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mLDNDCv1.0: A Machine Learning-based Surrogate of LandscapeDNDC for Optimising Cropping Systems in Denmark

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Abstract

Optimising Danish arable management is critical for reducing greenhouse-gas (GHG) emissions and nitrogen (N) losses while maintaining or even improving crop productivity and soil health. Process-based models such as LandscapeDNDC can simulate the effects of management on agroecosystem functioning. However, their computational demand limits large-scale optimisation. Here we present mLDNDCv1.0, a tree-based machine-learning surrogate of LandscapeDNDC that allows for the rapid exploration of large decision spaces without sacrificing mechanistic fidelity. We generated a synthetic training set of >45 million LandscapeDNDC simulations from a full factorial of soils, climate (2011-2020), and management options for winter wheat. We benchmarked gradient-boosted tree algorithms (LightGBM, XGBoost, CatBoost) on predictive performance. XGBoost delivered the most accurate and stable predictions for the core indicators in this study: soil N_2O emissions (R^2 = 0.81), NO_3^- leaching (R^2 = 0.84), yield (R^2 = 0.93), and for soil-organic-carbon stock changes (R^2 = 0.86). The model maintained high accuracy when confronted with real management and environmental settings that reflected true operating conditions. Coupling mLDNDC with the multi-objective evolutionary algorithm NSGA-II allowed us to optimise millions of management combinations across all winter wheat fields in Denmark. Pareto-optimal solutions reduced N_2O emissions by 27.5 ± 4.5 %, NO_3^- and leaching by 27 ± 3.0 %. These solutions also increased grain yield by 8.5 ± 1.5 % and soil-organic-carbon stocks by 1.2 ± 0.1 %, and improving nitrogen-use efficiency (NUE) by 10 ± 2 %, while turning the system into a net GHG sink (2200 ± 400 Mg CO_2-eq ha^{-1} yr^{-1}). These gains were achieved without increasing total fertiliser input. They arose from re-allocating mineral and organic fertliser N input, adjusting incorporation depth, and optimising residue, catch-crop, and irrigation practices. Thus, mLDNDC therefore provides a scalable, transparent framework for country-wide optimisation and real-time decision support in climate-smart agriculture.

1. Introduction

Optimising cropping systems is critical for increasing agricultural productivity while reducing environmental impacts. Agriculture accounts for 20–25 percent of global anthropogenic greenhouse gas (GHG) emissions and is a major driver of climate change (Vermeulen et al., 2012). In Denmark, where agriculture covers more than 55% of the total land area (Hansen et al., 2025), improving management practices is both necessary and urgent. The Danish agricultural sector plays a central role in national food, yet it is also responsible for about 23% of national greenhouse gas emissions (Nielsen et al., 2020), while being a major contributor to nutrient runoff and land-use pressures (Pugliese et al.,

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2023). As global demand for food continues to rise, Danish agriculture faces the dual challenge of sustaining high yields while meeting environmental and climate commitments.

Without optimisation, farming systems risk becoming inefficient and environmentally unsustainable (Wezel et al., 2020). Variability in soil conditions, weather patterns, and management intensity often leads to uneven resource use and suboptimal productivity (Abdu et al., 2023). Moreover, climate change is intensifying these challenges by altering growing conditions and increasing the frequency of extreme events such as droughts and floods **(Baker & Anttila-Hughes, 2020)**. This makes it increasingly important to identify management strategies that can maintain productivity, enhance resilience, and reduce environmental footprints.

For exploratory scenario testing, process-based models (PBMs) such as LandscapeDNDC (LDNDC) (Haas et al., 2013) — remain the tools of choice. PBMs represent the biophysical and biogeochemical processes that regulate crop growth, soil dynamics, water balance, and nutrient cycling (Zhang et al., 2022). By explicitly simulating interactions among crops, soils, and the atmosphere, they improve system understanding, challenge theoretical assumptions, and predict responses to management or climate drivers (Jeong et al., 2020). When run across diverse environments, PBMs quantify trade-offs among yield, nitrogen losses, GHG emissions, and soil-carbon dynamics, thereby providing a science-based foundation for sustainability assessments (Shi et al., 2025).

Yet the same mechanistic richness that gives PBMs their credibility also makes them computationally heavy, especially when thousands of management permutations must be tested at national scale (Lu et al., 2019). Machine-learning (ML) methods can overcome the runtime barrier, but, when used in isolation, they lack an intrinsic grasp of soil–plant–atmosphere processes. Merging ML with PBMs therefore offers an attractive compromise of process realism with substantial speed-ups (Droutsas et al., 2022). One promising avenue is surrogate (or meta-) modelling, in which an ML algorithm is trained on PBM outputs, and subsequently emulates the PBM at a fraction of the computational cost (Aderele et al., 2025).

Surrogate techniques are now being increasingly adopted across agri-environmental sciences (e.g., Aderele et al., 2025). Applications include predicting crop yield (Nguyen et al., 2019; Shahhosseini et al., 2019), gaseous-nitrogen fluxes such as nitrous oxide (N_2O) and ammonia (NH_3) (Perlman et al., 2014; Villa-Vialaneix et al., 2012), assessing nitrate-leaching (Piñeros Garcet et al., 2006), studying the terrestrial carbon-cycle (Luo et al., 2011; Xiao et al., 2022), investigating crop physiology and water dynamics (Attia et al., 2022), or grasslands (Pylianidis et al., 2022). However, these efforts have largely focused on field or landscape-scale applications and often target single sustainability indicators.

To date, no study has carried out a nationwide optimisation of agriculture that simultaneously considers yield, nitrous oxide (N_2O) emissions, nitrate (NO_3^-) leaching, and soil organic carbon (SOC) dynamics. Building on this gap, the present work addresses two questions: (i) can a functional machine learning–based surrogate model be developed for LandscapeDNDC, and (ii) can such surrogates be used to optimise Danish agriculture at national scale in a way that reduces environmental impacts while enhancing productivity and soil health, without compromising scientific rigour? Danish agriculture is used as a case study due to data availability, while the methodology is general and can be applied to other countries, continents, or even global-scale analyses. Filling these gaps demands both an accurate biogeochemical representation and an optimisation engine capable of searching a vast management decision space.

Exploratory scenario applications, where a range of management options are defined and simulated using PBMs, remain an interesting and potentially useful option (Aderele et al., 2025). While informative, such “fixed-scenario” approaches restrict discovery to strategies already envisioned. Search-based optimisation, by contrast, defines broad decision boundaries and allows an algorithm to find novel solutions within them. This paradigm has been applied to climate-smart crop production elsewhere (Xiao et al., 2024) and is adopted here.

Coupling an evolutionary optimiser with a PBM such as LandscapeDNDC would require thousands to millions of simulations, rendering the process impractical. Therefore we introduce mLDNDC, a machine-learning surrogate of LandscapeDNDC that preserves mechanistic fidelity while reducing computation

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time. mLDNDC allows for the thorough exploration of management options and, when paired with an optimiser, can identify strategies that improve productivity, resilience and environmental sustainability. This study showcases mLDNDC application to winter wheat, the most widely grown and economically important cereal in Denmark (Barua et al., 2014), accounting for over 23% of the cropping area, and demonstrate its use in optimising management under contemporary Danish conditions. The analysis tracks four core outputs: N_2O emissions, NO_3^- leaching, grain yield, and SOC change. Together, these variables capture the essential balance between productivity and environmental impact, forming the basis of our optimisation exercise.

2. Methods

This study was conducted through four main stages, summarized in Figure 1. The workflow comprised (i) Synthetic data generation for winter wheat at field level in Denmark, (ii) Simulation using LandscapeDNDC, (iii) Training of machine learning models on the synthetic input–output datasets produced by LandscapeDNDC, and (iv) Optimization, where the trained surrogate model was applied to achieve the study objectives.

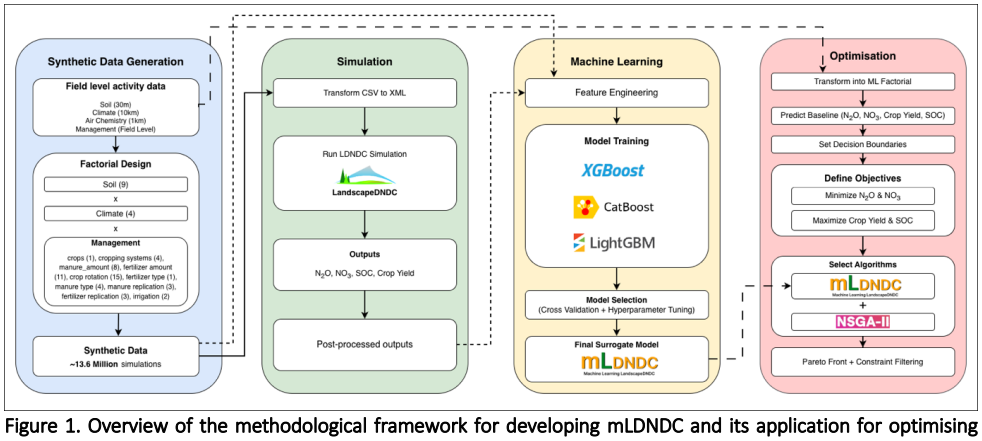

Figure 1. Overview of the methodological framework for developing mLDNDC and its application for optimising cropping systems in Denmark.

