Machine learning for optimizing complex site-specific management

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Abstract

Despite the promise of precision agriculture for increasing the productivity by implementing site-specific management, farmers remain skeptical and its utilization rate is lower than expected. A major cause is a lack of concrete approaches to higher profitability. When involving many variables in both controlled 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 optimization of site-specific management. We propose an algorithmic approach that enables each farmer to efficiently learn their own site-specific management through on-farm experiments. We test its performance in two simulated scenarios of medium complexity with 150 management variables and of high complexity with 864 management variables. Our results show that the learned site-specific management from, for example, 5-year experiments generates \$43/ha higher profits with 25 kg/ha less nitrogen fertilizer in the first scenario and \$40/ha higher profits with 55 kg/ha less nitrogen fertilizer in the second scenario 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, on-farm experiment

1 Introduction

Modern agriculture is faced with some of the most challenging problems in the 21st century such as farm profitability, food security, and environmental sustainability, all of which often require raising agricultural productivity. Site-specific management (SSM) emerges as an effective solution to the increased productivity [1–3] because, in principle, SSM can optimize a production system at a subfield level, which amounts to finer optimization of the overall system at a field level. Therefore, for both individual profitability and collective societal benefits, SSM has been advocated to farmers over the past two decades [4].

Despite the potential benefits for farmers, the adoption of SSM has been slower than expected [5, 6]. The most common reason for adopting SSM is, not surprisingly, relative advantage over the current management strategies [7]. In other words, the slower adoption is due largely to the lack of perceived profitability [8, 9]. Notice that there is a hidden assumption under this statement

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about profitability—farmers are able to optimally implement SSM. Even with the optimal SSM, there are not enough profits to justify the initial investment in equipment and the operational costs. However, since the advanced technologies used for implementing SSM are quite sophisticated and even intimidating, many farmers express their concerns about the complexity of the technologies and desires to keep things simple [10]. Consequently, we argue that, without concrete and proven procedures for optimal SSM, the profitability assessment is not reliable, and farmers cannot be fully convinced of the value of SSM [11–13]. This lack of actionable procedure or decision support systems for SSM is a serious problem in the existing literature [14].

The vast majority of SSM research investigates only a handful of management variables (often just one) in particular research environments, which is typically a total amount of nitrogen fertilizer [15–22], irrigation water [23, 24], or sowing densities [25, 26]. 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 [27, 28]. Within a single growing season, a number of decisions are made on types of activities (e.g., tillage, planting, fertilization, spraying, and harvest), their amounts, and their timings. Given that the overall effectiveness of SSM is determined by the totality of those decisions, independent studies of few management variables provide only partial knowledge and can be misleading as such complex systems typically involve significant nonlinearity [29, 30].

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 [31–33]. This problem is exacerbated in modern agriculture where the high dimensionality created by the advanced sensor technologies makes it even more difficult for selected cases to be representative, the problem called "the curse of dimensionality" in mathematics [34]. To give a sense of how specific a typical study setting is, note that Lo et al. [22] study nitrogen fertilizer SSM at the university extension research site in Nebraska which has been "under annual summer corn or soybean production without any tillage and any stover removal" with irrigation water applied through "a center pivot with sprayhead sprinklers positioned every other interrow at a height of 0.6 m above ground" using "GrowSmart Precision Variable Rate Irrigation system". Clearly, the problem is not each of these studies as it has a different objective even under the same topic of SSM. Rather, the problem is a lack of appropriate studies for optimizing complex SSM. In other words, since most of the existing studies 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 modern agriculture—how to optimize SSM with a large number of variables.

To address the multiplicity problem and offer an actionable procedure for SSM, we propose an algorithmic approach that enables each farmer to efficiently learn their own SSM through on-farm experiments. We emphasize the significance of on-farm experimentation [33, 35–37] to deal with both aspects of the multiplicity problem. First, on-farm experimentation allows farmers to adaptively design experiments and efficiently navigate a high-dimensional variable space [38]. Second, on-farm experimentation inherently circumvents the heterogeneity across farms. Particularly for SSM, use of field-scale experimentation is important to deal with spatial, infield variability [32, 39–41]. Our approach is not to construct a rigid empirical model that assumes a specific number and type of variables using a large observational dataset or so-called "big data". Big data in agriculture may be large in terms of sample size but, due to the very nature of observational data, unlikely contains sufficient variation in the high-dimensional space because without purposeful experimentation observed management choices mostly follow the standard recommendations from the existing low-dimensional representative studies. However, trials of unconventional management practices

are necessary for high-dimensional optimization with strong interactions among many variables, which can lead to unexpected optimal choices. To overcome the multiplicity problem, our approach is instead a machine learning algorithm that is versatile enough to be used for learning optimal SSM through on-farm experiments in a wide range of farming scenarios. The algorithm is based on Bayesian optimization [38], and capable to handle an arbitrary number of management and environmental variables and adapt to unexpected interaction effects. Moreover, if there exists historical data, large or small, it is simple to incorporate it as prior knowledge.

