The Voice of Optimization

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Abstract

We introduce the idea that using optimal classification trees (OCTs) and optimal classification trees with-hyperplanes (OCT-Hs), interpretable machine learning algorithms developed in [BD17, BD18], we are able to obtain insight on the strategy behind the optimal solution in any continuous and mixed-integer convex optimization problem as a function of key parameters that affect the problem. In this way, optimization is not a black box anymore. Instead, we redefine optimization as a multiclass classification problem where the predictor gives insights on the logic behind the optimal solution. In other words, OCTs and OCT-Hs give optimization a voice. We show on several realistic examples that the accuracy behind our method is in the 90%-100% range, while even when the predictions are not correct, the degree of suboptimality or infeasibility is very low. We compare optimal strategy predictions of OCTs and OCT-Hs and feed-forward neural networks (NNs) and conclude that the performance of OCT-Hs and NNs is comparable. OCTs are somewhat weaker but often competitive. Therefore, our approach provides a novel, reliable and insightful understanding of optimal strategies to solve a broad class of continuous and mixed-integer optimization problems.

1 Introduction

Optimization has a long and distinguished history that has had and continues to have genuine impact to the world. In a typical optimization problem in the real world, practitioners see optimization as a black-box tool where they
formulate the problem and they pass it to a solver to find an optimal solution. Especially in high dimensional problems typically encountered in real world applications, it is currently not possible to interpret or intuitively understand the optimal solution. However, independent from the optimization algorithm used, practitioners would like to understand how problem parameters affect the optimal decisions in order to get intuition and interpretability behind the optimal solution. Moreover, in almost all real world applications of optimization the main objective is not to solve just one problem but to solve multiple similar instances that vary little from each other. In fact, in most real-world applications we solve similar optimization problems multiple times with varying data depending on problem-specific parameters.

Our goal in this paper is to propose a framework to predict the optimal solution as parameters of the problem vary and do so in an interpretable way. A naive approach could be to learn directly the optimal solution from the problem parameters. However, this method is computationally intractable and imprecise: intractable, because it would require a potentially high dimensional predictor with hundreds of thousands of components depending on the decision variable size; imprecise, because it would involve a regression task that would naturally carry a generalization error leading to suboptimal or even infeasible solutions. Instead, our approach encodes the optimal solution with a small amount of information that we denote as strategy. Depending on the problem class, a strategy can have different meanings but it always corresponds to the complete information needed to efficiently recover the optimal solution.

In recent times, machine learning has also had significant impact to the world. Optimization methods has been a major driver of its success, see [HTF09] and [BD18]. In this paper, we apply machine learning to optimization with the objective to give a voice to optimization, that is to provide interpretability and intuition behind optimal solutions.

First, we solve an optimization problem for many parameter combinations and obtain the optimal strategy: the set of active constraints as well as the value of the discrete variables. Second, we encode the strategies with unique integer scalars. In this way, we have a mapping from parameters to the optimal solution strategies, which gives rise to a multiclass classification problem, see [HTF09]. We solve the multiclass classification problem using optimal classification trees (OCTs) and optimal classification trees with hyperplanes (OCT-Hs) developed in [BD17, BD18], very interpretable state of the art classification algorithms as well as neural networks (NNs) which,
while not interpretable, serve as a benchmark to compare the accuracy of OCTs and OCT-Hs.

1.1 Related Work

[MRN18] discuss the idea of learning the set of active constraints for parametric online optimization. They frame the learning procedure as a sampling scheme where they collect all the active sets appearing from the parameters. However, we found several limitations of their approach. First, in the online phase, they evaluate all the relevant active sets in parallel and pick the best one (ensemble policy in [MRN18]). Therefore, they do not solve the optimization problem as a multiclass classification problem and they are not able to gain insights on how the parameters affect the optimal strategy. In addition, they do not tackle mixed-integer optimization problems but only continuous convex ones. Finally, the sampling strategy in [MRN18] has to be tuned for each specific problem since it depends on at least four different parameters. This is because the authors compute the probabilistic guarantees based on how many new active sets appear over the samples in a window of a specific size [MRN18, Section 3]. In this work, instead, we provide a concise Good-Turing estimator [Goo53] for the probability of finding new unseen strategies which can be directly applied to many different problem instances.

Another related work in the field of model predictive control (MPC) appears in [KKK19] where the authors warm-start an online active set method for solving quadratic optimization problems (QOs). However, in that work there is no rigorous sampling scheme with probability bounds to obtain the different active sets. Instead, the authors either simulate the dynamical controlled system or provide an alternative gridding method to search for the relevant active sets. Furthermore, the method in [KKK19] is tailored to a specific linear control problem in the form of QO and cannot tackle any convex or mixed-integer convex problem.

1.2 Contributions

In this paper, we propose for the first time a learning framework to give a voice to continuous and mixed-integer convex optimization problems. With our approach we can reliably sample the occurring strategies using the Good-Turing estimator, learn an interpretable classifier using OCTs and OCT-Hs, interpret the dependency between the optimal strategies and the key
parameters from the resulting tree and solve the optimization problem with high accuracy.

Our specific contributions include:

1. We introduce a new framework for gaining insights on the solution of optimization problems as a function of their key parameters. We replace the optimizer with an interpretable machine learning classifier using OCTs and OCT-Hs highlighting the relationship between the optimal solution strategy and the problem parameters. In this way optimization is no longer a black box and our approach gives it a voice that provides intuition and interpretability on the optimal solution.

2. We show that our method can be applied to a broad collection of optimization problems including any convex continuous and convex mixed-integer optimization problem. We do not pose any assumption on the dependency of the cost and constraints on the problem parameters.

3. We introduce a new exploration scheme based on the Good-Turing estimator \[\text{Goo53}\] to discover the strategies arising from the problem parameters. This scheme allows us to reliably bound the probability of encountering unseen strategies in order to be sure our classifier accurately represents the optimization problem.

4. In several realistic examples we show that the sample accuracy of our method is in the 90%-100% range, while even in the cases where the prediction is not correct the degree of suboptimality or infeasibility is very low. We also compare the performance of OCTs and OCT-Hs to NNs obtaining comparable out of sample accuracy.

In other words, our approach provides a novel, reliable and insightful framework for understanding the strategies to compute the optimal solution of a broad class of continuous and mixed-integer optimization problems.

1.3 Paper Structure

The structure of the paper is as follows: In Section 2, we define an optimal strategy to solve continuous and mixed-integer optimization problems and present several concrete examples that demonstrate what we call the voice of optimization. In Section 3, we outline the core part of our approach of using multiclass classification to learn the mapping from parameters to
optimal strategies. We further present an approach to estimate how likely it is to encounter a parameter that leads to an optimal strategy that has not yet been seen. In Section 4, we outline our Python implementation MLOPT (Machine Learning Optimizer). In Section 5, we test our approach on multiple examples from continuous and mixed-integer optimization and present the accuracy of predicting the optimal strategy of OCTs and OCT-Hs in comparison with a NNs implementation. Section 6 summarizes our conclusions. Appendices A and B briefly present optimal classification trees (OCTs and OCT-Hs) and NNs, respectively to make the paper self-contained.

2 The Voice of Optimization

In this section, we introduce the notion of an optimal strategy to solve continuous and mixed-integer optimization problems. Given a parameter \( \theta \in \mathbb{R}^p \) we define *strategy* \( s(\theta) \) the complete information needed to efficiently compute the optimal solution of an optimization problem given the parameter \( \theta \). We assume that the problem is always feasible for every encountered value of \( \theta \).

