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Discrete Applied Mathematics 146 (2005) 233–243
DISCRETE APPLIED MATHEMATICS
www.elsevier.com/locate/dam

Data-independent neighborhood functions and strict local optima

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Received 15 October 2001; received in revised form 18 July 2003; accepted 13 September 2004
Available online 24 December 2004

Abstract

The paper proves that data-independent neighborhood functions with the smooth property (all strict local optima are global optima) for maximum 3-satisfiability (MAX 3-SAT) must contain all possible solutions for large instances. Data-independent neighborhood functions with the smooth property for 0–1 knapsack are shown to have size with the same order of magnitude as the cardinality of the solution space. Data-independent neighborhood functions with the smooth property for traveling salesman problem (TSP) are shown to have exponential size. These results also hold for certain polynomially solvable sub-problems of MAX 3-SAT, 0–1 knapsack and TSP.

Keywords: Computational complexity; Local search algorithm; Exponential neighborhood

1. Introduction

The effectiveness of local search algorithms [8] on discrete optimization problems is highly dependent on the choice of neighborhood function. This paper proves that the only data-independent neighborhood functions with the smooth property (all strict local optima are global optima) for maximum 3-satisfiability (MAX 3-SAT) [4] are neighborhood functions that contain all possible solutions for large instances. More precisely, if a given neighborhood function for MAX 3-SAT has the smooth property, then, for instances with

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0166-218X/$ - see front matter
doi:10.1016/j.dam.2004.09.007

$n \geqslant 4$ Boolean variables, the neighborhood of every solution $\boldsymbol{x}$ contains all possible solutions except for the solution $\boldsymbol{x}$ itself. A result for 0–1 knapsack shows that data-independent neighborhood functions with the smooth property must have size that is $\Theta(2^n)$, where n denotes the number of items in the problem instance. Furthermore, a neighborhood function η^{K} with the smooth property for 0–1 knapsack is given so that if $\eta(I, \boldsymbol{x}) \subset \eta^{\mathrm{K}}(I, \boldsymbol{x})$ for some instance I and solution $\boldsymbol{x}$, then η does not have the smooth property. The neighborhood function η^{K} is said to be the minimal data-independent neighborhood function with the smooth property for 0–1 knapsack. Note that a neighborhood function η^{MS} consisting of all solutions for instances of MAX 3-SAT (with $n \geqslant 4$ Boolean variables) also has the property that if $\eta(I, \boldsymbol{x}) \subset \eta^{\mathrm{MS}}(I, \boldsymbol{x})$ (for an instance I with $n \geqslant 4$ Boolean variables) and solution $\boldsymbol{x}$, then η does not have the smooth property. This paper also shows that if a given neighborhood function of traveling salesman problem (TSP) [6] has the smooth property, then the neighborhood of every solution has cardinality $\Omega(2^{n/3})$, where n denotes the number of cities in the problem instance.

The results in this paper are obtained by constructing instances of the discrete optimization problem such that specified data-independent neighborhood functions have a strict local optimum that is not a global optimum. In particular, instances are created where there is a unique global optimum and a unique solution with the second best objective function value. The solution with the second best objective function value is chosen such that the unique global optimum is not in its neighborhood. This implies that the solution with the second best objective function value is a strict local optimum. By construction, the classes of instances used in the proofs form polynomially solvable sub-problems of MAX 3-SAT, 0–1 knapsack and TSP. Therefore, the results listed in the first paragraph also hold for polynomially solvable sub-problems of MAX 3-SAT, 0–1 knapsack and TSP. For example, there exists a polynomially solvable sub-problem of MAX 3-SAT such that data-independent neighborhood functions with the smooth property must contain all possible solutions for instances with $n \geqslant 4$ Boolean variables.

A *neighborhood function* for problem Π in NP optimization (NPO) [3] is a rule that maps an instance and feasible solution pair $(I, \boldsymbol{x})$, where $I \in D$ and $\boldsymbol{x} \in \mathrm{SOL}(I)$, to a set of feasible solutions. Therefore, a neighborhood function η for problem Π satisfies $\eta(I, \boldsymbol{x}) \subseteq \mathrm{SOL}(I)$ for every instance $I \in D$ and every solution $\boldsymbol{x} \in \mathrm{SOL}(I)$. Given an instance and feasible solution pair $(I, \boldsymbol{x})$, where $I \in D$ and $\boldsymbol{x} \in \mathrm{SOL}(I)$, $\eta(I, \boldsymbol{x})$ is referred to as the neighborhood of solution $\boldsymbol{x}$. In this paper, a solution is not permitted to be a member of its own neighborhood (i.e., $\boldsymbol{x} \notin \eta(I, \boldsymbol{x})$ for all instances $I \in D$ and solutions $\boldsymbol{x} \in \mathrm{SOL}(I)$). This restriction is consistent and compatible with the local search algorithm formulation.

