Machine learning for optimizing complex site-specific management

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Abstract

Despite the promise of precision agriculture (PA) for increasing the efficiency of crop production by implementing site-specific management, farmers remain skeptical and its utilization rate is lower than expected. A major cause is, unsurprisingly, a lack of concrete approaches to higher profitability. Since PA involves many variables in both management and monitored environment, optimal site-specific management for such high-dimensional cropping systems is considerably more complex than the traditional low-dimensional cases widely studied in the existing literature, calling for a paradigm shift in approaches to the problem. We propose an algorithmic approach that enables each farmer to efficiently learn their own site-specific management through on-farm experiments. We demonstrate its performance in a simulated environment constructed with APSIM. According to our results, after 5-year experiments, the learned site-specific management generates \$40/ha higher profits with 21 kg/ha less nitrogen fertilizer than the benchmark uniform management. Thus, complex site-specific management can be learned very efficiently, which is indeed more profitable and environmentally sustainable than uniform management.

Keywords: Machine learning, Bayesian optimization, APSIM, precision agriculture, site-specific management

1 Introduction

Precision agriculture (PA) holds big promise of modern agriculture in addressing some of the most challenging problems in the 21st century, including farm profitability, food security, and environmental sustainability. All of them requires increase in yield without increase in farm inputs, in other words, higher productivity. Site-specific management emerges as a natural solution to the problem (Bongiovanni et al., 2004; Cassman, 1999; Gebbers et al., 2010) because, in principle, it can optimize production at a subfield level, which amounts to finer optimization at a field level.

Despite the big promise, many farmers have perceived PA as big disappointment, causing slow adoption of PA (Bramley, 2009; Schimmelpfennig, 2016). A major reason for the slow adoption is, understandably, a lack of profitability (Castle et al., 2016; Gandorfer et al., 2017). Since every other societal benefit of PA presumes farmers' adoption, convincing farmers is one of the first problems to solve. To be convinced, farmers need to see concrete procedures for utilizing complex technologies—how to implement site-specific management in their own fields and increase their profits from the conventional uniform management. However, farmers have received only partial answers to this request from the existing research (Antle, 2019; Antle et al., 2017; Leonard et al., 2017).

The vast majority of site-specific management research investigates only a single management variable, which is often a total amount of nitrogen fertilizer (Anselin et al., 2004; Boyer et al.,

2011; Jin et al., 2017b; Karatay et al., 2019; Thöle et al., 2013). However, multiplicity is the reality in farming where crop yield is an outcome of the complex interactions among a number of management and environmental factors (Bullock et al., 2000; Ruffo et al., 2006). Within a growing season, a farmer makes a number of decisions including many types of activities (e.g., tillage, planting, fertilization, spraying, and harvest), their amounts, and their timings. Since the overall profitability is determined by the totality of those decisions, profitability assessment requires more comprehensive analysis than the existing studies. In other words, independent studies of a single management variable provide only partial knowledge and can be misleading as such complex systems typically involve significant nonlinearity (Altieri, 2018; Gliessman, 1990). Thus, we must investigate effects of multiple variables simultaneously.

In addition to the large number of variables in each farm, the multiplicity of farming also implies heterogeneity, that is, a large variety of farms, each of which is unique and operates with different resources (e.g., machinery) in different environments (e.g., soil). Consequently, results from studying "representative" cases are useful for only farmers who face very similar managerial and environmental conditions. This problem is exacerbated in PA where the high dimensionality makes it even more difficult for selected cases to be representative, the problem called "the curse of dimensionality" in mathematics (Bellman, 2015). As mentioned above, since most studies in the current literature only examine low-dimensional scenarios, the representativeness issue is implicitly avoided. But, then, the research community has not genuinely faced up to the very question in the age of PA—how to optimize site-specific management with a large number of variables.

To address the multiplicity problem and facilitate profitability assessment, we propose an algorithmic approach that enables each farmer to efficiently learn their own site-specific management through on-farm experiments. We emphasize the significance of on-farm experimentation, which is a way to efficiently navigate a high-dimensional variable space and obtain useful information for each individual (Griffin, 2018; Panten et al., 2010; Wolfert et al., 2017). Our approach is not to construct a rigid empirical model that assumes a specific number and type of variables; instead, it is a machine learning algorithm that is versatile enough to be used for learning optimal site-specific management in a wide range of farming scenarios, including both low- and high-dimensional cases. First, we mathematically formulate the farmer's problem as profit maximization. Then, we describe our learning algorithm to solve it. We demonstrate the algorithm's performance in a simulated environment. According to our results, complex site-specific management can be learned very efficiently through on-farm experiments within a few years, which is indeed more profitable and more environmentally sustainable than uniform management.

