LETTER Special Section on Foundations of Computer Science - Algorithm, Theory of Computation, and their Applications -

# Exact Exponential Algorithm for Distance-3 Independent Set Problem 

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#### Abstract

SUMMARY Let $G=(V, E)$ be an unweighted simple graph. A distance-d independent set is a subset $I \subseteq V$ such that $\operatorname{dist}(u, v) \geq d$ for any two vertices $u, v$ in $I$, where $\operatorname{dist}(u, v)$ is the distance between $u$ and $v$. Then, Maximum Distance- $d$ Independent Set problem requires to compute the size of a distance- $d$ independent set with the maximum number of vertices. Even for a fixed integer $d \geq 3$, this problem is NP-hard. In this paper, we design an exact exponential algorithm that calculates the size of a maximum distance-3 independent set in $\mathrm{O}\left(1.4143^{n}\right)$ time. key words: exact exponential algorithm, independent set, distance-d independent set, maximum distance-d independent set


## 1. Introduction

Let $G=(V, E)$ be an unweighted simple graph with the vertex set $V$ and the edge set $E$. We denote by $n$ the numbers of vertices in $G$. An independent set of $G$ is a subset $I \subseteq V$ of vertices such that $\{u, v\} \notin E$ holds for all $u, v \in I$. Maximum Independent Set problem (MaxIS for short) asks to calculate the size of an independent set of $G$ with the maximum number of vertices. This problem is one of the most fundamental and important problems in theoretical computer science and is a classic NP-hard problem.

In this paper, we deal with a generalization of an independent set. A distance between two vertices $u, v$ of $G$, denoted by $\operatorname{dist}(u, v)$, is the number of edges on a shortest path between them. For an integer $d \geq 2$, a distance-d independent set is a subset $I \subseteq V$ such that $\operatorname{dist}(u, v) \geq d$ for any two vertices $u, v \in I$. Then, Maximum Distance- $d$ Independent Set problem (MaxD $d$ IS for short) requires to compute the size of a distance- $d$ independent set with the maximum number of vertices. Examples of distance-3 independent sets are shown in Fig. 1.


Fig. 1 (a) A distance-3 independent set and (b) a maximum distance-3 independent set of the graph.

[^0]When $d=2, \operatorname{MaxD} d \mathrm{IS}$ is equivalent to MaxIS. Hence, it is obvious that MaxDdIS is NP-hard. Furthermore, for a fixed integer $d \geq 3$, MaxD $d$ IS is NP-hard [1]. Hence, it seems to be hard to give a polynomial-time algorithm for MaxD $d \mathrm{IS}$. As existing results, approximation algorithms for MaxD3IS are presented by Eto et al. [2], [3].

In this paper, we focus on exact exponential algorithms for MaxD3IS. For MaxIS, there are a lot of existing exact exponential algorithms. However, to the best of our knowledge, our algorithm is the first exact exponential algorithm for the problem. Our algorithm calculates the size of a maximum distance- 3 independent set of a graph in $\mathrm{O}\left(1.4143^{n}\right)$ time.

## 2. Algorithm and Its Running Time Analysis

Let $G=(V, E)$ be a graph. We denote by $N(v)=\{u \mid\{v, u\} \in$ $E\}$ the set of the neighbors of $v$. We define $N^{d}(v)=\{u \mid$ $\operatorname{dist}(v, u) \leq d$ and $u \neq v\}$. The notation $N^{d}(v)$ is an extension of the set of neighbors of $v$. For a subset $V^{\prime} \subseteq V$, we denote $N^{d}\left(V^{\prime}\right)=\left\{u \mid u \in N^{d}(v)\right.$ for some $v \in V^{\prime}$ and $\left.u \notin V^{\prime}\right\}$

To solve MaxD $d \mathrm{IS}$, let us define a restricted variant of $\operatorname{MaxD} d \mathrm{IS}$. Suppose that we are given a graph $G=(V, E)$, a distance- $d$ independent set $I$ of $G$, and a subset $X \subseteq V$, where $I \cap X=\emptyset$, the problem ResMaxD $d$ IS asks for the size of a maximum distance- $d$ independent set of $G$ including $I$ and excluding $X$. If we set $I=\emptyset$ and $X=$ $\emptyset$, then ResMaxD $d \mathbf{I S}$ is equivalent to MaxD $d \mathbf{I S}$. We say that $(G, I, X)$ is an instance of ResMaxD $d \mathrm{IS}$. Let denote by $\alpha(G, I, X)$ the size of a maximum distance- $d$ independent set of $G$ including $I$ and excluding $X$. We denote by $F=V \backslash(I \cup X)$ and we say that a vertex in $F$ is free.

