Multi-objective optimization as a tool to identify possibilities for future agricultural landscapes

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1 # Multi-objective optimization as a tool to identify possibilities for future
2 agricultural landscapes.
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Abstract

14 Agricultural landscapes provide many functions simultaneously including food production, regulation

15 of water and regulation of greenhouse gases. Thus, it is challenging to make land management

16 decisions, particularly transformative changes, that improve on one function without unintended

17 consequences on other functions. To make informed decisions the trade-offs between different

18 landscape functions must be considered. Here, we use a multi-objective optimization algorithm with

19 a model of crop production that also simulates environmental effects such as nitrous oxide

20 emissions to identify trade-off frontiers and associated possibilities for agricultural management.

21 Trade-offs are identified in three soil types, using wheat production in the UK as an example, then

22 the trade-off for combined management of the three soils is considered. The optimisation algorithm

23 identifies trade-offs between different objectives and allows them to be visualised. For example, we

24 observed a highly non-linear trade-off between wheat yield and nitrous oxide emissions, illustrating

25   where small changes might have a large impact. We used a cluster analysis to identify distinct

26   management strategies with similar management actions and use these clusters to link the trade-off

27   curves to possibilities for management. There were more possible strategies for achieving desirable

28   environmental outcomes and remaining profitable when the management of different soil types was

29   considered together. Interestingly, it was on the soil capable of the highest potential profit that

30   lower profit strategies were identified as useful for combined management. Meanwhile, to maintain

31   average profitability across the soils, it was necessary to maximise the profit from the soil with the

32   lowest potential profit. These results are somewhat counterintuitive and so the range of strategies

33   supplied by the model could be used to stimulate discussion amongst stakeholders. In particular, as

34   some key objectives can be met in different ways, stakeholders could discuss the impact of these

35   management strategies on other objectives not quantified by the model.

Highlights

36

37   • Trade-offs between different objectives in agricultural landscapes are complex

38   • Cluster analysis helped visualise effects of management on trade-offs

39   • Minimum N_2O emissions scaled linearly with yield until ~85-90% of maximum yield

40   • A more fertile soil could be managed more flexibly and remain profitable

41   • Achieving profitability on the *least* fertile soil was key for overall profitability

Graphical Abstract

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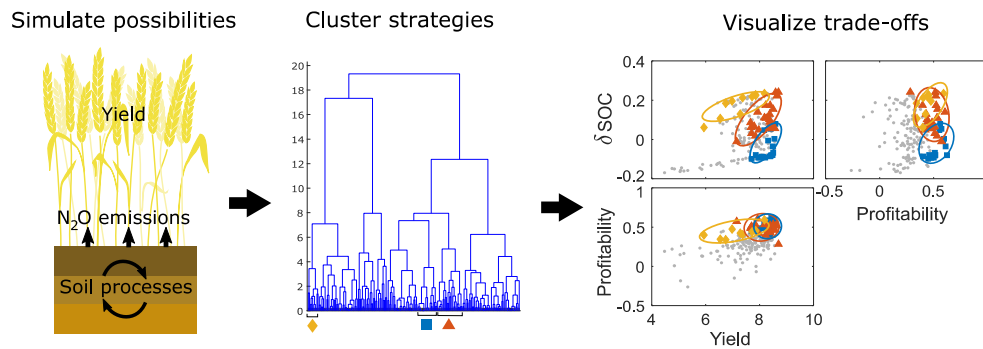
Introduction

The United Nations Sustainable Development Goals (SDGs) set out an ambitious suite of targets to stimulate effort to improve sustainability globally. Core to the SDGs is that these targets should not be considered in isolation, but that the interlinkages between the goals should be accounted for. The agricultural sector plays an important role in achieving many of the goals, most obviously 'zero hunger' which cannot be achieved without food production, but also impacts on goals relating to the environment (Gil et al., 2018) such as 'life on land', 'climate action' and 'end poverty'. Indeed, agricultural production systems have been identified as a major contributor to key global issues such as biodiversity loss, climate change and unsustainable nutrient cycling (Steffen et al, 2015; Burns et al., 2016; Campbell et al., 2017). This has led to increasing interest in understanding how agricultural production systems could be transformed to reduce negative environmental impacts whilst providing nutritious food and prosperous livelihoods within the sector (Kanter et al., 2018). Yet the complexity of these systems, their global scale and even their variability at local scale is a barrier to transformative change because it is difficult to identify alternatives to the current situation that take account of all the processes that might be affected by change and the multiple functions of agricultural landscapes.

One particular challenge is to stimulate informed stakeholder discussion about trade-offs within agricultural landscapes so that priorities can be identified collectively. This requires information about the likely trade-offs within agricultural systems and associated possibilities for managing these

64   systems to meet different combinations of objectives. Various methods have been used for

65   identifying trade-offs in agricultural systems, including participatory methods, empirical methods,

66   the use of multi-objective algorithms with models of agricultural systems and combinations of the

67   above (Klapwijk et al., 2014). Multi-objective algorithms are appealing because they can make use of

68   the current understanding of systems that is embedded in models. They may need to be combined

69   with other methods where key processes and objectives are not adequately represented in models.

70   Optimization algorithms strategically try different configurations of land management (the inputs to

71   a model of an agricultural system) to identify an optimal value of a quantifiable objective or

72   objectives (the outputs from the model). Multi-objective algorithms (e.g. Deb et al., 2002; Cao et al.,

73   2011; Huang et al., 2013) are particularly useful because they avoid the need to weight different

74   objectives. Such approaches have been used to identify scenarios of land-use change between an

75   agricultural use and a range of other uses (Polasky et al., 2008; Hu et al., 2015; Estes et al., 2016). In

76   these, the spatial configuration of the relevant land-use categories is optimised using objectives such

77   as agricultural production and environmental factors, including biodiversity and water retention.

78   However, the different possible practices within each land-use category are not considered. Other

79   studies, however, have also optimised the spatial configuration of agricultural land managed using

80   different practices using a multi-objective approach (Groot et al., 2007; Zhang et al., 2012; Kennedy

81   et al., 2016; Groot et al., 2018). Multi-objective algorithms therefore provide a useful way to explore

82   the effect of both land use and management practices on different objectives simultaneously.

83   Algorithms play a particularly interesting role in identifying possibilities because, whilst the

84   objectives and search options are set by people, within this range the computer algorithm can

85   search dispassionately and so consider options that might otherwise be discounted without due

86   consideration due to preconceptions. For example, in a study focussed on land use possibilities in

87   Iowa, Nassauer and Corry (2004) noted that whilst citizens might imagine future landscapes without

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88 perceiving unintended consequences, experts might limit their creativity based on what behavioural

89 change they deem possible.

90 One challenge in using multi-objective algorithms is that the results are complex and can be difficult

91 to interpret. If two objectives are considered and there is a trade-off between these two objectives,

92 the multi-objective algorithm will identify a number of optimal points along a trade-off frontier. The

93 points along this frontier have Pareto optimality, that is to say that at every point on the curve, an

94 improvement in one objective would be associated with a negative effect on the other objective (see

95 for example Lautenbach et al. 2013 for further explanation of pareto optimality). Such results can be

96 plotted easily on a 2-D plot (e.g. Zhang et al., 2012; Kennedy et al., 2016). If the algorithm considered

97 three objectives, the Pareto frontier could be shown as a 3-D surface. However. as more objectives

98 are included, the multi-dimensional surface becomes harder to plot and visualise. A variety of

99 approaches have been considered to visualise results, including the use of different colours and sizes

100 of points to represent additional dimensions and using heat maps (Lautenbach et al, 2013; Tušar and

101 Filipič, 2015; Ibrahim et al., 2016). For high dimensions, however, it is intuitive to project the surface

102 onto a series of 2-D plots representing the different pairs of dimensions (Groot et al., 2012). This

103 allows the frontiers between each pair of objectives to be visualised. Still, such plots do not show the

104 link from the land management actions to the associated outcomes (i.e. the associated point on the

105 trade-off frontier). This can be done to a limited extent by illustrating a few key points, for example

106 with a map of the land use that leads to a particular result (Polasky et al., 2008; Lautenbach et al.,

107 2013). However, it is not possible to do this for a frontier with hundreds of points; thus, new

108 approaches to enable this would aid interpretation of results.

