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On the Invariance of Ant Colony Optimization

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Abstract

Ant colony optimization (ACO) is a promising metaheuristic and a great amount of research has been devoted to its empirical and theoretical analysis. Recently, with the introduction of the *hyper-cube framework* [1], Blum and Dorigo have explicitly raised the issue of the invariance of ACO algorithms to transformation of units. They state [1] that the performance of ant colony optimization depends on the scale of the problem instance under analysis.

In this paper, we show that the ACO internal state—commonly referred to as the *pheromone*—indeed depends on the scale of the problem at hand. Nonetheless, we formally prove that this does not affect the sequence of solutions produced by the three most widely adopted algorithms belonging to the ACO family: ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system. For these algorithms, the sequence of solutions does not depend on the scale of the problem instance under analysis.

Moreover, we introduce three new ACO algorithms, the internal state of which is independent of the scale of the problem instance considered. These algorithms are obtained as minor variations of ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system. We formally show that these algorithms are *functionally equivalent* to their original counterparts. That is, for any given instance, these algorithms produce the same sequence of solutions as the original ones.

1 Introduction

Ant colony optimization (ACO) [2] is a metaheuristic inspired by the foraging behavior of ants [3]. In order to find the shortest path from the nest to a food source, ant colonies exploit a positive feedback mechanism: They use a form of indirect communication called stigmergy [4], which is based on the laying and detection of pheromone trails. In ant colony optimization, a generic combinatorial optimization problem is encoded into a constrained shortest path problem. A number of paths are generated in a Monte Carlo fashion on the basis of a probabilistic model whose parameters are called *artificial pheromone*—or more simply *pheromone*. In the ant colony optimization metaphor, these paths are said to be constructed by *artificial ants* walking on the graph that encodes the problem. The cost of the generated paths is used to modify the pheromone and therefore to bias the generation of further paths towards promising regions of the search space [5].

The ant colony optimization framework has been explicitly defined by Dorigo et al. in 1999 [6], and comprises a number of algorithms including the original ant system [7, 8, 9], ant colony system [10], and $\mathcal{MAX}$–$\mathcal{MIN}$ ant system [11, 12]. A vast literature exists on ant colony optimization and on its application to a large number of problems. We refer the reader to Dorigo and Stützle [2] for a comprehensive overview.

Recently, with the introduction of the *hyper-cube framework* [1], Blum and Dorigo have explicitly raised the issue of the invariance of ACO algorithms to transformation of units. In the hyper-cube framework, the cost of solutions is normalized on a per iteration basis. This entrains a number of desirable properties [1], among which the invariance to transformation of units. Blum and Dorigo [1] maintain that this property is peculiar to the hypercube framework:

> *in standard ACO algorithms the pheromone values and therefore the performance of the algorithms, strongly depend on the scale of the problem.* [1]

Here by "performance," the authors informally mean the sequence of solutions generated when solving a problem instance.

In this paper, we formally show that this statement is only partially correct: Indeed, in standard ant colony optimization algorithms the pheromone values (and the heuristic information) depend on the scale of the problem. Nonetheless, the sequence of solutions ACO algorithms find is independent of the scale of the problem. For concreteness, in this paper we focus on ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system, which are the three most representative algorithms in the ant colony optimization family.

As a second contribution, we propose variants of the aforementioned algorithms called *strongly-invariant ant system* (*si*AS), *strongly-invariant $\mathcal{MAX}$–$\mathcal{MIN}$ ant system* (*si*$\mathcal{MM}$AS), and *strongly-invariant ant colony system* (*si*ACS). These variants are equivalent to their original counterparts, but they enjoy the further property that the pheromone and the heuristic values do not depend on the scale of the problem. Although this property might be desirable in practical applications, the significance of the introduction of strongly-invariant ACO algorithms is mostly theoretical and speculative. Indeed, the fact of showing that it is possible to define algorithms enjoying the above invariance property provides new insight into ant colony optimization.

The rest of the paper is organized as follows. In Section 2, we introduce some preliminary concepts. In Sections 3, 4, and 5, we deal with ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system, respectively. In these sections, we formally define the three algorithms and we prove that the sequence of solutions they produce does not depend on the scale of the problem instance under analysis. Moreover, in these sections we propose the *strongly-invariant* versions of the three algorithms and we formally study their properties. In Section 6, we describe three combinatorial optimization problems—namely the traveling salesman problem, the quadratic assignment problem, and the open shop scheduling problem—and we illustrate how the theorems proved in Sections 3, 4, and 5 apply to these problems. In Section 7, we conclude the paper with some final remarks.

2 Preliminary definitions

In this section, we introduce a number of fundamental concepts that will be needed in the following.

Definition 1 (Linear transformation of units)**.** A linear transformation of units is a binary relation defined on the space of the instances of a combinatorial optimization problem. Two instances I and $\bar{I}$ are related via a linear transformation of units if they share the same space of solutions S and, for any solution $s \in S$, $\bar{f}(s) = g_1 f(s)$, where $g_1 > 0$ is a constant and $f(s)$ and $\bar{f}(s)$ are the value of the objective function in s for I and $\bar{I}$, respectively. In the following, the notation $\bar{I} = g_1 I$ will be adopted.

Being reflexive, symmetric, and transitive, a linear transformation of units is an equivalence relation. Accordingly, two instances I and $\bar{I}$ that meet the conditions given in Definition 1 will be said to be *equivalent up to a linear transformation of units* or more simply *equivalent*.

Algorithm 1 The Ant Colony Optimization Metaheuristic

Set parameters, set heuristic information, and initialize pheromone;
while termination condition not met **do**
  Construct solutions based on pheromone and heuristic information;
  Improve solutions via local search;[1] *(optional)*
  Update pheromone;
end while

Remark 1. In the following, if y is a generic quantity that refers to an instance I, then $\bar{y}$ is the corresponding quantity for what concerns instance $\bar{I}$, when $\bar{I}$ is equivalent to I up to a linear transformation of units.

Definition 2 (Construction graph, pheromone, and heuristic information)**.** In ant colony optimization, a combinatorial optimization problem is mapped on a graph $G = (N, E)$, where N is the set of nodes and E is the set of edges. The graph G is called *construction graph*.

The solutions of the original problem are mapped to paths on G. Variables called *pheromone* and *heuristic information* are associated with the edges in E.

Ant colony optimization algorithms are iterative. At each iteration, a number of solutions are built incrementally on the basis of stochastic decisions that are biased by pheromone and heuristic information. These solutions are used for updating the pheromone in order to bias future solutions towards promising regions of the search space. A pseudo-code of a generic ant colony optimization algorithm is given in Algorithm 1. The constraints of the optimization problem are implemented by enumerating the solution components that can be added at each step. This set typically depends on the partial solution constructed so far.

In the following, we will adopt the notation $\langle i, j\rangle$ to denote the edge connecting nodes i and j. With η_{ij} we denote the heuristic information on the desirability of constructing a path on G featuring node j immediately after i. Finally, with $\tau_{ij,h}$ we denote the pheromone on edge $\langle i, j\rangle$ at iteration h of the algorithm.

The following hypothesis will be used in the paper.

Hypothesis 1 (Pseudo-random number generator)**.** When solving two equivalent instances I and $\bar{I}$, the stochastic decisions taken while constructing solutions are made on the basis of random experiments based on pseudo-random numbers produced by the same pseudo-random number generator. We assume that this generator is initialized in the same way (for example, with the same seed) when solving the two instances so that the two sequences of pseudo-random numbers that are generated are the same in the two cases.

Similarly, when two algorithms A and $\tilde{A}$ solve the same instance I, we assume that the pseudo-random number generators adopted by the two algorithms are the same and are initialized in the same way.

Definition 3 (Weak-invariance)**.** An algorithm A is **weakly-invariant** (or more simply **invariant**) to linear transformation of units if the sequence of solutions $\mathcal{S}_I$ and $\mathcal{S}_{\bar{I}}$ generated when solving respectively the instances I and $\bar{I}$ are the same, whenever $\bar{I}$ is equivalent to I up to a linear transformation of units. If A is a stochastic algorithm, it is said to be invariant if it is so under Hypothesis 1.

[1]In this paper, we will not discuss the adoption of a local search to improve solutions constructed by ants. Nonetheless, it is worth noticing here that local search algorithms are typically invariant to transformation of units. Therefore, all the theorems presented in the paper hold true also when a local search is adopted.

