Data-driven Prediction of Relevant Scenarios for Robust Optimization

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Abstract

In this work we study robust one- and two-stage problems with discrete uncertainty sets which are known to be hard to solve even if the underlying deterministic problem is easy. Popular solution methods iteratively generate scenario constraints and possibly second-stage variables. This way, by solving a sequence of smaller problems, it is often possible to avoid the complexity of considering all scenarios simultaneously. A key ingredient for the performance of the iterative methods is a good selection of start scenarios. In this paper we propose a data-driven heuristic to seed the iterative solution method with a set of starting scenarios that provide a strong lower bound early in the process, and result in considerably smaller overall solution times compared to other benchmark methods. Our heuristic learns the relevance of a scenario by extracting information from training data based on a combined similarity measure between robust problem instances and single scenarios. Our experiments show that predicting even a small number of good start scenarios by our method can considerably reduce the computation time of the iterative methods.

Keywords: Robust optimization; two-stage robust optimization; data-driven optimization; machine learning for optimization

1 Introduction

Optimization under uncertainty is an important research field especially due to its relevance in practical applications from operations research. In the real world many parameters of an optimization problem can be uncertain, e.g. the demands, returns or traffic situations or any other parameters which are not precisely known due to measurement or rounding errors. It was shown that hedging against possible perturbations in the problem parameters is essential, since already small perturbations can lead to a large violation of the constraints \cite{BTEGN09}. Driven by the seminal works \cite{Soy73, KY96, BTN98, BTN99, BS04} robust optimization evolved to be one of the most popular approaches to tackle uncertainty in optimization problems by finding solutions which are worst-case optimal and feasible for all parameters of a pre-defined uncertainty set; see \cite{BBC11, BK18, GMT14} for a literature overview. Later the classical robust optimization approach was extended to the two-stage robust optimization approach (also called adaptive robust optimization) in \cite{BTGGN04} which has been extensively studied from then on; see e.g. \cite{BD16, PiH16, HKW15, KK20, GKZ21, YGdH19}. While most of the works mentioned above consider the case of convex uncertainty sets, discrete uncertainty sets naturally appear in practical applications where often a finite set of historical observations of the uncertain parameters is given; see \cite{ABV09, BK18, KY96}. Based on these historical observations uncertainty sets can be constructed by data-driven approaches from statistics or machine learning \cite{GK20, CDG19, SHY17, BGK18, CCCP21}.

While dualizing the robust constraint often leads to compact reformulations of the robust optimization problem, in some cases this derivation is not possible (e.g. in the two-stage case with integer recourse situation).
variables or for discrete uncertainty sets) or not desirable (see [FM12]). In this case the robust optimization problem can alternatively be solved by scenario generation approaches [BL21] while the two-stage robust problem can be solved by column-and-constraint algorithms [ZZ13]. In both cases the idea is to iteratively generate new scenarios by solving the adversarial problem and adding them to a master problem. While both approaches often perform well, one of the main drawbacks is that with an increasing number of iterations the size of the master problem increases, which often leads to master problems which cannot be solved in appropriate time; see [KK20]. Hence an important tool to improve the efficiency of the iterative methods is the choice of a good starting set of scenarios.

In this work we introduce what we call the Relevant Scenario Recognition Problem which aims at finding a set of \( k \) scenarios which maximizes the lower bound given by the master problem of the considered iterative algorithm. This is motivated by the fact that starting the iterative algorithms with the largest possible lower bound leads to a small optimality gap and to a reduced number of iterations. Additionally we can ensure that even if the algorithm does not terminate in an appropriate number of iterations we find a solution with small optimality gap after the first iteration.

Our contributions are the following. We introduce the Relevant Scenario Recognition Problem, where we aim at finding the strongest subset of scenarios in the master problem of a given size. We show that this problem is NP-hard and that it can be reformulated as a linear binary programming formulation. Since solving the problem exactly is intractable we develop a data-driven heuristic to identify relevant scenarios based on a combined similarity measure between robust problem instances and single scenarios. In computational experiments using two-stage shortest path and traveling salesperson problems with uncertain costs, we evaluate the effect of our heuristic in comparison with random starting scenarios and starting scenarios that maximize the sum of costs. We show that our method results in uncertainty sets that provide stronger lower bounds which lead to considerably reduced solution times in the subsequent iterative solution method. Our experiments show that the selection of the right start scenarios is crucial for the subsequent behaviour of the iterative method.

2 Preliminaries

2.1 Robust Optimization

We consider deterministic optimization problems of the form

\[
\begin{align*}
\min \ c^\top x \\
\text{s.t.} \quad Ax &\leq b \\
x &\in X
\end{align*}
\]

where \( c \in \mathbb{R}^n \) is a given cost vector, \( X \subseteq \mathbb{R}^n \) an arbitrary feasible region, \( A \in \mathbb{R}^{p \times n} \) and \( b \in \mathbb{R}^p \). We denote the \( i \)-th row of a matrix \( A \) by the corresponding lowercase variable indexed by \( i \), i.e. by \( a_i \in \mathbb{R}^n \). Note that we can choose \( X \subseteq \mathbb{Z}^n \) to model integer problems and for combinatorial optimization problems we often have \( X \subseteq \{0,1\}^n \). We assume that the parameters of the constraint matrix \( A \) are uncertain and all possible realizations of the constraint parameters are given by a discrete uncertainty set \( U = \{ A^1, \ldots, A^m \} \) where each \( A^i \in \mathbb{R}^{p \times n} \) is called a scenario. The aim in the classical robust optimization approach is to calculate a solution \( x^\star \in X \) which is feasible for all scenarios in \( U \) and which minimizes the objective function, i.e. we want to find an optimal solution of problem