109 Challenges in determining trade-offs within agricultural landscapes lie in the complexity of these

110 systems, both in terms of the need to consider multiple functions of the system from economic,

111 social and environmental perspectives and the need to consider different spatial scales. The spatial

112 component of these systems is important to consider both because of the connectivity of landscape

113   and landscape heterogeneity. The connectivity of the landscape means that altering a management

114   practice in one location may directly affect contiguous locations due to physical flows (e.g. water,

115   nutrients). Meanwhile the heterogeneity of landscapes means that actions taken to optimise

116   objectives in one place may not be optimal in another (e.g. due to differences in soil types).

117   However, this heterogeneity is also an opportunity, because different areas of land could be

118   managed to take best advantage of their specific characteristics. This is the idea behind the concept

119   of land sparing, the suggestion that environmental and food production might be best met by

120   removing some land from agricultural production and using it to meet environmental objectives

121   whilst increasing production on the land that remains in production (Phalan et al., 2011). Ultimately,

122   to identify trade-offs in agricultural landscapes using multi-objective optimization, it would be

123   desirable to use a single model that represents all relevant economic, social and environmental

124   objectives as well as spatial variability and interactions. Such a model does not exist, but

125   development of models and model frameworks that are able to represent multiple dimensions and

126   spatial interactions in agricultural landscapes simultaneously is ongoing (van Ittersum et al, 2008;

127   Schönhart et al., 2011; Groot et al., 2012; Schönhart et al., 2016). Meanwhile the Rothamsted

128   Landscape model (Coleman et al., 2017) captures another part of this complexity. It focusses on

129   agricultural production as well as the environmental component of agricultural landscapes,

130   specifically simulating nitrous oxide emissions and leaching from the soil, allowing the spatial

131   heterogeneity of the landscape to be considered.

132   In this paper the Rothamsted Landscape model (Coleman et al., 2017) is used to investigate and

133   visualise trade-offs, using wheat production in the south east of the United Kingdom (UK) as an

134   example. A specific aim is to consider the importance of spatial heterogeneity within the landscape,

135   which we do by comparing trade-offs in three soil types (clay, sandy clay and sandy loam) and then

136   identifying how the trade-offs change when these three soils are managed collectively, representing

137   a small heterogeneous landscape. This includes management approaches in which some soils are

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138   managed for production objectives and others for environmental objectives within the search space

139   for the multi-objective algorithm. The algorithm can then identify when objectives might be best

140   achieved by sharing production and environmental objectives across sites and when they might be

141   better achieved by reducing production at one site and maximising it at another to compensate thus

142   making use of landscape heterogeneity. The intention is that such results would be used to inform

143   and stimulate stakeholder discussion, although we do not report the results of such an interaction

144   here, focusing instead on the development of this modelling approach. We consider this as an

145   illustrative example, with a relatively simple set of possible management possibilities that could be

146   expanded in future work to further understand the importance of spatial heterogeneity and even

147   landscape connectivity in managing trade-offs across the landscape. Using this example of wheat

148   production in the UK, we develop a clustering approach to identify distinct management strategies

149   and how these relate to different outcomes for the multiple optimization objectives. This aims to

150   facilitate the interpretation of the results by associating possible land management strategies (i.e.

151   similar types of management actions) with different regions of the trade-off curves. This helps to

152   address the issue that for complex sets of objectives and land use and management options multi-

153   objective algorithms can identify numerous possibilities which may become overwhelming.

154   # Methods

155   *Optimization algorithm*

156   We coupled the Rothamsted Landscape model with an optimization algorithm to determine Pareto

157   optimal fronts between multiple objectives defined in terms of outputs from the model as has been

158   done previously (Coleman et al., 2017). The optimised Pareto fronts describe the synergies and

159   trade-offs between objective variables such as crop yield and nitrous oxide emissions. In order to use

160   such algorithms the user must define the optimization objectives and the control variables (in this

161   case a number of different farm management actions). The algorithm varies the control variables

162   and uses a simulation model (in this case the Rothamsted Landscape model) to calculate the effect

163   of these controls on the objectives. The algorithm must be able to identify which sets of control

164   variables result in better outcomes of the objectives and strategically identify new sets of control

165   variables to try to see if even better outcomes can be achieved. NSGA-II (Deb et al., 2002) is an

166   established algorithm to do this. Here, we combined the non-dominated sorting routine from NSGA-

167   II with differential evolution (Storn and Price, 1997) to identify new sets of options to try. Differential

168   evolution adds a directional component to the identification of new control variables which is useful

169   for numerical control variables, as gradients can be used to inform the search direction. This

170   approach is not relevant when the control variables are categorical and there is no 'gradient'

171   between categories as they are distinctly different options. In this application, as the controls were

172   numerical, the differential evolution approach was appropriate.

173   To run, the algorithm requires an initial list of management options to try; this forms the initial

174   population of management strategies. This initial population can be formed by randomly selecting

175   values for each of the management variables within each strategy. To do this a range or set of all the

176   values possible for each management variable is defined. Alternatively, the initial population could

177   be based on management strategies that are of interest, perhaps because they represent current

178   practice or an extreme management option. Here, the initial population was predominantly random

179   but was also seeded with some strategies representing current practice and extremes.

180   The algorithm then implements each of the management strategies from the initial population in the

181   simulation model and records the effect on each of the multiple objectives. Non-dominated sorting

182   then identifies the management options that result in the 'best' objectives, i.e. those that are non-

183   dominated. A point is said to be dominated by another if it is worse for every single objective.

184   The process is iterated in directions that the differential evolution algorithm suggests will be an

185   improvement, until the results converge and produce a similar Pareto front with each iteration. The

186   algorithm was run for 1500 iterations and convergence was judged manually by visually comparing

187   the frontier over multiple iterations. Running the algorithm for this application took around 1-2 days

188   for each soil, although the time depends on the control variables that are chosen as some

189   combinations take longer to run than others.

190   When considering the management of multiple units of land with different characteristics and

191   management possibilities, there was also a second stage of optimization to combine the three

192   frontiers across the land uses. This used the pareto fronts generated for each soil using the

193   simulation model as an input to the NSGA-II multi-objective optimization algorithm algorithm (i.e.

194   without differential evolution being implemented, as the control variables are categorical and a

195   directional search is not helpful in this context). By using the pareto frontiers identified in the first

196   step (i.e. the sets of points identified for each soil), we assumed that there were no interactions

197   between the sites and that what was optimal at one site was not affected by actions at other sites.

198   The algorithm was then used to consider how three sites with known individual trade-off curves

199   could be managed together to produce the best average values of the objectives. There was one

200   control variable for each unit of land, this control variable was an index value identifying the point

201   on the trade-off curve for that site. As the optimal trade-off curves for each soil consisted of 100

202   points, there are a million possible combinations of management practices. The algorithm thus

203   effectively searches for the best way in which the trade-off curves from different locations could be

204   combined by taking into account the strengths of each location and where they can best contribute

205   to specific objectives. A genetic population of 1000 points was used in this search, primarily to better

206   represent the resulting trade-off frontier as the shape of the surface becomes more complex.

