agronomy

MDPI

Article

Multitemporal and Multivariate Pedological Pattern Analysis of Machinery-Based Tillage Systems (No-Till and Chisel) Integrating Machine Learning Frameworks

Paola D'Antonio [1], Francesco Toscano [1,*], Antonio Scopa [1], Marios Drosos [1], Lucas Santos Santana [2], Luis Alcino Conceição [3], Felice Modugno [1], Mario Vitelli [1] and Costanza Fiorentino [1]

1 Department of Agricultural, Forestry, Food and Environmental Sciences (DAFE), University of Basilicata, Viale Dell'Ateneo Lucano 10, 85100 Potenza, Italy; paola.dantonio@unibas.it (P.D.); antonio.scopa@unibas.it (A.S.); marios.drosos@unibas.it (M.D.); felice.modugno@studenti.unibas.it (F.M.); mario.vitelli@studenti.unibas.it (M.V.); costanza.fiorentino@unibas.it (C.F.)
2 Agricultural Science Institute, Federal University of Vale do Jequitinhonha e Mucuri, Unaí 38610-000, MG, Brazil; santana.santos@ufvjm.edu.br
3 VALORIZA—Research Center for Endogenous Resource Valorization, Polytechnic Institute of Portalegre, 7300-110 Portalegre, Portugal; luis_conceicao@ipportalegre.pt
* Correspondence: francesco.toscano@unibas.it

Abstract

Long-term tillage management fundamentally reshapes soil's physical and chemical environment, yet an integrated, predictive characterization of the distinct chemical signatures induced by no-tillage (NT) versus chisel tillage (CT) remains limited. We analyzed an eight-year dataset (2010–2017) from a long-term experiment in Iowa, USA, focusing on pH, available phosphorus (Bray1-P), and macro- and micronutrients (K, Ca, Mg, Cu, Fe, Zn) at two depths (0–5 and 5–15 cm). A convergent multi-method framework combined robust univariate statistics, multivariate ordination (PCA, PERMANOVA), linear mixed-effects models, and machine learning (Random Forest and Firth-penalized logistic regression). Results reveal a clear stratification–homogenization pattern. NT is associated with surface accumulation of Zn (+14%), Fe (+16%), and Cu (+5%), with mild acidification (−0.4 pH units) and high temporal stability. CT favored vertical nutrient redistribution, marked by subsurface K enrichment (up to 6% higher than NT), progressive alkalinization, and greater temporal variability. Predictive modeling highlighted subsurface K and surface Zn/Fe as key discriminators, with Firth regression confirming their complementary effects. These findings indicate that long-term NT and CT are associated with distinct, depth-specific chemical configurations—integrated systems defined by concentration gradients, temporal stability, and element covariation—rather than isolated element changes. This work provides a robust, quantitative framework for diagnosing soil management history and characterizing the pedochemical imprint of tillage.

Keywords: no-tillage; chisel tillage; soil mechanization; soil chemistry; micronutrients; machine learning; soil stratification; multi-method analysis

Check for updates

Academic Editor: Guang-Wei Ding

Received: 3 February 2026
Revised: 23 February 2026
Accepted: 24 February 2026
Published: 25 February 2026

1. Introduction

The choice of soil tillage strategy—such as no-tillage (NT) or the use of disk harrows or chisels (conventional/reduced tillage, CT)—is a fundamental technical and mechanical decision that shapes the physical environment of the soil, with long-term implications for its chemical and biological properties. These management systems differ substantially in terms of the machinery used. In particular, the mechanization of NT systems uses coulters and disk openers capable of creating narrow slits, suitable for accommodating the seed while preserving the structure and stratigraphy of the soil. In contrast, CT mechanization applies the principle of controlled soil failure, employing shanks to induce fracturing and macro-porosity in the sub-surface layer (typically 15–30 cm depth) to alleviate compaction while inducing partial inversion and mixing of the surface horizon [1]. The distinction between NT and CT is now at the center of modern agronomic research, as the degree and mode of disturbance imposed by cultivation operations directly influence the reorganization of nutrients, organic matter, and redox gradients [2–4]. Several studies have shown that reduced or no tillage leads to a major reorganization of vertical gradients of nutrients and organic matter, with measurable effects on pH and the availability of redox-sensitive micronutrients such as iron (Fe), copper (Cu), and, to a lesser extent, zinc (Zn). In this context, conservation-oriented tillage practices have also been recognized as key drivers in the maintenance of High Nature Value Farmland (HNVF), as they contribute to preserving soil functionality, habitat heterogeneity, and long-term agroecosystem resilience [5]. An accumulation of organic carbon and nitrogen in the surface layers, resulting in stimulation of microbial activity and intensification of the redox cycles that regulate the mobility and speciation of these elements, has frequently been observed under conditions of reduced mechanical disturbance. These biogeochemical dynamics are strongly influenced by the type and intensity of mechanical intervention, as precision in field operations—including traction optimization and surface mapping—can modulate soil physical conditions and, indirectly, its chemical evolution [6]. Some studies have shown that prolonged NT management promotes marked stratification not only of macro-elements but also of redox-sensitive micronutrients. For example, Ref. [7], analyzing 21 years of management with different tillage systems, showed significantly higher concentrations of Fe and Cu in the surface layers under NT, with potential implications for their mobility and bioavailability. However, the effect of NT on soil chemistry is not uniform: while some medium- to long-term studies report limited variations in the main chemical parameters [8], decades-long experiments show more marked changes in pH stratification, cation exchange capacity, and nutrient distribution along the soil profile [9,10]. The decrease in surface pH observed in NT is commonly attributed to the accumulation of organic matter and nitrification dynamics concentrated in the most superficial layers. At the same time, the management of crop residues and the application of soil amendments and/or organic fertilizers in NT systems represent another key factor in modulating soil microenvironmental conditions by influencing pH dynamics [11,12]. The differences between tillage systems are also reflected in soil structural properties. NT is generally associated with an increase in soil organic carbon and a reduction in bulk density with a relative increase in biological microporosity [13]. As highlighted by [14,15], these structural changes improve pore connectivity and regulate oxygen diffusion, creating the physical context that supports alterations in redox potentials and, indirectly, the speciation and mobility of Fe and Cu. Long-term studies also indicate that NT can intensify bioturbation and macro-porosity connectivity [16], with possible effects on the vertical redistribution of nutrients and metals in the upper layers of the profile. Despite the growing availability of evidence on the effects of tillage on soil quality, the literature has focused mainly on carbon and nitrogen cycles, leaving the integrated dynamics of pH, available phosphorus (Bray1-P), K, Ca, Mg, and redox-sensitive micronutrients relatively unexplored from a quantitative and predictive perspective. Recent studies have highlighted the growing role of digital and mechanization-based approaches in supporting sustainable soil and nutrient management. In particular, Ref. [17] emphasized the importance of integrating modeling and digital tools for nitrogen management, while [18] demonstrated how advanced tractor guidance systems can improve operational efficiency and precision in field management. Furthermore, studies using time series of chemical variables to robustly discriminate between NT and CT systems are still limited. Most studies rely on classical multivariate statistics, such as PCA and PERMANOVA [19], without integrating modeling approaches capable of handling non-linear relationships, class imbalance, and quasi-separation phenomena. In this context, the combined use of penalized models, such as Firth's logistic regression, and non-parametric algorithms such as Random Forests represents a methodological evolution that is still largely unexplored in soil biogeochemistry applied to tillage systems. The integration of these tools with historical chemical data series allows us to assess whether the observed variations consistently reflect the cumulative effect of mechanical disturbance associated with different management regimes, without the aim of defining universal indicators, but rather to verify the consistency and discriminating power of the observed chemical patterns. Accordingly, we hypothesize that differential mechanical disturbance under no-tillage and chisel tillage is associated with modification in soil physical structure (stratification, porosity, and aeration), which may influence biogeochemical processes (redox dynamics, soil organic matter turnover, and acidification), and contribute to distinct, depth-specific, and temporally stable chemical signatures. In light of these considerations, this study adopts an integrated framework—combining exploratory multivariate analyses, longitudinal mixed-effects models, and machine-learning approaches (Random Forest and Firth logistic regression)—to investigate the 2010–2017 temporal dynamics of pH, Bray-1 P, K, Ca, Mg, Cu, Fe, and Zn in soils under NT and CT management. This framework enables not only the description of chemical differences between systems, but also a quantitative assessment of their temporal stability and predictive power in discriminating between management regimes. Unlike conventional studies based on isolated univariate comparisons, the present work conceptualizes tillage effects as an emergent, multivariate and depth-resolved system property. The theoretical advancement lies in the integration of inferential statistics, multivariate structure analysis, longitudinal modeling, and supervised classification within a unified framework that moves from detection of individual differences to the identification and validation of a reduced, management-specific pedochemical signature. The objective is to evaluate whether the observed patterns constitute a consistent and statistically supported multivariate reorganization of chemical signature attributable to the cumulative intensity of mechanical disturbance.

2. Materials and Methods

2.1. Study Site and Machinery

2.1.1. Study Area

The study was conducted at the Agricultural Engineering and Agronomy Research Farm of Iowa State University (42.017584° N, 93.76448° W) in central Iowa (Figure 1), USA, in collaboration with the National Laboratory for Agriculture and the Environment (USDA-ARS). The site hosts a long-term field experiment established in 2007–2008 to evaluate the effects of contrasting machinery-based tillage systems on soil functioning and agroecosystem sustainability. The experimental area comprises 88 plots subjected to contrasting tillage regimes, primarily NT and CT, applied either continuously or alternately over time. The plots are representative of the region's Mollisol soils and typical Midwest corn-based cropping systems. Treatments impose distinct modes and intensities of mechanical disturbance, creating gradients in soil structure, porosity, and surface stratification that form the basis for investigating long-term soil reorganization under different tillage management.