\[
\begin{align*}
\min \ c^\top x \\
\text{s.t.} \quad A^i x &\leq b \quad \forall \ i \in [m] \\
x &\in X.
\end{align*}
\]

where we use the notation \( [k] := \{1, \ldots, k\} \) for each \( k \in \mathbb{N} \). Note that we can assume w.l.o.g. that the cost parameters \( c \) are certain since otherwise by using a level set transformation we can shift the uncertain cost parameters into the constraint matrix.

Robust combinatorial optimization problems with discrete uncertainty are known to be computationally hard, even if the uncertainty only appears in the objective function and we have only two scenarios; see [KY96, BK18]. Despite this theoretical drawback these problems are often solved successfully using an iterative scenario generation approach. In this algorithm we alternately calculate an optimal solution \( x^i \in \{ x \in X : A^i x \leq b \ \forall \ i \in I \} \) of Problem (RP) for a subset of scenarios \( I \subset [m] \), which we call the master problem, and afterwards an adversarial problem is solved to find a new scenario for which \( x^i \) is not
feasible. This is often implemented by calculating the scenario which leads to the maximum constraint violation, i.e.

\[ i^* \in \arg \max_{i \in [m]} \max_{l \in [p]} \left\{ (a^l)^T x^* - b_l \right\} \]  

(1)

where \((a^l)\) is the l-th row of \(A^i\). Afterwards we set \(I := I \cup \{i^*\}\) and we iterate. If the optimal value of \((1)\) is smaller or equal to zero, then the current solution \(x^*\) is feasible for all scenarios in \(U\) and hence \(x^*\) is an optimal solution of \((RP)\). Finally note that the optimal values of the master problems define a non-decreasing sequence of lower bounds for the original robust problem \((RP)\).

### 2.2 Two-stage Robust Optimization

In the two-stage setting we consider deterministic optimization problems of the form

\[
\begin{align*}
\min & \ c^T x + d^T y \\
\text{s.t.} & \ Ax + Dy \leq b \\
& \ x \in X, \ y \in Y 
\end{align*}
\]

(2)

where \(c \in \mathbb{R}^n, d \in \mathbb{R}^q\) are given cost vectors, \(X \subset \mathbb{R}^n\) and \(Y \subset \mathbb{R}^q\) are arbitrary sets which can be integer or binary, \(A \in \mathbb{R}^{p \times n}, D \in \mathbb{R}^{p \times q}\) and \(b \in \mathbb{R}^p\). We assume that only the parameters of matrix \(A\) are uncertain (i.e., we consider fixed recourse problems), but all results from this work can easily be extended to the case of uncertain matrices \(D\). Again we may assume w.l.o.g. that uncertainty only appears in the constraint parameters. The variables \(x \in \mathbb{R}^n\) are the first-stage solutions which have to be fixed here-and-now. Variables \(y \in \mathbb{R}^q\) are the second-stage variables, also called wait-and-see variables, which can be adjusted flexibly after all uncertain parameters are known. Again we assume that all possible realizations of the uncertain constraint parameters are given by a discrete uncertainty set \(U = \{A^1, \ldots, A^m\}\) where \(A^i \in \mathbb{R}^{p \times n}\) are again called scenarios. The aim in two-stage robust optimization is then to calculate a first-stage solution \(x^*\) such that for every scenario \(A^i \in U\) there exists a feasible second-stage solution \(y^i\) such that the worst possible objective value over all scenarios is minimized. This can be modeled by problem

\[
\begin{align*}
\min & \ c^T x + \max_{i \in [m]} d^T y^i \\
\text{s.t.} & \ A^i x + Dy^i \leq b \quad \forall \ i \in [m] \\
& \ x \in X, y^i \in Y \quad \forall \ i \in [m].
\end{align*}
\]

(2RP)

One of the most popular methods to solve two-stage robust problems is the column-and-constraint generation algorithm (CCG), first introduced in [ZZ13] which can also be used in the case of discrete uncertainty sets. Similar to the scenario generation procedure described in the previous subsection, the idea is to iteratively generate new scenarios and add them to the master problem. Here each time we add a scenario we also have to add a new set of variables \(y^i\). More precisely, we alternately calculate an optimal solution \((x^*, \mu^*)\) of Problem \((2RP)\) for the current subset of scenarios given by indices \(I \subset [m]\), which we call the master problem, and afterwards an adversarial problem is solved to find a new scenario \(A^i\), where \(i^* \notin I\) such that either no feasible second-stage solution exists for the current solution \(x^*\) or the objective value is maximally increased. This if often implemented by solving the problem

\[
\begin{align*}
i^* \in \arg \min_{i \in [m]} \{ d^T y : A^i x^* + Dy \leq b, \ y \in Y \}.
\end{align*}
\]

(3)

Note that in the case where no feasible second-stage solution \(y\) exists for a scenario, the inner minimum-value is \(\infty\) and hence the scenario is a candidate to be chosen. Afterwards we set \(I := I \cup \{i^*\}\) and we iterate. If the optimal value of \((3)\) is smaller or equal to \(\mu^*\), then the current solution \(x^*\) is optimal for all scenarios in \(U\). Finally note that the optimal values of the master problems define a non-decreasing sequence of lower bounds for the original robust problem \((RP)\). On the other hand the optimal value of the adversarial problem always returns the objective value of solution \(x^*\) and is therefore a valid upper bound. Hence in each iteration of the CCG we can calculate an optimality gap to check how far we are at most from being optimal.