207   *Simulation model scenario*

208   The optimization algorithm used outputs from the Rothamsted Landscape model (Coleman et al.,

209   2017) to simulate the effect of the management options described by the control variables on the

210   objectives. This model has been calibrated and validated in South-East England, within the climatic

211   zone of the study, (Coleman et al., 2017). It operates at a daily time step and simulates agricultural

212   yield as well as the effect of production on environmental processes including nutrient leaching and

213   nitrous oxide emissions. The Landscape model is also able to simulate nutrient flows across the

214   landscape, however this feature of the model was not used here. Instead, the model was used to

215   simulate the trade-offs between multiple objectives at a single location at a time.

216   The model was used to simulate wheat production using weather data that represents conditions in

217   the climatic zones in the west and centre of England. To do this weather data from Chivenor, Devon,

218   was used. The simulations were initialised with soil textural data representing Clay, Sand Clay and

219   Sandy-Loam soils (Table 1).

220   In the second stage of the paper, when combined managements of the soils were considered, equal

221   areas of each of the three soil types were assumed. Thus the objectives were quantified by taking

222   the arithmetic means of the values at each site.

223   Table 1: Soil properties (0-23cm) of the three soil types used in simulations

	Clay	Sandy Clay	Sandy Loam
Clay (%)	76	36	14
Silt (%)	14	15	18
Sand (%)	10	49	68
SOC (%)	2.49	1.83	0.96
pH	7.63	7.14	6.03
Bulk density	1.23	1.38	1.33

224

225   *Control variables*

226   The identification and implementation of appropriate control variables is critical as it sets the range

227   of possibilities that the optimization algorithm can explore. Whilst it is therefore tempting to make

228   the scope wide, this can slow down the optimization algorithm or prevent it from finding global

229   optima. Here, we used 11 control variables – the first 9 of these represented the amounts of

230   ammonium nitrate fertiliser applications. Each application could vary between 0-100 kgN/ha. The

231   first application can be made on 1st March with possible subsequent applications at 2 week intervals.

232   If it rained on the day that any application was scheduled, that application was delayed until the next

233   day. The expectation here, was that several of the possible 9 applications would be 0. If the initial

234   values for these application rates were drawn from a uniform distribution it would be highly unlikely

235   that the value zero would be selected repeatedly. Thus, to improve the convergence of the

236   algorithm, up to half of the initial population was set to include members that had 6-8 zero values

237   for N application control variables whilst the remaining members of the population had 9 randomly

238   sampled application rates. The 10th control variable was a farm yard manure (FYM) application (0-3

239   t/ha) and the 11th control variable determined the time at which this manure application was applied

240   from 0-3 weeks before sowing.

241   *Objectives*

242   The optimization objectives were selected to represent indicators that are relevant to the

243   contribution of agriculture to the SDGs, either directly by production or due to the effects of

244   production on the surrounding environment. A number of possible SDG indicators for agriculture

245   have been proposed (Gil et al., 2018), here however, we focused on those for which it was possible

246   to quantify with the model. These were; crop yield, nitrogen use efficiency (NUE), nitrogen surplus,

247   nitrous oxide emissions, and change in soil organic carbon (SOC). The yield and nitrous oxide

248   emissions were simulated for each year and then calculated as the average over the nine seasons of

249   the simulation. The change in SOC was calculated as the difference between the value at the start

250   and the end of the simulation. These values are clearly sensitive to the initial SOC. The NUE and

251   nitrogen surplus objectives were calculated by first summing the inputs and outputs in the crop grain

252   and straw over the whole simulation. The NUE was then calculated as the ratio between the outputs

253 and inputs, and the surplus as the difference between inputs and outputs. All sources of nitrogen

254 entering the soil were accounted for, so including atmospheric deposition (Coleman et al., 2017).

255 In addition, a profit function is calculated, as the sum of the yield each year multiplied by the farm

256 price of the crop, minus the total cost of the N fertiliser applied (both the mineral N and N in FYM),

257 minus the total cost of the P fertiliser applied, minus the cost of applying the N fertiliser. This is

258 divided by the number of years to give the average profit.

259 *Clustering*

260 To identify common management strategies, the sets of control variables found to be optimal were

261 further analysed using a cluster analysis. Prior to clustering, the nine inorganic fertiliser application

262 values were summarised into 3 values; the total amount of N applied, the number of N applications

263 (i.e. number of non-zero values), and the timing of the first application. The cluster analysis was then

264 performed on sets of variables representing the three values summarising nitrogen fertiliser and the

265 amount of FYM applied. The cluster analysis used a minimum variance, hierarchical clustering

266 approach following the Ward (1963) method. This was implemented in MATLAB (version R2018a)

267 using the standardised Euclidean distance. To aid visualisation, the mean profitability factor for each

268 cluster was calculated, and only the most profitable strategies were highlighted in the trade-off

269 curves.

270 # Results

271 The optimization approach identified trade-off frontiers between the different objectives. Scatter

272 appears in the frontiers because the plots shown a multi-dimensional surface projected onto a 2-D

273 plot. Trade-offs occur when an improvement in one objective has a detrimental effect on another

274 objective. Meanwhile synergies occur when objectives improve concurrently. In the clay soil, this

275 approach identified trade-offs between the yield and N_2O emissions and the N_2O emissions and the

276 change in SOC (Fig 1a-f). As there were synergies between the N_2O emissions, NUE and the N surplus

277 (Fig. 2), the trade-offs between NUE and N surplus indicators with other objectives were the same as

278 those for the N_2O objective (Supplementary information, Fig. S2). Meanwhile synergies were

279 observed between the yield and profitability, yield and change in SOC, and the profitability and the

280 change in SOC. It is instructive to focus on the N_2O data because these results emphasise the non-

281 linearity of certain trade-offs (Fig 1d). Specifically, the line that would represent the 2-D frontier

282 between N_2O and each of the other objectives is non-linear. The frontier between the profitability

283 and the N_2O emissions suggests a synergy at high emission values and a trade-off at lower emission

284 values (Fig. 1e), however there is also a lot of scatter behind the frontier corresponding to the other

285 objectives. As such, to meet these other objectives it may not be desirable to optimise the N_2O

286 emissions per unit profit.

287 The cluster analysis approach was applied to look for similarities in the control variables from within

288 the optimal population identified by the optimization algorithm. We refer to these clusters as

289 'management strategies' as they group together similar sets of management actions allowing them

290 to be associated with their effect on the objectives. For the clay soil, hierarchical clustering was used

291 to divide the sets of management actions into 9 clusters (Fig 3). Looking at the mean of the

292 profitability objective in the clusters, three profitable strategies were identified:

293   1. Applying no FYM and relatively high fertiliser N over 3 applications

294   2. Applying a little FYM and a slightly less N fertiliser over 2 applications

295   3. Applying much FYM and rather less N fertiliser over 2 applications

296 Notably, in these strategies, fertiliser applications tended to start later (from the 4th possible

297 application date) than other less-profitable strategies (Supplementary Information, Fig S2). The first

298 two strategies were associated with high yield, whilst for the third profitable strategy the yield was

299 slightly less and the profitability arose from lower fertiliser costs. FYM application was,

300 unsurprisingly, associated with increases in SOC. Most of the profitable strategies were associated

301 with high N_2O emissions, except for a subset of the first strategy (when no FYM and lower amounts