To characterize properties of neighborhood functions, the following definitions are needed. Define the *size of a neighborhood function* η for an instance I to be $\max_{\boldsymbol{x} \in \mathrm{SOL}(I)} |\eta(I, \boldsymbol{x})|$. A neighborhood function η for Π is *complete* if $\eta(I, \boldsymbol{x}) = \mathrm{SOL}(I) - \{\boldsymbol{x}\}$ for every instance $I \in D$ (with length[I] sufficiently large, since the size of the neighborhood function is analyzed asymptotically) and $\boldsymbol{x} \in \mathrm{SOL}(I)$. A neighborhood function in which all local optima are global optima is said to have the *global search* (GS) *property*. A neighborhood function in which all strict local optima are global optima is said to have the *smooth property*. Suppose that for every solution if the neighborhood function η can be searched in polynomial time for an improving solution or else $\boldsymbol{x}$ is deemed a local optimum, then η is said to be *polynomially computable*.

The following definitions will be given for a maximization problem. A solution $\boldsymbol{x} \in \mathrm{SOL}(I)$ is a (*strict*) *local optimum* if $m(I, \boldsymbol{x})(>) \geqslant m(I, \boldsymbol{y})$ for all $\boldsymbol{y} \in \eta(I, \boldsymbol{x})$, and a solution $\boldsymbol{x} \in \mathrm{SOL}(I)$ is a *global optimum* if $m(I, \boldsymbol{x}) \geqslant m(I, \boldsymbol{y})$ for all $\boldsymbol{y} \in \mathrm{SOL}(I)$. Data-independent neighborhood functions are defined for discrete optimization problems in NPO that can be formulated as *consistent* optimization problems (i.e., there exists a sequence of sets $\{\Lambda_n\}_{n=1}^{\infty}$ such that $\Lambda_n \subseteq \{0, 1\}^n$ and every instance I can be represented as max $m(I, \boldsymbol{x})$ subject to $\boldsymbol{x} \in \Lambda_n$, where m is a polynomially computable objective function and n is a positive integer that is polynomial in the length of instance I). To be *independent* of the problem data, a neighborhood function η must satisfy the following property for all positive integers n:

> Let I_1 and I_2 be instances denoted as max $m(I_1, \boldsymbol{x})$ subject to $\boldsymbol{x} \in \Lambda_n$, and max $m(I_2, \boldsymbol{x})$ subject to $\boldsymbol{x} \in \Lambda_n$, respectively. Then $\eta(I_1, \boldsymbol{x}) = \eta(I_2, \boldsymbol{x})$ for all $\boldsymbol{x} \in \Lambda_n$.

The data-independent neighborhood function definition depends on the representation of the problem as a consistent optimization problem. Therefore, for the optimization problems discussed in this paper, the sets $\{\Lambda_n\}_{n=1}^{\infty}$ will be specified. In particular, MAX 3-SAT and 0–1 knapsack are consistent where $\{\Lambda_n\}_{n=1}^{\infty}$ are all Boolean vectors over n dimensions, while TSP is consistent where $\{\Lambda_{\binom{n}{2}}\}_{n=1}^{\infty}$ are the collection of distinct Hamiltonian tours over the n cities. A neighborhood function is *reasonable* if it is independent of the problem data and has polynomial size. Reasonable neighborhood functions have been studied since it is conjectured that their properties may indicate the difficulty of a discrete optimization problem [11]. Note that the restriction to polynomially sized neighborhood functions is not, in general, always necessary for iterations of a local search algorithm to be completed in polynomial time. In particular, there exist several exponentially large neighborhood functions for NP-hard discrete optimization problems, such as TSP, which can be searched in polynomial time [1].

A limited number of papers report results that prove that certain discrete optimization problems have no reasonable neighborhood function with the GS or smooth properties. Vizing [12] and Savage et al. [10] independently show that any problem parameter-independent neighborhood function of TSP for which all local optima are global optima must be exponentially large, hence there does not exist a reasonable neighborhood function for TSP that has the GS property. This result is extended here by showing that data-independent neighborhood functions with the smooth property must have size of $\Omega(2^{n/3})$, where n denotes the number of cities in the TSP instance. Papadimitriou and Steiglitz [7] show that all k-opt neighborhood functions for TSP do not have the GS property and their local optima can have cost that is arbitrarily worse than the cost of global optima. In particular, Papadimitriou and Steiglitz [7] show that there exist instances of TSP with $8n$ cities, for which there is a unique optimal tour and $2^{n-1}(n-1)!$ tours that are second best with arbitrarily high cost. Furthermore, all of these $2^{n-1}(n-1)!$ tours that are second best cannot be improved without changing fewer than $3n$ edges. Tovey [11] shows that every reasonable neighborhood function for maximum clique and MAX SAT does not have the smooth property. This MAX 3-SAT result is strengthened here by showing that all data-independent neighborhood functions for MAX 3-SAT do not have the smooth property, except for neighborhood functions that contain all possible solutions for instances with $n \geqslant 4$ Boolean variables. Rodl and Tovey [9] also demonstrate that for a maximum-independent set, there exists a graph

G (up to the relabeling of the vertices) such that all neighborhood functions of polynomial size have exponentially many local optima.