### 3 The Relevant Scenario Recognition Problem

Solving the robust counterpart \((RP)\) and especially the two-stage robust counterpart \((2RP)\) can be computationally challenging. In several methods (e.g. the constraint generation or column-and-constraint
Theorem 1. Let \( X \) be a polyhedron given by an outer description. Problem (RSRP-RO) can be solved in polynomial time if \( k \) is a constant value, but is NP-hard if \( k \) is part of the input.

Proof. Note that there are at most \( m^k \) possible subset \( I \) of \([m]\). Hence, if \( k \) is a constant value, Problem (RSRP-RO) can be solved by solving a polynomial number of linear programming problems since \( X \) is given by an outer description.

For the case that \( k \) is part of the input, consider any instance of the Set Cover problem, which is known to be NP-hard \([1] \). Given a set of items \( E = \{e_1, \ldots, e_N\} \) and sets \( S_i \subseteq E \) for \( i = 1, \ldots, M \), we need to decide if there exists a set of indices \( I \subseteq [M] \) with cardinality at most \( K \) such that each item from \( E \) is contained in at least one set \( S_i \), \( i \in I \).

Set \( n = N \), \( m = M \), \( k = K \), \( X = \mathbb{R}_+^n \) and consider constraints \(-A^i x \leq -1\), where \( 1 \) is the all-one vector and \( A^i \) is a diagonal matrix of size \( n \times n \), where the \( j \)th entry of the diagonal is equal to one if and only if \( e_j \in S_i \) and it is equal to two otherwise. Finally, set \( c = 1 \). Then it holds that there is a solution to Problem (RSRP-RO) with objective value equal to \( n \) if and only if there exists a set cover with cardinality at most \( K \). \( \square \)

Note that, if \( X \) is a polyhedron, we may dualize the inner minimization problem. Modelling the selection of the index set \( I \) by binary variables we can then reformulate the problem as a compact linear problem formulation by using standard linearization techniques for the product of binary and dual variables. On the other hand if \( X \) is a finite set the following theorem holds, which is proved in the appendix.

Theorem 2. If \( X \) is finite, Problem (RSRP-RO) can be reformulated as a binary linear program.

For the two-stage robust case we again assume we have a given discrete uncertainty set \( U = \{A^1, \ldots, A^m\} \). In the column-and-constraint generation method described in Section 2 we always obtain a lower bound to the original robust problem (RP) by solving the master problem which is given by

\[
\min \ c^\top x + \max_{i \in I} d_i^\top y^i \\
\text{s.t.} \quad A^ix + Dy^i \leq b \quad \forall \ i \in I \\
x \in X, y^i \in Y \quad \forall \ i \in I.
\] (MP2R)
for the current set of scenarios $I \subseteq [m]$. For a given $k \leq m$ the RSRP is then given by

$$\max_{k \leq I \subseteq [m]} \min_{|I| \leq k} \sum_{i \in I} c_i x_i + \max_{y \in Y} d^\top y.$$  \hfill (RSRP-2RO)

It follows directly from Theorem 1 that Problem (RSRP-2RO) is NP-hard under the same assumptions since we can reduce Problem (RSRP-RO) to it by choosing $D = 0$ and $d = 0$.

Note that similar to the single-stage case, Problem (RSRP-RO) can be reformulated as a binary linear program, which is proved in the appendix.

**Theorem 3.** If $X$ is finite, Problem (RSRP-2RO) can be reformulated as a binary linear program.

### 4 Data-driven Heuristic

In this section we present a machine learning method to extract information from given training data to find good solutions to Problem (RSRP-RO) (or (RSRP-2RO)). Here we assume that we have a given set of $N$ training samples where each training sample consists of an instance of Problem (RP) (or (2RP)), i.e. a finite uncertainty set $U = \{A^1, \ldots, A^n\}$ and an objective cost vector $c$. In the two-stage case we additionally have an objective cost vector $d$ for the second-stage variables and a recourse matrix $D \in \mathbb{R}^{|I| \times n}$. In the following we present all results for the two-stage case since it is the more general problem. Nevertheless all results can easily be adapted for classical robust optimization.

Denote the training set by $X = \{(c^1, d^1, U^1), \ldots, (c^N, d^N, U^N)\}$ where $U^1, \ldots, U^N$ are different uncertainty sets which can contain different numbers of scenarios. We denote by $c^1, \ldots, c^N$ the cost vectors of the first stage variables, and by $d^1, \ldots, d^N$ the cost vectors of the second-stage variables, while $D^1, \ldots, D^N$ are the recourse matrices of the problem. Furthermore we assume that each training sample is labeled, i.e. for each training instance $j$ we have a target vector $y^j \in \{0,1\}^{|U^j|$ where $y^j_i = 1$ if scenario $A^i \in U^j$ is a "relevant scenario" and $y^j_i = 0$ otherwise. We denote the set of corresponding label vectors for the training samples in $X$ by $Y = \{y^1, \ldots, y^N\}$.