Definition 4 (Strong-invariance)**.** An algorithm A is said to be **strongly-invariant** if, besides generating the same solutions on any two equivalent instances I and $\bar{I}$, it also enjoys the property that its internal state at each iteration is the same when solving I and $\bar{I}$. If A is stochastic, it is said to be strongly-invariant if it is so under Hypothesis 1.

Remark 2. An ant colony optimization algorithm is strongly-invariant if heuristic information and pheromone at each iteration are the same when solving any two equivalent instances.

Definition 5 (Functional equivalence)**.** Two algorithms A and $\tilde{A}$ are *functionally equivalent*, or simply *equivalent*, if for any instance I, the sequence of solutions $\mathcal{S}_I$ generated by A and the sequence of solutions $\tilde{\mathcal{S}}_I$ generated by $\tilde{A}$ are the same. If A and $\tilde{A}$ are stochastic, they are said to be equivalent if they are so under Hypothesis 1.

Definition 6 (Reference solution)**.** Let s_0 be a solution of instance I returned by some appropriate invariant algorithm. Such an algorithm, which is necessarily problem-specific, might be based either on a heuristic or more simply on a random sampling of the solution space. In this latter case, the invariance of the algorithm relies on Hypothesis 1. From this definition, it follows that $\bar{f}(s_0) = g_1 f(s_0)$, for any two equivalent instances I and $\bar{I}$ such that $\bar{I} = g_1 I$.

3 Ant system

Ant system is the original ant colony optimization algorithm proposed by Dorigo et al. [7, 8, 9]. In the following, we provide a formal definition of the algorithm.

Definition 7 (Random proportional rule)**.** At the generic iteration h, suppose that ant k is in node i. Further, let $\mathcal{N}_i^k$ be the set of feasible nodes that can be visited by ant k. In general, this set depends on the partial solution constructed so far by ant k. The node $j \in \mathcal{N}_i^k$, to which ant k moves, is selected with probability:

$$p_{ij,h}^k = \frac{[\tau_{ij,h}]^\alpha [\eta_{ij}]^\beta}{\sum_{l \in \mathcal{N}_i^k} [\tau_{il,h}]^\alpha [\eta_{il}]^\beta},$$

where α and β are parameters.

Definition 8 (Pheromone update rule)**.** At the generic iteration h, suppose that m ants have generated the solutions $s_h^1, s_h^2, \ldots, s_h^m$ of cost $f(s_h^1), f(s_h^2), \ldots, f(s_h^m)$, respectively. The pheromone on each edge $\langle i, j\rangle$ is updated according to the following rule:

$$\tau_{ij,h+1} = (1-\rho)\tau_{ij,h} + \sum_{k=1}^{m} \Delta_{ij,h}^k,$$

where ρ is a parameter called the *evaporation rate* and

$$\Delta_{ij,h}^k = \begin{cases} 1/f(s_h^k), & \text{if } \langle i, j\rangle \in s_h^k; \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

Definition 9 (Pheromone initialization)**.** At iteration $h = 1$, the pheromone is initialized to

$$\tau_{ij,1} = m/f(s_0), \text{ for all } \langle i, j\rangle \in E,$$

where m is the number of ants and s_0 is the reference solution.

Definition 10 (Ant system)**.** Ant system is an ant colony optimization algorithm in which solutions are constructed according to the random proportional rule given in Definition 7, the pheromone is initialized as in Definition 9 and updated according to the rule given in Definition 8. The evaporation rate ρ, the number of ants m, and the exponents α and β are parameters of the algorithm. The definition of the heuristic information is problem-specific.

The following theorem holds true.

Lemma 1. *The random proportional rule is invariant to concurrent linear transformation of the pheromone and of the heuristic information. Formally, for any two positive constants γ_1 and γ_2,*

$$(\bar{\tau}_{ij,h} = \gamma_1 \tau_{ij,h}) \wedge (\bar{\eta}_{ij} = \gamma_2 \eta_{ij}), \textit{ for all } \langle i,j \rangle \implies \bar{p}^k_{ij,h} = p^k_{ij,h}, \textit{ for all } \langle i,j \rangle,$$

where $\bar{p}^k_{ij,h}$ is obtained on the basis of $\bar{\tau}_{ij,h}$ and $\bar{\eta}_{ij}$, according to Definition 7.

Proof. According to Definition 7:

$$\begin{aligned}\bar{p}^k_{ij,h} &= \frac{[\bar{\tau}_{ij,h}]^\alpha [\bar{\eta}_{ij}]^\beta}{\sum_{l \in \mathcal{N}_i^k} [\bar{\tau}_{il,h}]^\alpha [\bar{\eta}_{il}]^\beta} = \frac{[\gamma_1 \tau_{ij,h}]^\alpha [\gamma_2 \eta_{ij}]^\beta}{\sum_{l \in \mathcal{N}_i^k} [\gamma_1 \tau_{il,h}]^\alpha [\gamma_2 \eta_{il}]^\beta} \\ &= \frac{[\gamma_1]^\alpha [\gamma_2]^\beta [\tau_{ij,h}]^\alpha [\eta_{ij}]^\beta}{[\gamma_1]^\alpha [\gamma_2]^\beta \sum_{l \in \mathcal{N}_i^k} [\tau_{il,h}]^\alpha [\eta_{il}]^\beta} = \frac{[\tau_{ij,h}]^\alpha [\eta_{ij}]^\beta}{\sum_{l \in \mathcal{N}_i^k} [\tau_{il,h}]^\alpha [\eta_{il}]^\beta} = p^k_{ij,h}.\end{aligned}$$

□

Theorem 1 (Weak invariance of ant system)**.** *Let I and $\bar{I}$ be two equivalent instances such that $\bar{I} = g_1 I$, with $g_1 > 0$. Further, let $G = (N, E)$ be the construction graph associated with I and $\bar{I}$. Ant system obtains the same sequence of solutions on I and $\bar{I}$ if*

(Condition 1) the heuristic information is such that:

$$[\bar{\eta}_{ij}]^\beta = [g_2 \eta_{ij}]^\beta, \textit{ for all } \langle i,j \rangle \in E,$$

where β is the parameter appearing in Definition 7 and $g_2 > 0$ is an arbitrary constant.

Proof. The theorem is proved by induction: We show that if at the generic iteration h some set of conditions $\mathcal{C}$ holds, then the solutions generated for the two instances I and $\bar{I}$ are the same, and the set of conditions $\mathcal{C}$ also holds at the following iteration $h+1$. The proof is concluded by showing that $\mathcal{C}$ holds at the very first iteration. With few minor modifications, this technique is adopted in the following for proving all theorems enunciated in the paper.

According to Lemma 1 and given Condition 1, if at the generic iteration h, $\bar{\tau}_{ij,h} = \frac{1}{g_1} \tau_{ij,h}$, for all $\langle i,j \rangle$, then $\bar{p}^k_{ij,h} = p^k_{ij,h}$, for all $\langle i,j \rangle$. Under Hypothesis 1,

$$\bar{s}^k_h = s^k_h, \text{ for all } k = 1, \ldots, m,$$

and therefore,

$$\bar{f}(\bar{s}^k_h) = g_1 f(s^k_h), \text{ for all } k = 1, \ldots, m.$$

According to Equation 1:

$$\begin{aligned}\bar{\Delta}^k_{ij,h} &= \begin{cases} 1/\bar{f}(\bar{s}^k_h), & \text{if } \langle i,j \rangle \in \bar{s}^k_h; \\ 0, & \text{otherwise;} \end{cases} = \begin{cases} 1/g_1 f(s^k_h), & \text{if } \langle i,j \rangle \in \bar{s}^k_h = s^k_h; \\ 0/g_1, & \text{otherwise;} \end{cases} \\ &= \frac{1}{g_1} \begin{cases} 1/f(s^k_h), & \text{if } \langle i,j \rangle \in s^k_h; \\ 0, & \text{otherwise;} \end{cases} = \frac{1}{g_1} \Delta^k_{ij,h},\end{aligned}$$

and therefore, for any edge $\langle i,j\rangle$:

$$\begin{aligned}\bar{\tau}_{ij,h+1} &= (1-\rho)\bar{\tau}_{ij,h} + \sum_{k=1}^{m}\bar{\Delta}^k_{ij,h} = (1-\rho)\frac{1}{g_1}\tau_{ij,h} + \sum_{k=1}^{m}\frac{1}{g_1}\Delta^k_{ij,h}\\ &= (1-\rho)\frac{1}{g_1}\tau_{ij,h} + \frac{1}{g_1}\sum_{k=1}^{m}\Delta^k_{ij,h} = \frac{1}{g_1}\left((1-\rho)\tau_{ij,h} + \sum_{k=1}^{m}\Delta^k_{ij,h}\right) = \frac{1}{g_1}\tau_{ij,h+1}.\end{aligned}$$

The proof is completed by observing that a basis for the above induction follows from Definition 9:

$$\bar{\tau}_{ij,1} = \frac{m}{\bar{f}(s_0)} = \frac{m}{g_1 f(s_0)} = \frac{1}{g_1}\tau_{ij,1},\ \text{for all } \langle i,j\rangle.$$

□

Remark 3. One notable case in which Condition 1 is satisfied is when $\beta = 0$, that is, when no heuristic information is used.

