Stochastic Runtime Analysis of a Cross-Entropy Algorithm for Traveling Salesman Problems

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Abstract

This article analyzes the stochastic runtime of a Cross-Entropy Algorithm mimicking a Max-Min Ant System with iteration-best reinforcement. It investigates the impact of magnitude of the sample size on the runtime to find optimal solutions for TSP instances.

For simple TSP instances that have a $\{1, n\}$-valued distance function and a unique optimal solution, we show that sample size $N \in \omega(\ln n)$ results in a stochastically polynomial runtime, and $N \in O(\ln n)$ results in a stochastically exponential runtime, where “stochastically” means with a probability of $1 - n^{-\omega(1)}$, and $n$ represents number of cities. In particular, for $N \in \omega(\ln n)$, we prove a stochastic runtime of $O(N \cdot n^6)$ with the vertex-based random solution generation, and a stochastic runtime of $O(N \cdot n^3 \ln n)$ with the edge-based random solution generation. These runtimes are very close to the best known expected runtime for variants of Max-Min Ant System with best-so-far reinforcement by choosing a small $N \in \omega(\ln n)$. They are obtained for

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the stronger notion of stochastic runtime, and analyze the runtime in most cases.

We also inspect more complex instances with \( n \) vertices positioned on an \( m \times m \) grid. When the \( n \) vertices span a convex polygon, we obtain a stochastic runtime of \( O(n^4m^{5+\epsilon}) \) with the vertex-based random solution generation, and a stochastic runtime of \( O(n^3m^{5+\epsilon}) \) for the edge-based random solution generation. When there are \( k \in O(1) \) many vertices inside a convex polygon spanned by the other \( n - k \) vertices, we obtain a stochastic runtime of \( O(n^4m^{5+\epsilon} + n^{6k-1}m^{\epsilon}) \) with the vertex-based random solution generation, and a stochastic runtime of \( O(n^3m^{5+\epsilon} + n^{3k}m^{\epsilon}) \) with the edge-based random solution generation. These runtimes are better than the expected runtime for the so-called \((\mu+\lambda)\) EA reported in a recent article, and again obtained for the stronger notion of stochastic runtime.

**Keywords:** probabilistic analysis of algorithms, stochastic runtime analysis of evolutionary algorithms, Cross Entropy algorithm, Max-Min Ant System, \((\mu+\lambda)\) EA.

1. Introduction

The Cross Entropy (CE) algorithm is a general-purpose evolutionary algorithm (EA) that has been applied successfully to many \( \mathcal{NP} \)-hard combinatorial optimization problems, see e.g. the book [1] for an overview. It was initially designed for rare event simulation by Rubinstein [2] in 1997, and thereafter formulated as an optimization tool for both continuous and discrete optimization (see [3]).

CE has much in common with the famous ant colony optimization (ACO, see [4]) and the estimation of distribution algorithms (EDAs, see [5]). They all belong to the so-called model-based search paradigm (MBS), see [6]. Instead of only manipulating solutions, which is very typical in traditional heuristics like Genetic Algorithms [7] and Local Search [8] and others, MBS algorithms attempt to optimize the solution reproducing mechanism. In each iteration, they produce new solutions by sampling from a probabilistic distribution on the search space. The distribution is often called a *model* in the literature (see e.g. [6] and [9]). This model evolves iteratively by incorporating information from some elite solutions occurring in the search history, so as to asymptotically model the spread of optimal solutions in the search...
space. See the recent Thesis [9] for more details on MBS algorithms and their mathematical properties.

An important issue for MBS algorithms is to determine a suitable size for the sampling in each iteration. A large sample size makes each iteration unwieldy, however a small sample size may mislead the underlying search due to the randomness in the sampling. Sample size reflects the iterative complexity (computational complexity in each iteration). Whether a large sample size is harmful depends on the required optimization time (i.e., the total number of iterations required to reach an optimal solution). This article aims to shed a light on this issue by theoretically analyzing the relation between sample size and optimization time for a CE variant that includes also some essential features of the famous Max-Min Ant System (MMAS [10]). To this end, a thorough runtime analysis is needed.

The theoretical runtime analysis of EAs has gained rapidly growing interest in recent years, see e.g. [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22], [23], [24], and [25]. In the analysis, an oracle-based view of computation is adopted, i.e., the runtime of an algorithm is expressed as the total number of solutions evaluated before reaching an optimal solution. Since the presence of randomness, the runtime of an EA is often conveyed in expectation or with high probability. Due to the famous No Free Lunch Theorem [26], the analysis must be problem-specific. The first steps towards this type of analysis were made for the so-called (1+1) EA [11] on some test problems that use pseudo boolean functions as cost functions, e.g., OneMax [15], LeadingOnes [27], and BinVar [11]. Recent research addresses problems of practical importance, such as the computing a minimum spanning trees (MST) [28], matroid optimization [29], traveling salesman problem [30], the shortest path problem [23], the maximum satisfiability problem [31] and the max-cut problem [32].

Runtime analysis generally considers two cases: expected runtime analysis and stochastic runtime analysis. Expected runtime is the average runtime of an algorithm on a particular problem, see, e.g., the runtime results of (1+1) EA reported in [11]. Expected runtime reflects the oracle-based average performance of an algorithm. A mature technique for expected runtime analysis is the so-called drift analysis [12]. However, this technique requires that the algorithm has a finite expected runtime for the underlying problem. By [33], drift analysis is not applicable to the traditional CE [3].

An algorithm with a smaller expected runtime need not be more efficient, see [34] for details. In contrast, stochastic runtime provides a better under-
standing of the performance of a (randomized) EA. Stochastic runtime is a runtime result conveyed with an overwhelming probability guarantee (see, e.g., the classic runtime result of 1-ANT in [15]), where an overwhelming probability means a probability tending to 1 superpolynomially fast in the problem size. It therefore reflects the efficiency of an algorithm for most cases in the sense of uncertainty. This article is concerned with stochastic runtime analysis, aiming to figure out the relation between stochastic runtime and magnitude of the sample size.

Runtime analysis of CE algorithms has been initiated in [33], where Wu and Kolonko proved a pioneering stochastic runtime result for the traditional CE on the standard test problem LEADINGONES. As a continuation of the study of [33], Wu et al [34] further investigated the stochastic runtime of the traditional CE on another test problem ONEMAX. The runtime results reported in [33] and [34] showed that sample size plays a crucial role in efficiently finding an optimal solution. In particular, Wu et al [34] showed that if the problem size $n$ is moderately adapted to the sample size $N$, then the stochastic runtime of the traditional CE on ONEMAX is $O(n^{1.5+\frac{3}{4}\epsilon})$ for arbitrarily small $\epsilon > 0$ and a constant smoothing parameter $\rho > 0$, which beats the best-known stochastic runtime $O(n^2)$ reported in [13] for the classic 1-ANT algorithm, although 1-ANT employs a much smaller sample size (i.e., sample size equals one). Moreover, by imposing upper and lower bounds on the sampling probabilities as was done in MMAS [10], Wu et al [34] showed further that the stochastic runtime of the resulting CE can be significantly improved even in a very rugged search space.

The present article continues the stochastic runtime analysis of [34], but now in combinatorial optimization with a study of CE on the traveling salesman problem (TSP). We emphasize the impact of the magnitude of $N$ on the stochastic runtime, put $\rho = 1$, and consider a CE variant resembling an MMAS with iteration-best reinforcement under two different random solution generation mechanisms, namely, a vertex-based random solution generation and an edge-based random solution generation.

Stochastic runtime for MMAS with iteration-best reinforcement on simple problems like ONEMAX has been studied in [20] and [25]. In particular, Neumann et al [20] showed that to obtain a stochastically polynomial runtime for ONEMAX, $N/\rho \in \Omega(\ln n)$ is necessary. We shall not only extend this to TSP for the case of $\rho = 1$, but also prove that $N \in \omega(\ln n)$ is already sufficient to guarantee a stochastically polynomial runtime for simple TSP instances.
TSP is a famous $\mathcal{NP}$-complete combinatorial optimization problem. It concerns finding a shortest Hamiltonian cycle on a weighted complete graph. Existing algorithms exactly solving TSP generally have a prohibitive complexity. For instance, the Held-Karp algorithm [35] solves the problem with a complexity of $O(n^{2.29})$. A well-known polynomial time approximation algorithm for metric TSP is the so-called Christofides algorithm [36], which finds a solution with a cost at most 3/2 times the cost of optimal solutions. As mentioned in [37], this is still the best known approximation algorithm for the general metric TSP so far. For Euclidean TSP there exists a famous polynomial-time approximation scheme (PTAS) by Arora, see [38]. To design a superior approximation algorithm, researchers in recent years tend to study TSP instances with particular structures, see, e.g., [39].

Due to the prohibitive running time of exact algorithms, heuristics are frequently employed in practice so as to efficiently compute an acceptable solution for a TSP problem, e.g., the Lin-Kernighan (LK) algorithm [40]. As a popular heuristic, CE has also been applied in practice to solve TSP instances, see [41] and [3]. The implementation there shows that CE can also efficiently compute an acceptable solution.

In view of the high complexity of general TSP, we consider in our analysis two classes of TSP instances with a particular structure. The first kind of instances has been used in [19] and [42] for analyzing the expected runtime of some $\mathcal{MMAS}$ variants with best-so-far reinforcement. These TSP instances have polynomially many objective function values and a unique optimal solution. Moreover, on these TSP instances, solutions containing more edges from the optimal solution have a smaller cost than those with fewer such edges. For more details on these instances, see Section 5.

For these simple instances, we prove in Theorem 2 that with a probability $1 - e^{-\Omega(n^\epsilon)}$, the runtime is $O(n^{6+\epsilon})$ with the vertex-based random solution generation, and $O(n^{3+\epsilon} \ln n)$ with the edge-based random solution generation, for any constant $\epsilon \in (0, 1)$ and $N \in \Omega(n^\epsilon)$. For the case of $N \in \omega(\ln n)$, we show that the runtimes (resp., $O(n^6 N)$ and $n^3 (\ln n) N$) are even smaller with probability $1 - n^{-\omega(1)}$, see Corollary 1. These results are very close to the known expected runtime $O(n^6 + \frac{n \ln n}{\rho})$ for (1+1) MMAA reported in [19], and the expected runtime $O(n^3 \ln n + \frac{n \ln n}{\rho})$ for MMAS$_{Arb}$ reported in [42] (where $\rho \in (0, 1)$ is an evaporation rate), if $N \in \omega(\ln n)$ is suitably small. But they give the stronger guarantee of achieving the optimal solution in the respective runtime with an overwhelming probability. Moreover, we show
a stochastically exponential runtime for a suitable choice of $N \in O(\ln n)$, see Theorem 3. This generalizes the finding in [20] for OneMax to TSP instances. Therefore, $N \in \Omega(\ln n)$ is necessary, and $N \in \omega(\ln n)$ is sufficient for a stochastically polynomial runtime for simple TSP instances.