Assume we have a given instance of Problem (2RP) with cost vectors $c, d$ and uncertainty set $U$ which we want to solve. The idea of our machine learning approach is to predict the relevant scenarios in $U$ by training a model on the given training data in $X$ with known relevant scenario vectors $Y$. We then predict a target vector $y \in [0,1]^{|U|$ for our given instance where a large entry of $y$ denotes that the corresponding scenario is more relevant. Hence after predicting the target vector $y$ we can choose the $k$ scenarios with largest target values as a solution for Problem (RSRP-RO).

The machine learning method we use in this work is based on the idea of $k$-nearest neighbor. In the following we always represent each matrix by its flattened vector, which we denote by the lowercase variable, e.g. the scenario matrix $A^i \in \mathbb{R}^{|I| \times n}$ is represented by the flattened vector $a^i \in \mathbb{R}^{|I| \times n}$. To implement a $k$-nearest neighbor approach we first have to define a similarity measure between two instances of (2RP) which we do as follows. First we calculate the center points of each uncertainty set

$$\bar{a} = \frac{1}{|U|} \sum_{a \in U} a, \quad \bar{d} = \frac{1}{|U|} \sum_{a \in U} d \quad \forall j \in [N]$$

and define the similarity between training sample $j$ and the instance to solve by

$$s \left((c, d, U), (c^j, d^j, U^j)\right) := \frac{c^\top c^j}{\|c\|\|c^j\|} \cdot \frac{d^\top d^j}{\|d\|\|d^j\|} \cdot \frac{\bar{a}^\top \bar{d}^j}{\|\bar{a}\|\|\bar{d}\|}.$$  

Note that the term $\frac{\bar{a}^\top \bar{d}^j}{\|\bar{a}\|\|\bar{d}\|}$ is equal to the cosine of the angle between the two vectors $\bar{a}$ and $\bar{d}$. Hence if the cost vectors and the center points point in a similar direction, the two instances have a large similarity value $s$ while if the directions are different the similarity is smaller. In Figure 1 we show an example for the classical robust optimization problem (i.e. $d = 0$) where on the left the similarity between the two instances is given by $s \left((c^1, 0, U^1), (c^2, 0, U^2)\right) = \cos(\alpha) \approx 0.59 \cdot 0.24 \approx 0.14$ and on the right the similarity is given by $s \left((c^1, 0, U^1), (c^2, 0, U^2)\right) = \cos(\alpha) \approx 1.0 \cdot 0.99 \approx 0.99$. The example shows that even if the uncertain region does not overlap the instances are considered similar if the direction of the center points is similar and if the optimization
direction is similar. This is motivated by the observation that if we optimize in a similar direction over
scenario sets both lying in a similar direction then the worst-case scenario will be located in a similar
region of the convex hull of the uncertainty set.

Having a measure for the similarity of two instances, we next want to define a measure for the similarity
of two scenarios. To this end we center each uncertainty set around the origin by subtracting the
center point from each scenario, i.e. for uncertainty set $U = \{a_1, \ldots, a_m\}$ we define the centered set
$\tilde{U} = \{\tilde{a}_1, \ldots, \tilde{a}_m\}$ where
\[
\tilde{a}_i = a_i - \frac{1}{|U|} \sum_{a \in U} a \quad \forall i \in [m].
\]

We now define the distance between scenario $a \in U$ and $a' \in U'$ by $d(a, a') := \|\tilde{a} - \tilde{a}'\|$, where $\tilde{a}$ and $\tilde{a}'$ are the corresponding centered scenarios from $\tilde{U}$ and $\tilde{U}'$ and $\|\cdot\|$ is the Euclidean norm. An example can be found in Figure 2.

Next we want to define an importance score $p_a$ for each scenario $a \in U$, where a larger value $p_a$ means
that the scenario is more likely to be a relevant scenario. To this end we use the two derived measures to
construct a $k$-nearest neighbor based scoring for each scenario. Denote by $W^\kappa_j$ the set of the $\kappa$ scenarios
in $U^j$ with smallest distances to $a \in U$ where $\kappa \in \mathbb{N}$ is a predefined hyperparameter. Note that in contrast
to the Pearson correlation the distance $d(a^i, a)$ is small if both scenarios lie in a similar region of their

Figure 1: Two examples of two different instances of the classical robust optimization problem (red and
blue) where the points denote the scenarios and $c_1$ and $c_2$ the cost vectors. We denote the angle
$\alpha$ between the center points vectors and the angle $\beta$ between the cost vectors.

Figure 2: On the left two scenario sets of two different instances (blue and red); on the right the centered
versions of the same scenario sets and the $\kappa = 3$ red scenarios with closest distance to a generic
blue scenario.
respective uncertainty sets. Finally the importance score of scenario $a \in U$ is defined as

$$p_a := \sum_{j=1}^{N} s \left( (c, d, U), (c^j, d^j, U^j) \right) \sum_{a' \in W^j} \frac{1}{D_j} \frac{1}{1 + d(a, a')} \kappa_{a'}$$

with normalization parameter $D_j = \sum_{a' \in W^j} \frac{1}{1 + d(a, a')}$. Note that the inner sum is just a weighted average of the labels of all scenarios in $W^j$ weighted by an inverse of its distance to the scenario $a$. Therefore the label values of the scenarios with closer distance to $a$ have a larger impact in the weighted average. The outer sum is then just a weighted sum of the latter weighted averages over all training samples where the weight for each instance is its similarity score. Hence the label values of more similar instances and the outer sum is then just a weighted sum of the latter weighted averages over all training samples where the label values of the scenarios with closer distance to $a$ in the first stage. We assume we have $m$ scenarios in the discrete uncertainty set $W$.