First, we mathematically formulate the farmer's problem as profit maximization. Then, we describe our machine learning algorithm to solve it. We test the algorithm's performance and versatility in two simulated environments with medium- and high-complexity. To underline the generality of our approach, we report all the results on a per-hectare basis so that they can be easily scaled. According to the results, complex SSM 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

Imagine a farmer who has access to some equipment for SSM but currently does not implement it due to the lack of knowledge, which is a typical story about SSM [14]. Suppose that the farmer is now interested in learning SSM through on-farm experiments. To conduct field-scale experiments, the farmer divides an entire field into a grid of sites of equal size according to the capacity of the 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:

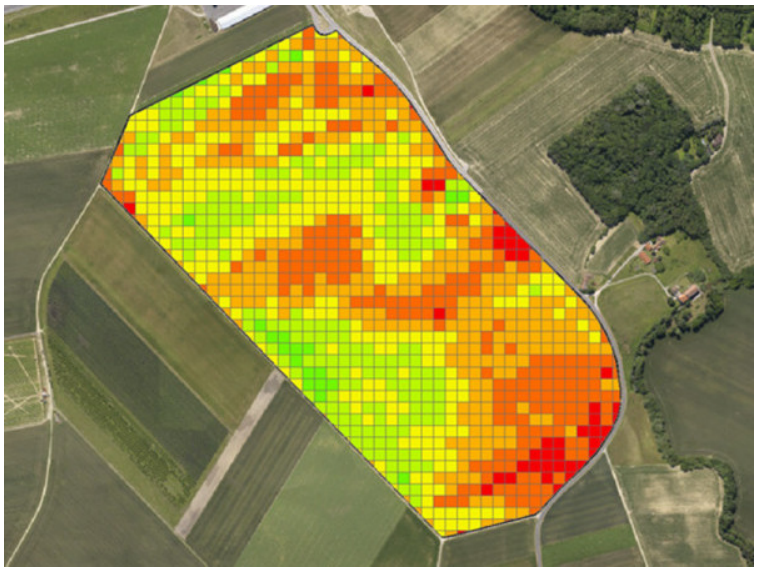


Figure 1: Example crop field divided into a grid of sites

Let M denote the total number of sites. Site $s \in \{1, 2, \ldots, M\}$ 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 SSM and the uniform management.

For conventional low-dimensional yield functions, it is common to use simple concave functions including quadratic [42–44], negative exponential [45, 46], and piecewise linear [47, 48]. 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 SSM, particularly zone delineation, in the literature [24, 49–55]. 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 SSM 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) [56, 57], 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 [38]. 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. [38] 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 SSM

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: $\quad\quad x_s \leftarrow \mathrm{argmax}_x\, \alpha(x; z_s)$
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: $\quad\quad\pi_s \leftarrow py_s - c \cdot x_s$
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 [58] being widely used for various

purposes such as generating synthetic datasets [59–64]. In each environment, we run the algorithm to learn optimal SSM over T years and compare the profit resulting from implementing the learned SSM 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 prior to 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 over the Monte Carlo samples.

Though the algorithm's applicability is by no means restricted to the scenarios described in this section, we rely on APSIM simulator and construct illustrative test beds within its capability. We simulate a maize production system in Ames, Iowa with the weather data in 2013, which is the most recent year available in APSIM. In terms of management variables, we follow Saikai et al. [38] 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:

$$(\bar{x}^1, \bar{x}^2, \bar{x}^3, \bar{x}^4, \bar{x}^5, \bar{x}^6) = (8, 50, 0.76, 67, 67, 67).$$

$\bar{x}^1 = 8$, $\bar{x}^2 = 50$, and $\bar{x}^3 = 0.76$ follow from Farnham [65] and Elmore [66]. The recommended total nitrogen amount is identified by using the Corn Nitrogen Rate Calculator [67], which gives us $\bar{x}^4 + \bar{x}^5 + \bar{x}^6 = 201$. We evenly split it into $\bar{x}^4 = \bar{x}^5 = \bar{x}^6 = 67$. Finally, for calculating profits, the output price is $p = \$0.177$/kg [68], and the input costs are $c^1 = \$3.64/1000$ seeds and $c^4 = c^5 = c^6 = \$1.29$/kg [69]. 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, in our demonstrations, datapoints resulting from the benchmark uniform management $\{(\bar{x}, z_s, \bar{\pi}_s)\}_{s=1}^{M}$ is the only existing dataset incorporated prior to the experimentation. Since they provide 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 uniform management.

2.3.1 Scenario A (medium complexity)

In this scenarios, we assume that a 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.

2.3.2 Scenario B (high complexity)

In this scenario, we imagine that the farmer possesses more precise equipment and capable to divide a field into more granular sites, namely, $16 \times 9 = 144$ sites. We also assume that the farmer has conducted more exhaustive soil tests, measuring four state variables (z^1, z^2, z^3, z^4) in each site:

- z^1: plant available water capacity (mm)
- z^2: organic carbon (%)
- z^3: nitrate-N (kg/ha)
- z^4: ammonium-N (kg/ha)

The addition of z^3 and z^4 is because of their significance [70] and availability in APSIM. Notice that nitrogen is also supplied by soil organic matter (z^1) through N-mineralization, creating stronger interactions among management and environmental variables [71]. Consequently, SSM in scenario B is even more complex than in scenario A. We generate a state vector for each site in a random but spatially correlated fashion, namely, random walk (see Appendices for details). Below are summary statistics of the generated state vectors for 144 sites.