Showing that particular NP-hard discrete optimization problems do not have a reasonable neighborhood function with the smooth property is important since it is conjectured that this condition is characteristic of all NP-hard discrete optimization problems. In other words, it is conjectured that all NP-hard discrete optimization problems have the property that every reasonable neighborhood function does not have the smooth property. This result is likely to be hard to prove in general since it implies that P $\neq$ NP [11]. Conversely, a discrete optimization problem is not necessarily hard if it does not have a reasonable neighborhood function with the smooth property, since there exist polynomially solvable such problems that do not have a reasonable neighborhood function with the smooth property. The results in this paper for MAX 3-SAT, 0–1 knapsack and TSP also hold for corresponding polynomially solvable sub-problems.

The results in this paper do not rely on complexity theoretic assumptions. The results in this paper show that a large collection of data-independent neighborhood functions for MAX 3-SAT, 0–1 knapsack, and TSP do not have the smooth property. This is in contrast to a similar result in Yannakakis [13] that relies on the assumption that P $\neq$ NP or NP $\neq$ co-NP. Suppose that Π is an optimization problem and η is a neighborhood function such that the local search problem (Π, η) is in PLS [5]. Yannakakis [13] shows that if Π is strongly NP-hard (NP-hard), then η cannot have the GS property unless P = NP (NP = co-NP). The MAX 3-SAT result in this paper implies that any neighborhood function (which can be searched in polynomial time) with the GS property for MAX 3-SAT must be data *dependent* or complete. Also, the 0–1 knapsack (TSP) result in this paper implies that any neighborhood function (which can be computed in polynomial time) with the GS property for 0–1 knapsack (TSP) must have size $\Theta(2^n)(\Omega(2^{n/3}))$ or else it must be data dependent, unless NP = co-NP (P = NP).

The paper is organized as follows: Section 2 provides formal definitions for MAX 3-SAT, 0–1 knapsack and TSP. Section 3 give results on the size of data-independent neighborhood functions for MAX 3-SAT, 0–1 knapsack and TSP with the smooth property. Section 4 provides concluding comments and directions for future research.

2. Definitions and background

Several discrete optimization problems are now formally described. Throughout the paper, let $\boldsymbol{x}$ denote a non-negated literal and $\bar{\boldsymbol{x}}$ denote the corresponding negated literal. Therefore, a truth assignment t satisfies the literal $\boldsymbol{x}(\bar{\boldsymbol{x}})$ if and only if $t(\boldsymbol{x}) = T(t(\boldsymbol{x}) = \text{F})$.

MAX SAT. Given m clauses, over n Boolean variables $X = \{x_1, x_2, \ldots, x_n\}$, find a truth assignment $t : X \to \{\text{T}, \text{F}\}$ that maximizes the number of satisfied clauses.

MAX 3-SAT is a special case of MAX SAT in which each clause has exactly three literals.

Given a knapsack with a finite capacity and a (finite) collection of items, where each item has two integers associated with it (i.e., size and value), the objective of 0–1 knapsack is to identify a subset of items that fit into the knapsack and have highest value. Instances of 0–1 knapsack are formulated with respect to the definition of a consistent optimization problem.

0–1 knapsack. Given vectors $\boldsymbol{s}=(s(1), s(2), \ldots, s(n))$, $\boldsymbol{v}=(v(1), v(2), \ldots, v(n))$, where $s(i), v(i) \in Z^+$, and capacity $B \in Z^+$, find the vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_n) \in \{0, 1\}^n$ that maximizes the objective function $-\sum_{i=1}^n v(i) \max\{0, \sum_{i=1}^n x_i s(i) - B\} + \sum_{i=1}^n x_i v(i)$.

In this definition, $s(i)$ denotes the size of item i, $v(i)$ denotes the value of item i, and B denotes the size of the knapsack. The term $-\sum_{i=1}^n v(i) \max\{0, \sum_{i=1}^n x_i s(i) - B\}$ is a penalty function that ensures that any solution of 0–1 knapsack, for which the collection of items exceeds the size of the knapsack, will have a nonpositive objective function value.

Symmetric TSP is now formally stated.

Traveling salesman problem (TSP). Given a collection of n cities $\{x_1, x_2, \ldots, x_n\}$ and distances $d(x_i, x_j)$ for each pair of cities x_i and x_j, where $x_i \neq x_j$, find a Hamiltonian circuit (permutation of the n cities, $y_1, y_2 \ldots, y_n$, where for each i, $y_i = x_j$ for some j and $y_i \neq y_k$ for all $i \neq k$) with smallest total length $(d(y_1, y_n) + \sum_{i=1}^{n-1} d(y_i, y_{i+1}))$.

3. Neighborhood results

This section gives results on the size of data-independent neighborhood functions for MAX 3-SAT, 0–1 knapsack and TSP that have the smooth property. Theorem 1 implies that the only data-independent neighborhood functions for MAX 3-SAT with the smooth property are the complete neighborhood functions.