2 Materials and methods

2.1 Farmer's problem

Suppose that a farmer defines a grid of sites of equal size according to the capacity of variable rate technologies and yield monitor. That is, in each site, the farmer can uniquely identify and collect a pair of data (x, y)—applying management x and observing the corresponding yield y. The divided field may look as follows:

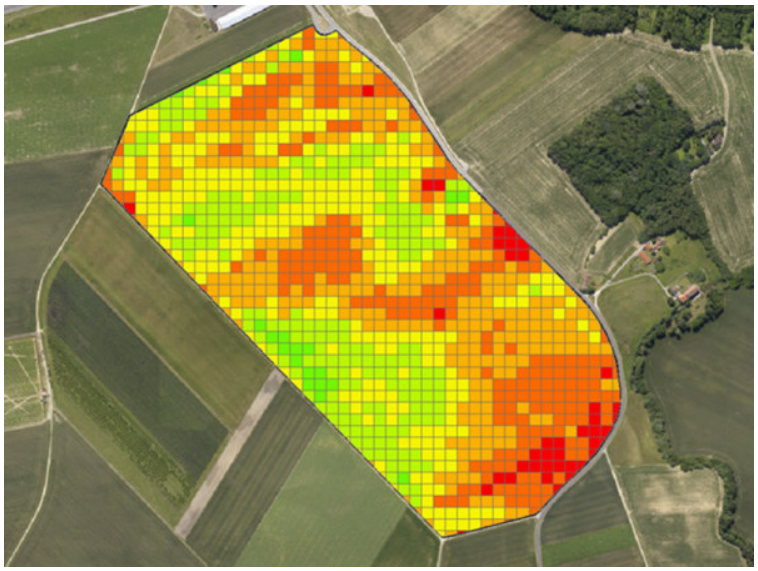

Figure 1: Example crop field divided into a grid of sites

Let M denote the total number of sites. Site $s \in \{1, 2, \dots, M\}$ is characterized by a state variable z_s, to which management x_s is applied. Then, a site-specific profit function is

$$\pi(x_s; z_s) = py(x_s; z_s) - c \cdot x_s,$$

where $y(x_s; z_s)$ is a site-specific yield function, p is an output price, and c is a vector of input prices. Notice that this is technically a partial profit as we subtract only the costs for modeled management x_s. Nonetheless, it is immaterial because our analysis is based on the difference between the profits of the site-specific management and the uniform management.

For conventional low-dimensional yield functions, it is common to use simple concave functions including quadratic (Bachmaier et al., 2009; Meyer-Aurich et al., 2010; Whelan et al., 2012), negative exponential (Edwards et al., 2005; Gaspar et al., 2015), and piecewise linear (Ouedraogo et al., 2018; Park et al., 2018). These simple functions may serve well for answering isolated questions such as optimality of a single management variable under a homogeneous condition. However, in high-dimensional cropping systems, the yield function is a fundamental source of the challenge because its uncertainty increases with the number of variables entering the function $y(\cdot; \cdot)$.

Note that each site need not be recognized as distinct or, equivalently, each z_s need not be distinct. A simple consequence of this assumption is that adjacent sites $\{s_1, s_2, \dots\}$ may have the same value $z_{s_1} = z_{s_2} = \dots$ and form a homogeneous "zone", which receives the same management. This is the framework commonly used to study site-specific management, particularly zone delineation, in the literature (Albornoz et al., 2018; Fraisse et al., 2001; Fridgen et al., 2004; Leroux et al., 2019; Li et al., 2007). Our formulation is more general and contains the existing one as a special case.

Having each site-specific profit defined, a field-level profit is simply the sum of the site-specific profits:

$$\sum_{s=1}^{M} \pi(x_s; z_s) = \sum_{s=1}^{M} py(x_s; z_s) - c \cdot x_s.$$

The farmer's objective is to learn optimal site-specific management x_s^* for all $s \in \{1, 2, \dots, M\}$:

$$(x_1^*, \dots, x_M^*) = \underset{x_1, \dots, x_M}{\operatorname{argmax}} \sum_{s=1}^{M} \pi(x_s; z_s).$$

In contrast, under the uniform management, a single management x is applied to every site s. Therefore, a field-level profit function is:

$$\sum_{s=1}^{M} \pi(x; z_s) = \sum_{s=1}^{M} py(x; z_s) - c \cdot x,$$

and the optimal uniform management $\bar{x}^*$ is:

$$\bar{x}^* = \underset{x}{\operatorname{argmax}} \sum_{s=1}^{M} \pi(x; z_s).$$

2.2 Solution algorithm

We construct an algorithm based on Bayesian optimization (BO) (Brochu et al., 2010; Shahriari et al., 2016), which is a class of numerical optimization techniques used for finding a global optimum of an unknown function. As with many other numerical optimization techniques, BO navigates the search space by examining a point at a time until it locates an acceptable point and halts. Since BO tries to optimize an unknown function, it needs a surrogate model to guide its search. For this purpose, Gaussian process (GP) statistical model is a standard choice in the literature.

