Learning optimization models in the presence of unknown relations

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Abstract

One of the difficulties in solving multiagent optimization problems is to construct an optimization algorithm describing the properties of a multiagent system that may be unknown to a centralized decision maker. For instance, in a sequential resource allocation problem with multiple buyer agents, it is highly challenging for the seller to decide on an optimal ordering of the resources to sell that maximizes the social welfare, as agents may be unwilling or it could be too expensive to share their own preferences over resources. In this paper, we demonstrate how to learn such an optimization model from data. Given the learned model, we propose several constructions to map it into integer linear programs that can directly be used for optimization.

We use an auction simulator and design several experiments to test the performance of the proposed method. Our experiments show that optimization based on historical data results in high social welfare. Furthermore, we compare our white-box approach with a black-box best first search approach and show its advantages over the black-box method. Our results indicate that the white-box method outperforms black-box when the models are not overly complex.

1 Introduction

One of the main challenges of mathematical optimization is to construct a mathematical model describing the properties of a system. In the mathematical optimization literature, when the structure of the system cannot be fully determined from the hypotheses at hand, machine learning and data mining techniques have been used to replace a decision model structure. For instance, Li and Olafsson [15] use a decision tree to learn dispatching rules that are then used to decide which job should be dispatched first. Brijs et al. [5] build a decision model as an integer program that maximizes product assortment of a retail store. The decision model is then refined by incorporating additional decision attributes that are the learned patterns from recorded sales data. Gabel and Riedmiller [9] show how reinforcement learning based on a neural network function

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approximation can be used to schedule the jobs in a distributed job-shop scheduling problem.

The challenges arising from unknown system structures for optimization are amplified in multiagent problems, due to the fact that agents are autonomous and their environment is changing and dynamic. Thus, in multiagent optimization problems, when agents are unwilling or impossible to share their local information, finding an optimal solution is difficult. In this paper, we adopt the idea of using machine learning and data mining techniques to construct a model for solving multiagent optimization problems. We demonstrate how to learn such models entirely from data by mapping the results from machine learning directly into integer linear programs (ILP) used for mathematical optimization.

Many studies have investigated the interplay of data mining and machine learning with mathematical modeling techniques, see e.g., [1, 17]. However, to the best of our knowledge, models learned from historical data have only been used in a black-box fashion, e.g., using only the predictions of learned models and not their internal structure. These predictions have for example been used as decision values [9], fitness functions [13], or model parameters [15]. In contrast to these black-box approaches, we propose a novel “white-box” optimization method, that is, we map a learned regression tree model entirely to a set of integer linear programming constraints. In our approach, therefore, all the properties of the learned models are visible as constraints to a mathematical problem solver. This solver can use sophisticated branching and cutting techniques on these constraints when finding solutions, which is impossible in black-box optimization. To the best of our knowledge, this promising way of using the results of machine learning is entirely novel. In addition, such a solver can provably find the optimal sequence given the learned model, without testing all possible solutions.

We illustrate our approach using a multiagent resource allocation problem. In this problem, the buyer agents require specific resources to achieve their goals and a seller is responsible for allocating resources. We assume that the resource allocation is done by sequential auctions, where the available resources are sold consecutively by the seller. A resource is rewarded to the buyer who values it most. There are many examples of such a sequential resource allocation problem in practice, such as sequential procurement for school milk [16], and the Dutch flower auction [24].

We measure the outcome of an allocation by the total values collected over all of the sold resources. Previous research has shown that such sequential resource allocation outcome is heavily dependent on the ordering of resources to be sold [8, 12, 20], especially when agents have budget or capacity constraints [18], or when agents have combinatorial preferences over bundles of resources [3, 23]. Budget or capacities constraints are often seen in real-world problems such as in industrial procurement [10]. Combinatorial preferences of agents are also commonplace. For example, obtaining one resource (i.e., a truck) without another resource (i.e., fuel) makes the first resource worthless. The optimization problem that we study here is therefore how to order a given set of resources to be allocated such that the expected allocation value is maximized, in the presence of unknown preferences and capacities of agents.

When agents represent different individuals or companies, their constraints and preferences are typically unshared. This poses a first hurdle for the optimization. A possible approach to tackle this difficulty would be to learn the constraints and the
preference functions of the agents. We could then use these estimated functions to try to find an ordering with the highest value. However, learning preferences of agents in combinatorial domains is hard [21], even when interacting with them as users, not to mention learning one for every agent. As historical data contains much less information than user queries, in this paper, we instead focus on learning the overall preferences of the group of buyer agents. First, we collect historical resource allocation data from an auction simulator. We then compute feature values that are linked with capacity constraints and combinatorial preferences, and learn regression trees from these feature values (Section 3). The optimization problem remains difficult (NP-complete) using this restricted representation of the agent’s constraints and preferences. To build an optimization model, we map the learned trees to an integer linear program (Section 4). An ILP-solver (CPLEX) is used to find a good ordering for a new set of items. We evaluate the found ordering using the regression tree models and the auction simulator (Section 5). Our results show that orderings with a high expected value according to the regression trees often correspond to actual high value orderings in the simulator. We compare our method with a black-box optimization approach: best-first search with dynamic programming cuts. Our ILP method outperforms the black-box method on problems where the models are not overly complicated. When the learned regression tree models become larger, the black-box method outperforms ILP. This is to be expected since the black-box approach does not model this complexity while the ILP models get significantly larger and thus more difficult to solve. In addition, both our white-box and black-box method significantly outperform existing (naive) ordering strategies suggested by the literature [23]: most valuable first and least valuable first.