Note that in the examples in this section we omit the details of the learning algorithm which we explain in Section 3. Instead, we focus on the interpretation of the resulting strategies which correspond to a decision tree. Note that for the illustrative examples in this section the accuracy of our approach to find the optimal solution was always 100%, confirming that the resulting models accurately recover the optimal solution. In all of the examples in this section we used OCTs since their accuracy was 100% and they are more interpretable than OCT-Hs. In the last example, we used both an OCT and an OCT-H for comparison.

2.1 Optimal Strategies in Continuous Optimization

Consider the continuous optimization problem

\[
\begin{align*}
\text{minimize} & \quad f(\theta, x) \\
\text{subject to} & \quad g(\theta, x) \leq 0,
\end{align*}
\]

where \( x \in \mathbb{R}^n \) is the vector of decision variables and \( \theta \in \mathbb{R}^p \) the vector of parameters affecting the problem data. Functions \( f : \mathbb{R}^p \times \mathbb{R}^n \rightarrow \mathbb{R} \) and \( g : \mathbb{R}^p \times \mathbb{R}^n \rightarrow \mathbb{R}^m \) are assumed to be convex in \( x \). Given a parameter \( \theta \) we
denote the optimal primal solution as $x^*(\theta)$ and the optimal cost function value as $f(\theta, x^*(\theta))$.

**Tight constraints.** Let us define the *tight constraints* $\mathcal{T}(\theta)$ as the set of constraints that are satisfied as equalities at optimality,

$$\mathcal{T}(\theta) = \{ i \in \{1, \ldots, m\} \mid g_i(\theta, x^*) = 0 \}. \quad (2)$$

Given the tight constraints, all the other constraints are redundant for the original problem.

For non-degenerate problems, the tight constraints correspond to the *binding constraints*, i.e., the set of constraints that, if removed, would allow a decrease in $f(\theta, x^*(\theta))$. In the case of linear optimization problems (LOs) the binding constraints are the linearly independent constraints defining a basic feasible solution [BT97, Definition 2.9]. Binding constraints are also referred to as *support constraints* in the literature [Cal10, Definition 2.1]. An important property of binding constraints is that they cannot be more than the dimension $n$ of the decision variable [Hof79, Proposition 1], [Cal10, Lemma 2.2]. This fact plays a key role in our method to reduce the complexity to predict the solution of parametric optimization problems. The benefits are more evident when the number of constraints is much larger than the number of variables, i.e., $n \ll m$.

For degenerate problems, there can be more active constraints than binding constraints. However, these situations are of minor importance because on the one hand, they can be avoided by perturbing the cost function and on the other hand the number of redundant active constraints is in practice way lower than the number of constraints.

**Solution strategy.** We can now define our strategy as the index of tight constraints at the optimal solution, i.e., $s(\theta) = \mathcal{T}(\theta)$. Given the optimal strategy, solving (1) corresponds to solving

$$\begin{align*}
\text{minimize} & \quad f(\theta, x) \\
\text{subject to} & \quad g_i(\theta, x) \leq 0, \quad \forall i \in \mathcal{T}(\theta). \quad (3)
\end{align*}$$

This problem is easier than (1), especially when $n \ll m$. Note that we can enforce the components $g_i$ that are linear in $x$ as equalities. This further simplifies (3) while preserving its convexity.
In case of LO and QU when the cost \( f \) is linear or quadratic and the constraints \( g \) are all linear, the solution of (3) corresponds to solving a linear system of equations defined by the KKT conditions [BV04, Section 10.2]. This means that we can solve these problems online without needing any optimization solver.

**Inventory management**

Consider an inventory management problem with horizon \( t = 0, \ldots, T - 1 \) with \( T = 30 \). The decision variables are \( u_t \) describing how much we order at time \( t \) and \( x_t \) describing the inventory level at time \( t \). \( c = 2 \) is the cost if ordering, \( h = 1 \) the holding cost and \( p = 3 \) the shortage cost. We define the maximum quantity we can order each time as \( M = 3 \). The parameters are the product demand \( d_t \) at time \( t \) and the initial value of the inventory \( x_{\text{init}} \).

The optimization problem can be written as follows

\[
\begin{align*}
\text{minimize} & \quad \sum_{t=0}^{T-1} \max(h x_t, -p x_t) + c u_t \\
\text{subject to} & \quad x_{t+1} = x_t + u_t - d_t, \quad t = 0, \ldots, T - 1 \\
& \quad x_0 = x_{\text{init}} \\
& \quad 0 \leq u_t \leq M, \quad t = 0, \ldots, T - 1.
\end{align*}
\]

Depending on \( d_t \) with \( t = 0, \ldots, T - 1 \) and \( x_{\text{init}} \), we need to adapt our ordering policy to minimize the cost. We assume that \( d_t \in [1, 3] \) and \( x_{\text{init}} \in [7, 13] \).

The strategy selection is summarized in Figure 1 and can be easily interpreted: \( u_t = 0 \) for \( t \leq t_0 \) and then \( u_t = d_t \) for \( t > t_0 \). A inventory level trajectory example can be seen in Figure 2. Let us outline the strategies depicted in Figure 1. For example, if the initial inventory level \( x_{\text{init}} \) is below 7.91, we should apply Strategy 4, where we wait only \( t_0 = 3 \) time steps before ordering. Otherwise, if \( 7.91 \leq x_{\text{init}} < 9.97 \) we should wait for \( t_0 = 5 \) time steps before ordering because the initial inventory level is higher. The other branches can be similarity interpreted. Note that for this problem instance the decision is largely independent from \( d_t \). The only exception comes with \( d_5 \) that determines the choice of strategies in the right-hand side of the tree.

The strategies we derived are related to the \((s, S)\) policies for inventory management, see [ZF91]: if the inventory level falls below value \( s \), we order so that the level becomes \( S \). The optimal decisions from our approach are as simple as the \((s, S)\) policies because we can describe them with if-then-else rules in Figure 1. However, they give better performance because they
Figure 1: Decision strategy for the inventory example. *Strategy 1:* do not order for the first 4 time steps, then order matching the demand. *Strategy 2:* do not order for the first 5 time steps, then order matching the demand. *Strategy 3:* do not order for the first 6 time steps, then order matching the demand. *Strategy 4:* do not order for the first 3 time steps, then order matching the demand.

2.2 Optimal Strategies in Mixed-Integer Optimization

When dealing with integer variables we address the following problem:

\[
\begin{align*}
\text{minimize} & \quad f(\theta, x) \\
\text{subject to} & \quad g(\theta, x) \leq 0 \\
& \quad x_I \in \mathbb{Z}^d.
\end{align*}
\]  

(5)

where \( I \) is the set of indices for the variables constrained to be integer and \(|I| = d|\).

**Tight constraints.** In this case the set of tight constraints does not uniquely define the optimal solution because of the integrality of some components of \( x \). However, when we fix the integer variables to their optimal values \( x_I^*(\theta) \), (5) becomes a continuous convex optimization problem of the form:

\[
\begin{align*}
\text{minimize} & \quad f(\theta, x) \\
\text{subject to} & \quad g(\theta, x) \leq 0 \\
& \quad x_I = x_I^*(\theta).
\end{align*}
\]  

(6)
Figure 2: Inventory behavior with Strategy 2. The lower bound on $u_t$ is active for the first 5 steps. Then $u_t = d_t$.

Note that the optimal cost of (6) and (5) are the same, however, optimal solutions may be different as there may be alternative optima. After fixing the integer variables, the tight constraints of problem (6) uniquely define an optimal solution.

