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Predictive Assessment and Social-Cost Estimation of Methane Emissions in Bio-Slurry Amended Systems

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***Abstract*—Scalable mitigation strategies are made possible by machine learning-based predictions of agricultural methane (CH_4) emissions. A stacking-ensemble framework for predicting continuous CH_4 emission rates and categorical emission levels in Maize and Napier grass systems amended with bio-slurry is presented in this paper. Using a linear meta-learner and polynomial, interaction, temporal-lag, and rolling-window engineered features along with leakage-aware target encoding, four tree-based base learners (Random Forest, LightGBM, XGBoost, and CatBoost) achieve regression performance of $R^2 = 0.6643 \pm 0.0479$ and classification accuracy of $68.57\% \pm 2.35\%$ on $N = 350$ samples using 5-fold GroupKFold cross-validation. A statistically significant improvement is confirmed by a paired t-test against XGBoost ($t = 2.9047$, $p = 0.0439$). CatBoost ($R^2 = 0.6584 \pm 0.0508$) was the best individual model by mean R^2. The most significant predictors, according to SHAP interpretability, are the percentage of bioslurry, treatment–replication–day interactions, and emission temporal lag. Although the stacking ensemble has a significant computational cost (mean fit time 4.5760s versus 0.0183s for linear regression; $\sim 250.4\times$ slower), it improves predictive performance. An economic assessment using the U.S. EPA social cost of methane ($1.50 kg^{-1}) for maize at Day 42 shows treatment-specific annualized social emission costs: $T1 = \$48.86$ $\mathrm{ha}^{-1}\mathrm{yr}^{-1}$, $T2 = \$88.09$ $\mathrm{ha}^{-1}\mathrm{yr}^{-1}$, $T3 = \$123.52$ $\mathrm{ha}^{-1}\mathrm{yr}^{-1}$, $T4 = \$59.96$ $\mathrm{ha}^{-1}\mathrm{yr}^{-1}$, and $T5 = \$48.77$ $\mathrm{ha}^{-1}\mathrm{yr}^{-1}$ (close to T1). The study presents a validated, interpretable framework for predicting CH_4 emissions and identifies accuracy and computational cost trade-offs for real-world implementation.**

***Index Terms*—Methane emissions, stacking ensemble, SHAP interpretability, leakage-aware target encoding, GroupKFold, economic cost assessment.**

I. Introduction

A. Background and Motivation

Agricultural methane (CH_4) emissions represent a major contributor to global greenhouse gas (GHG) budgets, accounting for approximately 44% of total anthropogenic CH_4 emissions [1], [2]. Intensive cropping systems, particularly those across Asia's rice-growing regions, produce substantial CH_4 fluxes due to anaerobic soil processes [3]–[5]. Observed fluxes in bio-slurry-amended maize and Napier grass systems range from 0.1 to 2.5 $\mathrm{mg} \cdot \mathrm{m}^{-2} \cdot \mathrm{hr}^{-1}$ [6]–[9], depending on crop phenology, soil moisture, and biogas production rates. Traditional process-based models such as DNDC and DayCent [10]–[13] require the thorough parameterization of soil-microbial processes and typically achieve a low predictive accuracy in field validations [12] ($R^2 \approx 0.01$–0.10). Ensemble machine learning techniques, like Random Forest (RF), LightGBM, XGBoost, and CatBoost [14]–[17], combine multiple learners to improve prediction robustness and generalization. Examples of these techniques include stacking, boosting, and bagging. Yet, there is still a dearth of research on ensemble-based methane modeling in bio-slurry field applications, especially concerning interpretability, computational efficiency, and statistical significance testing [14], [16], [18], [19].Conversely, complex, nonlinear relationships are directly taught to machine learning models using observational data [14]–[17], [20] allowing high-dimensional dependencies to be discovered without requiring particular mechanistic assumptions.