We also inspect more complex instances with $n$ vertices positioned on an $m \times m$ grid, and the Euclidean distance as distance function. These instances have been employed in [43] and [30] for analyzing the expected runtime of $(\mu + \lambda)$ EA and randomized local search (RLS). When the $n$ vertices span a convex polygon without vertices in the interior of the polygon (so they are the corners of that polygon), we prove a stochastic runtime of $O(n^4 m^{5+\epsilon})$ for the vertex-based random solution generation, and a stochastic runtime of $O(n^3 m^{5+\epsilon})$ for the edge-based random solution generation, see Theorem 4 for details. Similarly, the $\epsilon$ in the stochastic runtimes can be removed by slightly decreasing the probability guarantee, see Corollary 2. When the vertices span a convex polygon with $k \in O(1)$ vertices in the interior, we show a stochastic runtime of $O(n^4 m^{5+\epsilon} + n^{6k-1} m^\epsilon)$ with the vertex-based random solution generation, and a stochastic runtime of $O(n^3 m^{5+\epsilon} + n^{3k} m^\epsilon)$ with the edge-based random solution generation, see Theorem 5 for details. These runtimes are better than the expected runtime for the so-called $(\mu+\lambda)$ EA and RLS reported in the recent paper [30].

The remainder of this paper is arranged as follows. Section 2 defines the traditional CE and related algorithms, Section 3 defines the traveling salesman problem and provides more details of the used CE variants, Section 4 shows some important facts on the two random solution generation methods, and Section 5 reports the stochastic runtime results on the TSP instances. A short conclusion and suggestions for future work are given in Section 6.

Notations for runtime

Our analysis employs some commonly used notations from complexity theory. We use $O(f(n))$ to denote the class of functions which are bounded from above by the function $f(n)$, i.e., those functions $g(n)$ with $g(n) \leq c \cdot f(n)$ for large enough $n$ and some constant $c \geq 0$ not depending on $n$. Similarly, $\Omega(f(n))$ is the class of functions that are bounded from below by $f(n)$, i.e., for any $g(n) \in \Omega(f(n))$ there exists a constant $c > 0$ not depending on $n$ such that $g(n) \geq c \cdot f(n)$ for large enough $n$. Class $\Theta(f(n))$ is the intersection of $\Omega(f(n))$ and $O(f(n))$. Class $o(f(n))$ is the class of functions $g(n)$ with $g(n)/f(n) \to 0$ as $n \to \infty$, and class $\omega(f(n))$ is the class of functions
\( g(n) \) with \( g(n)/f(n) \to +\infty \) as \( n \to \infty \). Obviously, \( o(f(n)) \subset O(f(n)) \) and \( \omega(f(n)) \subset \Omega(f(n)) \).

2. The general cross entropy algorithm and related algorithms

We now introduce the traditional CE algorithm. The CE variant we will analyze inherits the framework of this traditional version. To compare our results with those in the literature, we shall give also details about some related algorithms.

2.1. The traditional cross entropy algorithm

Algorithm [1] lists the traditional CE that was proposed in [3], adapted to an abstract notion of combinatorial optimization problems. The algorithm assumes a combinatorial minimization problem \((S, f)\), where \( S \) is a finite search space of “feasible” solutions and \( f \) is the cost function. Every feasible solution \( s \in S \) is composed of elements from a fixed finite set \( A \), the ground set of the problem, i.e., we assume \( S \subseteq A^n \) for some integer \( n \in \mathbb{N} \). Furthermore there is a product distribution on the product space \( A^n \) that induces a distribution on \( S \subseteq A^n \). The distribution on \( A^n \) can usually be represented as a vector (or matrix) of real-valued probabilities. The convex combination of the two distributions in Step 6 of Algorithm [1] then corresponds to a convex combination of the two vectors (or matrices).

Specific to the TSP, the ground set \( A \) can be the set of nodes or edges, \( n \) is the number of nodes, and a feasible solution is a sequence of elements from \( A \) that forms a Hamiltonian cycle. The product distribution for the TSP is represented as an \( n \times n \) matrix.

When we consider the set of nodes as our ground set \( A \), each row \( i \) of the matrix is a marginal distribution that specifies choice probabilities for all nodes following the current node \( i \). A random Hamiltonian cycle is sequentially constructed from the product distribution by allowing only nodes not yet visited as continuations in each step, see Algorithm [2] for more details.

When we consider the set of edges as \( A \), marginals of the product distribution will be represented by the same \( n \times n \) matrix where the sum of the \((i, j)\)-th and \((j, i)\)-th entries reflects the probability that the edge \( \{i, j\} \) occurs in a random solution. A random Hamiltonian cycle is still constructed sequentially and only edges leading to a feasible solution are taken in each step, see Algorithm [3] for details.
Algorithm 1 The general Cross-Entropy algorithm

Input:
an initial distribution $\Pi_0$ on the solution space, a fixed smoothing parameter $\rho \in (0, 1]$, a sample size $N \in \mathbb{N}_+$, an elite size $M \in \mathbb{N}_+$ with $M \leq N$

1: $t = 0$
2: loop
3: independently generate $N$ random solutions $X_t^{(1)}, \ldots, X_t^{(N)}$ with the current distribution $\Pi_t$;
4: sort these $N$ solutions in non-decreasing order as $f(X_t^{[1]}) \leq \cdots \leq f(X_t^{[N]})$ according to the cost function $f$;
5: learn an empirical distribution $W_t$ from the $M$ best solutions $X_t^{[1]}, \ldots, X_t^{[M]}$;
6: set $\Pi_{t+1} = (1 - \rho)\Pi_t + \rho W_t$;
7: $t = t + 1$
8: end loop

Traditionally, CE sets a small elite ratio $\alpha \in (0, 1)$ and uses the best $\lfloor \alpha \cdot N \rfloor$ solutions in Step 5 to build the empirical distribution $W_t$. Here, we use the elite size $M$ instead. This does not intrinsically change the original algorithm. Steps 3 and 5 depend on the detailed definition of the underlying problem. We shall give details to them in Subsection 3.2.

Step 6 of Algorithm 1 plays a crucial role in the different theoretical analyses of the algorithm, see, e.g., [44], [33], [45], [9], [34]. The occurrence of good solutions are probabilistically enforced by incorporating the new information $W_t$ into $\Pi_{t+1}$. This idea, somehow, coincides with the reinforcement learning in [46]. The smoothing parameter $\rho$ reflects the relative importance of the new information $W_t$ in the next sampling. It balances global exploration and local exploitation to a certain degree. A larger $\rho$ makes the algorithm concentrate more on the particular area spanned by the elite solutions $X_t^{[1]}, \ldots, X_t^{[M]}$, while a smaller $\rho$ gives more opportunities to solutions outside that area.

However, balancing global exploration and local exploitation through tuning $\rho$ is ultimately limited. Wu and Kolonko [33] proved that the famous “genetic drift” [47] phenomenon also happens in this algorithmic scheme, i.e., the sampling (Step 3) eventually freezes at a single solution and that solution needs not to be optimal. This means that the algorithm gradually
loses the power of global exploration.

As a compensation for global exploration, Wu et al. [34] proved that a moderately large sample size \( N \) might be helpful. The results there showed that a moderately large \( N \) configured with a large \( \rho \) (e.g., \( \rho = 1 \)) can make the algorithm very efficient. Although a large \( N \) introduces a high computational burden in each iteration, the total number of iterations required for getting an optimal solution is considerably reduced.

Wu et al. [34] also indicated another way to compensate the global exploration, i.e., imposing a lower bound \( \pi_{\min} \in (0, 1) \) and an upper bound \( \pi_{\max} \in (0, 1) \) on the sampling distributions in each iteration. This idea is originated from MMAS [10]. In each iteration \( t \), after applying Step 6, the entries of distribution \( \Pi_{t+1} \) that are out of the range \([\pi_{\min}, \pi_{\max}]\) are reset to that range by assigning to them the nearest bounds, see (6) in Section 3 for more details. Wu et al. [34] have proved that this can make CE more efficient even in the case of a rugged search space.

To follow these theoretical suggestions made in [34], we shall in our stochastic runtime analysis use a CE that modifies the traditional CE (Algorithm 1) accordingly. We shall see that these modifications make the CE very efficient for the considered TSP instances.

2.2. Related evolutionary algorithms

Related evolutionary algorithms for TSP whose runtime has been extensively studied are RLS [28], \((\mu + \lambda)\) EA [30], and those theoretical abstractions of MMAS [10] including MMAS\(_b\) [17], (1+1) MMAA [19]. We now give algorithmic details of them. In order to facilitate the comparison, their runtimes for TSP instances will be discussed in Section 5.

\((\mu + \lambda)\) EA is an extension of the famous \((1+1)\) EA [11]. \((\mu + \lambda)\) EA randomly chooses \( \mu \) solutions as the initial population. In each iteration, \((\mu+\lambda)\) EA randomly chooses \( \lambda \) parents from current population, then produces \( \lambda \) children by applying randomized mutation to each of the selected parents, and forms the next population by taking the best \( \mu \) solutions from these \( \mu + \lambda \) solutions in the end of current iteration. The expected runtime of \((\mu + \lambda)\) EA on TSP instances is studied in [30], where Sutton et al uses a Poisson distribution to determine the number of randomized mutations (2-opt move or jump operation) should be taken by a selected parent in each iteration.

RLS is a local search technique [48]. It employs a randomized neighborhood. In each iteration, it randomly chooses a number of components of the
best solution found so far and then changes these components. The expected runtime of RLS for TSP instances is also studied in [30], where the neighborhood is taken to be a $k$-exchange neighborhood with $k$ randomly determined by a Poisson distribution.

$(1+1)$ MMAA is a simplified version of the famous $\text{MMAS}$ [10], where the sample size is set to 1 and pheromones are updated only with the best solution found so far (best-so-far reinforcement) in each iteration. In each iteration of $(1+1)$ MMAA, the ant which constructed the best solution found so far deposits an amount $\pi_{\text{max}}$ of pheromones on the traversed edges, and an amount $\pi_{\text{min}}$ of pheromones on the non-traversed edges, and the pheromones are updated by linearly combining the old and these newly added pheromones as in Algorithm [1]. The expected runtime of $(1+1)$ MMAA on simple TSP instances is studied in [19]. The expected runtime of its variant $\text{MMAS}^\ast_{\text{Arb}}$ on simple TSP instances is studied in [42].

3. The traveling salesman problem and details of the CE variant

Now, we formally define TSP, and give more details of the CE variant we will analyze.

3.1. The traveling salesman problem

We consider an undirected graph $G = (V,E)$ with vertex set $V = \{1, \ldots, n\}$ and edge set $E = \{\{i,j\} \mid i \in V, j \in V, i \neq j\}$. A Hamiltonian cycle is a sequence $\{(i_l, i_{l+1}) \mid l = 1, \ldots, n\}$ of edges such that

a) $i_1 = i_{n+1}$;

b) $(i_1, \ldots, i_n)$ is a permutation of $\{1, 2, \ldots, n\}$.

This definition actually considers $E$ as the ground set $\mathcal{A}$. As mentioned above, we can also put $\mathcal{A} = V$ and represent Hamiltonian cycles in a more compact way as permutations of $V$. Note that a Hamiltonian cycle corresponds to $n$ different permutations, whereas a permutation corresponds to a unique Hamiltonian cycle. However, the two representations are intrinsically the same. We shall use them interchangeably in the sequel. To facilitate our discussion, we shall refer to a Hamiltonian cycle by just referring to one of the $n$ corresponding permutations, and denote by $S$ the set of all possible permutations. We employ the convention that two permutations are said
to be same iff they form the same underlying Hamiltonian cycle. The notation \( \{k,l\} \in s \) shall mean that the edge \( \{k,l\} \) belongs to the underlying Hamiltonian cycle of the solution (permutation) \( s \).