$\kappa_{a'}$ have a larger impact in the weighted average. The importance score $p_a$. We can now derive a solution $\hat{Z}$ of Problem (RSRP-RO) by selecting the $k$ scenarios in $U$ with largest importance scores $p_a$.

Note that the latter procedure even works if the uncertainty sets of the training samples contain different numbers of scenarios. Hence to reduce the computational complexity the scenario set of each training instance could be clustered into a smaller number of scenarios e.g. by a classical k-means algorithm.

5 Experiments

5.1 Setup

In this section we perform several experiments to evaluate the efficiency and effectiveness of the proposed data-driven scenario prediction method introduced in Section 4. To this end, we consider two types of robust two-stage problems with objective uncertainty. Both problems have in common that, given a graph $G = (V, E)$, in the first-stage problem we need to decide which edges of the graph we want to buy. Once this decision is made, we obtain the costs of each edge and afterwards in the second-stage we have to find a feasible solution with minimal costs for a given network problem in the subgraph that was bought in the first stage. We assume we have $m$ scenarios in the discrete uncertainty set $U = \{d^1, \ldots, d^m\}$ that determine the second-stage costs. Our problems can then be modeled as follows:

$$\begin{align*}
\min & \quad \sum_{e \in E} c_e x_e + z \\
\text{s.t.} & \quad z \geq \sum_{e \in E} d^i_e y_e^i, \quad \forall i \in [m] \quad (4) \\
& \quad y_e^i \leq x_e, \quad \forall e \in E, i \in [m] \quad (5) \\
& \quad x_e \in \{0, 1\}, \quad \forall e \in E \quad (6) \\
& \quad y^i \in Y, \quad \forall i \in [m] \quad (7)
\end{align*}$$

with $Y$ denoting the set of feasible solutions for a given network problem. In the following experiments, we consider shortest path (SP) and traveling salesperson problems (TSP). Variable $x_e$ decides whether to buy edge $e$ or not, i.e., for known costs $c_e$, we can make an edge available for the second-stage problem. Due to Constraints (5), only edges bought this way may be used in the second-stage.

To model shortest path problems, we use standard flow constraints on each node. We generate layered graphs, where each node of one layer is connected to all nodes of the next layer. Additionally, the source node $s$ is connected to each node of the first layer, while all nodes of the last layer are connected to the sink node $t$. Each layer has a width of five nodes, while we vary the number of layers in $[10, 15, 20, 25]$.

For TSP, we use the classical Miller-Tucker-Zemlin formulation, see [MTZ60]. We note that more effective formulations have been developed to solve TSP, but as all scenario generation methods use the same formulation, this is not the focus of our experiment. We construct complete graphs with numbers of nodes in $\{6, 7, 8, 9\}$.

Note that there can be different criteria to label a scenario as relevant. One possibility is to define a scenario to be relevant if removing it from the uncertainty set leads to an decrease of the optimal value of Problem (2RP). A second possibility, which is computationally more demanding, is to calculate the smallest $k \leq m$ such that the objective value of Problem (RSRP-2RO) does not change anymore and choose the scenarios selected by the optimal solution $Z^*$ as relevant scenarios. Note that for each data point, i.e. each instance, we have to run the latter procedure. A third variant which is more accurate than the first one and computationally less demanding than the second one is the following: we solve the given instance of Problem (2RP) with uncertainty set $U$ by CCG and collect all scenarios which are
generated by the adversarial problem during this method in a new set \( U' \subseteq U \). After the algorithm has terminated \( U' \) is optimal for (2RP), i.e. if we solve (2RP) with uncertainty set \( U' \) we obtain an optimal solution of the same problem with complete uncertainty set \( U \). Now we label a scenario from \( U' \) as relevant if removing it from \( U' \) and solving (2RP) with this reduced set of scenarios has a smaller objective value than for the full set \( U' \). All other scenarios are labeled as zero. Note that the latter step is crucial since \( U' \) can contain irrelevant scenarios e.g. since the start scenario of the CCG can be irrelevant. Unfortunately our computations showed that all three data generation methods are too time consuming to build a relevant set of training instances since even solving (RSRP-2RO) once can be too time consuming for appropriate dimensions. Hence we decided to generate the instances as follows.

For each problem size, we generate 100 problem instances. Of these, 80 are used for training, and 20 are used for evaluation. To generate a problem instance, we sample five random scenarios and solve the resulting robust two-stage problem defined above. Let \( x \) be its optimal solution. We then check if the objective value remains the same if we remove any of the five scenarios. If this is the case (i.e., \( x \) remains optimal, as not all five scenarios are required), we start the process again. Having generated a problem with five relevant scenarios, we then sample additional scenarios, where we only keep those scenarios where the costs for the fixed first-stage solution \( x \) do not increase. We repeat this scenario generation until a total of 500 scenarios is obtained. By generating instances this way, we know that there are always exactly five relevant scenarios that determine the optimal objective value. Finding these five scenarios is now the task of the scenario prediction methods.