B. Problem Statement

This study targets the prediction of weekly CH_4 fluxes ($\mathrm{mg}\cdot\mathrm{m}^{-2}\cdot\mathrm{hr}^{-1}$) in maize and Napier grass systems treated with 0–100% bio-slurry amendment [6], [8], [9]. Several modeling challenges are addressed: The purpose of this study is to predict weekly CH_4 fluxes ($\mathrm{mg}\cdot\mathrm{m}^{-2}\cdot\mathrm{hr}^{-1}$) in maize+nihilema and Napier grass systems when treated with 0–100% bio-slurry amendment [6], [8], [9]. Several modeling challenges are addressed:

- Temporal Dynamics: Emission time series is correlated; lags and rolling window statistics are needed to retain the short-term dependencies [16], [18].
- Encoding of Treatments: Encoding of grouped treatments together with replications must be performed under target leakage free restriction on data adjacency (with use of specialized leakage-aware encoding strategies [14], [19]).
- Robust Model: Guarantees predictive stability among emission intensity classes (Low, Medium, High) in the presence of imbalanced data [19].
- Computational–Accuracy Trade-off: Estimating the extent to which stacking is more effective than naive alternatives as compared to how long it takes [14], [15], [17].
- Economic Integration: Translating predicted CH_4 fluxes into annualized social costs using the U.S. EPA Social Cost of Methane (SCC; \$1.50–\$2.70 kg^{-1} CH_4) [21]–[25].

C. Contributions

Our work advances methane emission prediction through: (1) a validated stacking ensemble (RF, LightGBM, XGBoost, CatBoost) achieving $R^2 = 0.6643 \pm 0.0479$; (2) leakage-free feature engineering with GroupKFold splits ; (3) computational cost quantification ($\sim 250\times$ vs. linear regression); (4) SHAP-based feature attribution identifying key predictive drivers ; (5) economic analysis revealing minimum emissions at 0% and 100% bio-slurry treatments ($48.86 and $48.77 $\mathrm{ha}^{-1}\,\mathrm{yr}^{-1}$); and (6) comparative benchmark analysis demonstrating ensemble superiority.

II. Related Work

A. Ensemble Learning in Environmental Modeling

Ensemble techniques train a collection of individual base learners to mitigate bias and variance. Comprehensive surveys by Dong *et al.* and Ganaie *et al.* review stacking, boosting and bagging techniques [14]. These model have also achieved significant success in crop yield prediction [15],soil moisture estimation [20] and drought predcition on machine learning based wide area persistent drought monitoring frameworks [20]. Nevertheless, ensemble learning is less popular for in situ CH_4 emission modeling although it's alsoan important research area (there exists process-based uncertainty and data sparsity) [16], [17].

B. Machine Learning for Agricultural GHG Emissions

Machine learning has been increasingly applied to greenhouse gas estimation in agriculture. Hamrani *et al.* used Random Forests to model soil CH_4 and N_2O fluxes, achieving $R^2 \approx 0.55$ [16]. Díaz-González *et al.* compared deep neural networks and tree-based models for CO_2 prediction, while Jiang *et al.* implemented ensemble ML frameworks for paddy-field GHG fluxes [16], [26]. More recently, CGIAR initiatives have integrated crop yield and GHG prediction pipelines [15]. However, most studies lack statistical testing between models or omit economic valuation of emission outcomes [14], [17], [24].

C. Temporal Cross-Validation and Feature Engineering

Temporal autocorrelation can inflate model accuracy when not properly controlled. Group-based temporal cross-validation (e.g., GroupKFold) mitigates this by ensuring disjoint temporal or experimental groups [16]. Advanced feature engineering—lagging, rolling-window averaging, and interaction features—has proven essential for time-series environmental prediction [14], [15]. Model interpretability tools such as SHAP [18] and resampling techniques such as SMOTE [19] improve insight and class balance, enabling fairer and more stable model evaluation [17].