2.1. Synthetic Data Generation

Developing a robust surrogate model demands a dataset that goes beyond what is available from field observations. Although empirical data is valuable, it only covers a narrow slice of the management practices currently used, missing much of the plausible decision space needed for trade-off analysis and optimisation. We bridge this gap by creating a synthetic dataset that combines observed and hypothetical management scenarios. This broader coverage enables the surrogate model to generalise beyond management boundaries of current management practices.

The construction of the dataset involved two steps. First, we defined plausible ranges for numeric predictors (e.g., fertiliser amount) and alternative possibilities for categorical (e.g., fertiliser type) options for all key management variables, drawing on field-level records and agronomic knowledge. Second, we varied these variables within their agronomic limits using a full factorial design to generate a large set of unique management combinations that represent both current practice and potential future strategies.

2.1.1. Field Level Activity Data

We used the harmonized field-level data from the SmartField project to drive the process-based model representing Danish agriculture. This dataset was developed to generate the Tier-3 GHG emission inventory (Rahimi et al., in preparation) and the dataset was used as baseline to represent variations in

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crop sequences and rotations and management practices (e.g., fertilisation, irrigation, tillage, cover cropping, and residue management).

The dataset is based on information on crop types and cropland boundaries available at field scale from 2011 to 2020 from the General Farm Register (Rolighed, 2023), combined with total amounts of synthetic (e.g., ammonium-based inputs) and organic (e.g., livestock slurry) fertilizers reported at the farm scale. The fertiliser inputs were distributed to fields within each farm based on the allowed rates for specific crop and soil types defined by the Danish AgriFish Agency to fulfill national regulations (Dalgaard et al., 2014).

Management boundaries were identified to represent the observed range of current agricultural practices in Denmark. These boundaries served as reference points for defining the limits of each management variable. A management library was then constructed, encapsulating all possible combinations of these management parameters for further use in the factorial design stage.

2.1.2. Factorial Design

The factorial design was developed to generate a comprehensive and representative set of synthetic management scenarios. This was accomplished by systematically combining soil, climate, crop management, and fertilisation.

Soil (9 levels): Soil properties, including texture, soil organic carbon (SOC) and bulk density (BD), were extracted as geospatial raster layers at 30.4 m resolution for five standard depth intervals (0–5, 5–15, 15–30, 30–60 and 60–100 cm). Soil pH for the same depths was obtained from a separate dataset at 100 m resolution. Saturated hydraulic conductivity (Ks) was derived using a pedotransfer function based on relevant soil attributes (Rahimi et al., 2024). The soil classes used for factorial design was derived from a 30 m resolution national soil map classified according to the Jordbær soil classification system in Denmark (Figure S.2). This classification system resulted in 9 distinct soil classes that represent the dominant soil types in Danish agricultural landscapes.

Climate (4 levels): Climate data, including (daily mean air temperature, global radiation, and precipitation) were obtained from the Danish Meteorological Institute (DMI) at a spatial resolution of 10 km (https://www.dmi.dk/). The DMI IDs were categorized into 4 climate zones based on the De Martonne aridity index (Figure S.3), capturing the spatial variability of moisture availability and its potential impact on crop growth and soil processes (e.g., potential evapotranspiration). To simulate the synthetic dataset, one DMI ID was randomly selected from each class. For atmospheric N deposition, regional-scale outputs from the atmospheric chemical transport model, the Danish Eulerian Hemispheric Model (Rahimi et al., 2024), were used to provide nitrogen deposition inputs for our model. For simulation purposes, the air-chemistry inputs were taken from the same randomly selected DMI ID.

Cropping Systems (4 levels): Cropping systems were adapted from Aderele et al. (2025) and represent different combinations of crop residue and catch crop management. Four distinct categories were defined: (i) complete residue removal without a catch crop, (ii) complete residue retention with a catch crop, (iii) complete residue removal with a catch crop, and (iv) complete residue retention without a catch crop. For all cropping systems, tillage was carried out five days before crop establishment to prepare the seedbed. These combinations capture the most relevant residue–catch crop interactions observed in Danish agricultural systems.

Fertilization amount (11×8 levels): Synthetic fertilizer application rates were defined in 30 kg N ha^{-1} increments from 0 to 330 kg N ha^{-1}, resulting in 11 levels. Organic fertilizer application rates followed a similar structure, ranging from 0 to 240 kg N ha^{-1} in 30 kg intervals, resulting in 8 levels. The upper bounds for both fertilizer types were intentionally set higher than the maximum levels typically observed in national practice to allow simulations beyond the baseline and support optimisation and sensitivity analyses.

Fertilization type (1x4 levels): Ammonium nitrate (NH_4NO_3-) was selected as the sole synthetic fertilizer type as it accounts for dominant share of the total synthetic fertilisers used in Denmark. Four organic fertilizer types were considered: compost, farmyard manure, slurry (injected), and slurry (surface applied).

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Fertilization splits (3x3 levels): Both synthetic and organic fertilization were represented by three application-frequency levels (one to three applications per growing season). For each synthetic scenario, the corresponding organic scenario was combined to create realistic split combinations. To ensure realistic application timing, data from the Danish catchments from the National Monitoring Program for Water Environment and Nature, NOVANA (LOOP-program; In Danish: Landovervågningsprogrammet) was used for the timing and per-split rates. One matching field-year was randomly selected from this dataset for each synthetic management record. For example, if a winter wheat scenario in 2017 required one organic split and two synthetic splits, a field-year with the same split structure (1 organic + 2 synthetic) would be randomly selected from the dataset and its observed timing and per-application rate pattern would be adopted. This approach preserves realistic within-season fertilization schedules while allowing for the systematic exploration of total N levels.

Crop Rotation (15 levels): Crop rotations were defined using a two-year rotation system that precede the main crop, winter wheat. Five primary crop categories were considered: cereals, legumes, leafy crops, root crops, and grasses. Combining these categories across two preceding years produced 15 unique rotation types, ensuring a broad range of agronomic sequences was represented (Figure S.4).

Irrigation (2 levels): We represented irrigation as a binary factor (irrigated vs. non-irrigated), and triggered applications based on crop water demand. This was preferred to dynamically calculating irrigation needs according to climate x management interactions to reduce the number of factorial scenarios and its computational demand both for LDNDC and ML.

Although a factorial design is comprehensive by nature, it can generate unrealistic or inconsistent combinations. For example, very high fertilization levels may not be agronomically plausible when represented with a single split as e.g. certain synthetic–organic pairings can produce excessively high total N inputs. When amount of organic fertilizer is zero, the "type" of an organic fertilizer is not meaningful. Therefore, the synthetic dataset was systematically screened and cleaned using rule-based plausibility checks to eliminate such combinations and ensure that the remaining scenarios reflect realistic and interpretable management configurations.

2.2. Simulation With LandscapeDNDC

The synthetic data generation process produced approximately 13.6 million rows, which were subsequently reduced to about 4.5 million rows per simulation year during preprocessing (Table S.3). This yielded a total of about 45 million rows spanning the ten-year period from 2011 to 2020. These rows served as the input dataset for the simulation stage. All simulations were performed using the LandscapeDNDC.

2.2.1. Process-based Model Description

LandscapeDNDC (LDNDC) is a process-based framework that simulates the coupled cycles of carbon, nitrogen, and water cycles in cropland, grassland, and forest systems (Haas et al., 2013). It links five core modules: (i) PlaMo^{x} for crop growth (Kraus et al., 2016; Liebermann et al., 2019); (ii) CanopyECM for micro-climate processes (Grote et al., 2009); (iii) WatercycleDNDC for soil water and hydrology (Kiese et al., 2011); (iv) AirchemistryDNDC for atmospheric chemistry; and (v) MeTr^{x} for soil biogeochemistry (Kraus et al., 2015).

The model has been applied and tested in a range of contexts. Across Europe, Haas et al. (2022) explored long-term residue-management effects on soil organic carbon (SOC) and N_2O emissions. Kraus et al. (2022) validated national-scale simulations in the Philippines for alternate wetting and drying in rice systems, while Smerald et al. (2023) used LDNDC to examine global nitrogen-redistribution options for closing yield gaps with minimal environmental damage.

For its application in Danish conditions, LDNDC has undergone detailed calibration and testing. Kollmer (2023) calibrated plant-physiological and soil parameters using data from the long-term Askov experiment and successfully reproduced the observed SOC accumulation in dependence of different field management regimes. Grados et al. (2024) compared modelled N_2O fluxes with field measurements from the Foulum and reported a standardised RMSE of 2.03 g N_2O-N ha^{-1} d^{-1}. Rahimi et al. (2024) evaluated LDNDC across the six LOOP catchments in Denmark and achieved an overall R^2 of 0.77 for yield predictions. The present study adopts the same parameter bounds and input settings as

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used in the listed studies. Finally, Aderele et al. (2025) assessed twelve alternative Danish cropping regimes combining fertiliser, residue, and catch-crop strategies. They analysed trade-offs among GHG emissions, nitrogen leaching, SOC changes, and yield.