We now explain the parameters that were used for these experiments. For shortest path problems the first-stage costs \( c \) are sampled uniformly iid from \([9, 11]^E\), while for the second-stage costs, we sample five midpoints \( \mu^t \in [25, 75]^E \) and deviations \( \delta^t \in [0, 1]^E, t = 1, \ldots, 5 \). The five relevant (required) scenarios are then set equal to the five midpoints. For each further scenario \( i \) that we sample, we use midpoint and deviation \( t = i \mod 5 \) and choose the cost of each edge \( e \) uniformly in \([\mu^t_e - \delta^t_e, \mu^t_e + \delta^t_e]^E\). For traveling salesperson problems the costs are generated in the same way, except first-stage costs \( c \), which are sampled uniformly iid from \([4, 6]^E\). The choice for the intervals of the first-stage costs are motivated by our observations that making the intervals too large can lead to trivial solutions where the edges bought in the first stage just form one feasible second-stage solution. Additionally the size of the boundary of the intervals had to be adjusted since for too small first-stage costs it can be beneficial to buy all edges of the graph, while for too large values again only one feasible second-stage solution is bought.

We apply the data-driven heuristic described in Section 4, in the following denoted as DDH. We reduce the size of the training uncertainty sets from 500 to 50 using a K-means clustering algorithm before we start DDH. Using DDH, we can order the scenarios of an uncertainty set from highest to lowest priority. As benchmark methods we use the following simple heuristics: In the method denoted by Random, the priorities are determined by a random shuffle of the uncertainty set. In the method denoted by Maxsum, the priority of a scenario is determined by its sum of cost values \( \sum_{e \in E} d^t_e \), i.e., scenarios with a higher sum are more likely to be relevant than scenarios with a smaller sum.

For each type of problem, we conduct two experiments. In the first experiment, the purpose is to determine the strength of the problem formulation when we only use the top \( k \) scenarios with highest priority, where we vary \( k \) in \( \{1, \ldots, 15\} \). Recall that the objective value of the resulting two-stage robust optimization problem is a lower bound on the actual objective value when using all scenarios; with a perfect choice of scenarios, \( k = 5 \) can already give an optimal bound by construction. We run each algorithm to determine the \( k \) most relevant scenarios, and solve the resulting problem formulation with a 15 minute time limit. If the problem cannot be solved to optimality, the best lower bound is reported.

In the second experiment, we would like to determine the time to find a certifiably optimal solution using the iterative method and \( k \) starting scenarios. For this experiment, we use a 60 minute time limit, where we include both the time required to rank scenarios, as well as the subsequent CCG time.

All experiments were conducted on a virtual server with Intel Xeon Gold 5220 CPU running at 2.20GHz. As a mixed-integer programming solver, we used Gurobi version 9.0.3. For better comparability, each run was restricted to one thread.

### 5.2 Results for Traveling Salesperson Problems

We first compare the lower bounds using \( k \) starting scenarios for \( k \in \{1, \ldots, 15\} \) in Figure 3. We show the optimality gap which is the difference between optimal value and lower bound, divided by the optimal value. All values are given in percent. We note that for \(|V| = 6\) to \(|V| = 9\), results are consistent. In each case, Random results in the largest gaps, followed by Maxsum, while DDH results in the smallest gaps. Each method benefits from adding more than five scenarios.
Figure 3: Average optimality gap in percent, depending on the number of starting scenarios, for traveling salesman problems on graphs of different sizes.
In Figure 4, we present average computation times when using the CCG with $k$ starting scenarios, for $|V| = 7$ and $|V| = 8$. Note that the values of the vertical axis are logarithmic. For Random and Maxsum, no training time is required, as the information of the training instances is not used. For DDH, we first need to calculate scenario scores to determine priorities. The solid line indicates the total time, consisting of calculating the scores by DDH and the subsequent CCG calculation time. The dashed line shows the solution time only, excluding the calculation of scores.

We can note that for smaller problems (Figure 4(a)), the solution times of DDH and Maxsum are similar. In a dashed line, we show the time spent only on CCG. This comparison shows that at this problem size, the iterative method using DDH reaches an optimal solution faster than Maxsum, but the additional overhead of calculating scores balances this benefit out. For larger problems (Figure 4(b)), this overhead becomes less relevant in the overall solution time, and DDH acquires a clear advantage over Maxsum. For both methods, solution times tend to decrease with more starting scenarios, indicating that scenarios are chosen that benefit that iterative solution process. This is different for Random, where additional starting scenarios lead to an overall increase in solution time, as master problems become larger.

![Figure 4: Average time in seconds to find an optimal solution, depending on the number of starting scenarios, for traveling salesperson problems. Dashed line shows CCG time only.](image)

5.3 Results for Shortest Path Problems

In Figure 5, we show average optimality gaps for shortest path problems. In comparison to TSP results (reported in Figure 3), the performance of Random and Maxsum has become more similar. While Maxsum has an advantage for small numbers of scenarios ($k \in \{1, 2, 3\}$), Random becomes the better choice for more scenarios. A possible explanation is that Maxsum is less able to diversify; if there is one base scenario $t$ with large midpoint values $\mu_t$, scenarios that are derived from $t$ may have large sums as well. Another difference to the previous results is that DDH has become even more effective in predicting relevant scenarios; for $k = 5$, gaps are already very close to zero.

