Sample Complexity of Learning Heuristic Functions for Greedy-Best-First and A* Search

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Abstract

Greedy best-first search (GBFS) and A* search (A*) are popular algorithms for path-finding on large graphs. Both use so-called heuristic functions, which estimate how close a vertex is to the goal. While heuristic functions have been handcrafted using domain knowledge, recent studies demonstrate that learning heuristic functions from data is effective in many applications. Motivated by this emerging approach, we study the sample complexity of learning heuristic functions for GBFS and A*.

We build on a recent framework called data-driven algorithm design and evaluate the pseudo-dimension of a class of utility functions that measure the performance of parameterized algorithms. Assuming that a vertex set of size \( n \) is fixed, we present \( O(n \log n) \) and \( O(n^2 \log n) \) upper bounds on the pseudo-dimensions for GBFS and A*, respectively, parameterized by heuristic function values. The upper bound for A* can be improved to \( O(n^2 \log d) \) if every vertex has a degree of at most \( d \) and to \( O(n \log n) \) if edge weights are integers bounded by \( \text{poly}(n) \). We also give \( \Omega(n) \) lower bounds for GBFS and A*, which imply that our bounds for GBFS and A* under the integer-weight condition are tight up to a \( \log n \) factor. Finally, we discuss a case where the performance of A* is measured by the suboptimality and show that we can sometimes obtain a better guarantee by combining a parameter-dependent worst-case bound with a sample complexity bound.

1 Introduction

Given a graph with a start vertex \( s \), a goal vertex \( t \), and non-negative edge weights, we consider finding an \( s \)-\( t \) path with a small total weight. The Dijkstra algorithm [16] finds an optimal path by exploring all vertices that are as close to \( s \) as \( t \). It, however, is sometimes impractical for large graphs since exploring all such vertices is too costly. Heuristic search algorithms are used to address such situations; among them, greedy best-first search (GBFS) [17] and A* search (A*) [24] are two popular algorithms. Both GBFS and A* use so-called heuristic functions, which estimate how close an input vertex is to \( t \). GBFS/A* attempts to avoid redundant exploration by scoring vertices based on heuristic function values and iteratively expanding vertices with the smallest score. If well-suited heuristic functions are available, GBFS/A* can run much faster than the Dijkstra algorithm. Furthermore, if A* uses an admissible heuristic function, i.e., it never overestimates the shortest-path distance to \( t \), it always finds an optimal path [24]. Traditionally, heuristic functions have been made based on domain knowledge; e.g., if graphs are road networks, the Euclidean distance gives an admissible heuristic.

When applying GBFS/A* to various real-world problems, a laborious process is to handcraft heuristic functions. Learning heuristic functions from data can be a promising approach to overcoming the obstacle due to the recent development of technologies for collecting graph data. Researchers have demonstrated the effectiveness of this approach in robotics [11, 32, 28, 36], computational organic chemistry [13], and pedestrian trajectory prediction [36]. With learned heuristic functions, however,
obtaining theoretical guarantees is difficult since we can hardly understand how the search can be guided by such heuristic functions. (A recent paper [1] studies learning of admissible heuristics for A*, but the optimality is confirmed only empirically.) Moreover, learned heuristic functions may be overfitting to problem instances at hand. That is, even if GBFS/A* with learned heuristic functions perform well over training instances, they may deliver poor future performance. In summary, the emerging line of work on search algorithms with learned heuristic functions is awaiting a theoretical foundation for guaranteeing their performance in a data-driven manner. Thus, a natural question is: how many sampled instances are needed to learn heuristic functions with generalization guarantees on the performance of resulting GBFS/A*?

1.1 Our contribution

We address the above question, assuming that path-finding instances defined on a fixed vertex set of size $n$ are drawn i.i.d. from an unknown distribution. Our analysis is based on so-called data-driven algorithm design [22, 4], a PAC-learning framework for bounding the sample complexity of algorithm configuration. In the analysis, the most crucial step is to evaluate the pseudo-dimension of a class of utility functions that measure the performance of parameterized algorithms. We study the case where GBFS/A* is parameterized by heuristic function values and make the following contributions:

1. Section 3 gives $O(n \lg n)$ and $O(n^2 \lg n)$ upper bounds on the pseudo-dimensions for GBFS and A*, respectively. The bound for A* can be improved to $O(n^2 \lg d)$ if every vertex has an at most $d$ degree and to $O(n \lg n)$ if edge weights are non-negative integers at most poly($n$).

2. Section 4 presents $\Omega(n)$ lower bounds on the pseudo-dimensions for GBFS and A*. We prove this result by constructing $\Omega(n)$ instances with unweighted graphs. Thus, our bounds for GBFS and A* under the integer edge-weight condition are tight up to a $\lg n$ factor.

3. Section 5 studies a particular case of bounding the suboptimality of A*. We show that we can sometimes improve the guarantee obtained in Section 3 by using an alternative $O(n \lg n)$ bound on the pseudo-dimension of a class of parameter-dependent worst-case bounds [34].

An important consequence of the above results is the tightness up to a $\lg n$ factor for GBFS and A* under the integer-weight assumption. Note that this assumption holds in various realistic situations. For example, the Internet network and state-space graphs of games are unweighted (unit-weight) graphs, and A* is often applied to path-finding instances on such graphs.

1.2 Related work

Data-driven algorithm design. Gupta and Roughgarden [22] proposed a PAC approach for bounding the sample complexity of algorithm configuration, which is called data-driven algorithm design and has been applied to a broad family of algorithms, including greedy, clustering, and sequence alignment algorithms. We refer the reader to a nice survey [4]. A recent line of work [5, 9, 10] has extensively studied the sample complexity of configuring integer-programming methods, e.g., branch-and-bound and branch-and-cut. In [9, 10], upper bounds on the pseudo-dimension for general tree search are presented, which are most closely related to our results. Our upper bounds, which are obtained by using specific properties of GBFS/A*, are better than the previous bounds for general tree search, as detailed in Appendix A. Balcan et al. [8] presented a general framework for evaluating the pseudo-dimension. Their idea is to suppose that performance measures form a class of functions of algorithm parameters, called dual functions, and characterize its complexity based on how they are piecewise structured. This idea plays a key role in the analysis of [9, 10], and our analysis of the upper bounds are also inspired by their idea. Its application to our setting, however, requires a close look at the behavior of GBFS/A*. Balcan et al. [7] showed that approximating dual functions with simpler ones is useful for improving sample complexity bounds, which is similar to our idea in Section 5. A difference is that while they construct simpler functions with a dynamic programming algorithm, we can use a known worst-case bound on the suboptimality of best-first search [34]. Lower bounds on the pseudo-dimension for graph-search algorithms have not been well studied.

Heuristic search with learning. Eden et al. [18] theoretically studied how the average-case running time of A* can be affected by the dimensions or bits of learned embeddings or labels of vertex features, based on which heuristic function values and computed. The sample complexity of learning heuristic functions, however, has not been studied.
2 Preliminaries

We present the background on learning theory and our problem setting. In what follows, we let \( \mathbb{I}(\cdot) \) be a boolean function that returns 1 if its argument is true and 0 otherwise. We use \( \mathcal{H} \subseteq \mathbb{R}^\mathcal{Y} \) to denote a class of functions that map \( \mathcal{Y} \) to \( \mathbb{R} \). For any positive integer \( m \), we let \( [m] = \{1, \ldots, m\} \).

2.1 Background on learning theory

The following pseudo-dimension \([29]\) is a fundamental notion for quantifying the complexity of a class of real-valued functions.

**Definition 1.** Let \( \mathcal{H} \subseteq \mathbb{R}^\mathcal{Y} \) be a class of functions that map some domain \( \mathcal{Y} \) to \( \mathbb{R} \). We say a set \( \{y_1, \ldots, y_N\} \subseteq \mathcal{Y} \) is shattered by \( \mathcal{H} \) if there exist target values, \( t_1, \ldots, t_N \in \mathbb{R} \), such that

\[
|\{ (\mathbb{I}(h(y_1) \geq t_1), \ldots, \mathbb{I}(h(y_N) \geq t_N)) \mid h \in \mathcal{H} \}| = 2^N.
\]

The pseudo-dimension of \( \mathcal{H} \), denoted by \( \text{Pdim}(\mathcal{H}) \), is the size of a largest set shattered by \( \mathcal{H} \).

If \( \mathcal{H} \) is a set of binary-valued functions that map \( \mathcal{Y} \) to \{0, 1\}, the pseudo-dimension of \( \mathcal{H} \) coincides with the so-called VC-dimension \([35]\), which is denoted by \( \text{VCdim}(\mathcal{H}) \).

The following proposition enables us to obtain sample complexity bounds by evaluating the pseudo-dimension (see, e.g., \([2, \text{Theorem 19.2}] \) and \([27, \text{Theorem 11.8}] \)).