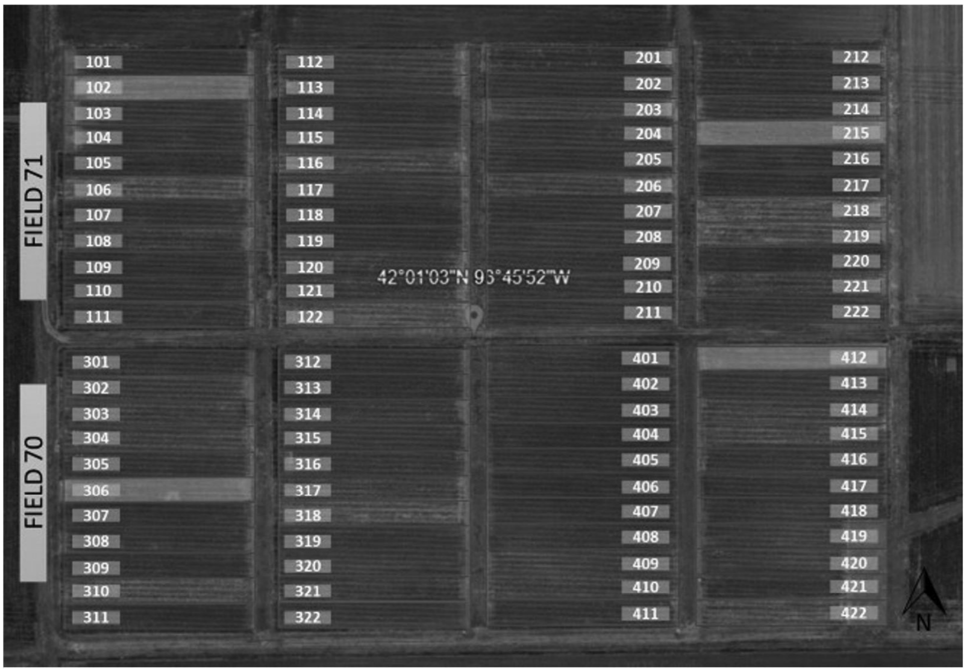

Figure 1. Satellite image of the Agricultural Engineering and Agronomy Research Farm at Iowa State University (42.017584° N, 93.76448° W), showing the layout of the long-term experimental area with 88 plots subjected to contrasting tillage regimes.

2.1.2. Tillage-Related Tractor Traffic

Within the broader experimental context (2008–2020), the mechanical characteristics of the topsoil (0–15 cm) were mainly determined by tillage and vehicle traffic associated with sowing, fertilization, and harvesting, with distinct effects between CT and NT. The present study focuses on the 2010–2017 interval, for which complete chemical data are available. In the CT plots, the soil was disturbed by autumn plowing with a John Deere 8230 chisel (Figure 2a) to a depth of 25 cm, followed by spring leveling with a field cultivator and surface disks affecting the top 10 cm, generating surface fracturing, nutrient redistribution, and differential compaction in the most heavily trafficked areas. In the NT plots, soil stratification was preserved, with disturbances limited to the passage of the John Deere 2955 tractor (Figure 2b) during sowing and side-dressing, causing localized compaction along the working rows (Table 1).

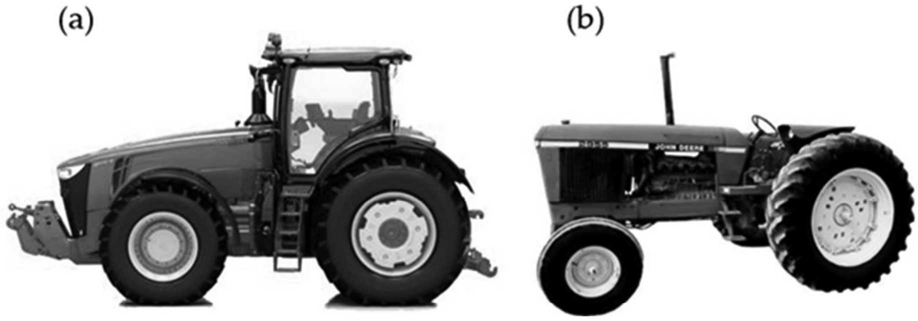

Figure 2. Agricultural machinery used in the experiment: (**a**) John Deere 8230 tractor; (**b**) John Deere 2955 tractor.

As highlighted in the long-term study by [20], at this same experimental site, traffic-induced compaction is highly dependent on the tillage system, with NT soils having a higher bearing capacity than CT soils and with effects mainly confined to the processed layer.

Table 1. Technical comparison of the main tractors used in the study, highlighting differences in power, mass, and potential soil mechanical impact.

Parameter	John Deere 8230	John Deere 2955
Tractor type	High-power row-crop	Utility tractor
Engine power	~240–245 hp	~97 hp
Drive	MFWD/ILS	2WD/MFWD
Operating weight	~11,000 kg	~4000–5000 kg
Wheelbase	~302 cm	~259 cm
Main field role	Primary tillage	Seeding, fertilization
Soil impact	High load, high compaction potential	Lower load, localized compaction

Although specific machinery parameters were not modeled quantitatively, the management systems are defined operationally by their mechanical disturbance regime (absence vs. presence of plowing), which represents the structural driver investigated in this study.

2.2. Dataset Structure and Preprocessing Data

The dataset characterizes each plot for a wide range of soil chemical properties measured over several years and at two depths: 0–5 cm and 5–15 cm. The variables included are OM (organic carbon); pH; Bray1-P; K, Ca, Mg, Cu, Fe, Mn, Zn, B, S; CEC; EC; Grain yield. Not all data are available for every year and depth. The original dataset was fragmented into several files and there were some missing data for certain depths or time intervals. It was therefore necessary to reorganize the dataset and define the most complete variables. Based on data completeness, the variables selected for subsequent analyses were pH, Bray1-P, K, Ca, Mg, Cu, Fe, and Zn. The selected time window (2010–2017) represents the interval with the greatest completeness and consistency of available measurements. A tillage index (Ti) was defined based on the cumulative number of chisel operations per plot (2010–2017). To isolate the distinct pedochemical signature of each system, we analyzed only plots under continuous NT (40 plots) or CT (36 plots) management. The 12 plots with alternating management were excluded due to their smaller, inconsistent sample size and temporally variable tillage history, which would introduce confounding signals and compromise statistical robustness. All statistical analyses were performed using R version 4.5.2.

Calculation of Baseline-Referenced Deviation Indicators (Δ)

To quantify temporal dynamics relative to initial conditions, annual deltas (Δ_{var}) were calculated as the difference between the value in each year "y" and the value in the baseline year (first available year for each variable-depth combination). The algebraic aggregation of annual deltas was computed as a synthetic index of directional persistence relative to baseline conditions, while the sum of absolute annual deltas was used as an indicator of temporal variability. These aggregated indices do not represent physically cumulative changes in a mass-balance sense, but rather comparative descriptors of temporal deviation patterns.

$$\Delta_{var,\ depth,\ y} = value_{var,\ depth,\ y} - value_{var,\ depth,\ baseline} \tag{1}$$

$$\Delta_{agg,\text{net},var,depth} = \sum_{y=baseline}^{2017} \Delta_{var,\text{depth},y} \tag{2}$$

$$\Delta_{agg,\ abs,var,\ depth} = \sum_{y=baseline}^{2017} |\Delta_{var,\text{depth},y}| \tag{3}$$

Consequently, inferential analyses presented in Sections 3.2 and 3.3 refer exclusively to annual baseline-referenced deviations ($\Delta_{var,depth,y}$), while aggregated indices (Δ_{agg}) are used only as descriptive indicators of temporal deviation patterns and are not employed for inferential testing.

2.3. Exploratory Analysis and Data Normality Testing

The choice of statistical approaches was guided by the distribution of the data. Although parametric tests offer greater statistical power when the assumptions of normality are met, soil chemical properties frequently exhibit non-Gaussian distributions, particularly in agricultural systems characterized by high spatial variability. Parameters such as macronutrients and micronutrients often show asymmetric log-normal distributions with high coefficients of variation, while pH and available phosphorus may approach normality only in specific pedoclimatic contexts, while still maintaining complex and variable distribution patterns [21–25]. In accordance with this evidence, a preliminary exploratory analysis was conducted to empirically verify the assumption of normality prior to inferential analyses. Normality was assessed for each combination of chemical variable, depth, and management system, using the Shapiro–Wilk and, where applicable, Anderson–Darling tests, supplemented by the calculation of asymmetry and kurtosis indices. Based on the results obtained and methodological recommendations for soil data, we adopted an analytical strategy predominantly based on non-parametric methods, which are more robust in the presence of non-Gaussian distributions and heterogeneous variances, including group comparison tests, rank correlations, and multivariate permutation analyses [26–28].

2.4. Statistical Analysis

To characterize both the state and dynamics of soil properties, all univariate statistical analyses described below were conducted on two distinct types of data: raw measured values and annual temporal differences (delta) calculated as described in Section Calculation of Baseline-Referenced Deviation Indicators (Δ). This approach allows us to distinguish differences in absolute values from differences in patterns of change over time between NT and CT systems. We evaluated the differences between the NT and CT groups—for each combination of chemical variable, depth (0–5 cm, 5–15 cm), and data type (raw values or temporal differences)—using the Wilcoxon–Mann–Whitney test for independent samples. To quantify the practical magnitude (effect size) of any detected difference, beyond its statistical significance, Cliff's Delta (δ) was calculated. This is a non-parametric and robust measure of the overlap between two distributions, ranging from -1 to +1. Its standard interpretation follows the magnitude categories proposed by [29] and adopted in subsequent methodological studies, e.g., [30]:

- $|\delta| < 0.147$ (or 14.7%): Negligible effect.
- $0.147 \leq |\delta| < 0.33$: Small effect.
- $0.33 \leq |\delta| < 0.474$: Medium effect.
- $|\delta| \geq 0.474$: Large effect.