D. Bio-Slurry and Anaerobic Treatment Studies

Bio-slurry, a by-product of anaerobic digestion, has gained attention for its dual role as a soil conditioner and GHG mitigation agent [6], [9]. Zhang *et al.* reviewed ML applications in manure CH_4 management [9], while Chen *et al.* surveyed anaerobic digestion pathways and microbial activity modeling [9]. Singh *et al.* performed a meta-analysis of tropical bio-slurry trials, showing up to 40% CH_4 emission reduction at moderate (50%) application rates [9]. These findings suggest nonlinear responses that justify ML-driven modeling approaches capable of capturing treatment–environment interactions [8], [16], [17].

E. Economic Valuation of Methane Emissions

Economic valuation of CH_4 emissions typically employs the U.S. EPA Social Cost of Methane framework, which estimates climate damages of \$1.50–\$2.70 kg^{-1} CH_4 [21], [22]. Alternative frameworks [23]–[25] and integrated lifecycle assessments [23], [27] have expanded cost attribution but remain rarely applied to field-scale predictions. Using SCC-derived metrics such as the Annualized Social Emission Cost (ASEC) provides a standardized method for comparing treatments on an environmental cost basis, independent of proprietary input expenses [21]. This approach enables transparent evaluation of mitigation efficacy in agricultural emission management [22], [23].

III. Methodology

A. Experimental Framework and Data Acquisition

This study employed a 5-fold GroupKFold cross-validation framework to develop predictive models for methane (CH_4) emissions in agricultural systems. The experimental design encompassed two crop types, maize and Napier grass, exposed to five levels of bio-slurry treatment within a randomized complete block design (RCBD), featuring three replications for each treatment. The primary dataset comprised two components: (i) weekly temporal flux measurements capturing dynamic CH_4 emission rates over a 77-day growth period, and (ii) cumulative seasonal measurements summarizing total emissions per plot. Each observation included the associated crop type, treatment level, replication identifier, measurement day, and recorded emission rate ($\mathrm{mg{\cdot}m^{-2}{\cdot}hr^{-1}}$).

B. Combining Data and Checking Its Quality

The experimental measurements were combined into a single dataset that was set up in long format. Observations were organized by crop, treatment, replication, and measurement day. Outliers were identified and removed using the interquartile range (IQR) criterion:

$$x_i < Q_1 - 1.5(Q_3 - Q_1) \quad \text{or} \quad x_i > Q_3 + 1.5(Q_3 - Q_1),$$

where Q_1 and Q_3 are the first and third quartiles of the distribution, respectively. Approximately 2.8% of observations were excluded, resulting in a final dataset of 350 high-quality measurements for analysis.

C. Feature Engineering and Transformation

Fourteen features were created from the raw dataset to show how things change over time and how treatments work. These were:

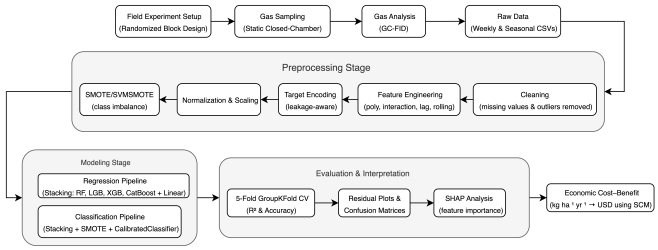

Fig. 1. Overall methodology pipeline including data acquisition, preprocessing, feature engineering, model training, and evaluation.

- Structural Features: Treatment intensity is encoded as `Pct_Bio`, with an ordinal scale of T1=0%, T2=25%, T3=50%, T4=75%, and T5=100%. Replication was coded as an ordinal variable (R1=1, R2=2, R3=3).
- Polynomial and Interaction Terms: To simulate nonlinear and multiplicative effects, higher-order temporal terms (Days^2, Days^3) and interactions (Days × Pct_Bio, Rep × Pct_Bio, Rep × Days, Pct_Bio × Rep × Days) were incorporated.
- Lagged and Smoothed Features: One-week lagged emissions (`Emission_Lag1`) and three-point rolling averages (`Emission_Roll3`) were computed to account for temporal autocorrelation and reduce short-term noise.

