# Theoretical Properties of Two ACO Approaches for the Traveling Salesman Problem

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**Abstract.** Ant colony optimization (ACO) has been widely used for different combinatorial optimization problems. In this paper, we investigate ACO algorithms with respect to their runtime behavior for the traveling salesperson (TSP) problem. We present a new construction graph and show that it has a stronger local property than the given input graph which is often used for constructing solutions. Later on, we investigate ACO algorithms for both construction graphs on random instances and show that they achieve a good approximation in expected polynomial time.

## 1 Introduction

Stochastic search algorithms such as evolutionary algorithms (EAs) [4] and ant colony optimization (ACO) [3] are robust problem solvers that have found a wide range of applications in various problem domains. In contrast to many successful application of this kind of algorithms, the theoretical understanding lags far behind their practical success. Therefore, it is highly desirable to increase the theoretical understanding of these algorithms.

The goal of this paper is to contribute to the theoretical understanding of stochastic search algorithms by rigorous runtime analyses. Such studies have been successfully applied for evolutionary algorithms and have highly increased the theoretical foundation of this kind of algorithms. In the case of ACO algorithms the theoretical analyses of their runtime behavior has been started only recently [12, 6, 7, 11, 10, 8]. We increase the theoretical understanding of ACO algorithms by investigating their runtime behavior on the well-known traveling salesperson (TSP) problem. For ACO the TSP problem is the first problem where this kind of algorithms has been applied. Therefore, it seems to be natural to study the behavior of ACO algorithms for the TSP problem from a theoretical point of view in a rigorous manner.

ACO algorithms are inspired by the behavior of ants to search for a shortest path between their nest and a common source of food. It has been observed that ants find such a path very quickly by using indirect communication via pheromones. This observed behavior is put into an algorithmic framework by considering artificial ants that construct solutions for a given problem by carrying out random walks on a so-called construction graph. The random walk (and the resulting solution) depends on pheromone values that are values on the edges of the construction graph. The probability of traversing a certain edge depends on its pheromone value. One widely used construction procedure for tackling the TSP has already been analyzed in [14]. It constructs a tour in an *ordered* manner, where the iteratively chosen edges form a path at all times. In this paper, we give new runtime bounds for ACO algorithms using this construction procedure. On the other hand, we propose a new construction procedure, where, in each iteration, an *arbitrary* edge not creating a cycle or a vertex of degree 3 may be added to extend the partial tour. We analyze both construction methods and point out their differences.

Our analysis of these two ACO variants goes as follows. We first examine the locality of changes made, i.e., how many edges of the current-best solution are also in the newly sampled tour, and how many are *exchanged* for other edges. We then use these results as upper bounds on the time until certain desired local changes are made to derive upper bounds on the optimization time.

In particular, we show the following results:

- The ordered edge insertion algorithm exchanges an expected number of  $\Omega(\log(n))$  many edges (Theorem 1) while the arbitrary edge insertion exchanges only an expected constant number of edges (Theorem 4).
- Arbitrary edge insertion has a probability of  $\Theta(1/n^2)$  for any specific exchange of two edges (Corollary 1), while ordered edge insertion has one of  $\Theta(1/n^3)$  [14].
- The simple TSP-instance analyzed in [14] is optimized by arbitrary edge insertion in an expected number of  $O(n^3 \log(n))$  steps (Theorem 5), while the best known bound for ordered edge insertion is  $O(n^6)$  ([14]).
- Both construction graphs lead in expected polynomial time to a good approximation on random instances.

In particular, arbitrary edge insertion allows for better runtime bounds thanks to its locality. It remains open whether there are TSP instances where the non-locality of ordered edge insertion provably gives better runtime bounds than the more local arbitrary edge insertion.

The rest of the paper is organized as follows. In Section 2, we introduce the problem and the algorithms that are subject to investigations. We investigate the number of edge exchanges for large pheromone updates in Section 3 and prove runtime bounds for certain classes of instances in Section 4. Finally, we finish with some concluding remarks and topics for future work.

#### 2 Problem and Algorithms

In this paper, we consider the symmetric Traveling Salesperson Problem (TSP). We are given a complete undirected graph G = (V, E) and a weight function  $w : E \to \mathbb{R}_+$  that assigns positive weights to the edges. The goal is to find a tour of minimum weight that visits every vertex exactly once and returns to the start vertex afterwards. We analyze an ACO algorithm called MMAS<sup>\*</sup> (Min-Max Ant System – see Algorithm 1), already used in different theoretical studies [11, 14]. MMAS<sup>\*</sup> works iteratively, creating one new candidate solution x in each iteration, and keeping track of the best-so-far solution  $x^*$ . A new candidate solution for a target graph G is constructed by an artificial ant that performs a random walk on an underlying graph, called the *construction graph*, step by

step choosing components of a new candidate solution. In this paper, we use edges of the given input as the components that influence this random walk. In each step of its random walk on the construction graph, we want the ant to choose an edge e in G with a probability based on *pheromone value*  $\tau(e)$ .<sup>1</sup> We use a procedure construct based on the pheromones  $\tau$  as given in Algorithm 2. In this paper, we consider two different approaches of constructing new solutions by specifying the neighborhood function Nof Algorithm 2 in Sections 2.1 and 2.2.