BO has two features that makes it suitable for agricultural experiments (Saikai et al., 2019). First, GP as a nonparametric Bayesian model is so flexible that it can adapt to cases in which the objective function takes a complex shape. In high-dimensional precision agriculture, this will likely happen due to strong interactions among many variables involved. Second, BO is in general known for its sample efficiency, which means that BO can locate a good enough point with relatively a small number of examinations. Since agricultural experiments take time before obtaining results, typically a year, the sample efficiency is a desirable feature.

We assume that a single sample is collected from each site, making up M samples in each year. Though depending on the size of a site, in reality, a farmer will likely collect more than one sample from each site. If this is the case, the average value of all samples from the site may be treated as the sample for that site. While the basic BO sequentially processes one sample at a time, we modify it using the "batch expected improvement'' acquisition function proposed by Saikai et al. (2019) in order to process M samples at a time. In each year, it proceeds as follows:

1. Prescribes x_s for each s by maximizing the acquisition function $\alpha(x; z_s)$
2. Observes a yield $y(x_s; z_s)$ for all s
3. Computes the corresponding $\pi(x_s; z_s)$ for all s
4. Updates GP with $\{(x_s, z_s, \pi_s)\}_{s=1}^{M}$ and the samples from the preceding years

After completing the planned number of years of experiments, a candidate for x_s^* for each s can be obtained by maximizing the mean function of the learned GP with fixed z_s. Below is the complete algorithm.

Algorithm 1 Batch BO for site-specific management

1: **require:** T, M, $\mathcal{S}$, GP, α
2: **for** $t \in \{1, 2, \ldots, T\}$ **do**
3: $\quad \mathcal{I} \leftarrow \{\ \}$
4: $\quad \widehat{GP} \leftarrow GP$
5: $\quad$ **for** $s \in \{1, 2, \ldots, M\}$ **do**
6: $\quad\quad x_s \leftarrow \text{argmax}_x\, \alpha(x; z_s)$
7: $\quad\quad \mathcal{I} \leftarrow \mathcal{I} \cup \{(x_s, z_s, \underline{\pi})\}$ where $\underline{\pi} = \min\{\mathcal{S}_\pi\}$
8: $\quad\quad$ Update $\widehat{GP}$ with $\mathcal{S} \cup \mathcal{I}$
9: $\quad$ **for** $s \in \{1, 2, \ldots, M\}$ **do**
10: $\quad\quad y_s \leftarrow Oracle(x_s; z_s)$
11: $\quad\quad \pi_s \leftarrow p y_s - c \cdot x_s$
12: $\quad\quad \mathcal{S} \leftarrow \mathcal{S} \cup \{(x_s, z_s, \pi_s)\}$
13: $\quad$ Update GP with $\mathcal{S}$
14: **return** $M \times T$ number of samples

In terms of notation, T is the total number of years used for experimentation, $\mathcal{S}$ is a set of samples, $\min\{\mathcal{S}_\pi\}$ implies the minimum realized profit, $\alpha(\,\cdot\,; z_s)$ is an acquisition function for site s defined based on GP, and $Oracle(x; z)$ returns an observed yield when x is applied to a site characterized by z. Notice that in Line 2-8 an interim $\widehat{GP}$ is updated with a hypothetical observation ($\underline{\pi}$) so that we can collect a batch of M samples while using the sequential sampling algorithm. As a small detail, in Line 5, site s is chosen in a random order to avoid a systematic bias arising from how we number the sites. Another detail is that, when updating GP, we fit the hyperparameters of GP only to observed data (Line 13) and not to hypothetical data (Line 8).

2.3 Simulation experiments

To construct simulation environments, we make use of the Agricultural Production Systems sIMulator (APSIM), an advanced simulator of cropping systems (Holzworth et al., 2014) being widely used for various purposes such as generating synthetic datasets (Jin et al., 2018, 2019, 2017a; Lobell et al., 2013, 2014, 2015). In each environment, we run the algorithm to learn optimal site-specific management over T years and compare the profit resulting from implementing the learned site-specific management against the benchmark profit resulting from some uniform management. We assume this uniform management to be the one recommended by university extension services.