Strongly-invariant ant system

In this section, we introduce *si*AS, which is a strongly-invariant version of ant system. We first define the algorithm, then we prove that it is functionally equivalent to ant system, and finally that it is indeed strongly invariant.

Definition 11 (Strongly-invariant pheromone update rule)**.** The pheromone is updated using the same rule given in Definition 8, with the only difference that $\Delta^k_{ij,h}$ is given by:

$$\Delta^k_{ij,h} = \begin{cases} f(s_0)/mf(s^k_h), & \text{if } \langle i,j\rangle \in s^k_h;\\ 0, & \text{otherwise;}\end{cases}$$

where m is the number of ants and s_0 is the reference solution.

Definition 12 (Strongly-invariant pheromone initialization)**.** At the first iteration $h = 1$, the pheromone is initialized to $\tau_{ij,1} = 1$, for all $\langle i,j\rangle$.

Definition 13 (Strongly-invariant ant system)**.** The strongly-invariant ant system (*si*AS) is a variation of ant system. In *si*AS, the random proportional rule is adopted for the construction of solutions, the pheromone is initialized according to Definition 12, and the update is performed according to Definition 11. The heuristic information is set in an invariant way through some appropriate problem-specific rule.

Theorem 2. *Ant system and siAS are functionally equivalent if*

(Condition 2) the heuristic information is such that:

$$[\tilde{\eta}_{ij}]^\beta = [\lambda\eta_{ij}]^\beta,\ \textit{for all } \langle i,j\rangle,$$

where β is the parameter appearing in Definition 7, $\tilde{\eta}_{ij}$ and η_{ij} are the heuristic information on edge $\langle i,j\rangle$ respectively in siAS and ant system, and $\lambda > 0$ is an arbitrary constant.

Proof. Let us consider a generic instance I. In this proof, a tilde placed above a symbol indicates that it refers to *si*AS. Let $\mu = f(s_0)/m$. According to Lemma 1 and given Condition 2, if at the generic iteration h, $\tilde{\tau}_{ij,h} = \mu\tau_{ij,h}$, for all $\langle i,j\rangle$, then $\tilde{p}^k_{ij,h} = p^k_{ij,h}$, for all $\langle i,j\rangle$. Under Hypothesis 1, $\tilde{s}^k_h = s^k_h$, for all $k = 1,\dots,m$. According to Definitions 8 and 11,

$$\tilde{\Delta}^k_{ij,h} = \begin{cases} f(s_0)/mf(\tilde{s}^k_h), & \text{if } \langle i,j\rangle \in \tilde{s}^k_h;\\ 0, & \text{otherwise;}\end{cases} = \mu\begin{cases} 1/f(s^k_h), & \text{if } \langle i,j\rangle \in s^k_h;\\ 0, & \text{otherwise;}\end{cases} = \mu\Delta^k_{ij,h}.$$

Therefore, for any edge $\langle i, j \rangle$:

$$\tilde{\tau}_{ij,h+1} = (1-\rho)\tilde{\tau}_{ij,h} + \sum_{k=1}^{m} \tilde{\Delta}^k_{ij,h} = (1-\rho)\mu\tau_{ij,h} + \sum_{k=1}^{m} \mu\Delta^k_{ij,h} = \mu\tau_{ij,h+1}.$$

The proof is completed by observing that a basis for the above induction is provided by

$$\tilde{\tau}_{ij,1} = \mu\tau_{ij,1}, \text{ for all } \langle i, j \rangle,$$

which follows from Definitions 9 and 12. □

Theorem 3. *siAS is strongly-invariant if*

(Condition 3) the heuristic information is such that:

$$[\bar{\eta}_{ij}]^\beta = [\eta_{ij}]^\beta, \textit{ for all } \langle i, j \rangle,$$

for any two instances I and $\bar{I}$ such that $\bar{I} = g_1 I$, with $g_1 > 0$.

Proof. Given Condition 3, according to Lemma 1 and Hypothesis 1, if at the generic iteration h, $\bar{\tau}_{ij,h} = \tau_{ij,h}$, for all $\langle i, j \rangle$, then $\bar{p}^k_{ij,h} = p^k_{ij,h}$, for all $\langle i, j \rangle$, and $\bar{s}^k_h = s^k_h$, for all $k = 1, \dots, m$, and therefore, $\bar{f}(\bar{s}^k_h) = g_1 f(s^k_h)$, for all $k = 1, \dots, m$. According to Definition 11:

$$\bar{\Delta}^k_{ij,h} = \begin{cases} \bar{f}(s_0)/m\bar{f}(\bar{s}^k_h), & \text{if } \langle i, j \rangle \in \bar{s}^k_h; \\ 0, & \text{otherwise;} \end{cases} = \begin{cases} f(s_0)/mf(s^k_h), & \text{if } \langle i, j \rangle \in s^k_h; \\ 0, & \text{otherwise;} \end{cases} = \Delta^k_{ij,h},$$

and therefore, for any edge $\langle i, j \rangle$:

$$\bar{\tau}_{ij,h+1} = (1-\rho)\bar{\tau}_{ij,h} + \sum_{k=1}^{m} \bar{\Delta}^k_{ij,h} = (1-\rho)\tau_{ij,h} + \sum_{k=1}^{m} \Delta^k_{ij,h} = \tau_{ij,h+1}.$$

The proof is completed by observing that Definition 12 provides a basis for the above induction. □

Remark 4. It is worth noticing that by initializing the pheromone to $\tau_{ij,1} = 1/m$, for all $\langle i, j \rangle$, and by defining $\Delta^k_{ij,h}$ as:

$$\Delta^k_{ij,h} = \begin{cases} f(s_0)/f(s^k_h), & \text{if } \langle i, j \rangle \in s^k_h; \\ 0, & \text{otherwise;} \end{cases}$$

one would have obtained nonetheless a strongly invariant algorithm. The advantage of the formulation given in Definitions 11 and 12 is that the magnitude of the pheromone deposited on the arcs does not depend on the number m of ants considered.

4 $\mathcal{MAX}$–$\mathcal{MIN}$ ant system

The results given for ant system can be extended to $\mathcal{MAX}$–$\mathcal{MIN}$ ant system [11, 12]. The characterizing element of $\mathcal{MAX}$–$\mathcal{MIN}$ ant system is the fact that the pheromone value is constrained between a minimum and a maximum, which possibly change iteration by iteration.

Definition 14 (Pheromone trail limits)**.** At iteration $h+1$, the pheromone value $\tau_{ij,h+1}$ on a generic edge $\langle i, j \rangle$ is constrained:

$$\tau^{min}_h \le \tau_{ij,h+1} \le \tau^{max}_h,$$

with $\tau^{max}_h = 1/\rho f(s^{bs}_h)$ and $\tau^{min}_h = a\tau^{max}_h$, where s^{bs}_h is the best solution found up to and including iteration h, ρ is the evaporation rate, and a is a parameter, with $0 \le a < 1$.

Remark 5. The following notation will be adopted:

$$[x]_{min}^{max} = \begin{cases} max, & \text{if } x > max; \\ x, & \text{if } min \leq x \leq max; \\ min, & \text{if } x < min. \end{cases}$$

It can be easily shown that, if $g > 0$,

$$[g \cdot x]_{g \cdot min}^{g \cdot max} = g\,[x]_{min}^{max}.$$

This property will be used in the following.