Solution strategy. For this class of problems the strategy corresponds to a tuple containing the index of tight constraints of the continuous reformulation (6) and the optimal value of the integer variables, i.e., $s(\theta) = (T(\theta), x_I^*(\theta))$. Compared to continuous problems, we must also include the value of the integer variables to recover the optimal solution $x^*(\theta)$.

Given the optimal strategy, problem (5) corresponds to solving the continuous problem

\[
\begin{align*}
\text{minimize} & \quad f(\theta, x) \\
\text{subject to} & \quad g_i(\theta, x) \leq 0, \quad \forall i \in T(\theta) \\
x_I = x_I^*(\theta).
\end{align*}
\]  

Solving this problem is much less computationally demanding than (5) because it is continuous, convex and has smaller number of constraints, especially when $n \ll m$. As for the continuous case (3), the components $g_i$ that
are linear in $x$ can be enforced as equalities further simplifying (7) while preserving its convexity.

Similarly to Section 2.1, in case of mixed-integer linear optimization problem (MILO) and mixed-integer quadratic optimization problem (MIQO) when the cost $f$ is linear or quadratic and the constraints $g$ are all linear, the solution of (3) corresponds to solving a linear system of equations defined by the KKT conditions [BV04, Section 10.2]. This means that we can solve these problems online without needing any optimization solver.

The knapsack problem

Consider the knapsack problem

$$
\begin{align*}
\text{maximize} & \quad c^T x \\
\text{subject to} & \quad a^T x \leq b \\
& \quad 0 \leq x \leq u \\
& \quad x \in \mathbb{Z}^n,
\end{align*}
$$

with $n = 10$. The decision variables are $x = (x_1, \ldots, x_{10})$ indicating the quantity to pick for each item $i = 1, \ldots, 10$. We chose the cost vector $c = (0.42, 0.72, 0, 0.3, 0.15, 0.09, 0.19, 0.35, 0.4, 0.54)$. The knapsack capacity is $b = 5$. The weights $a = (a_1, \ldots, a_{10})$ and the maximum order quantity $u = (u_1, \ldots, u_{10})$ are our parameters. We assume that $a$ is in a ball $B(a_0, r_0)$ and $u \in B(u_0, r_0)$ where $u_0 = a_0 = (2, 2, \ldots, 2)$ and $r_0 = 1$.

With this setup we obtain the solution strategy outlined in Figure 3. For this problem each strategy uniquely identifies the integer variables and is straightforward to analyze. For instance, the left part of the tree outlines what happens if the upper bound $u_2$ is strictly less than 2. Moreover, if the weight $a_1 < 1.4$, then it is easier to include $x_1$ in the knapsack solution and for this reason Strategy 3 has $x_1 = 2$ and $x_2 = 1$. On the contrary, if $a_1 \geq 1.4$, then Strategy 2 applies $x_1 = 0$ and $x_2 = x_{10} = 1$. Even though all these rules are simple, they capture the complexity of a hard combinatorial problem for the parameters that affect it. Note that only a few parameters affect the strategy selection, i.e., $u_2, a_1$ and $a_2$, while the others are not relevant for this class of problem instances that have $a \in B(a_0, r_0)$ and $u \in B(u_0, r_0)$.

Supplier selection

Consider the problem of selecting $n = 5$ suppliers in order to satisfy a known demand $d$. For each supplier $i$ we have a per-unit
Figure 3: Example knapsack decision strategies. 

**Strategy 1**: \( x_i = 0 \) for \( i \neq 2 \) and \( x_2 = 2 \).

**Strategy 2**: \( x_i = 0 \) for \( i \neq 2, 10 \) and \( x_2 = x_{10} = 1 \).

**Strategy 3**: \( x_i = 0 \) for \( i \neq 1, 2 \) and \( x_1 = 2 \) and \( x_2 = 1 \).

**Strategy 4**: \( x_i = 0 \) for \( i \neq 2, 10 \) and \( x_2 = 2 \) and \( x_{10} = 1 \).

The cost \( c = (0.42, 0.72, 0, 0.3, 0.15) \) and a maximum quantity to order \( m = (1.09, 1.19, 1.35, 1.4, 1.54) \), while \( \gamma = 0.1 \). We are interested to understand the optimal strategy as a function of the demand \( d \) and the supplier delivery times \( \tau_i \), which are the problem parameters. The optimization problem is as follows:

\[
\begin{align*}
\text{minimize} & \quad \sum_{i=1}^{n} c_i u_i + \gamma \max_i \{\tau_i x_i\} \\
\text{subject to} & \quad \sum_{i=1}^{n} u_i \geq d \\
& \quad 0 \leq u_i \leq x_i m_i \\
& \quad x \in \{0, 1\}^n, u_i \in \mathbb{R}.
\end{align*}
\]  

Specifically, we are interested in \( d \in [1, 3] \) and \( \tau = (\tau_1, \ldots, \tau_5) \in B(\tau_0, r_0) \) with the center of the ball being \( \tau_0 = (2, 3, 2.5, 5, 1) \) and radius \( r_0 = 0.5 \). With these parameters we obtain the solution described in Figure 4. As before, the decision rules are simple and the solution strategy is intuitive and interpretable.

In Figure 5 we show the tree that OCT-H gave for this example. Even though the accuracy of the OCT in Figure 4 is 100%, the OCT-H depth is smaller which can make some classification tasks possibly more interpretable despite the multiple coefficients on the hyperplanes.
Figure 4: Example vendor decision strategies using OCT. 

**Strategy 1:** $x = (1,0,1,0,1)$, $u_2 = u_4 = 0$. $u_3 = m_3, u_5 = m_5$ and $u_1$ is free. 

**Strategy 2:** 

$x = (0,0,1,0,1)$. $u_1 = u_2 = u_4 = 0$ and $u_3 = m_3$. $u_5$ is free. 

**Strategy 3:** 

$x = (0,0,1,0,0)$. $u_1 = u_2 = u_4 = u_5 = 0$ and $u_3$ is free. 

**Strategy 4:** 

$x = (0,0,0,0,1)$. $u_1 = u_2 = u_3 = u_4 = 0$. $u_5$ is free.

Figure 5: Example vendor decision strategies using OCT-H. The strategies are the same as in Figure 4 but accuracy is the same or higher and the tree depth is reduced. Smaller tree depth can make the classification easier to understand and interpret.
3 Machine Learning

In this section, we introduce the core part of our approach: learning the mapping from parameters to optimal strategies. This mapping is going to completely replace the hardest part of most optimization algorithms – the optimal strategy search – with a multiclass classification problem where each strategy corresponds to a class label.

3.1 Multiclass Classifier

We would like to solve a multiclass classification problem with data \((\theta_i, s_i), \ i = 1, \ldots, N\) where \(\theta_i \in \mathbb{R}^p\) are the parameters and \(s_i \in \mathcal{S}\) the corresponding labels identifying the optimal strategies. \(\mathcal{S}\) represents the set of strategies of cardinality \(|\mathcal{S}| = M\).

Two of the most successful supervised learning techniques for multiclass classification are optimal classification trees (OCTs, OCT-Hs) \([BD17, BD18]\) and neural networks (NNs) \([Ben09, LBH15]\). We apply both these methods to compare their predictive performance. As we mentioned earlier, OCTs, OCT-Hs are interpretable and can be described using simple rules as in the examples in the previous section, while NNs are not interpretable since they represent a composition of multiple nonlinear functions.

Optimal classification trees (OCTs). OCTs and OCT-Hs developed in \([BD17, BD18]\) are a recently proposed generalization of classification and regression trees (CARTs) developed in \([BFOS84]\) that construct decision trees that are near optimal with significantly higher prediction accuracy while retaining their remarkable interpretability. We present a more detailed description of OCTs and OCT-Hs in Appendix A.