Given the extensive international and Danish level validation, LDNDC provides a robust, well-tested foundation for the surrogate-modelling work carried out here.

2.2.1. Process-based Model Simulation

The simulations covered the period from 2011–2020 and focused on winter wheat. Next, we converted the generated synthetic management scenarios (Section 2.1.2) to LDNDC data requirements in Extensive Markup Language (XML). We took planting dates, harvest dates, and fertiliser schedules from the field-level activity dataset described in Section 2.1.1, so that model settings would reflect typical Danish practices across the main cropping regions. Every synthetic management combination from the factorial design was run as a separate LDNDC job. To manage the large workload, we used an HPC cluster, launching 40 parallel tasks, each with one (CPU cores each, 600 GB shared memory). With this setup the full batch finished in roughly seven days; running on a desktop machine would have taken several weeks.

LDNDC was configured for daily time steps, but the simulations were run at subdaily intervals, generating outputs for N_2O emissions, NO_3^- leaching, grain yield, and changes in soil organic carbon (SOC).

2.3. Machine Learning

2.3.1. Feature Engineering

Developing the surrogate model required a comprehensive set of predictor variables capturing the key biophysical, climatic, and management processes that regulate crop performance, nitrogen dynamics, and soil-carbon outcomes. These features were derived from LDNDC simulations and combined with processed soil and climate data. They were engineered to represent both long-term system characteristics and short-term, management-sensitive drivers.

Management practices: One primary management variable, additional feature such as total nitrogen input, was calculated by summing all mineral fertiliser nitrogen and manure nitrogen applied within a given year; this measure represents the total nitrogen supply entering the cropping system and is a critical determinant of crop productivity, nitrate leaching, and nitrous oxide emissions. To capture nonlinear response behaviour associated with nitrogen inputs, a squared term or second order polynomial of total nitrogen and each manure and synthetic fertiliser inputs were also included as an additional feature **(Sutton & Matheus, 1991)**.

Climate: To characterise rainfall patterns, we constructed a rainfall-frequency indicator by counting the number of days per year with measurable precipitation. This captures moisture intermittency which strongly influences soil mineralisation, denitrification, and crop-growth cycles. A suite of additional climate variables were engineered to capture both seasonal and crop-stage specific conditions, including annual precipitation, total precipitation during the crop's growing season, and seasonal precipitation for autumn, winter, and spring; equivalent temperature metrics—mean annual temperature and mean temperatures for the growing season and each major season—were generated to reflect the climatic environment governing crop development, soil biological activity, and nitrogen turnover.

Short-term climate effects: Short-term hydrological conditions surrounding nutrient applications were incorporated through event-based precipitation indicators that quantify accumulated rainfall in the seven days preceding each fertiliser and manure application. We also included rainfall in the three days following each application to capture conditions that influence nitrogen-loss pathways such as volatilisation, rapid infiltration, or surface runoff. These pathways are known to affect both nitrate leaching and nitrous oxide emissions.

Soil: We constructed soil features by aggregating the properties of the upper three soil layers (0-20cm depth), which represent the active root zone most relevant for crop growth and nutrient cycling. We calculated the mean values of field capacity, wilting point, sand, silt, and clay fractions, organic carbon, organic nitrogen, pH, bulk density, and saturated hydraulic conductivity for each field. These aggregated

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variables provide a representative profile of the soil's physical and biogeochemical characteristics to be used in the surrogate model.

Target variables: The target variables were transformed prior to training recognising that variable transformation is a well-established strategy for improving the performance of supervised-learning models when target variables are highly skewed or exhibit heteroscedasticity. Nitrous oxide emissions, nitrate leaching, and crop yield were log-transformed to address strong skewness.Soil-organic-carbon change was transformed using the Yeo–Johnson power-transformation method (Weisberg, 2001) to accommodate both positive and negative values, .

The full list of features used for the model training can be found in Table S.4.

2.3.1. Model training

2.3.1.1. Benchmarking

The dataset was split into two parts: 80 % used for model training, and the remaining 20 % was withheld for an independent test of generalisation performance. This ratio is widely adopted in machine-learning practice because it balances the data available for learning with the need for reliable evaluation (Kuhn & Johnson, 2013).

To identify the most suitable surrogate model for the target variables agro-ecosystem indicators, three gradient-boosting decision-tree algorithms (Section S.1) were benchmarked: LightGBM, XGBoost, and CatBoost. Light Gradient Boosting Machine (LightGBM; Ke et al., 2017) accelerates training via histogram-based splits and leaf-wise growth; Extreme Gradient Boosting (XGBoost; Chen & Guestrin, 2016) adds regularisation, parallel execution, and efficient sparse-matrix handling; and CatBoost (Prokhorenkova et al., 2017) employs ordered boosting with target statistics to mitigate overfitting and handle categorical inputs. First, each candidate model was initially trained using its default hyperparameters (Table S.1), and baseline performance was evaluated on the test set. Based on this initial comparison, the best-performing algorithm was selected and subsequently subjected to intensive hyperparameter tuning combined with further cross-validation. This staged workflow avoids unnecessary optimisation of weaker candidates and substantially reduces computational cost while maintaining methodological rigour in model selection and evaluation.

2.3.1.2. Hyperparameter Tuning

Hyper-parameter optimisation was carried out with Optuna (Akiba et al., 2019), which uses a Tree-structured Parzen Estimator (TPE) Bayesian-optimisation engine coupled with early-stopping "pruners" to traverse the search space efficiently. The objective function minimised the validation error, and wall-clock time was kept in check by running each trial on a random 1 % subsample of the training data to reduce the tuning time and computational requirements. This choice follows the findings of Kapoor and Amazon (2021), who showed that tuning on as little as 1 % of a large dataset yields validation-metric differences below 0.5% relative to tuning on the full dataset.

Once the hyperparameter search converged, the selected configuration was used to train the selected model using five-fold cross-validation on the full dataset. The data were randomly shuffled and partitioned into five equally sized folds; in each iteration, four folds were used for training and the remaining fold served as validation. This procedure ensured that every observation contributed to both model fitting and validation, providing robust estimates of predictive performance. Reported performance metrics were derived from the cross-validation results.

After confirming stable performance across folds, the final surrogate model was trained on the complete dataset using the optimised hyperparameters. This final refit maximised the use of available information and produced the mLDNDC model used for downstream large-scale prediction and management optimisation. This is consistent with standard practice when the objective is the operational deployment of a single, fully trained model (Hastie etal.,2009).

2.3.1.3. Model Explanation

To interpret the relative influence of management and environmental variables on each agro-ecosystem indicator, we computed SHapley Additive exPlanations (SHAP) values for the optimised XGBoost models. Using TreeSHAP (Lundberg & Lee, 2017), each prediction was decomposed into additive feature attributions whose magnitudes indicate the strength of the effect and whose signs

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indicate the direction (positive or negative) of the contribution, thereby offering a consistent, locally accurate measure of variable importance across the entire dataset.

2.3.1.4. Model Validation

To ensure the generalizability and external validity of the surrogate model, an independent validation was performed using data not involved in model training or simulation by LandscapeDNDC. For this purpose, national-scale crop yield data obtained from the National Statistics Denmark were employed as an external benchmark. This dataset represents real-world observations across diverse management and environmental conditions, providing a robust basis for evaluating model transferability beyond the simulation domain.

2.4. Optimisation

2.4.1. Decision Boundaries

The optimization process was constrained within predefined decision boundaries, representing the range of controllable management variables. These boundaries define the feasible search space for identifying optimal agroecosystem management strategies.

Specifically, the manure application rate was varied from 0 to 210 kg N ha^{-1}, and the synthetic fertilizer rate ranged from 0 to 300 kg N ha^{-1}. These ranges were selected to encompass the typical and extreme management practices observed in Danish cropping systems while ensuring agronomic plausibility.

Categorical management factors, as described in Section 2.1.2, were also included in the optimization search space. These comprised crop rotation, cropping systems, synthetic fertilizer types, manure types, replication schemes (for both manure and synthetic fertilizer, showing how many times they were applied), irrigation, and manure depth. Optimizing these continuous and categorical decision variables allows the optimization framework to capture a broad spectrum of feasible management combinations aimed that balance productivity and environmental outcomes.

The optimisation was conducted at the individual winter wheat field level across Denmark using national inventory data, with results subsequently aggregated to a 10 km × 10 km grid to facilitate spatial visualisation. Accordingly, the baseline represents the current, field-specific management practices and associated outcomes under current farming conditions.

2.4.2. Objectives

The optimization problem was formulated as a multi-objective task aimed at simultaneously improving environmental and agronomic outcomes. Specifically, the objectives were to minimize N_2O emissions and NO_3^- leaching, while maximizing crop yield and SOC change.