A positive value of δ indicates a tendency for values in the NT group to be greater than those in the CT group, while a negative value indicates the opposite. For univariate comparisons on raw data, the analyses were performed at the observation level. Given the repeated-measure structure, effect sizes were interpreted conservatively, and consistency across longitudinal mixed models was used as a robustness check to mitigate potential pseudo-replication bias. The monotonic relationship between the cumulative intensity of tillage, expressed by the original variable Till_count, and each chemical property was assessed by calculating Spearman's rank correlation coefficient (ρ). The correlation analysis was exploratory and aimed at identifying monotonic associations rather than establishing causal intensity effects. This method is appropriate for non-normally distributed data and for detecting monotonic, not necessarily linear, relationships.

To explore the multivariate structure of the data, we conducted a PCA on the chemical variables of the raw soil. The variables were standardized and the first five components were extracted and analyzed to identify global patterns of variation and the most influential variables. In particular, to identify the soil chemical indicators that best define each principal component, the percentage contribution of individual variables was calculated. To robustly assess the differences in soil chemical properties between the two management systems, a non-parametric ANOVA based on Aligned Rank Transformation (ART ANOVA) was applied, which is particularly suitable for data that violate the assumptions of normality and homoscedasticity required by traditional parametric ANOVA [31]. This approach proceeds by aligning the data to remove the effects of confounding factors, followed by transformation into ranks, preserving the original order of values and reducing the influence of non-Gaussian distributions. Subsequently, a normal analysis of variance is performed on the matrix of aligned ranks, from which F statistics and p-values are derived to test the main effect of the "Tillage" factor. The analysis was performed on each combination of chemical variable and depth using only "raw" data and considering only combinations with a sufficient number of observations ($n \geq 10$) to ensure reliable estimates. For each model, a robust measure of effect size was calculated based on the proportion of variance explained by the ranks. Finally, in order to control the risk of false positives resulting from multiple comparisons, the raw p-values were corrected using the Benjamin–Hochberg method (FDR), considering an effect to be statistically significant when the adjusted p-value was less than 0.05. This approach ensures robust and reliable inferences even in the presence of non-normal distributions typically observed in soil chemistry data [32].

A multivariate analysis was conducted to assess the overall differences in soil chemical signature between NT and CT systems, focusing on a set of seven key variables selected based on univariate results and biological relevance: pH, Zn, K, and Cu at both depths 0–5 cm and 5–15 cm (Cu_0to5, Cu_5to15, K_5to15, Zn_0to5, Zn_5to15, pH_0to5, pH_5to15). To obtain a stable chemical profile, median values were calculated for each plot over the entire study period. Missing values were imputed using column medians. Permutation multivariate analysis of variance (PERMANOVA) with 999 permutations was used to test for significant differences in multivariate centroids between management groups, using Euclidean distance [33]. Permutation multivariate dispersion analysis (PERMDISP) was applied to test for homogeneity of multivariate variances [34]. Principal component analysis (PCA) was performed on the standardized dataset to visualize the separation of groups [35]. The quality of clustering was quantified using silhouette analysis after k-means clustering (k = 2) on the first two principal components [36]. Finally, Hartigan's dip test was applied to the distributions of PC1 and PC2 scores to detect potential multimodality [37].

To evaluate the temporal trend of soil chemical properties and verify whether the evolutionary trajectories differed between NT and CT systems, a longitudinal analysis based on linear mixed-effects models was conducted [38,39]. The analysis was performed using only raw data in order to preserve the original information. Before modeling, the management history of each plot was verified to ensure consistency of treatment. Only variable $\times$ depth combinations that met minimum informativeness criteria were considered: at least 30 total observations, $\geq$5 distinct plots, and $\geq$3 years of sampling. For each estimated model, coefficients and significance were extracted and recorded for fixed effects (tillage, year, interaction), random effect parameters (intercept variance per plot), and model diagnostics (presence of singular fit and goodness-of-fit indices). This integrated approach allows robust inferences not only on the average differences between systems, but also on their distinctive temporal dynamics, revealing whether the effects of soil management are static or evolve differentially over the long term.

The analytical strategy follows a triangulation logic addressing complementary inferential dimensions. Univariate non-parametric tests (Wilcoxon–Mann–Whitney with Cliff's Delta) were applied as a distribution-free screening step, PCA explored latent covariance structure, and PERMANOVA tested overall multivariate separation between systems. Linear mixed-effects models accounted for the longitudinal and hierarchical data structure to evaluate temporal dynamics and Tillage $\times$ Year interactions. Finally, Random Forest and Firth-penalized logistic regression quantified predictive separability and provided parsimonious, interpretable effect estimates.

For a visual summary of the entire analytical framework—from data input to chemical signature identification—readers are referred to Appendix A, which provides a comprehensive workflow diagram illustrating the sequence of analyses and their interconnections. Model assumptions were evaluated through visual inspection of residual distributions and residual-versus-fitted plots. Given the moderate sample size and the robustness of mixed-effects models to mild deviations from normality, no additional transformations were applied.

2.5. Machine Learning Models

Machine learning models were implemented to integrate inferential analyses with a purely predictive approach and identify non-linear patterns typical of soil chemical systems. This strategy has two objectives: (i) to quantify the overall discriminating capacity of soil chemical properties in distinguishing NT and CT systems in a context free of distributional assumptions; (ii) to identify, through importance metrics, a reduced set of key variables with high informative power. To this end, the following were applied in sequence: a Random Forest algorithm for classification—maximizing predictive power and the identification of complex interactions—and Firth's penalized logistic regression—to refine the statistical interpretation of effects and manage potential quasi-separation problems.

2.5.1. Random Forest (RF)

To evaluate the ability of soil chemical properties to discriminate between NT and CT management systems, a supervised classification approach based on the Random Forest algorithm was applied [40–43]. This method, which is robust to multicollinearity and capable of capturing complex interactions, allows the predictive power of soil chemical variables to be quantified and the most discriminating ones to be identified. The analysis was conducted using a reduced set of original soil chemical variables selected based on prior multivariate evidence (PCA contribution and univariate screening). No synthetic composite variables (e.g., PCA scores) were used as predictors; only original measured chemical variables were included in the classification models. The Tillage classification factor was coded as a two-level categorical variable (NT and CT), starting from an internal binary coding. The overall dataset was divided into three independent subsets according to a 50–30–20% ratio, corresponding to the training, validation, and test sets, respectively. This division allowed the model to be trained, its intermediate performance to be evaluated, and its final predictive capacity to be estimated on data not used in the previous stages. The division was carried out randomly, setting a seed to ensure the reproducibility of the results. A model with 500 decision trees was trained, using bootstrap and random selection of predictors at each node. The number of variables randomly sampled at each split (mtry) was left at its default value ($\sqrt{p}$ predictors). No additional hyperparameter tuning was performed, and model stability was internally monitored through the out-of-bag (OOB) error estimate provided by the bootstrap aggregation procedure. Performance was evaluated on all three subsets using a comprehensive set of metrics: accuracy, Kappa, precision, sensitivity (recall), specificity, F1-score, area under the ROC curve (AUC), Log-Loss, and Brier Score. The combined use of metrics based on discrete classification and probabilistic calibration provides a robust and multidimensional assessment of performance. During training, the importance of the variables was calculated, quantified as Mean Decrease in Accuracy (average reduction in accuracy when the values of a variable are permuted). This ranking allows the identification of the soil parameters most closely associated with the distinction between the two management systems.

2.5.2. Firth Logistic Regression

To refine the statistical interpretation of the results and obtain robust estimates of the effects in the presence of moderate samples and potential quasi-separation of the data, a logistic regression with Firth's penalty was applied [44,45]. This method corrects the bias of maximum likelihood estimates in contexts with rare events or quasi-perfect predictors. Predictors were selected by integrating the results of previous analyses: importance in Random Forest (Mean Decrease Accuracy) and univariate evidence. Three nested models with varying complexity were defined:

- Model 1 (Simplified, 2 variables): Zn_0to5 + K_5to15. Combines the surface micronutrient (hypothesized negative association with CT probability) with the deeper macronutrient (positive association with CT probability), testing their potential synergy.
- Model 2 (Intermediate, 4 variables): Adds Bray1P_5to15 and Fe_0to5 to the previous ones, assessing the additional contribution of available phosphorus and surface iron.
- Model 3 (Univariate, 1 variable): Zn_0to5 only. Isolates the discriminating power of this single indicator.

For each model, the dataset was randomly divided into a training subset (70%) and a test subset (30%), setting a seed to ensure the reproducibility of the analyses. The models were estimated using penalized likelihood maximization, using Firth's correction and profiled likelihood tests to assess the significance of the coefficients. For each predictor, the regression coefficient, the associated odds ratio, and the 95% confidence interval were estimated. The predictive performance of the models was evaluated on the test set through classification accuracy and the area under the ROC curve (AUC), using a predicted probability of 0.5 as the decision threshold. The probabilistic output of the model was also used to analyze the practical effect of key variables, in particular surface Zn, translating the estimated odds ratios into relative changes in the probability of belonging to the till system along the observed gradient of concentration values. Finally, the comparison between the models was used to evaluate the trade-off between parsimony, statistical robustness, and discriminating power, allowing the identification of the minimum set of variables capable of effectively describing the differences between soil management systems.

In this study, a "chemical signature" is operationally defined as the subset of variables that (i) show significant between-management differences ($p < 0.05$), (ii) contribute to multivariate separation (PCA loadings and/or PERMANOVA), and (iii) retain predictive relevance in supervised classification models (Random Forest importance and/or significant Firth coefficients). Only variables meeting these criteria were considered components of the management-specific pedochemical signature.