Neural networks (NNs). NNs have recently become one of the most prominent machine learning techniques revolutionizing fields such as speech recognition (see \([HDY+12]\)) and computer vision (see \([KSH12]\)). The wide range of applications of these techniques recently extended to autonomous driving (see \([BDTD+16]\)) and reinforcement learning (see \([SSS+17]\)). The popularity of neural networks is also due to the widely used open-source libraries learning on CPUs and GPUs coming from both academia and industry such as TensorFlow \([AAB+15]\), Caffe \([JSD+14]\) and PyTorch \([PGC+17]\). We use
feedforward neural networks which offer a good tradeoff between simplicity and accuracy without resorting to more complex architectures such as convolutional or recurrent neural networks, see [LBH15]. A more detailed description of NNS can be found in Appendix B.

[BMS18] have shown that given a NN (feedforward, convolutional and recurrent), we can construct an OCT-H that has the same in sample accuracy, that is OCT-Hs are at least as powerful as NNS. The constructions, however, generate OCT-Hs with high depth. They report, however, computational results that show that OCT-Hs and NNS have comparable performance in practice even for depths of OCT-Hs below 10.

3.2 Strategies Exploration

In this section, we estimate how likely it is to find a new parameter \( \theta \) whose optimal strategy does not lie among the ones we have already seen. If it is unlikely to find new strategies, then we can be sure that our classification problem includes all the possible strategies arising in practice. Otherwise, we must collect more data to have a more representative classification problem.

**Estimating the probability of finding unseen strategies.** Given \( N \) independent samples \( \Theta_N = \{\theta_1, \ldots, \theta_N\} \) drawn from an unknown discrete distribution \( \mathcal{P} \) with the corresponding strategies \( (s(\theta_1), \ldots, s(\theta_N)) \), we find \( M \) unique strategies \( S(\Theta_N) = \{s_1, \ldots, s_M\} \). We are interested in bounding the probability of finding unseen strategies

\[
P(\theta_{N+1} \in \mathbb{R}^p \mid s(\theta_{N+1}) \notin S(\Theta_N)),
\]

with confidence at least \( 1 - \beta \) where \( \beta > 0 \).

This problem started from the seminal work by Turing and Good [Goo53] in the context of decrypting the Enigma codes during World War II. The Enigma machine was a German navy encryption device used for secret military communications. Part of Enigma’s encryption key was a three letter sequence (a word) selected from a book containing all the possible ones in random order. The number of possible words was so large that it was impossible to test all the combinations with the computing power available at that time. In order to decrypt the Enigma machine without testing all the possible words, Turing wanted to check only a subset of them while estimating that the likelihood of finding a new unseen word was low. This is how the
Good-Turing estimator was developed. It was a fundamental step towards the Enigma machine decryption which is believed to have shortened World War II of at least two years [Cop12]. In addition, this class of estimators have become standard in a wide range of natural language processing applications.

**Good-Turing estimator.** Let $N_r$ be the number of strategies that appeared exactly $r$ times in $(s(\theta_1), \ldots, s(\theta_N))$. The Good-Turing estimator for the probability of having an unseen strategy is given by [Goo53]

$$G = N_1/N,$$  \hspace{1cm} (11)

which corresponds to the ratio between the number of distinct strategies that have appeared exactly once, over the total number of samples. Despite the elegant result, Good and Turing did not provide a convergence analysis of this estimator for finite samples. Only few decades later the first theoretical work on that topic appeared in [MS00]. Using [McD89]'s inequality the authors derived a high probability confidence interval. That result can be directly applied to our problem with the following theorem.

**Theorem 3.1** (Missing strategies bound). The probability of encountering a parameter $\theta_{N+1}$ corresponding to an unseen strategy $s(\theta_{N+1})$ satisfies with confidence at least $1 - \beta$

$$P(\theta_{N+1} \in \mathbb{R}^p \mid s(\theta_{N+1}) \notin S(\Theta_N)) \leq G + c\sqrt{(1/N) \ln(3/\beta)},$$

where $G$ corresponds to the Good-Turing estimator (11) and $c = (2\sqrt{2} + \sqrt{3})$.

**Proof.** The result follows directly from [MS00, Theorem 9]. \(\square\)

**Exploration algorithm.** Given the bound in Theorem 3.1, we construct Algorithm 1 to compute the different strategies appearing in our problem.

The algorithm keeps on sampling until we encounter a large enough set of distinct strategies. It terminates when the probability of encountering a parameter with an unseen optimal strategy is less than $\epsilon$ with confidence at least $1 - \beta$. Note that in practice, instead of sampling one point per iteration $k$, it is more convenient to sample more points to avoid having to recompute the class frequencies which becomes computationally intensive with several thousands of samples and hundreds of classes. Algorithm 1 imposes no assumptions on the optimization problem nor the data distribution.
Algorithm 1 Strategies exploration

1: given $\epsilon, \beta, \Theta = \emptyset, S = \emptyset, u = \infty$
2: for $k = 1, \ldots,$ do
3: Sample $\theta_k$ and compute $s(\theta_k)$  \texttt{▷} Sample parameter and strategy.
4: $\Theta \leftarrow \Theta \cup \{\theta_k\}$  \texttt{▷} Update set of samples.
5: if $s(\theta_k) \notin S$ then
6: $S \leftarrow S \cup \{s(\theta_k)\}$  \texttt{▷} Update strategy set if new strategy found
7: if $G + c\sqrt{(1/k) \ln(3/\beta)} \leq \epsilon$ then
8: break  \texttt{▷} Break if bound less than $\epsilon$
9: return $k, \Theta, S$

4 Machine Learning Optimizer

We implemented our method in the Python software tool MLOPT (Machine Learning Optimizer). It is integrated with CVXPY \cite{DB16} to formulate and solve the problems. CVXPY allows the user to easily define mixed-integer convex optimization problems performing all the required reformulations needed by the optimizers while keeping track of the original constraints and variables. This makes it ideal for identifying which constraints are tight or not at the optimal solution.

We used the Gurobi Optimizer \cite{Gur16} to find the tight constraints because it provides a good tradeoff between solution accuracy and computation time. Note that from Section 2, in case of LO, MILO, QO and MIQO when the cost $f$ is linear or quadratic and the constraints $g$ are all linear, the online solution corresponds to solving a linear system of equations defined by the KKT conditions \cite[Section 10.2]{BV04} on the reduced subproblem. This means that we can solve those parametric optimization problems without the need to apply any optimization solver.

MLOPT performs the iterative sampling procedure outlined in Section 3.2 to obtain the strategies required for the classification task. We sample 5000 new points at each iteration and compute their strategies until the Good Turing estimate is below $\epsilon_{GT} = 0.005$. The strategy computation is fully parallelized across samples.

We interfaced MLOPT to the machine learning libraries Optimal-Trees.jl \cite{BD18} on multi-core CPUs and PyTorch \cite{PGC+17} for both CPUs and GPUs. In the training phase we automatically tune the predictor
parameters by splitting the data points in 90%/10% training/validation. We tune the OCTs and OCT-Hs with maximal depth for values 5, 10, 15 and minimum bucket size for values 1, 5, 10. For the NNs we validate the stochastic gradient descent learning rate for values 0.001, 0.01, 0.1, batch size for values 32, 128 and number of epochs for values 500, 1000.