We show the average solution time for the CCG in Figure 6 using only the smallest instances with 10 layers. The small computation times of DDH in comparison to Maxsum and Random show that the proposed method is highly effective in identifying relevant scenarios. From $k = 5$ onwards, we see a slight increase in computation times. This can be explained by the observation that for $k = 5$, the relevant scenarios are already part of the problem. Adding more scenarios only increases the solution time of the master problem. Interestingly, we see that Maxsum has smaller computation times than Random, despite the weaker lower bound. A possible explanation for this behavior is that Random adds more diverse scenarios to the starting set (which yields stronger lower bounds), but Maxsum can find at least one of the five relevant scenarios, which gives a faster convergence of the iterative method overall.

To summarize the findings of these experiments, we note that DDH is an effective method in identifying relevant scenarios, and clearly outperforms Random and Maxsum. Furthermore, it is also efficient in the sense that we do not only get stronger lower bounds when starting the iterative method, the iterative method also converges to an optimal solution in less time.
Figure 5: Average optimality gap in percent, depending on the number of starting scenarios, for shortest path problems on layered graphs of different sizes.

Figure 6: Average time in seconds to find an optimal solution, depending on the number of starting scenarios, for shortest path problems. Dashed line shows CCG time only.
6 Conclusions

Generating constraints and variables is a staple method to solve robust optimization problems, due to its simplicity and wide applicability. Most commonly, the starting set of scenarios is generated without optimization effort, e.g. by choosing them randomly. To the best of our knowledge, this paper explores for the first time the potential of more sophisticated methods of producing starting scenarios. This leads to the Relevant Scenario Recognition Problem, which asks for a subset of scenarios that maximizes the bound provided by the master problem. We show that this problem is NP-hard, even if the robust problem can be solved in polynomial time. Furthermore solving this problem directly is only possible for small instance sizes; however, in this case, predicting starting scenarios is of less relevance. By defining a suitable similarity measure, we show that it is possible to compare scenarios of a new problem instance with scenarios from previous problems, where a label that indicates scenario relevance is already available. Our computational experiments show that for two-stage shortest path and traveling salesperson problems, our method leads to considerably better optimality gaps which is especially beneficial for large problem dimensions where we cannot perform many iterations. Interestingly starting the iterative method with the right choice of start scenarios even leads to considerably reduced computation times for the iterative methods compared to the benchmark methods. Although one could expect that the iterative methods will find the most relevant scenarios after a few iterations, our experiments show that the selection of the right start scenarios still has a large impact on the subsequent behaviour of the algorithms.

For future work it is desired to build a data collection of labeled instances which can be made publicly available. Furthermore, the data-driven heuristic proposed in this paper does not cover the case where the dimension $n$ (and $q$) of the training instances is different to the dimension of the instance which has to be solved. Approaches that allow more flexibility in training and testing instance dimensions are desirable. Furthermore it would be interesting to extend our work to convex uncertainty sets.

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can be applied to arbitrary finite sets $X$ and $\delta$ is always chosen. However if we assume that all problem parameters are integer the minimum constraint violation is \(\delta_i\), where $\delta_i$ is the minimum possible constraint violation of constraint $i$ over all solutions in $X$, i.e.

\[ \delta_i = \min\{ b - (a_i)^{\top} x : x \in X, b - (a_i)^{\top} x > 0 \}. \]

The variables $u$ model the choice of scenarios, i.e. the optimal solution $u^*$ corresponds to the optimal index-set $I^* = \{ i \in [m] : u_i = 1 \}$ of Problem (RSRP-RO).

Constraint (11) ensures that at most $k$ scenarios can be chosen. Constraints (11) ensure that all $z$-variables are equal to zero if the scenario is not chosen. Otherwise it can be either zero or one. The crucial constraints are the big-M Constraints (9). Since we want to maximize $\tau$ in an optimal solution we always want to make the right-hand side as large as possible. Consider the constraint for a given $x \in X$ and a scenario $i \in [m]$ which was selected, i.e. we have $u_i = 1$. If $x$ is feasible for scenario $i$ then it must hold $A^i x \leq b$ and hence $(a_i)^{\top} x - b \leq 0$ for all $j \in [p]$. It follows that in an optimal solution we always want to set $z_{ij}^x = 0$ for all $j \in [p]$ to make the right-hand side as large as possible. If $x$ is feasible for all selected scenarios, then the constraint is equivalent to $\tau \leq c^T x$ since all $z_{ij}^x = 0$ for the non-selected scenarios $i$ due to Constraint (10). It follows that $\tau \leq c^T x$ for all $x \in X$ which are feasible for the selected scenarios. On the other hand if an $x \in X$ is not feasible for one of the selected scenarios $i$ we have to show that the corresponding constraint is switched off, i.e. it does not lead to any restriction on $\tau$. If $x$ is not feasible for scenario $i$ then at least for one $j \in [p]$ it holds $((a_i)^{\top} x - b) > 0$. In this case to maximize the right-hand side in an optimal solution we have $z_{ij}^x = 1$. It follows that for the right-hand side we have

\[
(c^T x + \sum_{i=1}^{m} \sum_{j=1}^{p} ((a_i)^{\top} x - b) M_i z_{ij}^x) \geq c^T x + \sum_{i=1}^{m} \sum_{j=1}^{p} \delta_i \sum_{i=1}^{n} c_i |z_{ij}^x| \geq c^T x + \sum_{i=1}^{m} c_i|z_{ij}^x|,
\]

where we used the definition of $M_i$ and $\delta_i$ for the first inequality and for the second inequality we used the fact that at least one $z_{ij}^x = 1$ for an infeasible $x \in X$. The last term can be bounded from below by $\max_{x \in X} c^T x$ since $X \subseteq \{0, 1\}^n$ and hence the corresponding constraint (9) leads to no restriction on $\tau$. In summary for a given solution $u$ we have that

\[
\tau \leq \min\{ c^T x : x \in X, A^i x \leq b \text{ if } u_i = 1 \}
\]

which proves the equivalence to (RSRP-RO).