Once a distance function \( d : E \mapsto \mathbb{R}_+ \) is given, the (total traveling) cost \( f(s) \) of a feasible solution \( s = (i_1, i_2, \ldots, i_n) \in S \) is then calculated by

\[
f(s) := \sum_{j=1}^{n-1} d(i_j, i_{j+1}) + d(i_n, i_1).
\]

We denote by \( S^* \subseteq S \) the set of feasible solutions (Hamiltonian cycles) that minimize the cost \( f \).

### 3.2. Details of the CE variant

The CE variant we consider in the analysis completely inherits the structure of Algorithm 1, and additionally employs a component from MMAS.

We now formalize the sampling distribution, and define Steps 3 and 5 in more detail. As mentioned, we represent a sampling distribution (a product distribution on \( A^n \)) for the TSP by a matrix \( \Pi = (\pi_{i,j})_{n \times n} \), such that

a) \( \sum_{j=1}^{n} \pi_{i,j} = 1 \), for all \( i = 1, \ldots, n \),

b) \( \pi_{i,i} = 0 \) for all \( i = 1, \ldots, n \),

c) \( \pi_{i,j} = \pi_{j,i} \) for each edge \( \{i,j\} \in E \).

For each edge \( \{i,j\} \in E \), \( \pi_{i,j} \) reflects the probability that a Hamilton cycle continues with vertex \( j \) when it is in vertex \( i \). In the sequel, we write the sampling distribution \( \Pi_t \) in iteration \( t \) as \( (\pi_{i,j}^t)_{n \times n} \), where the superscript \( t \) of \( \pi_{i,j}^t \) indicates the iteration. The initial distribution \( \Pi_0 = (\pi_{i,j}^0)_{n \times n} \) is, without loss of generality, set to be the uniform distribution, i.e., \( \pi_{i,j}^0 = \frac{1}{n-1} \) for all edges \( \{i,j\} \in E \).

We shall consider two random solution generation methods, a vertex-based random solution generation and an edge-based random solution generation. Algorithm 2 lists the vertex-based random solution generation method. This method uses \( V \) as the ground set \( \mathcal{A} \). A product distribution of \( \mathcal{A}^n \) is therefore represented as a matrix \( \Pi = (\pi_{i,j})_{n \times n} \) satisfying a)-c) above, i.e., each row of \( \Pi \) represents a sampling distribution on \( \mathcal{A} = V \). Directly sampling from \( \Pi \) may produce infeasible solutions from \( \mathcal{A}^n - S \). To avoid that, Algorithm 2 starts with a randomly fixed initial node, and then sequentially extends
a partial solution with an unvisited vertex until a complete permutation is obtained. This method is efficient and rather popular in practice, see, e.g., [11] and [4]. Here, “s + (v)” means that appends a vertex v to the end of a partial solution s.

Algorithm 2 Vertex-based random solution generation

Input:
- a distribution \( \Pi = (\pi_{i,j})_{n \times n} \)

Output:
- a permutation of 1, 2, ..., n

1: \( s = \emptyset \), and \( V_{\text{unvisited}} = V \);
2: randomly select \( v \) from \( V \), \( s = s + (v) \), and \( V_{\text{unvisited}} = V_{\text{unvisited}} - \{v\} \);
3: while \( \left| V_{\text{unvisited}} \right| \neq 0 \) do
4: select a random vertex \( v' \) from \( V_{\text{unvisited}} \) with a probability
\[
P[v' | s] = \frac{\pi_{v,v'}}{\sum_{k \in V_{\text{unvisited}}} \pi_{v,k}};
\] (2)
5: set \( s = s + (v') \), \( V_{\text{unvisited}} = V_{\text{unvisited}} - \{v'\} \);
6: \( v = v' \);
7: end while
8: return \( s \);

The edge-based random solution generation is listed in Algorithm 3. The idea is from [42]. This method considers edge set \( E \) as the ground set \( A \). A feasible solution is then a sequence of edges that form a Hamiltonian cycle, i.e. \( S \subseteq E^n \). To unify the notation of feasible solutions, Algorithm 3 translates its outcomes into permutations. As the actual ground set is \( E \), a product distribution is an \( n \times \frac{n(n-1)}{2} \) matrix such that each row is a marginal specifying a sampling distribution on \( E \). Algorithm 3 only considers those with identical marginals, a product distribution can be therefore fully characterized by one of its marginals and is therefore again represented by an \( n \times n \) matrix \( \Pi = (\pi_{i,j})_{n \times n} \) as above. An edge \( \{i,j\} \in E \) is then sampled from \( \Pi \) with probability \( \frac{(\pi_{i,j} + \pi_{j,i})}{\sum_{k=1}^{n} \sum_{l=1}^{n} \pi_{k,l}} = 2\pi_{i,j}/n \) since each row of \( \Pi \) sums up to 1. A random sequence \( \in E^n \) is generated by independently sampling from \( \Pi \) \( n \) times. To avoid infeasible solutions, Algorithm 3 considers in every sampling only edges that are \emph{admissible} by the edges selected before. Given a set \( B \) of edges such that the subgraph \((V,B)\) does neither contain a
cycle nor a vertex of degree $\geq 3$, an edge $e' \in E$ is said to be admissible by $B$ if and only if the subgraph $(V, B \cup \{e'\})$ still does neither contain a cycle nor a vertex of degree $\geq 3$. We denote by $B_{\text{admissible}}$ the set of edges $\notin B$ that are admissible by $B$.

**Algorithm 3** Edge-based random solution generation

**Input:**
- a distribution $\Pi = (\pi_{i,j})_{n \times n}$

**Output:**
- a permutation of $1, 2, \ldots, n$

1: $B = \emptyset$, $B_{\text{admissible}} = E$
2: while $(|B| \leq n - 1)$ do
3: select an edge $\{i, j\}$ from $B_{\text{admissible}}$ with a probability
4: \[ P[e \mid s] = \frac{\pi_{i,j} + \pi_{j,i}}{\sum_{(k,l) \in B_{\text{admissible}}} \pi_{k,l} + \pi_{l,k}}; \] (3)
5: set $B = B \cup \{\{i, j\}\}$;
6: update $B_{\text{admissible}}$;
7: end while
8: let $s = (1, i_2, i_3, \ldots, i_n)$ with $\{1, i_2\}, \{i_j, i_{j+1}\} \in B$ for $j = 2, \ldots, n - 1$;
9: return $s$;

The $N$ random solutions $X_t^{(1)}, \ldots, X_t^{(N)}$ in iteration $t$ are then generated by $N$ runs of Algorithm 2 or Algorithm 3 with the current distribution $\Pi_t = (\pi_{i,j}^t)_{n \times n}$. The empirical distribution $W_t = (w_{i,j}^t)_{n \times n}$ is then calculated from the $M$ elite solutions by setting

\[ w_{i,j}^t = \frac{\sum_{k=1}^M 1_{\{e' \in E \mid e' \in X_t^{[k]}\}(\{i, j\})}}{M}, \] (4)

where $1_A(\cdot)$ is the indicator function of set $A = \{e' \in E \mid e' \in X_t^{[k]}\}$ for each $\{i, j\} \in E$. The next distribution $\Pi_{t+1} = (\pi_{i,j}^{t+1})_{n \times n}$ is therefore obtained as

\[ \pi_{i,j}^{t+1} = (1 - \rho)\pi_{i,j}^t + \rho w_{i,j}^t \] (5)

for each $\{i, j\} \in E$.

We continue with the suggestions made in [34]. In the CE variant, we shall use a moderately large $N$ and a large $\rho = 1$. To fully use the best elite
solutions, we take $M = 1$. To prevent premature convergence (i.e., a possible stagnation at a non-optimal solution), we employ a feature from \textit{MMAS} [10], called \textit{max-min calibration}, in the construction of $\Pi_{t+1}$. We choose a lower bound $\pi_{\text{min}} \in (0, 1)$ and an upper bound $\pi_{\text{max}} \in (0, 1)$, and, after applying (5), adjust $\Pi_{t+1}$ by

\[ \pi_{i,j}^{t+1} = \begin{cases} 
\pi_{\text{min}} & \text{if } \pi_{i,j}^{t+1} < \pi_{\text{min}}, \\
\pi_{i,j}^{t+1} & \text{if } \pi_{i,j}^{t+1} \in [\pi_{\text{min}}, \pi_{\text{max}}], \\
\pi_{\text{max}} & \text{if } \pi_{i,j}^{t+1} > \pi_{\text{max}}, 
\end{cases} \tag{6} \]

for any edge $\{i, j\} \in E$. Note that the max-min calibration is the \textit{only} step that does not occur in the general CE (i.e., Algorithm 1).

This setting turns CE into an \textit{MMAS} with \textit{iteration-best reinforcement}, i.e., only the iteration-best solution $X^{[1]}_t$ is allowed to change the ‘pheromones’ $\Pi_t$. Stützle and Hoos [10] indicated in an empirical study that the practical performance of iteration-best reinforcement is comparable to best-so-far reinforcement for TSP instances. Thus, it should also be worthwhile to compare the theoretical runtime of iteration-best reinforcement with the known expected runtimes of best-so-far reinforcement for TSP instances presented in, e.g., [19] and [42].

4. Properties of the random solution generation methods

Before we start with our runtime analysis, we shall discuss some relevant properties of the two random solution generation methods, which concern the probability of producing a $k$-exchange move of the iteration-best solution in the next sampling.

Formally, a \textit{$k$-exchange move} on a Hamiltonian cycle is an operation that removes $k$ edges from the cycle and adds $k$ new edges to obtain again a cycle. A \textit{$k$-opt move} is a $k$-exchange move reducing the total travel cost. Figure 1a shows an example of a 2-exchange move, in which edges $\{i, j\}, \{k, l\}$ are removed, and edges $\{i, l\}, \{k, j\}$ are added. Figure 1b shows an example of a 3-exchange move.

In our analysis, we shall consider only iteration-best reinforcement with $\rho = 1$ and the max-min calibration [6]. The empirical distribution $W_t = (w_{i,j}^t)_{n \times n}$ for each iteration $t \in N$ in this particular case therefore satisfies

\[ \pi_{i,j}^{t+1} = \pi_{j,i}^{t+1} = \begin{cases} 
\min\{1, \pi_{\text{max}}\} = \pi_{\text{max}} & \text{if edge } \{i, j\} \in X^{[1]}_t, \\
\max\{0, \pi_{\text{min}}\} = \pi_{\text{min}} & \text{otherwise}, 
\end{cases} \tag{7} \]
for every edge \( \{i, j\} \in E \) and iteration \( t \in \mathbb{N} \). Furthermore, \( \Pi_{t+1} = W_t \).

Since \( \Pi_{t+1} \) is biased towards the iteration-best solution \( X_t^{[1]} \), \( k \)-exchanges of \( X_t^{[1]} \) with a large \( k \) are unlikely to happen among the \( N \) draws from \( \Pi_{t+1} \) by either of the two generation methods. Thus, an optimal solution is more likely to be reached by a sequence of repeatedly \( k \)-exchange moves with small \( k \) from iteration-best solutions. Therefore, it is necessary to estimate the probabilities of producing a \( k \)-exchange of \( X_t^{[1]} \) in the two generation methods, especially for the case of small \( k \).