These four objectives collectively represent the key dimensions of sustainable agricultural management, enhancing productivity while mitigating greenhouse gas emissions and nutrient losses The formulation can be expressed as:

$$\text{Minimize } (f1, f2) = (N_2\text{O emissions}, \text{N}O_3 - \text{ leaching})$$

$$\text{Maximize } (f3, f4) = (\text{Crop yield}, \text{SOC change})$$

There is no explicit weighting scheme applied to the target variables; in the current setup, none of the objectives is prioritized over the others, so N_2O, NO_3-, yield, and annual SOC are all treated equally.

The multi-objective optimization was conducted under the decision boundaries defined in Section 2.4.1, allowing the identification of Pareto-optimal solutions that represent trade-offs between environmental protection and agricultural productivity.

2.4.3. Optimisation Algorithm

The Non-dominated Sorting Genetic Algorithm II (NSGA-II) (Deb et al., 2002) was employed to solve the multi-objective optimization problem. NSGA-II is a widely adopted evolutionary algorithm designed for identifying Pareto-optimal solutions in problems with conflicting objectives. It maintains population diversity through a crowding distance mechanism and ensures computational efficiency via fast non-dominated sorting.

The implementation was carried out in Python using the pymoo optimization framework **(Blank & Deb, 2020)**. Each generation of the algorithm evolved candidate management strategies through processes of selection, crossover, and mutation, iteratively improving the trade-offs between environmental and productivity objectives. The algorithm efficiently explored the multi-dimensional decision space defined in Section 2.4.1, identifying optimal combinations of manure rate, fertilizer rate, and other categorical

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management variables that balanced N_2O emissions, NO_3^- leaching, crop yield, and SOC change. At the end of the optimization, the pareto front is returned which is the top 50 management practices that fulfils our objectives for a specific field.

2.4.4. Constraint Based Filtering

After generating the Pareto-optimal solutions for each field, a constraint-based filtering step was applied to identify management strategies that are both environmentally beneficial and agronomically feasible. Two sets of constraints were used in this study.

The first ensured that any selected management strategy outperformed the field's current baseline. Specifically, an optimised solution was retained only if it produced lower nitrous oxide emissions and lower nitrate leaching, while achieving a higher crop yield and greater soil organic carbon content than the baseline management for that field. This requirement ensured that the recommended solutions would deliver clear improvements in all key sustainability indicators rather than merely shifting environmental.

The second constraint addressed regional manure-use feasibility. To reflect realistic resource availability, the total manure applied in any optimised solution was required to remain at or below the total manure availability for the corresponding NUTS2 region in Denmark. This ensured that the optimisation results did not rely on manure inputs that exceed what is currently accessible within regional nutrient cycling systems.

These constraints guaranteed that the final set of optimised management strategies were both environmentally superior and grounded in practical resource limitations, thereby increasing the likelihood of real-world applicability and policy relevance.

2.5. Performance evaluation

Model performance was evaluated using the coefficient of determination (R^2) and the root mean square error (RMSE) to quantify both predictive accuracy and the magnitude of prediction error. It should be noted that this assessment was conducted in two phases, each of which aligned with the conceptual distinction between the possibility space and the actual space of management practices.

The first phase (possibility space) measured training accuracy by evaluating the model on the same synthetic dataset used for model development. This dataset represents the "possibility space", which encompasses the full range of management combinations that could theoretically occur. The aim was to determine how well the model captures relationships within this synthetic generated domain.

The second phase (actual space) measured validation accuracy using an independent dataset derived from reported national field management records for winter wheat. This dataset reflects the "actual space" i.e., the management practices that have been implemented under real-world conditions, and all the necessary response variables for this dataset were produced through LDNDC simulations. Consequently, this phase provides a more realistic test of the model's generalizability, since it evaluates performance under the management strategies that occur in practice rather than only in theory.

2.6. GHG Balance Calculation

The soil net greenhouse gas (GHG) balance was estimated to evaluate the overall climate impact of the baseline and optimised cropping system. The balance was calculated as the difference between soil organic carbon (SOC)–derived CO_2 sequestration and the sum of direct and indirect N_2O emissions, expressed on a CO_2-equivalent (CO_2equ) basis. A negative GHG balance indicates that the cropping system acts as a net sink of GHGs (i.e., net CO_2 removal). This approach allows for integrating changes in soil carbon storage with gaseous emissions to provide a comprehensive measure of the system's overall climate performance.

3. Results & Discussion

3.1. Model Performance

Table 1 summarises the predictive performance of the three tree-based models evaluated in this study and shows that all models achieved generally acceptable accuracy across the target variables. However, XGBoost and LightGBM consistently outperformed CatBoost, exhibiting higher coefficients of determination and lower error metrics. Although XGBoost and LightGBM achieved very similar

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predictive performance across all target variables, XGBoost was selected as the final model due to its substantially faster inference time. On average, XGBoost required approximately three minutes to generate predictions for all four variables, whereas LightGBM required nearly one hour to produce the same outputs under identical computational conditions. This difference in inference efficiency is critical given the scale of simulations in this study involving millions of management combinations and the need for timely generation of management scenario outcomes. The markedly lower inference cost makes XGBoost cheaper to deploy at scale and thus more suitable as a surrogate model within computationally intensive optimisation loops.

Table 1. Performance of CatBoost, XGBoost, and LightGBM across possibility and actual spaces

Variable	Model	R^2 (possibility)	R^2 (actual)	RMSE (possibility)	RMSE (actual)
N_2O (kg N ha^{-1})	CatBoost	0.73	0.63	0.59	0.39
	XGBoost	**0.81**	**0.70**	**0.50**	**0.35**
	LightGBM	0.81	0.71	0.49	0.35
NO_3- (kg N ha^{-1})	CatBoost	0.75	0.69	23.83	12.67
	XGBoost	**0.84**	**0.80**	**19.22**	**10.20**
	LightGBM	0.83	0.78	19.66	10.53
Yield (kg DM ha^{-1})	CatBoost	0.91	0.90	723.87	696.89
	XGBoost	**0.93**	**0.92**	**626.70**	**594.68**
	LightGBM	0.95	0.95	543.86	495.85
SOC (kg C ha^{-1})	CatBoost	0.79	0.66	359.94	341.33
	XGBoost	**0.86**	**0.76**	**288.72**	**286.76**
	LightGBM	0.86	0.74	293.30	299.39

Note: "Possibility space" refers to model evaluation on the synthetic dataset, and "actual space" refers to evaluation on an independent dataset that reflects real-world conditions.

Figure 2 (A & B) complements the quantitative metrics reported in Table 1 by providing a diagnostic comparison of predicted versus simulated values for all target variables across the three tree-based models. The scatter density plots show a strong alignment along the 1:1 line for yield and soil organic carbon, indicating stable predictions across the full value range. For nitrous oxide emissions and nitrate leaching, a wider dispersion is observed, particularly at higher values, reflecting the greater intrinsic variability of these processes and the presence of episodic extremes. Nevertheless, no pronounced systematic over or underestimation is evident, and prediction errors remain broadly symmetric.

A) Possibility Space

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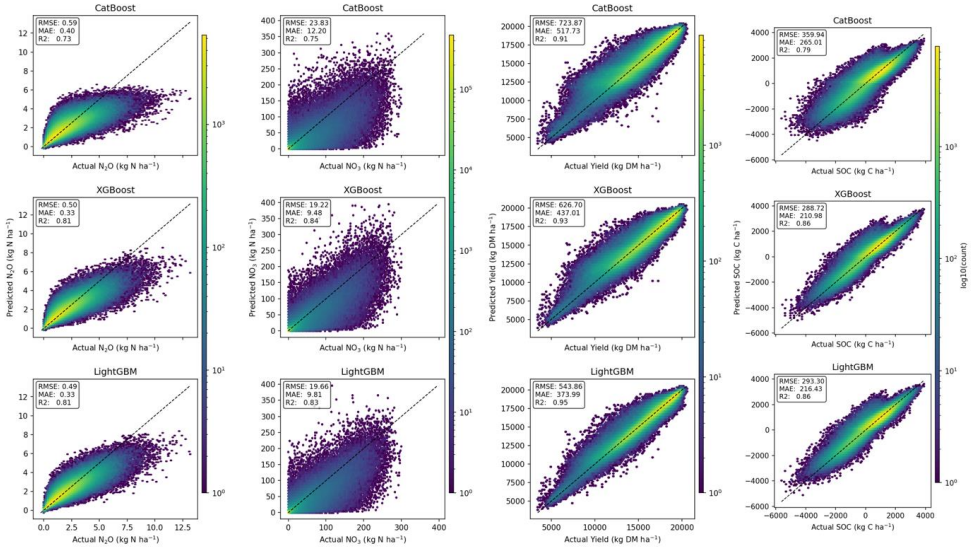