Theorem 1. *If η is a data-independent neighborhood function with the smooth property for MAX 3-SAT, then, for each instance I of MAX 3-SAT and truth assignment t over $n \geqslant 4$ variables, $\eta(I, t)$ consists of all truth assignments over the n variables, except for the truth assignment t itself.*

Proof. It is shown that for $n \geqslant 4$ and truth assignments $t_1, t_2 (t_1 \neq t_2)$ over n Boolean variables, there exists an instance I with n variables such that t_1 is the unique global optimum and t_2 is the unique solution with second best objective function value. This implies that $t_1 \in \eta(I, t_2)$ if η has the smooth property and the proof then follows since t_1, t_2 are arbitrary. Suppose that η is a data-independent neighborhood function and t_1, t_2 $(t_1 \neq t_2)$ are truth assignments over $n \geqslant 4$ Boolean variables $X = \{x_1, x_2, \ldots, x_n\}$. Given any truth assignment $t : X \rightarrow \{\mathrm{T}, \mathrm{F}\}$ define $h(t, x_i, x_j, x_k)$ to be the set of clauses over Boolean variables x_i, x_j, and x_k that t satisfies. For example, if $t(x_1) = \mathrm{F}$, $t(x_2) = \mathrm{F}$, and $t(x_3) = \mathrm{F}$, then

$$h(t, x_1, x_2, x_3) = \{(\bar{x}_1, \bar{x}_2, \bar{x}_3), (\bar{x}_1, \bar{x}_2, x_3), (\bar{x}_1, x_2, \bar{x}_3), (\bar{x}_1, x_2, x_3), (x_1, \bar{x}_2, \bar{x}_3), (x_1, \bar{x}_2, x_3), (x_1, x_2, \bar{x}_3)\}.$$

Choose $a, b, c \in Z^+$ $(1 \leqslant a, b, c \leqslant n)$ such that $t_1(x_a) \neq t_2(x_a)$ and $a \neq b$, $a \neq c$, $b \neq c$. Define a set of clauses

$$C = h(t_1, x_a, x_b, x_c) \cup \left(\bigcup_{i=1}^{n} \bigcup_{j=i+1}^{n} \bigcup_{k=j+1}^{n} (h(t_1, x_i, x_j, x_k) \cap h(t_2, x_i, x_j, x_k)) \right). \tag{1}$$

By construction, t_1 satisfies all the clauses in C. Also, t_2 satisfies all clauses in C, except for one clause in $h(t_1, x_a, x_b, x_c)$. Let $t : X \to \{T, F\}$ be a truth assignment such that $t \neq t_1$, $t \neq t_2$. To show that t does not satisfy as many clauses as t_2, let p and q be positive integers $(1 \leqslant p, q \leqslant n)$ such that $t(x_p) \neq t_1(x_p)$ and $t(x_q) \neq t_2(x_q)$. Therefore, there are two cases to consider.

Case 1: If $p \neq q$, then the truth assignment t does not satisfy one clause in $h(t_1, x_p, x_q, x_k) \cap h(t_2, x_p, x_q, x_k)$, where $k \neq p$ and $k \neq q$. It then follows that t does not satisfy at least $n - 2$ clauses in C.

Case 2: If $p = q$, then the truth assignment t does not satisfy one clause in $h(t_1, x_p, x_j, x_k) \cap h(t_2, x_p, x_j, x_k)$, where $j \neq p$, $k \neq p$, and $j \neq k$. Therefore, the truth assignment t does not satisfy at least $\binom{n-1}{2}$ clauses in C.

From Cases 1 and 2, t does not satisfy at least $n - 2$ clauses of C. Therefore, t_1 is the unique truth assignment that satisfies all clauses in C and t_2 is the unique truth assignment that satisfies all but one clause in C. □

The class MAX 3-SAT instances that can be specified according to (1) can be formulated into a polynomially solvable sub-problem of MAX 3-SAT. Instances of the form given in (1) can be recognized in polynomial time. Furthermore, given an instance of the form in (1), the optimal solution (truth assignment that satisfies all of the clauses) can be found in polynomial time. Therefore, Theorem 1 also holds for a polynomially solvable sub-problem of MAX 3-SAT.

In contrast to the result for MAX 3-SAT, there exists a data-independent neighborhood function with the smooth property for 0–1 knapsack that is not complete. The size of data-independent neighborhood functions for 0–1 knapsack can be given as a function of the number of possible items. Theorem 2 shows that there exists a data-independent neighborhood function η^{K} with the smooth property for 0–1 knapsack that has size $\Theta(2^n)$.

Theorem 2. *There exists a data-independent neighborhood function with the GS property for* 0–1 *knapsack with size*

$$f(n) = \begin{cases} 2^n - 2^{n/2+1} + n - k + 2 & for\ n\ even \\ 2^n - 2^{(n-1)/2} - 2^{(n+1)/2} + n - k + 2 & for\ n\ odd \end{cases} \quad for\ n \geqslant 1,$$

where n denotes the number of possible items.