13

of N fertiliser were applied). Also, in the clay soil the maximum yield was higher than the sandy clay
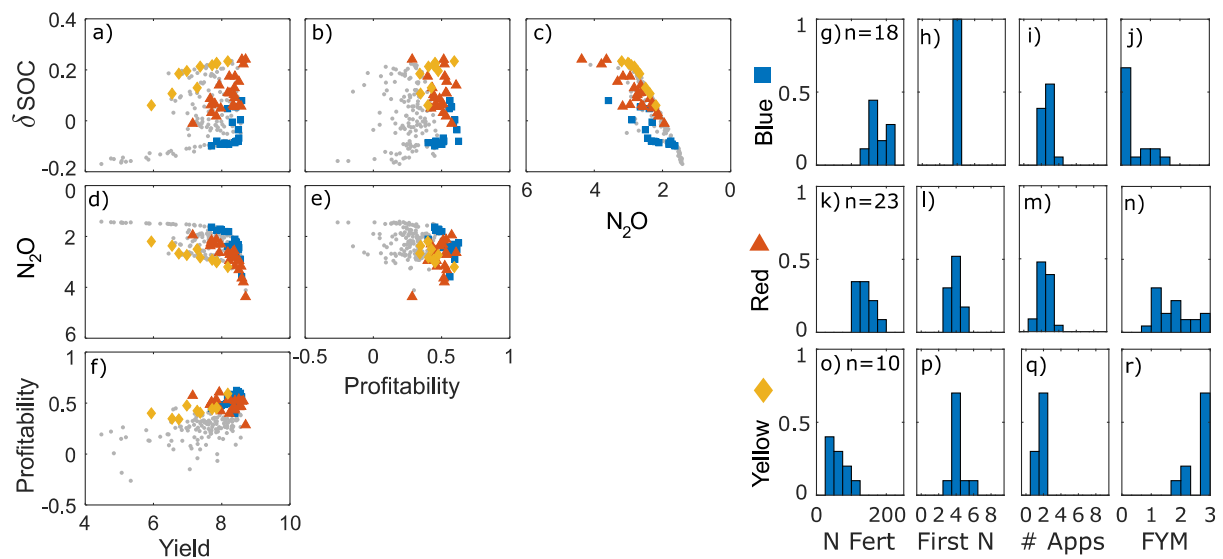
and sandy loam soils.

Figure 1: Trade-off frontiers (a-f) and cluster characteristics (g-r) in clay soil. Units are: Yield (t/ha), Profitability (x10^3 £ / ha /year), N_2O (x10^3 CO_2 equivalent yr^{-1}), change in SOC - δSOC (%). Note that for N_2O, increasing values are shown from right to left or top to bottom because this objective was minimised in the optimisation process. This means that, consistently across the plots, trade-offs show trends from the top left to the bottom right of the plots and synergies trends from the bottom left to the top right. Points within the most profitable clusters are highlighted; all other points are shown as small grey circles. Histograms of the cluster variates show the fraction of the points in each cluster with a particular management value, where n is the number of management strategies (i.e. points) in each cluster, N Fert is the total N applied in fertiliser, First N is the week of the first N application, # Apps is the number of fertiliser applications and FYM is the amount of farm yard manure applied.
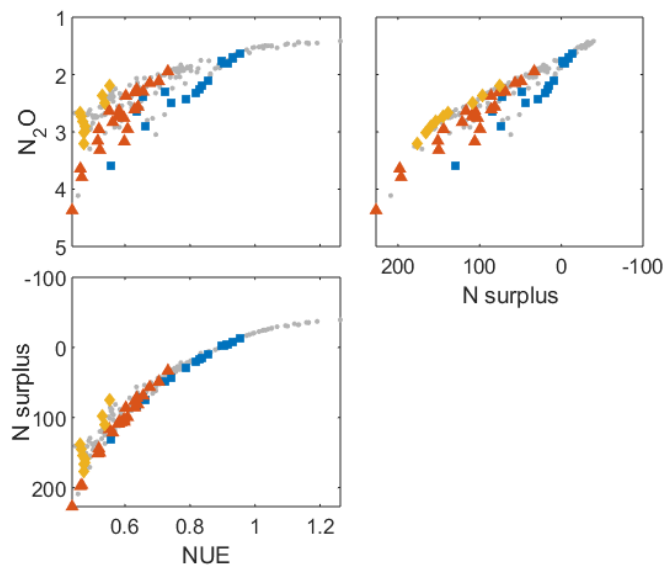
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317   Figure 2: Trade off frontiers between the objectives relating to nitrogen cycling for the clay soil.

318   Units are: N_2O ($x10^3$ CO_2 equivalent yr^{-1}), N surplus (kg ha^{-1} yr^{-1}), NUE (-). Yellow diamonds, red

319   triangle and blue squares indicate points in the frontier that correspond to the clusters detailed in

320   Fig. 1, g-r grey dots show all other points in the frontier. Note that for N_2O and N surplus, increasing

321   values are shown from right to left or top to bottom because these objectives were minimised in the

322   optimization process. This means that, consistently across the plots, trade-offs show trends from the

323   top left to the bottom right of the plots and synergies trends from the bottom left to the top right.
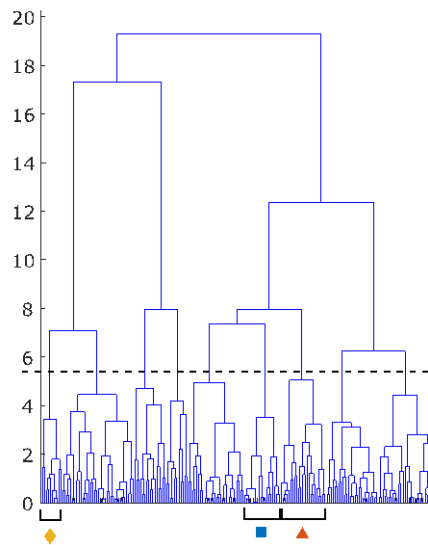
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Figure 3: Hierarchical cluster results for clay soil, with the profitable clusters highlighted. The dotted

line indicates the division of the dataset into 9 clusters.

In the sandy clay soil the same trade-offs and synergies between objectives were observed as in the

clay soil (Fig 4a-f). Two profitable management strategies were identified (Fig 4g-n):

1. High application of FYM, 1-3 applications of a small amount of N fertiliser
2. Low or Medium application of FYM, 1-3 applications of a medium amount of N fertiliser

In this soil, most of the points in the optimal set were high yielding (Fig 4f). Profitable strategies were