Definition 15 (Pheromone update rule)**.** If $\tau_{ij,h}$ is the value of the pheromone on edge $\langle i, j \rangle$ at the current iteration h, the value of the pheromone at iteration $h+1$ is given by:

$$\tau_{ij,h+1} = \Big[(1-\rho)\tau_{ij,h} + \Delta_{ij,h}\Big]_{\tau_h^{min}}^{\tau_h^{max}}, \tag{2}$$

where ρ is the evaporation rate. The quantity $\Delta_{ij,h}$ is given by:

$$\Delta_{ij,h} = \begin{cases} 1/f(s_h^{best}), & \text{if } \langle i, j \rangle \in s_h^{best}; \\ 0, & \text{otherwise}; \end{cases} \tag{3}$$

where s_h^{best} is either the *best-so-far* solution s_h^{bs}, that is, best solution found up to and including iteration h, or the *iteration-best* solution s_h^{ib}, that is, the best solution found in iteration h.

Remark 6. At a given iteration h, whether a *best-so-far* or an *iteration-best* update is to be performed is a design choice. In the typical implementation of $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, in the initial iterations the *iteration-best* update is mostly adopted, and the frequency with which the *best-so-far* update is employed increases iteration after iteration [12].

Definition 16 (Pheromone initialization)**.** At iteration $h = 1$, the pheromone on each edge is initialized to

$$\tau_{ij,1} = \frac{1}{\rho f(s_0)}, \text{ for all } \langle i, j \rangle \in E,$$

where ρ is the evaporation rate and s_0 is the reference solution.

Definition 17 ($\mathcal{MAX}$–$\mathcal{MIN}$ ant system)**.** $\mathcal{MAX}$–$\mathcal{MIN}$ ant system is an ACO algorithm in which solutions are constructed according to the random proportional rule given in Definition 7, the pheromone is initialized as in Definition 16, and it is updated according to Definition 15. The evaporation rate ρ, the exponents α and β, the number of ants m, and the factor a are parameters of the algorithm. The heuristic information is problem-specific.

Theorem 4. *Let I and $\bar{I}$ be two equivalent instances such that $\bar{I} = g_1 I$, with $g_1 > 0$. Further, let $G = (N, E)$ be the construction graph associated with I and $\bar{I}$. $\mathcal{MAX}$–$\mathcal{MIN}$ ant system obtains the same sequence of solutions on I and $\bar{I}$ if*

(Condition 1) the heuristic information is such that:

$$[\bar{\eta}_{ij}]^{\beta} = [g_2 \eta_{ij}]^{\beta}, \text{ for all } \langle i, j \rangle \in E,$$

where β is the parameter appearing in Definition 7 and $g_2 > 0$ is an arbitrary constant.

Proof. The proof follows the one given for Theorem 1. Let us assume that, at the beginning of the generic iteration h, $\bar{s}^{bs}_{h-1} = s^{bs}_{h-1}$ and $\bar{\tau}_{ij,h} = \frac{1}{g_1}\tau_{ij,h}$, for all $\langle i,j\rangle$. According to Lemma 1 and given Condition 1, $\bar{p}^k_{ij,h} = p^k_{ij,h}$, for all $\langle i,j\rangle$. Under Hypothesis 1, $\bar{s}^k_h = s^k_h$, for all $k = 1,\dots,m$, and therefore, $\bar{f}(\bar{s}^k_h) = g_1 f(s^k_h)$, for all $k = 1,\dots,m$. In particular, $\bar{s}^{ib}_h = s^{ib}_h$, and $\bar{f}(\bar{s}^{ib}_h) = g_1 f(s^{ib}_h)$. Moreover, whether or not an improvement is made on the *best-so-far* solution, $\bar{s}^{bs}_h = s^{bs}_h$. Indeed, since $\bar{s}^{bs}_{h-1} = s^{bs}_{h-1}$, then $\bar{f}(\bar{s}^{bs}_{h-1}) = g_1 f(s^{bs}_{h-1})$. If $f(s^{ib}_h) < f(s^{bs}_{h-1})$, then also $\bar{f}(\bar{s}^{ib}_h) < \bar{f}(\bar{s}^{bs}_{h-1})$, and $\bar{s}^{bs}_h = \bar{s}^{ib}_h = s^{ib}_h = s^{bs}_h$. On the other hand, if $f(s^{ib}_h) \geq f(s^{bs}_{h-1})$, then also $\bar{f}(\bar{s}^{ib}_h) \geq \bar{f}(\bar{s}^{bs}_{h-1})$, and $\bar{s}^{bs}_h = \bar{s}^{bs}_{h-1} = s^{bs}_{h-1} = s^{bs}_h$.

According to Equation 3,

$$\bar{\Delta}_{ij,h} = \begin{cases} 1/\bar{f}(\bar{s}^{best}_h), & \text{if } \langle i,j\rangle \in \bar{s}^{best}_h; \\ 0, & \text{otherwise;} \end{cases} = \begin{cases} 1/g_1 f(s^{best}_h), & \text{if } \langle i,j\rangle \in s^{best}_h; \\ 0/g_1, & \text{otherwise;} \end{cases} = \frac{1}{g_1}\Delta_{ij,h},$$

where $\bar{s}^{best}_h = s^{best}_h = s^{bs}_h$, in case of a *best-so-far* update; and $\bar{s}^{best}_h = s^{best}_h = s^{ib}_h$, in case of an *iteration-best* update. In both cases,

$$\bar{\tau}^{max}_h = \frac{1}{\rho \bar{f}(\bar{s}^{bs}_h)} = \frac{1}{g_1 \rho f(s^{bs}_h)} = \frac{1}{g_1}\tau^{max}_h,$$

and therefore,

$$\bar{\tau}^{min}_h = a\bar{\tau}^{max}_h = \frac{a}{g_1}\tau^{max}_h = \frac{1}{g_1}\tau^{min}_h.$$

It follows that,

$$\begin{aligned}\bar{\tau}_{ij,h+1} &= \Big[(1-\rho)\bar{\tau}_{ij,h} + \bar{\Delta}_{ij,h}\Big]^{\bar{\tau}^{max}_h}_{\bar{\tau}^{min}_h} = \Big[(1-\rho)\frac{1}{g_1}\tau_{ij,h} + \frac{1}{g_1}\Delta_{ij,h}\Big]^{\frac{1}{g_1}\tau^{max}_h}_{\frac{1}{g_1}\tau^{min}_h} \\ &= \Big[\frac{1}{g_1}\Big((1-\rho)\tau_{ij,h} + \Delta_{ij,h}\Big)\Big]^{\frac{1}{g_1}\tau^{max}_h}_{\frac{1}{g_1}\tau^{min}_h} = \frac{1}{g_1}\Big[(1-\rho)\tau_{ij,h} + \Delta_{ij,h}\Big]^{\tau^{max}_h}_{\tau^{min}_h} = \frac{1}{g_1}\tau_{ij,h+1}.\end{aligned}$$

The proof is completed by observing that, according to Definition 16, the pheromone is initialized as:

$$\bar{\tau}_{ij,1} = \frac{1}{\rho \bar{f}(s_0)} = \frac{1}{\rho g_1 f(s_0)} = \frac{1}{g_1}\tau_{ij,1}, \text{ for all } \langle i,j\rangle.$$

and the initial *best-so-far* solutions are $\bar{s}^{bs}_0 = s^{bs}_0 = s_0$, where s_0 is the reference solution. □

Remark 7. Condition 1 is trivially satisfied when no heuristic information is used, that is, when $\beta = 0$.

Strongly-invariant $\mathcal{MAX}$–$\mathcal{MIN}$ ant system

A strongly-invariant version of $\mathcal{MAX}$–$\mathcal{MIN}$ ant system (*si*$\mathcal{MM}$AS) can be defined. We first define the algorithm, then we prove that it is functionally equivalent to $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and finally that it is indeed strongly invariant.

Definition 18 (Strongly-invariant pheromone update rule)**.** The pheromone is updated as in Definition 15, with the difference that

$$\Delta_{ij,h} = \begin{cases} \rho f(s_0)/f(s^{best}_h), & \text{if } \langle i,j\rangle \in s^{best}_h; \\ 0, & \text{otherwise;} \end{cases} \tag{4}$$

where ρ is the evaporation rate, s_0 is the reference solution, and s^{best}_h is either the *best-so-far* or the *iteration-best* solution.

Definition 19 (Strongly-invariant pheromone initialization)**.** The pheromone is initialized to $\tau_{ij,1} = 1$, for all $\langle i, j\rangle$.