### 4.1. Probabilities of producing \( k \)-exchanges in the vertex-based random solution generation

The probability of producing \( k \)-exchanges with \( k = 2, 3 \) in the vertex-based random solution generation has been studied in Zhou [19]. With \( \pi_{\min} = \frac{1}{n} \) and \( \pi_{\max} = 1 - \frac{1}{n} \), Zhou [19] proved for (1+1) MMAA that with a probability of \( \Omega(1/n^5) \), Algorithm 2 produces a random solution having more edges from \( s^* \) than \( x_t^* \) (the best solution found so far) provided that \( x_t^* \) is not optimal. Zhou [19] actually showed that if \( x_t^* \neq s^* \), then there exists either a 2-opt move or a 3-opt move for \( x_t^* \), and Algorithm 2 produces an arbitrary 2-exchange of \( x_t^* \) with a probability of \( \Omega(1/n^3) \), and an arbitrary 3-exchange of \( x_t^* \) with a probability of \( \Omega(1/n^5) \).

Although we use \( \pi_{\min} = \frac{1}{n(n-2)} \) and consider iteration-best reinforcement, a similar result holds in our case. Claim 1 below gives a lower bound on the probability of producing a \( k \)-exchange move of the iteration-best solution in the next round with the vertex-based random solution generation.
Claim 1. Let $M = 1, \rho = 1$, and consider a $k$-exchange move of $X_t^{[1]}$ for some integer $k = 2, 3, \ldots, n$. Then, Algorithm 2 produces the given $k$-exchange move with a probability $\Omega(1/n^{2k-1})$ in every of the $N$ draws in iteration $t+1$.

Proof. Recall that in Algorithm 2, the probability to select a continuing edge $\{i, j\}$ is always bounded from below by $\pi^t_{i,j}$ (or, equivalently, $\pi^t_{j,i}$) for each iteration $t \in \mathbb{N}$, since each row of $\Pi_t$ sums up to 1. Given a $k$-exchange move of $X_t^{[1]}$, one possibility to generate it from $\Pi_{t+1} = W_t$ by Algorithm 2 is that one of the new edges is added in the last step. This happens with a probability at least $\frac{1}{n} \cdot \left(\frac{1}{n(n-2)}\right)^{k-1} \cdot (1 - \frac{1}{n})^{n-k} \geq \frac{1}{e^{n^{2k-1}}}$, where $e \approx 2.71828$ is Euler’s number, $\frac{1}{n}$ represents the probability to select the starting vertex, $\frac{1}{n(n-2)}$ is the common lower bound of the probability to select the remaining $k-1$ new edges, and $1 - \frac{1}{n}$ is the common lower bound of the probability to select one of the remaining $n-k$ edges from $X_t^{[1]}$.

Because of Claim 1, every 2-exchange of $X_t^{[1]}$ is produced from $\Pi_{t+1}$ by Algorithm 2 with a probability $\Omega(1/n^3)$, and every 3-exchange is produced by Algorithm 2 with a probability $\Omega(1/n^5)$. Note that for any $k = 2, 3, \ldots$, if a $k$-opt move of $X_t^{[1]}$ occurs among the $N$ draws in the next sampling, then $f(X_{t+1}^{[1]}) < f(X_t^{[1]})$ must hold. Thus, if we take a moderately large sample size, say $N = \Theta(n^{5+\epsilon})$ for some $\epsilon > 0$, with a probability $1 - (1 - \Omega(n^{-5}))^{\Omega(\ln n)} = 1 - e^{-\Omega(n^\epsilon)}$, $f(X_{t+1}^{[1]}) < f(X_t^{[1]})$ will hold, provided that there still exists a 2-opt or 3-opt move from $X_t^{[1]}$.

Claim 2. Suppose that $M = 1, \rho = 1$. Then, for iteration $t+1$, the probability that Algorithm 2 produces a solution with a cost not larger than $X_t^{[1]}$ in one application is in $\Omega(1)$.

Proof. Observe that the probability that $X_t^{[1]}$ is reproduced in one application of Algorithm 2 is larger than $(1 - 1/n)^{n-1} \in \Omega(1)$, which implies that the cost of the generated random solution is not larger than $f(X_t^{[1]})$.

Note that if $X_t^{[1]}$ is reproduced at least once among the $N$ draws in the next sampling, then $f(X_{t+1}^{[1]}) \leq f(X_t^{[1]})$. Thus, if the sample size $N \in \Omega(\ln n)$, then $f(X_{t+1}^{[1]}) \leq f(X_t^{[1]})$ with a probability $1 - (1 - \Omega(1))^N = 1 - O(1/n)$. Particularly, when $N \in \Omega(n^\epsilon)$ for some $\epsilon > 0$, $f(X_{t+1}^{[1]}) \leq f(X_t^{[1]})$ with an overwhelming probability $1 - e^{-\Omega(n^\epsilon)}$. 

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4.2. Probabilities of producing \(k\)-exchanges in the edge-based random solution generation

The behavior of the edge-based random solution generation is comprehensively studied in [42]. Kötzing et al [42] proved for MMAS\(^*\)\(_{Arb}\) and a constant \(k \in O(1)\) that, with a probability of \(\Omega(1)\), Algorithm 3 produces a random solution that is obtained by a \(k\)-exchange move from the best solution found so far.

Recall that in each iteration \(t\), either \(\pi^t_{i,j} = \pi^t_{j,i} = \pi_{\min}\) or \(\pi^t_{i,j} = \pi^t_{j,i} = \pi_{\max}\) for any edge \(\{i, j\} \in E\). For convenience, we will call an edge \(\{i, j\} \in E\) with \(\pi^t_{i,j} = \pi^t_{j,i} = \pi_{\max}\) a high edge, and otherwise a low edge. Kötzing et al [42] showed the probability of the event that Algorithm 3 chooses a high edge in an arbitrary fixed step conditioned on the event that \(l \leq \sqrt{n}\) low edges have been chosen in some \(l\) steps before this step is \(1 - O(1/n)\). Our setting is only slightly different with from theirs, i.e., we use \(\pi_{\min} = \frac{1}{n(n-2)}\) but they put \(\pi_{\min} = \frac{1}{n(n-1)}\). Thus, the result should also hold here. Claim 3 below formally asserts this, readers may also refer to [42] for a similar proof.

**Claim 3.** Assume \(M = 1, \rho = 1\). Then, the probability of choosing a high edge at any fixed step in Algorithm 3 is at least \(1 - \frac{12}{n}\) if at most \(\sqrt{n}\) low edges have been chosen before that step and there exists at least one high admissible edge to be added.

**Proof.** We now fix a step \(n-m\) for some \(m = 0, 1, \ldots, n-1\), and assume that \(l \leq \sqrt{n}\) low edges have been chosen before this step. Obviously, we still need to add \(m+1 \geq 1\) edges to obtain a complete solution. We now estimate the numbers of admissible high and low edges in this step. Note that every of the \(l\) low edges blocks at most 3 of the \(m+l\) remaining high edges (at most two which are incident to the end points of the low edge, and at most one that may introduce a cycle). So at least \(m+l-3l = m-2l \geq m-3l\) high edges are available for adding in this step. Of course, it may happen that there is no admissible high edges in this step. However, we are not interested in such a case. We consider only the case that there exists at least one admissible high edge in this step, i.e. the number of admissible high edges in this step is at least \(\max\{1, m-3l\}\). Note also that the \(n-m\) edges added before partition the subgraph of \(G = (V, E)\) with vertices \(V\) and edges from the partial solution constructed so far into exactly \(m\) connected components (here, we see an isolated vertex also as a connected component). For any two of the components, there are at most 4 admissible edges connecting them.
Therefore, there are at most \( \min\{4\binom{m}{2}, \binom{n}{2}\} \) admissible low edges. Observing \( l \leq \sqrt{n} \), the probability of choosing a high edge in this step is bounded from below by

\[
1 - \frac{\min\{4\binom{m}{2}, \binom{n}{2}\}}{\max\{1, m - 3l\}} \pi_{\min} \geq \begin{cases} 
1 - \frac{2m^2}{(m-3l)n(n-2)} \geq 1 - \frac{3}{(n-2)} & \text{if } m > 3\sqrt{n}, \\
1 & \text{if } m \leq 3\sqrt{n}, 
\end{cases}
\]

where the first inequality is obtained by observing that

\[
\min\{4\binom{m}{2}, \binom{n}{2}\} \leq \min\{2m^2, \binom{n}{2}\} \leq 2m^2,
\]

\( \tau_{\max} = 1 - 1/n, \pi_{\min} = \frac{1}{n(n-1)}, \) and \( \frac{2m^2}{m-3l} \leq \frac{2}{m - \frac{3m}{n}} \leq 3n. \)

With Claim 3, we can show that, for any \( t \in \mathbb{N} \) and any fixed \( k \in O(1) \), the probability of the event that a \( k \)-exchange of \( X_t^{[1]} \) is produced by one application of Algorithm 3 is \( \Omega(1) \), see Claim 4. Here, we shall use a different proof from the one presented by Kötzing et al [42], which appears to us as problematic.

**Claim 4.** Let \( M = 1, \rho = 1. \) For any \( k \in O(1), \) with probability \( \Omega(1) \), the random solution produced by Algorithm 3 is a \( k \)-exchange of \( X_t^{[1]} \).

**Proof.** Let \( k \in O(1) \) be arbitrarily fixed, and \( \mathcal{M} \) be the set of all \( k \)-element subsets of \( \{1, 2, \ldots, n/2\} \) (where we assume without loss of generality that \( n \) is even). Obviously, \( |\mathcal{M}| \in \Theta(n^k) \) since \( k \in O(1) \). Let \( \mathbb{M} \in \mathcal{M} \) be an arbitrarily fixed \( k \)-element subset. The probability of the event that Algorithm 3 selects \( k \) new edges (low edges) at steps \( i \in \mathbb{M} \) and \( n - k \) edges (high edges) from \( X_t^{[1]} \) at other steps, is bounded from below by

\[
(1 - O(\frac{1}{n}))^{n-k} \prod_{i \in \mathbb{M}} \frac{(\binom{n-i+1}{2} - (n-i+k+1))\pi_{\min}}{n(n-1)\pi_{\min} + (n-i+k+1)\pi_{\max}} \geq \Theta(\frac{1}{n^k}),
\]

where \( 1 - O(1/n) \) is a lower bound for the probability of selecting an edge from \( X_t^{[1]} \). In each step \( i \in \mathbb{M} \), the edges chosen before partition the graph into \( n-i+1 \) connected components, and for any two of the components there exists at least 2 edges connecting them without introducing a cycle. Hence, there are at least \( \binom{n-i+1}{2} \) admissible edges in each step \( i \in \mathbb{M} \). Notice also that the number of admissible high edges in this case is at most \( n-i+k+1 \).
(n – i + k + 1 is the maximal number of high edges that have not been chosen before). Therefore, each factor \( \frac{(n-i+1)-(n-i+k+1)\pi_{min}}{n(n-1)\pi_{min}+(n-i+k+1)\pi_{max}} \) of (9) is just the lower bound of the probability for choosing an admissible edge not belonging to \( X_t^{[1]} \) in a step \( i \in M \).

As a result, the probability of the random event that Algorithm 3 produces a \( k \)-exchange of \( X_t^{[1]} \) with \( k \in O(1) \) in any of the \( N \) independent draws in iteration \( t+1 \) is bounded from below by \( |M| \cdot \Theta(\frac{1}{n^k}) = \Theta(\frac{1}{n^k}) \cdot \Theta(\frac{1}{n^k}) \in \Omega(1) \), since new edges can also be added in steps \( l \geq \frac{n}{2} \).