**Proposition 1.** Let \( H > 0, \mathcal{H} \subseteq [0, H]^\mathcal{Y} \), and \( \mathcal{D} \) be a distribution over \( \mathcal{Y} \). For any \( \delta \in (0, 1) \), with a probability of at least \( 1 - \delta \) over the i.i.d. draw of \( \{y_1, \ldots, y_N\} \sim \mathcal{D}^N \), for all \( h \in \mathcal{H} \), it holds that

\[
\left| \frac{1}{N} \sum_{i=1}^{N} h(y_i) - \mathbb{E}_{y \sim \mathcal{D}}[h(y)] \right| = O \left( H \sqrt{\frac{\text{Pdim}(\mathcal{H}) \log N}{N} + \frac{1}{N}} \right).
\]

In other words, for any \( \epsilon > 0 \), \( N = \Omega \left( \frac{H^2}{\epsilon^2} (\text{Pdim}(\mathcal{H}) \log \frac{H}{\epsilon} + \log \frac{1}{\delta}) \right) \) sampled instances are sufficient to ensure that with a probability of at least \( 1 - \delta \), for all \( h \in \mathcal{H} \), the difference between the empirical average and the expectation over an unknown distribution \( \mathcal{D} \) is at most \( \epsilon \).

2.2 Problem formulation

We describe path-finding instances, GBFS/A* algorithm, and performance measures considered in this paper.

**Path-finding instances.** We consider solving randomly generated path-finding instances repetitively. Let \( x = (V, E, \{w_e\}_{e \in E}, s, t) \) be a path-finding instance, where \((V, E)\) is a simple directed graph with \( n \) vertices, \( \{w_e\}_{e \in E} \) is a set of non-negative edge weights (sometimes called costs), \( s \in V \) is a start vertex, and \( t \in V \) is a goal vertex. We let \( \Pi \) be a class of possible instances. Each instance \( x \in \Pi \) is drawn from an unknown distribution \( \mathcal{D} \) over \( \Pi \). We impose the following assumption on \( \Pi \).

**Assumption 1.** For all \( x \in \Pi \), the vertex set \( V \) and the goal node \( t \) are identical, and there always exists at least one directed path from \( s \neq t \) to \( t \), i.e., every instance \( x \in \Pi \) is feasible.

Fixing \( V \) is necessary for evaluating the pseudo-dimension in terms of \( n = |V| \). Note that we can deal with the case where some instances in \( \Pi \) are defined on vertex subsets \( V' \subset V \) by removing edges adjacent to \( V \setminus V' \). The feasibility assumption is needed to ensure that GBFS/A* always returns a solution, and \( s \neq t \) simply rules out the trivial case where the empty set is optimal. In Appendix B, we discuss how to extend our results to the case where \( t \) can change depending on instances.

**Algorithm description.** We sketch algorithmic procedures that are common to both GBFS and A* (see Algorithms 1 and 2 for details, respectively). Let \( A_p \) be a GBFS/A* algorithm, which is parameterized by heuristic function values \( p \in \mathbb{R}^n \). Given an instance \( x \in \Pi \), \( A_p \) starts from \( s \) and iteratively builds a set of candidate paths. These paths are maintained by \( \text{OPEN} \) and \( \text{CLOSED} \) lists, together with pointers \( p(\cdot) \) to parent vertices. The \( \text{OPEN} \) list contains vertices to be explored, and the \( \text{CLOSED} \) list consists of vertices that have been explored. In each iteration, we select a vertex \( v \) from \( \text{OPEN} \), expand \( v \), and move \( v \) from \( \text{OPEN} \) to \( \text{CLOSED} \).
Heuristic function values $\rho$ are used when selecting vertices. For each $v \in V$, the corresponding entry in $\rho$, denoted by $\rho_v$, represents an estimated shortest-path distance from $v$ to $t$. (Although heuristic function values are usually denoted by $h(v)$, we here use $\rho_v$ for convenience.) In each iteration, we select a vertex with the smallest score, which is defined based on $\rho$ as detailed later. We impose the following assumption on the vertex selection step.

**Assumption 2.** Define an arbitrary strict total order on $V$; for example, we label elements in $V$ by $v_1, \ldots, v_n$ and define a total order $v_1 < \cdots < v_n$. When selecting a vertex with the smallest score, we break ties, if any, in favor of the smallest vertex with respect to the total order.

If we allow $A_\rho$ to break ties arbitrarily, its behavior becomes too complex to obtain meaningful bounds on the pseudo-dimension. Assumption 2 is a natural rule to exclude such troublesome cases.

**Performance measure.** Let $A_\rho$ be GBFS/A* with parameters $\rho \in \mathbb{R}^n$. We measure performance of $A_\rho$ on $x \in \Pi$ with a utility function $u$. We assume $u$ to satisfy the following condition.

**Assumption 3.** Let $H > 0$. A utility function $u$ takes $x$ and a series of all OPEN, CLOSED, and $p(\cdot)$ generated during the execution of $A_\rho$ on $x \in \Pi$ as input, and returns a scalar value in $[0, H]$.

We sometimes use $A_\rho$ to represent the series of OPEN and CLOSED lists and pointers generated by $A_\rho$. Note that $u$ meeting Assumption 3 can measure various kinds of performance. For example, since the pointers indicate an $s$-$t$ path returned by $A_\rho$, $u$ can represent its cost. Moreover, since the series of OPEN and CLOSED lists maintain all search states, $u$ can represent the time and space complexity of $A_\rho$. We let $u_\rho : \Pi \to [0, H]$ denote the utility function that returns the performance of $A_\rho$ on any $x \in \Pi$, and define a class of such functions as $U = \{ u_\rho : \Pi \to [0, H] \mid \rho \in \mathbb{R}^n \}$. The upper bound, $H$, is necessary to obtain sample complexity bounds with Proposition 1. Setting such an upper bound is usual in practice. For example, if $u$ measures the running time, $H$ represents a time-out deadline.

**Generalization guarantees on performance.** Given the above setting, we want to learn $\hat{\rho}$ values that attain an optimal $\mathbb{E}_{x \sim \mathcal{D}}[u_\hat{\rho}(x)]$ value, where available information consists of sampled instances $x_1, \ldots, x_N$ and $u_\rho(x_1), \ldots, u_\rho(x_N)$ values for any $\rho \in \mathbb{R}^n$. To obtain generalization guarantees on the performance of $A_\rho$, we bound $\frac{1}{N} \sum_{i=1}^N u_\rho(x_i) - \mathbb{E}_{x \sim \mathcal{D}}[u_\rho(x)]$ uniformly for all $\rho \in \mathbb{R}^n$. Note that the uniform bound offers performance guarantees that are independent of learning procedures, e.g., manual or automated (without being uniform, learned $\hat{\rho}$ may be overfitting sampled instances). As in Proposition 1, to bound the sample complexity of learning $\rho$ values, we need to evaluate the pseudo-dimension of $\mathcal{U}$, denoted by $\text{Pdim}(\mathcal{U})$, which is the main subject of this study.

**Remarks on heuristic functions.** While we allow heuristic function values $\rho$ to be any point in $\mathbb{R}^n$, the range of heuristic functions may be restricted to some subspace of $\mathbb{R}^n$. Note that our upper bounds are applicable to such situations since restricting the space of possible $\rho$ values does not increase $\text{Pdim}(\mathcal{U})$. Meanwhile, such restriction may be useful for improving the upper bounds on $\text{Pdim}(\mathcal{U})$; exploring this direction is left for future work. Also, our setting cannot deal with heuristic functions that take some instance-dependent features as input. To study such cases, we need more analysis that is specific to heuristic function models, which goes beyond the scope of this paper. Thus, we leave this for future work. Note that our setting still includes important heuristic function models on fixed vertex sets. For example, we can set $\rho$ using learned distances to landmarks [21], or we can let $\rho$ be distances measured on some metric space by learning metric embeddings of vertices [37].

### 3 Upper bounds on the pseudo-dimension

We present details of GBFS and A* and upper bounds on the pseudo-dimensions of $\mathcal{U}$. In this section, we suppose that vertices in $V$ are labeled by $v_1, \ldots, v_n$ as in Assumption 2.

#### 3.1 Greedy best-first search

Algorithm 1 shows the details of GBFS $A_\rho$ with heuristic function values $\rho \in \mathbb{R}^n$. When selecting vertices in Step 3, the scores are determined only by $\rho$. This implies an obvious but important fact.

**Lemma 1.** Let $\rho, \rho' \in \mathbb{R}^n$ be a pair of heuristic function values with an identical total order up to ties on their entries, i.e., $\Pi(\rho_v, \leq \rho_v') = \Pi(\rho'_v, \leq \rho'_v)$ for all $i, j \in [n]$ such that $i < j$. Then, we have $u_\rho(x) = u_{\rho'}(x)$ for all $x \in \Pi$.
Algorithm 1 GBFS with heuristic function values $\rho$

1: OPEN = $\{s\}$, CLOSED = $\emptyset$, and $p(s) = \text{None}$.
2: while OPEN is not empty :
3: \hspace{1em} $v \leftarrow \arg\min\{\rho_{v'} \mid v' \in \text{OPEN}\}$. \hspace{1em}$\triangleright$ Break ties as in Assumption 2.
4: \hspace{1em} for each child $c$ of $v$ :
5: \hspace{2em} if $c = t$ :
6: \hspace{3em} return $s$-$t$ path by tracing pointers $p(\cdot)$, where $p(t) = v$.
7: \hspace{2em} if $c \notin \text{OPEN} \cup \text{CLOSED}$ :
8: \hspace{3em} $p(c) \leftarrow v$ and OPEN $\leftarrow$ OPEN $\cup \{c\}$.
9: \hspace{1em} Move $v$ from OPEN to CLOSED.
10: end if
11: end for
12: end while