- z^1: mean = 296, std = 32, min = 199, max = 365
- z^2: mean = 3.19, std = 0.31, min = 2.59, max = 3.90
- z^3: mean = 9.1, std = 0.98, min = 7.0, max = 11.5

- z^4: mean = 10.6, std = 1.6, min = 7.7, max = 14.1

Instead of writing down four numbers at each site, we illustrate the infield variability with a yield map arising from applying the uniform management to the generated field. Since each site receives the same management, the variability in yield indicates the variability in the underlying growing conditions.

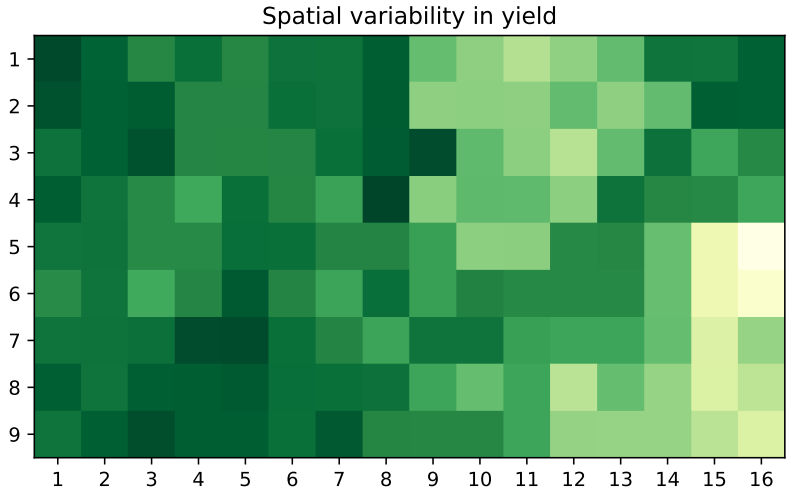


Figure 3: Yield map resulting from the uniform management in scenario B. Axis ticks are added to show the coordinates of each site. Since each site receives the same management, the variability in yield indicates the variability in the underlying growing conditions.

3 Results

3.1 Scenario A (medium complexity)

The following table and figure illustrate field-level profits ($/ha) from the SSM 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 SSM.

Years (T)	1	2	3	4	5	6	7	8	9	10
Learned	1103	1237	1266	1274	1277	1280	1283	1284	1285	1285
Uniform	1234	1234	1234	1234	1234	1234	1234	1234	1234	1234
Difference	-131	3	32	40	43	46	49	50	51	51
										($/ha)

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

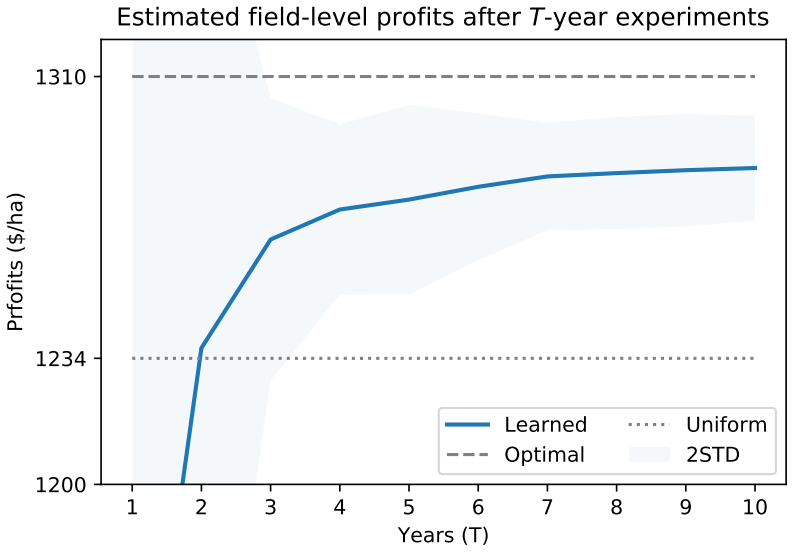


Figure 4: Learning curve of the algorithm with profits plotted against years of experiments in scenario A. The shaded areas indicate two standard deviations around each mean field-level profit over Monte Carlo samples.

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 SSM, 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 heatmaps illustrate the site-specific profits from the learned and uniform management.

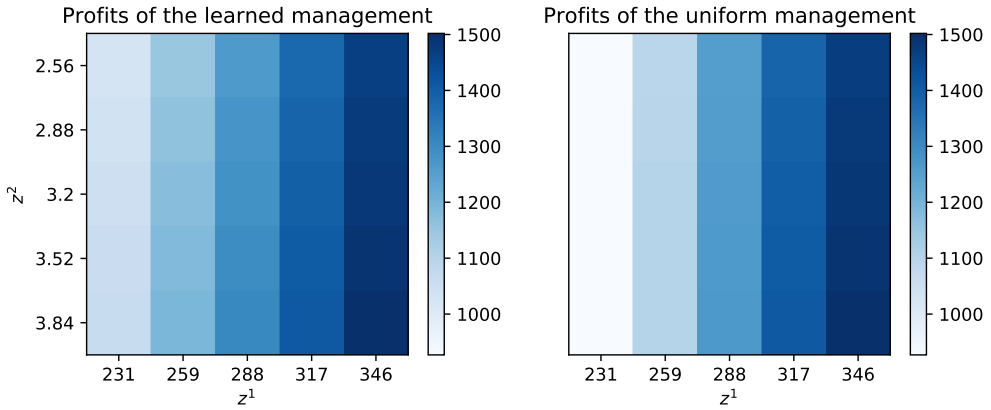


Figure 5: Site-specific profits for the learned and uniform management in scenario A

As 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). Since the overall patterns are quite similar, to highlight the difference, the following figure illustrates the difference at each site.