Although we use resource allocation by sequential auction to illustrate our method, all of our constructions are general and can be applied to any optimization setting where unknown relations can be represented using regression trees that have been learned from data. Furthermore, the feature values need to be computable using (integer) linear functions from intermediate solutions. We highlight that our approach tries to find an optimal ordering entirely before execution, instead of the more common approach of building a solution one-by-one in a sequential manner, see, e.g., [9, 25]. Our approach can thus be applied to complex optimization settings where entire orders, schedules, or plans need to be constructed beforehand. Our main contributions are as follows:

1. We provide the first translation from a learned regression tree model into an integer linear program that can be used directly as a component in mathematical optimization.

2. We demonstrate the feasibility of our approach using a challenging problem in multiagent resource allocation with unknown information. The obtained performance clearly shows the large potential of machine learning in these kinds of optimization problems.

2 The sequential resource allocation problem

We assume there is a finite set of agents. Let $R = \{r_1, \ldots, r_l\}$ denote the collection of the resource (or item) types, and the quantity of each resource type can be more than
1. When it is clear from the context, we will slightly abuse the notation and use $S = \{r_1, r_2, \ldots, r_1, \ldots\}$ to denote the multiset of all available resources. Each buyer agent $i$ has a valuation for each type of resource or each bundle of different resource types $v_i : 2^R \to \mathbb{R}^+$. We assume agents have combinatorial preferences over resources. The resources $r_1, r_2 \in R$ are complementary for agent $i$ if $v_i(r_1) + v_i(r_2) < v_i(r_1 \cup r_2)$, and substitutes if $v_i(r_1) + v_i(r_2) > v_i(r_1 \cup r_2)$. In addition, each agent has a budget constraint on purchasing resources.

In one allocation, a set of resources $S$ with type set $R' \subseteq R$ will be auctioned sequentially using a predetermined order. At the beginning of one sequential auction, each agent $i$ has a fixed amount of money which it can use to buy resources. For each resource $r_j$ that is being auctioned, agent $i$ puts a bid on $r_j$ based on its valuation function if its remaining money allows. The agent who bids highest on $r_j$ wins $r_j$. This sequential auction ends when all resources have been auctioned, or when all agents run out of their budgets.

There are many different options when detailing this auction setting. For ease of explanation, we simulate a simple auction setting where agents bid truthfully. The agents bid their true value based on the valuation function, which is determined by partitioning the set of resources that are in the agent’s possession and bundles such that the sum of their values is maximized. This difference in value before and after adding the current resource to the agent’s possessions is the agent’s true value.

We assume that the auction is repeated over time, and each auction sells possibly different resources $S$. At the end of each sequential auction, we have the following information at our disposal: (1) the ordering of auctioned resources; and (2) the allocation of resources to agents with their winning bids. The optimization problem in such sequential auctions is: given a set of resources $S$, deciding the ordering of resources such that the expected allocation value is maximized.

We use the following simple examples to demonstrate the importance of ordering on the total allocation value. The first example considers budget constrained agents.

**Example 1** Two agents $A_1$ and $A_2$ take part in a sequential resource allocation. For sale are resource $r_1$ and resource $r_2$. Agent $A_1$ values both resources $r_1$ and $r_2$ 5, and agent $A_2$ wants only $r_2$ with a value of 4. In addition, both $A_1$ and $A_2$ have a budget limit of 5. Consider one situation where the seller auctions first $r_1$ and then $r_2$. In this case $A_1$ will get $r_1$ with price 5, and then $A_2$ will win $r_2$ as $A_1$ has no money left. The total value collected is then 9. However, if $r_2$ is auctioned before $r_1$, $A_1$ will win $r_2$ with price 5, and $r_1$ will not be sold since $A_2$ is not interested in it. In this situation, the total value collected becomes 5.

In the second example, agents desire resources with complementarities.

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4In this paper, we simply assume that there exists a mechanism that incentivizes agents to bid based on their true valuation functions. We are not interested in the bidding strategies. Designing good bidding strategies for agents is topic of another line of research (see, e.g., [3]). Implementing such strategies would therefore only distract from our main contribution: the general ILP formulation of learned regression trees. However, our approach can be applied to other auction formats with more complex and realistic bidding strategies of agents. It works whenever regression trees are able to provide reliable predictions of the bidding values.
Example 2 Suppose given $r_1$ and $r_2$, agent $A_2$ only desires $r_2$ with value 5. $A_1$ has complementary resources, i.e., $A_1$ values $r_1$ and $r_2$ with 1 and 1 respectively if he wins only $r_1$ or $r_2$ at the end of the auction, however, if he wins both resources $r_1$ and $r_2$, the value $v(r_1 \cup r_2)$ goes up to 10. It is quite obvious that in this case, the auctioneer should sell $r_1$ first as it will end up with revenue 10, in contrast to 6 if $r_2$ is sold first.