Algorithm 1: The algorithm MMAS*.	
1 function $MMAS^*$ on $G = (V, E)$ is	
2	$\tau(e) \leftarrow 1/ V $ , for all $e \in E$ ;
3	$x^* \leftarrow \texttt{construct}(\tau);$
4	$ tupdate( au, x^*);$
5	while true do
6	$x \leftarrow \texttt{construct}(\tau);$
7	<b>if</b> $f(x) > f(x^*)$ <b>then</b>
8	$x^* \leftarrow x;$
9	$\tau \leftarrow \texttt{update}(\tau, x^*);$
,	

Algorithm 2: The algorithm construct.		
1 function construct based on $\tau$ is		
2	for $k = 0$ to $n - 2$ do	
3	$ R \leftarrow \sum_{y \in N(e_1, \dots, e_k)} \tau(y); $	
4	Choose one neighbor $e_{k+1}$ of $e_k$ where the probability of selection of any fixed	
	for $k = 0$ to $n - 2$ do $R \leftarrow \sum_{y \in N(e_1, \dots, e_k)} \tau(y);$ Choose one neighbor $e_{k+1}$ of $e_k$ where the probability of selection of any fixed $y \in N(e_1, \dots, e_k)$ is $\frac{\tau(y)}{R};$	
5	Let $e_n$ be the (unique) edge completing the tour;	
6	return $(e_1,\ldots,e_n);$	

For each edge  $e \in E$ , the pheromones are kept within upper and lower bounds  $\tau_{\max}$  and  $\tau_{\min}$ , respectively. The pheromone values change after each iteration of MMAS<sup>\*</sup> according to a procedure update and an *evaporation factor*  $\rho$ : For a tour x, let E(x) be the set of edges used in x; for each edge e, the pheromone values are updated such that the new pheromone values  $\tau' = \text{update}(\tau, x)$  are such that

$$\tau'(e) = \begin{cases} \min\left\{(1-\rho) \cdot \tau(e) + \rho, \tau_{\max}\right\}, & \text{if } e \in E(x);\\ \max\left\{(1-\rho) \cdot \tau(e), \tau_{\min}\right\}, & \text{otherwise.} \end{cases}$$

<sup>&</sup>lt;sup>1</sup> Note that, in this paper, we are not concerned with the use of *heuristic information*.

Here,  $\rho$ ,  $0 \le \rho \le 1$ , is the evaporation factor which determines the strength of an update. As in [14], we use  $\tau_{\min} = 1/n^2$  and  $\tau_{\max} = 1 - 1/n$  throughout this paper, where *n* is the number of nodes of the input graph; further, initial values for pheromones are 1/n. If in an iteration of MMAS<sup>\*</sup> the pheromone values are such that, for exactly the edges of the best-so-far tour the pheromone values are at  $\tau_{\max}$  and all others are at  $\tau_{\min}$ , we call the pheromones *saturated* at that iteration.

To measure the runtime of MMAS\*, it is common to consider the number of constructed solutions. Often we investigate the expected number of constructed solutions until an optimal tour or a good approximation of an optimal tour is obtained.

#### 2.1 The Input Graph as Construction Graph

To specify the construction graph, we need to introduce the neighborhood function N in Algorithm 2. The most common way of constructing a tour for TSP problem is to use the input graph as construction graph (see e. g. [2]). A tour is constructed by having an ant start at some vertex, visit all vertices by moving to a neighbor of the current vertex, and finally coming back to the start vertex. We model this behavior with a neighbor set as follows. For each sequence  $\sigma$  of chosen edges, let  $U(\sigma)$  be the set of unvisited nodes and  $l(\sigma)$  the most recently visited node (or, if  $\sigma$  is empty, some distinguished node); let

$$N_{Ord}(\sigma) = \{\{l(\sigma), u\} \mid u \in U(\sigma)\}.$$

This set has the advantage of being easily computable and of size linear in the number of edges needed to complete the tour. We will discuss drawbacks of this neighborhood set later. We will refer to MMAS<sup>\*</sup> using this neighborhood as  $MMAS^*_{Ord}$  ("Ord" is mnemonic for the "ordered" way in which edges are inserted into the new tour).