3. Results and Discussion

3.1. Data Characteristics, Normality, and Preliminary Effects of Tillage

Empirical analysis confirmed marked deviations from normality typical of soil chemistry data, justifying the predominant use of non-parametric methods for group comparisons and multivariate analyses. Shapiro–Wilk and Anderson–Darling tests indicated that

https://doi.org/10.3390/agronomy16050507

the vast majority of variables (98.4%) violated the assumptions of normality ($p < 0.001$). Micronutrients such as Cu and Zn, together with Bray1-P, showed particularly strong evidence of non-normality, while Ca was the only partial exception, with occasionally borderline or normal distributions in the surface layer. This non-normality, attributable to intrinsic log-normal distributions, management-induced spatial heterogeneity, and detection limits, guided the adoption of robust tests such as Wilcoxon–Mann–Whitney, Spearman correlations, and PERMANOVA for subsequent analyses. The relationship between soil tillage intensity (Till_count) and chemical properties was preliminarily assessed using Spearman's rank correlation, which is appropriate for monotonic relationships that are not necessarily linear. Table 2 summarizes the changes between NT and CT and the main response patterns.

Table 2. Summary of relative effects of tillage system on soil chemical properties at two depths.

Variable	0–5 cm	5–15 cm	Principal Pattern
Bray1P	+9.6%	−9.0%	Vertical P Gradient
Ca	−0.5%	−1.9%	Minimal Differences
Cu	+5.2%	+3.4%	NT ↑
Fe	+16.6%	+14.6%	NT higher concentrations
K	+2.3%	−6.5%	Depth redistribution under CT
Mg	−0.9%	+2.9%	Weak Effect
Zn	+14.0%	+3.6%	Surface higher concentrations
pH	−0.40 pH units	−0.46 pH units	Higher pH with TILL

Note: Percentage values refer to relative differences between NT and CT, except for pH, which is reported as absolute unit differences due to its logarithmic scale. "↑" indicates an increase.

The analysis shows that the NT system promotes a higher superficial concentration of micronutrients in the 0–5 cm layer (+14.0% Zn, +16.6% Fe, +5.2% Cu) and a slight acidification of the entire profile (approximately −0.43 pH units). In contrast, CT attenuates the vertical gradients of potassium (K: +2.3% at 0–5 cm vs. −6.5% at 5–15 cm) and available phosphorus (Bray1-P: +9.6% vs. −9.0%). Exchangeable cations (Ca, Mg) show minimal variations ($<\pm3\%$) between management systems. These trends were confirmed and quantified using non-parametric tests and effect size measures, as reported in the following section.

3.2. Univariate Comparisons: Static Differences and Temporal Dynamics

Wilcoxon–Mann–Whitney tests with Cliff's Delta (Table 3) revealed statistically significant differences between NT and CT in approximately 50% of comparisons (16/32, FDR-adjusted $p < 0.05$).

Raw Values (Static Chemical State):

- pH: CT showed small but significant alkalinization at both depths (0–5 cm: $\delta = -0.20$; 5–15 cm: $\delta = -0.28$, $p < 0.001$), indicating a modest alkalinizing effect of tillage.
- Micronutrients (Zn, Fe, Cu): NT exhibited statistically significantly higher surface concentrations with small effect sizes for Zn ($\delta = 0.19$) and Fe ($\delta = 0.26$), and a negligible effect for Cu ($\delta = 0.099$), reflecting a detectable yet modest surface stratification pattern.
- K: Small subsurface relative increase under CT (5–15 cm: $\delta = -0.18$, $p < 0.001$), suggesting modest vertical redistribution induced by tillage.
- Bray1-P, Ca, Mg: Effects were negligible ($|\delta| \leq 0.14$), indicating minimal influence of tillage on macronutrient availability.

Delta Values (Temporal Dynamics):

- CT exhibited greater temporal variability in pH and Bray1-P at both depths ($p < 0.01$), as well as in Ca and K at 5–15 cm ($p < 0.001$).
- NT maintained higher temporal stability, with lower aggregated absolute deviation values, particularly in the surface layer.

Overall, NT is associated with detectable but modest deviations in surface micronutrients and pH relative to baseline conditions, while CT promotes small-magnitude increases in temporal variability and subsurface redistribution of macronutrients.

Table 3. Significant effects of tillage system on soil chemical properties at two depths (p-adj < 0.05).

Variable	Depth	Value Type (Raw or Baseline-Referenced Δ)	δ (Cliff's Delta)	Effect Direction
pH	0–5 cm	raw	−0.20	NT < CT
	0–5 cm	delta	−0.15	NT < CT
	5–15 cm	raw	−0.28	NT < CT
	5–15 cm	delta	−0.25	NT < CT
Bray1-P	0–5 cm	raw	0.14	NT > CT
	5–15 cm	raw	−0.13	NT < CT
	5–15 cm	delta	−0.28	NT < CT
K	5–15 cm	raw	−0.16	NT < CT
	5–15 cm	delta	−0.18	NT < CT
Ca	5–15 cm	delta	−0.19	NT < CT
Cu	0–5 cm	raw	0.099	NT > CT
Fe	0–5 cm	raw	0.26	NT > CT
	5–15 cm	raw	0.26	NT > CT
Zn	0–5 cm	raw	0.19	NT > CT
	0–5 cm	delta	0.19	NT > CT

3.3. Multivariate Patterns and System Separation

3.3.1. Principal Component Analysis (PCA)

PCA performed on median raw values captured 89.9% of the total variance in the first five components (Table 4), highlighting the main gradients of soil chemical variation associated with tillage systems. PC1 (51.8% variance) was dominated by cations (Ca, Cu, Zn) at both depths, suggesting a general fertility gradient. The prominence of cations along this axis is consistent with the univariate differences observed between management systems, although PCA itself does not assign components to specific treatments. PC2 captures the acidity-solubility axis of metals, which is dominated by pH and Fe. Specifically, soils with high pH are associated with lower Fe values, while lower pH corresponds to higher Fe concentrations—a pattern coherent with Fe solubility dynamics and consistent with the univariate differences observed between management systems. This axis highlights the interactive effect of pH and micronutrient availability, consistent with how tillage practices may influence chemical balances. The remaining components explain a smaller percentage of the overall variance and reflect more specific and complex nutritional patterns and dynamics, with important influences related to depth. PC3 (9.9%) is mainly associated with K and Mg in the surface layer, confirming that their variability is largely limited to the 0–5 cm horizon and remains relatively stable in different tillage systems. PC4 (4.4%) highlights the distinct behavior of K in the subsoil, suggesting a tendency toward vertical redistribution in conventional tillage, while PC5 (2.9%) captures the residual variability in Bray1-P, supporting the sensitivity of phosphorus availability to soil mixing, particularly in deeper layers.

Table 4. PCA summary: variance explained and top contributing variables per component (raw median values).

PC	Variance Explained (%)	Cumulative (%)	Top Contributing Variables (Contribution %)
PC1	51.8	51.8	Ca_5–15 (9.5), Cu_0–5 (9.4), Zn_5–15 (9.0), Cu_5–15 (8.9), Ca_0–5 (8.7)
PC2	20.9	72.7	pH_5–15 (25.7), pH_0–5 (23.0), Fe_0–5 (17.0), Fe_5–15 (16.1), Ca_0–5 (4.9)
PC3	9.9	82.7	K_0–5 (29.0), Mg_0–5 (15.5), Mg_5–15 (12.3), Bray1P_0–5 (7.8), Cu_0–5 (6.5)
PC4	4.4	87	K_5–15 (65.6), Zn_0–5 (11.2), pH_0–5 (10.3), Bray1P_5–15 (4.2), Ca_0–5 (4.2)
PC5	2.9	89.9	Bray1P_5–15 (31.7), Bray1P_0–5 (30.1), Zn_5–15 (11.1), Zn_0–5 (9.0), K_5–15 (5.9)

Overall, PCA visualization suggests partial separation between NT and CT regimes along axes defined by cations, pH, and surface micronutrients. The pattern is consistent with NT tending toward higher concentrations and stability in the surface soil, while CT promotes vertical redistribution and greater variability along the profile. These results complement the univariate analysis and show that the effects of tillage are multidimensional, influencing both absolute concentrations and the covariance structure of soil chemical properties.

3.3.2. Robust ANOVA (ART)

In order to validate the considerations deriving from the results of the univariate and multivariate models identified in Sections 3.2 and 3.3.1, a robust ANOVA with aligned rank transformation (ART) was performed. This approach is ideal for deviations from normality and provides comparable estimates of the effect between variables. The analysis confirmed nine significant effects of tillage after FDR correction (p-adj < 0.05), highlighting the soil chemical properties most sensitive to management. In particular, it appears that the chemical changes induced by tillage are most pronounced for pH and key micronutrients. pH showed the strongest response at both depths, with CT increasing soil alkalinity compared to NT. Fe was highly sensitive throughout the profile, consistent with the relative surface increase associated with NT. Surface Zn and Cu also reflected significant relative increases with NT, while subsurface K and Bray1-P showed moderate but significant effects of tillage, indicating a redistribution of nutrients under CT (Figure 3).