B) Actual Space

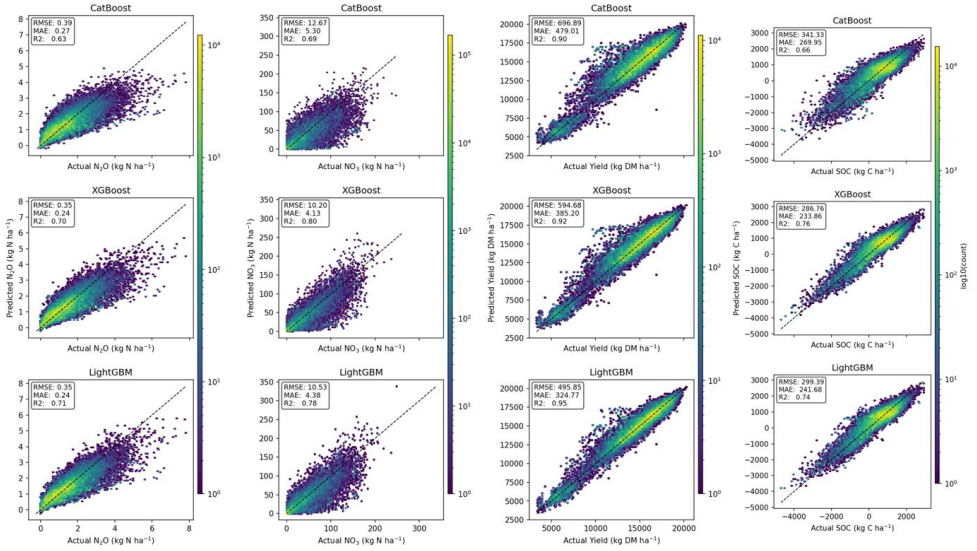

Figure 2. Performance metrics for CatBoost, XGBoost, and LightGBM across the four predicted variables (N_2O, NO_3^-, SOC, and yield). Panel A shows RMSE, MAE, and R^2 in the possibility space, and Panel B shows the corresponding metrics in the actual space.

Figure 3 presents the cross-validation results, indicating an extremely narrow range between the mean and standard deviation of the cross-validated R^2 values. This shows a consistent performance across folds, suggesting minimal overfitting and strong generalization capacity. When model predictions on national data were compared to Denmark national yield data for Winter Wheat from Statistics Denmark (https://www.dst.dk), the fully trained XGBoost model achieved a R^2 of 0.77 against the national yield data as shown in Figure S.1, indicating strong agreement between model predictions and independent observations. This level of performance demonstrates that the model capture´s key biophysical processes and its potential applicability for large-scale agroecosystem assessments.

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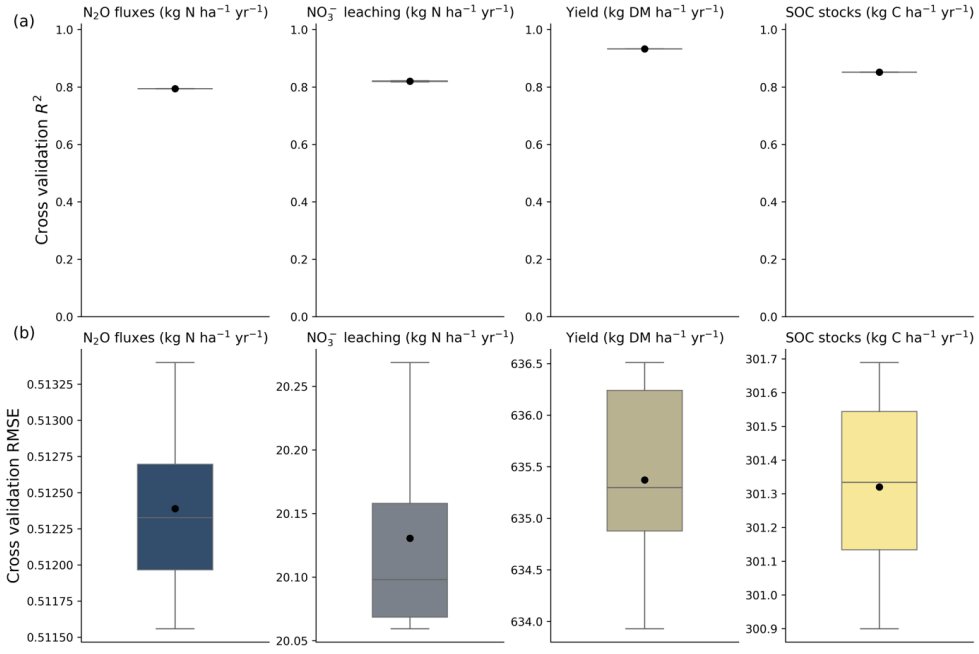

Figure 3. Stability of R^2 across 5-fold cross validation for N_2O, NO_3^-, yield, and SOC. It illustrates the variability and consistency of model performance within each fold, providing insight into the robustness and generalizability of the selected model across different subsets of the data. We highlight how in (b) the variability is artificial due to the extremely small variation (e.g., 0.51150 and 0.51325 kg N-N_2O ha^{-1} yr^{-1}).

An important highlight in the development of mLDNDC is the importance of incorporating seasonal climate descriptors and detailed soil variables into the feature set. Although the surrogate model produces annual predictions, several of the target variables, particularly nitrous oxide emissions, operate at much finer temporal scales and are strongly shaped by short term environmental fluctuations and episodic "hot moments". Without information that captures seasonal temperature and precipitation dynamics, as well as conditions immediately surrounding nutrient applications, the model was unable to fully represent the drivers of these sub-annual processes. Early versions of the model relied primarily on soil texture classes alongside a limited selection of soil physical and chemical properties. Under this simplified representation, the surrogate achieved moderate performance, with R^2 values of approximately 0.64 for N_2O emissions, 0.70 for nitrate leaching, 0.88 for yield, and 0.65 for soil organic carbon. When the feature set was expanded to include seasonal precipitation and temperature patterns, climatic conditions during the crop growth period, and rainfall events before and after fertiliser and manure applications, along with key soil variables such as available carbon, soil nitrogen concentration, field capacity, wilting point, bulk density, and pH; the performance improved substantially. The corresponding R^2 values increased to 0.81, 0.84, 0.93, and 0.86 for N_2O, NO_3^-, yield, and SOC respectively. These improvements reinforce the well-established understanding that soil nitrogen availability, soil carbon content, moisture status, aeration, temperature, and pH jointly regulate nitrogen cycling processes and N_2O production. This has been consistently reported in the literature, including (C. Wang et al., 2021), that highlight the strong direct and indirect influence of soil carbon, soil nitrogen concentration, soil moisture, temperature, and pH on N_2O emissions.

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Another important finding to consider with respect to feature engineering is that response variable transformation to deal with heteroscedasticity improved model performance. For gradient-boosted decision trees, stabilising the distribution of the response variable enhances model performance because the underlying optimisation uses a stage-wise additive framework that is sensitive to the scale and variance of residuals. (Friedman, 2001), who introduced gradient boosting, emphasised that reducing skewness and variance asymmetry in the target variable improves the convergence and stability of boosted models. **(Kuhn & Johnson, 2013)** similarly showed that transformations improve predictive accuracy by reducing the influence of extreme values and enabling tree-based models to make more effective splits. A more recent study by (Karwowska et al., 2025) show that data transformation can address data challenges in machine learning tasks.

The enhanced performance of mLDNDC after integrating these variables demonstrates that surrogate models can successfully capture the sensitivity of nitrogen and carbon processes to dynamic environmental conditions when provided with appropriately engineered features.

It is also important to note that neural networks were explored during the early stages of model development, but their performance was consistently poor across both the training and validation phases making them excluded from this study. This behaviour is consistent with observations in the broader machine learning literature, where conventional feed forward neural networks often struggle with tabular datasets, particularly when the underlying relationships are non-sequential and dominated by heterogeneous feature interactions rather than spatial or temporal dependency structures **(Borisov et al., 2024; Shwartz-Ziv & Armon, 2022)**. Deep learning architectures such as Long Short-Term Memory network (LSTM), Gated Recurrent Unit (GRU), and Transformers typically offer advantages when modelling sequential or high dimensional unstructured data, which was not the case in this study. In contrast, tree-based ensemble methods such as XGBoost are well known for their superior performance on structured agricultural and environmental datasets, which likely explains their substantial advantage in the present application.

3.2. Model Interpretation Using SHAP

To interpret the associations and interactions underlying the model predictions for each target variable, we computed SHAP values for samples drawn randomly from synthetic observations (Figure 4). The SHAP summary plots show the relative importance, intensity of influence, and model response on feature magnitude by showing the distribution of SHAP values for each feature across all samples. We interpret these results primarily as model-based associations inferred from the data, not as causal mechanisms. However, consistent and agronomically plausible SHAP patterns can be suggestive of underlying causal relationships and thus serve as a structured basis for formulating causal hypotheses.

