Using Machine Learning Predictions to Speed-up Dijkstra’s Shortest Path Algorithm

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Abstract. We study the use of machine learning techniques to solve a fundamental shortest path problem, which is also known as the single-source many targets shortest path problem (SSMTSP). Given a directed graph with non-negative edge weights, our goal is to compute a shortest path from a given source node to any of several designated target nodes. Basically, our idea is to combine a machine learning approach with an adapted version of Dijkstra’s algorithm to solve this problem: Based on the trace of Dijkstra’s algorithm, we design a neural network that predicts the shortest path distance after only a few iterations. The prediction is then used to prune the search space explored by Dijkstra’s algorithm, which allows us to save a significant fraction of operations on the underlying priority queue. Crucially, our approach always computes the exact shortest path distances, even if the prediction is inaccurate, and never uses more queue operations than the standard algorithm. In fact, we are able to prove a lower bound on the number of queue operations saved by our new algorithm, which depends on the accuracy of the prediction. Our bound applies to arbitrary graphs as long as (some of) the edge weights are drawn at random. Our experimental findings on random graphs confirm these bounds and show that the actual savings are oftentimes significantly higher.

Keywords: Machine Learning · Combinatorial Optimization · Supervised Learning · Algorithms

1 Introduction

Recently, techniques from machine learning (ML) have proven extremely powerful to tackle problems that were considered to be very difficult or even unsolvable. Success stories include contributions to health care, natural language processing, image recognition, board games, etc. ([5], [23], [22], [19], [27], [28]). As such, ML is intimately connected with optimisation because many learning algorithms are based on the optimisation of some loss function over a large set of training samples. Even though optimisation techniques play a vital role in the design of ML-approaches, the reverse direction of using ML-techniques to improve optimisation algorithms is much less explored.

In this paper, we contribute to the emerging research agenda of studying how ML-approaches can be used to design efficient algorithms for combinatorial optimisation problems. When designing such ML-based optimisation algorithms we ideally would like to meet the following requirements: (i) The algorithm provides a “proof of optimality” for the computed solution. (ii) The algorithm guarantees to compute a solution within its worst-case running time. While these are standard requirements which are satisfied...
by exact optimisation algorithms, it is unclear whether they can be achieved when using ML-techniques—typically, these techniques are shown to work well empirically, but providing provable performance guarantees oftentimes is infeasible.

The optimisation problem that we consider in this paper is a fundamental shortest path problem, known as the single-source many-targets shortest path problem (SSMTSP). In this problem, we are given a directed graph \( G = (V, E) \) with non-negative edge weights \( w : E \rightarrow \mathbb{R}_{\geq 0} \), a source node \( s \in V \) and a subset \( T \subseteq V \) of designated target nodes. Our goal is to compute a shortest path from \( s \) to any of the target nodes in \( T \). This problem can be solved efficiently by using the well-known shortest path algorithm due to Dijkstra [8]. Basically, this algorithm grows a shortest path tree rooted at the source node \( s \) by iteratively adding new nodes to the tree which are closest to it, until the first target node from \( T \) is included.\(^3\) Dijkstra’s algorithm guarantees a worst-case running time of \( O(m + n \log n) \), where \( n \) and \( m \) denote the number of nodes and edges of the graph, when Fibonacci heaps are used as the underlying data structure. This is also the (asymptotically) fastest shortest path algorithm known for arbitrary non-negative edge weights.

A heuristic improvement of Dijkstra’s algorithm, exploiting that there are potentially many target nodes, is as follows: Throughout the execution of the algorithm, we keep track of the best shortest path distance \( B \) to a node in \( T \) that was found so far. Based on \( B \), the algorithm can then prune all edges that lead to a node whose distance exceeds \( B \) (as these edges are irrelevant for the shortest path). Although this heuristic does not improve the worst-case running time of the algorithm, it may reduce the number of executed queue operations significantly. Bast et al. [2] analyse the effectiveness of this adaptation on random instances, both analytically and experimentally.

1.1 Our Contributions

The main contributions presented in this paper are as follows:

(1) We combine a ML-approach with the edge pruning idea sketched above to obtain a new algorithm for the SSMTSP problem. Basically, our idea is to develop a ML-algorithm that computes a prediction \( P \) of the final shortest path distance after a few iterations of the adapted Dijkstra algorithm. We then use this prediction in combination with the pruning idea above to further reduce the search space explored by Dijkstra’s algorithm. One of the challenges on the ML-side is to define features capturing the essence of the Dijkstra run which can be used to arrive at a good prediction. On the algorithm-design side, we need to take care of the fact that the prediction might actually be an underestimation of the actual shortest path distance.

(2) We prove that our new algorithm computes an optimal solution and has a worst-case running time of \( O(m + n \log n) \). Note that, in particular, our algorithm provides a proof of optimality and retains the worst-case running time of the original Dijkstra algorithm. That is, while our algorithm will never use more queue operations than the adapted Dijkstra algorithm, it can potentially save many queue operations additionally (depending on the accuracy of the prediction).

(3) We prove a lower bound on the number of queue operations saved by our algorithm, for randomly chosen edge weights. Intuitively, the closer the prediction \( P \) is to the

\(^3\)The attentive reader will have noted that the SSMTSP problem can be reduced to a single-source single-target shortest path problem simply by merging all target nodes into one super-target. However, for conceptual reasons (which will become clear below), we keep the viewpoint of having a set of target nodes here.
actual shortest path distance, the more edges will be pruned (leaving aside for now that underestimating predictions cause additional difficulties that need to be resolved). Our lower bound supports this intuition. Basically, our bound shows that the expected savings (i) are proportional to the number of edges that lead to “tentative distances” (defined below) exceeding the shortest path distance, and (ii) increase as the error of our prediction becomes smaller. Our lower bound applies to arbitrary instances of the SSMTSP problem as long as (some of) the edges are chosen independently uniformly at random from $[0, 1]$. We can also use our lower bound to derive a closed form expression for the expected savings on random instances (as introduced by Bast et al. [2]). Here our bound shows that the expected savings are proportional to the number of nodes inserted but never removed from the queue by Dijkstra’s algorithm.

We conduct extensive experimental studies comparing our new algorithm to the existing ones and evaluating different prediction algorithms. Our experimental findings on random instances show that our new algorithm, which combines a neural network ML-approach to compute the prediction with a smart restart procedure to handle possible underestimations, significantly outperforms all other algorithms (combinations of different prediction algorithms and restart procedures).

### 1.2 Related Work

Finding the shortest path in a graph is a classical problem in combinatorial optimisation, so it comes as no surprise that the classical methods to solve this problem come from a combinatorial perspective. Alternatives to Dijkstra’s method are goal-directed algorithms such as $A^*$-search (Hart et al. [13]), which use a heuristic approach to mostly search paths that lead to the goal, and landmark approaches, which use a pre-processing step to pre-compute distances between nodes and use these to speedup the shortest path computation (see, e.g., Goldberg and Werneck [11]). A third well-known approach uses the concept of reach (see Gutman [12]). Intuitively, the reach of a vertex encodes the lengths of shortest paths on which it lies, and can be used in combination with the $A^*$ algorithm to compute shortest paths. An extensive survey of combinatorial algorithms to solve the shortest path problem is given by Madkour et al. [20].

However, there has also been great interest from the field of ML in finding approximates for the shortest path distance, using a ML perspective. For example, Bagheri et al. [1] compute shortest paths by using a genetic algorithm. The crossover operation considers the set of current solutions and computes better ones, while the mutation operator introduces new shortest path solutions. Their algorithm works faster than Dijkstra, but they only test on small graphs with at most 80 nodes. Also, more recently, using ML techniques to approximate shortest path distances has lead to interesting results. For example, Rizi et al. [26] create a estimate for the shortest path distance between two nodes in a two step approach. In the first step, they create a vector embedding for each node, which is generated by deep learning techniques. In the second step, they then use the well-known landmark approach (see, e.g., [30, 31]), where a small set of nodes is chosen as landmark and all distances from each landmark to all of the remaining nodes are computed. These distances are used to compute sample pairs which samples are used to train a feed-forward neural network to approximate the distance between two new nodes. Rizi et al. [26] show results on large-scale real-world social networks (more than 1 million nodes). Their method differs from our approach in the sense that an algorithm is created to approximate shortest path distances in a specific large-scale real-world graph, opposed to an algorithm which can be used for any graph from a set of random graphs with similar properties. An advantage of the landmark-based approach is its scalability to
huge graphs, but Kleinberg et al. [14] show that strong theoretical guarantees on approximation quality are not provided for landmark-based methods. Qi et al. [24] use an idea similar to the one by Rizi et al. [26]. But instead of using a two step approach, a single model is used to predict vertex distances and also to create an embedding for a vertex. They demonstrate the efficiency of their approach on a real-world network.