Depending on specific scenarios, we can customize the algorithm in many ways. Among interesting modifications is how to incorporate observational data that is already collected before the experimentation. When comparing against the uniform management as a status quo, a natural dataset assumed is what arises from implementing the uniform management as it represents the existing knowledge. We do so by initializing the GP embedded in the algorithm. Specifically, let $\{(\bar{x}, z_s, \bar{\pi}_s)\}_{s=1}^{M}$ be a set of the uniform management ($\bar{x}$), site characteristics (z_s), and the corresponding profits ($\bar{\pi}_s$). Then, before the algorithm starts a learning process, we fit the GP to these M data points. Note that the use of the uniform management for both benchmark and prior knowledge is merely for simplifying the illustration. In practical applications, farmers may use any benchmark management of interest (either uniform or not) and any existing dataset. Finally, since the algorithm itself involves some randomness, we conduct Monte Carlo simulations and present averaged results.

Though the algorithm's applicability is by no means limited to the scenario described in this section, given the access to the APSIM simulator, we construct an illustrative test bed as follows. We assume that there is only a medium amount of information about the sites and, as a consequence, uniform management is a reasonable practice. However, given the narrow profit margins common in agriculture, a farmer still wonders whether there is room for increasing profits even by a small amount with site-specific management. Specifically, the square field is divided into a grid of 25 sites ($M = 25$). All the sites are distinct, each of which is characterized by a state vector $z_s = (z_s^1, z_s^2)$ where z_s^1 is plant available water capacity (mm) and z_s^2 is organic carbon (%). We set $z_s^1 \in \{231, 259, 288, 317, 346\}$ and $z_s^2 \in \{2.56, 2.88, 3.2, 3.52, 3.84\}$ (± 10 or 20% from the mid values, which are the default values in the APSIM soil module we use).

231, 2.56	259, 2.56	288, 2.56	317, 2.56	346, 2.56
231, 2.88	259, 2.88	288, 2.88	317, 2.88	346, 2.88
231, 3.2	259, 3.2	288, 3.2	317, 3.2	346, 3.2
231, 3.52	259, 3.52	288, 3.52	317, 3.52	346, 3.52
231, 3.84	259, 3.84	288, 3.84	317, 3.84	346, 3.84

Figure 2: Simulated maize field divided into a grid of 25 distinct sites. In each pair of numbers, the first indicates plant available water capacity (mm) and the second indicates organic carbon (%) at that site.

We simulate a maize production system in Ames, Iowa with the weather data in 2013. In terms of management variables, we follow Saikai et al. (2019) and identify six variables $x = (x^1, \ldots, x^6)$ in the APSIM maize module:

- x^1 : sowing density (seeds/m^2)
- x^2 : sowing depth (mm)
- x^3 : row spacing (m)
- x^4 : N fertilizer amount before sowing (kg/ha)
- x^5 : N fertilizer amount at sowing (kg/ha)
- x^6 : N fertilizer amount for top dressing (kg/ha)

Using the information from the research and extension services of Iowa State University, we specify the uniform management ($\bar{x}$) as follows:

$$(\bar{x}^1, \bar{x}^2, \bar{x}^3, \bar{x}^4, \bar{x}^5, \bar{x}^6) = (8, 50, 0.76, 60, 60, 60).$$

$\bar{x}^1 = 8$, $\bar{x}^2 = 50$, and $\bar{x}^3 = 0.76$ follow from Elmore (2013) and Farnham (2001). The recommended total nitrogen amount is identified by using the Corn Nitrogen Rate Calculator (Sawyer, 2019), which gives us $\bar{x}^4 + \bar{x}^5 + \bar{x}^6 = 180$. We evenly split it into $\bar{x}^4 = \bar{x}^5 = \bar{x}^6 = 60$. Finally, for calculating profits, the output price is $p = \$0.177$/kg (Duffy, 2013), and the input costs are $c^1 = \$0.00364$/seed and $c^4 = c^5 = c^6 = \$1.29$/kg (Johanns, 2019). We assume no cost for sowing depth and row spacing, which implies the cost vector $c = (c^1, 0, 0, c^4, c^5, c^6)$.

Given the domain knowledge as well as common sense, when the algorithm searches for the optimal management, we restrict the search space to the following:

- $x^1 \in [6.0, 10.0]$ (seeds/m^2)
- $x^2 \in [25, 150]$ (mm)
- $x^3 \in [0.4, 1.0]$ (m)
- $x^4, x^5, x^6 \in [0, 200]$ (kg/ha)

Finally, 25 datapoints resulting from the uniform management $\{(\bar{x}, z_s, \bar{\pi}_s)\}_{s=1}^{25}$ is the only existing dataset incorporated prior to the experimentation, which has no variation in management x. To build up smoothly, in the first year, the algorithm randomly chooses x for each s from the range defined by $\pm 50\%$ of the benchmark uniform management.

3 Results

The following table and figure illustrate field-level profits ($/ha) from the site-specific management learned after T-year experiments. That is, a value for each $T \in \{1, 2, \ldots, 10\}$ means a profit if the farmer terminates the experiments after T years and implements the learned site-specific management.

