Integrating mathematical optimization to enhance sustainability in a crop and dairy production agent-based model for Luxembourg

Supporting Information 3: Mathematical optimization

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1. Mathematical optimization problem formulation

Linear programming is one of the main Operations Research techniques [1]. The model contains sets of linear equations and inequalities. There should be a linear objective function that is maximized or minimized. Each linear equation is normally subject to constraints and the formulation of a MOO problem (MOOP) is written as follows:

|  |  |
| --- | --- |
|  | (S3.1) |

where, in farming activities, *z1* can be the objective function for profit, *p* is the profit vector of different types of production and *z2* can be the objective function for environmental impacts due to production. *x* is the vector that represents the amount of each production, *A* is the coefficient matrix and *b* is the vector that includes the resources available in a farm.

The weighted sum method can be used in LP to achieve MOO. In this method, each objective is assigned a weight before being combined into a single scalar objective function. For example, in a farm optimization problem, the multi‑objective function could be profit maximization while minimizing environmental impact. These goals are usually conflicting because maximizing profit may result in increased environmental impact. The weighted sum method has the following general form for a multi‑objective linear programming problem:

|  |  |
| --- | --- |
|  | (S3.2) |

Where *w1, w2, …, wn* are the weights assigned to each objective. It is important to note that the weighting method does not always find the best compromise solution because it assumes that the objectives can be ranked and traded against one another. Furthermore, this method may be limited because the decision maker may not know which weight to assign to each objective a priori.

Instead of assigning weights, GAs move from one set of solutions to the other using crossover, selection and mutation operators. Through the crossover process, two chromosomes, referred to as parents, are chosen and combined to create a new population, which is referred to as offspring. The search process does not reach a local optimal solution thanks to mutation operators. Several changes are made at the gene level by the mutation operator, which also generates new chromosomes. The new chromosomes will be very similar to those already present. In this way, a new population is produced through a selection procedure in the following step. A genetic algorithm (GA) searches the solution space for optimal values (based on objective functions and constraints) and will keep searching for the optimal solution until one of the termination conditions is met. The GA is terminated when one of the following criteria is attained:

1. The value of the objective function has reached a certain satisfactory level.
2. The maximum number of generations has been exceeded.
3. The time limit has been exceeded.
4. The results have not improved after a fixed number of iterations.

In our case, we represent a farm as a set of individuals, each representing a possible farm configuration. The fitness function assesses each individual's performance based on financial profitability, crop selection, livestock density and environmental factors such as greenhouse gases (GHG) emissions, land use, and water usage. Crossover and mutation are two genetic operators that can create new individuals from existing ones, allowing the GA to experiment with different farm configurations. Feed optimization, livestock density adjustment and manure management are examples of how GAs can optimize farms.

Crop rotation optimization is one example of GA application in farm optimization. Crop rotation is the practice of planting various crops in a specific order on the same field in consecutive years. This practice can improve soil health, reduce pest and disease pressure, and boost crop yields. A GA can be used to determine the best crop rotation schedule for maximizing crop yield while minimizing costs and minimizing environmental impacts. Another variable that can be optimized in a farm is livestock density, which is represented by several variables, including the number of animals per unit area, the types of animals, and the feeding schedule. In the case studies discussed in this paper, we apply the NSGA‑III algorithm [2].

The information readily available to manage farming operations is directly related to the degree to which those operations can be optimized. For example, we have data on farm properties, crop and livestock structures, cost and price information regarding those two categories, and lastly, information on subsidies. At the conclusion of each time step, the optimization module is activated to assist farmers in making decisions based on several criteria.