The aim of our paper is to bridge the gap between the combinatorial viewpoint and the ML perspective. Using ML techniques in combinatorial algorithms has been studied intensively recently, see Bengio et al. [4] for a survey paper on leveraging ML to solve combinatorial problems. In this survey, three different approaches of using ML components in combinatorial optimisation algorithms are given. Firstly, ML could be used to train a model to output solutions to combinatorial problems directly from the input instances (see, e.g., Vinyals et al. [29], Kool et al. [15], Bello et al. [3], Dai et al. [7]). A second approach is to learn meaningful properties of the optimisation problem at hand, and to augment the algorithm with these properties (see, e.g., Kruber et al. [16]). Also our approach, in which we use a prediction for the shortest path to prune our search space, can be categorised under this kind of combination. Thirdly, one could use ML repeatedly alongside the optimisation algorithm (see, e.g., Lodi and Zar primary text incomplete, please provide full text.
SSMTSP problem generalizes the single-source single-target shortest path problem (for which $T = \{t\}$ for a given target node $t \in V$) and the single-source all-targets shortest path problem (for which $T = V$).

We introduce some more notation that we use in this paper. We use $n$ and $m$ to refer to the number of nodes and edges of $G$, respectively. For every node $v \in V$, we use $\delta(v)$ to denote the total weight of a shortest path (with respect to $w$) from $s$ to $v$; if $v$ cannot be reached from $s$ we adopt the convention that $\delta(v) = \infty$. Given that all edge weights are non-negative, we thus have $\delta(v) \in \mathbb{R}_{\geq 0} \cup \{\infty\}$. Note that to solve the SSMTSP problem it is sufficient to compute the shortest path distances of all nodes $v \in V$ satisfying $\delta(v) \leq D$, where $D$ is the minimum shortest path distance of a target node, i.e.,

$$D = \min_{t \in T} \delta(t).$$

(1)

Once these distances are computed, the actual shortest path can be extracted in linear time $O(n + m)$ by computing the shortest path tree rooted at $s$; see, e.g., Cormen et al. [6] for more details. Throughout this paper, we assume that there is at least one target node in $T$ that is reachable from $s$.\(^4\)

### 2.2 Adapted Dijkstra Algorithm

Our algorithm combines an adaptation of Dijkstra’s algorithm by Bast et al. [2] with a machine learning prediction. We briefly review the adaptation by Bast et al. below and refer to it as **Dijkstra-Pruning**; our extension will be introduced in Section 3.

\(^4\) Note that this can easily be checked in linear time $O(n + m)$, simply by running a breadth-first search (BFS) (Cormen et al. [6]).
We conduct extensive experiments to assess the performance of our proposed algorithms. Rényi random graph model \[10\], also known as percolation model, performed by Dijkstra with Pruning. In each iteration, the algorithm removes from PQ an unsettled node \( u \) of minimum tentative distance, declares it to be settled and scans each outgoing edge \( (u, v) \in E \) to check whether \( d(v) \) needs to be updated; we also say that edge \( (u, v) \) is relaxed. The algorithm terminates when a node \( u \in T \) becomes settled.

In the worst case, Dijkstra performs \( n \) \text{REMOVE-MIN}, \( n \) \text{INSERT} and \( m \) \text{DECREASE-PRIORITIES} operations. Its running time crucially depends on how efficiently these operations are supported by the underlying priority queue data structure. In this context, Fibonacci heaps \[9\] are the (theoretically) most efficient data structure, supporting all these operations in (amortised) time \( O(m + n \log n) \). It is important to realise though that the actual time needed by the queue operations depends on the size (i.e., number of elements) of the priority queue. In general, a smaller queue size results in a better overall runtime of the algorithm.

Dijkstra with Pruning. Dijkstra-Pruning works the same way as Dijkstra, but additionally keeps track of an upper bound \( B \) on the shortest path distance to a node in \( T \). Initially, \( B = \infty \) and the algorithm lowers this bound whenever a shorter path to a node in \( T \) is encountered. Crucially, \( B \geq D \) always and a finite value of \( B \) witnesses the existence of a path from \( s \) to a node in \( T \) of distance \( B \). As a consequence, each edge \( (u, v) \in E \) that leads to a tentative distance \( d(v) \) with \( d(v) \geq B \) can be discarded from further considerations; we also say that edge \( (u, v) \) is pruned. The pseudocode of Dijkstra-Pruning is given in Algorithm 1.

Clearly, in the worst case Dijkstra-Pruning does not prune any edges. In particular, the worst-case running time of Dijkstra-Pruning remains \( O(m + n \log n) \). However, empirically Dijkstra-Pruning saves a significant fraction of the queue operations performed by Dijkstra. Bast et al. \[2\] use a random model (introduced below) to analyse the performance of Dijkstra-Pruning and show that the expected savings for these instances are significant.

2.3 Random Model

We conduct extensive experiments to assess the performance of our proposed algorithms and report on our findings in Section 6. The instances that we use in our experiments are constructed using the following random model, which was also used by Bast et al. \[2\] to analyze the performance of Dijkstra-Pruning.

We consider directed random graphs which are constructed according to the Erdös-Rényi random graph model \[10\], also known as \( G(n, p) \): In this model, there are \( n \) nodes and each of the \( n(n-1) \) possible (directed) edges is present independently with probability \( p = c/n \), where \( c \) is (roughly) the average degree of a node.\(^5\) Further, each node \( u \in V \)

\(^5\) Note that we implicitly assume that the graph does not contain any self-loops. The average degree of outgoing (or, equivalently, incoming) edges of a node is \((1 - \frac{1}{n})c\).
is chosen independently with probability \( q = f / n \) to belong to the target set \( T \), where \( f \) is the expected number of target nodes in \( T \). The weight \( w(e) \) of each edge \( e \) is chosen independently uniformly at random from the range \([0, 1]\).

### 3 Dijkstra’s Algorithm with Predictions

In this section, we describe our new algorithm to solve the SSMTSP problem and establish its correctness.

#### 3.1 High-level Idea

Our basic idea is to further amplify the effect of the edge prunings by using a machine learning approach to obtain a prediction of the shortest path distance at an early stage. More concretely, suppose we have a PREDICTION algorithm which, based on the execution of the algorithm so far, computes an estimate of the shortest path distance \( D \). We can then call this algorithm after a few iterations to obtain a prediction \( P \) of \( D \) and use it to prune all edges that lead to a tentative distance larger than \( P \).

There are different ways to realise such a PREDICTION algorithm. Some natural approaches are discussed in more detail in Section 5. Ideally, we would like to come up with an algorithm that provides a prediction \( P \) which comes close to the actual shortest path distance \( D \). In fact, both over- and underestimations of \( D \) can be harmful, though in different ways: If \( P \) overestimates \( D \) then edges which are irrelevant for the shortest path might not be pruned. If \( P \) underestimates \( D \) then edges which are essential for the shortest path might be pruned. Note that in the former case the algorithm might perform priority queue operations which are redundant—which is undesirable. However, in the latter case the algorithm might return an incorrect solution (claiming that there is no shortest path)—which is unacceptable.
Algorithm 4: **Naïve-Restart**

1. \( P = \beta \cdot P \) // inflate prediction
2. reinitialise \( d(\cdot) \) and \( PQ \) // leave \( B, P, X \) and \( i \) unchanged

Algorithm 5: **Smart-Restart**

1. \( P = \beta \cdot P \) // inflate prediction
2. foreach \( v \in R \) do // iterate over all reserve nodes in \( R \)
3. \[ \text{if } d(v) \leq \min \{ B, P \} \text{ then} \] // \( v \) is relevant for new prediction
4. \( R = R \setminus \{ v \} \) // move \( v \) from \( R \) to \( PQ \)
5. \( \text{PQ.INSERT}(v, d(v)) \)

To remedy the latter, we equip our algorithm with a \texttt{RESTART} procedure: If the prediction \( P \) turns out to be too small, it is increased and the algorithm continues with the new prediction. Clearly, such restarts should not happen too often as this might reduce the efficiency of the approach. We suggest two different \texttt{RESTART} procedures below, a naïve one and a smarter one.

There are several advantages from which our approach can (potentially) benefit when compared to the algorithms \texttt{Dijkstra} and \texttt{Dijkstra-Pruning}:

- Fewer queue operations may be performed because of the edges being pruned.
- Edge pruning might start after a few iterations only, potentially before having found any path to a target node.
- Queue operations may take less time because the size of the priority queue remains smaller.

### 3.2 More Detailed Description of Our Algorithm

We elaborate on our algorithm \texttt{Dijkstra-Prediction} in more detail. The pseudocode is given in Algorithm 3. The algorithm builds upon \texttt{Dijkstra-Pruning}, see Section 2. The three new input parameters \( i_0, \alpha \) and \( \beta \) will become clear below.

During the first \( i_0 \) iterations, an array \( X \) is maintained for storing the trace (as we term it) of the algorithm: \( X[i] \) stores the pair \((d(u), B)\) consisting of the distance of the settled node \( u \) and the upper bound value \( B \) in iteration \( i \). In iteration \( i_0 \), the constructed trace \( X \) is then used to compute an initial prediction by calling the \texttt{Prediction} procedure. We elaborate on the choice of \( X \) and compare different prediction methods in Section 5.