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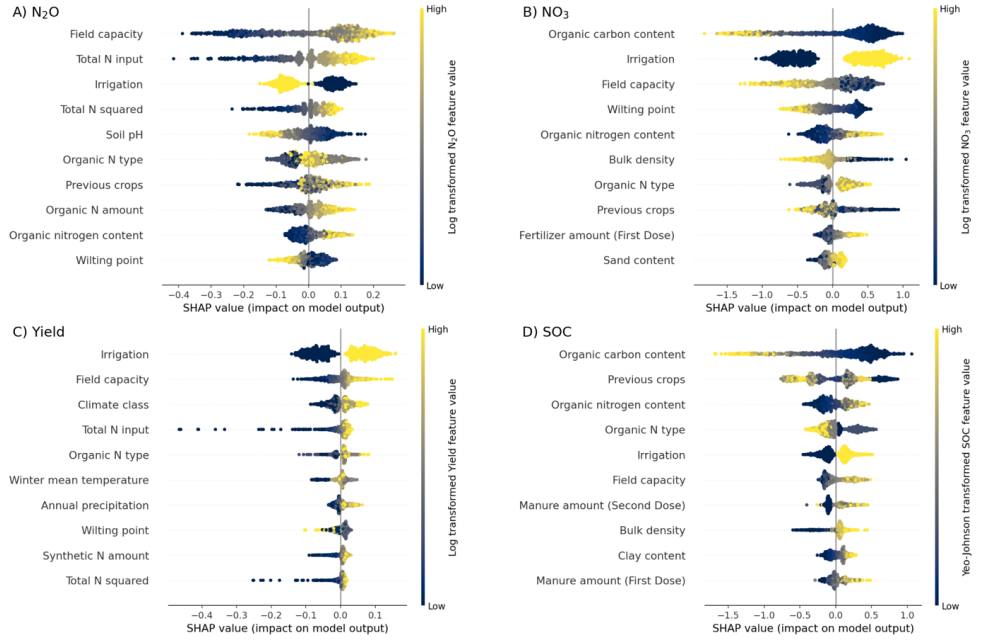

Figure 4. SHapley Additive exPlanations (SHAP) values of the four predicted variables (N_2O, NO_3^-, Crop Yield & SOC). The vertical position of a feature reflects its overall importance, while the horizontal spread and colour show the direction and strength of its effect across all observations.

Below we highlight the five key drivers per SHAP analysis for each one of the target variables:

N_2O. The five most influential predictors of N_2O emissions are field capacity, total N input (represented by both linear and squared terms to reflect the nonlinear increase in emissions at higher nitrogen application levels), irrigation, soil pH, and type of organic (e.g., slurry, farmyard manure).

Soils with high water holding capacity tend to have higher predicted N_2O emissions, as indicated by positive SHAP values. This is consistent with the central role of soil moisture in regulating nitrification and denitrification via controlling soil oxygen diffusion and redox conditions. N_2O fluxes increase as water-filled pore space approaches field capacity (Ciarlo et al., 2006; Diba et al., 2011). At this point, anaerobic microsites become more frequent but complete reduction to N_2 is still limited (Ciarlo et al., 2006).Total N input and its squared term show that higher fertiliser N rates significantly increase predicted N_2O emissions. The squared term captures the well-known non-linear, accelerating response of N_2O emissions to N addition. Global meta-analyses report that N_2O emissions rise disproportionately at high N rates, with emission factors increasing when fertiliser inputs exceed crop demand (Maaz et al., 2021; Shcherbak et al., 2014). Therefore, the model behaviour aligns with the established understanding that efficient N management is critical for N_2O mitigation.

Interestingly, Irrigation, encoded as a binary factor, shows that irrigated sites (high feature value) tend to have negative SHAP values, implying lower predicted N_2O emissions than non-irrigated sites. Many experiments report increased N_2O under excessive wetting, especially when soils remain close to saturation **(Huang & Gerber, 2015)**. However, there is also evidence that controlled irrigation around field capacity can suppress denitrification and N_2O emissions compared to extremes of very dry or very wet conditions, particularly in drip-irrigated systems where water is applied in small doses (Zhang et al., 2024).

Soil pH is strongly negatively associated with N_2O emissions: higher pH values produce negative SHAP values, indicating reduced predicted emissions. This aligns with experimental and meta-analytic evidence that liming acidic soils enhances the activity of N_2O reductase and shifts denitrification end-

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products from N_2O to N_2, reducing total N_2O emissions (Hénault et al., 2019; Y. Wang et al., 2021; Žurovec et al., 2021).

Organic N type, a categorical variable describing the form of organic fertiliser, also ranks among the leading predictors. Some organic N types are associated with positive SHAP values (higher N_2O), while others are associated with negative SHAP values. This is in line with comparative studies that show different fertiliser forms and C:N ratios alter N turnover and gaseous losses (Yao et al., 2022).

NO_3^- leaching. The dominant predictors of NO_3^- leaching are organic carbon content, irrigation, field capacity, wilting point, and organic N content. Low soil organic carbon content corresponds to positive SHAP values and higher predicted NO_3^- leaching losses, whereas high organic carbon content tends to reduce leaching. This agrees with experimental studies showing that increased soil organic matter can enhance microbial immobilisation of nitrate and improve soil structure, thereby reducing leaching losses (Malcolm et al., 2019).

The capacity to irrigate is strongly positively associated with NO_3^- leaching, with irrigated fields showing large positive SHAP values. Global meta-analyses of irrigated systems demonstrate that nitrate leaching risk is inherently high when water inputs exceed crop demand, and that both irrigation amount and timing are key determinants of leaching losses (Quemada et al., 2013). Thus, the model therefore captures the trade-off between yield benefits of irrigation and increased risk of leaching.

Both field capacity and wilting point, clearly demonstrates the effects of soil water holding properties and texture. Soils with low field capacity and low wilting point (i.e., coarse, free-draining soils) have positive SHAP values and higher predicted leaching. In contrast, finer textured soils with greater water holding ability tend to have lower NO_3^- losses. This is consistent with field and meta-analytic studies that link high leaching risks to sandy or structurally weak soils with poor water and nutrient retention, especially in areas of high rainfall or irrigation **(Pacheco & Sumreen Hina, 2024; Schuster et al., 2022)**.

Organic N content, representing the amount of organic N in the soil, is positively associated with NO_3^- leaching. High organic N content increases the pool of mineralisable N, which under moist conditions and sufficient aeration leads to increased nitrate formation and a larger leachable pool. Recent work has shown that soil C and N contents, and their ratios, are pivotal in regulating mineralisation, immobilisation, and nitrate availability (Kuśmierz et al., 2023; Ma et al., 2018).

Winter wheat yield. The five leading predictors of yield are irrigation, field capacity, climate class, total N input (including its squared term), and organic N type. Irrigation has large positive SHAP values when the field is irrigated, indicating substantial yield benefits relative to non-irrigated conditions. Meta-analyses of wheat production consistently show that well managed irrigation increases grain yield and water productivity compared to rainfed systems, especially in water-limited environments. Reported yield gains range from 10–30 percent depending on deficit level and environment (Li et al., 2022; Ren et al., 2025; Zhou et al., 2022). Therefore, the model performance is fully aligned with empirical evidence. Field capacity emerges as a critical soil property, with higher field capacity associated with positive SHAP values and higher predicted yields. Soils with greater plant-available water storage buffer crops against intra-seasonal drought, thereby stabilising and increasing yield. Recent analyses of long-term experiments and meta-studies on soil water storage(Lessmann et al., 2022; Slessarev et al., 2022) confirm that improved soil structure and water retention are strongly linked to wheat yield and stability. Climate class, which summarises the prevailing temperature and precipitation regime through aridity index classification, is also highly influential. This mirrors established knowledge that winter wheat yields in northern Europe are strongly constrained by temperature and water availability during critical growth stages, and that inter-annual climate variability is a major driver of yield variation.

Total N input, represented by both linear and squared terms, shows the expected yield response curve as moderate N rates increase predicted yield (positive SHAP values) while very high rates are associated with neutral or even negative contributions once the squared term dominates. Trials of yield response in Scandinavia including Denmark demonstrate that grain yield increases with N up to an economically optimal rate. Beyond this rate, additional N has little effect on yield but increases environmental losses (Styczen et al., 2020; Vogeler et al., 2022). The model captures this diminishing return and embeds it

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through the quadratic N term. In the case of Organic N type, the influence on the prediction is based on the different C:N ratios of the different organic manure applied.

Changes in soil organic carbon. The five most important predictors of SOC changes are initial organic carbon content, previous crops, organic nitrogen content, organic N type, and irrigation. The SHAP pattern for organic carbon content shows that soils with low initial SOC tend to have positive SHAP values, indicating a greater predicted SOC gain. In contrast, soils with high initial SOC often have negative contributions. This is consistent with recent global analyses demonstrating that SOC-poor soils generally exhibit higher sequestration potential and gain carbon more readily in response to improved management than SOC-rich soils, which are closer to saturation (Lessmann et al., 2022; Slessarev et al., 2022).

Previous crops, representing the two crops grown before winter wheat, have a strong effect on SOC. Long-term rotation experiments and recent global syntheses show that diversified rotations especially with legumes enhance SOC stocks and soil health relative to continuous cereal systems (Al-Musawi et al., 2025; Yang et al., 2024).