When we know the agent’s true preferences, this problem is NP-hard since the resource ordering can be used to simulate the allocation of goods to agents in a combinatorial auction, which is well-known to be NP-complete [6]. We now prove it remains hard when the agents only have budget constraints:

Theorem 1 Given a set of resources $R$ and non-combinatorial preferences $v_i : R \rightarrow \mathbb{R}^+$ and budgets $b_i$ for every bidder $i$. The problem of deciding whether there exists an ordering that obtains social welfare at least $K \in \mathbb{R}^+$ is NP-hard.

Proof 1 By reduction from the NP-hard partition problem \cite{11}: Given a set of integers $I = \{i_1, \ldots, i_n\}$, is $I$ dividable into two sets $A$ and $B$ such that $\sum A = \sum B$? We need two bidders with preferences such that $v_1(r_k) = i_k$ and $v_2(r_k) = 2 \cdot i_k$ for $1 \leq k \leq n$. The agents’ budgets are $b_1 = \frac{1}{2} \sum I$ and $b_2 = \sum I$. The set of resources $R$ is $\{r_1, \ldots, r_n\}$ and $K = \frac{3}{4} \sum I$. We claim that $I$ is partitionable into two sets with equal sums if and only if there exists an ordering that obtains an allocation value of $K$ (or more).

($\Rightarrow$) Given a partition of $I$ into sets $A$ and $B$, we order all resources in $A$ first, and those in $B$ later. In this case, agent 2 will buy all the $A$ resources because (s)he values these more than agent 1 and when they are auctioned, (s)he still has budget left. After buying all resources in $A$, (s)he will have spent $\sum_{i_k \in A} v_2(r_k) = 2 \cdot \sum_{i_k \in A} i_k$, which makes $\sum I$ in total (since $\sum_{i_k \in A} i_k = \frac{1}{2} \sum I$). This is the entire budget of agent 2, and all resources in $B$ are therefore sold to agent 1, with a total value of $\sum_{i_k \in B} v_1(r_k) = \sum_{i_k \in A} i_k = \frac{1}{2} \sum I$. This makes a total allocation value of $\frac{1}{2} \sum I + \frac{1}{2} \sum I = K$.

($\Leftarrow$) Given an ordering such that agent 1 and 2 spend all of their budget ($K$ in total), we let $A$ be the values of the resources sold to agent 1 and $B$ be half of the values of resources sold to agent 2. By construction, $I$ is the union of $A$ and $B$ and the sums of their values are equal.

The construction is clearly polynomial time.

Several related works deal with this type of ordering optimization problem. For example, in the Economics literature, the authors of \cite{23} investigate the optimal ordering strategy for the case where the auctioneer has two resources to sell. They show that when the resources are different in value, the higher valued resource should be auctioned first in order to increase the seller’s revenue. Pitchik \cite{13} points out that in the presence of budget constraints, in a sealed-bid sequential auction, if the bidder who wins the first good has a higher income than the other one, the expected revenue is

\footnote{We do not prove it NP-complete as deciding on which value the agents will bid is combinatorial as well and completeness would require that to be decided in polynomial time.}
maximized. As real-world auctions typically have more than two bidders or two resources, it is difficult to apply these results. Moreover, [21] show that it is difficult to construct a good model for the bidders’ combinatorial preferences even when interacting with them as users. Since historical data contains much less information than user queries, in this paper, we instead focus on learning the overall preferences of the group of bidders. In order to simplify this learning problem, we make the following modeling assumption.

**Assumption 1 (Bidder independence)** In every sequential auction, the set of participating bidders and their valuation functions are similar.

This assumption simplifies the problem of learning a good ordering. Instead of learning the individual valuation functions of agents, we can treat the agent population as a single entity for which we need to find a single global valuation function. Such an approach will fail if the valuations of the agents are radically different in every auction. However, we consider this assumption sensible in many auction settings. Although the different participants can be interested in different resource types, we assume the interests of the group of participants remain stable.

The assumption effectively reduces the difficulty of the learning problem to that of a standard machine learning setting: learn a single model from orderings and their rewards for predicting the expected reward for a given new input ordering. Because we can now generalize over all bids instead of only the bids of a single agent, the assumption significantly increases the amount of available data.

### 3 Representing orderings

We need to find a suitable way to model the expected values of such orderings. An ordering can be thought of as a sequence of items. However, to the best of our knowledge, none of the existing sequence models fits our auction setting. Language models such as deterministic automata [7] are too powerful since they can model every possible sequence independently and therefore require too much data to learn accurately. Short sequence models such as hidden Markov models or N-grams [2] do not model the dependence on items sold a long time (more than the sliding window length) before. What comes closest to our auction setting are models such as Markov decision processes (MDPs) [19]. These directly model the expected price per item, and we can build a state space that fits with our assumptions. However, none of the models we know of is capable of producing orderings for a given finite set of items (which is NP-hard). This given set of items determines both the available actions (which item to auction) and the goal state (when no items remain). Since this set is rarely the same in different auctions, representing and learning the values of auctions in an MDP is difficult. However, with a suitable factored representation of the states and/or function approximation [19] of the rewards, we could represent our auctioning problem as an MDP.