Our choice to use the pairs \((d(u), B)\) of the first \( i_0 \) iterations as the trace \( X \) of the algorithm is motivated as follows: The distances \( d(u) \) correspond to a lower bound on the shortest path distance, while the bound \( B \) represents an upper bound on the shortest path distance. The combination of both then (hopefully) conveys some information that can be used by the machine learning algorithms to predict the shortest path distance rather accurately. Note that the initial prediction is increased by a factor \( \alpha \geq 1 \). Intuitively, the idea here is that one may want to inflate the initial prediction (slightly) to bias it towards an overestimation of the distance \( D \) to reduce the number of times that the restarting procedure has to be called.

The algorithm keeps track of both the bound \( B \) on the smallest distance to a node in \( T \) encountered so far and the current prediction \( P \). An edge \((u, v)\) which is scanned
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Algorithm 6: RELAX-SMART($u, v, tent, P$)

1. if $d(v) > tent$ then // lower tentative distance
2. if $d(v) = \infty$ then // v reached for the first time
3. if $tent \leq P$ then PQ.INSERT($v, tent$) // add v to PQ
4. else $R = R \cup \{v\}$ // add v to R
5. else
6. if $v \notin R$ then PQ.DECREASE-PRIORITY($v, tent$)
7. else // v is in R already
8. if $tent > P$ then continue // v remains in R
9. $R = R \setminus \{v\}$ // move v from R to PQ
10. PQ.INSERT($v, tent$)
11. $d(v) = tent$ // update distance of v

by the algorithm is pruned whenever the tentative distance $d(u) + w(u, v)$ exceeds the minimum of $B$ and $P$ (unless we use a smarter book-keeping, as explained below).

There is a somewhat subtle point in the algorithm: Note that during the first $i_0$ iterations the prediction $P$ remains at $\infty$ as the trace is just being built. As a consequence, throughout this stage it could happen that nodes are inserted into the priority queue PQ, whose tentative distances are larger than the first prediction $P$ (determined in iteration $i_0$); after this stage, this is impossible due to the pruning. It is because of these nodes that we have to add the second condition to the while loop, which checks whether the minimum distance of a node in PQ is less than the current prediction $P$. If not, the respective restart procedure has to be initiated to increase the prediction and add all relevant nodes to PQ.

We turn to the restarting procedures. The idea of the first procedure, NAÏVE-RESTART (see Algorithm 4), is very simple: The current prediction is increased by a factor $\beta > 1$ and the tentative distances and the priority queue are reinitialised. The algorithm then starts a new trial with the updated prediction. This procedure is naïve in the sense that in each trial the algorithm basically starts from scratch, the only difference being that the (updated) prediction is used from the beginning.

Ideally, one would rather not start from scratch but do some smart book-keeping to keep track of the nodes (termed reserve nodes) that are pruned in the current trial, but might become relevant in subsequent trials. This is what our second procedure, SMART-RESTART (see Algorithm 5), does.

In order to incorporate this smart book-keeping, we have to make the following changes to DIJKSTRA-PREDICTION (all indicated by a “⋆” in Algorithm 3):

1. We maintain an additional set $R$ of the reserve nodes.
2. We only prune an edge $(u, v)$ when the tentative distance exceeds the bound $B$ (not $\min\{B, P\}$).
3. We use the RELAX-SMART routine (see Algorithm 6) to relax an edge $(u, v)$ (not RELAX).

The RELAX-SMART routine is similar to the standard RELAX routine (see Algorithm 2). The main difference is that the node $v$ is only inserted into the priority queue if its tentative distance is smaller than the prediction; otherwise, it is added to the reserve set $R$. $R$ will contain all nodes which have a finite tentative distance, but have not been added to the priority queue because their tentative distance exceeds the prediction in the current trial.
SMART-RESTART also first scales the current prediction by a factor $\beta > 1$. We then iterate over all reserve nodes in $R$ and move each relevant node $v \in R$ from $R$ to $PQ$. Here a node is considered relevant if its distance is smaller than the minimum of the upper bound $B$ and the (updated) prediction $P$. By proceeding this way, we do not need to start the algorithm from scratch, but can continue with the search after all relevant nodes were moved from $R$ to $PQ$ (we also refer to these kind of insertions as batch insertions).

### 3.3 Correctness Proofs

A point of vital importance is that our algorithms are correct in the sense that they

1. terminate in polynomial time, and
2. compute an optimal solution to the SSMTSP problem.

The correctness of DIJKSTRA-PREDICTION with the NAÏVE-RESTART procedure is straightforward once one realises that the algorithm keeps increasing the prediction $P$ until it exceeds the actual shortest path distance $D$. In the final trial, the algorithm thus relaxes all relevant edges and correctly determines the shortest path distance.

We are left to prove the following theorem.

**Theorem 1.** DIJKSTRA-PREDICTION with the SMART-RESTART procedure is correct.

We establish the correctness of this algorithm by showing that the following invariant holds true during the course of the algorithm. The invariant establishes a connection between DIJKSTRA-PREDICTION with SMART-RESTART and DIJKSTRA-PRUNING when run on the same input instance. We use $d$, $PQ$ and $R$ to refer to the respective data structures in DIJKSTRA-PREDICTION, and $d'$, $PQ'$ to the respective data structures in DIJKSTRA-PRUNING.

**Invariant 1.** Consider the runs of DIJKSTRA-PREDICTION with SMART-RESTART and DIJKSTRA-PRUNING on the same input instance. The following properties are satisfied in each iteration:

(P1) Both algorithms remove the same node $u$ from $PQ$ and $PQ'$, respectively.

(P2) The set of nodes in $PQ'$ can be partitioned into the set of nodes in $PQ$ and the set of nodes in $R$, with $d(v) > P$ for all $v \in R$.

(P3) The tentative distances are equal in both algorithms, i.e., $d(v) = d'(v)$ for all $v \in V$.

**Proof.** We assume that both algorithms employ a consistent tie-breaking rule for nodes with similar distances. It is easy to see that the invariant holds for the first iteration: the prediction is initialised to $P = \infty$ and thus the algorithms do exactly the same, and $R$ remains empty. Now, suppose by induction that the invariant holds at the beginning of iteration $i \geq 1$. We argue that the invariant holds at the end of iteration $i$:

(P1) Suppose that node $u$ is deleted from $PQ$ in iteration $i$. By the condition in the while-loop in Algorithm 3 it holds that $d(u) \leq P$, which together with (P2) gives that $d(u) < d(v)$ for all $v \in R$. By the REMOVE-MIN operation, $d(u) < d(v)$ for all $v \in PQ$, so $d(u) < d(v)$ for all $v \in PQ \cup R$. Since $PQ \cup R = PQ'$ (because of (P2)), we have $d(u) < d(v)$ for all $v \in PQ'$. From (P3), it follows that $d'(u) < d'(v)$ for all $v \in PQ'$, which proves that the same node is deleted in DIJKSTRA-PRUNING.

(P2) We consider each queue operation executed by the algorithms in this iteration separately and argue that the claim remains true. Firstly, if the claim holds at the beginning of an iteration, then it still holds after the REMOVE-MIN operation because the same node $u$ is deleted from $PQ$ and $PQ'$. Secondly, suppose that in iteration $i$ node $v$ is
We first show that in the worst case our algorithm does not prune any of the edges even while it actually only becomes available after $i$ (which is without loss of generality). Recall that $D$ then, before the priority is decreased, particular, we assume that the algorithm starts with this prediction from the beginning, perfect). This is unavoidable if the adversary (who defines the worst-case instance) can fix the entire input instance. If the prediction is perfect (i.e., $\varepsilon = 0$), then there is no overestimation, so the claim remains true. Further, note that we assume that the prediction starts with a prediction $P$ obtained from $I$-JSTRA algorithm. By (P3), we have $d(v) = \infty$ and $d(u) + w(u, v) < \infty$. This means that node $v$ is either inserted into PQ or R. A node $v$ is only added to R if $d(u) + w(u, v) > P$. So the claim still holds after an insertion when $d(v)$ is set to $d(u) + w(u, v)$. Finally, suppose that in iteration $i$ the priority of node $v$ in PQ is decreased because edge $(u, v)$ is relaxed. Then, before the priority is decreased, $d'(v) < \infty$ and $d'(u) + w(u, v) < d'(v)$. Again, edge $(u, v)$ will also be relaxed in the DIJKSTRA-PREDICTION algorithm, and by (P3) we have $d(v) < \infty$ and $d(u) + w(u, v) < d(v)$. This means that node $v$ will remain in PQ if it was already there, and will be moved from R to PQ if $d(u) + w(u, v) \leq P$. In both cases, the claim will remain true after the DECREASE-PRIOR operation when $d(v)$ is set to $d(u) + w(u, v)$. Lastly, the property also remains true when $P$ is inflated in the SMART-RESTART procedure, since all $v \in R$ with $d(v) \leq P$ are moved to PQ and removed from R.

(P3) Both algorithms remove the same node $u$, update the tentative distance of $u$'s neighbours based on the same condition and update it to the same value. So if the claim holds before the iteration, it will also hold at the end of the iteration.