#### 2.2 An Edge-Based Construction Graph

Alternatively, we can let the ant choose to add any edge to the set of edges chosen so far, as long as no cycle and no vertex are created. This is modeled by a neighbor set as follows. For each sequence  $\sigma$  of chosen edges, let  $V(\sigma)$  be the set of previously chosen edges and

$$N_{Arb}(\sigma) = (E \setminus V(\sigma)) \setminus \{e' \in E \mid (V, \{e'_1, \dots, e'_k, e'\}) \text{ contains a cycle or a vertex of degree} \ge 3\}.$$

This set has a size quadratic in the number of edges required to complete the tour. We will refer to MMAS<sup>\*</sup> using this neighborhood as  $MMAS^*_{Arb}$  ("Arb" is mnemonic for the "arbitrary" way in which edges are inserted into the new tour).

## **3** Number of Edge Exchanges

In this section, we consider the expected number of edges that a newly constructed solution x differs from the best-so-far solution  $x^*$  if the pheromone values are saturated.

In this case, the solution  $x^*$  can often be reproduced with constant probability and it is desirable that  $x^*$  and x only differ by a small (constant) number of edges. In such a situation, ACO algorithms are able to carry out improving steps by sampling solutions in their local neighborhood. In particular, for a tour t, we are interested in tours t' such that t and t' differ by exchanging 2 or 3 edges, called a 2-Opt or a 3-Opt neighbor, respectively.

#### 3.1 The Behavior of MMAS<sup>\*</sup><sub>Ord</sub>

In the following we examine  $MMAS^*_{Ord}$ . We show that the expected number of edges where  $x^*$  and x differ is  $\Omega(\log n)$ . Thus, the  $MMAS^*_{Ord}$  does not have the desired local property.

The reason for this large number of exchange operations is that if an ant has left the path corresponding the currently best solution then it will encounter paths of high pheromone that do not cover the rest of the tour. The rest of the tour needs to be discovered by joining different subpaths of high pheromone which implies the lower bound on the expected number of edge exchanges.

In the proof of the claimed result, we consider the following random process which captures the situation after an ant has left the high pheromone path for the first time. Let W be a walk on a sequence of t vertices. W starts at a random vertex, and will go to the just previous or following vertex in the sequence with equal probability, if both are available and unvisited. If only one is available and unvisited, W will go to this one. If none are available and unvisited, the walk will *jump* uniformly at random to an unvisited vertex. The walk ends as soon as all vertices are visited.

**Lemma 1.** For each t, let  $X_t$  be the random variable denoting number of jumps made by the walk W on a path of t vertices. Then we have

$$\forall t \ge 3 : E(X_t) \ge \frac{1}{6}\ln(t).$$

*Proof.* We start by giving a recursive definition of  $X_t$ . Clearly,  $X_1 = 0$  and  $X_2 = 0$ . Let  $t \ge 3$ . The walk can start with uniform probability in any vertex, and will not jump if the first or last vertex has been chosen. Otherwise, with equal probability, the walk will start up or down. After visiting all nodes in the chosen direction, the walk will jump once, and then perform a walk according to  $X_i$ , where *i* is the number of unvisited nodes just before the jump. Thus, we get, for all  $t \ge 3$ ,

$$E(X_t) = \frac{1}{t} \sum_{i=2}^{t-1} \left(\frac{1}{2} \left(1 + E(X_{i-1})\right) + \frac{1}{2} \left(1 + E(X_{t-i})\right)\right)$$
$$= \frac{t-2}{t} + \frac{1}{t} \left(\frac{1}{2} \sum_{i=2}^{t-1} E(X_{i-1}) + \frac{1}{2} \sum_{i=2}^{t-1} E(X_{t-1})\right)$$
$$= \frac{t-2}{t} + \frac{1}{t} \sum_{i=1}^{t-2} E(X_i) = \frac{t-2}{t} + \frac{1}{t} \sum_{i=3}^{t-2} E(X_i)$$

The claim is true for t = 3. We show the remainder of the claim of the lemma by induction on t. Let  $t \ge 4$  and for all  $i, 3 \le i < t$ ,  $E(X_i) \ge \frac{1}{6} \ln(i)$ . Using  $t \ge 3$ , we have  $(t-2)/t \ge 1/3$ . Thus, also using the induction hypothesis,

$$E(X_t) \ge \frac{1}{3} + \frac{1}{t} \sum_{i=3}^{t-2} \frac{1}{6} \ln(i)$$
  
=  $\frac{1}{3} + \frac{1}{t} \frac{1}{6} \ln(\prod_{i=3}^{t-2} i) = \frac{1}{3} + \frac{1}{t} \frac{1}{6} \ln((t-2)!/2) \ge \frac{1}{6} \ln(t).$ 

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Next we will give a lower bound on the expected number of edge exchanges which MMAS<sup>\*</sup><sub>Ord</sub> will make when saturated.