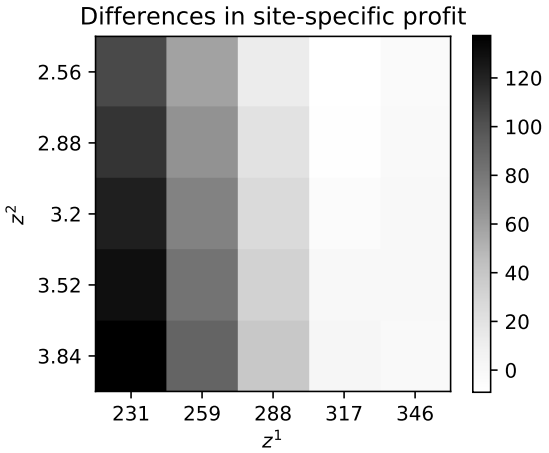


Figure 6: Differences in site-specific profit in scenario A. The maximum difference is \$138/ha at site (231,3.84), whereas the minimum difference is \$-9.4/ha at site (317,2.56).

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

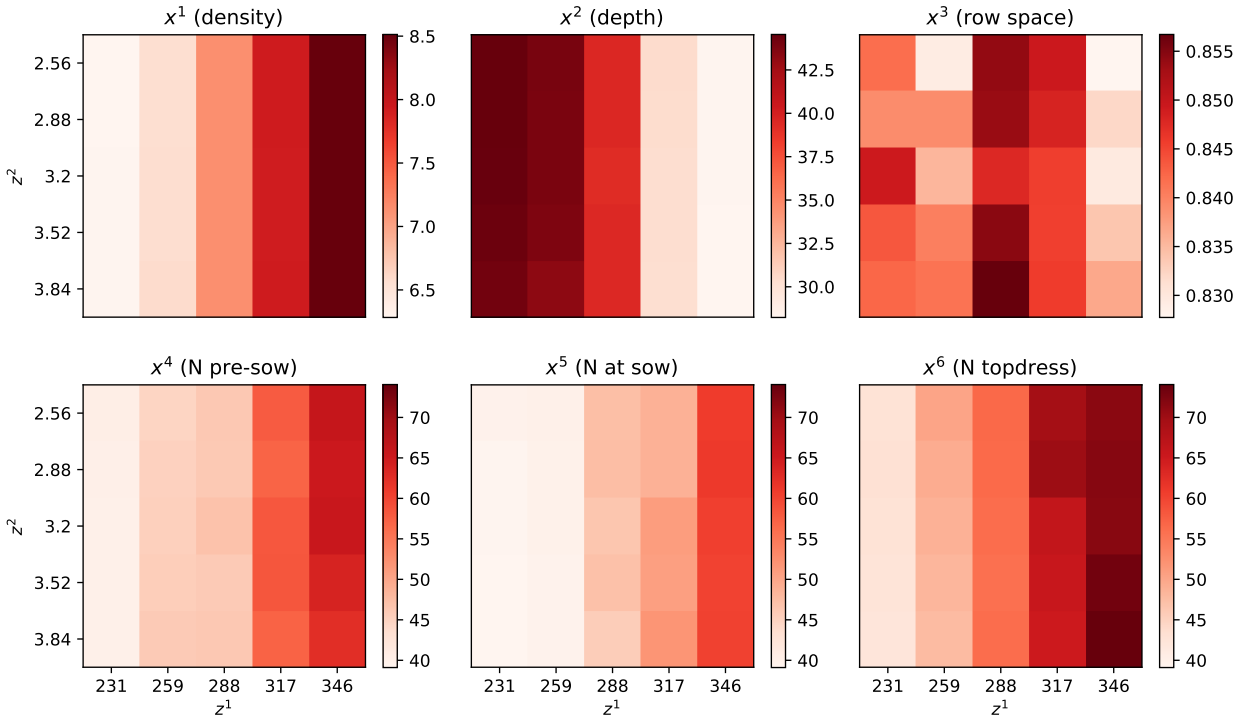


Figure 7: Learned SSM after 5-year experiments in scenario A. The average sowing density is 7.3 seeds/m^2, and the average amount of total nitrogen is 156 kg/ha.

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

$$\frac{1}{25}\sum_{s=1}^{25}\sum_{i=4}^{6} x_s^i = 156 \text{ kg/ha}.$$

As a result, \$43/ha higher profit is achieved by using 0.7 fewer seeds/m^2 and 45 kg/ha less nitrogen than the uniform management. To further emphasize the generality and robustness of our algorithmic approach, results from other years than 2013 are also provided in Appendices.