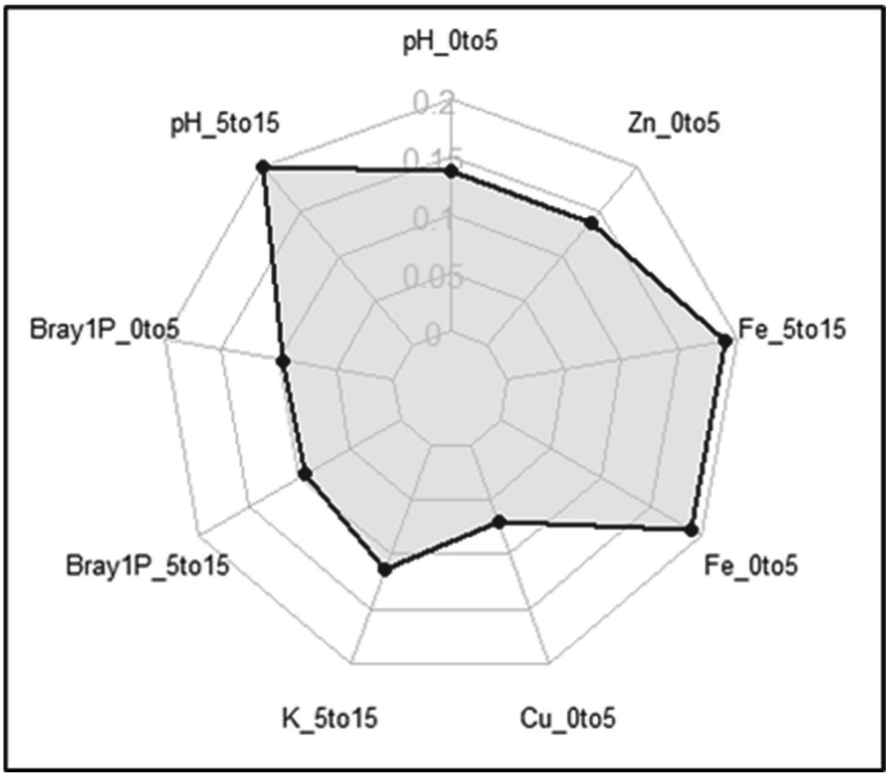

Figure 3. Radar plot of significant ART ANOVA effect sizes for tillage on soil chemical properties at 0–5 cm and 5–15 cm, with axes as Variable + Depth and distance from center proportional to effect magnitude. These results align with univariate and PCA, highlighting that surface micronutrients and pH are the most sensitive to tillage, whereas deeper macronutrients respond more moderately.

3.3.3. Internal Multivariate Analysis Based on Selected Features

To identify a minimum set of discriminating indicators, a multivariate analysis was conducted on seven variables selected based on converging evidence from previous analyses. The selection was made to represent the three key axes that emerged: (i) the higher concentrations and surface stratification of micronutrients (Cu and Zn at both depths); (ii) the redistribution at depth of a mobile macronutrient (K at 5–15 cm); and (iii) the alteration of acidity conditions throughout the profile (pH at both depths). PERMANOVA was then applied to this set to test whether these patterns, acting in synergy, generate significant multivariate differentiation.

The overall differentiation between management systems was assessed using multivariate permutational analysis of variance (PERMANOVA), applied to the set of seven selected indicators. The analysis showed a statistically significant effect of the tillage system ($p = 0.001$, $R^2 = 0.198$), indicating that approximately 20% of the total multivariate variability is explained by the soil tillage system. The multivariate dispersion homogeneity test (PERMDISP) showed no significant differences in the internal dispersion of the groups ($p = 0.053$), supporting the interpretation of the PERMANOVA result as an expression of a real difference between the multivariate centroids rather than an artifact due to dispersion heterogeneity.

Principal Component Analysis (PCA) corroborated these results, showing a partial visual separation between the NT and CT systems along the first two principal components. In particular, silhouette analysis, conducted after k-means clustering (k = 2) on PCA scores, returned a moderate mean value (0.32), indicative of a coherent but not clearly discrete group structure. Furthermore, the absence of significant multimodality in the principal component scores (Hartigan dip test; $p > 0.9$ for PC1 and PC2) suggests that the observed separation represents a continuous multivariate gradient rather than a clear categorical distinction. Overall, these results, summarized in Table 5, indicate that univariate differences translate into a consistent and statistically supported multivariate reorganization of the soil chemical profile associated with long-term tillage management.

Table 5. Summary of multivariate analyses (PERMANOVA, PERMDISP, PCA, clustering) for the selected seven-variable chemical signature.

Analysis	Test/Statistic	Result	*p*-Value
PERMANOVA (adonis2)	R^2 (variance explained)	0.198	0.001
	F statistic	18.26	0.001
PERMDISP	F statistic	3.88	0.053
PCA	Group separation	Visual	—
Silhouette (k = 2)	Mean silhouette width	0.323	—
Dip test (PC1)	Unimodality	—	0.917
Dip test (PC2)	Unimodality	—	0.958

3.3.4. Longitudinal Analysis: Temporal Stability and Diverging Subsurface Trajectories

To distinguish between static differences and temporally divergent trajectories induced by tillage, mixed-effects longitudinal models were applied to the raw chemical data. These models included tillage system, time (year), and their interaction as fixed effects, with plot as a random effect. Within this framework, temporal stability is explicitly defined and quantified through two complementary metrics: (i) the presence or absence of a significant Tillage × Year interaction, which indicates whether the temporal trends diverge between the two management systems; and (ii) the magnitude of between-year variance components from the mixed models, which reflects the overall interannual variability inherent to each soil property. All variables showed a strong common temporal signal (Year effect, $p < 0.05$ in all models), attributable to interannual climate variability and shared agronomic management. The main effect of tillage on the average level was significant only for pH, Ca, and Mg in the subsurface layer (5–15 cm). For surface micronutrients, the absence of a significant Tillage × Year interaction (discussed below) indicates that their marked differences represent stable long-term chemical states rather than transient contrasts. The most relevant information emerges from the interaction between tillage and year, which showed significantly divergent temporal trajectories only in the subsoil (5–15 cm) for pH, Ca, and Mg (p-adj < 0.05; Table 6). This indicates that, while the surface layer (0–5 cm) maintains higher temporal stability with no evidence of diverging trends, tillage continues to modulate chemical processes at depth over time.

Table 6. Summary of significant longitudinal findings (p-adj < 0.05) highlighting divergent temporal trajectories.

Variable	Depth	Tillage Effect (*p*)	Year Effect (*p*)	Tillage × Year Interaction	
				Effect (β)	*p*-Value
pH	5–15 cm	5.1×10^{-9}	4.2×10^{-7}	+0.058	4.7×10^{-9}
Ca	5–15 cm	1.6×10^{-5}	2.4×10^{-13}	+39.55	1.6×10^{-5}
Mg	5–15 cm	0.033	2.1×10^{-57}	−1.90	0.032

https://doi.org/10.3390/agronomy16050507

Specifically, CT amplified the positive temporal trend of pH and Ca in the subsoil, while NT was associated with a relative increase in subsurface Mg over time; Figure 4 shows the normalized values for the first year to allow comparison of the temporal trajectories.

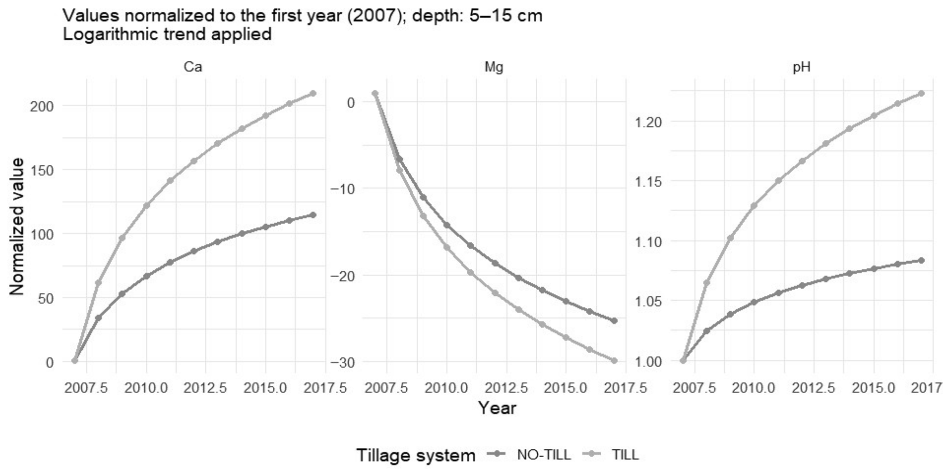

Figure 4. Normalized temporal trajectories (year "*i*" value/baseline year value) for pH, Ca, and Mg at 5–15 cm, illustrated to highlight significant Tillage × Year interactions. The progressive divergence of the trajectories underscores the dynamic and ongoing effect of tillage on subsoil chemistry.

On the contrary, no significant interactions were found for micronutrients (Cu, Zn, Fe) at any depth, nor for Bray1-P or K. This result indicates that the higher surface concentrations of Zn and Fe in the NT and the vertical redistribution of K and Bray1-P represent persistent differences over the observation period and have been maintained over time. Overall, the longitudinal analysis reinforces the conceptual model that emerged from the previous sections, highlighting a clear functional differentiation between the surface and subsoil: the 0–5 cm layer is dominated by stable chemical states linked to the presence or absence of mixing, while the 5–15 cm layer acts as a dynamic compartment, sensitive to mechanical disturbance and characterized by divergent chemical trajectories in the long term.

3.3.5. Random Forest Classification of Tillage Systems

To evaluate the predictive capacity of soil chemical characteristics in discriminating tillage systems, a Random Forest classifier was trained on a reduced set of original soil chemical variables, selected based on prior multivariate evidence from PCA and univariate screening. The dataset was divided into 50% training, 30% validation, and 20% test sets. Low-variance variables were removed before training. The model showed high accuracy on the training set (92.6%), demonstrating effective learning of discriminating patterns. Performance on independent validation and test sets was moderate, with accuracies of 78.3% and 73.3% respectively, though test recall for the TILL class was limited (0.50). The variable importance analysis (Mean Decrease Accuracy) identified K_5–15 as the single most important predictor, followed by Fe_0–5 and Zn_0–5 (Table 7). This ranking efficiently synthesizes the two key axes that emerged from the previous analyses: the redistribution of a mobile macronutrient (K) at depth associated with CT, and the detectable higher surface concentrations of micronutrients (Fe, Zn) characteristic of NT.

Table 7. Random Forest performance metrics and top variables for tillage classification.