Years (T)	1	2	3	4	5	6	7	8	9	10
Learned	1156	1259	1269	1280	1284	1285	1285	1287	1289	1289
Uniform	1244	1244	1244	1244	1244	1244	1244	1244	1244	1244
Difference	-88	15	25	36	40	41	41	43	45	45
										($/ha)

Table 1: Comparison of field-level profits from implementing the learned and uniform management.

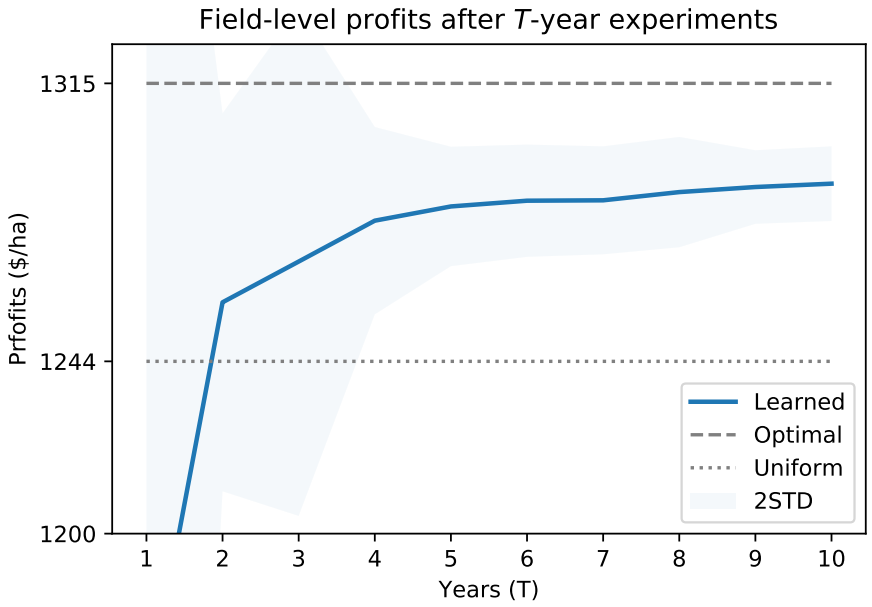

Figure 3: Learning curve of the algorithm with profits plotted against years of experiments. The shaded areas indicate two standard deviations around each mean field-level profit over Monte Carlo samples.

The shaded areas indicate two standard deviations around each mean field-level profit over the Monte Carlo samples. The dashed line indicates the profits from the optimal site-specific management, while the dotted line indicates the profits from the uniform management.

Since a field-level profit is the sum of the site-specific profits, next we provide a profit at each site. For the learned profits, we use $T = 5$ as the learning mostly levels off and the deviation from the mean prediction becomes small after four or five years. The following three heatmaps illustrate the site-specific profits from the learned and uniform management.

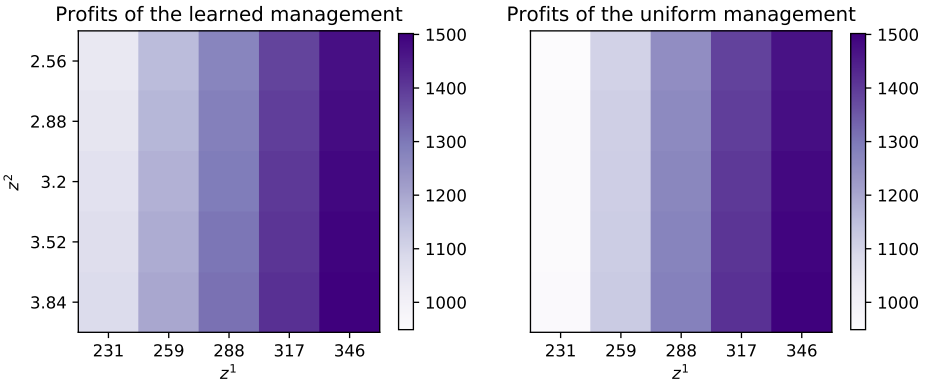

Figure 4: Site-specific profits for the learned and uniform management

The minimum and maximum profits from the learned management are \$1,037/ha and \$1,502/ha respectively, whereas those from the uniform management are \$949/ha and \$1,499/ha respectively. As clearly indicated in the panel for the uniform management, plant available water capacity (z^1) has much stronger influence on yield/profit than organic carbon (z^2). Also, in both state variables, the higher the values, the more fertile the site is (though hard to see in z^2).

Finally, we illustrate the learned site-specific management $(x^1, \ldots, x^6)$ after 5-year of experiments.