4 Lower Bound on Savings

In this section, we derive lower bounds on the savings that our algorithm DIJKSTRA-PREDICTION achieves by pruning edges. We start by giving two examples which illustrate that, in the worst case, our algorithm may not prune any edge (even if the prediction is perfect). This is unavoidable if the adversary (who defines the worst-case instance) can control the weights of all the edges. We therefore restrict the freedom of the adversary by considering partial random instances, where the edge weights of certain (relevant) edges are chosen at random. Based on this, we then derive lower bounds on the number of relevant edges that will be pruned by our algorithm. Finally, we use these insights to lower bound the number of saved queue operations for random instances constructed according to the model introduced in Section 2.3. Our results show that our DIJKSTRA-PREDICTION algorithm saves a significant number of queue operations compared to the standard DIJKSTRA algorithm.

We assume that all edge weights are normalised such that $w_e \in [0, 1]$ for all $e \in E$ (which is without loss of generality). Recall that $D$ denotes the shortest path distance from $s$ to any target node in $T$ as defined in (1). For the sake of the analysis, we make the following assumption throughout this section: The algorithm DIJKSTRA-PREDICTION starts with a prediction $P = D + \varepsilon$, where $\varepsilon \geq 0$ is the additive error of the prediction. In particular, we assume that the algorithm starts with this prediction from the beginning, while it actually only becomes available after $i_0$ many iterations. Given that $i_0$ is small, this assumption is negligible. Further, note that we assume that the prediction $P$ is an overestimation of the actual distance $D$. Clearly, $P$ might also be an underestimation of $D$ and our algorithm also saves on queue operations in this case. But at this stage we do not know how to estimate these savings analytically.

4.1 Worst-case Instances

We first show that in the worst case our algorithm does not prune any of the edges even if the prediction is perfect (i.e., $\varepsilon = 0$ and thus $P = D$). We assume that an adversary can fix the entire input instance.
Observe that the edges which our Dijkstra-Prediction algorithm might prune, either due to the bound \( B \) or the prediction \( P \), are those edges \((u,v) \in E\) for which \( u \) is removed from the priority queue at some point during the algorithm, i.e., \( d(u) \leq D \), and the new tentative distance for \( v \) exceeds \( D \), i.e., \( d(u) + w(u,v) > D \). We denote this set of edges by \( L \), i.e.,

\[
L := \{(u,v) \in E : d(u) \leq D \text{ and } d(u) + w(u,v) > D\}.
\]

Said differently, a necessary condition for pruning an edge is that it is contained in \( L \).

The first crucial observation is that nothing can be gained by our algorithm if the adversary has the power to construct the entire input instance, including the weights of all the edges. An illustrating example of such an instance is given in Figure 1a (with \( t \) being the only target node). Here, the set of edges \( L \) which are candidates for pruning consists of the edges \((u_i, v_i)\) for all \( i \) (indicated in grey). However, none of these edges will be pruned because of the bound \( B \), since it is only set to 1 once edge \((u_2,v)\) is scanned. Further, none of these edges will be pruned because of the prediction \( P \), since \( d(v_i) \) is \( 1 + \frac{\epsilon}{2} \) for all \( i \), which is smaller than \( P = 1 + \epsilon \). This example also illustrates that even if we are able to compute perfect predictions, i.e., \( \epsilon = 0 \), the algorithm might not prune any edges in the worst case.

In the example above, the reason why none of the edges \((u_i, v_i)\) in \( L \) is pruned is that the distance \( d(u_1) = \epsilon \) of the start node \( u_1 \) is small, and thus the tentative distance of \( v_i \) cannot exceed \( P \). Therefore, a necessary condition to prune an edge \((u,v)\) is that \( d(u) \) is larger than \( D - 1 + \epsilon \). Suppose we let the adversary create an instance again, but now we enforce it to have many edges which satisfy this condition. To do so, define a subset of \( L \), called \( L_\theta \), for some threshold \( \theta \) from the interval \([D - 1 + \epsilon, D]\), for which \( d(u) \) is larger than \( \theta \):

\[
L_\theta := \{(u,v) \in E : \theta \leq d(u) \leq D \text{ and } d(u) + w(u,v) > D\}. 
\]

We also say that the edges in \( L_\theta \) are relevant.

The second crucial observation is that we are still not able to guarantee any savings, even if there are many relevant edges. To see this, consider the illustration depicted in Figure 1b. Here, the nodes \( u_i \) removed from the priority queue are sorted by increasing distances \( d(u_i) \) (from left to right); only the \( u_i \)'s are shown for which \( d(u_i) > D - 1 + \epsilon \). Also, not all the edges of the graph are shown, but only the relevant edges in \( L_\theta \) (indicated in grey). Without further restrictions, the adversary can still fix the weights of the edges in \( L_\theta \) as indicated, and none of the edges will be pruned, neither by \( B \) nor by \( P \). Note that this holds even for \( P \) being arbitrarily close to \( D \).
4.2 Partial Random Instances

Based on the examples in the previous section, it is clear that we need to further restrict the power of the adversary. We therefore introduce randomness in the instances to obtain a more fine-grained understanding of the savings achieved by our algorithm. Generally speaking, we will do this by enforcing randomness on some of the edges, while allowing the adversary to still control the rest of the input instance.

The setup is as follows: We suppose that the adversary can fix the set \( Q = \{ u_1, \ldots, u_l \} \) of nodes that are removed from the priority queue, where \( u_i \) is the node removed in iteration \( i \), and the corresponding distances \( d(u_1) \leq \cdots \leq d(u_l) \) of these nodes. Further, the adversary can fix all outgoing edges of the nodes in \( Q \). Note that by doing so we implicitly allow that the adversary can fix the weights of certain edges to enforce this configuration (because these weights determine the order in which the nodes are removed from the priority queue). Crucially, however, we do not allow that the adversary can fix the weights of the relevant edges in \( L \); the weight of each relevant edge in \( L \) is random.

Now, in this partially random setting, the edge weights for all edges \((u, v) \in Q\) are independent and the distance labels \( d(u) + w(u, v) \) are uniform on \([D, d(u) + 1]\) (see also [2]). This is because \((u, v) \in Q\) implies \( d(u) + w(u, v) \geq D \) and \( d(u) + w(u, v) \leq d(u) + 1 \), but nothing else.

Given this partially random adversarial setting, we can lower bound the probability of pruning an edge in \( Q \). Like in the previous examples, the adversary still has enough power to setup the instance such that none of these edges are pruned based on the bound \( B \). In contrast, each of these edges is pruned with positive probability due to the prediction \( P \). For the edges in \( Q \) we know that the necessary condition for pruning, \( d(u) > D + 1 - \varepsilon \), holds. The next lemma shows that we can lower bound the probability of pruning a relevant edge in \( Q \).

**Lemma 1.** Suppose \( L_\theta \) is defined as above, with \( \theta = D + \gamma \varepsilon - 1 \), for some \( \gamma \in (1, \frac{1}{\varepsilon}] \). For each relevant edge \( e = (u, v) \in L_\theta \), let \( X_e \) be a random variable which equals 1 if edge \( e \) is pruned and zero otherwise. Then:

\[
P(X_e = 1) \geq 1 - \frac{1}{\gamma}.
\]

**Proof.** Let \( e = (u, v) \in L_\theta \) be a relevant edge and let \( d(v) \) be the distance of \( v \) at the end of the algorithm. Then \( e \) is pruned whenever the tentative distance \( \text{tent} := d(u) + w(u, v) \) exceeds the prediction \( P \). As argued before, \( e \in L_\theta \) implies that \( d(u) + w(u, v) \) is uniformly distributed on \([D, d(u) + 1]\). Furthermore, note that \( 1 - (D - d(u)) \geq \gamma \varepsilon \) follows from \( d(u) \geq \theta \) and the definition of \( \theta \) and note that \( D + \varepsilon \) is contained in the interval \([D, d(u) + 1]\), since \( D + \varepsilon \leq D + \gamma \varepsilon \leq d(u) + 1 \). We can simply apply the cumulative distribution function for the uniform distribution:

\[
P(X_e = 1) = P(\text{tent} \geq P) = P(d(u) + w(u, v) \geq D + \varepsilon) = \frac{d(u) + 1 - (D + \varepsilon)}{d(u) + 1 - D} = 1 - \frac{\varepsilon}{1 - (D - d(u))} \geq 1 - \frac{1}{\gamma}.
\]

We give some intuition for the lemma, which shows the interplay between the number of edges in \( L_\theta \) and the probability that an edge is pruned. The number of edges in \( L_\theta \) is largest when \( \gamma \) is close to 1, and the lemma shows there is a small positive probability for each of those to be pruned by the prediction. As \( \gamma \) increases to \( \frac{1}{\varepsilon} \), the threshold \( \theta \)
approaches $D$ and the size of $L_{\theta}$ decreases. So the number of relevant edges decreases, while the probability that each such edge is pruned increases.

Define $X$ as the total number of pruned edges in $L_{\theta}$, i.e., $X = \sum_{e \in L_{\theta}} X_e$. We can now lower bound $X$.