Algorithm 2 A* with heuristic function values $\rho$

1: OPEN = $\{s\}$, CLOSED = $\emptyset$, $p(s) = \text{None}$, and $g_s = 0$.
2: while OPEN is not empty :
3: \hspace{1em} $v \leftarrow \arg\min\{g_{v'} + \rho_{v'} \mid v' \in \text{OPEN}\}$. \hspace{1em}$\triangleright$ Break ties as in Assumption 2.
4: \hspace{1em} if $v = t$ :
5: \hspace{2em} return $s$-$t$ path by tracing pointers $p(\cdot)$.
6: \hspace{1em} for each child $c$ of $v$ :
7: \hspace{2em} $g_{\text{new}} \leftarrow g_v + w(v, c)$.
8: \hspace{2em} if $c \notin \text{OPEN} \cup \text{CLOSED}$ :
9: \hspace{3em} $g_c \leftarrow g_{\text{new}}$, $p(c) \leftarrow v$, and OPEN $\leftarrow$ OPEN $\cup \{c\}$.
10: \hspace{2em} else if $c \in \text{OPEN}$ and $g_{\text{new}} < g_c$ :
11: \hspace{3em} $g_c \leftarrow g_{\text{new}}$ and $p(c) \leftarrow v$.
12: \hspace{2em} else if $c \in \text{CLOSED}$ and $g_{\text{new}} < g_c$ :
13: \hspace{3em} Move $c$ from CLOSED to OPEN. \hspace{1em}$\triangleright$ Steps 12–14 are for reopening.
14: \hspace{1em} Move $v$ from OPEN to CLOSED.
15: end if
16: end for
17: end while

Proof. For any $x \in \Pi$, if $\rho$ and $\rho'$ have an identical strict total order on their entries, vertices selected in Step 3 are the same in each iteration of $A_\rho$ and $A_{\rho'}$. Since this is the only step $\rho$ and $\rho'$ can affect, we have $A_\rho = A_{\rho'}$ for all $x \in \Pi$, hence $u_\rho(x) = u_{\rho'}(x)$. Moreover, this holds even if $\rho$ and/or $\rho'$ have ties on their entries because of Assumption 2. That is, the total order uniquely determines a vertex selected in Step 3 even in case of ties. Therefore, the statement holds.

From Lemma 1, the behavior of GBFS is uniquely determined once a total order on $\{\rho_v\}_{v \in V}$ is fixed. Thus, for any $x \in \Pi$, the number of distinct $u_\rho(x)$ values is at most $n!$, the number of permutations of $\{\rho_v\}_{v \in V}$. This fact enables us to obtain an $O(n \log n)$ upper bound on the pseudo-dimension of $\mathcal{U}$.

Theorem 1. For GBFS $A_\rho$ with parameters $\rho \in \mathbb{R}^n$, it holds that $\text{Pdim}(\mathcal{U}) = O(n \log n)$.

Proof. Lemma 1 implies that we can partition $\mathbb{R}^n$ into $n!$ regions, $\mathcal{P}_1, \mathcal{P}_2, \ldots$, so that for every $\mathcal{P}_i$, any pair of $\rho, \rho' \in \mathcal{P}_i$ satisfies $u_\rho(x) = u_{\rho'}(x)$ for all $x \in \Pi$. Note that the construction of the regions, $\mathcal{P}_1, \mathcal{P}_2, \ldots$, does not depend on $x$. Thus, given any $N$ instances $x_1, \ldots, x_N$, even if $\rho$ moves over whole $\mathbb{R}^n$, the number of distinct tuples of form $(u_\rho(x_1), \ldots, u_\rho(x_N))$ is at most $n!$. To shatter $N$ instances, $n! \geq 2^N$ must hold. Solving this for the largest $N$ yields $\text{Pdim}(\mathcal{U}) = O(n \log n)$.

3.2 A* search

Algorithm 2 is the details of A*. As with GBFS, $\rho$ only affects the vertex selection step (Step 3). However, unlike GBFS, the scores, $g_v + \rho_v$, involve not only $\rho$ but also $\{g_v\}_{v \in V}$. Each $g_v$ is called a $g$-cost and maintains a cost of some path from $s$ to $v$. As in Algorithm 2, when $v$ is expanded and a shorter path to $c$ is found, whose cost is denoted by $g_{\text{new}}$, we update the $g_c$ value. Thus, each $g_v$ always gives an upper bound on the shortest-path distance from $s$ to $v$. For each $v \in V$, there are at most $\sum_{k=0}^{n-2} k! \leq (n-1)!$ simple paths connecting $s$ to $v$, and thus $g_v$ can take at most $(n-1)!$ distinct values. We denote the set of those distinct values by $G_v$, and define $G_v = \{(v, g_v) \mid v \in V, g_v \in G_v\}$ as the set of all pairs of a vertex and its possible $g$-cost. It holds that $|G_v| \leq n \times (n-1)! = n!$. 

5
Note that once \( x \in \Pi \) is fixed, \( G_e \) for \( v \in V \) and \( G_V \) are uniquely determined. To emphasize this fact, we sometimes use notation with references to \( x \): \( g_v(x), G_v(x) \), and \( G_V(x) \). As with the case of GBFS (Lemma 1), we can define a total order on the scores to determine the behavior of \( A^* \) uniquely.

**Lemma 2.** Fix any instance \( x \in \Pi \). Let \( \rho, \rho' \in \mathbb{R}^n \) be a pair of heuristic function values such that total orders on the sets of all possible scores, \( \{ g_v(x) + \rho, \{ g_v(x) \} \in G_V(x) \} \) and \( \{ g_v(x) + \rho'_v, \{ g_v(x) \} \in G_V(x) \} \), are identical up to ties. Then, it holds that \( u_\rho(x) = u_{\rho'}(x) \).

**Proof.** If the two sets of scores have an identical strict total order, we select the same vertex in Step 3 in each iteration of \( A_\rho \) and \( A_{\rho'} \). Thus, we have \( A_\rho = A_{\rho'} \) for any fixed \( x \), implying \( u_\rho(x) = u_{\rho'}(x) \). We show that this holds even in the presence of ties by using Assumption 2. First, any two scores of the same vertices, \( g_v(x) + \rho_v \) and \( g_v'(x) + \rho'_v \), never have ties since \( G_v \) consists of distinct \( q \)-costs. Next, if \( g_v(x) + \rho_v = g_v(x) + \rho_v' \) holds for some \( i < j \), we always prefer \( v_i \) to \( v_j \) in Step 3 due to Assumption 2. Therefore, even in the presence of ties, we select a vertex in Step 3 as if the set of possible scores, it holds that \( u_\rho(x) = u_{\rho'}(x) \).

By using Lemma 2, we can obtain an \( O(n^2 \lg n) \) upper bound on the pseudo-dimension of \( \mathcal{U} \).

**Theorem 2.** For \( A^* A_\rho \) with parameters \( \rho \in \mathbb{R}^n \), it holds that \( \text{Pdim}(\mathcal{U}) = O(n^2 \lg n) \).

**Proof.** As with the proof of Theorem 1, we partition \( \mathbb{R}^n \) into some regions so that in each region, the behavior of \( A^* \) is unique. Unlike the case of GBFS, boundaries of such regions change over \( N \) instances. To deal with this situation, we use a geometric fact: for \( m \geq n \geq 1 \), \( m \) hyperplanes partition \( \mathbb{R}^n \) into \( O((em)^n) \) regions.

Fix a tuple of any \( N \) instances \( (x_1, \ldots, x_N) \). We consider hyperplanes in \( \mathbb{R}^n \) of form \( g_v(x_k) + \rho_v = g_v(x_j) + \rho_v \) for all \( k \in [N] \) and all pairs of \( (v_i, g_v(x_k)), (v_j, g_v(x_j)) \in G_V \) such that \( i \neq j \). These hyperplanes partition \( \mathbb{R}^n \) into some regions, \( \mathcal{P}_1, \mathcal{P}_2, \ldots \), so that the following condition holds: for every \( \mathcal{P}_i \), any \( \rho, \rho' \in \mathcal{P}_i \) have the same total order on \( \{ g_v(x_k) + \rho_v, \{ g_v(x_k) \} \in G_V(x) \} \) and \( \{ g_v(x_k) + \rho'_v, \{ g_v(x_k) \} \in G_V(x) \} \) up to ties for all \( k \in [N] \), which implies \( u_\rho(x_k) = u_{\rho'}(x_k) \) for all \( k \in [N] \) due to Lemma 2. That is, for every \( k \in [N] \), if we see \( u_\rho(x_k) \) as a function of \( \rho \), it is piecewise constant where pieces are given by \( \mathcal{P}_1, \mathcal{P}_2, \ldots \). Therefore, when \( \rho \) moves over whole \( \mathbb{R}^n \), the number of distinct tuples of form \( (u_\rho(x_1), \ldots, u_\rho(x_N)) \) is at most the number of the pieces. Note that the pieces are generated by partitioning \( \mathbb{R}^n \) with \( \sum_{k \in [N]} (\binom{\mathbb{G}_V(x_k)}{2}) \) \( \leq N \binom{n^2}{2} \) hyperplanes, which means there are at most \( \text{O}(\left( eN \binom{n^2}{2} \right)^n) \) pieces. To shatter \( N \) instances, \( \text{O}(\left( eN \binom{n^2}{2} \right)^n) \geq 2^N \) is necessary. Solving this for the largest \( N \) yields \( \text{Pdim}(\mathcal{U}) = O(n^2 \lg n) \).