Proof. Let $n \geqslant 1$. Construct a neighborhood function η for 0–1 knapsack as follows: for each instance I over n Boolean variables, $\boldsymbol{x} \in \{0,1\}^n$, and $\boldsymbol{x} \neq \boldsymbol{0}$,

$$\eta^{\mathrm{K}}(I,\boldsymbol{x}) = \{0,1\}^n - \left\{\boldsymbol{y} \in \{0,1\}^n : \sum_{i=1}^{n} y_i - x_i \geqslant 2 \quad \text{and} \quad \boldsymbol{y}-\boldsymbol{x} \in \{0,1\}^n\right\},$$
$$- \ \{\boldsymbol{y} \in \{0,1\}^n : \boldsymbol{y} \neq \boldsymbol{0} \quad \text{and} \quad \boldsymbol{x}-\boldsymbol{y} \in \{0,1\}^n\}.$$

For $\boldsymbol{x} = \boldsymbol{0}$, define $\eta^{\mathrm{K}}(I,\boldsymbol{x}) = \{\boldsymbol{y} = (y_1, y_2, \ldots, y_n) \in \{0,1\}^n : \sum_{i=1}^{n} y_i = 1\}$. Suppose that $\boldsymbol{x}$ has exactly $k \geqslant 1$ elements equal to one. Then, $|\eta^{\mathrm{K}}(I,\boldsymbol{x})| = 2^n - 2^{n-k} - 2^k + n - k + 2$. The value of $|\eta^{\mathrm{K}}(I,\boldsymbol{x})|$ is maximized when there are $k = n/2$ elements equal to one, for n even, and $k = (n-1)/2$ elements equal to one, for n odd. Given $\boldsymbol{x} \in \{0,1\}^n$, $\boldsymbol{x} \neq \boldsymbol{0}$, if there exists a solution with better objective function value (as defined in Section 2) than $\boldsymbol{x}$ in the set $\{\boldsymbol{y} \in \{0,1\}^n : \boldsymbol{y}-\boldsymbol{x} \in \{0,1\}^n\}$, then there exists an improving solution to $\boldsymbol{x}$ in the set $\{\boldsymbol{y} \in \{0,1\}^n : \sum_{i=1}^{n} x_i - y_i = 1$ and $\boldsymbol{y}-\boldsymbol{x} \in \{0,1\}^n\}$. Also, if a solution in the set $\{\boldsymbol{y} \in \{0,1\}^n : \boldsymbol{x}-\boldsymbol{y} \in \{0,1\}^n\}$ has objective function value greater than $\boldsymbol{x}$, then the solution $\boldsymbol{y}=\boldsymbol{0}$ has a better objective function value than $\boldsymbol{x}$. It then follows that η^{K} has the GS property (and hence the smooth property) since η^{K} has no local optima, except for global optima. □

Theorem 3 shows that the neighborhood function η^{K} described in the proof of Theorem 2 is the minimal data-independent neighborhood function with the smooth property. Therefore, Theorem 3 implies that a data-independent neighborhood function with the smooth property for 0–1 knapsack must have size $\Theta(2^n)$.

Theorem 3. *Let η^{K} be the neighborhood function for* 0–1 *knapsack that is given in the proof of Theorem* 2. *If η is a data-independent neighborhood function such that $\eta(I,\boldsymbol{x}) \subset \eta^{\mathrm{K}}(I,\boldsymbol{x})$ for some $\boldsymbol{x} \in \{0,1\}^n$ $(n \geqslant 1)$ and instance I, then η does not have the smooth property.*

Proof. The proof follows by showing that η does not have the smooth property. By definition, any data-independent neighborhood function for 0–1 knapsack is independent of the instance I and depends only on the solution $\boldsymbol{x} \in \{0,1\}^n$. Therefore, the neighborhood of a solution $\boldsymbol{y}$ for a data-independent neighborhood function η may be written as $\eta(\boldsymbol{y})$. Suppose that $\boldsymbol{x}^* \in \{0,1\}^n$ such that $\boldsymbol{x}^* \in \eta^{\mathrm{K}}(\boldsymbol{x}) - \eta(\boldsymbol{x})$. The proof follows by showing that there exists an instance of 0–1 knapsack over n variables such that $\boldsymbol{x}^*$ has better objective function value than $\boldsymbol{x}$ and no other solution in $\eta(\boldsymbol{x})$ has objective function value greater than or equal to $\boldsymbol{x}$. In the following, for any $\boldsymbol{y} \in \{0,1\}^n$, define $\Delta(\boldsymbol{y}) = \{i : y_i = 1\}$. There are three possibilities for the solution $\boldsymbol{x}^*$.

Case 1: $\boldsymbol{x}^* - \boldsymbol{x} \in \{0,1\}^n$ and $\sum_{i=1}^{n} x_i^* - x_i = 1$. Suppose that $\sum_{i=1}^{n} x_i = k$. In this case, let $B = k+1$, $v(i) = 2$ for $i \in \Delta(\boldsymbol{x})$, $v(i) = 1$ for $i \notin \Delta(\boldsymbol{x})$, $s(i) = 1$ for $i \in \Delta(\boldsymbol{x}^*)$, and $s(i) = B+1$ for $i \notin \Delta(\boldsymbol{x}^*)$. It then follows that $\boldsymbol{x}^*$ is the unique global optimum and $\boldsymbol{x}$ is the unique solution with second best objective function value.