Now, let us assume that $d=3$. Let $(G, I, X)$ be an instance of ResMaxD3IS. First, we give the following simple reduction.

Reduction D3IS. 1. Add all the vertices in $N^{2}(I)$ into $X$.
Let $X^{\prime}$ be the subset obtained by applying Reduction D3IS. 1. Obviously, $\alpha(G, I, X)=\alpha\left(G, I, X^{\prime}\right)$ holds.

The second reduction is as follows.
Reduction D3IS. 2. Remove all the vertices of degree-1 in $X$.

Let ( $G^{\prime}, I, X^{\prime}$ ) be the instance obtained by applying Reduction D3IS. 2 to $(G, I, X)$. Then, $\alpha(G, I, X)=\alpha\left(G^{\prime}, I, X^{\prime}\right)$ holds, because any distance-3 independent set of $(G, I, X)$ is
also a distance-3 independent set of $\left(G^{\prime}, I, X^{\prime}\right)$.
The third reduction is as follows.
Reduction D3IS. 3. Remove every edge between two vertices in $X$.

Now, we prove that Reduction D3IS. 3 is correct.
Lemma 1: Let $(G, I, X)$ be an instance of ResMaxD3IS, and let $\left(G^{\prime}, I, X\right)$ be an instance obtained by applying Reduction D3IS. 3. Then, $\alpha(G, I, X)=\alpha\left(G^{\prime}, I, X\right)$ holds.

Proof. Since edges are removed from $G$, clearly $\left.\alpha(G, I, X)) \leq \alpha\left(G^{\prime}, I, X\right)\right)$ holds. We assume for a contradiction that $\alpha(G, I, X)<\alpha\left(G^{\prime}, I, X\right)$ holds. Let $I_{M}^{\prime}$ be a maximum distance-3 independent set of ( $G^{\prime}, I, X$ ). Namely, $\left|I_{M}^{\prime}\right|=\alpha\left(G^{\prime}, I, X\right)$ holds. Let $e=(u, v)$ be a removed edge in the reduction. Recall that $u, v \in X$. If $I_{M}^{\prime}$ has no vertex in $N(u) \cap F$ and $I_{M}^{\prime}$ has no vertex in $N(v) \cap F$, then $I_{M}^{\prime}$ is also a distance-3 independent set of $(G, I, X)$. Assume that $I_{M}^{\prime}$ includes a vertex $x$ in $N(u) \cap F$. Again $I_{M}^{\prime}$ is also a distance-3 independent set of $(G, I, X)$, because, for every vertex $y$ in $N(v)$, the length of any path from $x$ to $y$ along $e$ is 3 . Hence, $\alpha(G, I, X) \geq\left|I_{M}^{\prime}\right|=\alpha\left(G^{\prime}, I, X\right)$, which is a contradiction.

The last reduction is as follows.
Reduction D3IS. 4. Remove all the isolated vertices in $X$.
Let ( $G^{\prime}, I, X^{\prime}$ ) be the instance obtained by applying Reduction D3IS. 4. Clearly, we have $\alpha(G, I, X)=\alpha\left(G^{\prime}, I, X^{\prime}\right)$.

Let $\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$ be the instance obtained by exhaustively applying Reduction D3IS. 1-4 for a given instance $(G, I, X)$ (actually $I^{\prime}=I$ holds, however, we use $I^{\prime}$ to unify the notations). In ( $G^{\prime}, I^{\prime}, X^{\prime}$ ), we can observe that every vertex in $I^{\prime}$ is an isolated vertex in $G^{\prime}$ and the other connected components consist of free vertices and the vertices in $X^{\prime}$. For a vertex $v$, we denote by $f(v)$ and $\#_{f}(v)$ the set and number of the free vertices in $N^{2}(v)$. A connected component $C$ is cyclic if $C$ includes four or more free vertices and $\#_{f}(v)=2$ for every free vertex $v$ in $C$. In what follows, we show that ResMaxD3IS is polynomial-time solvable on cyclic connected components. This is a key observation of our algorithm.