Definition 20 (Strongly-invariant pheromone trail limits)**.** At iteration $h+1$, the value $\tau_{ij,h+1}$ of the pheromone on a generic edge $\langle i, j\rangle$ is constrained: $\tau_h^{min} \leq \tau_{ij,h+1} \leq \tau_h^{max}$, with $\tau_h^{max} = f(s_0)/f(s_h^{bs})$ and $\tau_h^{min} = a\tau_h^{max}$, where s_0 is the reference solution, $f(s_h^{bs})$ is the best solution found up to and including iteration h, and a is a parameter.

Definition 21 (Strongly-invariant $\mathcal{MAX}$–$\mathcal{MIN}$ ant system)**.** The strongly-invariant $\mathcal{MAX}$–$\mathcal{MIN}$ ant system (*si*$\mathcal{MM}$AS) is a variation of $\mathcal{MAX}$–$\mathcal{MIN}$ ant system. In *si*$\mathcal{MM}$AS, the random proportional rule given in Definition 7 is adopted for the construction of solutions. The pheromone is initialized according to Definition 19, limited according to Definition 20, and the update is performed according to Definition 18. The heuristic information is set in an invariant way through some appropriate problem-specific rule.

Theorem 5. *$\mathcal{MAX}$–$\mathcal{MIN}$ ant system and si$\mathcal{MM}$AS are functionally equivalent if*

(Condition 2) the heuristic information is such that:

$$[\tilde{\eta}_{ij}]^{\beta} = [\lambda\eta_{ij}]^{\beta}, \text{ for all } \langle i, j\rangle,$$

where β is the parameter appearing in Definition 7, $\tilde{\eta}_{ij}$ and η_{ij} are the heuristic information on edge $\langle i, j\rangle$ respectively in si$\mathcal{MM}$AS and $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and $\lambda > 0$ is an arbitrary constant.

Proof. As in the proof of Theorem 2, a tilde placed above a symbol indicates that the latter refers to *si*$\mathcal{MM}$AS. Let $\mu = \rho f(s_0)$. According to Lemma 1 and given Condition 2, if at the generic iteration h, $\tilde{s}_{h-1}^{bs} = s_{h-1}^{bs}$ and $\tilde{\tau}_{ij,h} = \mu\tau_{ij,h}$, for all $\langle i, j\rangle$, then $\tilde{p}_{ij,h}^{k} = p_{ij,h}^{k}$, for all $\langle i, j\rangle$. Under Hypothesis 1, $\tilde{s}_h^k = s_h^k$, for all $k = 1, \dots, m$. In particular, $\tilde{s}_h^{ib} = s_h^{ib}$. Moreover, whether or not an improvement is made on the *best-so-far* solution, $\tilde{s}_h^{bs} = s_h^{bs}$—see the proof of Theorem 4. According to Equation 4:

$$\tilde{\Delta}_{ij,h} = \begin{cases} \rho f(s_0)/\tilde{f}(\tilde{s}_h^{best}), & \text{if } \langle i, j\rangle \in \tilde{s}_h^{best}; \\ 0, & \text{otherwise}; \end{cases} = \mu \begin{cases} 1/f(s_h^{best}), & \text{if } \langle i, j\rangle \in s_h^{best}; \\ 0, & \text{otherwise}; \end{cases} = \mu\Delta_{ij,h},$$

where s_h^{best} is either the *best-so-far* s_h^{bs}, or the *iteration-best* solution s_h^{ib}. In both cases, according to Definitions 14 and 20, $\tilde{\tau}_h^{max} = f(s_0)/f(s_h^{bs}) = \rho f(s_0)/\rho f(s_h^{bs}) = \mu\tau_h^{max}$ and $\tilde{\tau}_h^{min} = a\tilde{\tau}_h^{max} = a\mu\tau_h^{max} = \mu\tau_h^{min}$. It follows that, for all $\langle i, j\rangle$:

$$\tilde{\tau}_{ij,h+1} = \Big[(1-\rho)\tilde{\tau}_{ij,h} + \tilde{\Delta}_{ij,h}\Big]_{\tilde{\tau}_h^{min}}^{\tilde{\tau}_h^{max}} = \Big[(1-\rho)\mu\tau_{ij,h} + \mu\Delta_{ij,h}\Big]_{\mu\tau_h^{min}}^{\mu\tau_h^{max}} = \mu\tau_{ij,h+1}.$$

The proof is completed by observing that at the first iteration $h = 1$, $\tilde{\tau}_{ij,1} = 1 = \rho f(s_0)/\rho f(s_0) = \mu\tau_{ij,1}$, for all $\langle i, j\rangle$; and the initial *best-so-far* solutions are $\tilde{s}_0^{bs} = s_0^{bs} = s_0$. □

Theorem 6. *si$\mathcal{MM}$AS is strongly-invariant if*

(Condition 3) the heuristic information is such that:

$$[\bar{\eta}_{ij}]^{\beta} = [\eta_{ij}]^{\beta}, \text{ for all } \langle i, j\rangle,$$

for any two instances I and $\bar{I}$ such that $\bar{I} = g_1 I$, with $g_1 > 0$.

Proof. Given Condition 3, according to Lemma 1 and Hypothesis 1, if at the generic iteration h, $\bar{\tau}_{ij,h} = \tau_{ij,h}$, for all $\langle i,j\rangle$, and if $\bar{s}^{bs}_{h-1} = s^{bs}_{h-1}$, then $\bar{p}^k_{ij,h} = p^k_{ij,h}$, for all $\langle i,j\rangle$, $\bar{s}^k_h = s^k_h$ and $\bar{f}(\bar{s}^k_h) = g_1 f(s^k_h)$, for all $k = 1,\ldots,m$. It follows that $\bar{s}^{bs}_h = s^{bs}_h$ and, due to Definition 20, $\bar{\tau}^{max}_h = \tau^{max}_h$ and $\bar{\tau}^{min}_h = \tau^{min}_h$. Moreover, it can be easily observed that, as a consequence of Definition 18, $\bar{\Delta}_{ij,h} = \Delta_{ij,h}$, for all $\langle i,j\rangle$; therefore, $\bar{\tau}_{ij,h+1} = \tau_{ij,h+1}$, for all $\langle i,j\rangle$. The proof is completed by observing that, according to Definition 19, $\bar{\tau}_{ij,1} = \tau_{ij,1}$, for all $\langle i,j\rangle$, and the initial *best-so-far* solutions are $\bar{s}^{bs}_0 = s^{bs}_0 = s_0$. □

5 Ant colony system

The weak invariance property holds also for ant colony system [10]. In ant colony system, the concept of *local* pheromone update is introduced: When an ant traverses edge $\langle i,j\rangle$ while constructing a solution, that is, when the solution component encoded by edge $\langle i,j\rangle$ is included in the solution being constructed, the pheromone on $\langle i,j\rangle$ is decreased [10, 2]. In order to describe this feature, a slightly modified notation is needed: With $s^k_{h,t}$ we denote the partial solution constructed by ant k, at iteration h, in the first t steps of the solution construction process. Further, $s^k_{h,t}(t')$, with $t' \leq t$, is the solution component added at step t'. Similarly, $\tau^k_{ij,h,t}$ is the value of the pheromone on edge $\langle i,j\rangle$ at iteration h, when ant k is performing step t of the solution construction process. Finally, if ant k is in node i at construction step t of iteration h, $p^k_{ij,h,t}$ is the probability that it moves to node j.

Definition 22 (Local pheromone update rule)**.** At the generic iteration h, in turn, the m ants perform a step of the solution construction by traversing an edge, the pheromone on which is then decreased. This process is iterated until each of the m ants has constructed its complete solution. After the generic ant k has performed step t of the construction of its solution, the pheromone is modified according to:

$$\tau^{k+1}_{ij,h,t} = \begin{cases} (1-\xi)\,\tau^k_{ij,h,t} + \xi\,\tau^1_{ij,1,1}, & \text{if } s^k_{h,t}(t) = \langle i,j\rangle; \\ \tau^k_{ij,h,t}, & \text{otherwise;} \end{cases}$$

where ξ is a parameter called the *local pheromone evaporation rate*, and $\tau^1_{ij,1,1}$ is the initial value of the pheromone—see Definition 25. When all m ants have completed step t of the solution construction process, step $t+1$ is started with $\tau^1_{ij,h,t+1} = \tau^{m+1}_{ij,h,t}$.