Instead of representing our problem with a sequence model, we view the prediction of an auction’s outcome as a regression problem. We split this problem into the
subproblems of predicting the value of the auctioned items. We then sum these up to obtain the overall objective function:

\[ V(r_1 \ldots r_n) = \sum_{1 \leq k \leq n} R(r_k, \{ r_j | j < k \}, \{ r_l | k < l \}) \]

where \( R(r_k, J, L) \) is a regression function that determines the expected value of \( r_k \) given that \( J \) was auctioned before and \( L \) will be auctioned afterwards. We use regression trees [4] as a regression function and train it using features based on the items auctioned before and after the current item \( r_k \). Currently, we provide the following features:

**Feature 1: sold** For every item type \( r \), the amount of \( r \) items already auctioned.

**Feature 2: diff** For every pair of item types \( r \) and \( r' \), the difference between the amount of \( r \) and \( r' \) items already auctioned.

**Feature 3: sum** For every item type \( r \), the amount of value obtained from auctioning \( r \) items, and the overall sum.

These features are sufficient to model the influence of utility functions with complementarities. For instance, if many agents desire both \( A \) and \( B \) types, and if the amount of \( B \) items already auctioned is large when auctioning an \( A \) item, then we expect the value for this \( A \) item to be high. Other sequential features such as sliding windows and N-grams can of course be added to the model. Since they are to be computed by an ILP solver, the only requirement is that they can be represented using an integer linear formulation. Although the second feature can be determined using the first, it is added for convenience of learning a regression tree, which requires many nodes to represent such values. The influence of budget constraints is modeled by the third feature: once the amount paid for sold \( A \) items reaches a certain (to be learned) bound, we can expect all agents that only want \( A \) items to be out of budget.

A data set obtained in this way can be given as input to any regression method from machine learning. In our case, we learn a regression tree for every item type using recursive partitioning techniques [4]. The result is a set of predictive models for the expected value of items, and by summing up these values we obtain the expected value of an auction. Below we give an example of how an ordering and its obtained values is transformed into a data set using these 3 types of features.

**Example 3** Two agents 1 and 2 take part in a sequential auction of resources. The valuations of the agents for resources \( A \) and \( B \) are given as follows: \( v_1(A) = 1, v_1(B) = 1, v_1(\{A, B\}) = 10, v_2(A) = 5 \). Two auctions have been carried out. One sold \( A \) first to agent 2 (as agent 2 values \( A \) higher than agent 1), and then \( B \) to agent 1, which ended up with a social welfare of 6. The second auction sold \( B \) first and then \( A \), both to agent 1, which had social welfare 10. We compute feature values from these two auctions as depicted in Table 1. Subsequently, we learn regression trees for both item types \( A \) and \( B \), as shown in Figure 1.

\[ \square \]
Table 1: The data set created from the past two auctions \{A, B\} and \{B, A\} in Example 3.

| type | value | soldA | soldB | diffAB | sumA | sumB | sum |
|------|-------|-------|-------|--------|------|------|-----|
| A    | 5     | 0     | 0     | 0      | 0    | 0    | 0   |
| B    | 1     | 1     | 0     | 1      | 5    | 0    | 5   |
| B    | 1     | 0     | 0     | 0      | 0    | 0    | 0   |
| A    | 9     | 0     | 1     | -1     | 0    | 1    | 1   |

Figure 1: Two regression trees for the two item types from Example 3. Since item B always sells with a value of 1, the tree for B consists of a single leaf node.

## 4 Finding an optimal allocation

Given the predictive model for the expected value per item, it is not straightforward to compute a good ordering. In fact, the problem is NP-complete.

**Lemma 1** Using regression trees, the problem of whether there exists an ordering that has a total predicted value of at least \(K\) is NP-complete.

**Proof 2** The proof follows from the fact that we can use simple regression trees to model the preferences of the two agents from Theorem 1, and evaluating an ordering using these trees can be done in polynomial time. The regression tree for every item type \(r_i\) is shown in Figure 2.

In spite of this hardness result, we present two optimization methods for finding an optimal allocation of the given items: (1) a novel “white-box” optimization (i.e., ILP model), and (2) a “black-box” heuristic (i.e., best-first search).

### 4.1 A white-box optimization: ILP model

Given the regression tree models for the expected value per item type, we automatically formulate the problem of finding an optimal ordering as an integer linear program (ILP).