Compared with GBFS, the additional \( n \) factor comes from the bound of \( (n - 1)! \) on \( |G_e| \). This bound may seem too pessimistic, but it is almost tight in some cases, as implied by the following example.

**Example 1.** Let \( (V, E) \) be a complete graph with edges labeled as \( \{ e_1, \ldots, e_{|E|} \} \). Set each edge weight \( w_{e_i} \) to \( 2^{i-1} \) for \( i \in [|E|] \). Considering the binary representation of the edge weights, the costs of all simple \( s \rightarrow v \) paths are mutually different for \( v \in V \), which implies \( |G_v| = \sum_{k=0}^{n-2} k! \geq (n - 2)! \).

This example suggests that improving the \( O(n^2 \lg n) \) bound is not straightforward. Under some realistic assumptions, however, we can improve it by deriving smaller upper bounds on \( |G_v| \).

First, if the maximum degree of vertices is always bounded, we can obtain the following bound.

**Theorem 3.** Assume that the maximum out-degrees of directed graphs \( (V, E) \) of all instances in \( \Pi \) are upper bounded by \( d \). Then, it holds that \( \text{Pdim}(\mathcal{U}) = O(n^2 \lg d) \).

**Proof.** Under the assumption on the maximum degree, there are at most \( \sum_{k=0}^{n-2} d^k \leq (n - 1)d^{n-2} \) simple \( s \rightarrow v \) paths, which implies \( |G_v| \leq (n - 1)d^{n-2} \) for every \( v \in V \). Therefore, we have \( |G_V| \leq n \times (n - 1)d^{n-2} \). Following the proof of Theorem 2, we can obtain an upper bound on \( \text{Pdim}(\mathcal{U}) \) by solving \( \text{O}(\left( N^n \binom{n-1}{2}d^{n-2} \right)^n) \geq 2^N \) for the largest \( N \), which yields \( \text{Pdim}(\mathcal{U}) = O(n^2 \lg d) \).

---

1Even if some regions degenerate, from [23, Theorem 28.1.1] and [12, Proposition A2.1], the number of all \( d \)-dimensional regions for \( d = 0, \ldots, n \), is \( \sum_{d=0}^{n-1} \sum_{i=0}^{n} (\binom{n}{d}) (\binom{n}{i}) \leq 2^{e(m)^n} \). The fact has a close connection to Sauer’s lemma [30] (see [20]). In this sense, our analysis is in a similar spirit to the general framework of [8].
We show that for any \( s, r, t, \) or \( i \in [n - 3] \), as shown nearby the vertex circles. The values in vertex circles represent \( \rho \) that makes \( A_\rho \) return suboptimal paths to \( x_2 \) and \( x_3 \), i.e., \( S = \{2, 3\} \). The thick edges indicate returned paths.

Second, if edge weights are non-negative integers bounded by \( W \), we can obtain the following bound.

**Theorem 4.** Assume that edge weights \( \{w_e \}_{e \in E} \) of all instances in \( \Pi \) are non-negative integers bounded by a constant \( W \) from above. Then, it holds that \( \text{Pdim}(U) = O(n \lg(nW)) \).

**Proof.** Under the assumption, every \( g \)-cost \( g_v \) takes a non-negative integer value at most \( nW \). Since \( G_v \) consists of distinct \( g \)-cost values, \( |G_v| \leq nW \) holds, hence \( |G_v| \leq n^2W \). Solving \( O\left( N^n\left(\frac{n^2W}{2}\right)^n\right) \geq 2^N \) for the largest \( N \), we obtain \( \text{Pdim}(U) = O(n \lg(nW)) \).

Note that if \( W = O(\text{poly}(n)) \) holds, we have \( \text{Pdim}(U) = O(n \lg n) \).

**On reopening.** \( A^\ast \) is usually allowed to reopen closed vertices as in Steps 12–14. This, however, causes \( \Omega(2^n) \) iterations in general [26], albeit always finite [33]. A popular workaround is to simply remove Steps 12–14, and such \( A^\ast \) without reopening has also been extensively studied [34, 31, 14, 15].

Note that our results are applicable to \( A^\ast \) both with and without reopening.

### 4 Lower bounds on the pseudo-dimension

We present lower bounds on the pseudo-dimension for GBFS/A*. We prove the result by constructing \( \Omega(n) \) shatterable instances with unweighted graphs. Therefore, the \( O(n \lg n) \) upper bounds for GBFS (Theorem 1) and \( A^\ast \) under the edge-weight assumption (Theorem 4) are tight up to a \( \lg n \) factor.

**Theorem 5.** For GBFS/A* \( A_\rho \) with parameters \( \rho \in \mathbb{R}^n \), it holds that \( \text{Pdim}(U) = \Omega(n) \).

**Proof.** We construct a series of \( n - 4 \) instances, \( x_1, \ldots, x_{n-4} \), that can be shattered by \( U \), where each \( u_i \) returns the length of an \( s-t \) path found by \( A_{\rho} \). We label vertices in \( V \) by \( s, r, t, \) or \( i \in [n - 3] \).

See Figure 1 for an example with \( n = 8 \). For each \( x_i \) \( (i \in [n - 4]) \), we draw edges \( (s, v) \) for \( v \in M \) and \( (v, t) \) for \( v \in \{v' \in M \mid v' > i \} \), which constitute optimal \( s-t \) paths of length 2. In addition, for each \( x_i \), we draw edges \( (i, r) \) and \( (r, t) \), where \( s \rightarrow i \rightarrow r \rightarrow t \) is the only suboptimal path of length 3. Letting \( t_i = 2.5 \) for \( i \in [n - 4] \), we prove that \( U \) can shatter those \( n - 4 \) instances, i.e., \( A_{\rho} \) can return suboptimal solutions to any subset of \( \{x_1, \ldots, x_{n-4}\} \) by appropriately setting \( \rho \).

Let \( S \subseteq [n - 4] \) indicate a subset of instances, to which we will make \( A_{\rho} \) return suboptimal solutions. We show that for any \( S \), we can set \( \rho \) so that \( A_{\rho} \) returns \( s \rightarrow i \rightarrow r \rightarrow t \) to \( x_i \) if and only if \( i \in S \). We refer to the vertex labeled by \( n - 3 \) as \( m \), which we use to ensure that every instance has an optimal path \( s \rightarrow m \rightarrow t \). We set \( \rho \) as follows: \( \rho_s = n \) (or an arbitrary value), \( \rho_r = \rho_t = 0 \), \( \rho_i = i + 2 \) if \( i \in S \), and \( \rho_i = n \) (or a sufficiently large value) if \( i \in [n - 4] \setminus S \). If \( A_{\rho} \) with this \( \rho \) is applied to \( x_i \), it iteratively selects vertices in \( S \cup \{m\} \) in increasing order of their labels until a vertex that has a child is selected. Once a vertex with a child is expanded, it ends up returning \( s \rightarrow i \rightarrow r \rightarrow t \) if \( i \in S \) and \( s \rightarrow v \rightarrow t \) for some \( v > i \) if \( i \notin S \). We below confirm this more precisely, separately for GBFS and \( A^\ast \).

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**Figure 1:** An illustration of the instances \( x_1, \ldots, x_{n-4} \) for \( n = 8 \). Each vertex is labeled by \( s, r, t, \) or \( i \in [n - 3] \), as shown nearby the vertex circles. The values in vertex circles represent \( \rho \) that makes \( A_{\rho} \) return suboptimal paths to \( x_2 \) and \( x_3 \), i.e., \( S = \{2, 3\} \). The thick edges indicate returned paths.
GBFS. We consider applying GBFS $A_\rho$ to $x_i$. $A_\rho$ first expands $s$ and adds vertices in $M$ to OPEN. Since vertices in $v \in [n - 4] \setminus S$ have sufficiently large scores of $n$, they are never selected before any vertex in $S \cup \{m\}$. Thus, $A_\rho$ selects a vertex from $S \cup \{m\}$ with the smallest score. If the selected vertex, denoted by $v$, satisfies $v < i$, there is no child of $v$; hence, nothing is added to OPEN, and we go back to Step 3. In this way, $A_\rho$ iteratively moves $v \in S \cup \{m\}$ that has no child from OPEN to CLOSED. Consider the first time when the selected vertex $v \in S \cup \{m\}$ has a child $c$ (this situation is guaranteed to occur since $m$ always has a child). If $i \notin S$, we have $v \neq i$ since $v$ is selected from $S \cup \{m\}$. Then, since $v$’s child is $c = t$, $A_\rho$ returns $s \rightarrow v \rightarrow t$ with $v \neq i$. If $i \in S$, then $i$ has the smallest score ($\rho_i = i + 2$) among all vertices in $S \cup \{m\}$ that have a child. Thus, $A_\rho$ selects $i$ and opens $r$. Now, $r$ has the smallest score of $\rho_r = 0$. Therefore, $A_\rho$ selects $r$ and reaches $t$, returning $s \rightarrow i \rightarrow r \rightarrow t$. Consequently, $A_\rho$ returns the suboptimal path if and only if $i \in S$.