Organic nitrogen content, which reflects cumulative organic inputs and soil organic N, contributes positively to SOC predictions when high. This is consistent with evidence that increased organic inputs from manure, crop residues, or combined mineral-organic fertilisation increase soil C stocks while also supporting higher yields (Ma et al., 2018). The influence of organic N type is based on the C:N ratios of the applied manure.

Finally, there is positive relationship between irrigation and SOC. Irrigated sites showed higher predicted SOC than non-irrigated sites. Meta-analyses of irrigated agriculture indicate that irrigation generally increases SOC stocks, especially in surface soils, by promoting greater biomass production and residue return. However, the magnitude of this effect depends on climate and management practices(Antón et al., 2022; Emde et al., 2021; Sun et al., 2024). The SHAP result suggests that, in the Danish context considered here, irrigation contributes to higher SOC through enhanced primary productivity and associated organic input.

3.2. Baseline-to-Optimised Differences at the National Scale

3.2.1. Changes in N_2O Emissions, NO_3^- Leaching, Grain Yield, and SOC

Figure 5a illustrates the spatial distribution of the optimisation benefits for N_2O emissions across Denmark. Because the optimisation objective for both N_2O and NO_3^- is minimisation, the percentage changes shown on the map indicate the extent to which emissions can be reduced relative to the baseline (Figure S.6). Depending on their location within the 10 × 10 km grid, many grid cells across the country show reductions ranging from approximately 15 percent to more than 35 percent. Figure 5e's national-level summary further confirms this pattern. The N_2O emission bar indicates that an average reduction of about 26 percent can be achieved through optimised cropping system management.

Similarly, Figure 5b shows that nitrate leaching can also be substantially reduced. In some grid cells, reductions reach up to about 40 percent, while most areas show improvements of roughly 30 percent. The national aggregation in Figure 5e indicates an average reduction of approximately 27 percent. These reductions in both N_2O emissions and NO_3^- leaching is achieved without compromising yield or soil organic carbon, demonstrating the potential for environmentally beneficial optimisation of Danish cropping systems.

The optimization objective for yield and SOC is maximisation. The spatial pattern in Figure 5c reveals that crop yield can increase by up to 16 percent in some grid cells, with most areas showing improvements of around 10 percent. The national average, shown in Figure 5e, is approximately 8 percent. Importantly, these gains are achieved without increasing N_2O emissions or NO_3- leaching, indicating that higher productivity can coexist with reduced environmental impacts.

SOC shows a similar pattern of improvement. As illustrated in Figure 5d, SOC can be increased by up to 3 percent in some areas, with most regions showing increases of around 2 percent. The national mean, as reflected in Figure 5e, is about 1 percent, which is close to the noise level of measurement and should be interpreted as marginal improvements rather than large changes. Although this magnitude is smaller

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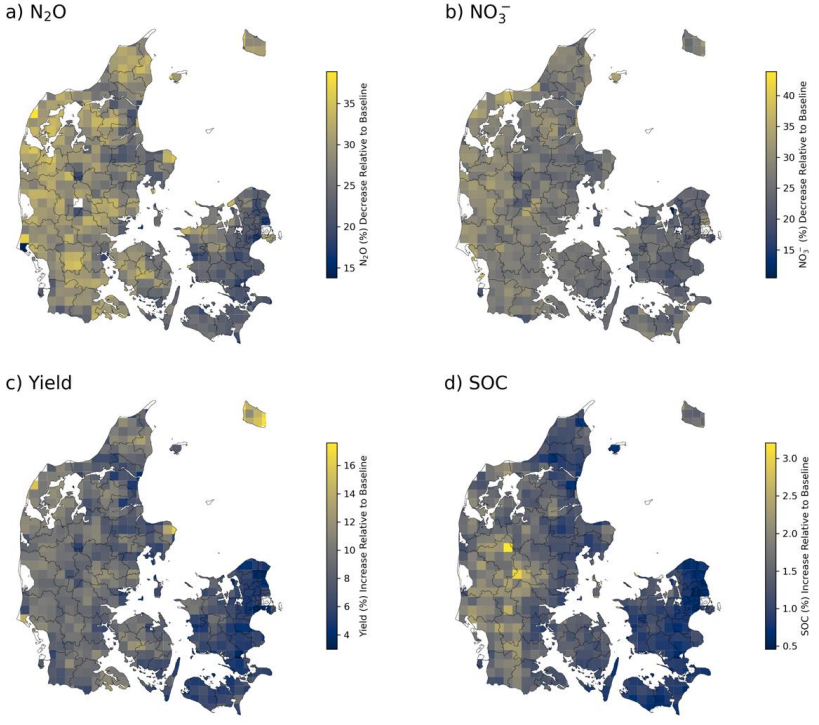
than the yield response, it represents a meaningful improvement given the slow dynamics of soil carbon accumulation.

These results demonstrate that optimised management strategies can simultaneously reduce N_2O emissions and NO_3^- leaching while enhancing crop yield and SOC. It further highlights the potential for integrated, multi-objective optimisation to support both environmental and agronomic goals within Danish cropping systems. The percentage of specific management changes in each 10 x 10km grid are shown in (Figure S.5)



e) National

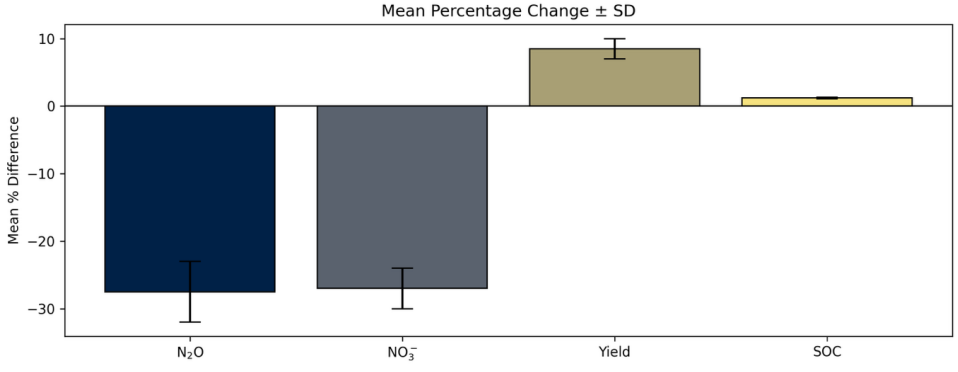


Figure 5. Panels (a–d) show the percentage difference between optimised management and the baseline scenario over the 10-year period from 2011 to 2020, aggregated to a 10 × 10 km grid, with decreases shown for N_2O emissions and NO_3^- leaching and increases shown for yield and soil organic carbon. Panel (e) presents the corresponding mean percentage change at the national scale.

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3.2.2 Nitrogen and Greenhouse Gas Performance Indicators

A) Nitrogen Use Efficiency

In addition to the environmental and productivity gains identified in the multi-objective optimisation, the results also demonstrate clear improvements in nitrogen use efficiency (NUE) defined as follows:

$$NUE = \frac{Y}{FN} * 100$$

where *Y* is the crop yield (kg N ha^{-1}), and *FN* is the amount of fertiliser nitrogen applied (kg N ha^{-1}).

As shown in Figure 6, optimised management strategies increase NUE across most regions of Denmark, with national level gains averaging approximately 10 percent relative to the baseline. This indicates that the optimised cropping systems can produce more yield per unit of nitrogen applied, reflecting more efficient nitrogen utilisation without increasing N_2O emissions or nitrate leaching. Such improvements in NUE align with the broader goals of enhancing nitrogen productivity while reducing surplus nitrogen in agricultural landscapes.

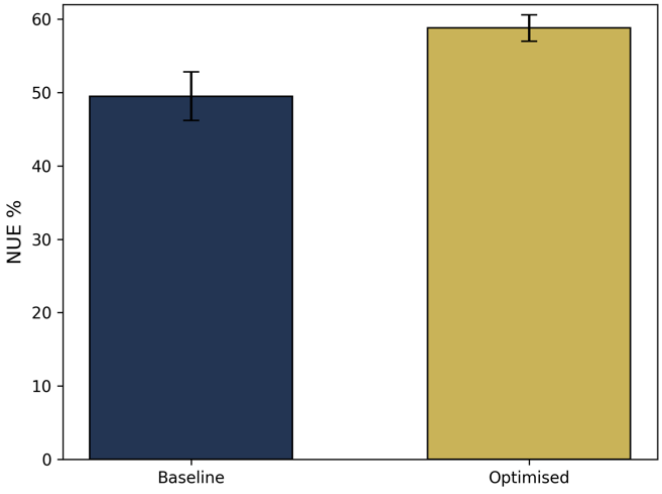

Figure 6. Nitrogen Use Efficiency of baseline and optimized management over 10 years (2011-2020).

B) Soil Net GHG Balance

Figure 7 compares the CO_2-equivalent (CO_2-eq) soil-net GHG balance of the baseline and optimised management scenarios over the 10-year period 2011–2020. The optimised scenario exhibits a substantially more negative CO_2-eq value than the baseline, indicating greater net climate benefits through enhanced carbon sequestration and reduced emissions. Moreover, the wider negative range shown by the error bar suggests that optimisation improves mitigation potential consistently across spatial and inter-annual variability over the 10-year period. Overall, the results demonstrate that systematically optimising management practices can meaningfully strengthen the climate mitigation capacity of Danish cropping systems.