5 Computational Benchmarks

In this section, we test our approach on multiple examples from continuous and mixed-integer optimization. We benchmarked the predictive performance of OCTs, OCT-Hs (see Appendix refsec:trees) and NNs (see Appendix B) depending on the problem type and size. We executed the numerical tests on a Dell R730 cluster with 28 Intel E5-2680 CPUs with a total of 256GB RAM and a Nvidia Tesla K80 GPU. We evaluated the performance metrics on 100 unseen samples drawn from the same distribution of $\theta$.

**Infeasibility and suboptimality.** After the learning phase, we compared the predicted solution $\hat{x}_i^*$ to the optimal one $x_i^*$ obtained by solving the instances from scratch. Given a parameter $\theta_i$, we say that the predicted solution is infeasible if the constraints are violated more than a predefined tolerance $\epsilon_{\text{inf}} = 10^{-3}$ according to the infeasibility metric

$$p(\hat{x}_i^*) = \left\| (g(\theta_i, \hat{x}_i^*))_+ \right\|_2 / r(\theta_i, \hat{x}_i^*),$$

where $r(\theta, x)$ normalizes the violation depending on the size of the summands of $g$. For example, if $g(\theta, x) = A(\theta)x - b$, then $r(\theta, x) = \max(\|A(\theta)x\|_2, \|b\|_2)$. If the predicted solution $\hat{x}_i$ is feasible, we define its suboptimality as

$$d(\hat{x}_i^*) = (f(\hat{x}_i^*) - f(x_i^*)) / |f(x_i^*)|.$$  

Note that $d(\hat{x}_i^*) \geq 0$ by construction. We consider a predicted solution to be accurate if it is feasible and if the suboptimality is less than the tolerance $\epsilon_{\text{sub}} = 10^{-3}$. For each instance we report the maximum infeasibility $\max_i p(\hat{x}_i^*)$ and the maximum suboptimality $\max_i d(\hat{x}_i^*)$. Note that for notation ease and to simplify the max operation, if a point is infeasible we consider its suboptimality 0 and ignore it.
Predicting the optimal strategy. Once the learning phase is completed, the predictor outputs the three (3) most likely optimal strategies and picks the best one according to infeasibility and suboptimality after solving the associated reduced problems.

5.1 Transportation Optimization

Consider a standard transportation problem with \( n \) warehouses and \( m \) retail stores. Let \( x_{ij} \) be the quantity we ship from warehouse \( i \) to store \( j \). \( s_i \) denotes the supply for warehouse \( i \) and \( d_j \) the demand from store \( j \). We define the cost of transporting a unit from warehouse \( i \) to store \( j \) as \( c_{ij} \). The optimization problem can be formulated as follows:

\[
\begin{align*}
\text{minimize} & \sum_{i=1}^{n} \sum_{j=1}^{m} c_{ij} x_{ij} \\
\text{subject to} & \sum_{j=1}^{m} x_{ij} \leq s_i, \quad \forall i \\
& \sum_{i=1}^{n} x_{ij} \geq d_j, \quad \forall j \\
& x_{ij} \geq 0 \quad \forall i, j.
\end{align*}
\]

The first constraint ensures we respect the supply for each warehouse \( i \). The second constraint enforces the sum of all the shipments to match at least the demand for store \( j \). Finally, the quantity of shipped product has to be nonnegative. Our learning parameters are the demands \( d_j \).

Problem instances We generate the transportation problem instances by varying the number of warehouses \( n \) and stores \( m \). The cost vectors \( c_i \) are distributed as \( \mathcal{U}(0,5) \) and the supplies \( s_i \) as \( \mathcal{U}(3,13) \). The parameter vector \( d = (d_1, \ldots, d_m) \) was sampled from a uniform distribution within the ball \( B(\bar{d}, 0.75) \) with center \( \bar{d} \sim \mathcal{N}(3,1) \).

Results. The results appear in Table 1. Independently from the problem instances the prediction accuracy is very high for both optimal trees and neural networks. Note that even though we solve problems with thousands of variables and constraints, the number of strategies is always within few tens or less. Moreover, both NNS and OCT-Hs provide optimal and feasible
Table 1: Transportation benchmarks.

| n   | m   | nvar | nconstr | learner | N    | |S| | accuracy [%] | max, p(\bar{x}_i) | max, d(\bar{x}_i) |
|-----|-----|------|---------|---------|------|-----|----------------|------------------|------------------|
| 20  | 20  | 400  | 440     | NN      | 10000| 0.0001| 10             | 100.0            | 8.88 × 10^{-5}   | 0.00             |
| 20  | 20  | 400  | 440     | OCT     | 10000| 0.0001| 10             | 100.0            | 8.88 × 10^{-5}   | 0.00             |
| 20  | 20  | 400  | 440     | OCT-H   | 10000| 0.0001| 9              | 100.0            | 8.88 × 10^{-5}   | 0.00             |
| 20  | 10  | 200  | 230     | NN      | 10000| 0.0004| 9              | 100.0            | 0.00             | 0.00             |
| 20  | 10  | 200  | 230     | OCT     | 10000| 0.0004| 9              | 99.0             | 1.00             | 0.00             |
| 20  | 10  | 200  | 230     | OCT-H   | 10000| 0.0004| 9              | 100.0            | 0.00             | 0.00             |
| 40  | 40  | 1600 | 1680    | NN      | 10000| 0.0003| 9              | 100.0            | 1.29 × 10^{-16}  | 0.00             |
| 40  | 40  | 1600 | 1680    | OCT     | 10000| 0.0003| 9              | 100.0            | 1.29 × 10^{-16}  | 0.00             |
| 40  | 40  | 1600 | 1680    | OCT-H   | 10000| 0.0003| 9              | 100.0            | 1.29 × 10^{-16}  | 0.00             |
| 20  | 20  | 800  | 860     | OCT     | 10000| 0.0001| 7              | 100.0            | 0.00             | 0.00             |
| 20  | 20  | 800  | 860     | OCT-H   | 10000| 0.0001| 7              | 100.0            | 0.00             | 0.00             |
| 60  | 60  | 3600 | 3720    | NN      | 10000| 0.0006| 17             | 100.0            | 1.86 × 10^{-5}   | 0.00             |
| 60  | 60  | 3600 | 3720    | OCT     | 10000| 0.0006| 17             | 100.0            | 1.59 × 10^{-16}  | 0.00             |
| 60  | 60  | 3600 | 3720    | OCT-H   | 10000| 0.0006| 17             | 100.0            | 1.59 × 10^{-16}  | 0.00             |
| 60  | 30  | 1800 | 1890    | NN      | 10000| 0.0001| 13             | 100.0            | 0.00             | 0.00             |
| 60  | 30  | 1800 | 1890    | OCT     | 10000| 0.0001| 13             | 100.0            | 0.00             | 0.00             |
| 60  | 30  | 1800 | 1890    | OCT-H   | 10000| 0.0001| 13             | 100.0            | 0.00             | 0.00             |
| 80  | 80  | 6400 | 6560    | NN      | 16200| 0.0016| 93             | 92.0             | 7.34 × 10^{-3}   | 0.00             |
| 80  | 80  | 6400 | 6560    | OCT     | 16200| 0.0016| 93             | 73.0             | 1.00             | 0.00             |
| 80  | 80  | 6400 | 6560    | OCT-H   | 16200| 0.0016| 93             | 96.0             | 1.00             | 0.00             |
| 80  | 40  | 3200 | 3320    | NN      | 10000| 0.0000| 7              | 100.0            | 0.00             | 0.00             |
| 80  | 40  | 3200 | 3320    | OCT     | 10000| 0.0000| 7              | 100.0            | 0.00             | 0.00             |
| 80  | 40  | 3200 | 3320    | OCT-H   | 10000| 0.0000| 7              | 100.0            | 0.00             | 0.00             |

Solutions with almost perfect accuracy. OCT performed comparably, except in one instance.