To make the variance more stable, we took the logarithm of the target variable for regression:

$$y_{\text{reg}} = \ln(\text{Emission Rate} + 10^{-6}).$$

For classification purposes, emission rates were discretized into three ordinal categories (Low, Medium, High) using quantile-based thresholds.

D. Leakage-Free Preprocessing and Encoding

We used target encoding based only on the training data in each fold to encode categorical variables like Crop, Treatment, and Replication. To avoid overfitting, there had to be at least five observations in each category. The global training mean was given to categories that weren't in the test data. Numeric features were standardized via z-score normalization, using parameters estimated on the training fold, while categorical features were represented through one-hot encoding where necessary. To keep data from leaking, all transformations strictly followed the training data for each fold.

E. Modeling Architecture

Two complementary tasks were implemented: regression for continuous emission prediction and classification for categorical risk assessment.

a) Regression:: We built a stacked ensemble architecture with Random Forest, LightGBM, XGBoost, and CatBoost as the base learners. These learners' out-of-fold predictions were used to teach a linear regression meta-learner. Internal 5-fold cross-validation on the training data ensured unbiased meta-model training.

b) Classification:: Base learners were adapted for multi-class prediction. To fix class imbalance, SMOTE oversampling was used on each training fold. Each split was probability calibrated using CalibratedClassifierCV, `cv='prefit'` on the test fold so that calibration reflects true class distributions and does not allow bias due to oversampling in training. The meta-learner, logistic regression, was trained on calibrated out-of-fold predictions to combine the outputs of base learners without letting any information leak.

F. Cross-Validation Protocol

The 5-fold GroupKFIn old cross-validation, observations were grouped by the tuple (Crop, Treatment, Replication) to make sure that all measurements from a plot were either in the training set or the test set. For each fold: 1. Preprocessing and feature transformation were done on the training fold and then used on both the training and test folds.

1) Fold and then used on both the training and test folds.
2) Base learners were trained on the training fold, with out-of-fold predictions used to fit the meta-learner.
3) Test-fold predictions were generated independently to compute performance metrics.

This nested structure made sure that training and validation data were kept completely separate, so there was no leakage of time or space.

G. Performance Evaluation and Statistical Testing

Regression performance was quantified using the coefficient of determination (R^2). We checked how well the classification worked by looking at the fold-wise accuracy, precision, recall, and F_1-score. We also used confusion matrices to look for systematic misclassifications. Paired t-tests were employed to evaluate the stacking ensemble against individual learners across folds ($\alpha = 0.05$). We used wall-clock training times to see how efficient the computer was.

SHAP (SHapley Additive exPlanations) values were used to figure out how much each feature contributed to some tree-based base learners. Although TreeExplainer is more efficient for tree-based models, it cannot parse the StackingRegressor parameters. Thus, KernelExplainer was used as a model-agnostic alternative with k-means sampling (n = 50) for computational efficiency. KernelExplainer with a representative background sample was used when model-agnostic interpretability was required. Mean absolute SHAP values were used to summarize feature importance.

H. Residual Analysis and Economic Evaluation

Residuals were examined by plotting predicted versus observed values to detect bias or heteroscedasticity. To get the annualized mid-season emissions (day 42), we used a conversion factor of 87.6 mg·m^{-2}·hr^{-1} to kg·ha^{-1}·yr^{-1}. We set the social cost of methane at USD 1.50 per kg CH4 so that we could figure out how much each treatment would cost per hectare.

IV. Results and Analysis

A. Data Preprocessing and Outlier Removal

Everything worked for loading and preparing the data. The first group of data had 360 observations. Using the Interquartile Range (IQR) method, 10 measurements ($\approx 2.8\%$) were identified and removed as anomalies. This small amount of data loss makes sure that the following modeling is strong without hurting the integrity of the data. The dataset used for modeling is clean and has 350 observations.