Case 2: $\boldsymbol{x}^* = \boldsymbol{0}$. Let $B = 1$, $v(i) = 1$ for $i = 1, 2, \ldots, n$, and $s(i) = 2$ for $i \in \Delta(\boldsymbol{x})$ and $s(i) = 2n$ for $i \notin \Delta(\boldsymbol{x})$. Therefore, there is no solution in $\eta(\boldsymbol{x})$ with better objective function value than $\boldsymbol{x}$.

Case 3: $\boldsymbol{x}^* - \boldsymbol{x} \notin \{0, 1\}^n$ and $\boldsymbol{x} - \boldsymbol{x}^* \notin \{0, 1\}^n$. Let $k_1 = |\Delta(\boldsymbol{x}^*) - \Delta(\boldsymbol{x})|$, $k_2 = |\Delta(\boldsymbol{x}) - \Delta(\boldsymbol{x}^*)|$, $k_3 = k_1 + k_2$ and $k_4 = |\Delta(\boldsymbol{x}^*) \cap \Delta(\boldsymbol{x})|$. Also, let $\Delta(\boldsymbol{x}^*) - \Delta(\boldsymbol{x}) = \{\delta_{11}, \delta_{12}, \ldots, \delta_{1k_1}\}$ and $\Delta(\boldsymbol{x}) - \Delta(\boldsymbol{x}^*) = \{\delta_{21}, \delta_{22}, \ldots, \delta_{2k_2}\}$. Note that $k_1, k_2 \geqslant 1$. Define the values and sizes for the items as follows:

$$v(\delta_{11}) = s(\delta_{11}) = 2^{k_3}, \quad v(\delta_{21}) = s(\delta_{21}) = 2^{k_3-1} + 2\sum_{i=1}^{k_1-1} 2^{k_1-i} + 1,$$

$$v(\delta_{1i}) = s(\delta_{1i}) = 2^{k_1-i+1} \quad \text{for } i = 2, 3, \ldots, k_1,$$

$$v(\delta_{2i}) = s(\delta_{2i}) = 2^{k_3-i} \quad \text{for } i = 2, 3, \ldots, k_2,$$

$$v(i) = s(i) = 2^{k_3+2} \quad \text{for } i \in \Delta(\boldsymbol{x}^*) \cap \Delta(\boldsymbol{x})$$

and

$$v(i) = 1, \quad s(i) = B = k_4 2^{k_3+2} + 2^{k_3} + \sum_{i=1}^{k_1-1} 2^{k_1-i} \quad \text{for } i \notin \Delta(\boldsymbol{x}^*) \cup \Delta(\boldsymbol{x}).$$

For the remainder of the proof, let $V(\boldsymbol{y}) = \sum_{i=1}^{n} v(i) y_i$ and $S(\boldsymbol{y}) = \sum_{i=1}^{n} s(i) y_i$ for any $\boldsymbol{y} \in \{0, 1\}^n$. Then

$$V(\boldsymbol{x}^*) = S(\boldsymbol{x}^*) = k_4 2^{k_3+2} + 2^{k_3} + \sum_{i=1}^{k_1-1} 2^{k_1-i}$$

and

$$V(\boldsymbol{x}) = S(\boldsymbol{x}) = k_4 2^{k_3+2} + \sum_{i=1}^{k_2} 2^{k_3-i} + 2\sum_{i=1}^{k_1-1} 2^{k_1-i} + 1$$
$$= k_4 2^{k_3+2} + 2^{k_3} + \sum_{i=1}^{k_1-1} 2^{k_1-i} - 1 = V(\boldsymbol{x}^*) - 1.$$

Now, $\boldsymbol{x}^*$ and $\boldsymbol{x}$ will be shown to be the unique global optimum and unique solution with second best objective function value, respectively. Suppose that $\boldsymbol{y} \in \{0, 1\}^n$ such that $V(\boldsymbol{y}) \geqslant V(\boldsymbol{x})$ and $S(\boldsymbol{y}) \leqslant B$, and show that $\boldsymbol{y} = \boldsymbol{x}^*$ or $\boldsymbol{y} = \boldsymbol{x}$. For $i \in \Delta(\boldsymbol{x}^*) \cap \Delta(\boldsymbol{x})$, $v(i) = 2^{k_3+2} > \sum_{i=1}^{k_1} v(\delta_{1i}) + \sum_{i=1}^{k_2} v(\delta_{2i})$. Therefore, $y_i = 1$ for all $i \in \Delta(\boldsymbol{x}^*) \cap \Delta(\boldsymbol{x})$. Furthermore, since $s(i) = B$ for $i \notin \Delta(\boldsymbol{x}^*) \cup \Delta(\boldsymbol{x})$, then $y_i = 0$ for all $i \notin \Delta(\boldsymbol{x}^*) \cup \Delta(\boldsymbol{x})$. Since $V(\boldsymbol{y}) \geqslant V(\boldsymbol{x})$, then $y_{\delta_{11}} = 1$ or $y_{\delta_{21}} = 1$. However, it is impossible that $y_{\delta_{11}} = y_{\delta_{21}} = 1$, since this implies that $S(\boldsymbol{y}) \geqslant k_4 2^{k_3+2} + 2^{k_3} + 2^{k_3-1} + 2\sum_{i=1}^{k_1-1} 2^{k_1-i} + 1 > B$. Therefore, there are two possibilities:

Case 3a: $y_{\delta_{11}} = 1$ and $y_{\delta_{21}} = 0$. In this case, $y_{\delta_{2i}} = 0$ for all $i = 1, 2, \ldots, k_2$, since otherwise $S(\boldsymbol{y}) \geqslant k_4 2^{k_3+2} + 2^{k_3} + 2^{k_3-k_2} > B$. Also, since $V(\boldsymbol{y}) \geqslant V(\boldsymbol{x})$ and $v(\delta_{1i}) \geqslant 2$ $(i = 1, 2, \ldots, k_1)$, then $y_{\delta_{1i}} = 1$ for all $i = 1, 2, \ldots, k_1$. Therefore, $\boldsymbol{y} = \boldsymbol{x}^*$.

Case 3b: $y_{\delta_{11}} = 0$ and $y_{\delta_{21}} = 1$. Since $V(\boldsymbol{y}) \geqslant V(\boldsymbol{x})$ and $v(\delta_{1i}) \leqslant 2^{k_1-i}$ $(i = 2, 3, \ldots, k_1)$, then $y_{\delta_{2i}} = 1$ for all $i = 1, 2, \ldots, k_2$. Furthermore, if $y_{\delta_{1i}} = 1$ for some $i = 1, 2, \ldots, k_1$, then $S(\boldsymbol{y}) \geqslant B + 1$. Therefore, $\boldsymbol{y} = \boldsymbol{x}$. $\square$

Theorem 4 shows that for every reasonable neighborhood function of TSP, there exists an instance of TSP with *strict* local optima that are not global optima; hence TSP has no reasonable neighborhood function with the smooth property. Furthermore, Theorem 4 shows that many exponentially sized and data-independent neighborhood functions do not have the smooth property. The proof of Theorem 4 follows by starting with an arbitrary solution ω and choosing another solution $\omega_{A'}$ (that is not a neighbor of ω) from an exponential set of solutions A' (Hamiltonian circuits) such that there does not exist any solution using edges from only ω and $\omega_{A'}$, except for the solutions ω and $\omega_{A'}$ themselves. The distances between the cities are then defined so that $\omega_{A'}$ and ω are the unique global optimum and unique second best solution (Hamiltonian circuit), respectively. For TSP, the size of data-independent neighborhood functions can be given as a function of the number of cities n in an instance.

Theorem 4. *If η is a data-independent neighborhood function for the TSP with the smooth property, then* $\min_{\mathbf{x}\in \mathrm{SOL}(I)} |\eta(I,\mathbf{x})| = \Omega(2^{n/3})$, *where n denotes the number of cities.*

Proof. The proof follows by showing that any data-independent neighborhood function η for TSP such that $|\eta(I,\omega)| < 2^{\lfloor (n-2)/3\rfloor} - 1$, where I is a n ($\geqslant 5$) city TSP instance, does not have the smooth property. Let η be a data-independent neighborhood function for TSP such that $|\eta(I,\omega)| < 2^{\lfloor (n-2)/3\rfloor} - 1$ for some TSP instance I with n ($\geqslant 5$) cities and solution ω. Consider the collection of $\lfloor (n-2)/3\rfloor$ pairs of cities

$$\Delta = \{(i, i+1) : i = 2 + 3k,\ \ k = 0, 1, \ldots, \lfloor (n-2)/3\rfloor - 1\}.$$

Let $A = \{(k_i, k_i + 1) : i = 1, 2, \ldots, p\}$ (where $k_i < k_{i+1}$ for $i = 1, 2, \ldots, p-1$) be a subset of size p of the set Δ and define the solution (Hamiltonian circuit):

$\omega_A = 12\ldots(k_1-1)(k_1+1)k_1(k_1+2)\ldots(k_2-1)(k_2+1)k_2(k_2+2)\cdots(k_p-1)(k_p+1)k_p(k_p+2)(k_p+3)\cdots n$.

Suppose A and B are two non-empty subsets of Δ such that $A \neq B$, then $\omega_A \neq \omega_B$. Also, note there are $2^{\lfloor (n-2)/3\rfloor} - 1$ different non-empty subsets of Δ. Without loss of generality, suppose $\omega = 123\ldots n$. Since $|\eta(I,\omega)| < 2^{\lfloor (n-2)/3\rfloor} - 1$, where I denotes an n-city TSP instance, choose a subset $A' \subset \Delta$ such that $\omega_{A'} \notin \eta(I,\omega)$. Let $A' = \{(k_i, k_i+1) : i = 1, 2, \ldots, p\}$ (where $k_i < k_{i+1}$ for $i = 1, 2, \ldots, p-1$) for some positive integer p ($1 \leqslant p \leqslant \lfloor (n-2)/3\rfloor$). Define the distance function

$$d(k_i - 1, k_i + 1) = d(k_i, k_i + 2) = 1 \quad \text{for all } i = 1, 2, \ldots, p,$$

$$d(i, i+1) = 1 \quad \text{for all } i = 1, 2, \ldots, n-1,\ \ i \neq k_1 - 1, \quad d(n, 1) = 1,$$

$$d(k_1 - 1, k_1) = 2.$$

Suppose that all of the remaining edges have length three. It then follows that the length of ω is $n+1$ and the length of $\omega_{A'}$ is n.