Notice that in the edge-based random solution generation, for any \( k = 2, 3, \ldots, n \), any two \( k \)-exchanges of \( X_t^{[1]} \) are generated with the same probability, since the generation does not require adding the edges in a particular order. Therefore, by Claim 4, for any \( k \in O(1) \), any specified \( k \)-exchange of \( X_t^{[1]} \) will be produced with a probability \( \Theta(1/n^k) \). Since reproducing \( X_t^{[1]} \) can be seen as a 0-exchange of \( X_t^{[1]} \), we can thus derive the following conclusion.

**Claim 5.** Let \( M = 1, \rho = 1 \). With probability \( \Omega(1) \), the random solution generated by Algorithm 3 has a cost not larger than that of \( X_t^{[1]} \).

Claim 6 shows that it is unlikely that the random solution generated by Algorithm 3 is “very” different from the last iteration-best solution \( X_t^{[1]} \). This will be fundamental for deriving the runtime lower bound.

**Claim 6.** Let \( M = 1, \rho = 1 \). For any \( \delta \in (0, 1] \), with an overwhelming probability \( 1 - e^{-\omega(n^{-\min(\delta, 1/4)})/2)} \), the random solution generated by Algorithm 3 is a \( k \)-exchange move from \( X_t^{[1]} \) for some \( k < n^\delta \).

**Proof.** Let \( \delta \in (0, 1] \) be arbitrarily fixed, and put \( \gamma = \min\{\delta, 1/4\} \). To prove the claim, we just need to show that with an overwhelming probability, the random solution generated by Algorithm 3 is a \( k \)-exchange of \( X_t^{[1]} \) for some \( k \leq n^\gamma \leq n^{1/4} \). This is again implied by the fact that with an overwhelming probability, at most \( n^{\gamma/2} \) low edges are chosen within the first \( T := n - \frac{3n^\gamma}{4} \) steps in Algorithm 3, since the best case \( n^{\gamma/2} + \frac{3n^\gamma}{4} \) is still smaller than \( n^\gamma \).

By Claim 3 for any \( k \leq n^{\gamma/2} \) and any \( m \leq T \), Algorithm 3 chooses high edges with a probability at least \( 1 - 12/n \) at step \( m \) if at most \( k \) edges have been chosen before step \( m \), since there exist at least \( n - m - 3k \geq \frac{3n^\gamma}{4} - 3n^{\gamma/2} \geq 3 \) admissible high edges at step \( m \).
Let $P$ denote the probability of the random event that at most $n^{\gamma/2}$ low edges are chosen within $T$ steps, and $Q$ the probability of the random event that at least $n^{\gamma/2} + 1$ low edges are chosen within the same $T$ steps. Then $P = 1 - Q$. We shall bound $Q$ from above, which will give a lower bound for $P$.

Let $E$ be the random event that at least $n^{\gamma/2} + 1$ low edges are chosen within $T$ steps. Then $Q = P[E]$. For each $l = 1, \ldots, n^{\gamma/2} + 1$, we define a random variable $v_l$ denoting the first step $m \leq T$ such that $l$ low edges are chosen within $m$ steps. Obviously, $E$ implies the random event $E_1$ that $v_1 < v_2 < \cdots < v_{n^{\gamma/2}+1} \leq T$. Thus, $Q \leq P[E_1]$, and $P \geq 1 - P[E_1]$.

Observe that

$$P[E_1] = \sum_{a_1 < a_2 < \cdots < a_{n^{\gamma/2}+1} \leq T} P[v_1 = a_1, \ldots, v_{n^{\gamma/2}+1} = a_{n^{\gamma/2}+1}],$$

and $v_1 = a_1, \ldots, v_{n^{\gamma/2}+1} = a_{n^{\gamma/2}+1}$ is equivalent to the random event that before step $a_1$ only high edges are chosen, that at any step between $a_l$ and $a_{l+1}$ only high edges are chosen for any $l$ with $1 \leq l \leq n^{\gamma/2}$, and that at steps $a_1, \ldots, a_{n^{\gamma/2}+1}$ only low edges are chosen. Thus, we have by Claim 3 that

$$P[v_1 = a_1, \ldots, v_{n^{\gamma/2}+1} = a_{n^{\gamma/2}+1}] \leq \left(\frac{12}{n}\right)^{n^{\gamma/2}+1},$$

since at each step $a_l$, there exists at least one admissible high edge and we do not care about what happens after step $v_{n^{\gamma/2}+1}$.

There are at most $\left(\frac{T}{n^{\gamma/2}+1}\right)$ different combinations for $a_1 < a_2 < \cdots < a_{n^{\gamma/2}+1}$. Therefore, $P \geq 1 - P[E_1] \geq 1 - \left(\frac{T}{n^{\gamma/2}+1}\right)\left(\frac{12}{n}\right)^{n^{\gamma/2}+1}$.

By Stirling’s formula, and observing that $n^{\gamma/2} + 1 \in o(T), T \in \Theta(n)$, we have $\left(\frac{T}{n^{\gamma/2}+1}\right)\left(\frac{12}{n}\right)^{n^{\gamma/2}+1} = e^{-\omega(n^{\gamma/2})}$. Hence, $P \geq 1 - e^{-\omega(n^{\gamma/2})}$ is overwhelmingly large.

5. Main results

We shall now analyze the stochastic runtime of our two different random solution generation methods for two classes of TSP instances that have been well studied in the literature.
5.1. Stochastic runtime analysis for simple instances

We first consider a class of simple TSP instances that is defined by the following distance function \( d : E \to \mathbb{R} \) on a graph with \( n \) vertices.

\[
d({i,j}) = \begin{cases} 
1 & \text{if } \{i,j\} = \{i,i+1\} \text{ for each } i = 1,2,\ldots,n-1, \\
1 & \text{if } \{i,j\} = \{n,1\}, \\
n & \text{otherwise.}
\end{cases}
\]  

(10)

Obviously, TSP instances with this distance function have a unique optimal solution \( s^* = (1,2,\ldots,n) \) (in the sense of the underlying Hamiltonian cycle), and \( s^* \) has a cost of \( n \). The cost of an arbitrary feasible solution \( s \) equals \( k + (n-k) \cdot n \), where \( k \) is the number of edges \( \in s \) that are also in \( s^* \). We shall refer to these instances as \( G_1 \) in the sequel.

The class \( G_1 \) has been used in [19] and [42] for analyzing the expected runtime of variants of MMAS. Zhou [19] proved that the \( (1+1) \) MA algorithm has an expected runtime of \( O(n^6 + \frac{n \ln n}{\rho}) \) on \( G_1 \) in the case of non-visibility (i.e., without the greedy distance information in the sampling), and has an expected runtime of \( O(n^5 + \frac{n \ln n}{\rho}) \) in the case of visibility (i.e., with considering the greedy distance information in the sampling). Kötzing et al [42] continued the study in [19]. They investigated the expected runtime of \((1+1) \) MA and its variant MMAS\(_{\text{Arb}}^*\) on \( G_1 \) and other TSP instances on which both \((1+1) \) MA and MMAS\(_{\text{Arb}}^*\) have exponential expected runtime. MMAS\(_{\text{Arb}}^*\) differs with \((1+1) \) MA only in the random solution generation. MMAS\(_{\text{Arb}}^*\) uses Algorithm 3 as its random solution generation method, while \((1+1) \) MA used Algorithm 2. Kötzing et al [42] proved that MMAS\(_{\text{Arb}}^*\) has an expected runtime of \( O(n^3 \ln n + \frac{n \ln n}{\rho}) \) on \( G_1 \).

Theorem 1 shows a stochastic runtime of \( O(n^{6+\epsilon}) \) for the CE variant with the add-on, i.e., Algorithm 1 with max-min calibration (6), the vertex-based random solution generation, and a stochastic runtime of \( O(n^{4+\epsilon}) \) for the edge-based random solution generation. These results are comparable with the above known expected runtimes. Although we are not able to get strictly superior runtimes, our results are actually stronger and more informative.

**Theorem 1** (Stochastic runtime of Algorithm 1 with max-min calibration on \( G_1 \)). Assume that we set \( M = 1, \rho = 1, \) and use Algorithm 1 with the max-min calibration (6) for the values \( \pi_{\text{min}} = \frac{1}{n(n-2)}, \pi_{\text{max}} = 1 - \frac{2}{n}. \) Then

a) if we use the vertex-based random solution generation method (Algorithm 2), and take a sample size \( N \in \Omega(n^{5+\epsilon}) \) for any constant \( \epsilon \in \)
(0, 1), then with a probability at least $1 - e^{-\Omega(N/n^5)}$ the optimal solution $s^*$ can be found within $n$ iterations;

b) if we use the edge-based random solution generation method (Algorithm 3), and take a sample size $N \in \Omega(n^{3+\epsilon})$ for a constant $\epsilon \in (0, 1)$, then with a probability at least $1 - e^{-\Omega(N/n^5)}$, the optimal solution can be found within $n$ iterations.

Proof. We prove the Theorem by showing that the probability of the random event that before the optimal solution is met, the number of edges shared by the iteration-best and optimal solution strictly increases is overwhelmingly large. This implies that the optimal solution is found within $n$ iterations, since the optimal solution has only $n$ edges. Furthermore, the runtimes presented in the Theorem hold. We only discuss the case of $a)$, $b)$ follows with an almost identical argument.

By [19] (see also proof of Theorem 2), if $X_t^{[1]}$ is not optimal, it has at least either a 2-opt move or a 3-opt move. Note that for $G_1$, any $k$-opt move of the iteration-best solution increases the number of its edges shared with the optimal solution. By Claim 1 any 2-opt move is generated by Algorithm 2 with probability $\Omega(n^{-3})$, and any 3-opt move is generated with probability $\Omega(n^{-5})$. Thus, if $X_t^{[1]}$ is not optimal, $X_{t+1}^{[1]}$ shares more edges with the optimal solution than $X_t^{[1]}$ with a probability at least $1 - (1 - n^{-5})^N = 1 - e^{-\Omega(N/n^5)} \leq 1 - e^{-\Omega(n^{5+\epsilon})}$ if $N \in \Omega(n^{5+\epsilon})$ for any $\epsilon > 0$. Thus, this repeatedly happens within polynomially many number of iterations with overwhelming probability $1 - e^{-\Omega(N/n^5)}$. This completes the proof.

The stochastic runtimes of Theorem 1 are derived for a relatively large sample size, namely $N = \Omega(n^{5+\epsilon})$ and $N = \Omega(n^{3+\epsilon})$. Actually, Theorem 1 may still hold for a smaller sample size. Theorem 2 partially asserts this. It states that the total number of iterations required to reach the optimal solution for both generation schemes may increase considerably if a smaller sample size is used. However, the stochastic runtime does not increase. Interestingly, one can obtain a smaller stochastic runtime with a small sample size for the edge-based random solution generation.

Theorem 2 (Stochastic runtime of Algorithm 1 on $G_1$ for a small sample size). Assume the conditions in Theorem 1 but set $N \in \Omega(n^\epsilon)$ for any $\epsilon \in (0, 1)$. Then:
a) For the vertex-based random solution generation, Algorithm 1 finds the optimal solution $s^*$ within $n^6$ iterations with a probability of $1 - e^{-\Omega(N)}$.

b) For the edge-based random solution generation, Algorithm 1 finds the optimal solution $s^*$ within $n^3 \ln n$ iterations with a probability of $1 - e^{-\Omega(N)}$.