Crop production and animal husbandry are the two primary forms of farm production activities in our model. Multiple crop types can be cultivated on a farm. After the harvest, they are either sold in the market or used as animal feed on the farm. The production of milk and meat are examples of animal products sold on the market; however, manure can also be considered an essential product for crop production due to the value it possesses as a fertilizer. Farmers buy inorganic fertilizers if they need to fulfil the fertilizer requirements. Because farmers typically trade their excess manure for digestate, a byproduct of biogas production, manure is considered part of the biogas feedstock. This feedstock has an economic value for biogas producers, but this value is not passed on to the farmers. In addition, the nitrogen content of digestate is exceptionally high, and unlike manure, it is much simpler to store.

The characteristics that define a crop are its yield, requirements for fertilizer, price, production costs, and effect on the environment. On the other hand, animals are sorted into different groups based on their age, gender, and the kind of offspring they produce (dairy or suckler). Each livestock category is described in terms of its milk or meat production capability, prices for milk and meat, costs to maintain the livestock and the impact on the environment, meaning the level of nitrogen excretion into the soil. Crop production is constrained due to several different factors. The model considers the typical crop rotation schemes in the region and the seeding and harvesting seasons of each crop during the land allocation phase of the simulations. The model aims to determine the quantity of each production activity in vector *x* in (Eq. 1) that will result in the most efficient operation of the farm system. In our model, each farm's performance is optimized individually, and farms do not collaborate by exchanging products or pooling resources. There are two optimization criteria in our model, where the first one is economic optimization, where we maximize the gross margin of animal and crop production. The second is environmental optimization, where we minimize the selected environmental indicator.

The way in which NSGA‑III deals with multiple objectives is the primary factor that sets it apart from other GAs. NSGA‑III makes use of a non‑dominated sorting mechanism to sort the solutions in accordance with the values of the objective function. This enables the algorithm to find a set of non‑dominated solutions, where the definition of a non‑dominated solution is that it is the only solution that satisfies all the objectives better than any other solution. Environmental selection is a novel operator that has been added to NSGA‑III. This operator is used to determine who will be a part of the generation after this one. This operator seeks to maintain the diversity of the solutions available and is based on the crowding distance metric.

NSGA‑III for farm optimization can be utilized through the following steps. In addition, a summary of these steps can be found in Figure A1.

**Problem representation:** Represent the farm as a collection of individuals, where each individual represents a distinct arrangement of the farm that could be used. This may involve considerations such as the schedule for crop rotation.

1. **Objective functions:** Define the objective functions that will be used to evaluate the performance of each individual. These objective functions will be used to evaluate their performance. These could include the production of crops and livestock, as well as the environmental and financial impacts of these activities.
2. **Non‑dominated sorting:** Using the non‑dominated sorting mechanism, sort the individuals into groups according to the values of the objective functions they possess. This will result in a set of solutions that are not dominated by any other solutions.
3. **Genetic operators:** It is possible to generate new individuals from existing ones by making use of genetic operators such as crossover and mutation. This will enable the algorithm to explore various configurations of the farm.
4. **Stopping criterion:** Determine when the algorithm should stop running by deciding on a stopping criterion, such as a fixed number of generations or a threshold value of the fitness function. Stopping criteria can be anything from a fixed number of generations to a threshold value.
5. **Initial population:** The first step is to produce an initial population of individuals, which is typically done in a random fashion. The effectiveness of the algorithm is directly related to the degree of diversity present in the initial population.
6. **Running the algorithm:** Start the algorithm and repeat steps 4 through 5 until the termination criteria are satisfied. The final group of non‑dominated solutions will represent a set of trade-off solutions that can be utilized in the process of making decisions pertaining to the farm.

Diagram

Description automatically generated

**Figure S1.** NSGA‑III optimization scheme.

**References**

1. Hillier, F.; Lieberman, G. *Introduction to Operations Research*; 2015; ISBN 978-0-07-352345-3.

2. Deb, K.; Jain, H. An Evolutionary Many-Objective Optimization Algorithm Using Reference-Point-Based Nondominated Sorting Approach, Part I: Solving Problems With Box Constraints. *IEEE Transactions on Evolutionary Computation* **2014**, *18*, 577–601, doi:10.1109/TEVC.2013.2281535.