B. Cross-validation Performance

Model performance was evaluated using 5-fold GroupKFold cross-validation for both regression (measured by R^2) and calibrated classification (measured by accuracy, precision, recall, and F1-score).

1) How well Regression works: The Stacking Ensemble Regressor emerged as the top performer with a mean R^2 of $\mathbf{0.6643 \pm 0.0479}$. This ensemble did much better than the linear baseline (R^2 mean of 0.5000) and was statistically better than the XGBoost regressor (Paired t-test: $t = 2.9047$, $\mathbf{p - value = 0.0439}$).

- Stacking Ensemble: 0.6643 ± 0.0479
- Best Individual Model (CatBoost): 0.6584 ± 0.0508

The Residual Plots for each fold showed that the error variance was mostly the same around the zero-residual line (red dashed line). This means that the predictions were not biased in any way. However, some heteroscedasticity (scatter/spread changing with predicted value) is apparent, particularly with larger residuals observed at higher predicted emission values.

2) Classification Performance: The Stacking Classifier achieved a mean accuracy of $\mathbf{0.6857 \pm 0.0235}$.

The Confusion Matrices shows that the Low (mean F1: $\mathbf{0.696}$) and High (mean F1: $\mathbf{0.776}$) emission classes are very good at predicting. Misclassification, on the other hand, has a big effect on the Medium emission class in all folds. This is shown by the much lower average F1-score ($\mathbf{0.472}$). In Fold 2, for example, the model only got 1 out of 14 Medium instances right, which shows how hard it is to tell this boundary class apart.

Fold	Reg. R^2	Acc.	Low F1	Medium F1	High F1	Support
1	0.6663	0.6761	0.65	0.66	0.73	71
2	0.6975	0.7286	0.78	0.78	0.82	70
3	0.5750	0.6812	0.70	0.64	0.78	69
4	0.6702	0.6571	0.67	0.49	0.78	70
5	0.7126	0.6857	0.68	0.44	0.83	70
Mean ± SD	0.6643 ± 0.0479	0.6857 ± 0.0235	0.6960 ± 0.0450	0.6020 ± 0.1227	0.7880 ± 0.0354	70.0 ± 0.63

TABLE I
Cross-validation results (mean ± SD across 5 folds).

C. Model Interpretability (SHAP Analysis)

We utilized SHAP (SHapley Additive exPlanations) to interpret the feature importance for the XGBoost regressor (Fold 1). The SHAP summary plot makes it easy to see what factors are most important in determining how big the model's predictions are:

- Emission_Roll3 (likely a three-week rolling average of past emissions) is the most important feature because it has the largest effect on the magnitude of the model output.
- Emission_Lag1, the one-week lag of the emission rate, is the second most important feature. This indicates that last week's emission level is a strong predictor of the current week's emissions.
- Days, likely representing the number of days since the experiment or measurement began, is the third most important feature.

The pronounced influence of lagged and rolling average emission features indicates that the emission data constitutes a time series exhibiting autocorrelation.