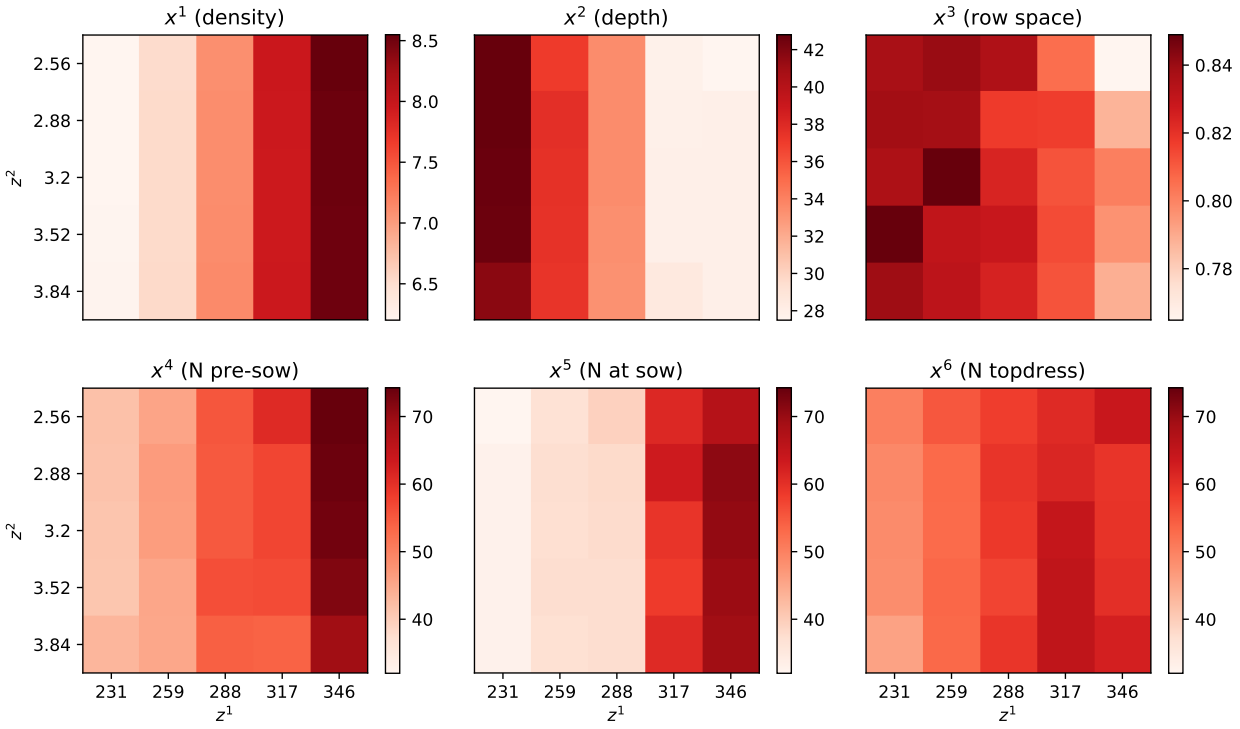

Figure 5: Learned site-specific management after 5-year experiments

The average sowing density is

$$\frac{1}{25}\sum_{s=1}^{25} x_s^1 = 7.3 \text{ seeds/m}^2,$$

and the average amount of total nitrogen fertilizer is

$$\frac{1}{25}\sum_{s=1}^{25}\sum_{i=4}^{6} x_s^i = 159 \text{ kg/ha}.$$

As a result, \$40/ha higher profit is achieved by using 0.7 fewer seeds/m^2 and 21 kg/ha less nitrogen than the uniform management.

4 Discussion

The results for field-level profit are aligned with our intuition. With only 1-year experiments, the farmer has little site-specific data, and therefore the algorithm has to explore for good candidate management. As a result, the profit for $T = 1$ is below that of the uniform management. Nonetheless, the algorithm quickly learns and its performance reaches the performance of the uniform management with only 2-year experiments. Thereafter, it continues to learn and widen the performance difference. With the 5-year learning, the estimated profit reaches \$1,289 or 98% of the maximum possible profit (\$1,315) in this environment. Considering the complexity of the site-specific management, which involves $25 \times 6 = 150$ choice variables, this is considered to be very efficient learning.

As seen in the large shaded area formed by two standard deviations around each mean prediction in Figure 3, due to the random sampling used in the first year, the mean prediction is not precise during the first two years. However, it dramatically improves after three years, and thereafter its spread continues to shrink.

The higher field-level profit of the learned management is due mainly to its higher profits from low-yielding sites ($z^1 \in \{231, 259\}$). In other words, the uniform management is excessively tailored to the high-yielding conditions ($z^1 \in \{317, 346\}$) leading to the decrease in profitability in the low-yielding sites where the optimal amounts are lower. As to the overall pattern in the learned site-specific management, we can see in Figure 5 that the higher plant available water capacity (z^1), the more inputs it receives. That is, in the heatmaps for x^1, x^4, x^5, and x^6, the color becomes darker as we move to the right.