**Theorem 1.** If in an iteration of  $MMAS^*_{Ord}$  the pheromone values are saturated, then, in the next iteration of  $MMAS^*_{Ord}$ , the newly constructed tour will exchange an expected number of  $\Omega(\log(n))$  of edges.

*Proof.* It is easy to see that an ant leaves the path corresponding the currently best solution  $x^*$  with probability  $\Omega(1)$  after having visited at most n/2 vertices. After the ant has left the path it performs on the remaining  $r \ge n/2$  vertices as a walk similar to W on a path of length r. In fact, with constant probability, the ant will never leave the path again unless necessary, so that we get the result by applying Lemma 1.  $\Box$ 

However, constructing new solutions with few exchanged edges is still somewhat likely. In [14] it is shown that the probability for a particular 2-Opt step is  $\Omega(1/n^3)$ . Taking a closer look at the analysis presented in this paper a matching upper bound on this probability can be extracted. In summary, we get the following result.

**Theorem 2** ([14]). Let t be a tour found by  $MMAS^*_{Ord}$  and let t' be a tour which is a 2-Opt neighbor of t. Suppose that the pheromone values are saturated. Then  $MMAS^*_{Ord}$  constructs t' in the next iteration of with probability  $\Theta(1/n^3)$ .

## 3.2 The Behavior of MMAS<sup>\*</sup><sub>Arb</sub>

In this section we examine the expected number of edge exchanges of  $MMAS^*_{Arb}$ . In Theorem 4 we show that the expected number of edges where  $x^*$  and x differ is  $\Theta(1)$ . Thus, the  $MMAS^*_{Arb}$  does have the desired local property.

**Theorem 3.** Let k be fixed. If in an iteration of  $MMAS^*_{Arb}$  the pheromone values are such that, for exactly the edges of the best-so-far tour the pheromone values are at  $\tau_{max}$ and all others are at  $\tau_{min}$ , then, in the next iteration of  $MMAS^*_{Arb}$  with probability  $\Theta(1)$ , the newly constructed tour will choose k new edges and otherwise rechoose edges of the best-so-far tour as long as any are admissible.

*Proof.* We call an edge with pheromone level  $\tau_{\text{max}}$  a "high" edge, the others are "low" edges. Let *P* be the set of all high edges (the edges of the best-so-far tour). We consider an iteration of MMAS<sup>\*</sup><sub>Arb</sub>. We analyze the situation where, out of the *n* edges to be

chosen to create a new tour, there are still *i* edges left to be chosen. In this situation, the edges chosen so far partition the graph into exactly *i* components. For each two components, there are between 1 and 4 edges to connect them (each component is a path with at most 2 endpoints, only the endpoints can be chosen for connecting with another component); thus, there are between  $\binom{i}{2}$  and  $\min(4\binom{i}{2}, \binom{n}{2})$  edges left to be chosen. Further, when there are *i* edges left to be chosen for the tour, at most *k* of which are low edges, there are between *i* and *i* + *k* high edges and between  $\binom{i}{2} - (i + k)$  and  $\min(4\binom{i}{2}, \binom{n}{2})$  low edges left to choose from.

For a fixed k-element subset M of  $\{1, \ldots, n\}$ , and any choice of edges at positions M, we use the union bound to analyze the probability to rechoose as many other high edges as possible in all the other postions. This probability is lower bounded by

$$1 - \sum_{i=1}^{n} \min\left(4\binom{i}{2}, \binom{n}{2}\right) \tau_{\min} \cdot \frac{1}{i\tau_{\max}}$$
$$= 1 - \frac{\tau_{\min}}{\tau_{\max}} \left(\sum_{i=1}^{n/2} 4\binom{i}{2} \cdot \frac{1}{i} + \sum_{i=n/2+1}^{n} \binom{n}{2} \cdot \frac{1}{i}\right) \ge \frac{1}{4} > 0.$$

For each k-element subset M of  $\{1, \ldots, n\}$ , the probability of choosing a low edge on all positions of M, and choosing a high edge on all other positions is lower bounded by

$$\frac{1}{4} \prod_{i \in M} \left( \binom{i}{2} - (i+k) \right) \tau_{\min} / ((i+k)\tau_{\max} + n^2 \tau_{\min}) \\ \ge \frac{\tau_{\min}^k}{4} \prod_{i \in M} \left( \frac{i^2 - i}{2} - (i+k) \right) / (i+k+1) \ge \frac{\tau_{\min}^k}{4} \prod_{i \in M} \left( \frac{i}{2k+4} - 2 \right)$$