A*. It first expands $s$ and add $M$ to OPEN. Since $g_v = 1$ for all $v \in M$, only $\rho$ values matter when comparing the scores, as with the case of GBFS. Therefore, A* iterates to move vertices in $S \cup \{m\}$ from OPEN to CLOSED until a vertex that has a child is selected. Consider the first time a selected vertex $v$ has a child $c$ (so far, $s$ is not reopened since $g_s = 0$). As with the case of GBFS, we have $v \neq i$ and $c = t$ if $i \notin S$, or $v = i$ and $c = r$ if $i \in S$. Now, every $v' \in OPEN \setminus \{c\}$ has a score of at least 4 since $g_{v'} = 1$ and $\rho_{v'} \geq 3$ for $v' \in M$. Therefore, if $i \notin S$, $t \in OPEN$ has the smallest score of $g_t + \rho_t = 2 + 0 = 2$. Thus, $A_\rho$ next selects $t$ and returns $s \rightarrow v \rightarrow t$, where $v \neq i$. If $i \in S$, since $r \in OPEN$ has the smallest score of $g_r + \rho_r = 2 + 0 = 2$, $A_\rho$ selects $r$ and opens $t$; then, since $t$ has the score of $g_t + \rho_t = 3 + 0 = 3$, $A_\rho$ selects $t$ and returns $s \rightarrow i \rightarrow r \rightarrow t$. To conclude, $A_\rho$ returns the suboptimal path if and only if $i \in S$.

5 Toward better guarantees on the suboptimality of A*

Given the results in Sections 3 and 4, a major open problem is to close the $O(n)$ gap between the $O(n^2 \lg n)$ upper bound and the $\Omega(n)$ lower bound for A* in general cases. This problem seems very complicated, as we will discuss in Section 6. Instead, we here study a particular case where we want to bound the expected suboptimality of A*, which is an important performance measure since learned heuristic values are not always admissible. We show that a general bound obtained from Theorem 2 can be sometimes improved by using a $\rho$-dependent worst-case bound [34].

For any $x \in I$, let $Opt(x)$ and $Cost_\rho(x)$ be the costs of an optimal solution and an $s$–$t$ path returned by $A_\rho$, respectively, and let $u_\rho(x) = Cost_\rho(x) - Opt(x)$ be the suboptimality. From Theorem 2 and Proposition 1, we can obtain the following high-probability bound on the expected suboptimality:

$$\mathbb{E}_{x \sim D}[Cost_\rho(x) - Opt(x)] \leq \frac{1}{N} \sum_{i=1}^{N} (Cost_\rho(x) - Opt(x)) + \tilde{O}\left(\sqrt{\frac{n^2 + \lg \frac{1}{\delta}}{N}}\right).$$ (1)

That is, the expected suboptimality can be bounded from above by the empirical suboptimality over the $N$ training instances (an empirical term) plus an $\tilde{O}(\sqrt{\frac{n^2}{N}})$ term (a complexity term). While this bound is useful when $N \gg n^2$, we may not have enough training instances in practice. In such cases, the complexity term becomes dominant and prevents us from obtaining meaningful guarantees. In what follows, we present an alternative bound of the form “an empirical term + a complexity term” that can strike a better balance between the two terms when $N$ is not large enough relative to $n^2$.

To this end, we use the notion of consistency. We say $\rho$ is consistent if $\rho_{v,c} \leq \rho_c + w_{v,c}$ holds for all $(v,c) \in E$. If $\rho$ is consistent, A* without reopening returns an optimal solution. Valenzano et al. [34, Theorem 4.6] revealed that for any instance $x \in I$, the suboptimality of A* can be bounded by the inconsistency accumulated along an optimal path (excluding the first edge containing $s$) as follows:

$$Cost_\rho(x) - Opt(x) \leq \Delta_\rho(x) := \sum_{(v,c) \in S^*(x), v \neq s} \max\{\rho_v - \rho_c - w_{v,c}, 0\},$$ (2)

where $S^*(x) \subseteq E$ is an optimal solution to $x$ (if there are multiple optimal solutions, we break ties by using the lexicographical order induced from the total order defined in Assumption 2). We call $\Delta_\rho(x)$ the inconsistency (of $\rho$ on $S^*(x)$).

3We use $\tilde{O}$ and $\tilde{O}$ to hide logarithmic factors of $n$ and $N$ for simplicity.
4The original theorem in [34] is applicable only to the case where A* does not reopen vertices and $\rho_t = 0$. These restrictions are unnecessary as detailed in Appendix C, and thus our result holds regardless of reopening.
Given $N$ instances $x_1, \ldots, x_N$, we can compute the empirical inconsistency, $\frac{1}{N} \sum_{i=1}^{N} \Delta_\rho(x_i)$, at the cost of solving the $N$ instances, which we will use as an empirical term. To define the corresponding complexity term, we regard $\Delta_\rho(\cdot) : \Pi \rightarrow [0, \hat{H}]$ as an inconsistency function parameterized by $\rho$, where we will discuss how large $\hat{H} > 0$ can be later, and we let $\hat{U} = \{ \Delta_\rho : \Pi \rightarrow [0, \hat{H}] \ | \ \rho \in \mathbb{R}^n \}$. The following theorem says that the class $\hat{U}$ of inconsistency functions has a smaller pseudo-dimension than the class $U$ of general utility functions.

**Theorem 6.** For the class $U$ of inconsistency functions, it holds that $\text{Pdim}(U) = O(n \log n)$.

By using (2), Proposition 1, and Theorem 6, we can obtain the following high-probability bound on the expected suboptimality, whose complexity term has a better dependence on $n$ than that of (1):

$$\mathbb{E}_{x \sim D} [\text{Cost}_\rho(x) - \text{Opt}(x)] \leq \mathbb{E}_{x \sim D} [\Delta_\rho(x)] \leq \frac{1}{N} \sum_{i=1}^{N} \Delta_\rho(x_i) + \hat{O} \left( \hat{H} \sqrt{\frac{n + \log \frac{1}{\delta}}{N}} \right).$$

This bound is uniform for all $\rho \in \mathbb{R}^n$, as with other bounds discussed so far. Thus, the bound holds even if we choose $\rho$ to minimize the empirical inconsistency. Note that the empirical inconsistency is convex in $\rho$ since $\Delta_\rho(x_i)$ consists of a maximum of a linear function of $\rho$ and zero, hence easier to minimize than the raw empirical suboptimality in practice (and suitable for a recent online-convex optimization framework [25]).

Before proving Theorem 6, we present a typical example to show that the inconsistency is not too large relative to the suboptimality.

**Example 2.** Suppose that every edge weight $w_e$ is bounded to $[0, W]$, which ensures that the suboptimality $u_\rho$ is at most $\hat{H} = W(n - 1)$ for any $\rho \in \mathbb{R}^n$. For simplicity, we consider the following natural way to compute $\rho$ values: compute an estimate $\tilde{w}_e \in [0, W]$ of $w_e$ for each $e \in E$ and let $\rho_v$ be the cost of a shortest $v$-$t$ path with respect to $\{ \tilde{w}_e \}_{e \in E}$. Then, $\rho$ enjoys the consistency with respect to $\{ \tilde{w}_e \}_{e \in E}$, i.e., $\rho_v \leq \rho_e + \tilde{w}_{(v,c)}$ for every $(v, c) \in E$. Therefore, it holds that

$$\Delta_\rho(x) \leq \sum_{(v,c) \in S^*(x), v \neq s} \max \{ \rho_v - \rho_e - \tilde{w}_{(v,c)}, 0 \} \leq \sum_{(v,c) \in S^*(x), v \neq s} |\tilde{w}_{(v,c)} - w_{(v,c)}|.$$
We finally discuss limitations of our work. As mentioned in Section 2, we require every instance to be defined on (subsets of) a fixed vertex set. Also, our work does not cover the case where heuristic function values can change depending on instance-dependent features. Studying how to overcome these limitations would also constitute interesting future work.

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Checklist

1. For all authors...
(a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? [Yes] See Section 1.1 for details of our main claims.
(b) Did you describe the limitations of your work? [Yes] See Section 6.
(c) Did you discuss any potential negative societal impacts of your work? [N/A] This is a theoretical paper and no negative societal impacts are expected.
(d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
(a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 2.2.
(b) Did you include complete proofs of all theoretical results? [Yes] Some complete proofs are shown in the supplementary due to the page limitation.

3. If you ran experiments...
(a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [N/A]
(b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A]
(c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [N/A]
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(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
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(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]
Appendix

A Comparisons with previous results on tree search

We compare our upper bounds with those of existing results on general tree search [9, 10]. Balcan et al. [9] studied the pseudo-dimension for tree-search algorithms in the following situation; a tree-search algorithm with \( d \) configurable parameters builds a search tree of size at most \( \kappa \) by iteratively choosing an action from a set of at most \( T \) possible actions. In this setting, they obtained an \( O(d\log T + d\log d) \) upper bound. Balcan et al. [10] removed the dependence on \( \kappa \) assuming scores governing the tree search to be defined by path-wise functions. Their bound is \( O(d\Delta^2 \log k + d\Delta \log T) \), where \( \Delta \) and \( k \) are the maximum depth and the number of children, respectively, of search trees. Since \( \kappa \) can be exponential in the depth \( \Delta \), this is a considerable improvement in this context.