**Ordering an auction** Given a multiset of \(n\) items \(S\), each from a set of possible types \(R\), we use the following free variables to encode any possible ordering of \(S\):

\[ x_{i,r} \in \{0, 1\}: \text{item } i \text{ is of type } r \text{ iff } x_{i,r} = 1. \]
Thus, if $x_{3,A}$ is equal to 1, it means that the third auctioned item is of type $A$. We require that at every index $i$ at most one item type is auctioned, and that the total number of auctioned items of type $r$ is equal to the number $n_r$ of type $r$ items in $S$.

\[
\sum_{r \in R} x_{i,r} = 1 \quad \text{for all } 1 \leq i \leq n
\]
\[
\sum_{1 \leq i \leq n} x_{i,r} = n_r \quad \text{for all } r \in R
\]

Any assignment of ones and zeros to the $x$ variables that satisfies these two types of constraints corresponds to a valid ordering of the items in $S$. The value of such an ordering is determined by the learned regression tree models.

### 4.1.1 Translating feature values

In order to compute the prediction of a regression tree model, we not only need to translate these models into ILP constraints, but also the values of the features used by these models. Feature 1 and Feature 2 can be computed using linear functions from the $x$ variables:

\[
\text{sold}_{i,r} = \sum_{j < i} x_{j,r} \quad \text{for all } 1 \leq i \leq n, r \in R
\]
\[
\text{diff}_{i,r,r'} = \text{sold}_{i,r} - \text{sold}_{i,r'} \quad \text{for all } 1 \leq i \leq n, r \in R, r' \neq r, r' \in R
\]

For the last type of feature, we need to sum over the predicted values, determined by the regression tree models, described next.

### 4.1.2 The regression tree ILP model

We translate the regression tree models into ILP using carefully constructed linear functions. These functions constrain the values of two new sets of $\{0, 1\}$ variables $d_{i,r}$ and $l_{i,r}$ such that they are equal to 1 if and only if in the learned tree, a binary decision in a decision node is true ($d_{i,r} = 1$) and a leaf node is reached ($l_{i,r} = 1$). We first explain our representation of the binary decision nodes in the regression tree models.

**Representing decision nodes** Let $D$ be the set of all decision nodes in all trees. Every decision in $D$ is a boolean constraint $f \leq c$, which is true if and only if feature $f$ has a value less than or equal to a constant $c$. We represent every such decision using a $\{0, 1\}$ variable: $g_{i,f \leq c} \in \{0, 1\}$: decision $f \leq c$ is true for item $i$. Every $g$ variable is constrained by the value of a feature $f$ and a constant $c$ as follows:
regression trees: only one leaf can be reached for every item. We force this by adding: The objective is to maximize the expected values.

4.1.3 The objective function

Example 4 Given the learned trees in Example 3, suppose we are asked to order a new multiset of items \{A, B, B\}. We translate this new set, together with the learned trees, into the following integer linear program with the following \{0,1\} decision variables (for all \(1 \leq i \leq 3\)): \(x_{i,A}, x_{i,B}, y_{i,<olid>B>0.5}, z_{i,1,A}, z_{i,2,A}, z_{i,1,B}\):
\[
\max \sum_{1 \leq i \leq 3} v_i, A + v_i, B, \\
\text{where } v_i, A = 5z_{i,1}, A + 9z_{i,2}, A, v_i, B = z_{i,1}, B \\
\text{subject to (for all } 1 \leq i \leq 3 \text{ and } l \in \{1, 2\})
\]

- \(x_{1,A} + x_{2,A} + x_{3,A} = 1, \quad x_{1,B} + x_{2,B} + x_{3,B} = 2, \quad x_{i,A} + x_{i,B} = 1,\)
- \(-100 \cdot y_{1, soldB} > 0.5 \leq 0.5, \quad 100 \cdot y_{1, soldB} > 0.5 \leq 99.5,\)
- \(-100 \cdot y_{2, soldB} > 0.5 + x_{1,B} \leq 0.5, \quad 100 \cdot y_{2, soldB} > 0.5 - x_{1,B} \leq 99.5,\)
- \(-100 \cdot y_{3, soldB} > 0.5 + x_{1,B} + x_{2,B} \leq 0.5, \quad 100 \cdot y_{3, soldB} > 0.5 - x_{1,B} - x_{2,B} \leq 99.5,\)
- \(z_{i,l}, A \leq x_{i,A}, \quad z_{i,1}, A \leq 1 - y_{i, soldB} > 0.5, \quad z_{i,2}, A \leq y_{i, soldB} > 0.5,\)
- \(z_{i,1}, B \leq x_{i,B}, \quad z_{i,1}, A + z_{i,2}, A + z_{i,1}, B = 1.\)

We set \(M = 100\) in this example. A satisfying assignment to the \(x\) variables is \(x_{1,A}, x_{2,B}, x_{3,B}\) set to 1, the rest to 0. This leads to \(100 \cdot y_{1, soldB} > 0.5 = 100 \cdot y_{2, soldB} > 0.5 \leq 99.5,\) forcing \(y_{1, soldB} > 0.5\) and \(y_{2, soldB} > 0.5\) to be 0, and similarly -100 \(y_{3, soldB} > 0.5 + 1 \leq 0.5,\) forcing \(y_{2, soldB} > 0.5 = 1.\) This makes \(z_{1,2}, A = z_{2,2}, A = 0\) and \(z_{3,1}, A = 0.\) Since \(z_{1,1}, B \leq x_{1,B} = 0,\) \(z_{2,1}, A \leq x_{2,A} = 0,\) and \(z_{3,2}, A \leq x_{3,A} = 0,\) the last constraint makes \(z_{1,1}, A, z_{2,1}, B,\) and \(z_{3,1}, B\) equal to 1, and all other \(z_{i,1}, l\) variables equal to 0. This results in an objective value of 5 + 1 + 1 = 7.