**Theorem 2.** Suppose $L_{\theta}$ is defined as above, with $\theta = D + \gamma \varepsilon - 1$, for some $\gamma \in \left(1, \frac{1}{\varepsilon}\right]$. Then the expected number of edges pruned by our algorithm is

$$E[X] \geq \left(1 - \frac{1}{\gamma}\right) |L_{\theta}|.$$

**Proof.** By linearity of expectation,

$$E[X] = E \left[ \sum_{e \in L_{\theta}} X_e \right] = \sum_{e \in L_{\theta}} E[X_e] = \sum_{e \in L_{\theta}} P(X_e = 1).$$

The proof follows from Lemma 1. \qed

We can use a standard Chernoff bound argument to prove that with high probability the number of pruned edges is at least $\frac{1}{2}(1 - \frac{1}{\gamma})|L_{\theta}|$.

**Theorem 3.** Suppose $L_{\theta}$ is defined as above, with $\theta = D + \gamma \varepsilon - 1$, for some $\gamma \in \left(1, \frac{1}{\varepsilon}\right]$. Let $X$ be the number of pruned edges and assume that $(1 - \frac{1}{\gamma})|L_{\theta}| \geq 8 \ln n$, where $n$ is the number of nodes. Then:

$$P \left( X \geq \frac{1}{2} \left(1 - \frac{1}{\gamma}\right) |L_{\theta}| \right) \geq 1 - \frac{1}{n}.$$

**Proof.** Note that $X = \sum_{e \in L_{\theta}} X_e$ is a sum of $|L_{\theta}|$ independent random variables. Let $\mu := E[X]$ be the expected value of $X$. The following (standard) Chernoff bound holds for every $\delta \in (0, 1)$:

$$P(X \leq (1 - \delta)\mu) \leq e^{-\mu \delta^2 / 2}.$$ \n
By choosing $\delta = \frac{1}{2}$, we obtain

$$P \left( X \leq \frac{1}{2} \mu \right) \leq e^{-\mu / 8} \leq \frac{1}{n},$$

where the second inequality holds because $\mu = E[X] \geq (1 - \frac{1}{\gamma})|L_{\theta}| \geq 8 \ln n$ by Theorem 2 and our assumption.

Using this, we conclude that

$$P \left( X \geq \frac{1}{2} \left(1 - \frac{1}{\gamma}\right) |L_{\theta}| \right) \geq P \left( X \geq \frac{1}{2} \mu \right) \geq 1 - \frac{1}{n}.$$ \hspace{1cm} \qed

### 4.3 Random model

In this section, we consider random instances which are created according to the random model introduced in Section 2.3. We are able to show how that, on these instances, we save a significant number of queue operations compared to the **DIJKSTRA-PRUNING** algorithm.
In the random model, it is not straightforward to compute the size of $L_\theta$. Therefore, we will consider a specific subset of $L_\theta$ for which we are able to compute the size. More specifically, we only consider the edges $(u, v)$ from $L_\theta$ for which the final distance $d(v)$ is larger than $D$, i.e., edges from $L_\theta$ that lead to a node $v$ which is not in $Q$. Note that there could be multiple edges in $L_\theta$ that lead to such a node $v \not\in Q$. In that case, we only consider the edge in $L_\theta$ which has led to an insertion of $v$ into the priority queue in the standard Dijkstra algorithm, and not the edges which have led to decrease priority operations. We use $L'_\theta$ to denote this subset of $L_\theta$:

$$L'_\theta := \{(u, v) \in E : \theta \leq d(u) \leq D \text{ and } d(v) > D \text{ and } (u, v) \text{ leads to insertion of } v \text{ in PQ of Dijkstra}\}.$$ 

In the Dijkstra algorithm, all the end nodes of edges in $L'_\theta$ are inserted in the priority queue, but they are never removed. Dijkstra-Prediction can actually save a number of these insert operations by pruning the edges in $L'_\theta$. We will lower bound these savings by computing an upper bound for the number of these nodes which are still inserted in our Dijkstra-Prediction algorithm. Consequently, all the edges which lead to nodes which are not inserted in Dijkstra-Prediction are pruned.

First, we will prove the following Key Lemma which will help us to upper bound the probability of inserting an edge below.

**Lemma 2 (Key Lemma).** Let $X_j, j = 1, \ldots, k + 1$, be $k + 1$ uniform random variables, with $X_j$ uniform on $[a, b_j]$ and $b_1 \leq \cdots \leq b_{k+1}$. Let $P > 0$ be a real number, which is contained in all intervals, i.e., $a < P < b_1$. Let $E_1$ be the event $\{X_{k+1} \leq X_j, \forall j\}$ and let $E_2$ be the event $\{X_{k+1} \leq P\}$. Then:

$$P(E_1 \cap E_2) \leq \frac{1}{k+1} \left(1 - \left(1 - \frac{P - a}{b_k - a}\right)^{k+1}\right).$$

**Proof.** We will upper bound the probability by conditioning on values of $X_{k+1}$, using the law of total probability and applying the density function of $X_{k+1}$: $f_{X_{k+1}}(s) = \frac{1}{b_{k+1} - a}$.

$$P(E_1 \cap E_2) = \int_a^{b_{k+1}} P(E_1 \cap E_2 \mid X_{k+1} = x)f_{X_{k+1}}(x)dx
= \frac{1}{b_{k+1} - a} \int_a^{b_{k+1}} P(E_1 \cap E_2 \mid X_{k+1} = x)dx$$

Note that $L_\theta$ may contain edges $(u, v)$ with tentative distance $d(u) + w(u, v) > D$, but whose final distance $d(v) \leq D$. These are relevant edges having both endpoints in $Q$ that might be pruned. However, we do not account for these savings in our analysis here.
Since $\mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2 \mid X_{k+1} = x) = 0$ if $x > P$, we can write:
\[
\mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2 \mid X_{k+1} = x) = \mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2 \mid \{X_{k+1} = x\} \land \{x \leq P\}) \\
= \mathbb{P}(\{X_{k+1} \leq X_j, \forall j\} \land \{X_{k+1} \leq P\} \mid \{X_{k+1} = x\} \land \{x \leq P\}) \\
= \mathbb{P}(x \leq X_j, j = 1, \ldots, k \mid \{X_{k+1} = x\} \land \{x \leq P\}) \\
= \mathbb{P}(x \leq X_j, j = 1, \ldots, k \mid x \leq P)
\]
\[
= \prod_{j=1}^{k} \mathbb{P}(x \leq X_j \mid x \leq P) \\
= \prod_{j=1}^{k} \left(1 - \frac{x - a}{b_j - a}\right) \\
\leq \left(1 - \frac{x - a}{b_k - a}\right)^{k}.
\]

The third equality holds because the conditioning already implies that $X_{k+1} \leq P$. The fourth equality holds since the value of $X_j, j = 1, \ldots, k$ is independent of the value of $X_{k+1}$. Thereafter we use that all the $X_j$’s are identically distributed, and we use the cumulative distribution function of the uniform distribution. In the last inequality we exploit that $b_j - a \leq b_k - a$ for all $j$. We can use this, together with $\frac{b_k - a}{b_{k+1} - a} \leq 1$, to upper bound the expectation of $\mathcal{E}_1 \cap \mathcal{E}_2$:
\[
\mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2) \leq \frac{1}{b_{k+1} - a} \int_{a}^{P} \left(1 - \frac{x - a}{b_k - a}\right)^{k} \, dx
\]
\[
= \frac{1}{b_{k+1} - a} \int_{a}^{P} \left(-\frac{b_k - a}{k + 1} \left(1 - \frac{x - a}{b_k - a}\right)^{k+1}\right) \, dx
\]
\[
= \frac{1}{b_{k+1} - a} \left[-\frac{b_k - a}{k + 1} \left(1 - \frac{x - a}{b_k - a}\right)^{k+1} \left|_{a}^{P}\right. \right. \\
= \frac{b_k - a}{b_{k+1} - a} \left[1 - \left(1 - \frac{P - a}{b_k - a}\right)^{k+1}\right]
\]
\[
\leq \frac{1}{k + 1} \left[1 - \left(1 - \frac{P - a}{b_k - a}\right)^{k+1}\right].
\]

We will continue to lower bound the expected number of end nodes of edges in $L'_\theta$, which are inserted in the Dijkstra-Prediction algorithm, despite the prunings. We call this quantity $\text{INRP}_\theta$. We condition on the event $E_l$, which implies not only the adversarial setting introduced in the previous section, but also that the size of $L'_\theta$ equals $l$.

**Theorem 4.** Suppose $L'_\theta$ is defined as above, with $\theta = D + \gamma e - 1$, for some $\gamma \in (1, \frac{1}{2}]$. Let $\text{INRP}_\theta$ be the number of end nodes of edges in $L'_\theta$ which are inserted but never removed in the Dijkstra-Prediction algorithm. Under the conditioning of the event $E_l$, i.e. $|L'_\theta| = l$ and the adversarial setting, we have that:
\[
\mathbb{E}[\text{INRP}_\theta \mid E_l] \leq \frac{1}{q} \left(1 + \ln \left(\frac{ld}{\gamma}\right)\right).
\]
Proof. Let $l$ be the size of $L'_0$ and let $e_1 = (u_1,v_1), e_2 = (u_2,v_2), \ldots, e_l = (u_l,v_l)$ be all the edges in $L'_0$. Note that there might be repetitions in the $u_i$’s, but all the $v_i$’s are distinct. For $i = 1, \ldots, l$, define $X_i = d(u_i) + w(e_i)$. We observed in the previous section that for all edges $e_i$ in $L'_0$ it holds that $X_i$ is random uniform on $[D,d(u_i) + 1]$.