Split	Accuracy	Kappa	Precision	Recall	F1	Principal Features (Mean Decrease Accuracy)
Train	0.926	0.787	0.962	0.897	0.90	(1) K_5–15, (2) Fe_0–5, (3) Zn_0–5, (4) Bray1P_5–15, (5) Fe_5–15
Validation	0.783	0.563	0.769	0.833	0.80	
Test	0.733	0.412	0.750	0.500	0.60	

The Random Forest results provide predictive support for the inferential evidence. They demonstrate that NT and CT systems are distinguishable with **moderate accuracy** based on an established chemical profile. The model independently identifies the same key variables (subsurface K and surface micronutrients), reinforcing the ecological relevance of stratification and redistribution patterns as indicators of long-term soil management.

3.3.6. Firth Logistic Regression—Model Refinement

To ensure comparable effect sizes across variables with different measurement scales, all predictors were standardized (mean = 0, standard deviation = 1) prior to Firth logistic regression. Odds Ratios (OR) are thus interpreted as the change in odds per one standard deviation increase in the predictor.

Three models were trained and compared (Table 8):

Table 8. Comparison of Firth's logistic regression models and odds ratio estimates.

Model (n Variables)	Variables	Accuracy (%)	AUC	Odds Ratio (OR) [IC 95%]
Model 1 (2)	Zn_0to5 + K_5to15	73.9	0.900	Zn_0to5: 0.37 [0.18–0.74] K_5to15: 4.74 [2.42–9.27]
Model 2 (4)	Zn_0to5 + K_5to15 + Fe_0to5 + Bray1P_5to15	78.3	0.923	K_5to15: 3.63 [1.37–9.62] Fe_0to5: 0.31 [0.11–0.85] Zn_0to5: 0.53 [0.21–1.31]
Model 3 (1)	Zn_0to5	73.9	0.750	Zn_0to5: 0.78 [0.45–1.34]

Note: Variables standardized to mean = 0, SD = 1. OR represent multiplicative change in odds per SD increase.

Model 1 (Zn_0to5 + K_5to15): Showed moderate performance (Accuracy = 73.9%, AUC = 0.900). Standardized surface Zn exhibited a negative association with CT probability (OR = 0.37 per SD increase, 95% CI [0.18–0.74], $p = 0.007$), while subsurface K showed a strong positive association with CT probability (OR = 4.74 per SD, 95% CI [2.42–9.27], $p < 0.001$).

Model 2 (4 variables): Achieved the best predictive performance (Accuracy = 78.3%, AUC = 0.923). In this multivariate context, K_5to15 (OR = 3.63, $p = 0.010$) and Fe_0to5 (OR = 0.31, $p = 0.019$) remained significant, while Zn_0to5 attenuated and lost statistical significance (OR = 0.53, $p = 0.170$).

Model 3 (Zn_0to5 only): Confirmed Zn's limited univariate discriminating power (OR = 0.78 per SD, $p = 0.356$, Accuracy = 73.9%, AUC = 0.750).

The results of the Firth regression reveal two fundamental concepts:

Complementary additive effects: Zn_0to5 and K_5to15 provide complementary classification information with opposing directions (negative vs. positive association with CT probability), but their effects are additive rather than synergistic (interaction $p = 0.534$).

https://doi.org/10.3390/agronomy16050507

Context-dependent significance: The significance of surface Zn depends on model specification, being strong in bivariate models (OR = 0.37, p = 0.007) but attenuated in multivariate contexts (OR = 0.53, p = 0.170).

Robust multivariate predictors: Subsurface K consistently associates with conventional tillage (OR $\approx$ 3.6–4.7 per SD), while surface Fe shows consistent negative association with CT probability (OR = 0.31 per SD).

This analysis provides interpretable, scale-invariant effect estimates that confirm the complementary roles of surface micronutrients (Zn, Fe) and subsurface macronutrients (K) in distinguishing tillage systems, while demonstrating that their combined predictive power arises from additive rather than interactive effects.

3.4. Brief Synthesis of Evidence: A Convergent Multidimensional Signature

The univariate, multivariate, longitudinal, and machine-learning analyses presented here, while methodologically independent, converge to delineate a coherent and consistent picture of tillage-induced pedochemical reorganization. The univariate tests (Wilcoxon, Cliff's Delta) established the core static differences in key elements (pH, Zn, Fe, K). Multivariate ordination (PCA, PERMANOVA) contextualized these differences within a broader chemical covariance structure, revealing the stratification–homogenization duality as the dominant organizational gradient. Crucially, the longitudinal mixed models indicated that these differences are not transient but represent stable states (for surface micronutrients) or divergent temporal trajectories (for subsoil pH and cations). Finally, the predictive models (Random Forest, Firth regression) provided convergent support for these patterns, with subsurface K (OR $\approx$ 3.6–4.7 per SD) and surface Zn (OR $\approx$ 0.37–0.78 per SD) emerging as complementary, additively acting classifiers of tillage management history. This methodological triangulation provides a high degree of confidence in the results. It supports the interpretation that the observed chemical signature is not an artifact of a single statistical approach but a recurrent pattern consistently associated with contrasting long-term management. From a mechanistic perspective, these convergent statistical patterns can be interpreted in light of the physical processes induced by tillage. The higher surface concentrations of Zn, Fe, and Cu under NT are consistent with reduced mechanical mixing, which favors higher residue concentrations and the subsequent mineralization/release of nutrients at the soil surface. The mild acidification observed under NT is likely attributable to the build-up of soil organic matter and associated nitrification processes in the absence of tillage mixing. Furthermore, the stable and moist micro-environment at the NT surface may promote the mobilization and re-deposition of redox-sensitive elements such as Fe and Zn, although, as no direct measurements of soil redox status were made, this interpretation remains a hypothesis supported by recent literature [7,15]. Conversely, the mechanical action under CT physically dilutes surface nutrients and redistributes them throughout the plow layer, as evidenced by the relative increase in subsurface K. The disruption of macro-aggregates under CT can expose previously protected organic matter, contributing to greater temporal variability and distinct pH dynamics compared to the more stable NT system. This multi-method approach aligns with the growing body of literature applying machine learning to tillage discrimination and soil management diagnostics. Several recent studies have leveraged Random Forest and ensemble classifiers on remote sensing data to map tillage practices at regional and national scales [46], demonstrating the discriminative power of spectral and temporal signatures. Similarly, ML-based frameworks have been employed to classify soil properties under contrasting tillage and straw management regimes from sensor arrays [47] and to predict soil organic carbon dynamics following the transition to no-till [48]. More recently, multi-sensor features fusion approaches have achieved near-perfect classification of tillage systems from ground-based soil imaging [49], while novel ensemble architectures have improved the prediction of soil-mediated biogeochemical fluxes under different tillage and fertilization treatments [50]. In this broader context, the present study offers a complementary and distinctive contribution: whereas these studies rely predominantly on spectral signatures, satellite-derived indices, or emission fluxes, we demonstrate that depth-resolved soil chemical properties alone—measured through conventional soil analysis—can effectively discriminate long-term tillage history. This finding underscores the diagnostic value of integrating vertical chemical gradients as interpretable features, an aspect largely underexplored in the ML-for-tillage literature. Our integration of Random Forest with Firth regression further addresses the recognized need for robust, interpretable classifiers applicable to imbalanced agricultural datasets [51,52], providing methodological transparency alongside predictive performance.

4. Conclusions

This multi-method analysis demonstrates that long-term tillage management imposes distinct, depth-specific chemical signatures on the soil profile, primarily driven by the mechanical manipulation of the soil environment. NT, by eliminating soil disturbance, shows high temporal stability and tends to favor the arrangement of a stabilized surface layer characterized by detectable yet modestly higher concentrations of micronutrients (Zn, Fe and Cu) and mild acidification. These surface patterns are consistent with reduced mixing, higher residue concentrations, and the creation of a stable micro-environment that may influence micronutrient dynamics, though the specific biogeochemical pathways (e.g., redox cycling) require direct experimental validation. Conversely, the mechanical action in CT tends to homogenize the profile by redistributing nutrients, leading to a distinct pedochemical trajectory characterized by a relative potassium increase in the subsurface, progressive alkalinization, and greater temporal variability. These features are coherent with physical mixing, aggregate disruption, and the exposure of organic matter to decomposition. While the fundamental dichotomy of stratification versus homogenization is a universal response to tillage intensity, the specific magnitudes of surface micronutrients' relative increases and subsurface macronutrient redistribution are contingent on the local pedoclimatic context, here represented by Mollisols in a continental climate. Further studies across diverse soil types, climatic zones, and cropping systems are needed to validate and contextualize these chemical signatures and assess their broader applicability as diagnostic tools for tillage management history. The convergence of analytical evidence identifies mechanical tillage management as a major structuring factor of soil chemical dynamics through its long-term effects on soil physical structure. These physical modifications—stratification versus homogenization—create structural conditions that are consistent with observed differences in nutrient distribution and may plausibly influence biogeochemical processes such as organic matter turnover and element mobilization. Surface Zn and subsurface K emerge as complementary discriminators, reflecting additive rather than synergistic consequences of mechanical soil handling—defined by altered vertical gradients, diverging temporal dynamics, and specific elemental covariation. The identified chemical patterns offer objective criteria for distinguishing the long-term effects of conventional and conservation tillage, supporting agronomic decisions, such as fertilizer placement, that take these predictable gradients into account. The complementary signature identified here—surface Zn negatively associated with CT probability and subsurface K positively associated with CT probability—provides a practical imprint of mechanization choices, offering a practical basis for rapid, cost-effective soil tests. Thus, this work provides an analytically supported diagnostic framework where soil chemistry becomes a partially readable record of past mechanical management and a guide for its future optimization.

https://doi.org/10.3390/agronomy16050507

Author Contributions: Conceptualization, P.D., C.F., A.S. and F.T.; methodology, P.D., C.F. and F.T.; software, C.F., F.M. and F.T.; validation, L.A.C., M.D., A.S. and L.S.S.; formal analysis, P.D., C.F. and F.T.; investigation, L.A.C., P.D. and A.S.; resources, P.D., C.F., A.S. and M.V.; data curation, P.D., C.F. and F.T.; writing—original draft preparation, F.T.; writing—review and editing, P.D., C.F., M.D. and F.T.; visualization, L.S.S.; supervision, L.A.C., P.D., C.F., F.M., L.S.S., M.V. and F.T.; project administration, P.D., C.F. and F.T.; funding acquisition, P.D., C.F. and F.T. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the University of Basilicata; "Casa delle Tecnologie Emergenti" of Matera (CTEMT), "Laboratorio del Giardino delle tecnologie emergenti" (CUP: I14E20000020001); the "Territorial Pacts" (Patti Territoriali) doctoral research project of F.T. (CUP: C42C24000220001); the Smart@Irrifert Project (PSR Basilicata 2014–2020—Sottomisura 16.2, CUP: G19J21004870006); and the "Vertical gaRdens with Digital twin of plants" (Viridiis) Project, PRIN 2022 (CUP: C53D23000480006).