5.2 Portfolio Optimization

Consider the problem of allocating assets to minimize the risk adjusted return considered in [Mar52] who formulated it as a QO

\[
\begin{align*}
\text{maximize} & \quad \mu^T x - \gamma (x^T \Sigma x) \\
\text{subject to} & \quad 1^T x = 1 \\
& \quad x \geq 0,
\end{align*}
\]

where the variable \( x \in \mathbb{R}^n \) represents the investments to make.

Our learning parameter is the vector of expected returns \( \mu \in \mathbb{R}^n \). In addition we denote the risk aversion coefficient as \( \gamma > 0 \), and the covariance matrix for the risk model as \( \Sigma \in S_+^n \). \( \Sigma \) is assumed to be

\[
\Sigma = FF^T + D,
\]
where $F \in \mathbb{R}^{n \times p}$ is the factor loading matrix and $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix describing the asset-specific risk.

**Problem instances.** We generated portfolio instances for different number of factors $p$ and assets $n$. We chose the elements of $F$ with 50% nonzeros and $F_{ij} \sim \mathcal{N}(0, 1)$. The diagonal matrix $D$ has elements $D_{ii} \sim \mathcal{U}(0, \sqrt{p})$. The return vector parameters were randomly sampled from a uniform distribution within the ball $B(\mu, 0.15)$ with $\mu \sim \mathcal{N}(0, 1)$. The risk-aversion coefficient is $\gamma = 1$.

**Results.** Results are shown in Table 2. The prediction accuracy for OCTs, OCT-Hs and NNs is 100%, the number of strategies is less than 15, and the infeasibility and suboptimality are very low.

### 5.3 Facility location

Let $i \in I$ the set of possible locations for facilities such as factories or warehouses. We denote as $j \in J$ the set of delivery locations. The cost of transporting a unit of goods from facility $i$ to location $j$ is $c_{ij}$. The construction cost for building facility $i$ is $f_i$. For each location $j$, we define the demand $d_j$. The capacity of facility $i$ is $s_i$. The main goal of this problem is to find the best tradeoff between transportation costs versus construction costs.
costs. We can write the model as a MILO

$$\text{minimimize} \sum_{i \in I} \sum_{j \in J} c_{ij} x_{ij} + \sum_{i \in I} f_i y_i$$

subject to

$$\sum_{i \in I} x_{ij} \geq d_j, \quad \forall j \in J$$

$$\sum_{j \in J} x_{ij} \leq s_i y_i, \quad \forall i \in I$$

$$x_{ij} \geq 0$$

$$y_i \in \{0, 1\}.$$  \hspace{1cm} (12)

The decision variables $x_{ij}$ describe the amount of goods sent from facility $i$ to location $j$. The binary variables $y_i$ determine if we build facility $i$ or not.

**Problem instances.** We generated the facility location instances for different values of facilities $n$ and warehouses $m$. The costs $c_{ij}$ are sampled from a uniform distribution $\mathcal{U}(0, 1)$ and $f_i$ from $\mathcal{U}(0, 10)$. We chose capacities $s_i$ as $\mathcal{U}(8, 18)$ to ensure the problem is always feasible. The demands parameters $d = (d_1, \ldots, d_m)$ were sampled from a uniform distributions within the ball $B(\bar{d}, 0.25)$ with $\bar{d} \sim \mathcal{N}(3, 1)$.

**Results.** Table 3 shows the benchmark examples. We notice a predictive performance degradation when the number of strategies is higher. We suspect this is related to more samples needed to properly train the models. However, the infeasibility and suboptimality measures are low even when the prediction is not correct. As before OCTs and OCT-Hs are comparable except in one instance where OCT-H significantly outperformed.

### 5.4 Hybrid Vehicle Control

Consider the hybrid-vehicle control problem in [TMBB17, Section 3.2]. The model consists of a battery, an electric motor/generator and an engine. We assume to know the demanded power $P_{\text{des}}^t$ over the horizon $t = 0, \ldots, T - 1$. The goal is to plan the battery and the engine power outputs $P_{\text{batt}}^t$ and $P_{\text{eng}}^t$ so that they match at least the demand,

$$P_{\text{batt}}^t + P_{\text{eng}}^t \geq P_{\text{des}}^t.$$
Table 3: Facility location benchmarks.

| n  | m  | n_var | n_constr | learner | N   | |S| | accuracy [%] | max$_i$ p($\bar{x}_i$) | max$_i$ d($\bar{x}_i$) |
|----|----|-------|----------|---------|-----|------|------|--------------|-----------------|-----------------|
| 20 | 20 | 420   | 480      | NN      | 10000 | 0.0000 | 3    | 100.0        | 1.14 × 10$^{-16}$ | 1.19 × 10$^{-7}$ |
| 20 | 20 | 420   | 480      | OCT     | 10000 | 0.0000 | 3    | 100.0        | 1.14 × 10$^{-16}$ | 8.56 × 10$^{-8}$ |
| 20 | 20 | 420   | 480      | OCT-H   | 10000 | 0.0000 | 3    | 100.0        | 1.14 × 10$^{-16}$ | 8.57 × 10$^{-8}$ |
| 20 | 20 | 220   | 270      | NN      | 10000 | 0.0000 | 1    | 100.0        | 0.00            | 1.22 × 10$^{-16}$ |
| 20 | 20 | 220   | 270      | OCT     | 10000 | 0.0000 | 1    | 100.0        | 0.00            | 0.00            |
| 20 | 20 | 220   | 270      | OCT-H   | 10000 | 0.0000 | 1    | 100.0        | 0.00            | 1.22 × 10$^{-16}$ |
| 40 | 40 | 1640  | 1760     | NN      | 10000 | 0.0000 | 12   | 95.0         | 1.53 × 10$^{-2}$  | 2.02 × 10$^{-16}$ |
| 40 | 40 | 1640  | 1760     | OCT     | 10000 | 0.0000 | 12   | 93.0         | 2.01 × 10$^{-2}$  | 2.02 × 10$^{-16}$ |
| 40 | 40 | 1640  | 1760     | OCT-H   | 10000 | 0.0000 | 12   | 99.0         | 2.78 × 10$^{-3}$  | 2.02 × 10$^{-16}$ |
| 40 | 20 | 840   | 940      | NN      | 10000 | 0.0000 | 2    | 100.0        | 2.54 × 10$^{-16}$ | 4.86 × 10$^{-8}$  |
| 40 | 20 | 840   | 940      | OCT     | 10000 | 0.0000 | 2    | 100.0        | 2.54 × 10$^{-16}$ | 4.58 × 10$^{-8}$  |
| 40 | 20 | 840   | 940      | OCT-H   | 10000 | 0.0000 | 2    | 100.0        | 2.54 × 10$^{-16}$ | 1.09 × 10$^{-8}$  |
| 60 | 60 | 3660  | 3840     | NN      | 10000 | 0.0008 | 28   | 100.0        | 8.28 × 10$^{-5}$  | 2.25 × 10$^{-16}$ |
| 60 | 60 | 3660  | 3840     | OCT     | 10000 | 0.0008 | 28   | 100.0        | 2.74 × 10$^{-16}$ | 2.25 × 10$^{-16}$ |
| 60 | 60 | 3660  | 3840     | OCT-H   | 10000 | 0.0008 | 28   | 100.0        | 2.74 × 10$^{-16}$ | 2.25 × 10$^{-16}$ |
| 60 | 30 | 1860  | 2010     | NN      | 10000 | 0.0000 | 2    | 100.0        | 1.90 × 10$^{-16}$ | 1.40 × 10$^{-16}$ |
| 60 | 30 | 1860  | 2010     | OCT     | 10000 | 0.0000 | 2    | 100.0        | 1.90 × 10$^{-16}$ | 1.40 × 10$^{-16}$ |
| 60 | 30 | 1860  | 2010     | OCT-H   | 10000 | 0.0000 | 2    | 100.0        | 1.90 × 10$^{-16}$ | 1.40 × 10$^{-16}$ |
| 80 | 80 | 6480  | 6720     | NN      | 10000 | 0.0005 | 25   | 64.0         | 2.72 × 10$^{-2}$  | 5.63 × 10$^{-3}$  |
| 80 | 80 | 6480  | 6720     | OCT     | 10000 | 0.0005 | 25   | 66.0         | 2.72 × 10$^{-2}$  | 5.45 × 10$^{-3}$  |
| 80 | 80 | 6480  | 6720     | OCT-H   | 10000 | 0.0005 | 25   | 88.0         | 5.46 × 10$^{-3}$  | 5.39 × 10$^{-3}$  |
| 80 | 40 | 3280  | 3480     | NN      | 10000 | 0.0001 | 10   | 98.0         | 4.27 × 10$^{-3}$  | 6.26 × 10$^{-4}$  |
| 80 | 40 | 3280  | 3480     | OCT     | 10000 | 0.0001 | 10   | 93.0         | 4.41 × 10$^{-3}$  | 2.65 × 10$^{-3}$  |
| 80 | 40 | 3280  | 3480     | OCT-H   | 10000 | 0.0001 | 10   | 99.0         | 3.47 × 10$^{-16}$ | 6.26 × 10$^{-4}$  |
The status of the battery is modeled with the internal energy $E_t$ evolving as