Let $C$ be a cyclic connected component in $G^{\prime}$. We define a cyclic order $\left(v_{1}, v_{2}, \ldots, v_{k}\right)$ among the free vertices in $C$, as follows. Let $v$ be any free vertex in $C$, and let $u, w$ be the two free vertices in $N^{2}(v)$. Then, it can be observed that $u$ and $w$ are non-adjacent, because if $u$ and $w$ are adjacent, $C$ includes only three free vertices $v, u$, and $w$ (recall that $\#_{f}(v)=2$ for every free vertex $v$ in $C$ ). Now, we choose $v$ as $v_{1}$ and $u$ as $v_{2}$ (we can choose $u$ or $w$ arbitrary). Next, let $x$ be a free vertex in $N^{2}(u)$ except $v$. Then, we choose $x$ as $v_{3}$. We repeat the same process. This process assigns an order to each free vertex in $C$ and ends up with $w$. We call the obtained order a cyclic order of the free vertices in $C$. In the cyclic order $\left(v_{1}, v_{2}, \ldots, v_{k}\right)$, we denote by $\operatorname{succ}\left(v_{i}\right)$ the successor of $v_{i}$ for each $i=1,2, \ldots, k$ in $C$. Note that $v_{1}=\operatorname{succ}\left(v_{k}\right)$. We also denote $\operatorname{succ}\left(\operatorname{succ}\left(v_{i}\right)\right)$ by $\operatorname{succ}^{2}\left(v_{i}\right)$.

Now, let us have observations for two consecutive free


Fig. 2 (a) An adjacent pair, (b) a non-adjacent pair, and (c) an adjacent pair. The white vertices are free vertices and the black vertices are vertices in $X$.
vertices in the cyclic order. For a vertex $v_{i}$ and $\operatorname{succ}\left(v_{i}\right)$, they are adjacent (Fig. 2 (a)) or have one or more common adjacent vertices in $X$ (Fig. 2 (b)). They may be adjacent and have one or more common adjacent vertices in $X$ (Fig. 2 (c)). We say that a pair $\left(v_{i}, \operatorname{succ}\left(v_{i}\right)\right)$ is adjacent if $v_{i}$ and $\operatorname{succ}\left(v_{i}\right)$ are adjacent and is non-adjacent if $v_{i}$ and $\operatorname{succ}\left(v_{i}\right)$ are not adjacent. Note that, if $\left(v_{i}, \operatorname{succ}\left(v_{i}\right)\right)$ is non-adjacent, $v_{i}$ and $\operatorname{succ}\left(v_{i}\right)$ have one or more common adjacent vertices in $X$, that is $\operatorname{dist}\left(v_{i}, \operatorname{succ}\left(v_{i}\right)\right)=2$. We have the following lemma.

Lemma 2: Let $C$ be a cyclic connected component, and let $\left(v_{1}, v_{2}, \ldots, v_{k}\right)$ be a cyclic order of the free vertices in $C$. Then, if a pair $\left(v_{i}, \operatorname{succ}\left(v_{i}\right)\right)$ is adjacent for some $i, 1 \leq i \leq k$, then $\left(\operatorname{succ}\left(v_{i}\right), \operatorname{succ}^{2}\left(v_{i}\right)\right)$ is non-adjacent.
Proof. Assume for a contradiction that $\left(\operatorname{succ}\left(v_{i}\right), \operatorname{succ}^{2}\left(v_{i}\right)\right)$ is adjacent. Then, $f\left(v_{i}\right)=\left\{\operatorname{succ}\left(v_{i}\right), \operatorname{succ}^{2}\left(v_{i}\right)\right\}, f\left(\operatorname{succ}\left(v_{i}\right)\right)=$ $\left\{v_{i}, \operatorname{succ}^{2}\left(v_{i}\right)\right\}$, and, $f\left(\operatorname{succ}^{2}\left(v_{i}\right)\right)=\left\{v_{i}, \operatorname{succ}\left(v_{i}\right)\right\}$. This implies that $C$ includes only 3 free vertices, which contradicts the definition of cyclic connected components.
From the above lemma, two adjacent pairs do not appear consecutively in a cyclic order. Hence, we immediately have the following corollary.
Corollary 1: Let $C$ be a cyclic connected component, and let $\left(v_{1}, v_{2}, \ldots, v_{k}\right)$ be a cyclic order of the free vertices in $C$. Then, $\operatorname{dist}\left(v_{i}, \operatorname{succ}^{2}\left(v_{i}\right)\right) \geq 3$ holds.