Proof of Theorem 2. The proof shares a similar idea with that of Theorem 1. However, we consider here the random event that the number of edges shared by the iteration-best and optimal solution does not decrease and strictly increases enough times within a specified polynomial number of iterations.

For a), we shall consider the first $n^6$ iterations. By Claim 2, the number of edges shared by the iteration-best and optimal solution does not decrease with a probability $1 - (1 - \Omega(1))^N = 1 - e^{-\Omega(N)}$ (for $N \in \Omega(n^k)$). Therefore, the number does not decrease within the first $n^6$ iterations with probability $\prod_{t=0}^{n^6} (1 - e^{-\Omega(N)}) = 1 - e^{-\Omega(N)}$. By Claim 1, for every consecutive $n^5$ iterations, if the starting iteration-best solution is not optimal, then with probability $1 - (1 - n^{-k})^N = 1 - e^{-\Omega(N)}$, the number will strictly increase at least once within these $n^5$ iterations. Therefore, with overwhelming probability $1 - e^{-\Omega(N)}$, the optimal solution will be reached within the period of the first $n^6$ iterations, since there are $n$ many consecutive $n^5$ iterations within that period.

b) can be proved by a similar way with a). We shall consider the first $n^3 \ln n$ iterations. By Claim 4, with probability $1 - (1 - \Omega(1))^N = 1 - e^{-\Omega(N)}$, the number of shared edges does not decrease in consecutive two iterations. To complete the proof, we need an extra fact on 2,3-exchanges.

Kötzing et al [42] showed for MMAS*$_{arb}$ that if the best solution $s^*_t$ found so far has $n-k$ edges from the optimal solution $s^*$, then the probability of the event that $s^*_{t+1}$ has at least $n-k+1$ edges from $s^*$, is in $\Omega(k/n^3)$. We shall use a different but simpler proof to show that this also holds in our case of iteration-best reinforcement. And with this fact, if $|X_{[t]} \cap s^*| = n-k$ for some $0 < k \leq n$, then with probability $1 - (1 - k \cdot n^{-3})^N = 1 - e^{-\Omega(N)}$, the number of edges shared by the iteration-best solution and $s^*$ will strictly increase at least once within the period $[t, t + n^3/k]$. This implies that $s^*$ is sampled within the first $n^3 \ln n$ iterations with overwhelming probability $1 - e^{-\Omega(N)}$, since $n^3 \ln n$ iterations can be partitioned into $n$ many consecutive phases $[0, n^2), [n^2, n^2 + n^3/(n-1)), [n^2 + n^3/(n-1), n^2 + n^3/(n-1) + n^3/(n-2)), \ldots$. We now prove that fact.
We first show that when $|X_t^{[1]} \cap s^*| = n - k$ with $k > 0$, then there exists a 2-opt move or a 3-opt move for $X_t^{[1]}$ (see also [19] for a similar proof). Assume that $X_t^{[1]}$ contains exactly $n - k$ edges from $s^*$ for some integer $k > 0$. Let $e^* = \{i, i+1\}$ be an edge in $s^*$ but not in $X_t^{[1]}$. Note that each node of the graph is exactly incident to two edges of $s^*$ and $X_t^{[1]}$, respectively. Therefore there exists an edge $e_0 \in X_t^{[1]}$ incident to $i$, an edge $e'_0 \in X_t^{[1]}$ incident to $i+1$, and $e_0, e'_0$ are not in $s^*$. Figure 2 shows an example, where $e_0$ is either $\{i, u\}$ or $\{i, v\}$, and $e'_0$ is either $\{i+1, w\}$ or $\{i+1, y\}$. If $e_0 = \{i, u\}$ and $e'_0 = \{i+1, w\}$ or $\{i, v\}$ and $e'_0 = \{i+1, y\}$, then there exists a 2-opt move of $X_t^{[1]}$ which removes $e_0, e'_0$ of distance $n$ and adds $e^*$ and another edge (either $\{u, w\}$ or $\{v, y\}$) of distance at most $n + 1$ together. If $e_0 = \{i, u\}$, $e'_0 = \{i+1, y\}$ or $e_0 = \{i, v\}, e'_0 = \{i+1, w\}$, there is a 3-opt move of $X_t^{[1]}$ which removes $e_0, e'_0$, and an edge $e_1 \notin s^*$, and adds edge $e^*$ and another two edges, this replacing 3 edges of distance $n$ by 3 edges of distance at most $2n + 1$ together. Here, observe the fact that adding $e^*$ to $X_t^{[1]}$ and removing $e_0, e'_0$ from $X_t^{[1]}$ results in graph containing a cycle, and there must be an edge $e_1 \in X_t^{[1]}$ on that cycle that does not belong to $s^*$. We choose this edge as the edge $e_1$. Therefore, for each $e^*$ of the $k$ remaining edges in $s^*$ that are not in $X_t^{[1]}$, there exists a 2-opt or 3-opt move of $X_t^{[1]}$ that adds $e^*$.

By Claim 4, for any $l \in O(1)$, the probability of producing an $l$-exchange of the iteration-best solution $X_t^{[1]}$ by Algorithm 3 in iteration $t + 1$ is $\Omega(1)$. Since any two $l$-exchanges are produced with the same probability, the probability of producing a particular $l$-exchange in iteration $t + 1$ is $\Omega(1/n^l)$. As a result, Algorithm 3 produces for each edge $e^* \in s^* - X_t^{[1]}$ a 2-opt or 3-opt move of $X_t^{[1]}$ that adds edge $e^*$ with probability at least $\Omega(1/n^3)$.
Note that the generation of a 2-exchange (or a 3-exchange) with two newly added edges \( e_2, e_3 \) by Algorithm 3 includes two mutually exclusive cases (3! cases for a 3-exchange): \( e_2 \) is chosen before \( e_3 \), or \( e_3 \) is chosen before \( e_2 \). It is not difficult to see that these two cases (3! cases for 3-exchange) have the same probability. Therefore, the probability of the event that Algorithm 3 generates a 2-opt or 3-opt move of \( X_t^{[1]} \) that \( e^* \) as one of the newly added edges and selects \( e^* \) before the other newly added edges, is bounded from below by \( \Omega(1/3!) = \Omega(1/n^3) \). Since \( X_t^{[1]} \) has \( k \) such \( e^* \) and the corresponding \( k \) events are also mutually exclusive, we obtain that the probability that \( X_{t+1}^{[1]} \) has more edges from \( s^* \) than \( X_t^{[1]} \) if \( X_t^{[1]} \) has exactly \( n-k \) edges from \( s^* \) for a constant \( k > 0 \) is \( \Omega(k/n^3) \).

Corollary 1 further improves the stochastic runtime for an even smaller sample size. It can be proved by an argument similar to the proof of Theorem 1, where we observe that

\[
(1 - (1 - p(n)))^{\omega(ln n)} n^l = 1 - n^{-\omega(1)} \text{ for any constant } l > 0 \text{ and probability } p(n) \in \Omega(1), \text{ and that } 1 - e^{-\omega(ln n)} = 1 - n^{-\omega(1)}.
\]

**Corollary 1.** Assume the conditions in Theorem 1, but let \( N \in \omega(ln n) \). Then:

a) For the vertex-based random solution generation, Algorithm 1 finds the optimal solution \( s^* \) within \( n^6 \) iterations with a probability of \( 1 - n^{-\omega(1)} \). Particularly, if \( N = (ln n)^2 \), the runtime is \( n^6(ln n)^2 \) with probability \( 1 - n^{-\omega(1)} \).

b) For the edge-based random solution generation, Algorithm 1 finds the optimal solution \( s^* \) within \( n^3 \ln n \) iterations with a probability of \( 1 - n^{-\omega(1)} \). Particularly, if \( N = (ln n)^2 \), the runtime is \( n^3(ln n)^3 \) with probability \( 1 - n^{-\omega(1)} \).

Theorem 2 tells that, for any \( \epsilon \in (0, 1) \), a sample size of \( N \in \Theta(n^\epsilon) \) is already sufficient for iteration-best reinforcement to efficiently find an optimal solution of simple TSP instances with an overwhelming probability. Corollary 1 further shows that \( N \in \omega(ln n) \) even leads to a better runtime with a slightly smaller but still overwhelming probability. Theorem 3 below shows that with an overwhelming probability, the runtime of iteration-best reinforcement will be exponential if \( N \in O(ln n) \), even if the instances are as simple as those in \( G_1 \).
**Theorem 3.** Assume the conditions of Theorem 1, but set \( N < \frac{1}{220} \ln n \). Then, with probability \( 1 - e^{-\Omega(n^{1/200})} \), Algorithm 1 with edge-based solution generation does not find the optimal solution \( s^* \) within \( e^{\Theta(n^{1/300})} \) iterations.

**Proof.** We prove the Theorem by inspecting the probability of the random event that, before the optimal solution is found, the cost of the iteration-best solution \( X_t^{[1]} \) will oscillate for exponentially many iterations with an overwhelming probability. We shall consider this in the last stages of the optimization process.

Let \( T_0 \) be the first iteration which samples a solution containing at least \( n - n^{1/4} + n^{1/5} \) edges from the optimal solution. We show that with an overwhelming probability, the number of common edges in the iteration-best and optimal solution will drop below \( n - n^{1/4} + n^{1/5} \) and the optimal solution is not sampled before that. This will imply the conclusion of Theorem 3, since, with an overwhelming probability, this phenomenon can repeatedly occur exponentially many times before optimal solution is found.

To that end, we need to show the following:

1) For any \( 1/4 > \delta > 0 \), if \( X_t^{[1]} \) contains at least \( n - n^\delta \) edges from the optimal solution, then with a probability \( O(\frac{1}{\sqrt{n}}) \), the random solution generated by Algorithm 3 will contain more edges from the optimal solution than \( X_t^{[1]} \) in iteration \( t + 1 \);

2) For any \( 1/4 > \delta > 0 \), if \( X_t^{[1]} \) contains at least \( n - n^\delta \) edges from the optimal solution, then with a probability \( \Omega(1) \) (at least \( e^{-5} \)), the random solution generated by Algorithm 3 will contain fewer edges from the optimal solution than \( X_t^{[1]} \) in iteration \( t + 1 \).

However, we first use these two facts and show them afterwards.

By Claim 6, with probability \( 1 - e^{-\omega(n^{1/200})} \), \( X_{T_0}^{[1]} \) contains at most \( n - n^{1/4} + n^{1/5} + n^{1/10} \) edges from the optimal solution, since the random event that the number of common edges from the iteration-best and optimal solution increases more than \( n^{1/10} \) in one iteration implies an occurrence of a \( \Omega(n^{1/10}) \)-exchange. Similarly, by Claim 6 again, with probability \( 1 - e^{-\omega(n^{1/200})} \), the iteration-best solution contains \( k \in [n - n^{1/4} + n^{1/5} - n^{1/6+1/100}, n - n^{1/4} + n^{1/5} + n^{1/10} + n^{1/6+1/100}] \) edges from the optimal solution in each iteration \( t \in [T_0, T_0 + n^{1/6}] \). This means that the optimal solution is not found in the period \( [T_0, T_0 + n^{1/6}] \) with an overwhelming probability. With the help of 1) and 2), we are now to show that within this period, the number of edges
shared by the iteration-best and optimal solution is significantly reduced with an overwhelming probability. This will complete the proof.