In Dijkstra-Pruning $e_i$ leads to an insertion only if $X_i$ is smaller than $X_j$ for every free $v_j$, with $j < i$. Suppose that there are $k$ of these free $v_j$’s preceding $v_i$ in the endpoints of $L'_0$. In Dijkstra-Prediction, an extra condition must be met, namely that $X_i$ does not exceed the prediction. To lower bound the expectation of $\text{INRP}_{b_i}$, we partition over $k$, the number of free $v_j$ preceding $v_i$:

$$E[\text{INRP}_{b_i} \mid E_i] \leq \sum_{1 \leq i \leq l} \sum_{0 \leq k < i} \binom{i-1}{k} (1 - q)^{i-1-k} \mathbb{P}(\{X_i \leq X_j, j = 1, \ldots, k \} \land \{X_i \leq P\})$$

To be able to apply our Key Lemma (Lemma 2), we need that the variables $X_j$ must be random uniform. We have already shown that they are random uniform on $[D,d(u_j) + 1]$, for which the upper bounds increase as $j$ increases. Moreover, we need that $P < b_i$, which holds since for all edges in $L'_0$ we have $d(u_i) + 1 > P$. Therefore, we can apply our Key Lemma to bound the probability in the sum to obtain:

$$\mathbb{P}(\{X_i \leq X_j, j = 1, \ldots, k \} \land \{X_i \leq P\}) \leq \frac{1}{k+1} \left[1 - \left(1 - \frac{P - D}{d(u_k) + 1 - D}\right)^{k+1}\right]$$

$$\leq \frac{1}{k+1} \left[1 - \left(1 - \frac{1}{\gamma}\right)^{k+1}\right],$$

which gives

$$E[\text{INRP}_{b_i} \mid E_i] \leq \sum_{1 \leq i \leq l} \sum_{0 \leq k < i} \binom{i-1}{k} (1 - q)^{i-1-k} \frac{1}{k+1} \left(1 - \left(1 - \frac{1}{\gamma}\right)^{k+1}\right)$$

$$= \sum_{1 \leq i \leq l} \sum_{0 \leq k < i} \binom{i-1}{k} (1 - q)^{i-1-k} \frac{1}{k+1} \left(1 - \left(1 - \frac{1}{\gamma}\right)^{k+1}\right)$$

$$- \sum_{1 \leq i \leq l} \sum_{0 \leq k < i} \binom{i-1}{k} (1 - q)^{i-1-k} \frac{1}{k+1} \left(1 - \frac{1}{\gamma}\right)^{k+1}. \quad (3)$$

We know from Bast et al. [2] that $\sum_{1 \leq i \leq l} \frac{1}{iq} \left(1 - (1 - q)^i\right)$.

$$E[\text{INRP}_{b_i} \mid E_i] \leq \sum_{1 \leq i \leq l} \sum_{0 \leq k < i} \binom{i-1}{k} (1 - q)^{i-1-k} \frac{1}{k+1} \left(1 - \left(1 - \frac{1}{\gamma}\right)^{k+1}\right)$$

(3) = \sum_{1 \leq i \leq l} \frac{1}{iq} \left(1 - (1 - q)^i\right).
We will use similar techniques to obtain such an expression for (4). Like in Bast et al. [2] we use \( \binom{i-1}{k} \frac{1}{k+1} \approx \frac{1}{7} \binom{i}{k+1} \), and we use the binomial of Newton to rewrite the sum.

\[
(4) = \sum_{1 \leq i \leq l} \frac{1}{iq} \sum_{0 \leq k < i} \binom{i}{k+1} \left( q \left( 1 - \frac{1}{\gamma} \right) \right)^{k+1} (1 - q)^i (1 - q)^{i-(k+1)} \\
= \sum_{1 \leq i \leq l} \frac{1}{iq} \sum_{1 \leq k \leq i} \binom{i}{k} \left( q \left( 1 - \frac{1}{\gamma} \right) \right)^{k} (1 - q)^i (1 - q)^{i-k} \\
= \sum_{1 \leq i \leq l} \frac{1}{iq} \left[ \sum_{0 \leq k \leq i} \binom{i}{k} \left( q \left( 1 - \frac{1}{\gamma} \right) \right)^{k} (1 - q)^{i-k} - (1 - q)^i \right] \\
= \sum_{1 \leq i \leq l} \frac{1}{iq} \left[ \left( 1 - \frac{q}{\gamma} \right)^i - (1 - q)^i \right].
\]

We can combine those two results to obtain the following bound for \( \mathbb{E}[\text{INRP}_\theta \mid E_i] \):

\[
\mathbb{E}[\text{INRP}_\theta \mid E_i] \leq \sum_{1 \leq i \leq l} \frac{1}{iq} \left( 1 - (1 - q)^i \right) - \sum_{1 \leq i \leq l} \frac{1}{iq} \left[ \left( 1 - \frac{q}{\gamma} \right)^i - (1 - q)^i \right] \\
= \sum_{1 \leq i \leq l} \frac{1}{iq} \left[ 1 - (1 - q)^i - \left( 1 - \frac{q}{\gamma} \right)^i + (1 - q)^i \right] \\
= \sum_{1 \leq i \leq l} \frac{1}{iq} \left[ 1 - \left( 1 - \frac{q}{\gamma} \right)^i \right].
\]

Like in Bast et al. [2], we split the sum at a yet to be determined index \( i_0 \). For \( i < i_0 \), we estimate \( 1 - (1 - \frac{q}{\gamma})^i \leq \frac{iq}{\gamma} \), and for \( i \geq i_0 \), we use \( 1 - (1 - \frac{q}{\gamma})^i \leq 1 \).

\[
\mathbb{E}[\text{INRP}_\theta \mid E_i] \leq \frac{i_0}{\gamma} + \frac{1}{q} \sum_{i_0 \leq i \leq l} \frac{1}{i} \\
\approx \frac{i_0}{\gamma} + \frac{1}{q} \ln \left( \frac{l}{i_0} \right).
\]

Taking the derivative with respect to \( i_0 \) gives that \( i_0 = \frac{q}{\gamma} \) minimizes this expression:

\[
\mathbb{E}[\text{INRP}_\theta \mid E_i] \leq \frac{1}{q} \left( 1 + \ln \left( \frac{1}{\gamma} \right) \right).
\]

\( \square \)

Now, suppose \( D \) lies in \([0, 1 - \varepsilon]\) and let \( \gamma \) be \( \frac{1-D}{\varepsilon} \), which makes \( \theta \) equal to 0. This means that all the edges which lead to nodes that are inserted but not removed by Dijkstra are in the set \( L'_0 \). So the size of \( |L'_0| \) is exactly equal to the number of nodes which are inserted but never removed in Dijkstra; this quantity is denoted by \( \text{INRS} \) in [2]. Bast et al. [2] estimate the expected value of \( \text{INRS} \). We summarise their findings in the following proposition.

**Proposition 1 (Bast et al. [2])**. Consider an instance from the random model introduced in Section 2.3. Let \( R \) be the number of reachable nodes from \( s \) in the random graph. Then if \( c \geq 8 \) and \( f \geq 4 \ln(n) \), it holds that \( R \) is large, i.e. \( R \geq (1 - \delta)an \), for some \( \alpha \) such that \( \alpha = 1 - \exp(-ca) \).
and δ small like 0.01. Moreover, the expected number of nodes that are inserted but never removed in the priority queue by the DIJKSTRA algorithm, given that R is large, is approximately:

\[ E[\text{INRS} | R \text{ is large}] \approx \frac{c-1}{q}. \]

We can use this expectation to upper bound the expected value of INRP given in Theorem 4 as follows: Since \( \ln \left( \frac{lq}{c-1} \right) \) is a convex function of \( l \), we can replace \( l \) simply by the expectation of \( \text{INRS} \). We obtain the following theorem.