We dismiss the patchy looking in x^3 as an artifact of numerical optimization, which strictly distinguishes two values whenever one results in even a minuscule amount higher than the other. Indeed, the color bar for x^3 has a very small range (0.78 – 0.84 in meter), indicating little practical significance.

Despite \$40/ha higher profit, the 5-year learned management uses only 154 kg/ha nitrogen fertilizer in total, which is much smaller than 180 kg/ha of the uniform management. In terms of the total yield, the learned management produces 9,933 kg/ha, whereas the uniform management produces 9,987 kg/ha. While the management optimization is guided by profit maximization, it turns out to be environmentally more friendly as well. This makes sense because both costs of fertilizer (i.e., to the profitability and to the environment) are aligned and simply the less, the better. However, higher yield does not necessarily coincide with higher profit as yield typically increases with more inputs, which reduces profit.

We have set out to learn site-specific management for maximizing profits because, to realize the other societal benefits of PA (i.e., food security and environmental sustainability), farmers' adoption

of PA must precede, which is in turn driven by profitability of PA. So, we have simplified the problem by exclusively focusing on learning profitable management. However, the balance between many benefits of PA need not be this extreme, and it is certainly possible to have a different goal and design an appropriate objective function that guides machine learning in a effective and efficient way.

Finally, despite the promising results, there are several clarifications and limitations to note for real-world implementations and future research.

- We assume no costs for switching management. In reality, however, there will likely be some forms of costs when changing management from site to site. For example, if a management choice is not an amount but a type of fertilizer, it may require human labor and incur non-trivial costs. Also, a high frequency for switching seeding rates may put a excessive strain on and damage an electric motor. For real-world applications, we need to incorporate these costs.
- When variables are theoretically continuous (e.g., seeding rate), we assume that it is possible to choose any arbitrary level and run the algorithm accordingly. In reality, however, choices of continuous variables are constrained for various practical reasons. For example, for a technical reason, we cannot change a fertilizer amount precisely by a fraction of a kilogram. Even though technically possible, it is economically infeasible to change row spacing every time an algorithm recommends a different value. Therefore, for real-world implementations, we need to modify those continuous factors into discrete ones.
- Considering the gap between the learned and the optimal profit (e.g., \$27 for $T = 10$), it is certainly possible to narrow the gap by engineering more sophisticated algorithms such as ones that evolves the search strategies as time goes. We have kept it simple so that we can highlight the generality of our approach and focus on the relative advantage against the uniform management.
- Our approach is limited to one-shot optimization. In other words, a farmer makes all the management decisions at the beginning of the year and wait to see results until the end of the year. In agriculture, many management choices are sequentially made within the year. To handle such more realistic situations, we need dynamic models in which feedback information and learning take place both within and across years.
- As to the temporal variation, we assume a single weather condition and stable site characteristics that prevail over T years. While this may hold or be acceptable in certain circumstances, it will be strong restriction in other circumstances. We are currently developing a model that incorporate temporal variations.
- In addition, we assume out spatial dependency, which means management x_{s_1} for site s_1 affects site s_2, which in turn affects back site s_1, and so on. This may not be negligible under some environments and/or with a very fine grid of sites. Combined with the temporal consideration above, ultimately we need to construct spatiotemporally dynamic models.

5 Conclusions

We have proposed an algorithmic approach to optimizing complex site-specific management with many management and environmental variables. It enables each farmer to efficiently learn their own site-specific management through on-farm experiments. We have also demonstrated its performance using a simulated environment. Our results have provided a positive answer to both the learnability

of complex site-specific management and the higher profitability than the uniform management. We hope that our approach will incentivize many farmers to utilize their own PA equipment and find more profitable management, which will in turn lead to the greater societal benefits.

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Appendices

Gaussian process

Gaussian process is a Bayesian nonparametric model, and its behavior is largely dependent on a choice of kernel and its hyperparameters (Rasmussen et al., 2006). A kernel is a function that returns a similarity measure $k(x, x')$ between two points x and x'. We use the Matérn kernel—a popular class of isotropic stationary kernels.