To facilitate our discussion, we call an iteration a successful iteration if its iteration-best solution contains more edges from the optimal solution than the last iteration-best solution, and an iteration a failure iteration if its iteration-best solution contains fewer edges from the optimal solution than the last iteration-best solution.

By 1) and the subsequent discussion, the expected number of successful iterations within \([T_0, T_0 + n^{1/6}]\) is \(O\left(\frac{\ln n}{n^{1/3}}\right)\), since \(N < \frac{1}{220} \ln n\). Thus, by the Chernoff bound, with probability \(1 - e^{-\Omega(n^{1/6})}\), at most \(n^{1/100}\) successful iterations can occur within \([T_0, T_0 + n^{1/6}]\). By 2) and the subsequent discussion, the expected number of failure iterations in \([T_0, T_0 + n^{1/6}]\) is \(\Omega(n^{1/6})\), since \(N < \frac{1}{220} \ln n\). By the Chernoff bound, it happens that with probability \(1 - e^{-\Omega(n^{1/6})}\), at least \(n^{1/7}\) failure iterations will occur in \([T_0, T_0 + n^{1/6}]\). Since a successful iteration can add at most \(n^{1/100}\) edges from the optimal solution with probability \(1 - e^{-\Omega(n^{1/200})}\), it totally adds at most \(n^{1/100} \times n^{1/100} = n^{1/50}\) edges from the optimal solution to the iteration-best solution within \([T_0, T_0 + n^{1/6}]\) with probability \(1 - e^{-\Omega(n^{1/200})}\). Note that within \([T_0, T_0 + n^{1/6}]\), with probability \(1 - e^{-\Omega(n^{1/6})}\), at least \(n^{1/7} \times 1 = n^{1/7}\) “good” edges are removed from the iteration-best solution. Therefore, with overwhelming probability \(1 - e^{-\Omega(n^{1/200})}\), \(X_{[1]}^{[1]} t_{0 + n^{1/6}}\) will contain at most

\[
\begin{align*}
n - n^{1/4} + n^{1/5} + n^{1/10} - n^{1/7} + n^{1/50} < n - n^{1/4} + n^{1/5}
\end{align*}
\]

edges from the optimal solution, since \(X_{[1]}^{[1]} t_{0}\) contains at most \(n - n^{1/4} + n^{1/5} + n^{1/10}\) iterations with probability \(1 - e^{-\Omega(n^{1/200})}\). As a result, with probability \(1 - e^{-\Omega(n^{1/200})}\), the number of common edges in the iteration-best and optimal solution will again be smaller than \(n - n^{1/4} + n^{1/5}\) in some iteration after \(T_0\), and the optimal solution is not found before that. And this will repeatedly happen \(e^{\Theta(n^{1/300})}\) times with probability \(1 - e^{-\Omega(n^{1/200})}\).

To finish the proof, we now formally prove 1) and 2). We first consider 2). By taking \(k = 2\) and considering the \(\binom{2}{2}\) 2-exchanges that happen in the first \(n - 3\sqrt{n}\) steps in the proof of Claim 4, one can show a tighter probability lower bound \(\frac{1}{e^2}\) for producing 2-exchanges of \(X_{[1]}^{[1]} t\) by Algorithm 3. Here, we observe that the probability of choosing a high edge at a step before \(n - 3\sqrt{n}\) is at least \(1 - 3/(n - 2)\), see the proof of Claim 3.

Note that if 2-exchanges deleting 2 edges from the optimal solution happen \(N\) times in an iteration, then the iteration will be a failure iteration.
By the above and the fact that any two \( k \)-exchanges happen with the same probability, a failure iteration then occurs with a probability at least

\[
\left( \frac{1}{e^5} \left( \frac{n-n^\delta}{2} \right) \right)^N \geq \left( \frac{1}{e^5} \left( \frac{n-n^\delta}{2} \right) \right)^{\frac{1}{220} \ln n} \in \Omega(n^{-1/44}),
\]

where \( \delta \in (0, 1/4) \) and \( N < \frac{1}{220} \ln n \). This asserts 2).

1) follows with a similar discussion. Since \( X^{[1]}_t \) is assumed to contain at least \( n - n^\delta \) edges from the optimal solution for some \( \delta \in (0, 1/4) \), and since \( \Omega(n^\delta) \)-exchanges happen with an overwhelmingly small probability, we need to consider only \( O(n^\delta) \)-exchanges when we estimate the probability of a successful iteration. For each \( k \in \Omega(n^\delta) \), the proportion of failure \( k \)-exchanges is bounded from below by

\[
\left( \frac{n-n^\delta}{k} \right) \geq e^{-2k n^\delta} + o(1) \geq e^{-2n^{-1/2}} + o(1),
\]

since \( 0 < \delta < 1/4 \), and \( k \)-exchanges removing \( k \) edges shared by the iteration-best and optimal solution are not “successful” \( k \)-exchanges. Since for any \( k \in \Omega(n^\delta) \), any two \( k \)-exchanges happen with the same probability, and since the sum of the probabilities of successful and failure \( k \)-exchanges is smaller than 1, we conclude that successful \( O(n^\delta) \)-exchanges happen with a probability smaller than \( 1 - e^{2n^{-1/2}} \in O(\frac{1}{\sqrt{n}}) \). Therefore, a successful iteration happens with a probability

\[
1 - (1 - O(\frac{1}{\sqrt{n}}))^N \in O(\frac{\ln n}{\sqrt{n}})
\]

since \( N < \frac{1}{220} \ln n \).

Theorem \( \text{[3]} \) generalizes the finding of \( \text{[20]} \) to simple TSP instances. It formally states that for \( \rho = 1 \), \( N \in \Omega(\ln n) \) is necessary to efficiently find an optimal solution to TSP. By Theorem \( \text{[3]} \), Theorem \( \text{[1]} \), Theorem \( \text{[2]} \) and its Corollary \( \text{[1]} \), we have clearly analyzed the impact of the size of \( N \) on the resulting stochastic runtime for the simple TSP instances in the case of that \( \rho = 1 \). \( N \in \omega(\ln n) \) is sufficient to find the optimal solution in a stochastically polynomial runtime, and the degree of the polynomial may increase with \( N \), but the probability guaranteeing the runtime is also increasing with \( N \).

5.2. Stochastic runtime analysis for grid instances

Now, we consider more general TSP instances. Herein, the \( n \) vertices are positioned on an \( m \times m \) grid for some integer \( m \in \mathbb{N}_+ \). The vertices are positioned in a way that no three of them are collinear. Figure \( \text{[3]} \) gives an
example of such an instance where $m = 5$ and $n = 8$. The weight of an edge \( \{l, k\} \in E \) in this case is defined as the usual Euclidean distance \( d(l, k) \) between vertex \( l \) and vertex \( k \) for every \( l, k = 1, \ldots, n \). In this section, we shall refer to these TSP instances as grid instances.

Grid instances have been studied in [43] and [30]. Sutton and Neumann [43] investigated the expected runtime of \((1+1)\) EA and RLS for these instances. As a continuation of [43], Sutton et al [30] further proved that the more extensive algorithm \((\mu + \lambda)\) EA finds an optimal solution for the instances expectedly in

\[
O((\mu/\lambda)n^3 m^5 + nm^5 + (\mu/\lambda)n^{4k}(2k-1)!)
\]

iterations if every of the \( \lambda \) selected parents is mutated by taking a random number of consecutive 2-exchange moves, and expectedly in

\[
O((\mu/\lambda)n^3 m^5 + nm^5 + (\mu/\lambda)n^{2k}(k-1)!)\]

iterations with a mixed mutation operator, where \( k \) denotes the number of vertices that are not on the boundary of the convex hull of \( V \). Sutton et al [30] also studied general Euclidean TSP instances (without collinearity) and showed similar results in terms of the maximum distance value \( d_{\text{max}} \), the minimum distance value \( d_{\text{min}} \), \( k \) and the minimum angle in the triangles formed by the vertices.

Before we present our stochastic runtime, we summarize some structural properties of grid instances (some just follow from properties of general Euclidean instances). We say that two different edges \( \{i, j\} \) and \( \{k, l\} \) intersect with each other if there exists a point \( p \) such that \( p \notin \{i, j, k, l\} \) locates on both of the two edges, see, e.g., Figure 4a. We say that a solution is
intersection-free if the corresponding Hamiltonian cycle does not contain intersections, see, e.g., Figure 4b.

![Figure 4: Example for intersections](image)

Figure 4: Example for intersections

Obviously, the triangle inequality holds for grid instances. Therefore, removing an intersection by a (unique) 2-exchange move in a solution strictly reduces the total traveling cost, see Figure 4a. Lemma 1 states the well known fact that an optimal solution of grid instances is intersection-free.

**Lemma 1.** Optimal solutions of grid instances are intersection-free.

![Figure 5: Example for a 2-opt move](image)

Figure 5: Example for a 2-opt move

We now restrict 2-opt moves to 2-exchange moves that remove an intersection. For example, removing edges \( \{i, j\}, \{k, l\} \) in Figure 5 and adding new edges \( \{i, l\}, \{k, j\} \) form such a 2-opt move. Lemma 2 below says that for grid instances, removing one intersection may reduce the total traveling cost \( \Omega(m^{-4}) \) if it is applicable. We omit the simple proof here. Interested readers may refer to [30] for a proof.

**Lemma 2.** If a feasible solution to a grid instance contains intersections, then removing the intersection can reduce the total traveling cost \( \Omega(m^{-4}) \).
The convex hull $\mathcal{Y}(V)$ of the vertex set $V$ is the smallest convex set in $\mathbb{R}^2$ that contains $V$. Its boundary is a convex polygon spanned by some vertices with possibly other vertices in the interior of that polygon. Let $V^b$ denote the set of vertices on the boundary of $\mathcal{Y}(V)$. Figure 6 illustrates this.

![Figure 6: Example of a convex hull](image)

Quintas and Supnick [50] proved that if a solution $s$ is intersection-free, then the solution respects the hull-order, i.e., any two vertices in the subsequence of $s$ induced by the boundary (the outer polygon) of $\mathcal{Y}(V)$ are consecutive in $s$ if and only if they are consecutive on the boundary of $\mathcal{Y}(V)$. Therefore, if $V^b = V$, i.e., all of the vertices are on the convex hull, then every intersection-free solution is optimal.

Theorem 4 below analyzes the stochastic runtime of Algorithm 1 for grid instances for the case that $V^b = V$, i.e., every vertex in $V$ is on the convex hull $V^b$, that we apply the max-min calibration (6) with $\pi_{\max} = 1 - \frac{1}{n}$, $\pi_{\min} = \frac{1}{n(n-2)}$, $\rho = 1$, $M = 1$ and $N \in \Omega(m^\epsilon)$ for some constant $\epsilon > 0$. Then:

a) With an overwhelming probability of $1 - e^{-\Omega(N)}$, Algorithm 4 finds the optimal solution within at most $n^4 \cdot m^5$ iterations with the vertex-based random solution generation.

b) With an overwhelming probability of $1 - e^{-\Omega(N)}$, Algorithm 4 finds an optimal solution within at most $n^3 \cdot m^5$ iterations with edge-based random solution generation.
Proof of Theorem 4. Note that under the conditions of Theorem 4, every intersection free solution is optimal. By Lemma 2, we know that a 2-opt move reduces the total traveling cost by $\Omega(m^{-4})$. Therefore, $n \cdot m^5$ consecutive 2-opt moves turn a feasible solution into an optimal one, since the worst solution in this case has a total traveling cost smaller than $n \cdot m$ and the optimal solution has total traveling cost larger than $n$. Notice also that $m \geq n/2$, since the $n$ vertices are positioned on the $m \times m$ grid and no three of them are collinear. With these facts, we prove the Theorem by a similar argument to the one used in the proof of Theorem 2.