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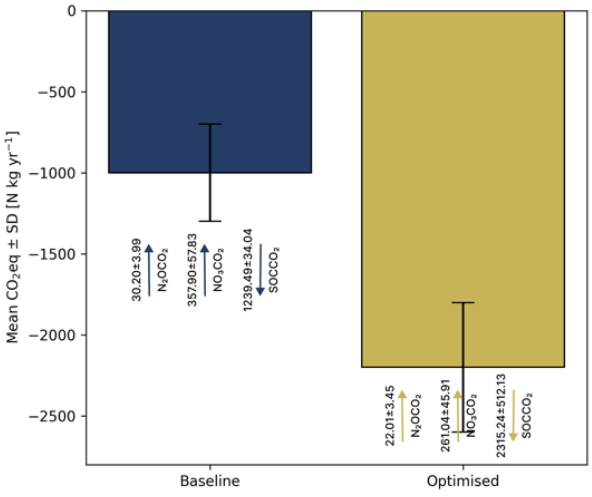

Figure 7. Soil-net GHG balance (Mg CO_2-eq ha^{-1} yr^{-1}) under baseline and optimised management scenarios, averaged over the 10-year period 2011–2020; negative values indicate greater net climate-mitigation potential.

C) Total N_2O and NO_3- per Nitrogen Yield

Figure 8 illustrates the relationship between total nitrogen exported as yield and the corresponding annual N_2O emissions and NO_3^- losses for both the baseline and optimised scenarios. The optimised management consistently shifts observations upward and to the right, indicating higher nitrogen export through increased yield while simultaneously reducing N_2O emissions and NO_3^- leaching relative to the baseline. This pattern shows that the optimised system achieves greater nitrogen productivity without incurring additional gaseous or leaching losses, demonstrating improved overall nitrogen stewardship in Danish cropping systems.

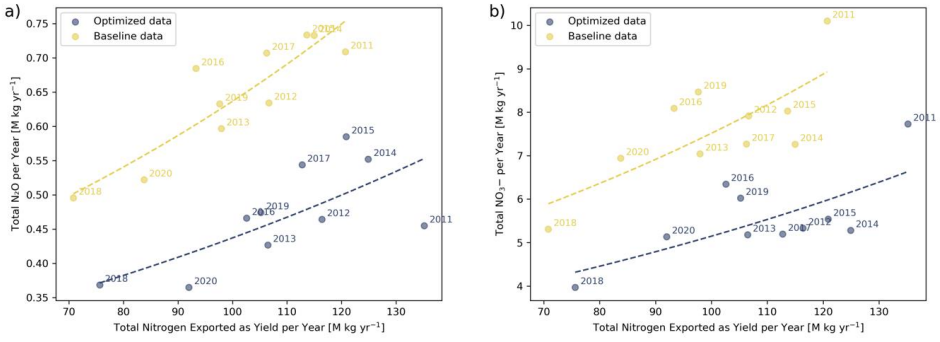

Figure 8. Total nitrogen exported as yield per year compared with (a) total N_2O emissions per year and (b) total NO_3^- leaching per year for baseline and optimised management.

4. Conclusion

The development of the surrogate model mLDNDC was motivated by the need for a computationally efficient alternative to full process-based simulations when conducting multi-objective optimisation at scale. While process-based models provide detailed mechanistic representations of agroecosystem dynamics, they remain computationally demanding when thousands of management scenarios must

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be evaluated repeatedly. mLDNDC preserves the core behavioural response of the LandscapeDNDC model while reducing runtime by several orders of magnitude. This computational gain enables optimisation across large spatial domains, allows the evaluation of a far broader range of management combinations, and supports systematic exploration of trade-offs and synergies among multiple environmental and productivity outcomes.

Importantly, the surrogate model does not replace the process-based model but supplements it by making national-scale optimisation feasible in practice. As a data-driven approximation, the surrogate can reliably predict only the outputs and objectives included in its training data. If additional objectives, such as new biogeochemical indicators or management goals, are introduced, the surrogate must be retrained using corresponding simulations from the process-based model. In contrast, process-based models explicitly simulate the underlying biophysical processes governing system behaviour. They embed mathematical representations of physical, chemical, and biological processes, including soil water dynamics, plant growth, nutrient cycling, and greenhouse gas fluxes. As a result, they generate intermediate state variables, such as microbial activity or nitrification and denitrification rates, that provide explanatory insight into system functioning beyond final outputs like yield or emissions (Kim et al., 2025). This fundamental difference in model design leads to distinct but complementary roles. Process-based models offer broad scope, interpretability, and flexibility, whereas surrogate models provide speed and scalability but limited process transparency.

This study was designed as a multi-objective optimisation experiment to assess whether agronomic management can simultaneously sustain high crop productivity while delivering substantial environmental co-benefits at national scale. The underlying premise is that sustainable arable systems must balance yield with reductions in greenhouse gas emissions, nitrogen losses, and soil degradation, rather than optimising any single outcome in isolation. A single-objective formulation, such as yield maximisation alone, would have obscured potential win-win solutions and provided limited insight into trade-offs or synergies among productivity, nitrogen use efficiency, and environmental performance relative to current practice in Denmark.

To the best of current knowledge, no previous study in Denmark has applied a standard multi-objective optimisation framework to crop management using a surrogate-based approach capable of evaluating thousands of spatially explicit management combinations. In contrast to studies based on a limited set of predefined scenarios, this work demonstrates that more balanced outcomes are achievable. The optimisation identified management strategies that reduced N_2O emissions by 27.5 ± 4.5 percent and NO_3^- leaching by 27 ± 3.0 percent, while simultaneously increasing grain yield by 8.5 ± 1.5 percent and soil organic carbon stocks by 1.2 ± 0.1 percent, alongside a 10 ± 2 percent improvement in nitrogen use efficiency. These improvements were achieved without increasing total fertiliser inputs. Instead, gains arose from reallocating mineral and organic nitrogen, adjusting incorporation depth, and optimising residue management, catch-crop use, and irrigation practices. Collectively, these changes shifted the system towards a substantially lower net greenhouse gas balance relative to current practices.

Despite its strengths, the surrogate modelling approach has limitations. Model performance depends on the breadth and quality of the synthetic training data generated from the process-based model, and gaps in the simulation design may reduce accuracy when the surrogate extrapolates beyond the training domain. In addition, the optimisation framework does not currently account for economic costs, labour availability, or machinery constraints, which are important determinants of real-world adoption. Incorporating these factors in future work would improve the practical relevance of the results. Furthermore, while the present study focuses on winter wheat systems, extending the surrogate framework to full crop rotations would provide a more comprehensive representation of Danish arable agriculture.

The development of mLDNDC also highlighted the importance of including detailed seasonal climate information and soil variables to faithfully replicate the behaviour of the full process-based model. The marked improvement in surrogate performance following the inclusion of these variables demonstrates that careful feature engineering is essential when using machine learning to emulate complex biogeochemical processes.

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Collectively, the results show that mLDNDC is an effective and computationally efficient tool for exploring management scenarios and supporting multi-objective optimisation at national scale. When coupled with appropriate decision-making frameworks, it offers substantial potential to inform policy development, advisory services, and strategic planning aimed at balancing agricultural productivity with environmental sustainability.

Several avenues for future research emerge from this work. Linking mLDNDC with socioeconomic and land-use models would enable assessment of national-scale policy interventions, including nitrogen quotas, carbon pricing mechanisms, fertiliser price changes, and incentives for manure redistribution. The computational efficiency of the surrogate makes it well suited for integration with economic optimisation or agent-based modelling frameworks to explore behavioural responses across farming systems. In addition, incorporating climate change scenarios would allow evaluation of the robustness of optimised management strategies under projected changes in temperature and precipitation, which is essential for designing resilient cropping systems.

Finally, the strong spatial heterogeneity observed in optimisation outcomes highlights the need for regionalised advisory tools and policy support. mLDNDC could serve as the computational core of interactive decision-support systems that provide grid-specific recommendations tailored to local soils, climate, and management histories. Overall, the methodological framework developed in this study provides a scalable and robust foundation for next-generation agricultural assessment and optimisation. With further integration of socioeconomic factors and climate projections, mLDNDC has the potential to support Denmark's transition toward climate-smart and resource-efficient agricultural systems.

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Code and data availability

The code used for training all machine learning models presented in this manuscript are publicly available on Zenodo at https://doi.org/10.5281/zenodo.18278474 (Aderele et al., 2026a). The datasets are publicly available on Zenodo at https://doi.org/10.5281/zenodo.18573225 (Aderele et al., 2026b)

Author Contribution

M.O.A and J.R. conceived and designed the study, prepared model input data, performed the analysis. M.O.A and J.R. wrote the first draft, while all co-authors (E.H., L.L., J.S., and K.B.B.) have contributed to improving the manuscript.

Competing Interests

The contact author has declared that none of the authors has any competing interests.

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