$$k_\nu(x, x') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{d}{\rho} \right)^\nu B_\nu \left(\sqrt{2\nu} \frac{d}{\rho} \right),$$

where Γ is the gamma function, B_ν is the modified Bessel function of the second kind, and d is a metric often induced by the Euclidean norm, i.e. $d = \|x - x'\|$. The Matérn kernel is characterized by two hyperparameters ν and ρ, which control, respectively, the smoothness and the scaling of distance. As standard in applied work, we do not estimate but rather handpick ν and write as Matérn_ν or $k_\nu(x, x')$. To simplify the notation, let r denote the scaled distance, $r = d/\rho$. An important property of the Matérn kernel is that when $\nu = p + 1/2, p \in \mathbb{N}$, it can be written as a product of an exponential and a polynomial of order p:

$$k_{p+1/2}(x, x') = \sigma^2 \exp\left(-\sqrt{2p+1} r \right) \frac{p!}{(2p)!} \sum_{i=0}^{p} \frac{(p+i)!}{i!(p-i)!} (2\sqrt{2p+1} r)^{p-i}.$$

Common choices of ν are $1/2, 3/2, 5/2$ and ∞, with each of which the kernel reduces to, respectively,

$$\begin{aligned}
k_{1/2}(x, x') &= \sigma^2 \exp(-r) \\
k_{3/2}(x, x') &= \sigma^2 \exp\left(-\sqrt{3} r \right) \left(1 + \sqrt{3} r \right) \\
k_{5/2}(x, x') &= \sigma^2 \exp\left(-\sqrt{5} r \right) \left(1 + \sqrt{5} r + \frac{5}{3} r^2 \right) \\
k_\infty(x, x') &= \lim_{\nu \to \infty} k_\nu(x, x') = \sigma^2 \exp\left(-\frac{1}{2} r^2 \right).
\end{aligned}$$

Matérn$_\infty$ is also known as squared exponential kernel or radial basis function. Following Snoek et al. (2012) and Stein (1999), we avoid squared exponential and use Matérn with $\nu = 3/2$ for our algorithm. The following figure plots $k_\nu(x, x')$ with $\sigma^2 = \rho = 1$ for $\nu \in \{1/2, 3/2, \infty\}$.

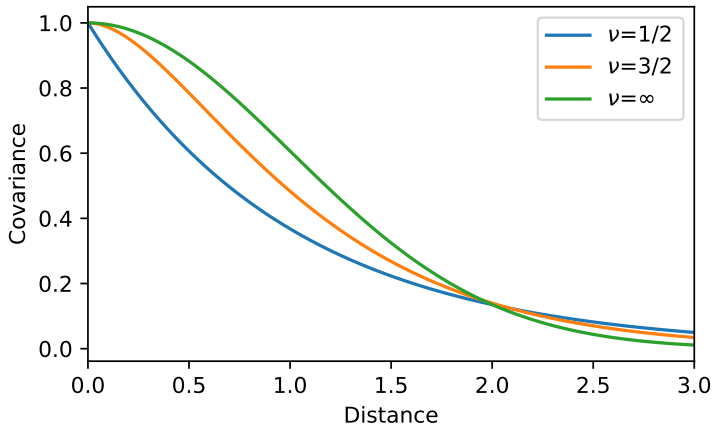

Figure 6: Matérn$_\nu$ kernels

Expected improvement acquisition function

In Bayesian optimization, an algorithm prescribes the next sampling point x based on how we value the mean and variance at x estimated by the accompanying GP. Specifically, the recommendation x_t for the next round t is determined by maximizing an acquisition function $\alpha(x|D_{t-1})$:

$$x_t = \operatorname*{argmax}_x \alpha(x|D_{t-1}),$$

where D_{t-1} is the data used to fit the GP at round $t-1$. The acquisition function is a reflection of the underlying utility of the next sample or our preference in selecting the next sampling point. It is heuristic and designed to trade off exploration of the search space and exploitation of the current promising areas. There are a number of acquisitions functions proposed in the literature. One of the popular acquisition functions is called expected improvement, which is constructed based on the following intuitive idea. Let y^* be the maximum value observed up until round $t-1$, i.e. $y^* = \max\{y_1, \ldots, y_{t-1}\}$. Then, we may define "improvement" at point x at round t to be

$$\max\{0, GP(x) - y^*\},$$

which is random as $GP(x)$ is a random function. Thus, the expected improvement acquisition function is defined to be:

$$\alpha_{EI}(x|D_{t-1}) = \mathbb{E}[\max\{0, GP(x) - y^*\}|D_{t-1}].$$

When using Gaussian process, at each point x in the domain, we have $GP(x) \sim \mathcal{N}(\mu(x), \sigma(x))$, which allows the expected improvement to have a closed form (Jones et al., 1998; Moćkus et al., 1978):

$$\alpha_{EI}(x|D_{t-1}) = \begin{cases} (\mu(x) - y^*)\Phi\left(\frac{\mu(x)-y^*}{\sigma(x)}\right) + \sigma(x)\phi\left(\frac{\mu(x)-y^*}{\sigma(x)}\right) & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0 \end{cases},$$

where Φ is the standard normal cumulative distribution function and ϕ is the standard normal probability density function.