also associated with high yields. The greatest possible profitability was less than in the clay soil.
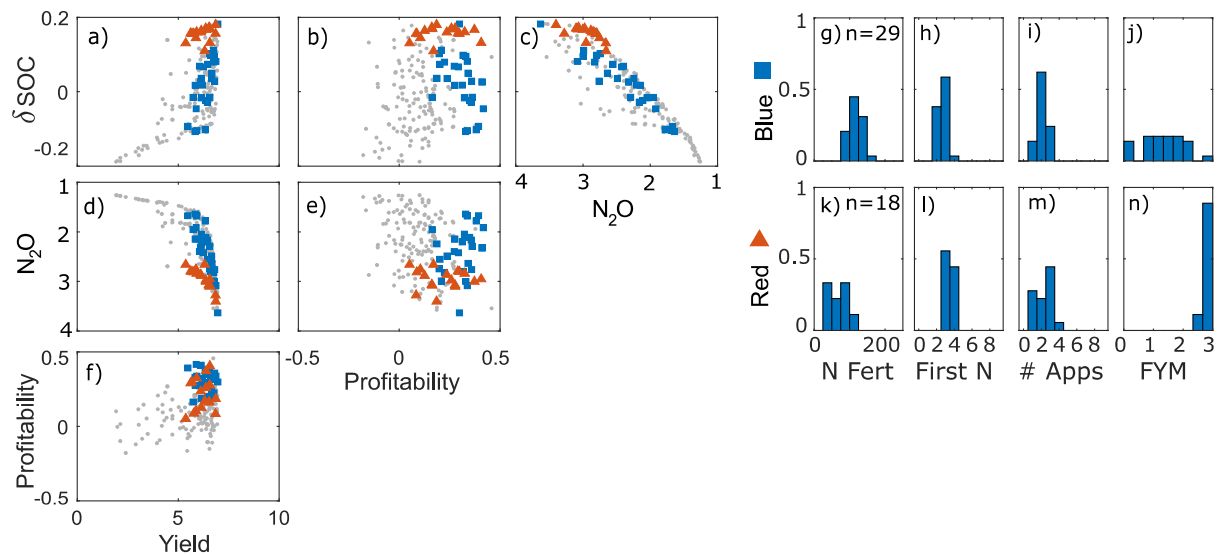
Figure 4: Trade-off frontiers (1-f) and cluster characteristics (g-r) in sandy clay soil. Units are: Yield (t/ha), Profitability (x10³ £ / ha / year), N₂O (x10³ CO₂ equivalent), Change in SOC - δSOC (%). Note that for N₂O, increasing values are shown from right to left or top to bottom because this objective was minimised in the optimisation process. This means that, consistently across the plots, trade-offs show trends from the top left to the bottom right of the plots and synergies trends from the bottom left to the top right. Points within the most profitable clusters are highlighted; all other points are shown as small grey circles. Histograms of the cluster variates show the fraction of the points in each cluster with a particular management value, where n is the number of management strategies (i.e. points) in each cluster, N Fert is the total N applied in fertiliser, First N is the week of the first N application, # Apps is the number of fertiliser applications and FYM is the amount of farm yard manure applied.

For the sandy loam soil (Fig. 5), the highest possible profitability was £390 ha⁻¹ yr⁻¹, lower than the sandy clay and clay soils (£458 and £624 ha⁻¹ yr⁻¹ respectively). Meanwhile, the maximum possible yield 7.5 t ha⁻¹ for the sandy loam soil, was higher than possible for the sand clay (7.0 t ha⁻¹) but lower than for the clay soil (8.7 t ha⁻¹).

The 3 profitable strategies identified were:

352   1.   High FYM, high N fertiliser in 2-3 applications, starting early

353   2.   High FYM, medium N fertiliser, typically 2-3 applications, starting slightly later

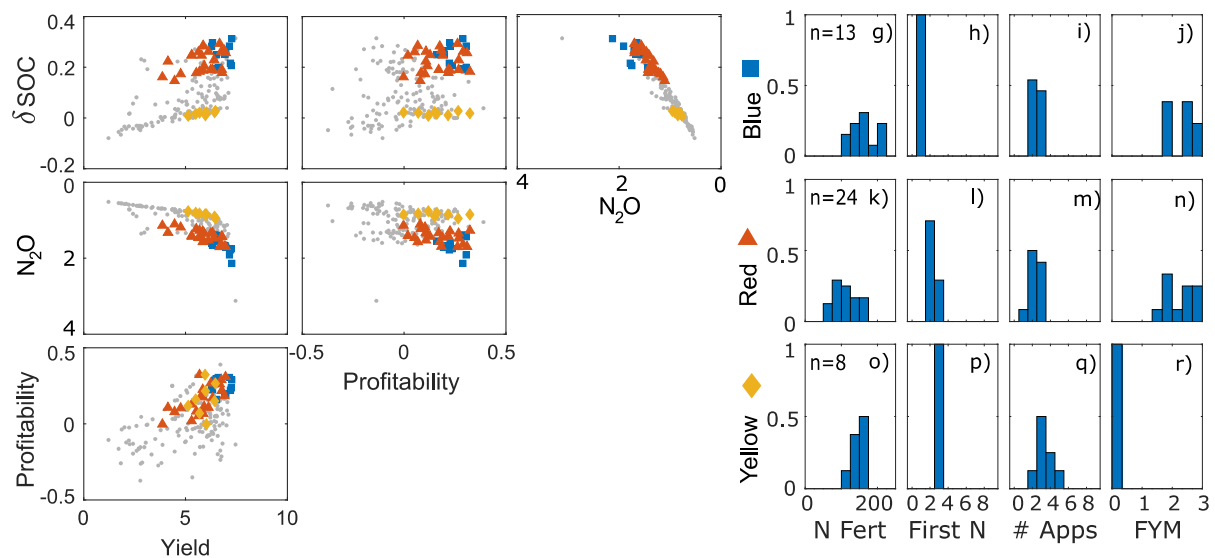354   3.   No FYM, medium N fertiliser, typically 3-4 applications, starting even later

355

356

357   Figure 5: Trade-off frontiers (1-f) and cluster characteristics (g-r) in sandy loam soil. Units are: Yield

358   (t/ha), Profitability (x10^3 £ / ha / year), N_2O (x10^3 CO_2 equivalent), Change in SOC - δSOC (%). Note

359   that for N_2O, increasing values are shown from right to left or top to bottom because this objective

360   was minimised in the optimisation process. This means that, consistently across the plots, trade-offs

361   show trends from the top left to the bottom right of the plots and synergies trends from the bottom

362   left to the top right. Points within the most profitable clusters are highlighted; all other points are

363   shown as small grey circles. Histograms of the cluster variates show the fraction of the points in each

364   cluster with a particular management value, where n is the number of management strategies (i.e.

365   points) in each cluster, N Fert is the total N applied in fertiliser, First N is the week of the first N

366   application, # Apps is the number of fertiliser applications and FYM is the amount of farm yard

367   manure applied.

368   Combining the objectives across three fields of equal area but differing in soil texture (clay, sandy

369   clay, sandy loam) led to a combined trade-off frontier (Fig. 6). Notably, for the combined

370   management, it becomes more clear that the frontier is a multi-dimensional surface with the Pareto

371   optimal points more spread out compared to the management for each of the soils individually (Figs.

372   1, 4 and 5). The relationship between the profitability and N_2O emissions was synergistic for high

373   emissions, but becomes a trade-off at lower emissions. This change at the frontier, from synergy to

374   trade-off, was clearer than in the individual soils and indicated that a reduction in nitrous oxide

375   emissions beyond a certain point would be associated with a large reduction in profitability (Fig. 6e).

376   Multiple profitable strategies perform similarly with respect to multiple objectives (e.g. green and

377   yellow clusters in Fig. 6) meaning that there is freedom to make choices between these strategies

378   based on additional objectives not captured by the model. The most profitable strategies (the blue

379   cluster in Fig. 6) produced lower nitrous oxide emissions than the other profitable clusters, all of

380   which resulted in an increase in SOC.

381   Interestingly, all of the more profitable clusters in the combined management included the most

382   profitable management strategies for the sandy clay soil, which had the lowest maximum yield (Fig.

383   8). Furthermore, only one of the five management strategies on the sandy loam soil (which had the

384   medium maximum yield) included less profitable management strategies on this soil. On the clay soil

385   (which had the highest maximum yield), there were a wider range of management strategies that

386   resulted in profitable overall management. Compared to the strategies identified for the clay soil

387   alone (Fig 1.), the strategies that were profitable on clay in the case of combined management

388   included more in which manure was applied to the clay soil, and more numerous fertiliser

389   applications (Fig. 7).