$$E_{t+1} = E_t - \tau P_{\text{batt}}^t,$$

where $\tau > 0$ is the time interval discretization. The battery capacity is limited by $E_{\text{max}}$ and its initial value is $E_{\text{init}}$.

We now model the cost function. We penalize the terminal energy state of the battery with the function

$$g(E) = \eta (E_{\text{max}} - E)^2,$$

with $\eta \geq 0$. At each time $t$ we model the on-off state of the engine with the binary variable $z_t$. When the engine is off ($z_t = 0$) we do not consume any energy, thus we have $0 \leq P_{t}^{\text{eng}} \leq P_{\text{max}} z_t$. When the engine is on ($z_t = 1$) it consumes $\alpha P_{t}^{\text{eng}} + \beta P_{t}^{\text{eng}} + \gamma$ units of fuel, with $\alpha, \beta, \gamma > 0$. We define the stage power cost as

$$f(P, z) = \alpha P^2 + \beta P + \gamma z.$$

We also introduce a cost of turning the engine on at time $t$ as $\delta(z_t - z_{t-1})$.

The hybrid vehicle control problem can be formulated as a mixed integer quadratic optimization problem:

$$\begin{align*}
\text{maximize} & \quad \eta(E_T - E_{\text{max}}) + \sum_{t=0}^{T-1} f(P_t^{\text{eng}}, z_t) + \delta(z_t - z_{t-1})_+ \\
\text{subject to} & \quad E_{t+1} = E_t - \tau P_{t}^{\text{batt}}, \quad t = 0, \ldots, T - 1 \\
& \quad 0 \leq E_t \leq E_{\text{max}}, \quad t = 0, \ldots, T \\
& \quad E_0 = E_{\text{init}} \\
& \quad 0 \leq P_{t}^{\text{eng}} \leq P_{\text{max}}, \quad t = 0, \ldots, T - 1 \\
& \quad P_{t}^{\text{batt}} + P_{t}^{\text{eng}} \geq P_{t}^{\text{des}}, \quad t = 0, \ldots, T - 1 \\
& \quad z_t \in \{0, 1\}, \quad t = 0, \ldots, T - 1.
\end{align*}$$

The initial state $E_0$ and demanded power $P_{t}^{\text{des}}$ are our parameters.

**Problem instances.** We generated the control instances with varying horizon length $T$. The discretization time interval is $\tau = 4$. We chose the cost function parameters parameters $\alpha = \beta = \gamma = 1$, and $\delta = 0.1$. The maximum charge is $E_{\text{max}} = 50$ and the maximum power $P_{\text{max}} = 1$. The parameter $E_0$ was sampled from a uniform distribution within the ball $B(40, 0.5)$. The demand $P_{t}^{\text{des}}$ also comes from a uniform distribution within the ball $B(P_{t}^{\text{des}}, 0.5)$.
Table 4: Hybrid control benchmarks.

| \(T\) | \(n_{\text{var}}\) | \(n_{\text{constr}}\) | learner | \(N\) | GT | \(|S|\) | accuracy [%] | \(\max_t p(\bar{x}_t)\) | \(\max_t d(\bar{x}_t)\) |
|---|---|---|---|---|---|---|---|---|---|
| 5  | 21  | 43  | NN  | 10000 | 0.0002 | 10 | 99.0 | \(9.43 \times 10^{-15}\) | \(2.84 \times 10^{-3}\) |
| 5  | 21  | 43  | OCT | 10000 | 0.0002 | 10 | 97.0 | \(9.43 \times 10^{-15}\) | \(9.83 \times 10^{-2}\) |
| 5  | 21  | 43  | OCT-H | 10000 | 0.0002 | 10 | 100.0 | \(9.43 \times 10^{-15}\) | \(1.20 \times 10^{-15}\) |
| 10 | 41  | 83  | NN  | 10000 | 0.0003 | 14 | 100.0 | \(1.17 \times 10^{-14}\) | \(3.81 \times 10^{-15}\) |
| 10 | 41  | 83  | OCT | 10000 | 0.0003 | 14 | 100.0 | \(1.17 \times 10^{-14}\) | \(3.53 \times 10^{-15}\) |
| 10 | 41  | 83  | OCT-H | 10000 | 0.0003 | 14 | 100.0 | \(1.17 \times 10^{-14}\) | \(3.53 \times 10^{-15}\) |
| 20 | 81  | 163 | OCT | 10000 | 0.0006 | 14 | 99.0 | \(2.92 \times 10^{-4}\) | \(6.26 \times 10^{-15}\) |
| 20 | 81  | 163 | OCT-H | 10000 | 0.0006 | 14 | 99.0 | \(1.51 \times 10^{-4}\) | \(6.33 \times 10^{-15}\) |
| 20 | 81  | 163 | OCT  | 10000 | 0.0006 | 14 | 100.0 | \(6.18 \times 10^{-5}\) | \(6.33 \times 10^{-15}\) |
| 30 | 121 | 243 | NN  | 10000 | 0.0002 | 22 | 94.0 | \(2.34 \times 10^{-3}\) | \(9.86 \times 10^{-4}\) |
| 30 | 121 | 243 | OCT | 10000 | 0.0002 | 22 | 83.0 | \(6.42 \times 10^{-3}\) | \(5.31 \times 10^{-4}\) |
| 30 | 121 | 243 | OCT-H | 10000 | 0.0002 | 22 | 94.0 | \(1.55 \times 10^{-13}\) | \(5.23 \times 10^{-4}\) |
| 40 | 161 | 323 | NN  | 10000 | 0.0001 | 34 | 91.0 | \(3.78 \times 10^{-3}\) | \(4.24 \times 10^{-4}\) |
| 40 | 161 | 323 | OCT | 10000 | 0.0001 | 34 | 65.0 | \(2.59 \times 10^{-2}\) | \(1.97 \times 10^{-3}\) |
| 40 | 161 | 323 | OCT-H | 10000 | 0.0001 | 34 | 80.0 | \(1.07 \times 10^{-2}\) | \(6.19 \times 10^{-4}\) |

where

\[
\mathcal{P}_t^{\text{des}} = (0.05, 0.30, 0.55, 0.80, 1.05, 1.30, 1.55, 1.80, 1.95, 1.70, 1.45, 1.20, 1.02, 1.12, 1.22, 1.32, 1.42, 1.52, 1.62, 1.72, 1.73, 1.38, 1.03, 0.68, 0.33, -0.02, -0.37, -0.72, -0.94, -0.64, -0.34, -0.04, 0.18, 0.08, -0.02, -0.12, -0.22, -0.32, -0.42, -0.52)
\]

is the desired power in [TMBB17]. Depending on the horizon length \(T\) we choose only the first \(T\) elements of \(\mathcal{P}_t^{\text{des}}\) to sample \(\mathcal{P}^{\text{des}}\).