Let  $c_{i,k} = i/(2k+4)-2$ . Note that, for any set M with  $|M| \le k$ , we have  $\sum_{i=1,i \notin M}^{n} c_{i,k} = \Theta(n^2)$ . Now we have that the probability of choosing low edges on *any* k positions is lower bounded by

$$\frac{\tau_{\min}^{k}}{4} \sum_{\substack{M \subseteq \{1,\dots,n\}\\|M|=k}} \prod_{i \in M} c_{i,k} \\
= \frac{1}{4k! n^{2k}} \sum_{i_{1}=1}^{n} \left( \sum_{i_{2}=1,i_{2} \notin \{i_{1}\}}^{n} \left( \dots \left( \sum_{i_{k}=1,i_{k} \notin \{i_{1},\dots,i_{k-1}\}}^{n} \prod_{j=1}^{k} c_{i_{j},k} \right) \right) \right) \\
= \frac{1}{4k! n^{2k}} \left( \sum_{i_{1}=1}^{n} c_{i_{1},k} \right) \left( \sum_{i_{2}=1,i_{2} \notin \{i_{1}\}}^{n} c_{i_{2},k} \right) \dots \left( \sum_{i_{k}=1,i_{k} \notin \{i_{1},\dots,i_{k-1}\}}^{n} c_{i_{k},k} \right) \\
= \Theta(1).$$

As a corollary to the proof just above, we get the following.

**Theorem 4.** If in an iteration of  $MMAS^*_{Arb}$  the pheromone values are such that, for exactly the edges of the best-so-far tour the pheromone values are at  $\tau_{max}$  and all others are at  $\tau_{min}$ , then, in the next iteration of  $MMAS^*_{Arb}$ , the newly constructed tour will exchange an expected number of O(1) of edges.

As a further corollary to Theorem 3, we get the following.

**Corollary 1.** Let t be a tour found by  $MMAS^*_{Arb}$  and let t' be a tour which is a 2-Opt neighbor of t. Suppose that the pheromone values are such that for exactly the edges of t the pheromone values are at  $\tau_{max}$  and all others are at  $\tau_{min}$ . Then  $MMAS^*_{Arb}$  constructs t' in the next iteration with probability  $\Theta(1/n^2)$ .

*Proof.* The tour t has  $\Theta(n^2)$  many 2-Opt neighbors. By Theorem 3,  $\text{MMAS}^*_{Arb}$  will construct, with constant probability, a tour that exchanges one edge and otherwise rechooses edges of t as long as possible. This new tour is a 2-Opt neighbor of t. As all 2-Opt neighbors of t are constructed equiprobably (thanks to the symmetry of the construction procedure), we obtain the desired result.

## 4 Runtime Bounds

#### 4.1 A Simple Instance

An initial runtime analysis of ACO algorithms for the TSP problem has been carried out by Zhou in [14]. In that paper, the author investigates how ACO algorithms can obtain optimal solutions for some simple instances. The basic ideas behind these analyses is that ACO algorithms are able to imitate 2-Opt and 3-Opt operations.

A simple instance called  $G_1$  in [14] consists of a single optimum, namely a Hamiltonian cycle where all edges have cost 1 (called light edges), while all remaining edges get a large weight of n (called heavy edges). The author shows that  $MMAS^*_{Ord}$  for arbitrary  $\rho > 0$  obtains an optimal solution for  $G_1$  in expected time  $O(n^6 + (1/\rho)n \log n)$ . The proof idea is as follows: As long as an optimal solution has not been obtained, there is always a 2-Opt or 3-Opt operation that leads to a better tour. Having derived a bound of  $\Omega(1/n^5)$  for the probability of performing an improving 2- or 3-Opt step, the result follows since at most n improvements are possible and  $O(\log n/\rho)$  is the so-called freezing time, i. e., the time to bring all pheromone values to upper or lower bounds.

In this section, we prove a bound of  $O(n^3 \log n + (n \log n)/\rho)$  on the expected optimization time of  $\text{MMAS}^*_{Arb}$  for the instance  $G_1$ . This bound is considerably better than the  $O(n^6)$  proved before in [14] for  $\text{MMAS}^*_{Ord}$ . At the same time, the analysis is much simpler and saves unnecessary case distinctions.

The following lemma concentrates on a single improvement. Following the notation in [14], let  $A_k$ ,  $k \le n$ , denote the set of all tours of total weight n - k + kn, i. e., the set of all tours consisting of exactly n - k light and k heavy edges.