390   This shift to less profitable strategies occurs in the clay soil but not in the sandy clay when combined

391   management is considered. The reasons for this are complex but occur because of the effect that a

392   decrease in profitability has on the other objectives in each of the soils. For example, in the sandy

393   clay soil, most of the possible reduction in N₂O emissions can be achieved whilst remaining

394   profitable (i.e. the frontier has a fairly straight vertical edge in Fig. 4e). In the clay soil however, there

395   is a discernible trade-off that emerges to reach the lowest possible emissions (i.e. the top edge of

396   the frontier is more rounded in Fig. 1e). Additionally, in the clay soil the differences between

397   profitability of the more profitable strategies was smaller than in the sandy clay soil (i.e. with respect

398   to profitability, the points are grouped together predominantly in the high profitability region for the

399   clay soil – Fig. 1, but are more spread out for the sandy clay soil – Fig. 4). This means that, to

400   maintain overall profitability for a decrease in the profitability in the sandy clay soil, a relatively large

401   increase in profitability on another soil would be necessary. Hence optimal combined strategies

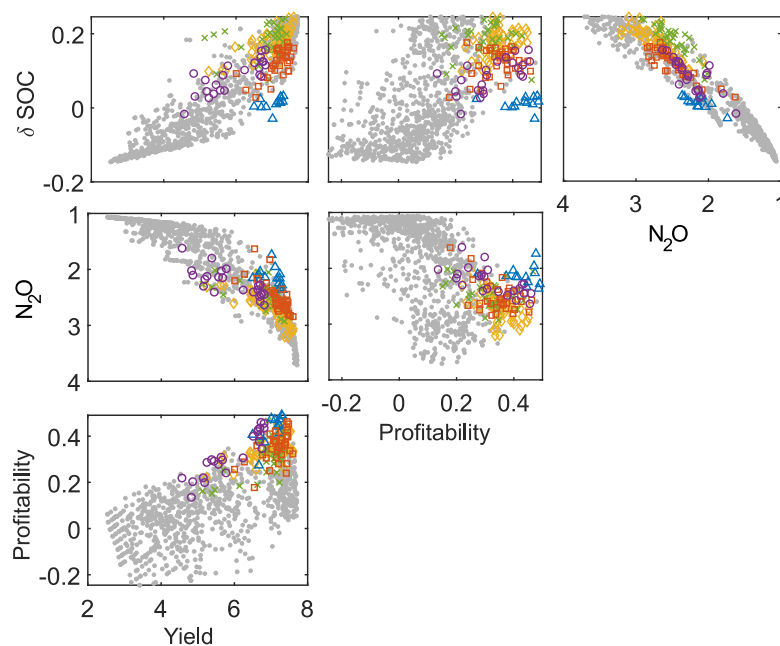402   maintain profit in the sandy clay soil.

403

404   Figure 6: Trade-off frontiers when managing three fields each of equal area but each of a different

405   soil texture (clay, sandy clay, sandy loam). Units are: Yield (t/ha), Profitability (x10³ £ / ha / year), N₂O

406   (x10³ CO₂ equivalent), Change in SOC - δSOC (%). Note that for N₂O, increasing values are shown

407   from right to left or top to bottom because this objective was minimised in the optimisation process.

408   This means that, consistently across the plots, trade-offs show trends from the top left to the

409   bottom right of the plots and synergies trends from the bottom left to the top right. Points within

410   the most profitable clusters are highlighted; all other points are shown as small grey circles.

411   Histograms of the cluster characteristics for the most profitable clusters are shown in Fig. 7.

412
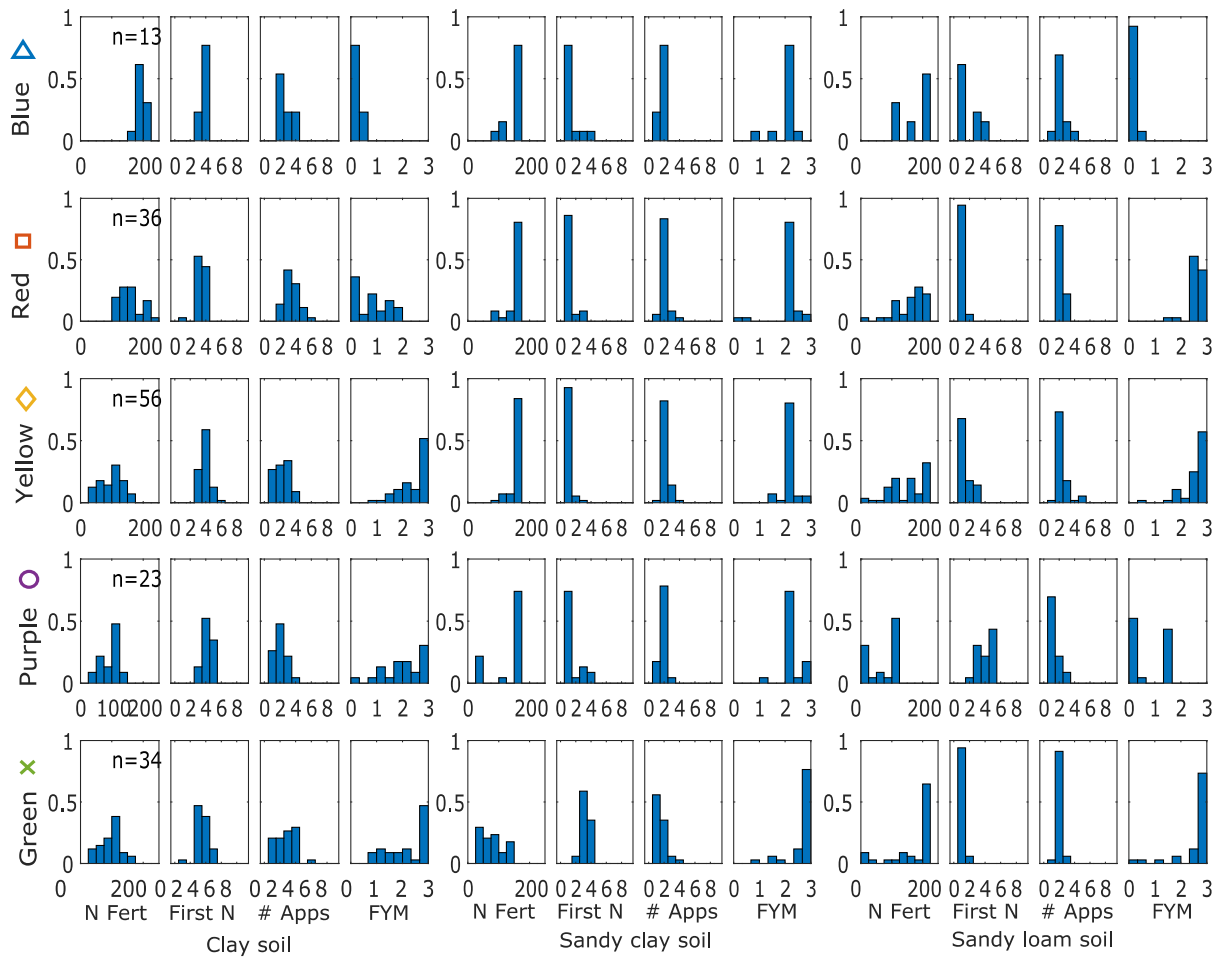
Figure 7: Characteristics of the profitable clusters for the combined management of three soil types.

414   Histograms of the cluster variates show the fraction of the points in each cluster with a particular

415   management value, where n is the number of management strategies (i.e. points) in each cluster, N

416   Fert is the total N applied in fertiliser, First N is the week of the first N application, # Apps is the

417   number of fertiliser applications and FYM is the amount of farm yard manure applied.