**Results.** We present the results in Table 4. Also in this case the number of strategies \(|S|\) is much less than the number of variables or the worst case number of control input combinations. The maximum infeasibility and suboptimality are low even when the predictions are not exact and the performance of OCT-Hs and NNs is comparable, except on one instance where NNs were stronger. The performance of OCT was weaker especially as the dimension of the problem increased.
6 Conclusions

We introduced the idea that using OCTs and OCT-Hs we obtain insight on the strategy of the optimal solution in many optimization problems as a function of key parameters. In this way, optimization is not a black box anymore, but rather it has a voice, i.e., we are able to provide insights on the logic behind the optimal solution. The class of optimization problems that these ideas apply to is rather broad since it includes any continuous and mixed-integer convex optimization problems without any assumption on the parameters dependency. The accuracy of our approach is in the 90%-100%, while even when it does not provide the optimal solution the degree of suboptimality or infeasibility is extremely low. Comparisons on several examples show that the out of sample strategy prediction accuracy of OCT-Hs is comparable to the NNs. Therefore our method provides a reliable and insightful understanding of optimal solutions in a broad class of optimization problems.

A Optimal Classification Trees

Architecture. OCTs recursively partition the feature space $\mathbb{R}^p$ to construct hierarchical disjoint regions. A tree can be defined as a set of nodes $t \in \mathcal{T}$ of two types $\mathcal{T} = \mathcal{T}_B \cup \mathcal{T}_L$:

Branch nodes Nodes $t \in \mathcal{T}_B$ at the tree branches describe a split of the form $a_t^T \theta < b_t$ where $a_t \in \mathbb{R}^p$ and $b_t \in \mathbb{R}$. They partition the space in two subsets: the points on the left branch satisfying the inequality and the remaining ones points on the right branch. If splits involve a single variable we denote them as parallel and we refer to the tree as optimal classification tree (OCT). This is achieved by enforcing all components of $a_t$ to be all 0 except from one. Otherwise, if the components of $a_t$ can be freely nonzero, we denote the splits as hyperplanes and we refer to the tree as optimal classification tree with-hyperplanes (OCT-H).

Leaf nodes Nodes $t \in \mathcal{T}_L$ at the tree leaves make a class prediction for each point falling into that node.

An example OCT for the Iris dataset appears in Figure 6, see [BD18]. For each new data point it is straightforward to follow which hyperplanes are
satisfied and to make a prediction. This characteristic makes OCTs and OCT-Hs highly interpretable. Note that the level of interpretability of the resulting trees can be also tuned by changing minimum sparsity of $a_t$. The two extremes are maximum sparsity OCTs and minimum sparsity OCT-Hs but we can specify anything in between.

**Learning.** With the latest computational advances in mixed-integer optimization (MIO) [BD18] were able to exactly formulate the tree training as a MIO problem and solve it in a reasonable amount of time for problem sizes arising in real-world applications.

The OCT cost function is a tradeoff between the misclassification error at each leaf and the tree complexity

$$\mathcal{L}_{OCT} = \sum_{t \in T_L} L_t + \alpha \sum_{t \in T_B} \|a_t\|_1,$$

where the $L_t$ is the misclassification error at node $t$ and the second term represents the complexity of the tree measured as the sum the norm of the hyperplane coefficients in all the splits. The parameter $\alpha > 0$ regulates the tradeoff. For more details about the cost function and the constraints of the problem, we refer the reader to [BD18, Section 2.2, Section 3.1].

Bertsimas and Dunn apply a local search method [BD18, Section 2.3] that manages to solve OCT problems for realistic sizes in fraction of the time an off-the-shelf optimization solver would take. The algorithm proposed iteratively improves and refines the current tree until a local minimum is
reached. By repeating this search from different random initialization points the authors compute several local minima and then take the best one as the resulting tree. This heuristic showed remarkable performance both in terms of computation time and quality of the resulting tree becoming the algorithm included in the OptimalTrees.jl Julia package [BD18].

B Neural Networks

Architecture. Given \( L \) layers, a neural network is a composition of functions of the form

\[
\hat{s} = f_L(f_{L-1}(\cdots f_1(\theta))),
\]

where each function consists of

\[
y_l = f(y_{l-1}) = g(W_ly_{l-1} + b_l).
\]

(13)

The number of nodes in each layer is \( n_l \) and corresponds to the dimension of the vector \( y_l \in \mathbb{R}^{n_l} \). Layer \( l = 1 \) is defined as the input layer and \( l = L \) as the output layer. Consequently \( y_1 = \theta \) and \( y_L = \hat{s} \). The linear transformation in each layer is composed of an affine transformation with parameters \( W_l \in \mathbb{R}^{n_l \times n_{l-1}} \) and \( b_l \in \mathbb{R}^{n_l} \). The activation function \( g : \mathbb{R}^{n_l} \to \mathbb{R}^{n_l} \) models nonlinearities. We chose as activation function the rectified linear unit (ReLU) defined as

\[
g(x) = \max(x, 0),
\]

for all the layers \( l = 1, \ldots, L - 1 \). Note that the max operator is intended element-wise. We chose a ReLU because on the one hand it provides sparsity to the model since it is 0 for the negative components of \( x \) and because on the other hand it does not suffer from the vanishing gradient issues of the standard sigmoid functions [GBC16]. An example neural network can be found in Figure 7.

For the output layer we would like the network to output not only the predicted class, but also a normalized ranking between them according to
how likely they are to be the right one. This can be achieved with a softmax activation function in the output layer defined as

\[
g(x)_j = \frac{e^{x_j}}{\sum_{j=1}^{M} e^{x_j}},
\]

where \( j = 1, \ldots, M \) are the elements of \( g(x) \). Hence, \( 0 \leq g(x) \leq 1 \) and the predicted class is \( \text{argmax}(\hat{s}) \).

**Learning.** Before training the network, we rewrite the labels for the neural network learning using a one-hot encoding, \( i.e. \), \( s_i \in \mathbb{R}^M \) where \( M \) is the total number of classes and all the elements of \( s_i \) are 0 except the one corresponding to the class which is 1.

We define a smooth cost function amenable to algorithms such as gradient descent, \( i.e. \), the cross-entropy loss

\[
L_{\text{NN}} = \sum_{i=1}^{N} -s_i^T \log(\hat{s}_i),
\]

where \( \log \) is intended element-wise. The cross-entropy loss \( L \) can also be interpreted as the distance between the predicted probability density of the labels compared to the true one.

The actual training phase consists of applying stochastic gradient descent using the derivatives of the cost function using the back-propagation rule. This method works very well in practice and provides good out of sample performance with short training times.

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