**Lemma 2.** Let  $\alpha = 1$  and  $\beta = 0$ ,  $\tau_{\min} = 1/n^2$  and  $\tau_{\max} = 1 - 1/n$ . Denote by  $X^t$  the best-so-far tour sequence produced by  $MMAS^*_{Arb}$  on TSP instance  $G_1$  until iteration t > 0 and assume that  $X_t$  is saturated. Then the probability of an improvement, given  $1 \le k \le n$  heavy edges in  $X_t$ , satisfies  $s_k = P(X^{t+1} \in A_{k-1} \cup \ldots \cup A_0 \mid X^t \in A_k) = \Omega(k/n^3)$ .

*Proof.* Consider an arbitrary light edge  $e = \{u, v\} \notin T$  outside the best-so-far tour. Each vertex of  $G_1$  is incident to 2 light edges, so both u and v are incident to exactly one light edge different from e. Since  $e \notin T$ , this implies the existence of two different heavy edges  $e_0, e_1 \in T$  on the tour such that  $e_0$  is incident on u and  $e_1$  incident on v. Let  $e'_0, e'_1 \in T$  with  $e'_0 \neq e_0$  and  $e'_1 \neq e_1$  be the other two edges on the tour that are incident to u and v, respectively. The aim is to form a new tour containing e and still  $e'_0$  and  $e'_1$  but no longer  $e_0$  and  $e_1$ . Note that the set of edges  $(T \cup \{e\}) \setminus \{e_0, e_1\}$ has cardinality n - 1 but might contain a cycle. If that is the case, there must be a heavy edge  $e_2 \in T$  from the old tour on that cycle (since there is a unique cycle of light edges in  $G_1$ ). Then we additionally demand that the new tour does not contain  $e_2$ . Since the undesired edges  $e_0, e_1$  and possibly  $e_2$  are heavy and e is a light edge outside the previous tour, any tour being a superset of  $(T \cup \{e\}) \setminus \{e_0, e_1, e_2\}$  is an improvement compared to T.

For  $1 \leq j \leq n/4$ , we consider the following intersection of events, denoted by  $M_e(j)$  and prove that  $\operatorname{Prob}(M_e(j)) = \Omega(1/n^4)$ ; later, a union over different j and e is taken to get an improved bound.

- 1. the first j 1 steps of the construction procedure choose edges from  $T^* := T \setminus \{e_0, e_1, e_2\}$  and the *j*-th step chooses  $e_i$ ,
- 2.  $e'_0$  is chosen before  $e_0$  and  $e'_1$  before  $e_1$ ,
- 3. all steps except the first one choose from  $T^*$  as long as this set contains applicable edges.

Note that  $e_0$  and  $e_1$  are no longer applicable once  $\{e, e'_0, e'_1\}$  is a subset of the new tour. For the first subevent, assume that the first i < j steps have already chosen exclusively from  $T^*$ . Then there n-i edges from T and n-i-3 edges from  $T^*$  left. Finally, there are at most  $n^2/2$  edges outside T. Using that  $X_t$  is saturated, the probability of choosing another edge from  $T^*$  is then at least

$$\frac{(n-i-3)\tau_{\max}}{(n-i)\tau_{\max} + n^2\tau_{\min}/2} \ge \frac{n-i-3}{n-i+1}$$

(assuming  $n \ge 2$ ). Altogether, the probability of only choosing from  $T^*$  in the first j-1 steps is at least

$$\prod_{i=0}^{j-2} \frac{n-i-3}{n-i+1} \ge \left(\frac{3n/4-1}{3n/4+3}\right)^{n/4-1} = \Omega(1)$$

since  $j \le n/4$ . The probability of choosing e in the j-th step is at least at least  $\tau_{\min}/n = 1/n^3$  since the total amount of pheromone in the system is at most n. Altogether, the first subevent has probability  $\Omega(1/n^4)$ .

The second subevent has probability at least  $(1/2)^2 = 1/4$  since all applicable edges in T are chosen with the same probability (using that  $X_t$  is saturated).

For the third subevent, we study a step of the construction procedure where there are i applicable edges from T left and all edges chosen so far are from  $T \cup \{e\}$ . Now we need a more precise bound on the number of applicable outside T. Taking out  $k \ge 1$  edges from T breaks the tour into k connected components, each of which has at most two

vertices of degree less than 2. Since  $e \notin T$  has been chosen, at most two edges from T are excluded from our consideration. Altogether, the number of connected components in the considered step of the construction procedure is at most i + 2, which means that there are at most  $\binom{2(i+2)}{2} \leq 2(i+2)^2 \leq 18i^2$  edges outside T applicable. The probability of neither choosing  $e_2$  nor an edge outside T in this situation is at least