418

419   Figure 8: Proportion of the points within each cluster that correspond to profitable management of
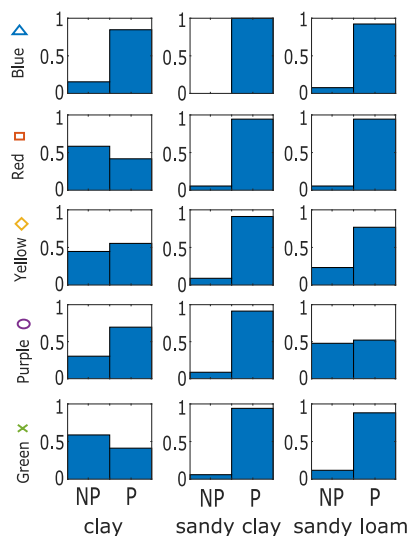
420   that soil type. On the x-axis, P corresponds to profitable and NP to not profitable. Profitable points

421   are defined as the 30% of most profitable points for that soil type.

Discussion

422

Trade-offs between objectives

423

424   One distinctive feature of the results is the non-linearity of the trade-off between yield and N_2O

425   emissions. This is not unexpected as high yields are associated with high N application, either in the

426   form of fertiliser or manure, but is important to note because many national greenhouse gas

427   inventories follow an emissions factor approach that effectively assumes this relationship is linear

428   (Eggleston et al., 2006; Shcherbak et al., 2014).. Recent work has suggested that the increase in N_2O

429   emissions with increasing N application is non-linear (Shcherbak et al., 2014), and here, when the

430   trade-off is considered with respect to yield, this non-linearity is exacerbated as at high N application

431   further increases in N applied result in only a marginal increase in yield. Linquist et al. (2012)

432   considered the trade-off between greenhouse gas and cereal crop production. They concluded that

433   the lowest global warming potential per unit yield occurred at 91% of potential yield for wheat. This

434 is comparable to the point at which we observed the non-linear increase in GHG production (90% of

435 the maximum yield in the clay soil, 85% in the sandy clay and 88% in the sandy loam soil). A similar

436 finding was also reported by Nguyen et al., (2018) who suggested that 90% of potential production

437 can be achieved with minimal impacts, including greenhouse gas emissions. It is interesting to note

438 that this non-linear point is comparable to the 80% of potential yield that is often considered as the

439 'exploitable yield' in yield gap analysis (Lobell et al., 2009; van Ittersum et al., 2013). Whilst this

440 exploitable yield has been reached from a resource use and profitability perspective, in our analysis

441 is corresponds more to the threshold that limits a negative environmental impact, as some of these

442 high emission management strategies still appear to be profitable in our analysis.

443 The results also highlight a trade-off between N_2O emissions and increasing SOC in the soil. This is in

444 part due to the control options by which the SOC can be increased in the simulations; either by

445 manure addition or by increasing N application in such a way that yield increased and hence crop

446 residues also. Both mechanisms are typically associated with an increase in N_2O emissions. Bos et al.

447 (2017) showed that net GHG emission reductions could not be obtained with manure application,

448 and only the application of compost resulted in larger emission reductions because of SOC increase

449 compared to N_2O emission increase. There are also indications that N_2O emissions may be inherently

450 higher from soils with higher SOC (Palmer et al., 2017; Charles et al., 2017), as this would reduce the

451 chance that N_2O emissions are limited by C availability in soil (Charles et al., 2017). Other studies,

452 however, have not found a significant effect of SOC (Buckingham et al., 2014). When considering

453 carbon sequestration to mitigate GHG production, the net effect of sequestration and emissions

454 must be considered. Other studies have also suggested that, in terms of global warming potential

455 carbon sequestration may be offset by N_2O emissions (Powlson et al. 2011; Zhou et al., 2017). A

456 systems perspective is also clearly necessary as, if manure was not applied to the soil, it would still

457 emit greenhouse gases elsewhere (Hou et al., 2015). However, increases in SOC are also desirable

458   for other reasons such as increasing future soil fertility (Garratt et al., 2018) and reducing erosion

459   risk.

460   The EU nitrogen panel has made recommendations for NUE and N surplus (EU Nitrogen Expert

461   Panel., 2015), suggesting a range of NUE from 0.5 - 0.9 combined with an N surplus of less than 80 kg

462   ha^{-1} yr^{-1}. In our study these ranges were met by using strategies in which very little manure was

463   applied, for example the blue square cluster (Fig. 2) in which no manure was applied or very few of

464   the red triangle cluster in which a small amount of manure was applied. This corresponds to the fact

465   that manure applications were associated with an increase in N_2O emissions in the simulations, and

466   also with increased N leaching. Some thought must be given to how NUE and N surplus is calculated

467   when applying organic matter to the soil, as nitrogen applied in one year may benefit crops in future

468   years. For this reason N inputs and outputs were calculated for the whole simulation, however,

469   there was also likely a build up of soil nitrogen in this period. Indeed, an increase in SOC would

470   require this (Van Groenigen et al., 2017); So if increasing SOC is an objective, the NUE and N surplus

471   targets or calculation approaches may need to be reconsidered concurrently.

472   *Management across soil types*

473   As expected, the model simulated differences between the soils in terms of the yield and N_2O

474   emissions. The N_2O emissions from the sandy loam soil were notably less than from the other two

475   soils, particularly at greater N application rates. This corresponds to the findings from other studies

476   which suggest that emissions from fine textured soils are greater than from coarse textures (Charles

477   et al., 2017) and that water filled pore space is a key factor affecting emissions (García-Marco et al.,

478   2014). Thus soils which retained more water, emitted more N_2O. The lower NUE values and higher N

479   surplus values in this soil also suggest that more N is lost from the soil profile by leaching, as would

480   be expected.

481   Interestingly, the maximum possible increase in SOC was comparable for all three soils. The

482   simulated potential is of course related to the initial SOC in the simulations. In this case, the

483   simulations were based on soils under long-term arable management with low initial SOC and in this

484   situation it seems that, for the soil textures we considered, the soil texture had little effect on the

485   possible increase in SOC.

486   In general, profitable strategies were associated with large yields. At the highest yields, we might

487   have expected to see a trade-off between these two objectives; indeed, in yield gap analysis, 80% of

488   the potential yield is considered as the 'exploitable yield' (Lobell et al., 2009; van Ittersum et al.,

489   2013), representing a point at which there starts to be a trade-off between the two objectives

490   because the cost of inputs outweighs the increase in sale price due to the increase in yield. Here,

491   however, as in other studies (Silva et al., 2017), we did not observe this trade-off. Nevertheless, in

492   the clay soil, a reduction of yield to around 70% of the maximum could be achieved with very little

493   impact on the profitability (Fig. 1). In the sandy clay, reductions in yield resulted in a linear reduction

494   in profitability (Fig. 4). In both case, strategies that reduced yield but maintained profitability were

495   associated with large manure application rates and small amounts of N fertiliser. This strategy was

496   not identified as a possibility in the sandy clay soil, which also had the lowest yield potential. In this

497   soil, all the profitable strategies were associated with high yields. This suggests that there is less

498   opportunity to adapt management strategies whilst remaining profitable.

499   On many farms, such as those in the UK, different soil types are present and these soils must be

500   managed simultaneously. Considering the combined options across these different soils means that

501   additional strategies can be identified to deliver the same objectives overall. Here, for example, the

502   clay soil could be managed in a way that was not necessarily the most profitable for that soil, but

503   contributed to improving the other objectives. The loss in the likely profit from this soil could then

504   be compensated for on another soil in which the other objectives were less desirable.