3.2 Scenario B (high complexity)

The following table and figure illustrate field-level profits (\$/ha) from the SSM 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 SSM.

Years (T)	1	2	3	4	5	6	7	8	9	10
Learned	1319	1324	1331	1333	1335	1335	1336	1337	1338	1339
Uniform	1295	1295	1295	1295	1295	1295	1295	1295	1295	1295
Difference	24	29	36	38	40	40	41	42	43	44
										(\$/ha)

Table 2: Comparison of field-level profits from implementing the learned and uniform management in scenario B.

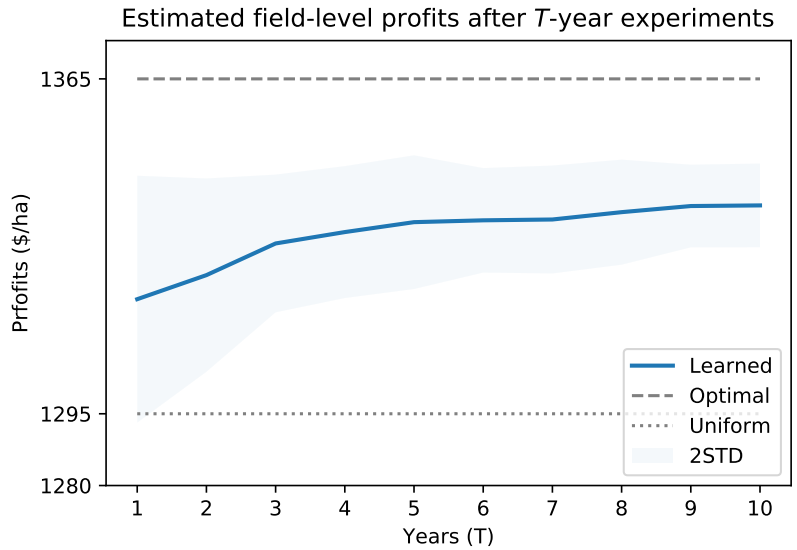


Figure 8: Learning curve of the algorithm with profits plotted against years of experiments in scenario B. The shaded areas indicate two standard deviations around each mean field-level profit over Monte Carlo samples.

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 SSM, while the dotted line indicates the profits from the uniform management.

The following heatmaps compare the site-specific profits from the learned at $T = 5$ and uniform management.

Figure 9: Site-specific profits for the learned and uniform management in scenario B

As in scenario A, the overall patters are very similar. The SSM, however, has higher profits (darker colors) in low-yielding sites. The following figure illustrates the difference at each site.

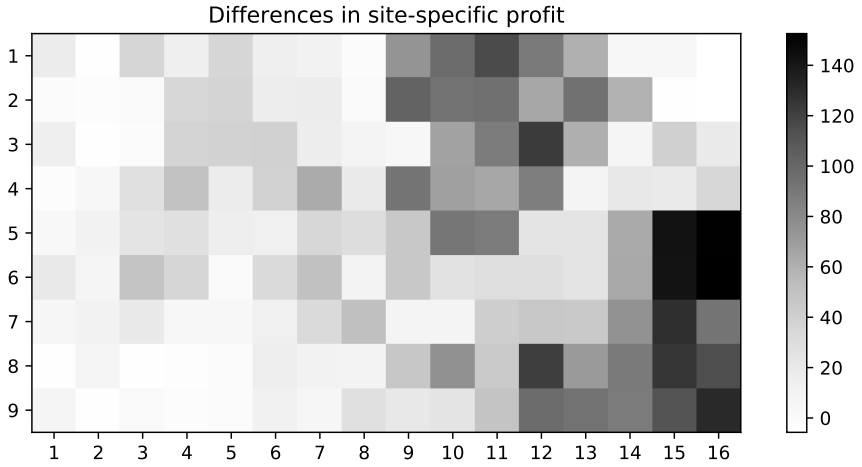
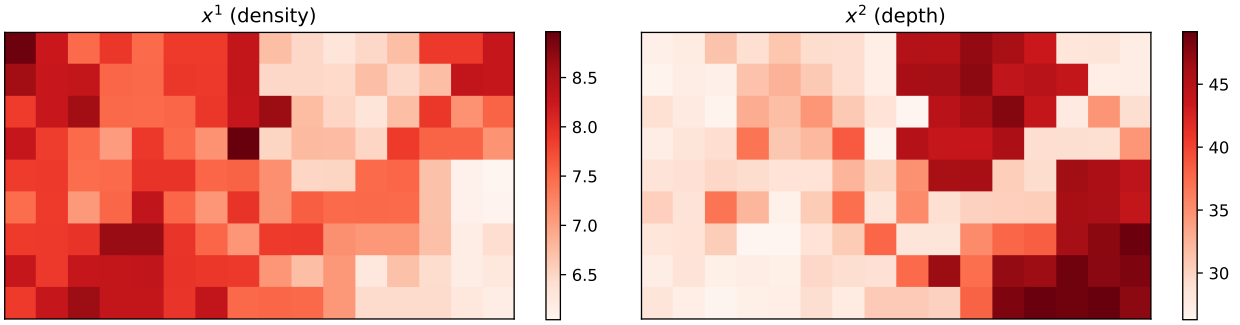


Figure 10: Differences in site-specific profit in scenario B. The maximum difference is \$153/ha at site (16,6), whereas the minimum difference is \$-5.7/ha at site (8,1).