$$\frac{i\tau_{\max}}{(i+1)\tau_{\max} + 18i^2\tau_{\min}}$$

Hence, given the second subevent, the probability of the third subevent is at least

$$\begin{split} \prod_{i=1}^{n-1} \frac{i \cdot \tau_{\max}}{(i+1)\tau_{\max} + 18i^2 \tau_{\min}} &= \prod_{i=1}^{n-1} \left( \frac{i}{i+1} \cdot \frac{(i+1) \cdot \tau_{\max}}{(i+1)\tau_{\max} + 18i^2 \tau_{\min}} \right) \\ &\geq \frac{1}{n} \prod_{i=1}^{n-1} \frac{i+1}{(i+1) + 18(i+1)^2/(\tau_{\max} \cdot n^2)} \geq \frac{1}{n} \left( \prod_{i=1}^n 1 + \frac{18i}{(\tau_{\max} \cdot n^2)} \right)^{-1} \\ &\geq \frac{1}{n} \left( 1 + \frac{18}{n-1} \right)^{-n} = \Omega(1/n), \end{split}$$

altogether, the intersection  $M_e(j)$  of the three subevents happens with probability  $\Omega(1/n^4)$ .

Finally, consider the union  $M_e := \bigcup_{j \le n/4} M_e(j)$ , which refers to including e in any of the first n/4 steps. Since the  $M_e(j)$  are disjoint for different j, we obtain  $\operatorname{Prob}(M_e) = (n/4) \cdot \Omega(1/n^4) = \Omega(1/n^3)$ . Similarly, for all light edges  $e \notin T$  (of which there are k), the events  $M_e$  are disjoint (as a different new edge is picked in the first step). Thus, the probability of an improvement is  $\Omega(k/n^3)$  as desired.  $\Box$ 

**Theorem 5.** Let  $\alpha = 1$  and  $\beta = 0$ ,  $\tau_{\min} = 1/n^2$  and  $\tau_{\max} = 1 - 1/n$ . Then the expected optimization time of MMAS<sup>\*</sup><sub>Arb</sub> on  $G_1$  is  $O(n^3 \log n + n(\log n)/\rho)$ .

*Proof.* Using Lemma 2 and the bound  $O(\log n/\rho)$  on the freezing time, the waiting time until a best-so-far solution with k heavy edges is improved is bounded by  $O((\log n)/\rho) + s_k = O((\log n)/\rho + n^3/k)$ . Summing up, we obtain a total expected optimization time of  $O(n(\log n)/\rho) + \sum_{k=1}^{n} (1/s_k) = O(n^3 \log n + n(\log n)/\rho)$ .  $\Box$ 

#### 4.2 Random Instances

The 2-Opt heuristic, which starts with an arbitrary tour and performs 2-Opt steps until a local optimum is reached, is known to perform well in practice in terms of running time and approximation ratio [9]. In contrast to this, it has been shown to have exponential running time in the worst case [5] and it has been shown that there are instances with local optima whose approximation ratio is  $\Omega(\log n/\log \log n)$  [1]. To explain this discrepancy between theory and practice, 2-Opt has been analyzed in a more realistic model of random instances reminiscent of smoothed analyis [13]. In this model, n points are placed independently at random in the d-dimensional Euclidean space, where each point  $v_i$  (i = 1, 2, ..., n) is chosen according to its own probability density  $f_i: [0, 1]^d \rightarrow [0, \phi]$ , for some parameter  $\phi \ge 1$ . It is assumed that these densities are chosen by an adversary, and hence, by adjusting the parameter  $\phi$ , one can interpolate between worst and average case: If  $\phi = 1$ , there is only one valid choice for the densities and every point is chosen uniformly at random from the unit hypercube. The larger  $\phi$  is, the more concentrated can the probability mass be and the closer is the analysis to a worst-case analysis. We analyze the expected running time and approximation ratio of MMAS<sup>\*</sup><sub>Arb</sub> and MMAS<sup>\*</sup><sub>Ord</sub> on random instances. For this, we have to take a closer look into the results from [5] which bound the expected number of 2-Opt steps until a good approximation has been achieved. We show the following theorem.

**Theorem 6.** For  $\rho = 1$ ,  $MMAS^*_{Arb}$  finds in time  $O(n^{6+2/3} \cdot \phi^3)$  with probability 1 - o(1) a solution with approximation ratio  $O(\sqrt[4]{\phi})$ .

*Proof.* As we have argued in Corollary 1, if all edges are saturated and there is an improving 2-Opt step possible, then this step is performed with probability at least  $\Omega(1/n^2)$ . From [5] we know that from any state, the expected number of 2-Opt steps until a tour is reached that is locally optimal for 2-Opt is at most  $O(n^{4+1/3} \cdot \log(n\phi) \cdot \phi^{8/3})$  even if in between other changes are made to the tour that do not increase its length. Hence, using Markov's inequality we can conclude that MMAS<sup>\*</sup><sub>Arb</sub> has reached a local optimum after  $O(n^{6+2/3} \cdot \phi^3)$  steps with probability 1 - o(1).