505   One ongoing debate regarding sustainable agriculture relates to the notion of sharing or sparing land

506   in agricultural production (Phalan et al., 2011; Fischer et al., 2014). This relates to considering

507   whether environmental objectives might be best achieved by reducing production (and thus

508   negative environmental impacts) across all agricultural land (sharing) or whether it would be

509   preferable to remove some agricultural land from production entirely and use remaining agricultural

510   land even more intensively (sparing). Most research in this area has focussed on the trade-off

511   between biodiversity and production. However, recent studies suggest that land-sparing might help

512   mitigate leaching and GHG emissions as well (Lamb et al., 2016; Balmford et al., 2018).

513   Generally, for land sparing it might be expected that the least productive agricultural land be

514   removed from production because the focus is on yield and profit. Contrary to this, however, the

515   results here suggest that it is management of the most productive soil that should be targeted to

516   improve the multi-objective performance. Biodiversity is not a part of this analysis, nor is carbon

517   sequestration in spared land. In this study, land cannot be entirely removed from production in the

518   way the control variables in this study have been implemented, and the environmental objectives

519   focus mainly on nitrogen. However, given the typical nitrogen response curve of crops, it is

520   unsurprising that spreading nitrogen thinly over a larger area will be preferable to putting the same

521   amount on a smaller area. This takes advantage of the larger yield increase per unit nitrogen that

522   occurs at low application rates compared to those that occur at higher application rates. This means,

523   however, that in a land sparing scenario, the agricultural land that is managed more intensively is

524   likely to result in higher nitrous oxide emissions per unit yield. A natural extension of this work

525   would therefore be to include biodiversity objectives within the optimization. Any trade-off between

526   these objectives and nitrogen cycling objectives should then become apparent.

527   *Envisioning future landscapes*

528   One core aim of this paper is to illustrate the potential of of this approach to identify possibilities for

529   possible strategies for managing agricultural landscapes. Notably the approach identifies many

530   possibilities, the intention being that these can be presented to and discussed with stakeholders.

531   Specifically, this approach could be used as a tool within a visioning and backcasting exercise (i.e.

532   envisioning the future and then working backwards from this vision until the current state is

533   reached). Visioning and backcasting is an approach that was developed in the energy sector as a tool

534   to identify transformation pathways (Robinson, 1982) and has subsequently been used in other

535   sectors as a tool for considering transformative change within complex systems (Dreborg, 1996;

536   Vergragt and Quist, 2011). The first step is to envisage a desirable future and this is often done using

537   a participatory that brings together multiple stakeholders with different perspectives. The idea in the

538   visioning step is to focus on the key factors that are important to the different stakeholders for the

539   future, rather than discussing the current problems and barriers to change (as can easily happen in a

540   forecasting approach, or when the current situation is the focus of discussion). Gil et al. (2018)

541   represent an example, where priorities for SDG-2 ('End Hunger') were set by comparing SDG-2

542   indicator target values for 2030 with current values. With the end vision in sight, the backcasting

543   process then allows stakeholders to be more creative in considering how any barriers might be

544   overcome. Thus, in theory, the approach should allow more room for a truly transformative pathway

545   to be identified.

546   Such approaches encourage idealism, the philosophy being that our visions provide the motivation

547   to develop new approaches and therefore reshape what is possible (Wright, 2010). Yet this idealism

548   must be balanced with realism in order to generate visions that are also plausible and tangible so

549   that action can be taken (Wiek and Iwaniec, 2014). Without this, there is a risk that an idealistic

550   future vision may include multiple objectives that are not physically possible to achieve concurrently.

551   Trade-off frontiers identified by multi-objective algorithms could therefore be used as a tool to

552   encourage stakeholders to discuss trade-offs whilst they are developing this future vision. This would

553   allow challenging discussions about trade-offs to occur during the visioning process, rather than

554   during the backcasting process, thus with less focus on challenges that occur within the current

555   system and more focus on what would be desirable in future. For instance, the example presented in

556   this study could be used to inform stakeholder discussion about the relative importance of

557   minimising nitrous oxide emissions from soil compared to maximising yield, without the idealistic

558   assumption that both can be achieved simultaneously and without apportioning blame with regards

559   to the current state of the system.

560   In this example the focus was on wheat production in a small landscape and with a defined set of

561   control variables relating to fertiliser and manure application. Thus, there is clearly scope to expand

562   the method to consider more diverse agricultural practices in more complex landscapes as the scale

563   and context will affect the trade-offs that can be achieved. These could include practices that are of

564   interest to stakeholders within a particular context and things that are technically possible and the

565   scales (field, farm, region) at which different options could be implemented. Even so, the approach

566   highlighted the range of possibilities that might be achievable with simple changes and the

567   opportunities in considering the heterogeneity of the landscape.

568   There are various technical challenges in the optimization approach, including the risk of the

569   algorithm becoming stuck in local minima and the inconvenience of the algorithm converging slowly

570   because extreme control variables are selected and are difficult to simulate. These risks would be

571   even more present in more complex modelling scenarios considering more complex landscapes and

572   management possibilities. However, we found that seeding some of the initial population with a

573   number of likely scenarios was effective at reducing the number of steps needed for convergence,

574   an approach that has been useful elsewhere (Milne et al., in review). Within the initial population,

575   several possible fertiliser applications were set to a rate of zero. When using more complex sets of

576   control variables, subgroups of these control could be optimised initially in order to be able to seed

577   optimization of the complete set.

578   The cluster analysis was used as a tool to relate the control variables to the resulting sets of

579   objectives. This allowed the management strategies to be associated with different regions of the

580   Pareto front. It is particularly interesting that for some pairs of objectives similar trade-offs can be

581   achieved by alternative strategies (e.g. those from different clusters). For example, similar yields and

582   GHG emissions occur for strategies identified by the clusters of red squares and green crosses in Fig.

583   6. In this case, more points occur in the red square cluster and fewer in green cross cluster. In

584   general, the points in the green cross cluster dominate those in the red square cluster with respect

585   to the indicators of SOC. Without this dominance in another factor, it is likely that this management

586   strategy would occur less frequently in the population. Indeed, if the algorithm were optimised

587   based on yield and GHG objectives alone it may even be overlooked entirely, if a strategy from the

588   red square cluster marginally outperforms the strategy of the green cross cluster. Thus inclusion of

589   another objective enabled the identification of an alternative management approach with similar

590   performance for another objective.

591   To capture the complexity and the multiple stakeholder objectives and to identify a diverse range of

592   strategies, it may seem desirable to include more objectives. However, with more objectives it

593   becomes increasingly difficult to visualise the results and communicate them clearly. Additionally,

594   models are unlikely to be able to simulate all of stakeholders' priorities. We suggest, therefore, that

595   the objectives simulated and optimised by the model are viewed as a subset of the stakeholders'

596   priorities. In this case the objectives used in the model were a subset of those identified by Gil et al.

597   (2018) which included NUE, N surplus and greenhouse gas emissions intensity as priorities for

598   agriculture in the Netherlands as well as pesticide use and genetic diversity which cannot currently

599   be represented in the model. In most situations there will also exist additional objectives that have

600   not been quantified by the model which stakeholders will be considering when they interpret the

601   results. For each management strategy, another analysis exercise (e.g. a participatory method with

602   the stakeholders or empirical evidence) could then be used to identify how the management

603   strategies would likely affect unmodelled objectives. However, there may also be distinct

604   management strategies that are appealing to stakeholders that exist close to the frontier but are

605 neglected by the optimization algorithm. Although it is likely to increase convergence time, future

606 algorithms should retain solutions that are 'almost' optimal within a chosen tolerance, particularly if

607 they are associated with distinctly different management strategies. Given complex control

608 variables, this should increase the number of distinct management strategies that might be of

609 interest for stakeholder discussion and might meet other, untested objectives such as those relating

610 to biodiversity.

611

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622

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