To complete the proof, to show that ω is the unique solution of length $n+1$ and $\omega_{A'}$ is the unique solution of length n, suppose that there exists a solution $\omega' = x_1x_2\ldots x_n$ of length less than or equal to $n+1$. Then, by the distance definition, every edge that is part of solution ω' must be an edge on ω or $\omega_{A'}$. Therefore, $\omega' = 12\ldots(k_1-1)x_{k_1}x_{k_1+1}\ldots x_n$; hence there are two possibilities: $x_{k_1} = k_1$ or $x_{k_1} = k_1 + 1$. If $x_{k_1} = k_1$, then $x_{k_1+1} = k_1 + 1$

since otherwise, $x_{k_1+1} = k_1 + 2$ and it is impossible to visit both cities $k_1 + 1$ and $k_1 + 3$ using edges only on ω or $\omega_{A'}$. Similarly, if $x_{k_1} = k_1 + 1$, then $x_{k_1+1} = k_1$ since otherwise, $x_{k_1+1} = k_1 + 2$ and it is impossible to visit both cities k_1 and $k_1 + 3$ by using edges only on ω or $\omega_{A'}$. Therefore,

$$\omega' = 12 \ldots (k_2 - 1)x_{k2} \ldots x_n \quad \text{or}$$
$$\omega' = 12 \ldots (k_1 - 1)(k_1 + 1)k_1(k_1 + 2) \ldots (k_2 - 1)x_{k_2}x_{k_2+1} \ldots x_n.$$

Iteratively applying this argument results in $\omega' = \omega$ or $\omega' = \omega_{A'}$. Therefore, ω is the unique solution of length $n + 1$ and $\omega_{A'}$ is the unique solution of length n. Since $\omega_{A'} \notin \eta(I, \omega)$, then ω is a strict local optimum that is not a global optimum. □

Similar to Theorems 1 and 3, the class of instances used in the proof of Theorem 4 can be formulated into a polynomially solvable sub-problem. It follows that there exists a polynomially solvable sub-problem of TSP such that a data-independent neighborhood function η with the smooth property must satisfy $\min_{x \in \mathrm{SOL}(I)} |\eta(I, \boldsymbol{x})| = \Omega(2^{n/3})$. The results in this section demonstrate a drawback of local search algorithms that use data-independent neighborhood functions for MAX 3-SAT, 0–1 knapsack and TSP. These results also provide a first step towards showing that a large class of NP-hard discrete optimization problems has the property that every reasonable neighborhood function does not have the smooth property.

4. Conclusions and directions for future research

A difficulty with local search algorithms is that neighborhood functions for NP-hard discrete optimization problems typically have many (strict) local optima that are not global optima. This paper shows that a large class of neighborhood functions for MAX 3-SAT, 0–1 knapsack and TSP do not have the smooth property. In particular, the complete neighborhood functions are shown to be the only data-independent neighborhood functions with the smooth property for MAX 3-SAT. The smallest data-independent neighborhood function for 0–1 knapsack is proven to have size with the same order of magnitude as the solution space size. Furthermore, the results demonstrate the minimal data-independent neighborhood functions with the smooth property for 0–1 knapsack and MAX 3-SAT. Every reasonable neighborhood function (and many exponentially sized data-independent neighborhood functions) for TSP is shown to not have the smooth property.

Directions for future research include studying the properties of data-independent neighborhood functions for other discrete optimization problems. By doing this, it may be possible to develop a general proof that would show that every reasonable neighborhood function for a large class of discrete optimization problems has at least one strict local optimum that is not a global optimum. In particular, one future direction of research focuses on determining if transformations between discrete optimization problems can be used to show that problems do not have reasonable neighborhood functions with the smooth property. That is, developing transformations from a problem Π_A to a problem Π_B so that if problem Π_A does not have a reasonable neighborhood function with the smooth property, then problem Π_B does not have a reasonable neighborhood function with the smooth property. Armstrong and Jacobson [2] have defined a transformation between discrete optimization problems that preserves semi-reasonable neighborhood functions in this manner. A semi-reasonable neighborhood function is a neighborhood function that is independent of the problem data, except that it may depend on the maximum absolute value of a number in an instance. It would be useful to obtain similar results as reported in [2] for data-independent neighborhood functions. The overall objective of this research is to develop an understanding of the properties of neighborhood functions for discrete optimization problems.

Acknowledgements

The authors would like to thank Dr. Peter L. Hammer (the Editor-in-Chief), as well as two anonymous referees for their insightful feedback and suggestions for the paper, resulting in a significantly improved manuscript. This research has been supported in part by the National Science Foundation (DMI-9907980) and the Air Force Office of Scientific Research (F49620-01-1-0007, FA9550-04-1-0110).

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