Note that calculating the minimum constraint violations $\delta_i$ for each constraint may be a challenging task. However if we assume that all problem parameters are integer the minimum constraint violation is always $\delta_i \geq 1$ and we can choose $\delta_i = 1$. On the other hand in practical computations it often suffices to choose $\delta_i = \varepsilon$ where $\varepsilon$ is an appropriately selected accuracy parameter. Also note that the same approach can be applied to arbitrary finite sets $X$ after adjusting the big-M parameters $M_i$ appropriately.

The binary linear reformulation can be solved by any state-of-the-art integer programming solver as CPLEX or Gurobi. However the problem contains one constraint for each $x \in X$, hence the number of constraints can be exponential in the problem parameters if $X$ has exponential size. We can circumvent this problem by using an iterative constraint generation approach. Unfortunately, the Big-M constraints may still make the problem challenging to solve. To avoid these computational problems, we present an efficient data-driven heuristic to solve Problem (RSRP-RO) in Section 4.

**Appendix**

**Proof of Theorem 2**

In the following we assume that $X \subseteq \{0, 1\}^n$ but the proof can be easily adjusted to the more general case that $X$ is an arbitrary finite set. We show that Problem (RSRP-RO) is equivalent to problem

\[
\begin{align*}
\text{max } & \tau \\
\text{s.t. } & \tau \leq c^T x + \sum_{i=1}^{m} \sum_{j=1}^{p} ((a_i)^{\top} x - b) M_i z_{ij}^x \quad \forall x \in X \\
& z_{ij}^x \leq u_i \quad \forall i \in [m], j \in [p], x \in X \\
& \sum_{i=1}^{m} u_i \leq k \\
& u \in \{0, 1\}^m, z^x \in \{0, 1\}^{m \times p} \forall x \in X
\end{align*}
\]

(8)

where $M_i \geq \frac{1}{\varepsilon} \sum_{i=1}^{n} |c_i|$ and $\delta_i$ is the minimum possible constraint violation of constraint $i$ over all solutions in $X$, i.e.

\[
\delta_i = \min\{ b - (a_i)^{\top} x : x \in X, b - (a_i)^{\top} x > 0 \}.
\]

This proves the equivalence to (RSRP-RO).
Proof of Theorem 3

The idea of the proof is similar to the one of Theorem 2 and hence the details are omitted. We show that Problem (RSRP-2RO) is equivalent to

\[
\begin{align*}
\max & \quad \tau \\
n & \leq c^T x + \sum_{i \in [m]} d_i^T y_i^u + \sum_{i=1}^{m} \sum_{j=1}^{p} ((a_i^j)^T x + d_j^i y_i^u - b) M_i z^x_{ij} \\
\forall x & \in X, y = (y_1^1, \ldots, y^m) \in Y^m \\
\sum_{i \in [m]} t_i^u & = 1 \quad \forall y = (y_1^1, \ldots, y^m) \in Y^m \\
t_i^u & \leq u_i \quad \forall y = (y_1^1, \ldots, y^m) \in Y^m, \ i \in [m] \\
z_i^x & \leq u_i \quad \forall i \in [m], j \in [p], x \in X \\
\sum_{i=1}^{m} u_i & \leq k \\
u & \in \{0, 1\}^m, z^x & \in \{0, 1\}^{m \times p} \forall x \in X
\end{align*}
\]

where \( M_i \geq \frac{1}{\delta_i} \left( \sum_{i=1}^{m} |c_i| + \sum_{j=1}^{n} |d_j| \right) \) and \( \delta_i \) is the minimum possible constraint violation of constraint \( i \) over all solutions in \( X \), i.e.

\[
\delta_i = \min_{j \in [p]} \{ b - (a_i^j)^T x - d_j^i y_i^u : \ x \in X, y \in Y, \ b - (a_i^j)^T x - d_j^i y > 0 \}.
\]

As in the proof of Theorem 2, the \( u \)-variables define the indices for the solution \( I \) of Problem (RSRP-2RO). Again the big-M constraints (14) ensure that only the objective values of solutions \( (x, y) \) which are feasible for the selected scenarios influence the optimal value of \( \tau \). The main difference is that we have to model the maximum expression \( \max_{t \in T} d^T y^u \) appearing in the objective value which is implemented by using the variables \( t_i^u \) which for each solution \( y \) select the maximum value due to Constraint (15) and since we always want the right-hand side of Constraint (14) as large as possible. Constraints (16) ensure that for the maximum we can only choose solutions \( y_i^u \) for a scenarios which are selected by the \( u \)-variables. \( \square \)