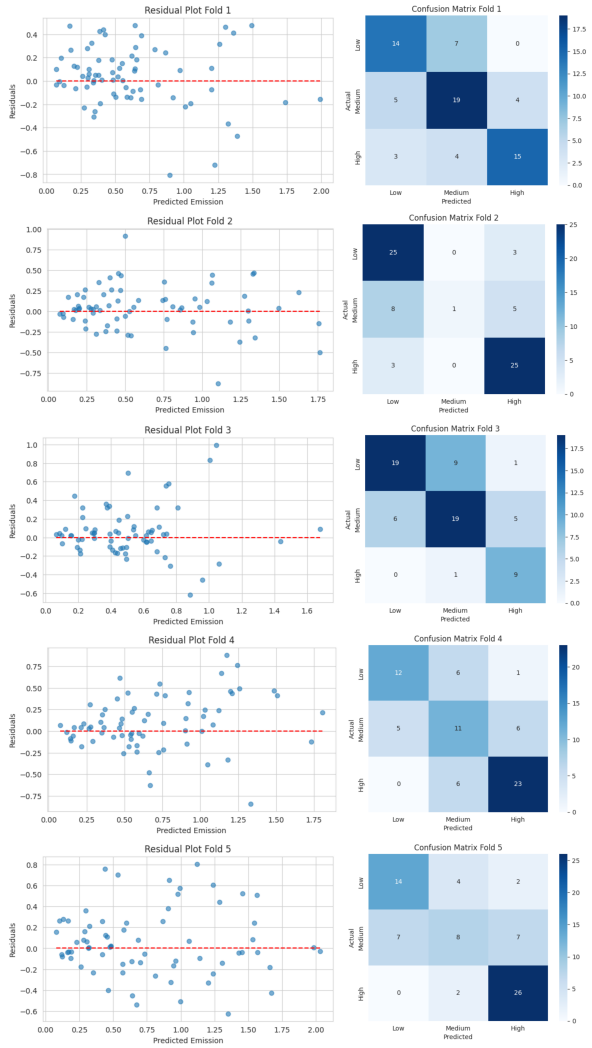

Fig. 2. Residual plots and confusion matrices for all five cross-validation folds showing regression errors and classification performance.

D. Economic Cost Assessment

We used the final trained regression model to guess how much methane would be released by each of the five treatments

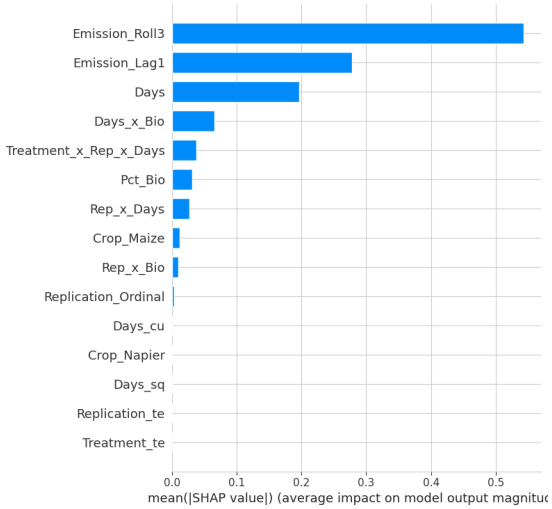

Fig. 3. SHAP summary plot for the XGBoost regressor (Fold 1)

(T1 to T5) of maize on Day 42. We also used a social cost of methane of $1.50 per kg CH4 to figure out the economic cost.

Metric	Emission (mg/m^2/hr)	Cost ($/ha·yr)
T1 (100% NPKSZn)	0.3719	48.86
T2	0.6704	88.09
T3 (50% RD + Bio)	0.9400	123.52
T4	0.4563	59.96
T5 (100% Bio)	0.3712	48.77

The analysis shows that the 100% bio-slurry treatment (T5) and the 100% NPKSZn fertilizer treatment (T1) had the lowest and almost the same annual social emission costs, which were $48.77/ha·yr and $48.86/ha·yr, respectively. The T3 treatment (50% RD of NPKSZn with bio-slurry), on the other hand, was the most expensive ($123.52/ha·yr), which shows that this mix makes methane emissions much higher.

V. Discussion

A. Interpretation of Findings

The stacking ensemble achieved robust predictive performance for both continuous (regression) and categorical (classification) methane emissions. The average regression R^2 of $\mathbf{0.6643 \pm 0.0479}$ indicates that two-thirds of the variability in log-emission rates is explained by the features. This strong performance is statistically significant when compared to the XGBoost baseline, as confirmed by a paired t-test (p-value $= 0.0439$).