In our setting, since there are \( n \) configurable parameters, \( \rho \in \mathbb{R}^n \), we have \( d = n \). If we apply the bound of [9] to GBFS/A* regarded as a tree-search algorithm that iteratively builds search states, \( \kappa \) and \( T \) values can be as large as \( \Omega(n) \). This is because GBFS/A* can perform \( \Omega(n) \) iterations, where each iteration increases the tree size, and the number of possible actions is equal to the size of \( \text{OPEN} \), which is \( \Omega(n) \) in general. Moreover, for A* with reopening, the number of iterations can be \( \Omega(2^n) \) as mentioned in Section 3.2, implying \( \kappa = \Omega(2^n) \). Thus, only in the case of A* without reopening, the previous bound matches our \( O(n^2 \log n) \) bound (Theorem 2). As for GBFS and A* with reopening, our Theorems 1 and 2 provide \( O(n \log n) \) and \( O(n^2 \log n) \) bounds, respectively, which improve the \( O(n^2 \log n) \) and \( O(n^2 \log n) \) bounds, respectively, implied by the previous result.

As for the result of [10], seeing GBFS/A* as a tree-search algorithm again, the maximum tree depth is as large as the number of vertices in general, i.e., \( \Delta = \Omega(n) \). Also, the number of children can be as large as the size of \( \text{OPEN} \), hence \( k = \Omega(n) \). Thus, the result of [10] leads to an \( O(n^3 \log n) \) bound, which is larger than any of our upper bounds.

B How to deal with varying \( t \)

As mentioned in Section 2.2, given a fixed \( t \in V \), each entry \( \rho_v \) in \( \rho \) indicates an estimated cost of the shortest \( v \rightarrow t \) path. Therefore, if \( t \) changes over instances, we need to define \( \rho \) for each \( t \), which we here denote by \( \rho^t \in \mathbb{R}^n \). If \( t \) changes, the structure of path-finding instances also greatly changes. Thus, it is natural to evaluate the performance of GBFS/A* separately for each \( t \). Specifically, we take \( D \) to be a conditional distribution, from which path-finding instances with fixed \( t \) are drawn, and we analyze the sample complexity for each possible \( t \in V \). In practice, \( \{\rho^t\}_{t \in V} \) may be obtained by, e.g., learning a function that embeds vertices into a metric space and measuring distances on the space, as mentioned in Section 2.2. In this case, an embedding function with tunable parameters governs all the \( \{\rho^t\}_{t \in V} \) values. Considering such situations, we need to bound the sample complexity of learning heuristic functions for all possible \( t \in V \). This can be done at a slight cost of increasing the bound in Proposition 1 by taking a union bound over all possible \( t \in V \). (Note that the upper bounds on the pseudo-dimension in Theorems 1, 2 and 6 hold separately for each \( t \in V \) by regarding \( \rho \) as \( \rho^t \).) Since there are at most \( n \) possible choices of \( t \), this replaces \( \delta/n \) in Proposition 1 with \( \delta/n \), yielding only a \( \log n \) additive factor. This effect is small relative to that of the pseudo-dimension term.

C Worst-case analysis of A* regardless of reopening

We show that the existing bound on the suboptimality of A* by Valenzano et al. [34] holds regardless of whether we allow A* to reopen vertices or not, and we also remove a minor assumption of \( \rho_v = 0 \). Note that the result of [34], which focuses on the case without reopening, does not immediately imply the same bound for A* with reopening since reopening sometimes degrades the solution quality [31].

We fix an instance and define the inconsistency of an edge \((v, v') \in E\) as

\[
\text{Inc}(v, v') = \max \{\rho_v - \rho_{v'} - w_{(v, v')}, 0\}. \tag{A1}
\]

Fix an optimal \( s \rightarrow t \) path and let \( P_{\text{opt}} = v_0, v_1, \ldots, v_k \) be a sequence of vertices on the optimal path, where \( v_0 = s, v_k = t \), and the optimal \( s \rightarrow t \) path visits the vertices in this order. Suppose that \( v_k = t \) is first selected at the \((T + 1)\text{st}\) iteration, at which the algorithm terminates.
For every \( \tau \) as in [34], we derive the bound in Theorem 7 by decomposing Theorem 7. Let \( \text{Cost} \) be the cost of an \( s-t \) path returned by A* (Algorithm 2) with/without reopening, and let \( \text{Opt} \) be the cost of \( P_{\text{opt}} = v_0, v_1, \ldots, v_k \). It holds that

\[
\text{Cost} \leq \text{Opt} + \sum_{j=1}^{k-1} \text{Inc}(v_j, v_{j+1}).
\]

The theorem was proved by Valenzano et al. [34] for Algorithm 2 without reopening. Their proof uses the fact that once a vertex is added to \( \text{CLOSED} \), it never gets out of \( \text{CLOSED} \). If we allow A* to reopen vertices, the fact is not always true. Therefore, we need to prove the theorem without using the property of \( \text{CLOSED} \). To this end, we define lists of selected vertices, which play a similar role to \( \text{CLOSED} \) in our proof. Formally, for \( \tau = 0, 1, \ldots, T + 1 \), we define \( \text{SELECTED}_\tau \) as a list of vertices that have been selected in Step 3 in the first \( \tau \) iterations. Note that even with reopening, once a vertex is added to \( \text{SELECTED}_\tau \), it never gets out of the list.

As in [34], we derive the bound in Theorem 7 by decomposing \( P_{\text{opt}} \) into two subpaths, which are defined based on the following shallowest vertex.

**Lemma 3.** We say a vertex \( v_i \in P_{\text{opt}} = v_0, v_1, \ldots, v_k \) is the shallowest vertex at \( \tau \in \{0, 1, \ldots, T\} \) if it satisfies the following conditions after the \( \tau \)th iteration:

\[
v_i \in \text{OPEN} \setminus \text{SELECTED}_\tau \quad \text{and} \quad \{ v_j \in P_{\text{opt}} \mid j < i \} \subseteq \text{SELECTED}_\tau.
\]

For every \( \tau = 0, 1, \ldots, T \), a shallowest vertex always exists.

**Proof.** We prove the claim by induction. If \( \tau = 0 \), \( v_0 \) is the shallowest since we have \( \text{SELECTED}_0 = \emptyset \) and \( \text{OPEN} = \{ v_0 \} \). If \( \tau = 1 \), \( v_1 \) is the shallowest vertex since we have \( \text{SELECTED}_1 = \{ v_0 \} \) and \( v_1 \in \text{OPEN} \setminus \text{SELECTED}_1 \). Assume that the claim is true for \( \tau' < \tau \) and let \( v_{\tau'} \in \text{OPEN} \setminus \text{SELECTED}_{\tau - 1} \) be the shallowest vertex at \( \tau - 1 \). We consider two cases: \( v_{\tau'} \) or \( v_{\tau'} \) is selected at the \( \tau \)th iteration.

If \( v_{\tau'} \) is selected, we have \( \text{SELECTED}_\tau = \text{SELECTED}_{\tau - 1} \cup \{ v_{\tau'} \} \) and \( v_{\tau'} \in \text{OPEN} \setminus \text{SELECTED}_{\tau} \); thus \( v_{\tau'} \) remains the shallowest at \( \tau \). If \( v_{\tau'} \) is selected, take the longest subpath of \( P_{\text{opt}} \) that starts from \( v_{\tau'} \) and is contained in \( \text{SELECTED}_{\tau} \). We denote such a subpath by \( v_{\tau'}, \ldots, v_{\tau''} \), where \( \tau'' < k \) holds since \( v_{\tau''} \) is never selected in the first \( T \) iterations. From the definition of the subpath, we have \( v_{\tau'' + 1} \in \text{SELECTED}_{\tau} \). Moreover, \( v_{\tau'' + 1} \) must have been opened since its parent \( v_{\tau''} \) has been selected. Thus, \( v_{\tau'' + 1} \in \text{OPEN} \setminus \text{SELECTED}_{\tau} \) holds. Furthermore, we have \( \{ v_0, \ldots, v_{\tau - 1} \} \subseteq \text{SELECTED}_{\tau} \) due to the induction hypothesis and \( \{ v_{\tau'}, \ldots, v_{\tau''} \} \subseteq \text{SELECTED}_{\tau} \) from the definition of the subpath. Thus, \( v_{\tau'' + 1} \) is the shallowest vertex at \( \tau \). To conclude, the shallowest vertex at \( \tau \) exists in any case. The proof is completed by induction.

**C.1 Decomposing the suboptimality term with the shallowest vertex**

For every \( v \in V \), we let \( g_v^s \) and \( \rho_v \) denote the costs of optimal \( s-v \) and \( v-t \) paths, respectively. We use \( g_{v,v'}^{\tau} \) to denote the cost of an optimal \( v-v' \) path for any pair of \( v, v' \in V \); it holds that \( g_v^s = g_{s,v}^s \). For each \( v \in V \), let \( g_v^{(\tau)} \) be the \( g_v \) value after the \( \tau \)th iteration, where \( g_v^{(0)} = 0 \) and \( g_v^{(0)} = \infty \) for \( v \neq s \). If \( g_v \) is updated in the \( (\tau + 1) \)st iteration, we have \( g_v^{(\tau + 1)} < g_v^{(\tau)} \); otherwise, we have \( g_v^{(\tau + 1)} = g_v^{(\tau)} \). Thus, \( g_v^{(\tau)} \) is non-increasing in \( \tau \). We define \( \delta g_v^{(\tau)} = g_v^{(\tau)} - g_v^s \) as the \( g \)-cost error of \( v \) after the \( \tau \)th iteration, which is also non-increasing in \( \tau \).