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



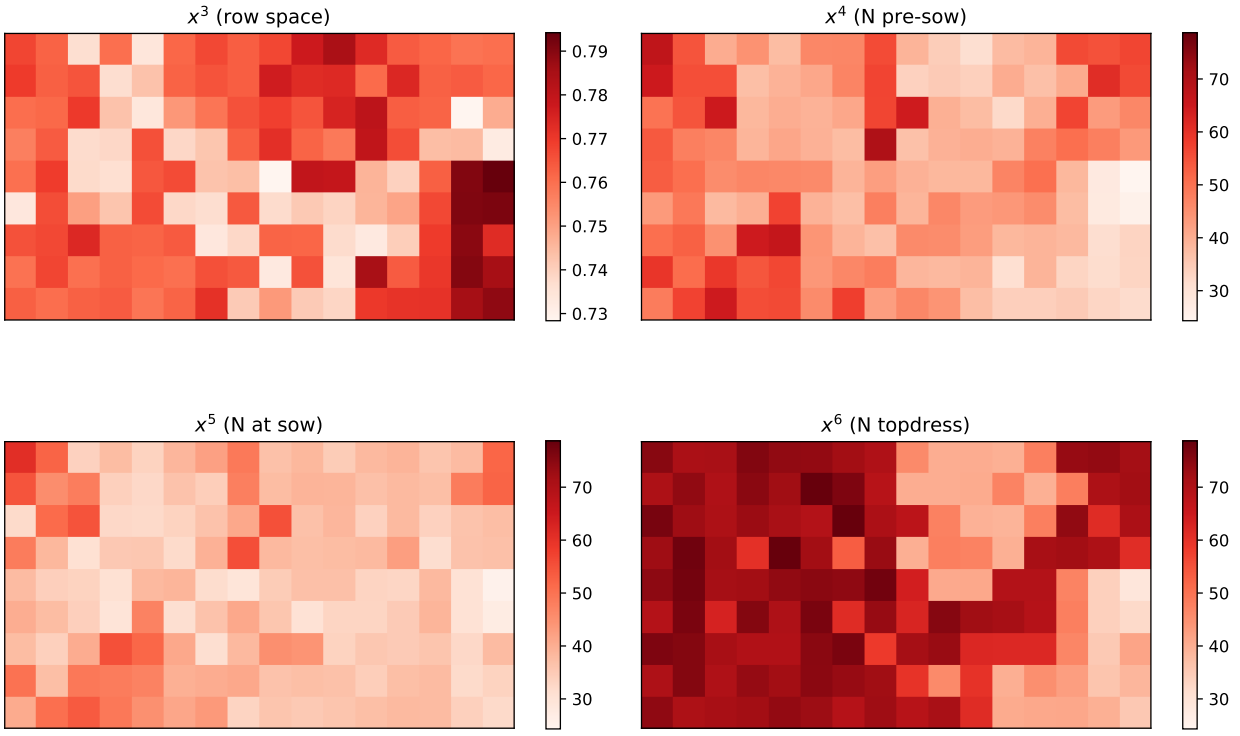


Figure 11: Learned SSM after 5-year experiments in scenario B. The average sowing density is 7.4 seeds/m^2, and the average amount of total nitrogen is 146 kg/ha.

The average sowing density is

$$\frac{1}{144}\sum_{s=1}^{144} x_s^1 = 7.4 \text{ seeds/m}^2,$$

and the average amount of total nitrogen fertilizer is

$$\frac{1}{144}\sum_{s=1}^{144}\sum_{i=4}^{6} x_s^i = 146 \text{ kg/ha}.$$

As a result, \$40/ha higher profit is achieved by using 0.6 fewer seeds/m^2 and 55 kg/ha less nitrogen than the uniform management.

4 Discussion

The results for field-level profit in Table 1,2 and Figure 4,8 are well aligned with our intuition. When the algorithm starts with little existing data incorporated, it is difficult to identify good management. This is particularly the case in scenario A, in which the profit from the learned management after 1-year experiment is far below that of the uniform management. In contrast to scenarios A, good management is found even after 1-year experiment in scenario B because, although most sites are technically distinct, some sites are similar and provide mutual information. As a result, the greater number of sites in the field, the more information collected each year. Despite the low performance in the first year in scenario A, the algorithm quickly learns and its performance surpasses the performance of the uniform management after 2-year experiments. Both scenarios, the algorithm continues to learn and widen the performance gap. With 5-year learning,

the estimated profit reaches \$1,274 or 97% of the maximum possible profit (\$1,310) in scenario A and \$1,335 or 98% of the maximum possible profit (\$1,365) in scenario B. Given the complexity of the SSM, which involves $25 \times 6 = 150$ (scenario A) and $144 \times 6 = 864$ (scenario B) management variables, this is considered to be very efficient learning.