An optimal assignment would be to order one \(B\) first by setting \(x_{1,B}, x_{2,A}, x_{3,B}\) to 1, this will make \(y_{2, soldB} > 0.5 = 1,\) and therefore \(z_{1,2}, A = 1,\) resulting in a total allocation value of 1 + 9 + 1 = 11. Finding this assignment can be done using an ILP-solver. 

4.2 A black-box heuristic: best-first search algorithm

We now provide a black-box heuristic for solving the ordering problem. The traditional method to overcome the computational blowup caused by sequential decision making in MDPs is to use a dynamic programming method. Although this lessens the computational load by combining the different paths that lead to the same sets of auctioned items, the search space is still too large and waiting for a solution will take too long. Instead, we therefore employ a best-first search strategy that can be terminated anytime in order to return the best found solution so far. We show how this best-first search strategy works in Algorithm 1.

The algorithm uses a hashtable and a priority queue. The hashtable is used to exclude the possibility of visiting the same nodes twice if the obtained value is less than before (just like a dynamic programming method). These dynamic programming cuts are sensible but lose optimality as on rare occasions it could be better to sell earlier items for less, leaving more budget for the remaining ones. The priority queue provides promising candidate nodes for the best-first strategy. By computing random orderings of the remaining items, the learned models can evaluate complete orderings of all items.
Algorithm 1 Computing a good ordering

Require: A set of items $S$, historical data on orderings and their values $D$, a maximum number of iterations $m$

Ensure: Returned is a good (high expected value) ordering

Transform $D$ into a data set

for every item type $r_T$ do
    Learn a regression model from $D$ for predicting the value of item type $r_T$ 
end for

Initialize a hashtable $H$ and a priority queue $Q$

Add the empty data row to $Q$

while $Q$ is not empty and the size of $H$ is less than $m$ do
    Pop the row of features $F$ with highest value $v$ from $Q$
    if $H$ does not contain $F$ with a value $\geq v$ then
        Add $F$ with value $v$ to $H$
        Let $L$ be the set of remaining items in $F$
        for every item type $r_T$ of items in $L$ do
            Let $i_k$ be an item of Type $r_T$ in $L$
            Let $L'$ be a random ordering of $L - i_k$
            Use the models to evaluate the value $v'$ of auctioning the ordering $i_kL'$ after $F$
            Create new features $F'$ for auctioning $i_k$ after $F$
            Add $F'$ to $Q$ with value $v + v'$
        end for
    end if
end while

return The highest evaluated ordering

The best one found is stored and returned if the algorithm is terminated. Unfortunately, this does not result in an admissible heuristic for an A* search procedure. Hence, even if the algorithm pops a solution from the queue, this is not necessarily optimal. In our experience, using random orderings of the remaining items in this heuristic provides a good spread over the search space. Although some nodes can be ‘unlucky’ and obtain a bad ordering of the remaining items, there are always multiple ways to reach nodes in the search space and it is very unlikely that all possibilities will be ‘unlucky’.

4.3 White-box or black-box optimization?

Both black-box and white-box approaches have their advantages. The main advantage of black-box is that its performance is for a large part independent of the complexity of the used regression model. In contrast, by explicitly modeling the regression model as constraints, a more complex regression model potentially leads to much more constraints, which can lead to an increase in the time needed to solve it in a white-box fashion.

In our opinion, however, the advantages of white-box optimization largely outweigh those of black-box optimization and make it a very interesting topic for research in machine learning and optimization. Most importantly, a white-box formulation provides a new way of modeling in mathematical optimization. We show how to construct
an ILP formulation entirely from data in this paper. Such constructions can also be easily integrated into existing LP formulations that have been used in a wide range of applications in for instance Operations Research. In this way, one can combine the vast amount of expert knowledge available in these applications with the knowledge in the readily available data. Our white-box method is the first we know of that makes the results of machine learning directly available to mathematical modeling in this fashion.

5 Experiments

We created an auction simulator of a sealed-bid, second-price auction, where agents have a simple bidding strategy, i.e., they bid as soon as the asking price reaches their true value. If multiple agents have the same true value, one of these is selected as winner uniformly at random. We used this simulator to generate data sets, which are orderings of item-price pairs, and tested whether the ILP model could produce good orderings. Now we will describe how we generated an auction which contains 40 agents who are bidding for 40 items from 10 item types.