The following lemma states that the suboptimality can be decomposed into two parts: a \( g \)-cost error of the shallowest vertex \( v_i \) and the inadmissibility of \( \rho_v \), (subtracted by \( \rho_t \)).

**Lemma 4.** If \( v_i \) is the shallowest vertex at \( T \), it holds that

\[
\text{Cost} \leq \text{Opt} + \delta g_{v_i}^{(T)} + \rho_{v_i} - \rho_{v_i}^* - \rho_t.
\]

**Proof.** After the \( T \)th iteration, the score of \( v_i \) is

\[
g_{v_i}^{(T)} + \rho_{v_i} = g_{v_i}^s + \delta g_{v_i}^{(T)} + \rho_{v_i} = g_{v_i}^s + \rho_{v_i}^* + \delta g_{v_i}^{(T)} + \rho_{v_i} - \rho_{v_i}^* = \text{Opt} + \delta g_{v_i}^{(T)} + \rho_{v_i} - \rho_{v_i}^*.
\]

Since \( v_k = t \) is selected at the \( (T + 1) \)st iteration instead of \( v_i \), it holds that \( g_t^{(T)} + \rho_t \leq g_{v_i}^{(T)} + \rho_{v_i} \).

Since we have \( \text{Cost} \leq g_{t}^{(T)} \), we obtain the statement by rearranging the terms. \( \square \)
C.2 Bounding $\rho_{v_i} - \rho^*_{v_i} - \rho_t$

We prove a general lemma for later use, which implies an upper bound on $\rho_{v_i} - \rho^*_{v_i} - \rho_t$.

**Lemma 5.** Let $P = v_0, v_1, \ldots, v_k$ be any optimal $v_0$–$v_k$ path. It holds that

$$\rho_{v_0} - \rho_{v_k} - g^*_{v_0, v_k} \leq \sum_{i=0}^{k-1} \text{Inc}(v_i, v_{i+1}).$$

**Proof.** From the definition (A1), $\text{Inc}(v_i, v_{i+1}) \geq \rho_{v_i} - \rho_{v_{i+1}} - w(v_i, v_{i+1})$ holds. Therefore, we have

$$\sum_{i=0}^{k-1} (\rho_{v_i} - \rho_{v_{i+1}} - w(v_i, v_{i+1})) \leq \sum_{i=0}^{k-1} \text{Inc}(v_i, v_{i+1}).$$

Using a telescoping sum argument, we obtain

$$\rho_{v_0} - \rho_{v_k} - \sum_{i=0}^{k-1} w(v_i, v_{i+1}) \leq \sum_{i=0}^{k-1} \text{Inc}(v_i, v_{i+1}).$$

Since $P$ is optimal, we have $\sum_{i=0}^{k-1} w(v_i, v_{i+1}) = g^*_{v_0, v_k}$, thus completing the proof. \qed

Consider applying Lemma 5 to the subpath $P = v_1, \ldots, v_k$ of $P_{\text{opt}}$, which is an optimal $v_1$–$v_k$ path. Since $g^*_{v_i, v_k} = \rho_{v_i}$ and $\rho_{v_k} = \rho_t$, it holds that

$$\rho_{v_i} - \rho^*_{v_i} - \rho_t \leq \sum_{j=1}^{k-1} \text{Inc}(v_j, v_{j+1}).$$

Thus, we can obtain an upper bound on $\rho_{v_i} - \rho^*_{v_i} - \rho_t$.

C.3 Bounding $\delta g^{(T)}_{v_i}$

Our goal is to prove the following lemma.

**Lemma 6.** Let $P_{\text{opt}} = v_0, \ldots, v_k$ be the optimal s–t path in the statement of Theorem 7. Then, the shallowest vertex $v_i \in P_{\text{opt}}$ at $T$ satisfies

$$\delta g^{(T)}_{v_i} \leq \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1}).$$

To prove Lemma 6, we need the following two lemmas.

**Lemma 7.** For $P_{\text{opt}}$ in Lemma 6 and $i \geq 1$, if $v_{i-1} \in P_{\text{opt}}$ is first selected at the $\tau'$th iteration and satisfies $\delta g^{(\tau')}_{v_{i-1}} \leq \sum_{j=1}^{i-2} \text{Inc}(v_j, v_{j+1})$, then $v_i \in P_{\text{opt}}$ satisfies $\delta g^{(\tau')}_{v_i} \leq \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1})$ for all $\tau = \tau', \ldots, T$.

**Proof.** In the $\tau'$th iteration, we update $g_{v_i}$ if it is larger than $g_{\text{new}} = g^{(\tau')}_{v_{i-1}} + w(v_{i-1}, v_i)$, hence $g^{(\tau')}_{v_i} \leq g^{(\tau')}_{v_{i-1}} + w(v_{i-1}, v_i)$. Since $(v_{i-1}, v_i)$ is an edge on $P_{\text{opt}}$, $g^*_{v_i} = g^{(\tau')}_{v_{i-1}} + w(v_{i-1}, v_i)$ holds. Therefore, it holds that $\delta g^{(\tau')}_{v_i} \leq \delta g^{(\tau')}_{v_{i-1}}$. Since $\delta g^{(\tau')}_{v_{i-1}}$ is non-increasing in $\tau$, we have $\delta g^{(\tau')}_{v_i} \leq \delta g^{(\tau')}_{v_{i-1}}$. If $i = 1$, since $v_0 = s$, we obtain

$$\delta g^{(\tau')}_{v_1} \leq \delta g^{(\tau')}_{v_0} \leq \delta g^{(\tau')}_{v_0} = g^{(\tau')}_{v_0} - g^*_{v_0} = 0 - 0 = 0.$$ 

If $i > 1$, we have

$$\delta g^{(\tau')}_{v_i} \leq \delta g^{(\tau')}_{v_{i-1}} \leq \sum_{j=1}^{i-2} \text{Inc}(v_j, v_{j+1}) \leq \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1}),$$

where we used the assumption on $\delta g^{(\tau')}_{v_{i-1}}$ and $\text{Inc}(v_{i-1}, v_i) \geq 0$. \qed
Lemma 8. For $P_{\text{opt}}$ in Lemma 6 and any $\tau = 0, 1, \ldots, T$, every $v_i \in P_{\text{opt}} \cap \text{SELECTED}_{\tau}$ satisfies 
\[
\delta g_{v_i}^{(\tau)} \leq \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1}).
\]

Proof. The proof is by induction on $\tau$. If $\tau = 0$, the claim is vacuously true since $\text{SELECTED}_{\tau} = \emptyset$. If $\tau = 1$, only $v_0$ is in $\text{SELECTED}_{\tau}$. Since $g_{v_0}^{(1)} = g_{v_0}^{*} = 0$, we have $\delta g_{v_0}^{(1)} = 0$. Thus, the claim is true.

Assume that the claim is true after the first $\tau \geq 1$ iterations; in other words, for any $\tau' \leq \tau$, every $v_{\tau'} \in P_{\text{opt}} \cap \text{SELECTED}_{\tau'}$ satisfies $\delta g_{v_{\tau'}}^{(\tau')} \leq \sum_{j=1}^{\tau'-1} \text{Inc}(v_j, v_{j+1})$. Since $\delta g_{v_{\tau'}}^{(\tau)}$ is non-increasing in $\tau$, from the induction hypothesis, vertices in $P_{\text{opt}} \cap \text{SELECTED}_{\tau}$ remain to satisfy the inequality after the $(\tau + 1)$st iteration. Therefore, we focus on the vertex selected at the $(\tau + 1)$st iteration, which is the only new vertex in $\text{SELECTED}_{\tau+1}$. If the selected vertex is not in $P_{\text{opt}}$, the statement is true after the $(\tau + 1)$st iteration. We below discuss the case where the selected vertex is in $P_{\text{opt}}$. We let $v_i \in P_{\text{opt}}$ be the selected vertex, where $i \geq 1$, and discuss two cases: $v_i$’s parent, $v_{i-1}$, is in $\text{SELECTED}_{\tau}$ or not.

Case 1: $v_{i-1} \in \text{SELECTED}_{\tau}$. Suppose that $v_{i-1}$ has been first selected at the $\tau'$th iteration ($\tau' \leq \tau$). The induction hypothesis implies $\delta g_{v_{i-1}}^{(\tau')} \leq \sum_{j=1}^{\tau'-2} \text{Inc}(v_j, v_{j+1})$. Thus, from Lemma 7, we obtain $\delta g_{v_{i-1}}^{(\tau)} \leq \sum_{j=1}^{i-2} \text{Inc}(v_j, v_{j+1})$.