Data Availability Statement: The data presented in this study are available in Data.gov at https://catalog.data.gov/dataset/thirteen-year-stover-harvest-and-tillage-effects-on-corn-agroecosystem-sustainability-in-i-be5ae (accessed on 14 November 2025), reference number [21]. These data were derived from the following resources available in the public domain: "Thirteen-year Stover Harvest and Tillage Effects on Corn Agroecosystem Sustainability in Iowa" (surface soil test data from 2007–2021, Iowa State University) and specifically the file "Field 70–71 Surface Soil Test Data 2007–2021.xlsx", focusing on continuous no-tillage and chisel tillage plots for the period 2010–2017. Custom R scripts and code used for data preprocessing, statistical analysis (ART ANOVA, mixed-effects models, PCA, PERMANOVA), and machine learning (Random Forest, Firth logistic regression) are available from the corresponding author upon reasonable request.

Acknowledgments: This work was carried out within the framework of research activities and scientific collaboration between the University of Basilicata and international institutions, including the Federal University of Vale do Jequitinhonha e Mucuri (Brazil) and the VALORIZA—Research Center for Endogenous Resource Valorization at the Polytechnic Institute of Portalegre, Portugal. This research falls within the scientific-disciplinary fields of **Agricultural Engineering**. During the preparation of this work, the authors used generative AI tools exclusively for non-substantive tasks related to language editing, technical refinement, and code debugging. All scientific reasoning, model selection, data interpretation, and conclusions remain entirely the responsibility of the authors. No generative AI was used to generate data, formulate hypotheses, or produce original scientific content. The authors have reviewed and edited the output and take full responsibility for the content of this publication.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CT	Chisel Tillage
NT	No-Tillage
Bray1-P	Available Phosphorus (Bray-1 extraction method)
CEC	Cation Exchange Capacity
EC	Electrical Conductivity
OM	Organic Matter
SOC	Soil Organic Carbon
Ca	Calcium
Cu	Copper
Fe	Iron
K	Potassium
Mg	Magnesium
Mn	Manganese
Zn	Zinc

0–5	0–5 cm depth
5–15	5–15 cm depth
NN	Non-Normal
Δ%	Percentage Change
ANOVA	Analysis of Variance
ART	Aligned Rank Transformation
AUC	Area Under the (ROC) Curve
FDR	False Discovery Rate
ML	Machine Learning
OR	Odds Ratio
PCA	Principal Component Analysis
PERMANOVA	Permutational Multivariate Analysis of Variance
PERMDISP	Permutational Analysis of Multivariate Dispersions
RF	Random Forest
ROC	Receiver Operating Characteristic
δ (delta)	Cliff's Delta (non-parametric effect size measure)
ρ (rho)	Spearman's Rank Correlation Coefficient
Δvar (delta)	Temporal difference (annual change) for a variable
Δagg	Aggregated delta (net or absolute cumulative deviation)
PC1, PC2, . . .	Principal Component 1, 2, . . .
Ti	Tillage Index
USDA-ARS	United States Department of Agriculture-Agricultural Research Service
VALORIZA	Research Center for Endogenous Resource Valorization
hp	Horsepower
ILS	Integrated Load Sensing (hydraulic system)
kg	Kilograms
cm	Centimeters
MFWD	Mechanical Front-Wheel Drive
2WD	Two-Wheel Drive

Appendix A

The Appendix A (Analytical Workflow) provides a schematic overview of the analytical framework adopted in this study, from data input through to the identification of the management-specific pedochemical signature. The diagram shows how preprocessing, normality assessment, and three parallel analytical tracks—univariate, multivariate, and longitudinal—converge into the machine learning stage and ultimately into the final chemical characterization of NT and CT soils. It is intended as a visual companion to the methodological description provided in Section 2.

References

1. Ma, Y.; Li, Z.; Xu, Y.; Li, C.; Ding, H.; Li, C.; Tang, Q.; Liu, M.; Hou, J. The Development of No-Tillage Seeding Technology for Conservation Tillage—A Review. *Sustainability* **2025**, *17*, 1808. [CrossRef]
2. Blevins, R.L.; Smith, M.S.; Thomas, G.W. Changes in Soil Properties Under No-Tillage. In *No-Tillage Agriculture*; Phillips, R.E., Phillips, S.H., Eds.; Springer: Boston, MA, USA, 1984; pp. 123–145. [CrossRef]
3. Limousin, G.; Tessier, D. Effects of No-Tillage on Chemical Gradients and Topsoil Acidification. *Soil Tillage Res.* **2007**, *92*, 167–174. [CrossRef]
4. Rhoton, F.E.; Bruce, R.R.; Buehring, N.W.; Elkins, G.B.; Langdale, C.W.; Tyler, D.D. Chemical and Physical Characteristics of Four Soil Types under Conventional and No-Tillage Systems. *Soil Tillage Res.* **1993**, *28*, 51–61. [CrossRef]
5. Fiorentino, C.; D'Antonio, P.; Toscano, F.; Donvito, A.; Modugno, F. New Technique for Monitoring High Nature Value Farmland (HNVF) in Basilicata. *Sustainability* **2023**, *15*, 8377. [CrossRef]
6. Santana, L.S.; Santos, L.G.M.; Silva, J.M.; Filho, A.C.M.; Toscano, F.; Silva, E.F.; Jardim, A.M.; Silva, T.G.F.; Zanella, M.A. Surface Mapping by RPAs for Ballast Optimization and Slip Reduction in Plowing Operations. *AgriEngineering* **2025**, *7*, 332. [CrossRef]
7. Engell, I.; Gerigk, J.; Linsler, D.; Joergensen, R.G.; Potthoff, M. Tillage and Land Use Management Effects on Soil Organic Matter and Soil Microbial Biomass in a Field Network of Practical Farms in France, Romania, and Sweden. *Appl. Soil Ecol.* **2024**, *202*, 105584. [CrossRef]