**Theorem 5.** Suppose \( D \) lies in \([0, 1-\varepsilon)\). The expected number of nodes inserted but never removed by DIJKSTRA-PREDICTION is upper bounded by

\[ E[\text{INRP} | R \text{ is large}] \leq \frac{1}{q} \left( 1 + \ln(c-1) - \ln \left( 1 - \frac{D}{\varepsilon} \right) \right). \]

**Proof.**

\[ E[\text{INRP} | R \text{ is large}] \leq \frac{1}{q} \left( 1 + \ln \left( \frac{(c-1)q\varepsilon}{q(1-D)} \right) \right) = \frac{1}{q} \left( 1 + \ln(c-1) - \ln \left( 1 - \frac{D}{\varepsilon} \right) \right). \]

\( \Box \)

It is shown by Bast et al. [2] that the number of insert but never removed operations of the DIJKSTRA-PRUNING algorithm, denoted \( \text{INRR} \) in [2], is at most

\[ E[\text{INRR} | R \text{ is large}] \leq \frac{1}{q} \left( 1 + \ln(c-1) \right). \]

That is, compared to the DIJKSTRA-PRUNING algorithm, our DIJKSTRA-PREDICTION algorithm saves \( \ln \left( \frac{1-D}{q} \right) \) insertions of such nodes. So even though DIJKSTRA-PRUNING already saves a significant number of insertions, DIJKSTRA-PREDICTION is able to further improve on this. Naturally, these savings grow whenever the prediction becomes more accurate and \( \varepsilon \) decreases. In our experiments, we have considered instances where \( n = 1000, c = 8 \) and \( q = 0.02 \). For these instances, \( D \) is approximately 0.55. With a prediction \( P = D + \varepsilon \) which overpredicts \( D \) by at most \( \varepsilon = 0.1 \) (which seems reasonable from the experiments), the expected number of \( \text{INRP} \) of DIJKSTRA-PREDICTION is at most 63. In comparison, the expected number of \( \text{INRS} \) of DIJKSTRA is 350; so our algorithm saves at least 287 of these insertions. The expected number of \( \text{INRR} \) of DIJKSTRA-PREDICTION is at most 137; so our algorithms significantly improves upon this by exploiting the prediction.

## 5 Prediction Methods

The PREDICTION algorithm used in our algorithm DIJKSTRA-PREDICTION can be obtained in numerous ways. Below, we first explain how we obtain a prediction algorithm based on a machine learning approach. We elaborate on two different machine learning models and compare them to a benchmark prediction. After that two alternative prediction methods based on breadth-first search (BFS) are given.
5.1 Machine Learning

In order to make a prediction after $i_0$ iterations, we need to be able to describe the current optimisation run by means of some characteristic features. One of the challenges here is to come up with features that capture the essence of the current run such that they can be used by the machine learning model to make a good prediction of the shortest path distance. We do this by keeping track of a lower and upper bound on the shortest path distance in each iteration. More precisely, in iteration $i \leq i_0$, the distance $d(u)$ of the node $u$ extracted from the priority queue serves as the lower bound $d_i$ and the current value of the pruning bound $B$ is used as the upper bound $B_i$. The resulting sequence $X = ((d_1, B_1), (d_2, B_2), \ldots, (d_{i_0}, B_{i_0}))$ of these lower and upper bounds for the first $i_0$ iterations then constitutes what we call the trace of the algorithm.

A training sample and target for the machine learning algorithm then consists of the trace $X$ and the corresponding shortest path distance $D$, respectively. The set of samples for the machine learning models can be created by executing a run of Dijkstra-pruning on each problem instance of the training set. During this run, both the trace $X$ and the final shortest path distance $D$ need to be stored. Before the traces are used to train the machine learning models, we normalise each feature to ensure that it has mean 0 and standard deviation 1. For each feature, we subtract the mean and divide by the standard deviation. Of course, the mean and standard deviation are computed using the training data only. To prevent blowing up the mean value of the upper bound feature, all bounds $B_j$ which are equal to the initial value of $B = \infty$ are set to 0.

We implemented and compared two standard machine learning models, namely a neural network model and a linear regression model. The neural network model that we use is a straightforward multilayer perceptron network consisting of two hidden layers, for which we optimise the number of nodes per layer by a k-fold cross validation (see, e.g., [25] for more details). To verify whether anything has been learned by these models at all, the results for these models are compared with a straightforward benchmark prediction. This benchmark prediction, which is independent of the instance, is computed by taking the average of the shortest path distance for each instance in the training set.

5.2 BFS-based Predictions

As an alternative to the machine learning models, we implement two prediction methods that are based on breadth-first search (BFS). For each instance, we can simply run a BFS from the source node $s$ to determine a path $p_{\text{BFS}}$ to any of the target nodes having the smallest number of edges. We also call $p_{\text{BFS}}$ a BFS-path and use $L_{\text{BFS}}$ to denote its length (i.e., number of edges). Note that, equivalently, $L_{\text{BFS}}$ is the shortest path distance to any of the target nodes if all edge weights are set to 1. We use this BFS-path to derive two different predictions of the actual shortest path distance $D$: (i) BFS: We define the prediction $P$ as $L_{\text{BFS}} \cdot \mu_w$, where $\mu_w$ is the expected edge weight. (ii) $w$-BFS: We define the prediction $P$ as the sum of the actual weights on $p_{\text{BFS}}$, i.e., $P = \sum_{e \in p_{\text{BFS}}} w(e)$. Note that the latter prediction might overestimate but never underestimate the actual distance $D$.

6 Experimental Findings

In this section, we present our experimental findings. We first introduce our experimental setup and then discuss the results and insights we obtained from the experiments.
Table 1: Statistics on different shortest path parameters for 20,000 instances (validation and test set).

| EDGES | MEAN | MIN | MAX | UP-MEAN |
|-------|------|-----|-----|--------|
| RAND  | 4.363| 0.553| 0.065| 1.848  |
| UNIT  | 2.225| 1.154| 0.129| 3.217  | 1.000  |

6.1 Experimental Setup

We generated 100,000 instances of the SSMTSP problem using the random model described in Section 2.3 with \( n = 1000 \) nodes, edge probability \( p = c/n \) with \( c = 8 \), and target probability \( q = f/n \) with \( f = 20 \). The edge weights were chosen independently uniformly at random from \([0, 1]\). Further, we fixed the length of the constructed traces to \( i_0 = 10 \). We only accepted an instance if DIJKSTRA-PRUNING executed more than \( i_0 \) iterations to ensure that DIJKSTRA-PREDICTION reaches the point where a prediction is made. This set of 100,000 instances was split into a training set of 80,000 instances used for building the machine learning models, a validation set of 10,000 instances used for parameter tuning and a test set of 10,000 instances used for the final experiments.

To get an idea of a few parameters related to the shortest path distance in the generated instances, we provide some statistical data for the validation and test set in Table 1. We computed the average number of edges on a shortest path, the average, minimum and maximum cost of a shortest path, and the average weight of an edge on a shortest path. Note that the first row refers to these parameters with respect to the actual random weights, while the second row refers to the case when all edge weights are set to 1.

6.2 Machine Learning Results

For each of the 80,000 graphs in the training set, we executed a run of DIJKSTRA-PRUNING, during which we stored both the features \( X \) and the final returned shortest path distance \( y \). After running this, we had a training set of 80,000 samples, where each sample was of shape \((X, y)\). We used these 80,000 samples to built both a neural network and a linear regression model (as described in Section 5).

The number of nodes in the two hidden layers of the neural network was optimised by minimising the mean absolute error (MAE) in a \( k \)-fold cross validation with \( k = 4 \) and a batch size of 256. We tested layer sizes 8, 16, 32, 64 and 128; see Figure 2 for the results. We decided to use 16 nodes per layer and train for 47 epochs. We did not use the validation set of 10,000 instances in the \( k \)-fold cross validation, since it was used to tune parameters \( \alpha \) and \( \beta \). The results for the performance of the neural network, linear regression and the benchmark are given in Table 2. Both machine learning models perform better than the benchmark prediction, in both the training and test set. Moreover, the neural network outperforms the linear regression model on both the training and the test set.

6.3 Benchmark Algorithm ORACLE

In order to assess the performance of the different algorithms, we decided to use the following (idealised) benchmark algorithm to compare against: We run DIJKSTRA-PRUNING with the pruning bound \( B \) being initialised with the actual shortest path distance \( D \). We refer to this algorithm as ORACLE.

Note that this algorithm only inserts nodes into the priority queue which are necessary for finding the shortest path distance \( D \). Said differently, the algorithm spends the
minimum possible amount of work to provide a “certificate” of optimality for the shortest path distance $D$; no other algorithm could spend less work (as long as we insist that the shortest path distance is computed correctly always).