Definition 23 (Global pheromone update rule)**.** At each iteration h, after all m ants have built their solution and performed the local pheromone update, the pheromone on the edges belonging to the *best-so-far* solution s^{bs}_h found up to and including iteration h, are reinforced:

$$\tau^1_{ij,h+1,1} = \begin{cases} (1-\rho)\tau^{m+1}_{ij,h,T} + \rho\Delta_{ij,h}, & \text{if } \langle i,j\rangle \in s^{bs}_h; \\ \tau^{m+1}_{ij,h,T}, & \text{otherwise;} \end{cases}$$

where $\Delta_{ij,h} = 1/f(s^{bs}_h)$, and T is the number of construction steps needed to obtain a complete solution. The quantity $\tau^{m+1}_{ij,h,T}$ is the value of the pheromone on edge $\langle i,j\rangle$ after all m ants have completed the T construction steps of iteration h, while $\tau^1_{ij,h+1,1}$ is the quantity of pheromone on edge $\langle i,j\rangle$ right before the first ant performs the first construction step of iteration $h+1$.

Definition 24 (Pseudorandom proportional rule)**.** At the generic iteration h and generic construction step t, suppose that ant k is in node i and $\mathcal{N}^k_i$ is the set of feasible nodes. The node to be visited next is selected according to the following rule: With a probability given by the parameter q_0, the ant moves to the feasible node that maximizes $\tau^k_{il,h,t}[\eta_{il}]^\beta$, where $l \in \mathcal{N}^k_i$; with probability

$1 - q_0$ a node is selected according to the random proportional rule given in Definition 7, with $\alpha = 1$.[2] Formally:

$$p^k_{ij,h,t} = \begin{cases} q_0 + (1-q_0)\dfrac{\tau^k_{ij,h,t}[\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}\tau^k_{il,h,t}[\eta_{il}]^\beta}, & \text{if } j = \arg\max_{l\in\mathcal{N}_i^k}\tau^k_{il,h,t}[\eta_{il}]^\beta; \\ (1-q_0)\dfrac{\tau^k_{ij,h,t}[\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}\tau^k_{il,h,t}[\eta_{il}]^\beta}, & \text{otherwise;} \end{cases}$$

where β and q_0 are parameters, with $0 \le q_0 \le 1$.

Definition 25 (Pheromone initialization)**.** At iteration $h = 1$, the pheromone on each edge is initialized to

$$\tau^1_{ij,1,1} = \frac{1}{nf(s_0)}, \text{ for all } \langle i,j\rangle \in E,$$

where $n = |N|$ is the number of nodes in the construction graph G, and s_0 is the reference solution.

Definition 26 (Ant colony system)**.** Ant colony system is an ACO algorithm in which solutions are constructed according to the pseudorandom proportional rule given in Definition 24, the pheromone is initialized as in Definition 25 and updated according to Definitions 22 and 23. The local and global evaporation rates ξ and ρ, the number of ants m, the exponent β, and the probability q_0 are parameters of the algorithm. The definition of the heuristic information is problem-specific.

Lemma 2. *The pseudorandom proportional rule is invariant to concurrent linear transformation of the pheromone and of the heuristic information. Formally, for any two positive constants g_1 and g_2,*

$$\bar\tau^k_{ij,h,t} = g_1\tau^k_{ij,h,t} \wedge \bar\eta_{ij} = g_2\eta_{ij}, \textit{ for all } \langle i,j\rangle \implies \bar p^k_{ij,h,t} = p^k_{ij,h,t}, \textit{ for all } \langle i,j\rangle.$$

where $\bar p^k_{ij,h,t}$ is obtained on the basis of $\bar\tau^k_{ij,h,t}$ and $\bar\eta_{ij}$, according to Definition 24.

Proof. Indeed:

$$\bar p^k_{ij,h,t} = \begin{cases} q_0 + (1-q_0)\dfrac{\bar\tau^k_{ij,h,t}[\bar\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}\bar\tau^k_{il,h,t}[\bar\eta_{il}]^\beta}, & \text{if } j = \arg\max_{l\in\mathcal{N}_i^k}\bar\tau^k_{il,h,t}[\bar\eta_{il}]^\beta; \\ (1-q_0)\dfrac{\bar\tau^k_{ij,h,t}[\bar\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}\bar\tau^k_{il,h,t}[\bar\eta_{il}]^\beta}, & \text{otherwise;} \end{cases}$$

$$= \begin{cases} q_0 + (1-q_0)\dfrac{g_1\tau^k_{ij,h,t}[g_2\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}g_1\tau^k_{il,h,t}[g_2\eta_{il}]^\beta}, & \text{if } j = \arg\max_{l\in\mathcal{N}_i^k}g_1\tau^k_{il,h,t}[g_2\eta_{il}]^\beta; \\ (1-q_0)\dfrac{g_1\tau^k_{ij,h,t}[g_2\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}g_1\tau^k_{il,h,t}[g_2\eta_{il}]^\beta}, & \text{otherwise;} \end{cases}$$

$$= \begin{cases} q_0 + (1-q_0)\dfrac{\tau^k_{ij,h,t}[\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}\tau^k_{il,h,t}[\eta_{il}]^\beta}, & \text{if } j = \arg\max_{l\in\mathcal{N}_i^k}\tau^k_{il,h,t}[\eta_{il}]^\beta; \\ (1-q_0)\dfrac{\tau^k_{ij,h,t}[\eta_{ij}]^\beta}{\sum_{l\in\mathcal{N}_i^k}\tau^k_{il,h,t}[\eta_{il}]^\beta}, & \text{otherwise;} \end{cases} = p^k_{ij,h,t}.$$

□

Theorem 7. *Let I and $\bar I$ be two equivalent instances such that $\bar I = g_1 I$, with $g_1 > 0$. Further, let $G = (N,E)$ be the construction graph associated with I and $\bar I$. Ant colony system obtains the same sequence of solutions on I and $\bar I$ if*

[2] In the original ant colony system, α is set to 1 and is not a free parameter.

(Condition 1) the heuristic information is such that:

$$[\bar{\eta}_{ij}]^{\beta} = [g_2 \eta_{ij}]^{\beta}, \text{ for all } \langle i, j\rangle \in E,$$

where β is the parameter appearing in Definition 7 and $g_2 > 0$ is an arbitrary constant.

Proof. The proof follows those given for Theorems 1 and 4. Let us assume that, at the beginning of the generic iteration h, $\bar{s}^{bs}_{h-1} = s^{bs}_{h-1}$ and $\bar{\tau}^1_{ij,h,1} = \frac{1}{g_1}\tau^1_{ij,h,1}$, for all $\langle i, j\rangle$. Let us consider the first construction step at iteration h. According to Lemma 2, for the first ant, $\bar{p}^1_{ij,h,1} = p^1_{ij,h,1}$, for all $\langle i, j\rangle$. Under Hypothesis 1, $\bar{s}^1_{h,1} = s^1_{h,1}$. On the basis of Definition 22,

$$\begin{aligned}
\bar{\tau}^2_{ij,h,1} &= \begin{cases} (1-\xi)\,\bar{\tau}^1_{ij,h,1} + \xi\,\bar{\tau}^1_{ij,1,1}, & \text{if } \bar{s}^1_{h,1}(1) = \langle i, j\rangle; \\ \bar{\tau}^1_{ij,h,1}, & \text{otherwise;} \end{cases} \\
&= \begin{cases} (1-\xi)\,\frac{1}{g_1}\tau^1_{ij,h,1} + \xi\,\frac{1}{g_1}\tau_{ij,1,1} & \text{if } s^1_{h,1}(1) = \langle i, j\rangle; \\ \frac{1}{g_1}\tau^1_{ij,h,1}, & \text{otherwise;} \end{cases} = \frac{1}{g_1}\tau^2_{ij,h,1}.
\end{aligned}$$