Again, we consider the random event that the cost of the iteration best solution does not increase within a specified period of polynomially many iterations and strictly decreases sufficiently many times within that period. For $a)$, we consider the first $n^4m^5$ iterations. For $b)$, we consider the first $n^3m^5$ iterations.

For $a)$ : By Claim 2, with probability $(1 - (1 - 1/n)^N)^{n^4m^5} = 1 - e^{-\Omega(N)}$, the cost of the iteration-best solution does not increase within $n^4m^5$ iterations. By Claim 1 for a phase consisting of consecutive $n^3$ iterations, with probability $1 - (1 - n^{-3})^N \cdot n^3 = 1 - e^{-\Omega(N)}$, in at least one iteration of that phase an intersection is removed from the iteration-best solution, provided the phase starts with an iteration-best solution containing at least one intersection. Since the first $n^4m^5$ iterations can have $nm^5$ such phases, $a)$ follows.

$b)$ follows with an almost identical discussion. We therefore omit the proof. 

Corollary 2. Consider a TSP instance with $n$ vertices located on an $m \times m$ grid such that no three of them are collinear. Assume that $V^b = V$, i.e., every vertex in $V$ is on the convex hull $V^b$, that we apply the max-min calibration (6) with $\pi_{\max} = 1 - 1/n$, $\pi_{\min} = \frac{1}{n(n-1)}$, $\rho = 1$, $M = 1$ and $N \in \omega(\ln m)$. Then:

a) With probability $1 - m^{-\omega(1)}$, Algorithm 1 finds the optimal solution within at most $n^4 \cdot m^5$ iterations with the vertex-based random solution generation.

b) With probability $1 - m^{-\omega(1)}$, Algorithm 1 finds an optimal solution within at most $n^3 \cdot m^5$ iterations with the edge-based random solution generation.

Now, we consider the more interesting case that $|V| - |V^b| = k \in O(1)$, i.e., $k$ vertices are not on the convex hull. Note that we can turn an arbitrary
intersection-free solution to an optimal solution only by rearranging the positions of those $k$ interior points in that solution, and this requires at most $k$ consecutive jump moves (see [30] for a proof). A jump move $\delta_{i,j}$ transforms a solution into another solution by shifting positions $i$, $j$ as follows. Solution $s$ is transformed into solution $\delta_{i,j}(s)$ by moving the vertex at position $i$ into position $j$ while vertices at positions between $i$ and $j$ are shifted appropriately, e.g.,

$$\delta_{2,5}(i_1, i_2, i_3, i_4, i_5, i_6, i_7) = (i_1, i_3, i_5, i_2, i_6, i_7) \quad \text{and} \quad \delta_{5,2}(i_1, i_2, i_3, i_4, i_5, i_6, i_7) = (i_1, i_5, i_2, i_3, i_4, i_6, i_7).$$

It is not difficult to see that a jump move $\delta_{i,j}$ can be simulated by either a 2-exchange move (in the case that $|i-j|=1$) or a 3-exchange move (in all other cases). Therefore, we can actually turn an intersection-free solution into an optimal one by a sequence of at most $k$ consecutive 2-exchange or 3-exchange moves. Furthermore, a sequence of $k$ consecutive 2-exchange or 3-exchange moves can be simulated by a $\kappa$-exchange move with an integer $\kappa \leq 3k$. This means that any intersection-free solution can be turned into an optimal solution by a $\kappa$-exchange move with $\kappa \leq 3k$. We shall call such a $\kappa$-exchange move in the sequel a $3k$-opt move, although $\kappa$ may be smaller than $3k$. Recall that a $3k$-opt move is produced with a probability of $\Omega\left(\frac{1}{n^{6k-1}}\right)$ by Algorithm 2 (see Claim 1), and with a probability of $\Omega\left(\frac{1}{n^3}\right)$ by Algorithm 3 (see Lemma 6 of [42], or Claim 4) in any of the $N$ independent draws in iteration $t$, if $X_{t-1}$ is intersection-free and not optimal. As a result, we obtain by a similar proof as above Theorem 5 below.

**Theorem 5.** Consider a TSP instance with $n$ vertices located on an $m \times m$ grid such that no three of them are collinear. Assume that $|V| - |V^b| = k \in O(1)$ ($k$ vertices are not on the convex hull $V^b$), that we apply the max-min calibration $\widetilde{\mathcal{D}}$ with $\pi_{\max} = 1 - \frac{1}{n}$, $\pi_{\min} = \frac{1}{n(n-2)}$, and set $\rho = 1$, $M = 1$, for some constant $\epsilon > 0$. Then:

a) If we set $N \in \Omega(n^3 \cdot m^4)$, then with an overwhelming probability of $1 - e^{-\Omega(N/n^3)}$, Algorithm 4 finds an optimal solution within at most $n \cdot m^5 + n^{5k-4}$ iterations with the vertex-based random solution generation;

b) If we set $N \in \Omega(n^2 \cdot m^4)$, then with an overwhelming probability of $1 - e^{-\Omega(N/n^2)}$, Algorithm 4 finds an optimal solution within at most $n \cdot m^5 + n^{3k-2}$ iterations with the edge-based random solution generation.
Proof of Theorem 5. We only prove a), b) can be derived by a very similar argument. We define two random events as following:

\( \mathcal{E}_1 : \) for each \( t \leq n \cdot m^5 + n^{6k-4} \), \( f(\mathbf{X}_{t-1}^{[1]}) \geq f(\mathbf{X}_t^{[1]}) \);

\( \mathcal{E}_2 : \) for each \( t \leq n \cdot m^5 + n^{6k-4} \), if \( \mathbf{X}_t^{[1]} \) is not intersection-free, then a 2-opt move happens in iteration \( t \).

By a similar argument as the one for Theorem 4, we obtain that \( \mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2) \geq 1 - e^{-\Omega(N/n^3)} \). Let \( \eta \) be a random variable denoting the number of iterations for which \( \mathbf{X}_{t-1}^{[1]} \) is intersection-free. Notice that, conditioned on \( \mathcal{E}_1 \cap \mathcal{E}_2 \), \( \eta \geq n \cdot m^5 \) implies that an optimal solution occurs within \( n \cdot m^5 + n^{6k-4} \) iterations.

Conditioned on \( \mathcal{E}_1 \cap \mathcal{E}_2 \) and \( \eta < n \cdot m^5 \), there are at least \( \Omega(n^{6k-4}) \) iterations in which \( \mathbf{X}_{t-1}^{[1]} \) is intersection-free, and not optimal, a 3k-opt move that turns \( \mathbf{X}_{t-1}^{[1]} \) into an optimal solution happens with probability of at least \( 1 - (1 - \Omega(n^{6k-4}))^N \). This means for any fixed \( \eta \in \mathbb{N} \), if \( \mathbf{X}_{t-1}^{[1]} \) is intersection-free, then the probability of the event that \( \mathbf{X}_t^{[1]} \) is optimal is bounded from below by \( 1 - (1 - \Omega(n^{6k-4}))^N \). Therefore, for any fixed \( \Omega(n^{6k-4}) \) iterations in which the iteration-best solution \( \mathbf{X}_{t-1}^{[1]} \) is intersection-free and not optimal, the probability of the event that the corresponding \( \Omega(n^{6k-4}) \) \( \mathbf{X}_t^{[1]} \)'s are still not optimal, is bounded from above by \( (1 - \Omega(n^{6k-4}))^{n \cdot n^{6k-4}} = e^{-\Omega(N/n^3)} \). This means that, conditioned on \( \mathcal{E}_1 \cap \mathcal{E}_2 \) and \( \eta < n \cdot m^5 \), an optimal solution occurs within \( n \cdot m^5 + n^{6k-4} \) iterations with a probability of \( 1 - e^{-\Omega(N/n^3)} \).

As a result, an optimal solution occurs within the first \( n \cdot m^5 + n^{6k-4} \) iterations with a probability of \( 1 - e^{-\Omega(N/n^3)} \).

Theorem 3 shows a stochastic runtime of \( n^3m^{5+\epsilon} + n^{6k-1}m^\epsilon \) for Algorithm 1 equipped with the vertex-based solution generation, and a stochastic runtime of \( n^3m^{5+\epsilon} + n^{3k}m^\epsilon \) for Algorithm 1 equipped with edge-based solution generation, in the case of that \( |V| - |V^b| = k \in O(1) \). This is much better than the expected runtime

\[ O(\mu \cdot n^3m^5 + nm^5 + \mu \cdot n^4k(2k-1)!) \]

for (\( \mu+\lambda \)) EA with sequential 2-opt mutations reported by Sutton et al [30]. However, we are not able to analyze the stochastic runtime in the case that
6. Conclusion

We have analyzed the stochastic runtime of a CE algorithm on two classes of TSP instances under two different random solution generation methods. The stochastic runtimes are comparable with corresponding expected runtimes reported in the literature.

Our results show that the edge-based random solution generation method makes the algorithm more efficient for TSP instances in most cases. Moreover, \( N \in \Omega(\ln n) \) is necessary for efficiently finding an optimal solution with iteration-best reinforcement. For simple instances, \( N \in \omega(\ln n) \) is sufficient to efficiently find an optimal solution with an overwhelming probability, and \( N \in O(\ln n) \) results in an exponential runtime with an overwhelming probability. However, for more difficult instances, one may need to use a relatively large sample size.

Our stochastic runtimes are better than the expected runtimes of the \((\mu + \lambda)\) EA on the grid instances. The EA randomly changes local structures of some of its current solutions by a Poisson distributed number of consecutive 2-exchange moves in every iteration, while our algorithm refrains from local operations on current solutions and only refreshes solutions by sampling from an evolving distribution. The solution reproducing mechanism in the EA stays the same throughout the optimization, only the current solutions in every iteration vary. However, the solution reproducing mechanism (sampling distribution) of our algorithm also evolves. This is the essential difference of MBS with traditional EAs. The comparison of our results with the expected runtimes in [30] therefore show that using a self-adaptive dynamic solution reproducing mechanism is helpful (in efficiently finding an optimal solution) when the search space becomes rugged. The stochastic runtimes in Theorem 4 are only valid for instances with a bounded number of interior points. In the future, it should be interesting to analyze the case that \( |V| - |V^b| \in \omega(1) \). This might also give more insight to the problem of \( \mathcal{RP} \) v.s. \( \mathcal{P} \) [51].

Our analysis is actually a kind of worst-case analysis, which is rather pessimistic. We analyze the optimization progress by only checking some very particular random events. This may not only underestimate the probability
of finding an optimal solution with our algorithm, but also overestimate the required number of iterations. In the future, it should be of great interest to consider a smoothed runtime analysis over an $\epsilon$-neighborhood of the $n$ nodes in the real plane as has been done for the Simplex method by Spielman and Teng in their famous paper [52].

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