### 6.4 Discussion of Results

We start by considering how the queue sizes differ for the different algorithms; see Figure 3 (top layer, three distinctive instances). As to be expected, the queue size of Dijkstra-Prediction with Smart-Restart is always between the ones of Dijkstra-Pruning and Oracle. The improvement of our Dijkstra-Prediction with respect to Dijkstra-Pruning varies and depends on the instance. Next, we comment on the efficiency of the different restarting procedures; see Figure 3 (middle layer, three figures for same instance). On the left, we see Dijkstra-Prediction needed to do a Smart-Restart after (roughly) 85 iterations because the initial prediction turned out to be too small. In the middle, we see the difference between the restart procedure Naive-Restart and Smart-Restart. Observe that Naive-Restart starts from scratch (queue size drops to 0); while Smart-Restart only adds some nodes from the reserve list (queue size increases) and continues. On the right, we clearly see that the prediction obtained after $i_0 = 10$ iterations was too low, triggering a restart later on. However, the inflation with $\beta$ was sufficient to find the shortest path distance in the second trial. This plot also indicates
Fig. 3: (In all plots the $x$-axis refers to the number of iterations.) Top layer (three distinctive instances): Queue size of the algorithms. Middle layer (same instance): Queue size of the algorithms (left) with different restart procedures (middle), and distance $d(u)$ together with $B$ and $P$ (right) for the smart algorithm. Bottom layer (same instance): Queue size for fixed $\beta = 1.3$ and varying $\alpha$ (left) and fixed $\alpha = 1.4$ and varying $\beta$ (right) for the smart algorithm.
Table 3: Average number of queue operations, number of trials and cumulative queue sizes for Dijkstra, Dijkstra-Pruning, Dijkstra-Prediction with Smart-Restart and Naive-Restart and the oracle algorithm for the test set.

|          | Oracle | Dijkstra Prune | Smart | Naive |
|----------|--------|----------------|-------|-------|
| RM       | 59.39  | 59.39          | 59.39 | 59.39 | 152.77 |
| IS       | 59.39  | 335.50         | 122.91| 91.73 | 186.53 |
| DP       | 0.78   | 43.96          | 5.87  | 2.89  | 3.37   |
| Q        | 119.55 | 438.85         | 188.17| 154.01| 342.66 |
| T        | 1.00   | 1.00           | 1.00  | 2.28  | 2.28   |
| Ĉ         | 1456   | 13949          | 5246  | 2476  | 4973   |
| ĉ         | 1.00   | 9.57           | 3.60  | 1.70  | 3.42   |

the interplay of the prediction $P$ and the pruning bound $B$; first the former and later the latter providing the better bound.

If we zoom in to obtain a more fine-grained picture of the different queue operations executed by the algorithms, the results are as specified in Table 3 (test set). The respective rows state the number of REMOVE-MIN (RM), INSERT (IS) and DECREASE-PRIOR (DP) operations, the total number of queue operations (Q), the number of trials (T), the cumulative queue size $C$ (over all iterations), and the cumulative queue size relative to the Oracle $\bar{C}$. As to be expected, Oracle inserts and removes the minimum possible number of nodes only. Also, as we already inferred from Invariant 1 before, Dijkstra, Dijkstra-Pruning and Dijkstra-Prediction with Smart-Restart have the same number of REMOVE-MIN operations, whereas Dijkstra-Prediction with Naive-Restart needs many more.

Observe that the results show that our algorithm Dijkstra-Prediction with Smart-Restart outperforms all other algorithms, both in terms of the total number of queue operations and cumulative queue size. The smart algorithm outperforms Dijkstra-Pruning mostly on the number of insertions, as expected from the analysis in Section 4. In terms of cumulative queue size, our algorithm Dijkstra-Prediction with Smart-Restart even comes close to the benchmark Oracle, the average cumulative queue size being only 1.7 times larger then the one of Oracle (which is impossible to achieve); both Dijkstra-Prediction with Naive-Restart and Dijkstra-Pruning perform much worse, being off by factors 3.42 and 3.6, respectively.

6.5 Parameter Tuning

There are two parameters in the restarting procedures which decide how to handle the machine learning prediction. The first one is $\alpha$, which specifies the amount by which the initial prediction is inflated. The second one is $\beta$, the amount by which the prediction is inflated due to a restart. We investigate the impact of these parameters on the queue size; see Figure 3 (bottom layer, both figures for same instance). On the left, we fix $\beta = 1.3$ and vary $\alpha$; on the right we fix $\alpha = 1.4$ and vary $\beta$. As is visible from these plots, a larger $\alpha$ means that the first restart occurs later. Also, a larger $\beta$ leads to a large number of nodes inserted during a restart.

We tested several configurations for $\alpha$ and $\beta$ on the instances in the validation set. Table 4 and Table 5 state the respective number of queue operations $Q$ and the cumulative queue size $C$ for various choices. As it turns out, for both these performance indicators it is best to choose $\alpha$ and $\beta$ small.
Table 4: Average number of queue operations (Q) for Dijkstra-Prediction with Smart-Restart for different values of $\alpha$ and $\beta$ on the validation set.

| $\alpha$ \ $\beta$ | 1.05 | 1.10 | 1.20 | 1.50 | 2.00 |
|---------------------|------|------|------|------|------|
| 1.00                | 153.08 | 153.59 | 154.90 | 158.55 | 160.20 |
| 1.05                | 154.37 | 154.80 | 155.83 | 158.08 | 158.84 |
| 1.10                | 156.06 | 156.37 | 157.06 | 158.39 | 158.74 |
| 1.20                | 160.38 | 160.82 | 161.20 | 161.30 | 161.30 |
| 1.50                | 172.57 | 172.58 | 172.58 | 172.61 | 172.61 |
| 2.00                | 182.27 | 182.27 | 182.27 | 182.27 | 182.27 |

Table 5: Average cumulative queue size (C) for Dijkstra-Prediction with Smart-Restart for different values of $\alpha$ and $\beta$ on the validation set.

| $\alpha$ \ $\beta$ | 1.05 | 1.10 | 1.20 | 1.50 | 2.00 |
|---------------------|------|------|------|------|------|
| 1.00                | 2446.0 | 2561.9 | 2740.4 | 3115.7 | 3274.6 |
| 1.05                | 2573.5 | 2669.2 | 2815.5 | 3067.5 | 3150.1 |
| 1.10                | 2732.6 | 2805.3 | 2914.2 | 3065.1 | 3104.4 |
| 1.20                | 3112.6 | 3148.4 | 3197.7 | 3251.9 | 3266.3 |
| 1.50                | 4104.3 | 4106.6 | 4109.5 | 4114.2 | 4114.2 |
| 2.00                | 4809.9 | 4809.9 | 4809.9 | 4809.9 | 4809.9 |

### 6.6 Fine-grained Results for Different Algorithms

We present some more fine-grained results for all algorithms in Table 6. In addition to the basic queue operations stated in Table 3, we also keep track of various other operations. The meaning of the labels are as follows: INR indicates the number of nodes that are inserted into but never removed from the priority queue. RRM1 is the number of nodes that are moved from $R$ to PQ not due to a restart, while RRM2 is the number of nodes that are moved from $R$ to PQ due to a restart (batch insertion). RIS is the number of nodes added to $R$ and RDP is the number of times the distance of a node in $R$ is updated.

The number of nodes that are inserted into but never removed from the queue (INR) is where one would expect the most savings by our Dijkstra-Prediction algorithms (see also Section 4). The experiments indeed confirm this: our algorithm saves a significant fraction of these operations (both with Smart-Restart and Naive-Restart) compared to Dijkstra-Pruning (which in turn already saves a large fraction of these operations with respect to Dijkstra). In the Dijkstra-Prediction with Smart-Restart algorithm, some extra book-keeping needs to happen in order to perform the restart. For our test set, there are approximately $\sim$46 insertions into $R$ and $\sim$15 moves from a node from $R$ to PQ. The amount of extra work that is needed to realise the book-keeping necessary for Smart-Restart (see rows RRM1, RRM2, RIS and RDP) is not very significant and seems acceptable given the overall better performance. Finally, the alternative prediction means based on BFS are inferior to the machine learning approach, both for BFS and $w$-BFS.

### 7 Conclusion

We proposed an algorithm in which a ML prediction of a shortest path further reduces the search space explored by Dijkstra’s algorithm. The universal idea of using a ML viewpoint to augment CO algorithms works in the case of the SSMTSP, and we believe that this combination can be successfully applied in other problems as well.
Table 6: Average number of various operations of the algorithms and using different prediction algorithms (ML, BFS, $w$-BFS).

|       | ORACLE | Dijks | Prune | Smart | Naive | BFS  | $w$-BFS |
|-------|--------|-------|-------|-------|-------|------|---------|
| $RM$  | 59.39  | 59.39 | 59.39 | 59.39 | 152.77| 59.39| 59.39   |
| $IS$  | 59.39  | 335.50| 122.91| 91.73 | 186.53| 117.66| 118.86  |
| $INR$ | 0.00   | 276.12| 63.53 | 32.34 | 33.76 | 58.27| 59.47   |
| $DP$  | 0.78   | 43.96 | 5.87  | 2.89  | 3.37  | 5.29 | 5.46    |
| $RRM1$| 0.00   | 0.00  | 0.00  | 0.82  | 0.00  | 0.45 | 0.33    |
| $RRM2$| 0.00   | 0.00  | 0.00  | 14.05 | 0.00  | 1.30 | 0.00    |
| $RIS$ | 0.00   | 0.00  | 0.00  | 46.06 | 0.00  | 7.00 | 4.39    |
| $RDP$ | 0.00   | 0.00  | 0.00  | 2.16  | 0.00  | 0.14 | 0.08    |
| $Q$   | 119.55 | 438.85| 188.17| 154.01| 342.66| 182.33| 183.70  |
| $T$   | 1.00   | 1.00  | 1.00  | 2.28  | 2.28  | 1.23 | 1.00    |
| $C$   | 1456.16| 13949.37| 5245.96| 2476.35| 4973.46| 4825.09| 4980.69 |
| $ar{C}$ | 1.00   | 9.58  | 3.60  | 1.70  | 3.42  | 3.31 | 3.42    |
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