Now, we are ready to prove the key lemma below.
Lemma 3: Let $C$ be a cyclic connected component, and let $k$ be the number of free vertices in $C$. Then, the size of a maximum distance-3 independent set of $C$ is $\lfloor k / 2\rfloor$.
Proof. First, we show that one can construct a distance-3 independent set $I_{C}$ with $\left|I_{C}\right|=\lfloor k / 2\rfloor$. Let $S=\left(v_{1}, v_{2}, \ldots, v_{k}\right)$ be a cyclic order of the free vertices in $C$. From Corollary 1, $\operatorname{dist}\left(v_{i}, \operatorname{succ}^{2}\left(v_{i}\right)\right) \geq 3$ holds for each $i$. Hence, we can observe that the set $\left\{v_{2 i-1} \mid i=1,2, \ldots,\lfloor k / 2\rfloor\right\}$ is a distance-3 independent set of $C$.

Next, we prove that the size $\lfloor k / 2\rfloor$ is the maximum. Let us assume for a contradiction that $I_{C}^{\prime}$ is a distance- 3 independent set of $C$ and $\left|I_{C}^{\prime}\right|>\lfloor k / 2\rfloor$. Then, $I_{C}^{\prime}$ contains two consecutive free vertices on $S$. Hence $I_{C}^{\prime}$ is not a distance-3 independent set of $C$.

Now, we present our algorithm in Algorithm 1 and AIgorithm 2. Algorithm 1 is the main routine ResMaxD3IS and Algorithm 2 is the subroutine Helper. We are given an instance $(G, I, X)$, ResMaxD3IS $(G, I, X)$ returns the size of a maximum distance-3 independent set of $G$ including $I$ and excluding $X$. Note that $\operatorname{ResMaxD} 3 \operatorname{IS}(G, \emptyset, \emptyset)$ returns the size of a maximum distance-3 independent set of $G$. The

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Algorithm 1: ResMaxD3IS( \(G, I, X\) )
    begin
        Repeat to apply Reduction D3IS. 1-4 exhaustively, and let
        ( \(G^{\prime}, I^{\prime}, X^{\prime}\) ) be the obtained instance. Let \(F^{\prime}\) be the set of
        free vertices of \(\left(G^{\prime}, I^{\prime}, X^{\prime}\right)\).
        if \(F^{\prime}=\emptyset\) then
            return \(\left|I^{\prime}\right|\)
        if \(\exists v \in F^{\prime}\) with \(\#_{f}(v)=0\) then
            return \(\operatorname{ResMaxD} 3 I S\left(G^{\prime}, I^{\prime} \cup\{v\}, X^{\prime}\right)\)
        if \(\exists v \in F\) with \(\#_{f}(v)=1\) then
            Let \(u\) be the vertex in \(f(v)\).
            return max \(\left\{\operatorname{ResMaxD} 3 \operatorname{IS}\left(G^{\prime}, I^{\prime} \cup\{v\}, X^{\prime} \cup\{u\}\right)\right.\),
                \(\left.\operatorname{ResMaxD} 3 \operatorname{IS}\left(G^{\prime}, I^{\prime} \cup\{u\}, X^{\prime} \cup N^{2}(u)\right)\right\}\)
        if \(\exists v \in F^{\prime}\) with \(\#_{f}(v) \geq 3\) then
            return max \(\left\{\operatorname{ResMaxD} 3 \operatorname{IS}\left(G^{\prime}, I^{\prime} \cup\{v\}, X^{\prime} \cup N^{2}(v)\right)\right.\),
                \(\left.\operatorname{ResMaxD3IS}\left(G^{\prime}, I^{\prime}, X^{\prime} \cup\{v\}\right)\right\}\)
        if \(\forall v \in F^{\prime}\) with \(\#_{f}(v)=2\) then
            Let \(C_{1}, C_{2}, \ldots, C_{\ell}\) be the connected components of \(G^{\prime}\)
            each of which contains free vertices and vertices in \(X^{\prime}\).
            return \(\left|I^{\prime}\right|+\sum_{1 \leq i \leq \ell} \operatorname{Helper}\left(C_{i}, I^{\prime} \cap V\left(C_{i}\right), X^{\prime} \cap V\left(C_{i}\right)\right)\)
            /* \(V\left(C_{i}\right)\) is the set of the vertices in
            \(C_{i}\)
                                    */
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Algorithm 2: \(\operatorname{Helper}(G, I, X)\)
    begin
        if \(G\) has 3 or less free vertices then
            Calculate \(\alpha(G, I, X)\) using an exhaustive search.
            return \(\alpha(G, I, X)\)
        else /* \(G\) is a cyclic connected component. */
            return \(\lfloor V(G) / 2\rfloor\)
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algorithm is a branching algorithm. The algorithm repeats to either select or discard each vertex in $V$. The set of selected vertices is a distance- 3 independent set of $G$ and denoted by $I$. The set of the discarded vertices is denoted by $X$.