The random sampling used in year 1 crates the large shaded area formed by two standard deviations around the mean predictions over the first few years in scenario A (Figure 4), indicating that imprecise mean prediction. However, it dramatically improves after four years, and thereafter its spread continues to shrink. Combined with the increasing mean profits, this is a desirable feature because it implies that no matter how the algorithm starts off, after several years, good SSM is consistently learned. This impreciseness is mostly absent in scenario B due to the the larger sample size from the beginning (Figure 8).

As seen in Figure 5,6,9, and 10, the higher field-level profits of the learned management are due mainly to their higher profits from the low-yielding sites (e.g., sites with $z^1 \in \{231, 259\}$ in scenario A and sites around (11,2) and (15,7) in scenario B). In other words, the uniform management is excessively tailored to the high-yielding conditions—$z^1 \in \{317, 346\}$ in scenario A and the left half of the field in scenario B—leading to the decrease in profitability in the low-yielding sites where it is optimal to put less inputs. Overall, albeit not necessarily true in other environments, in these particular scenarios, the algorithm discovers that it is profitable to put more inputs in the high-yielding sites and less in the low-yielding sites as indicated in panels for x^1, x^4, x^5, and x^6 in Figure 7 and 11.

We dismiss the patchy looking of x^3 in Figure 7 and Figure 11 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 (0.830–0.855 in scenario A and 0.73–0.79 in scenario B), indicating little practical significance.

In both scenarios, the learned SSM is evidently more efficient than the benchmark uniform management. After 5-year experiments, the learned management generates \$43/ha higher profit with 25 kg/ha less nitrogen in scenario A and \$40/ha higher profit with 55 kg/ha less nitrogen in scenario B. In terms of the total yield, the learned management produces 210 kg/ha less maize in scenario A and 278 kg/ha less maize in scenario B. While the SSM optimization is guided by profit maximization, it turns out to be environmentally more sustainable 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 SSM for maximizing profits because, to realize the other societal benefits of SSM (i.e., food security and environmental sustainability), farmers' adoption of SSM must precede, which is in turn driven by profitability of SSM. So, we have simplified the problem by exclusively focusing on learning profitable management. However, the balance between many benefits of SSM 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 an 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 in profit between the learned and the optimal management (e.g., \$23 in scenario A and \$26 in scenario B 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 individual farmers to efficiently learn their own site-specific management through on-farm experiments. We have demonstrated its performance using simulated environments. Our results have provided a positive answer to both the learnability of complex site-specific management and the higher profitability than the uniform management. Given the strong support for our approach, real-world field experiments seem warranted to empirically validate the simulated results. We also hope that our approach will empower and incentivize many farmers to utilize their own equipment and find more profitable management, which will in turn lead to the greater societal benefits such as food security and environmental sustainability.

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Appendices

APSIM configuration

As a basis, we use the Continuous Maize module in APSIM. Then, we modify its default settings as follows. To simulate maize production in Ames, Iowa.

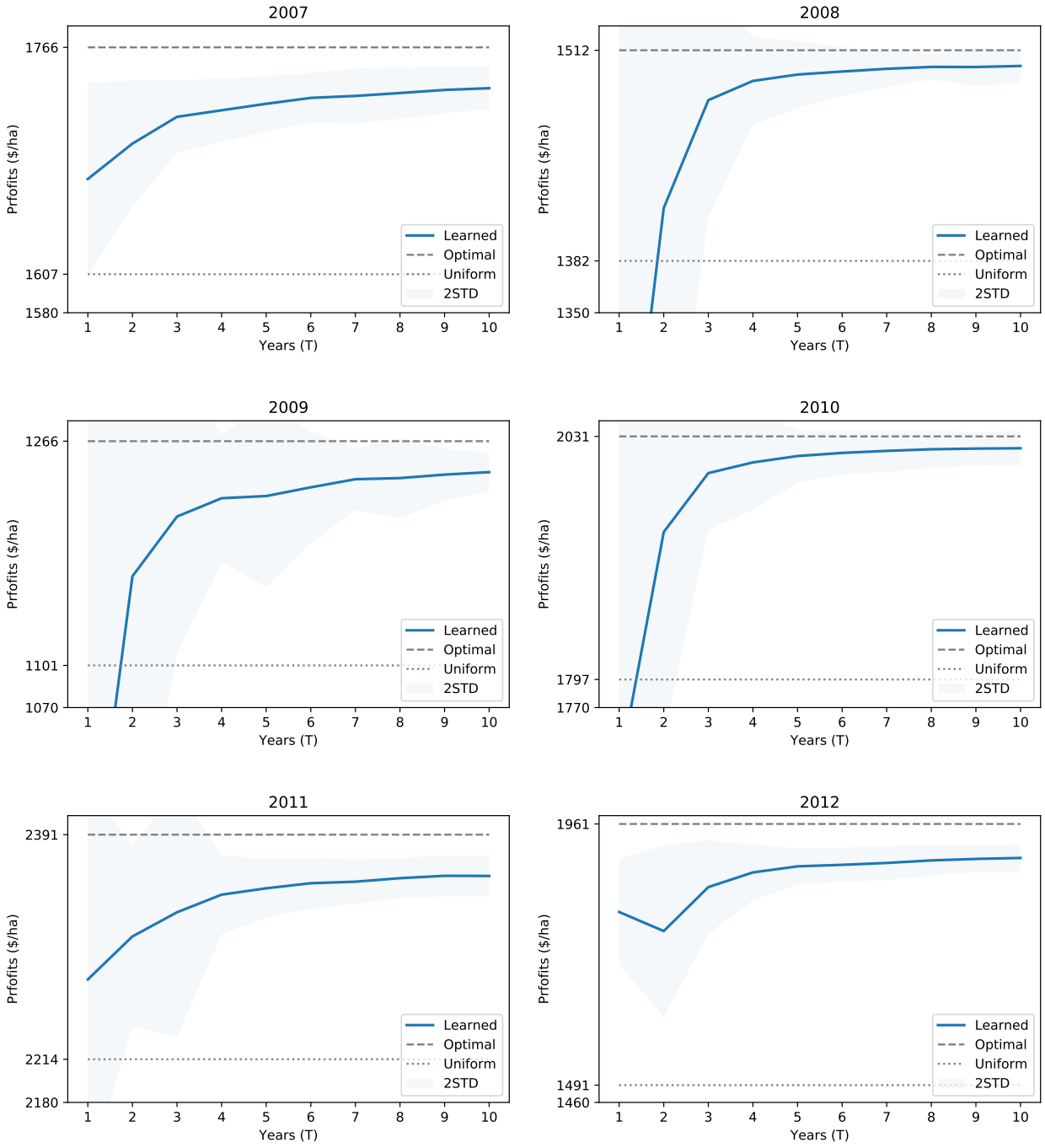
- Metfile: USA_Iowa_Ames.met
- Calendar: Jan 1, 2013 - Dec 31, 2013
- Cultivar: Pioneer 3394
- Sowing window START data: 15-apr
- Sowing window END data: 2-may
- Soil: Iowa Nicollet soil series
- Initial nitrogen: 0 kg/ha for both NO3 and NH4 for scenario A
- Initial water: 80% filled from top