5.1 Generating auctions

We use a given set of items \( S \) to initialize the auction simulator. Every type in \( S \) gets assigned an average value of \( 5 + (5 \cdot i) \), for \( 1 \leq i \leq 10 \). Every type is assigned a random popularity, which is the probability of being desired by an agent. Furthermore, every possible subset of types is assigned a complementarity probability drawn uniformly from \( \{1.5, 2.0, 2.5\} \). Every type is assigned a sparsity value drawn uniformly from \([2, 10]\). In every auction, 40 items are generated using a roulette wheel drawing scheme using the sparsity values.

Every agent is generated at random using a similar scheme. They get assigned a budget between 50 and 250 at random. They may desire any of the 10 item types, where popular types have a higher probability of being selected. Every desired item type is assigned the average type value multiplied by a value between 0.75 and 1.5, drawn uniformly at random. For every possible subset of an agent’s desired types, the agent also desires this subset with probability equal to the subset’s complementarity probability. The value of such a subset is equal to the sum of its individual type’s values multiplied by the subset complementarity value. If necessary, the additional budget is drawn from 50 to 250 for the agent in order to supersede the value of its most valuable desired subset. The following is for example four agents generated for the experiments, with different budgets and valuations:

- Budget: 142, \( v(C) = 19 \)
- Budget: 78, \( v(A) = 13 \), \( v(C) = 17 \), \( v(AC) = 75 \)
- Budget: 197, \( v(A) = 12 \), \( v(C) = 20 \), \( v(F) = 31 \), \( v(ACF) = 126 \)
- Budget: 239, \( v(A) = 8 \), \( v(D) = 37 \), \( v(F) = 30 \), \( v(AD) = 90 \), \( v(ADF) = 150 \)

When deciding what value to bid, the agents compute the largest possible value of its obtained items and the new item over its complementary valuations, while keeping its remaining budget in mind. We learn regression tree models that uncover the hidden structure underlying the winning bids in these auctions. We then use the learned models to construct a mathematical optimization model in order to find the highest value ordering for a new set of items. In the next section, we describe the methods we use to test the quality of this ordering.
5.2 Experimental setup

We use the auction simulator to evaluate the performance of our method. We generate a set of 40 agents and run simulations of 1000 random orderings of 40 randomly selected items. From these 1000 orderings and their achieved values, we obtain a data set, which is then provided to the regression tree learner. We use an implementation of regression trees from the scikit-learn machine learning module [22] in Python. We range the maximum depth of the tree and set the minimum number of samples required to split an internal node to 10. The resulting tree then gets translated to an ILP, which in turn gets solved by an ILP-solver (CPLEX [14]) that returns an ordering for a new set of randomly generated items. We set a time limit on the ILP solver of 10 minutes on an Intel core i-5 with 8GB RAM and record the best ordering of items that the ILP solver has obtained, the last minute is spent on solution polishing (a local search procedure in CPLEX). We apply our best-first search method on the same problem instance. We then run a simulation of this ordering and obtain the corresponding allocation value. We also use the learned regression tree to evaluate the ordering, to see whether it corresponds with the found objective value in the ILP. We generate 10 sets of agents. For each set of agents we generate and run new sets of items 5 times.

We compare the solutions returned by the ILP-solver and best-first search with three ordering methods: (i) a fixed ordering: auction the least valuable item first; (ii) another fixed ordering suggested by the literature [23]: auction the most valuable item first; and (iii) a random ordering.

5.3 Results

Table 2: The performance difference between the white-box and black-box methods (LP - best first), evaluated using the regression tree models. The numbers are averaged over 5 runs using different items and the same set of agents and trees.

| tree depth | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|------------|----|----|----|----|----|----|----|----|----|----|
| 3          | 53 | 1.4| 66.6| 40.8| 37.8| 45.6| -14.4| 9.8| 21.6| 35.8|
| 5          | 13.4| 23.2| -37.8| -57.0| 35.0| -6.4| -94.4| -20.4| 3.8| -126.0|
| 8          | -62.6| 0.0| -56.2| -78.0| -56.4| -89.4| -110.2| -3.4| -13.6| -78.4|

In this challenging setting (ordering 40 items from 10 types, potentially \(40! \prod_{i=1}^{10} 4!\) distinct orderings assuming there are 4 indistinguishable items of each type), we compare the performance of the white-box and black-box methods for different settings of the maximum tree depth in the scikit-learn regression tree learner. The results are shown in Table 2. The results are very interesting in that our white-box method outperforms black-box when the regression tree models are small (10 models of depth 3, making \(10 \cdot (2^4 - 1) = 150\) decision and leaf nodes), and is outperformed when the models are large. This is what we would intuitively expect, and thus confirms that our white-box encoding performs well. Unfortunately, the current regression tree learning in scikit-learn does not include a pruning method, so the tree will expand as long as its leaves
are reached more frequently than 10 times. In the 1000 auctions with 40 items every item corresponds to a row in the data set. This results in 4000 rows on average for every item type. For the large trees, there will thus be approximately 400 leaf nodes in the worst case (an even distribution), making about 800 nodes in total. When the trees are limited to a depth of 5, the performance of both methods is comparable with a slight favor for black-box over white-box. In our future work, we would like to investigate the effect of pruning methods on these results.