Under the condition $\bar{\tau}^2_{ij,h,1} = \frac{1}{g_1}\tau^2_{ij,h,1}$, Lemma 2 applies also to the second ant at the first step of the solution construction at iteration h: $\bar{p}^2_{ij,h,1} = p^2_{ij,h,1}$, for all $\langle i, j\rangle$. Therefore, $\bar{s}^2_{h,1} = s^2_{h,1}$ and finally $\bar{\tau}^3_{ij,h,1} = \frac{1}{g_1}\tau^3_{ij,h,1}$, for all $\langle i, j\rangle$. This procedure is repeated for all m ants at the first step of the solution construction at generation h, with the net result that $\bar{s}^k_{h,1} = s^k_{h,1}$, for all $k = 1, \ldots, m$, and $\bar{\tau}^{m+1}_{ij,h,1} = \frac{1}{g_1}\tau^{m+1}_{ij,h,1}$ for all $\langle i, j\rangle$. The same reasoning holds also for the second step of the solution construction. Indeed, according to Definition 22, $\bar{\tau}^1_{ij,h,2} = \bar{\tau}^{m+1}_{ij,h,1} = \frac{1}{g_1}\tau^{m+1}_{ij,h,1} = \frac{1}{g_1}\tau^1_{ij,h,2}$, for all $\langle i, j\rangle$. Eventually, after T construction steps, $\bar{\tau}^{m+1}_{ij,h,T} = \frac{1}{g_1}\tau^{m+1}_{ij,h,T}$, for all $\langle i, j\rangle$, and $\bar{s}^k_h = s^k_h$, for all $k = 1, \ldots, m$. Therefore, $\bar{f}(\bar{s}^k_h) = g_1 f(s^k_h)$, for all $k = 1, \ldots, m$. In particular, $\bar{f}(\bar{s}^{ib}_h) = g_1 f(s^{ib}_h)$. Moreover, whether or not an improvement is made on the *best-so-far* solution, $\bar{s}^{bs}_h = s^{bs}_h$ and therefore $\bar{f}(\bar{s}^{bs}_h) = g_1 f(s^{bs}_h)$—see the proof of Theorem 4—which results in $\bar{\Delta}_{ij,h} = \frac{1}{g_1}\Delta_{ij,h}$. According to Definition 23,

$$\begin{aligned}
\bar{\tau}^1_{ij,h+1,1} &= \begin{cases} (1-\rho)\bar{\tau}^{m+1}_{ij,h,T} + \rho\bar{\Delta}_{ij,h}, & \text{if } \langle i, j\rangle \in \bar{s}^{bs}_h; \\ \bar{\tau}^{m+1}_{ij,h,T}, & \text{otherwise;} \end{cases} = \begin{cases} (1-\rho)\frac{1}{g_1}\tau^{m+1}_{ij,h,T} + \rho\frac{1}{g_1}\Delta_{ij,h}, & \text{if } \langle i, j\rangle \in s^{bs}_h; \\ \frac{1}{g_1}\tau^{m+1}_{ij,h,T}, & \text{otherwise;} \end{cases} \\
&= \frac{1}{g_1}\begin{cases} (1-\rho)\tau^{m+1}_{ij,h,T} + \rho\Delta_{ij,h}, & \text{if } \langle i, j\rangle \in s^{bs}_h; \\ \tau^{m+1}_{ij,h,T}, & \text{otherwise;} \end{cases} = \frac{1}{g_1}\tau^1_{ij,h+1,1}.
\end{aligned}$$

The proof is completed by observing that, according to Definition 25, the pheromone is initialized as:

$$\bar{\tau}^1_{ij,1,1} = \frac{1}{n\bar{f}(s_0)} = \frac{1}{ng_1 f(s_0)} = \frac{1}{g_1}\tau^1_{ij,1,1}, \text{ for all } \langle i, j\rangle.$$

and the initial *best-so-far* solutions are $\bar{s}^{bs}_0 = s^{bs}_0 = s_0$, where s_0 is the reference solution. □

Remark 8. Condition 1 is trivially satisfied when no heuristic information is used, that is, when $\beta = 0$.

Strongly-invariant ant colony system

A strongly-invariant version of ant colony system (*si*ACS) can be defined. We first define the algorithm, then we prove that it is functionally equivalent to ant colony system, and finally that it is indeed strongly invariant.

Definition 27 (Strongly-invariant global pheromone update rule)**.** The global pheromone update is performed as in Definition 23, with the difference that $\Delta_{ij,h} = nf(s_0)/f(s_h^{bs})$, where $n = |N|$ and s_0 and s_h^{bs} are the reference and the *best-so-far* solution, respectively.

Definition 28 (Strongly-invariant pheromone initialization)**.** The pheromone is initialized to $\tau_{ij,1,1}^1 = 1$, for all $\langle i, j\rangle$.

Definition 29 (Strongly-invariant ant colony system)**.** The strongly-invariant ant colony system (*si*ACS) is a variation of ant colony system. In *si*ACS, the pseudorandom proportional rule is used for the construction of solutions, the pheromone is initialized according to Definition 28 and the local and global pheromone updates are performed according to Definitions 22 and 27, respectively. The heuristic information is set in an invariant way through some appropriate problem-specific rule.

Theorem 8. *Ant colony system and siACS are functionally equivalent if*

(Condition 2) the heuristic information is such that:

$$[\tilde{\eta}_{ij}]^\beta = [\lambda\eta_{ij}]^\beta, \textit{ for all } \langle i, j\rangle,$$

where β is the parameter appearing in Definition 7, $\tilde{\eta}_{ij}$ and η_{ij} are the heuristic information on edge $\langle i, j\rangle$ respectively in siACS and ant colony system, and $\lambda > 0$ is an arbitrary constant.

Proof. As in the proofs of Theorems 2 and 5, a tilde placed above a symbol indicates that the latter refers to *si*ACS. Let $\mu = nf(s_0)$. According to Lemma 2, given Condition 2, and under Hypothesis 1, if at the beginning of the generic iteration h, $\tilde{s}_{h-1}^{bs} = s_{h-1}^{bs}$ and $\tilde{\tau}_{ij,h,1}^1 = \mu\tau_{ij,h,1}^1$, for all $\langle i, j\rangle$, then, $\tilde{p}_{ij,h,t}^k = p_{ij,h,t}^k$, for all $\langle i, j\rangle$, for all ants $k = 1, \dots, m$, and for all construction steps $t = 1, \dots, T$. Further, $\tilde{\tau}_{ij,h,t}^k = \mu\tau_{ij,h,t}^k$ and therefore $\tilde{s}_h^k = s_h^k$—see the proof of Theorem 7. In particular, $\tilde{\tau}_{ij,h,T}^{m+1} = \mu\tau_{ij,h,T}^{m+1}$. Moreover, $\tilde{s}_h^{ib} = s_h^{ib}$. Finally, whether or not an improvement is made on the *best-so-far* solution, $\tilde{s}_h^{bs} = s_h^{bs}$—see the proof of Theorem 4. The global pheromone update takes place on the basis of the quantities:

$$\tilde{\Delta}_{ij,h} = \frac{nf(s_0)}{f(\tilde{s}_h^{bs})} = \frac{\mu}{f(s_h^{bs})} = \mu\Delta_{ij,h}.$$

It follows that, for all $\langle i, j\rangle$:

$$\tilde{\tau}_{ij,h+1,1}^1 = \begin{cases} (1-\rho)\tilde{\tau}_{ij,h,T}^{m+1} + \rho\tilde{\Delta}_{ij,h}, & \text{if } \langle i,j\rangle \in \tilde{s}_h^{bs}; \\ \tilde{\tau}_{ij,h,T}^{m+1}, & \text{otherwise}; \end{cases} = \begin{cases} (1-\rho)\mu\tau_{ij,h,T}^{m+1} + \rho\mu\Delta_{ij,h}, & \text{if } \langle i,j\rangle \in s_h^{bs}; \\ \mu\tau_{ij,h,T}^{m+1}, & \text{otherwise}; \end{cases}$$

$$= \mu \begin{cases} (1-\rho)\tau_{ij,h,T}^{m+1} + \rho\Delta_{ij,h}, & \text{if } \langle i,j\rangle \in s_h^{bs}; \\ \tau_{ij,h,T}^{m+1}, & \text{otherwise}; \end{cases} = \mu\tau_{ij,h+1,1}^1.$$

The proof is completed by observing that at the first iteration $h = 1$, $\tilde{\tau}_{ij,1,1}^1 = 1 = nf(s_0)/nf(s_0) = \mu\tau_{ij,1,1}^1$, for all $\langle i, j\rangle$; and the initial *best-so-far* solutions are $\tilde{s}_0^{bs} = s_0^{bs} = s_0$. □

Theorem 9. *siACS is strongly-invariant if*

(Condition 3) the heuristic information is such that:

$$[\bar{\eta}_{ij}]^\beta = [\eta_{ij}]^\beta, \textit{ for all } \langle i, j\rangle,$$

for any two instances I and $\bar{I}$ such that $\bar{I} = g_1 I$, with $g_1 > 0$.