First, the algorithm applies Reduction D3IS. 1-4 exhaustively. Let ( $G^{\prime}, I^{\prime}, X^{\prime}$ ) be the obtained instance. Let $I_{M}\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$ be a maximum distance-3 independent set for $\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$. Let us assume that there is a free vertex $v$ with $\#_{f}(v)=0$ in $\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$. Then, $v$ is always included in $I_{M}\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$. In this case, we always select $v$ and recursively call ResMaxD3IS $\left(G^{\prime}, I^{\prime} \cup\{v\}, X^{\prime}\right)$. Next, let us assume that there is a free vertex $v$ with $\#_{f}(v)=1$. Let $u$ be the free vertex in $f(v)$. If we select $v$, then $u$ is discarded into $X$. On the other hand, if we discard $v$, we have to select $u$. Because otherwise, $v$ and $u$ are both discarded, then we cannot obtain a maximum distance-3 independent set for ( $G^{\prime}, I^{\prime}, X^{\prime}$ ). In this case, the branching vector is $(2,2)$, since the number of free vertices decreases by 2 in each case. Then, its branching factor is $\tau(2,2)<1.4143$. Intuitively, this means that the number of nodes in a search tree is bounded above by $\tau(2,2)^{n}$. (See [4] for the formal definitions of branching vectors and branching factors.) Next, let us assume that
there is a free vertex $v$ with $\#_{f}(v) \geq 3$. If we select $v$, then $v$ is selected and at least 3 vertices in $f(v)$ are discarded. If we discard $v$, then $v$ is inserted into $X^{\prime}$. Hence, the branching vector is $(4,1)$ and its branching factor is $\tau(4,1)<1.3803$. Finally, let us assume that every vertex $v$ holds $\#_{f}(v)=2$. In this case, one can compute $\alpha\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$ in polynomial time. For each connected component $C$ of $G^{\prime}$, we compute the size of a maximum distance- 3 independent set of $C$ using Helper procedure. Let $n_{C}$ be the number of free vertices in $C$. Helper procedure calculates the size of a maximum distance-3 independent set of $C$ in an exhaustive manner if $n_{C} \leq 3$ holds. Otherwise, since $C$ is a cyclic connected component, the size of its maximum distance-3 independent set of $C$ is $\left\lfloor n_{C} / 2\right\rfloor$ from Lemma 3. Hence, in this case, one can obtain $\alpha\left(G^{\prime}, I^{\prime}, X^{\prime}\right)$ in polynomial time.

Consequently, the worst case branching factor is $\tau(2,2)<1.4143$. Therefore, we obtain the main theorem below.

Theorem 1: One can solve MaxD3IS in $\mathrm{O}\left(1.4143^{n}\right)$ time.
By slightly modifying the algorithm, we also have the following corollary.

Corollary 2: One can find a maximum distance-3 independent set in $\mathrm{O}\left(1.4143^{n}\right)$ time.

## 3. Conclusions

We have designed an algorithm that calculates the size of a maximum distance-3 independent set of a given graph in $\mathrm{O}\left(1.4143^{n}\right)$ time, where $n$ is the number of vertices. By slightly modifying the algorithm, we can construct a maximum distance- 3 independent set in $\mathrm{O}\left(1.4143^{n}\right)$ time. Our algorithm uses a basic technique, called branching, for designing exact algorithms. Our future work includes designing more efficient exact algorithms using other techniques. For example, we may use the measure and conquer technique.

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