Sensitivity analysis

In addition to two simulated environments with medium- and high-complexity, to further emphasize the generality and robustness of our algorithmic approach, we conducted simulation experiments in different years than 2013. Since output price, input prices, and weather are all dependent on a particular year, the differences in year provide different environments for profit maximization. The price information for each year was obtained from the same sources [68, 69].

Year	2007	2008	2009	2010	2011	2012
Output price ($/kg)	0.17	0.16	0.14	0.21	0.24	0.27
Seed price ($/1000 seeds)	1.82	2.10	3.13	3.44	3.25	3.40
Nitrogen price ($/kg)	0.69	1.02	1.51	0.73	1.13	1.40

Note that all sensitivity analysis was conducted under the environments with medium complexity, because of the significantly greater computational resources required in environments with high complexity. While there were considerable variations in both the growing and economic conditions across the different years, overall, the algorithm is quite versatile and able to learn good SSM within a few years in every environment. Similar to Figure 4, for each environment, we plot estimated field-level profits after T-year experiments.



Constructing scenario B

To generate a state vector $z = (z^1, z^2, z^3, z^4)$ for each site, we need to choose which site s and what values for $(z_s^1, z_s^2, z_s^3, z_s^4)$. For both purposes, we use random walk. Start from the mid site $(9, 5)$ with the initial values $(288, 3.2, 10, 10)$ assigned. Then, with probability of $1/3$, randomly either move right, move left, or stay. Similarly, with probability of $1/3$, randomly either move up, move down, or stay. This gives us the next site to consider. If the move means hitting a boundary, it stays at the site. Once moving into the new site, see if the site has already been assigned a state

vector. If not, with probability of 1/3, randomly perturb the state vector at the originating site by either -5%, 0%, or 5%. Continue the process until all sites are assigned a state vector.

Gaussian process

Gaussian process is a Bayesian nonparametric model, and its behavior is largely dependent on a choice of kernel and its hyperparameters [72]. 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_∞ is also known as squared exponential kernel or radial basis function. Following Snoek et al. [73] and Stein [74], 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 $\nu \in \{1/2, 3/2, \infty\}$.

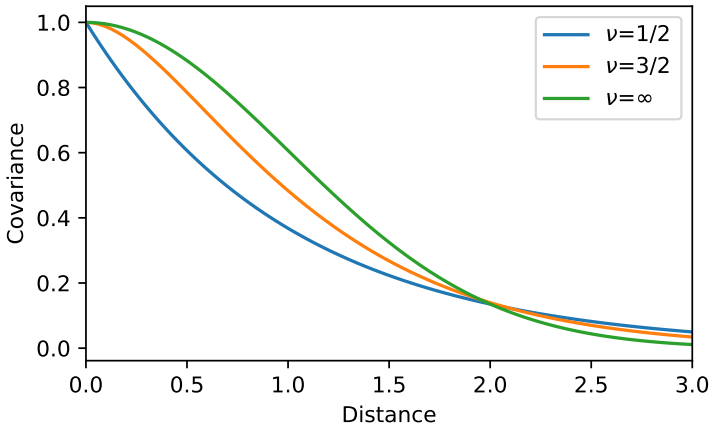


Figure 12: Matérn$_\nu$ kernels

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 $\alpha(x|D_{t-1})$:

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

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 [75, 76]:

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

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