Table 3: The performance of the different methods in the auction simulator, divided by the performance of a lower bound of the optimum (i.e., the best run found over 500 random orderings in the simulator). The numbers are averaged over 5 runs using different items and the same set of agents and trees.

| method         | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|----------------|----|----|----|----|----|----|----|----|----|----|
| best first 3   | 0.947 | 0.977 | 0.956 | 0.973 | 0.926 | 0.969 | 0.911 | 0.935 | 0.976 | 0.955 |
| best first 5   | 0.957 | 0.966 | 0.978 | 0.956 | 0.949 | 0.947 | 1.008 | 0.964 | 0.975 | 0.987 |
| best first 8   | 0.972 | 0.975 | 0.931 | 0.928 | 0.986 | 0.939 | 0.936 | 0.983 | 0.973 | 0.969 |
| LP 3           | 0.988 | 0.963 | 0.963 | 0.909 | 0.985 | 0.983 | 0.952 | 0.945 | 0.983 | 0.941 |
| LP 5           | 0.970 | 0.964 | 0.957 | 0.933 | 0.968 | 0.949 | 1.009 | 0.959 | 0.973 | 0.935 |
| LP 8           | 0.999 | 0.979 | 0.936 | 0.961 | 1.030 | 0.980 | 0.963 | 0.985 | 0.973 | 0.973 |
| random         | 0.922 | 0.899 | 0.923 | 0.916 | 0.907 | 0.952 | 0.969 | 0.917 | 0.940 | 0.946 |
| least valuable | 0.761 | 0.817 | 0.852 | 0.855 | 0.788 | 0.826 | 0.754 | 0.806 | 0.900 | 0.878 |
| most valuable  | 0.872 | 0.884 | 0.826 | 0.875 | 0.823 | 0.870 | 0.824 | 0.848 | 0.859 | 0.735 |

Our second set of results concern the actual performance of the discovered orderings in practice, evaluated using our simulator and the generated agents (see Table 3). Strangely, learning larger trees does seem to help in practice for the white-box LP method, but this cannot be concluded for the results of the best first method. Note that the trees used in these methods are learned from exactly the same data set. Also, the 8 tree LP method seems to perform slightly better in practice than any of the best first methods. We believe this is an artefact due to the fact that the trees are not perfect predictors. The 8 tree LP method does find significantly worse orderings when evaluated using the trees themselves (Table 2). More interestingly, all results are very close to optimal, at least close to the best solution found by running 500 random orderings in the auction simulator which we use as a lower bound on the optimal value. The performance of both our methods is frequently within 5% of this value and sometimes even outperforms it. Furthermore, the methods suggested by literature of using a fixed ordering with the most valuable item first or the least valuable item first clearly perform not very well in the complex auction setting in our experiments. In fact, using a random ordering already outperforms both of these methods, achieving values within 10% of the lower bound. This result clearly demonstrates the significant impact that machine learning based approaches can have in areas of optimization where most results are based on pure mathematical analysis and (often unrealistic) assumptions.
6 Conclusions

We demonstrate how to construct decision support models entirely from data by mapping learned regression tree models to integer linear programs, which can be used for optimization. To the best of our knowledge, ours is the first white-box optimization method of its kind. The main advantage of our approach is that all the properties of the learned models are visible as constraints to a mathematical problem solver. This solver can use sophisticated branching and cutting techniques on these constraints, which cannot be used in more traditional black-box optimization approaches. Our constructions are general and can be applied to any settings where regression trees can be learned from data, and their feature values can be computed as linear functions from solutions.

We demonstrate our approach by transforming historical auctions into data sets for learning regression trees, which then can be used to predict the expected value of orderings for new auctions. Although optimizing the orderings in sequential allocations is a hard problem, our method obtains very high values, significantly outperforming the naive methods proposed in the literature. We choose a simple auction model for ease of explanation in this paper. However, our approach works whenever regression trees are able to provide reliable predictions of the bidding values. Hence we believe it can be applied to other auction formats with more complex and realistic bidding strategies.

In the future, we plan to test our method on real auction data. The main purpose of the experiments in this paper is to demonstrate the use and feasibility of our method. In addition, we compare it to a black-box best first search approach with dynamic programming cuts. Our results show that the method is promising, outperforming the black-box method when the models are not overly complex. The more complex the learned models become, however, the better the black-box method performs in comparison. This is to be expected since explicitly modeling the learned models as constraints, a more complex regression model potentially leads to much more constraints, which can lead to an increase in the time needed to solve it in a white-box fashion. It would therefore be very interesting to investigate the effect of pruning methods on the performance of our methods.

Our white-box formulation provides a new way of modeling in mathematical optimization. Our method therefore has many other potential application areas, especially in multiagent problems where more and more data is being collected in many different domains such as logistics, transportation, and marketing. Even in cases where there already exists a handcrafted optimization model, a model that is learned and translated using our method can easily be included in the objective function in order to determine part of the objective function based on data.

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