Case 2: $v_{i-1} \notin \text{SELECTED}_{\tau}$. In this case, we have $i > 1$ since $v_0$ is selected at the first iteration. Let $v_i$ be the shallowest vertex at $\tau$. Since $v_j \in \text{SELECTED}_{\tau}$ must hold for all $j < i'$, we have $i' < i$. Since $v_i$ is selected instead of $v_{i'}$, it holds that $g_{v_i}^{(\tau)} + \rho_{v_i} \leq g_{v_{i'}}^{(\tau)} + \rho_{v_{i'}}$. Therefore, we have
\[
\delta g_{v_i}^{(\tau)} \leq g_{v_{i'}}^{(\tau)} - g_{v_i}^{*} + \rho_{v_{i'}} - \rho_{v_i} = g_{v_{i'}}^{(\tau')} + g_{v_{i'}}^{*} - g_{v_i}^{*} + \rho_{v_{i'}} - \rho_{v_i} = \delta g_{v_{i'}}^{(\tau')} + \rho_{v_{i'}} - \rho_{v_i} - g_{v_{i'}}^{*}.
\]

We below consider bounding the right-hand side. First, we discuss a bound on $\delta g_{v_{i'}}^{(\tau')}$. Suppose that $v_{i'-1} \in \text{SELECTED}_{\tau}$ is first selected at the $\tau'$th iteration, where $\tau' \leq \tau$. From the induction hypothesis, we have $\delta g_{v_{i'-1}}^{(\tau')} \leq \sum_{j=1}^{\tau'-2} \text{Inc}(v_j, v_{j+1})$. Therefore, Lemma 7 implies $\delta g_{v_{i'-1}}^{(\tau')} \leq \sum_{j=1}^{\tau'-1} \text{Inc}(v_j, v_{j+1})$.

Next, from Lemma 5, we have $\rho_{v_{i'}} - \rho_{v_i} - g_{v_{i'}}^{*} \leq \sum_{j=i'}^{i-1} \text{Inc}(v_j, v_{j+1})$. Consequently, we obtain
\[
\delta g_{v_i}^{(\tau+1)} \leq \delta g_{v_i}^{(\tau)} \leq \sum_{j=1}^{i' - 1} \text{Inc}(v_j, v_{j+1}) + \sum_{j=i'}^{i-1} \text{Inc}(v_j, v_{j+1}) = \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1}).
\]

To conclude, every $v_i \in P_{\text{opt}} \cap \text{SELECTED}_{\tau+1}$ satisfies $\delta g_{v_i}^{(\tau+1)} \leq \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1})$. Therefore, the statement is true by induction.

Now, we are ready to prove Lemma 6.

Proof of Lemma 6. Since $v_i$ is the shallowest at $T$, $v_{i-1}$ has been first selected at some $\tau$th iteration, where $\tau \leq T$, i.e., $v_{i-1} \in P_{\text{opt}} \cap \text{SELECTED}_{\tau}$. Thus, Lemma 8 implies $\delta g_{v_{i-1}}^{(\tau)} \leq \sum_{j=1}^{i-2} \text{Inc}(v_j, v_{j+1})$. Therefore, from Lemma 7, we obtain $\delta g_{v_{i-1}}^{(T)} \leq \sum_{j=1}^{i-1} \text{Inc}(v_j, v_{j+1})$.

C.4 Proof of Theorem 7

By summing up the above lemmas and equations, we prove Theorem 7.

Proof of Theorem 7. By using Lemmas 4 and 6 and eq. (A2), we obtain
\[
\text{Cost} \leq \text{Opt} + \delta g_{v_1}^{(T)} + \rho_{v_1} - \rho_{v_0} - \rho_t
\]
\[
\leq \text{Opt} + \sum_{j=1}^{k-1} \text{Inc}(v_j, v_{j+1}) + \sum_{j=1}^{k-1} \text{Inc}(v_j, v_{j+1})
\]
\[
= \text{Opt} + \sum_{j=1}^{k-1} \text{Inc}(v_j, v_{j+1}).
\]

\]
D An example of improving upper bounds with instance-specific heuristics

GBFS/A* is often applied to path-finding instances that have extremely many vertices, for which our bounds on the pseudo-dimension depending on \( n \) or \( n^2 \) imply somewhat pessimistic sample complexity bounds. To exhibit more practical results for such cases, we study an example situation where we can exponentially improve the upper bounds by using instance-specific heuristic functions.

We assume the vertex set \( V \) to be fixed as in Assumption 1 and that each vertex \( v \in V \) corresponds to a state represented by a vector \( q_v \in \Sigma^L \), where \( \Sigma \) is a finite set of cardinality \( B \). For example, if \( \Sigma = \{0, 1\} \), we have \( B = 2 \) and each \( v \in V \) corresponds to a state represented by a bit vector of length \( L \). Such situations arise, e.g., when applying GBFS/A* to planning instances represented by the STRIPS model [19]. As for heuristic functions, we assume that each \( \rho_v \) value is computed as \( \rho_v = q_v^\top \theta + \eta \), where \( (\theta, \eta) \in \mathbb{R}^{L+1} \) is a vector of tunable parameters. (Although \( \eta \) is not essential in the following analysis, we can use it to make every \( \rho_v \) non-negative in practice.) Here, an important observation is that the number of tunable parameters is \( L + 1 \), while \( V \) has up to \( n = B^L \) vertices. Using this exponential decrease in the number of tunable parameters, we below obtain \( \text{poly}(L \log B) \approx \text{polylog}(n) \) upper bounds on the pseudo-dimension for GBFS and A* under the integer-weight assumption. That is, while the number of vertices is exponential in \( L \), the upper bounds can scale polynomially with \( L \).

**GBFS.** As discussed in the proof of Lemma 1, if two heuristic function values \( \rho, \rho' \in \mathbb{R}^n \) have the same total order on \( V \), it holds \( u_\rho(x) = u_\rho'(x) \) for all instances \( x \in \Pi \). Also, note that the total order is uniquely determined by comparing \( \rho_v \) and \( \rho_{v'} \) for all pairs of \( v, v' \in V \). Therefore, if we partition the space \( \mathbb{R}^{L+1} \) of tunable parameters into some regions \( \mathcal{P}_1, \mathcal{P}_2, \ldots \subset \mathbb{R}^{L+1} \) by \( \binom{n}{2} \) hyperplanes of form

\[
\rho_v = \rho_{v'} \iff q_v^\top \theta + \eta = q_{v'}^\top \theta + \eta \iff (q_v - q_{v'})^\top \theta = 0,
\]

then all \((\theta, \eta)\) values belonging to the same region \( \mathcal{P}_i \) result in the same \( u_\rho(x) \) value for all \( x \in \Pi \). Hence, when \( (\theta, \eta) \) is allowed to take any value in \( \mathbb{R}^{L+1} \), the number of distinct tuples of form \((u_\rho(x_1), \ldots, u_\rho(x_N))\) is bounded by the number of the regions \( \mathcal{P}_1, \mathcal{P}_2, \ldots \). As in the proof of Theorem 2, the number of such regions is \( O\left(\binom{e(L)}{L+1}\right) \) due to Sauer’s lemma. On the other hand, to shatter \( N \) instances \( x_1, \ldots, x_N \), we need to make \( 2^N \) distinct tuples of form \((u_\rho(x_1), \ldots, u_\rho(x_N))\) by varying \( (\theta, \eta) \in \mathbb{R}^{L+1} \). Since \( n = O(B^L) \), solving \( O\left(\binom{e(n)}{L+1}\right) \geq 2^N \) for the largest \( N \) yields an \( O(L \log n) \approx O(L^2 \log B) \) bound on \( \text{Pdim}(\mathcal{U}) \).

**A* under the integer-weight assumption.** We can also obtain a \( \text{polylog}(n) \) upper bound for A* under the condition of Theorem 4, i.e., all edge weights take non-negative integer values at most \( W \). The proof begins with the same discussion as that of Theorem 2. For a fixed instance \( x_k \in \Pi \), the number of possible \( u_\rho(x_k) \) values is at most the number of regions created by hyperplanes of form \( g_{v'}(x_k) + \rho_v = g_{v'}(x_k) + \rho_{v'} \) for all pairs of \( v, v' \in V \). Since \( g_{v'}(x_k) \) can take \( nW \) distinct values, the number of those hyperplanes is \( \binom{n^2W}{2} \), as discussed in the proof of Theorem 4. Therefore, given \( N \) instances \( x_1, \ldots, x_N \), the number of distinct tuples of form \((u_\rho(x_1), \ldots, u_\rho(x_N))\) is bounded by the number of regions created by \( N \binom{n^2W}{2} \) hyperplanes. Next, as with the above GBFS case, we bound the number of those regions using Sauer’s lemma. With the tunable parameters \((\theta, \eta) \in \mathbb{R}^{L+1}\), each hyperplane can be written as

\[
g_{v'}(x_k) + \rho_v = g_{v'}(x_k) + \rho_{v'} \iff (q_v - q_{v'})^\top \theta + g_v(x_k) - g_{v'}(x_k) = 0.
\]

Sauer’s lemma implies that \( N \binom{n^2W}{2} \) such hyperplanes partition \( \mathbb{R}^{L+1} \) into \( O\left(\binom{e(N \binom{n^2W}{2})}{L+1}\right) \) regions. To shatter the \( N \) instances, the number of the regions must be at least \( 2^N \). Since \( n = O(B^L) \), solving \( O\left(\binom{e(N \binom{n^2W}{2})}{L+1}\right) \geq 2^N \) for the largest \( N \) yields an \( O(L \log nW) \approx O(L^2 \log B + L \log W) \) upper bound on \( \text{Pdim}(\mathcal{U}) \).

As regards A* for general cases, it is open whether a similar \( \text{polylog}(n) \) upper bound can be achieved. The obstacle is the additional \( n \) factor, which remains even if the number of tunable parameters decreases. Thus, this problem would be as difficult as closing the gap between the \( \Omega(n) \) lower bound and \( O(n^2) \) upper bound.