8. De Santiago, A.; Quintero, J.M.; Delgado, A. Long-Term Effects of Tillage on the Availability of Iron, Copper, Manganese, and Zinc in a Spanish Vertisol. *Soil Tillage Res.* **2008**, *98*, 200–207. [CrossRef]
9. Battaglia, M.L.; Thomason, W.; Ozlu, E.; Rezaei-Chiyaneh, E.; Fike, J.H.; Diatta, A.A.; Uslu, O.S.; Babur, E.; Schillaci, C. Short-Term Crop Residue Management in No-Tillage Cultivation Effects on Soil Quality Indicators in Virginia. *Agronomy* **2023**, *13*, 838. [CrossRef]
10. Mestelan, S.; Smeck, N.; Sprunger, C.; Dyck, A.; Dick, W. Four Decades of Continuously Applied Tillage or No-Tillage on Soil Properties and Soil Morphology. *Agrosyst. Geosci. Environ.* **2021**, *4*, e2021. [CrossRef]
11. Neugschwandtner, R.W.; Száková, J.; Pachtrog, V.; Tlustoš, P.; Černý, J.; Kulhánek, M.; Kaul, H.; Euteneuer, P.; Moitzi, G.; Wagentristl, H. Basic Soil Chemical Properties after 15 Years in a Long-Term Tillage and Crop Rotation Experiment. *Int. Agrophys.* **2020**, *34*, 133–140. [CrossRef]
12. He, Z.; Tazisong, I.; Yin, X.; Watts, D.; Senwo, Z.; Torbert, H. Long-Term Cropping System, Tillage, and Poultry Litter Application Affect the Chemical Properties of an Alabama Ultisol. *Pedosphere* **2019**, *29*, 180–194. [CrossRef]
13. Mara, S.; Fontoura, V.; Pias, H.; Cherubin, M.; Moraes, R.; Bayer, C.; Tiecher, T. Effect of Gypsum Rates and Lime with Different Reactivity on Soil Acidity and Crop Grain Yields in a Subtropical Oxisol under No-Tillage. *Soil Tillage Res.* **2019**, *193*, 27–41. [CrossRef]
14. Dewi, R.K.; Fukuda, M.; Takashima, N.; Yagioka, A.; Komatsuzaki, M. Soil Carbon Sequestration and Soil Quality Change between No-Tillage and Conventional Tillage Soil Management after 3 and 11 Years of Organic Farming. *Soil Sci. Plant Nutr.* **2021**, *68*, 133–148. [CrossRef]
15. Dong, H.; Zeng, Q.; Sheng, Y.; Chen, C.; Yu, G.-H.; Kappler, A. Coupled Iron Cycling and Organic Matter Transformation across Redox Interfaces. *Nat. Rev. Earth Environ.* **2023**, *4*, 659–673. [CrossRef]
16. Keshavarz Afshar, R.; Cabot, P.; Ippolito, J.; Dekamin, M.; Reed, B.; Doyle, H.; Fry, J. Corn Productivity and Soil Characteristic Alterations Following Transition from Conventional to Conservation Tillage. *Soil Tillage Res.* **2022**, *220*, 105351. [CrossRef]
17. Schlüter, S.; Albrecht, L.; Schwärzel, K.; Kreiselmeier, J. Long-Term Effects of Conventional Tillage and No-Tillage on Saturated and Near-Saturated Hydraulic Conductivity—Can Their Prediction Be Improved by Pore Metrics Obtained with X-ray CT? *Geoderma* **2020**, *361*, 114082. [CrossRef]
18. Silva, L.; Conceição, L.A.; Lidon, F.C.; Patanita, M.; D'Antonio, P.; Fiorentino, C. Digitization of Crop Nitrogen Modelling: A Review. *Agronomy* **2023**, *13*, 1964. [CrossRef]
19. D'Antonio, P.; Mehmeti, A.; Toscano, F.; Fiorentino, C. Operating Performance of Manual, Semi-Automatic, and Automatic Tractor Guidance Systems for Precision Farming. *Res. Agric. Eng.* **2023**, *69*, 179–188. [CrossRef]
20. Stellacci, A.M.; Castellini, M.; Diacono, M.; Rossi, R.; Gattullo, C.E. Assessment of Soil Quality under Different Soil Management Strategies: Combined Use of Statistical Approaches to Select the Most Informative Soil Physico-Chemical Indicators. *Appl. Sci.* **2021**, *11*, 5099. [CrossRef]
21. Phillips, C.L.; Tekeste, M.Z.; Ebrahimi, E.; Logsdon, S.D.; Malone, R.W.; O'Brien, P.L.; Emmett, B.D.; Karlen, D. Thirteen-Year Stover Harvest and Tillage Effects on Soil Compaction in Iowa. *Agrosyst. Geosci. Environ.* **2023**, *6*, e20361. [CrossRef]
22. Yang, J.; Sun, J.; Hammer, D.; Blanchar, R. Distribution Normality of pH and H+ Activity in Soil. *Environ. Chem. Lett.* **2004**, *2*, 159–162. [CrossRef]
23. Gonzalez, J.P.; Jarvis, A.; Cook, S.E.; Oberthür, T.; Rincon-Romero, M.; Bagnell, J.A.; Dias, M.B. Digital Soil Mapping of Soil Properties in Honduras Using Readily Available Biophysical Datasets and Gaussian Processes. In *Digital Soil Mapping with Limited Data*; Hartemink, A.E., McBratney, A., Mendonça-Santos, M.d., Eds.; Springer: Dordrecht, The Netherlands, 2008; pp. 385–396. [CrossRef]
24. Sharma, V.; Irmak, S.; Padhi, J. Effects of Cover Crops on Soil Quality: Part I. Soil Chemical Properties—Organic Carbon, Total Nitrogen, pH, Electrical Conductivity, Organic Matter Content, Nitrate-Nitrogen, and Phosphorus. *J. Soil Water Conserv.* **2018**, *73*, 637–651. [CrossRef]
25. Rostampour, M.; Azarmi Atajan, F. Comparison of Normality Test Methods for Some Soil Properties in the Arid Land of South Khorasan. *Desert* **2023**, *28*, 95765. [CrossRef]
26. Mishra, P.; Pandey, C.M.; Singh, U.; Gupta, A.; Sahu, C.; Keshri, A. Descriptive Statistics and Normality Tests for Statistical Data. *Ann. Card. Anaesth.* **2019**, *22*, 67–72. [CrossRef] [PubMed]
27. Liang, J.; Tang, M.-L.; Chan, B. A Generalized Shapiro-Wilk W Statistic for Testing High-Dimensional Normality. *Comput. Stat. Data Anal.* **2009**, *53*, 3883–3891. [CrossRef]
28. Rochon, J.; Gondan, M.; Kieser, M. To Test or Not to Test: Preliminary Assessment of Normality When Comparing Two Independent Samples. *BMC Med. Res. Methodol.* **2012**, *12*, 81. [CrossRef] [PubMed]
29. Razzaq, A.; Le Gear, A.; Exton, C.; Buckley, J. An Empirical Assessment of Baseline Feature Location Techniques. *Empir. Softw. Eng.* **2020**, *25*, 266–321. [CrossRef]

30. Romano, J.; Kromrey, J.D.; Coraggio, J.; Skowronek, J. Appropriate Statistics for Ordinal Level Data: Should We Really Be Using t-Test and Cohen's d for Evaluating Group Differences on the NSSE and Other Surveys. In Proceedings of the Annual Meeting of the Florida Association of Institutional Research, Cocoa Beach, FL, USA, 1–3 February 2006; pp. 1–33.
31. Wobbrock, J.O.; Findlater, L.; Gergle, D.; Higgins, J.J. The Aligned Rank Transform for Nonparametric Factorial Analyses Using Only ANOVA Procedures. In Proceedings of the SIGCHI Conference on Human Factors in Computing Systems, Vancouver, BC, Canada, 7–12 May 2011; pp. 143–146. [CrossRef]
32. Benjamini, Y.; Hochberg, Y. Controlling the False Discovery Rate: A Practical and Powerful Approach to Multiple Testing. *J. R. Stat. Soc. Ser. B* **1995**, *57*, 289–300. [CrossRef]
33. Anderson, M.J. A New Method for Non-Parametric Multivariate Analysis of Variance. *Austral Ecol.* **2001**, *26*, 32–46. [CrossRef]
34. Anderson, M.J. Distance-Based Tests for Homogeneity of Multivariate Dispersions. *Biometrics* **2006**, *62*, 245–253. [CrossRef]
35. Jolliffe, I.T.; Cadima, J. Principal Component Analysis: A Review and Recent Developments. *Philos. Trans. R. Soc. A* **2016**, *374*, 20150202. [CrossRef]
36. Rousseeuw, P.J. Silhouettes: A Graphical Aid to the Interpretation and Validation of Cluster Analysis. *J. Comput. Appl. Math.* **1987**, *20*, 53–65. [CrossRef]
37. Hartigan, J.A.; Hartigan, P.M. The Dip Test of Unimodality. *Ann. Stat.* **1985**, *13*, 70–84. [CrossRef]
38. Pinheiro, J.C.; Bates, D.M. *Mixed Effects Models in S and S PLUS*; Springer: New York, NY, USA, 2000. [CrossRef]
39. Bolker, B.M.; Brooks, M.E.; Clark, C.J.; Geange, S.W.; Poulsen, J.R.; Stevens, M.H.H.; White, J.S.S. Generalized Linear Mixed Models: A Practical Guide for Ecology and Evolution. *Trends Ecol. Evol.* **2009**, *24*, 127–135. [CrossRef] [PubMed]
40. Breiman, L. Random Forests. *Mach. Learn.* **2001**, *45*, 5–32. [CrossRef]
41. Padarian, J.; Minasny, B.; McBratney, A.B. Machine Learning and Soil Sciences: A Review Aided by Machine Learning Tools. *Soil* **2020**, *6*, 35–52. [CrossRef]
42. Ballabio, C.; Robinson, D.A. Modelling and Prediction of Major Soil Chemical Properties with Random Forest: Machine Learning as Tool to Understand Soil-Environment Relationships in Antarctica. *Catena* **2024**, *235*, 107677. [CrossRef]
43. Fiorentino, C.; D'Antonio, P.; Toscano, F.; Capece, N.; Conceição, L.A.; Scalcione, E.; Modugno, F.; Sannino, M.; Colonna, R.; Lacetra, E.; et al. Smart Sensors and Artificial Intelligence Driven Alert System for Optimizing Red Peppers Drying in Southern Italy. *Sustainability* **2025**, *17*, 1682. [CrossRef]
44. Firth, D. Bias Reduction of Maximum Likelihood Estimates. *Biometrika* **1993**, *80*, 27–38. [CrossRef]
45. Heinze, G.; Schemper, M. A Solution to the Problem of Separation in Logistic Regression. *Stat. Med.* **2002**, *21*, 2409–2419. [CrossRef]
46. Pasut, C.; Li, M.; Armour, B.; Asanopoulos, C.; Brown, G.; Crawford, D.; Farrell, M.; Garrard, M.; Hoyle, F.; McCaskill, M.; et al. Integrating soil monitoring and machine learning to map historical tillage and stubble management across Australian cropping systems (2001–2023). *Comput. Electron. Agric.* **2026**, *243*, 111408. [CrossRef]
47. Liu, S.; Chen, X.; Huang, D.; Wang, J.; Jiang, X.; Meng, X.; Gao, X. The discrete taxonomic classification of soils subjected to diverse treatment modalities and varied fertility grades utilizing machine olfaction. *Agriculture* **2024**, *14*, 291. [CrossRef]
48. Anand, S.K.; Singh, R.; Mohanty, B.P.; Rajan, N.; Calabrese, S. Classifying the potential for soil organic carbon gain under regenerative agriculture. *Environ. Res. Lett.* **2025**, *20*, 044045. [CrossRef]
49. He, J.H.; Mickelson, S.K.; Hatfield, J.L.; Tekeste, M.Z. Tillage-induced soil feature extraction and multi-sensors fusion for tillage system classification. *Biosyst. Eng.* **2026**, *261*, 104329. [CrossRef]
50. Lussich, F.R.; Ackett, R.; Dhaliwal, J.K.; Gan, H.; Saha, D. Enhancing predictions of nitrous oxide emissions from agricultural soils using a classification-swap machine learning approach. *J. Environ. Qual.* **2026**, *55*, e70126. [CrossRef]
51. Mo, Y.; Bier, R.L.; Li, X.; Daniels, M.D.; Smith, A.H.; Yu, L.; Kan, J. Agricultural practices influence soil microbiome assembly and interactions at different depths identified by machine learning. *Commun. Biol.* **2024**, *7*, 1349. [CrossRef]
52. Fiorentini, M.; Schillaci, C.; Denora, M.; Zenobi, S.; Deligios, P.A.; Santilocchi, R.; Perniola, M.; Ledda, L.; Orsini, R. Fertilization and soil management machine learning based sustainable agronomic prescriptions for durum wheat in Italy. *Precis. Agric.* **2024**, *25*, 2853–2880. [CrossRef]