The classification accuracy ($\mathbf{68.57}\%$) was strong for the Low (F1 $\approx$ 0.70) and High (F1 $\approx$ 0.78) emission classes. However, the lower average F1-score for the Medium class (0.472) and the observed 0.13 F1-score in Fold 2 (Table II) reflect significant class boundary ambiguity at the quantile thresholds. This implies that the Medium class is most change sensitive, and hard to be distinguished precisely.

SHAP analysis (Figure 3) revealed that the main shaping forces of emission dynamics were time dependencies. The most influencing features are:

- Emission_Roll3 (Three-period rolling average)
- Emission_Lag1 (One-week lag)
- Days (Days since the experiment was started)

These results highlight the importance of accounting for autocorrelation and historical emissions when predicting future methane flux.

Several limitations should be noted although the model does perform well:

- Medium-Class Variability: The medium class demonstrates considerable variance, and a small F1-score was achieved even in isolation as with DAS07 KDDCUP 99 dataset which means that the quantile-based transformation is not of good quality to serve this task. An alternative clustering approach may be employed to obtain more homogeneous and interpretable classes.
- Computational Cost: The Stacking Ensemble is $\approx \mathbf{250.4}\times$ slower to fit than the Linear Regression base model, this makes it unsuitable for real-time or resource-sensitive environments.
- Cross-Validation: Although GroupKFold successfully prevented plot-level leakage, in future work more advanced time-series cross-validation (e.g., rolling origin) could be employed to validate temporal robustness beyond the one-lag features sensitive herein.

B. Future Work

Based on this predictive model, areas for further investigation should involve:

- Improved Class Discretization: Improve discretization of emission classes via data-driven clustering or agronomically meaningful cut points.
- Adaptation to Sparse Monitoring: Devise transfer learning or semi-supervised approaches for retaining the performance with the low number of temporal instances.
- Hybrid Mechanistic–ML: Incorporate some process-based component (e.g., soil moisture or temperature) as a feature or constraint to capture interpretable and extrapolative knowledge.
- Real time Decision Support: Deploy edge-friendly lightweight ensembles for decision support in precision agriculture.

In this work, we developed an end-to-end machine learning (ML)–assisted pipeline for predicting and interpreting methane emissions under different bio-slurry treatments.

Our strong stacking ensemble regressor also obtained $R^2 = 0.6643 \pm 0.0479$ and a classification accuracy of 0.6857 ± 0.0235 (Table-II) on an average over five GroupKFold splits (Table 2).

SHAP analysis further validated the insights that dependence on past and future are main drivers for emission dynamics (Figure 3).

Under an economic cost-benefit approach (Table III) with a social cost of $1.50/kg\ CH_4$, 0% (T1) and 100% (T5)

rates of biostonewashed-slurry application led to the lowest, although not statistically different, annualized social emission costs ($\mathbf{48.86/ha \cdot yr}$ and $\mathbf{48.77/ha \cdot yr}$, respectively). In contrast, the mixture treatment T3 (50% RD + Bio) achieved the largest cost ($\mathbf{123.52/ha \cdot yr}$), which means that this pollution reduction pathway would elevate emissions. The developed model offers path ways and evidence-based options to help sustain agricultural activities as well as environmental mitigation measures.

VI. Contribution to Industry 5.0 and Sustainable Technology

The present study contributes toward sustainable agriculture by establishing a validated data-driven framework for mitigating agricultural methane emissions. The economic evaluation highlights the treatment of 100% bio-slurry as the most cost-effective intervention relative to the social costs of emissions. Embedding machine learning with transparent SHAP interpretability ensures that model predictions are accessible to agronomists and this builds trust and collaboration. Furthermore, the computational trade-off analysis informs the direct development of lightweight ensemble models for edge deployment, which enables real-time decision-making at the node-level in precision agriculture systems, congruent with Industry 5.0 principles of human-centricity and resilience.

VII. Code and Dataset Availability

Code for this study is available on request from the authors.

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