From [5], we also know that every locally optimal tour has an expected approximation ratio of  $O(\sqrt[d]{\phi})$ . Implicitly, the proof of this result also contains a tail bound showing that with probability 1 - o(1) every local optimum achieves an approximation ratio of  $O(\sqrt[d]{\phi})$ . The theorem follows by combining the previous observations and taking into account that for our choice of  $\rho$  all edges are saturated after the first iteration of MMAS<sup>\*</sup><sub>Arb</sub>.

Taking into account that a specific 2-Opt operation in  $MMAS^*_{Ord}$  happens with probability of  $\Omega(1/n^3)$  in the next step, we get the following results.

**Theorem 7.** For  $\rho = 1$ ,  $MMAS^*_{Ord}$  finds in time  $O(n^{7+2/3} \cdot \phi^3)$  with probability 1 - o(1) a solution with approximation ratio  $O(\sqrt[d]{\phi})$ .

## 5 Conclusions

Our theoretical results show that the usual construction procedure leads to solutions that are in expectation far away from the currently best one in terms of edge exchanges even if the pheromone values have touched their corresponding bounds. Due to this, we have examined a new construction graph with a stronger locality. On the other hand, this construction procedure has a high probability of carrying out a specific 2-opt operation which is important for successful stochastic search algorithms for the TSP problem. Afterwards, we have shown that both algorithms perform well on random instances if the pheromone update is high.

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## References

- 1. B. Chandra, H. J. Karloff, and C. A. Tovey. New results on the old k-Opt algorithm for the traveling salesman problem. *SIAM J. Comput.*, 28(6):1998–2029, 1999.
- M. Dorigo and L. M. Gambardella. Ant colony system: a cooperative learning approach to the traveling salesman problem. *IEEE Trans. Evolutionary Computation*, 1(1):53–66, 1997.
- 3. M. Dorigo and T. Stützle. Ant Colony Optimization. MIT Press, Cambridde, MA, 2004.
- 4. A. Eiben and J. Smith. *Introduction to Evolutionary Computing*. Springer, Berlin, Germany, 2nd edition, 2007.
- M. Englert, H. Röglin, and B. Vöcking. Worst case and probabilistic analysis of the 2-opt algorithm for the tsp: extended abstract. In N. Bansal, K. Pruhs, and C. Stein, editors, SODA, pages 1295–1304. SIAM, 2007.
- 6. W. J. Gutjahr. Mathematical runtime analysis of ACO algorithms: Survey on an emerging issue. *Swarm Intelligence*, 1:59–79, 2007.
- 7. W. J. Gutjahr and G. Sebastiani. Runtime analysis of ant colony optimization with best-so-far reinforcement. *Methodology and Computing in Applied Probability*, 10:409–433, 2008.
- C. Horoba and D. Sudholt. Running time analysis of ACO systems for shortest path problems. In T. Stützle, M. Birattari, and H. H. Hoos, editors, *SLS*, volume 5752 of *Lecture Notes in Computer Science*, pages 76–91. Springer, 2009.
- D. S. Johnson and L. A. McGeoch. The traveling salesman problem: A case study in local optimization. In E. H. L. Aarts and J. K. Lenstra, editors, *Local Search in Combinatorial Optimization*. Wiley, 1997.
- F. Neumann, D. Sudholt, and C. Witt. Rigorous analyses for the combination of ant colony optimization and local search. In M. Dorigo, M. Birattari, C. Blum, M. Clerc, T. Stützle, and A. F. T. Winfield, editors, *ANTS Conference*, volume 5217 of *Lecture Notes in Computer Science*, pages 132–143. Springer, 2008.
- 11. F. Neumann, D. Sudholt, and C. Witt. Analysis of different MMAS ACO algorithms on unimodal functions and plateaus. *Swarm Intelligence*, 3(1):35–68, 2009.
- 12. F. Neumann and C. Witt. Runtime analysis of a simple ant colony optimization algorithm. *Algorithmica*, 54(2):243–255, 2009.
- 13. D. A. Spielman and S.-H. Teng. Smoothed analysis of algorithms: Why the simplex algorithm usually takes polynomial time. *J. ACM*, 51(3):385–463, 2004.
- 14. Y. Zhou. Runtime analysis of an ant colony optimization algorithm for TSP instances. *IEEE Transactions on Evolutionary Computation*, 13(5):1083–1092, 2009.