Proof. Under Hypothesis 1 and given Condition 3, according to Lemma 2 and Definition 22, if at the generic iteration h, $\bar{s}^{bs}_{h-1} = s^{bs}_{h-1}$ and $\bar{\tau}^1_{ij,h,1} = \tau^1_{ij,h,1}$, for all $\langle i,j \rangle$, then $\bar{\tau}^k_{ij,h,t} = \tau^k_{ij,h,t}$ and $\bar{p}^k_{ij,h,t} = p^k_{ij,h,t}$, for all $\langle i,j \rangle$, for all ants $k = 1,\ldots,m$, and for all construction steps $t = 1,\ldots,T$. It follows that $\bar{s}^k_h = s^k_h$ and $\bar{f}(\bar{s}^k_h) = g_1 f(s^k_h)$, for all $k = 1,\ldots,m$. In particular, $\bar{s}^{bs}_h = s^{bs}_h$ from which, as a consequence of Definition 27, $\bar{\Delta}_{ij,h} = \Delta_{ij,h}$, for all $\langle i,j \rangle$; therefore, $\bar{\tau}^1_{ij,h+1,1} = \tau^1_{ij,h+1,1}$, for all $\langle i,j \rangle$.

The proof is completed by observing that, according to Definition 28, $\bar{\tau}^1_{ij,1,1} = \tau^1_{ij,1,1} = 1$, for all $\langle i,j \rangle$, and the initial *best-so-far* solutions are $\bar{s}^{bs}_0 = s^{bs}_0 = s_0$. □

6 Problems

In this section, we illustrate how the theorems proved in Sections 3, 4, and 5 apply to some well known combinatorial optimization problems. In particular, Section 6.1 deals with the traveling salesman problem, Section 6.2 with the quadratic assignment problem, and Section 6.3 with the open shop scheduling problem. Further examples of how the proposed theorems apply to other combinatorial optimization problems are given in Pellegrini and Birattari [13] and can be found on-line at `http://iridia.ulb.ac.be/supp/IridiaSupp2006-008/`.

6.1 Traveling salesman problem

The traveling salesman problem (TSP) consists in finding a Hamiltonian circuit of minimum cost on an edge-weighted graph $G = (N,E)$, where N is the set of nodes, and E is the set of edges. If a directed graph is considered, the problem is known as the *asymmetric* traveling salesman problem [14].

Let $x_{ij}(s)$ be a binary variable taking value 1 if edge $\langle i,j \rangle$ is included in tour s, and 0 otherwise. Let c_{ij} be the cost associated to edge $\langle i,j \rangle$. The goal is to find a tour s such that the function

$$f(s) = \sum_{i \in N} \sum_{j \in N} c_{ij} x_{ij}(s)$$

is minimized.

1) Transformation of units: If the cost of all edges is multiplied by a constant ζ, the resulting instance $\bar{I}$ is equivalent to the original I, that is, $\bar{I} = g_1 I$, with $g_1 = \zeta$. Indeed, $\bar{c}_{ij} = \zeta c_{ij}$, for all $\langle i,j \rangle \implies \bar{f}(s) = \zeta f(s)$, for all s.

2) Reference solution: Many constructive heuristics exist for the TSP [15] that can be conveniently adopted here.

3) Heuristic information: The typical setting is $\eta_{ij} = 1/c_{ij}$, for all $\langle i,j \rangle$. This meets Condition 1 with $g_2 = 1/\zeta$.

Therefore, the theorems on the weak invariance of ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system hold. In the literature, the three variants of ant colony optimization considered in this paper have been applied to the traveling salesman problem with the setup just described [2].

4) Strongly-invariant heuristic information: $\eta_{ij} = f(s_0)/nc_{ij}$, for all $\langle i,j \rangle$, where $n = |N|$. It is worth noting that the term n is not needed for the invariance to transformation of units. It has been included for achieving another property: the above defined η_{ij} does not depend on the size of the instance under analysis—that is, on the number n of cities. This definition meets Condition 2 with $\lambda = f(s_0)/n$, and Condition 3.

Therefore, *si*AS, *si*$\mathcal{MM}$AS, and *si*ACS are indeed strongly invariant and are functionally equivalent to their original counterparts.

6.2 Quadratic assignment problem

In the quadratic assignment problem (QAP), n facilities and n locations are given, together with two $n \times n$ matrices $A = [a_{ij}]$ and $B = [b_{uv}]$, where a_{ij} is the *distance* between locations i and j, and b_{uv} is the *flow* between facilities u and v. A solution s is an assignment of each facility to a location. Let $x_i(s)$ denote the facility assigned to location i. The goal is to find an assignment that minimizes the function:

$$f(s) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} b_{x_i(s) x_j(s)}.$$

1) Transformation of units: If all distance are multiplied by a constant ζ_1 and all flows by a constant ζ_2, the resulting instance $\bar{I}$ is equivalent to the original I, that is, $\bar{I} = g_1 I$, with $g_1 = \zeta_1 \zeta_2$.

2) Reference solution: The construction of the reference solution is typically stochastic: a number of solutions are randomly generated and improved through a local search. The best solution obtained is adopted as the reference solution [16]. It is worth noting that a local search is an invariant algorithm.

3) Heuristic information: Often, the heuristic information is not adopted [16], that is, $\beta = 0$. In this case, Condition 1 is trivially met. Some authors [17] set $\eta_{ij} = 1/\sum_{l=1}^{n} a_{il}$. This meets Condition 1 with $g_2 = 1/\zeta_1$.

Therefore, the theorems on the weak invariance of ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system hold.

4) Strongly-invariant heuristic information: If the heuristic information is adopted, $\eta_{ij} = f(s_o)/\sum_{l=1}^{n} a_{il}$, for all $\langle i, j \rangle$. This meets Condition 2 with $\lambda = f(s_o)$, and Condition 3. On the other hand, if no heuristic information is adopted as suggested in [16], Conditions 2 and 3 are trivially met.

Therefore, *si*AS, *si*$\mathcal{MM}$AS, and *si*ACS are indeed strongly invariant and are functionally equivalent to their original counterparts.

6.3 Open shop scheduling problem

In open shop scheduling problems (OSP) [18], a finite set $\mathcal{O}$ of operations is given, which is partitioned into a collection of subsets $\mathcal{M} = \{M_1, M_2, \ldots, M_U\}$ and a collection of subsets $\mathcal{J} = \{J_1, J_2, \ldots, J_V\}$. Each M_u is the set of operations that have to be performed by machine u; and each J_v is the set of operations belonging to job v. A non-negative *processing time* $t(o_j)$ and an *earliest possible starting time* $e(o_j)$ are associated with operation $o_j \in \mathcal{O}$. A solution s is a collection of schedules $\mathcal{X}(s) = \{X^1(s), X^2(s), \ldots, X^U(s)\}$, where $X^u(s)$ is the sequence of operations scheduled for machine u and $X^u_r(s)$ is the operation in position r in sequence $X^u(s)$. The completion time $c^u_r(s)$ of operation $X^u_r(s)$ is computed recursively from $c^u_{r'}(s) = t\big(X^u_{r'}(s)\big) + \max\big[e\big(X^u_{r'}(s)\big), c^u_{r'-1}(s)\big]$, with $c^u_0(s) = 0$. The goal is to minimize the *makespan*, which is given by:

$$f(s) = \max_u c^u_{|M_u|}(s).$$

1) Transformation of units: If all processing times and earliest possible starting times are multiplied by a constant ζ, the resulting instance $\bar{I}$ is equivalent to the original I, that is, $\bar{I} = g_1 I$, with $g_1 = \zeta$.

2) Reference solution: The construction of the reference solution is typically stochastic.

3) Heuristic information: The heuristic information is typically $\eta_{ij} = 1/e(o_j)$, for all $\langle i, j \rangle$, which meets Condition 1 with $g_2 = 1/\zeta$.

Therefore, the theorems on the weak invariance of ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system hold.

4) Strongly-invariant heuristic information: $\eta_{ij} = f(s_0)/e(o_j)$, for all $\langle i, j \rangle$. This meets Condition 2 with $\lambda = f(s_0)$, and Condition 3.

Therefore, *si*AS, *si*$\mathcal{MM}$AS, and *si*ACS are indeed strongly invariant and are functionally equivalent to their original counterparts.

7 Conclusions

Contrary to what previously believed [1], at least three of the most representative and most widely adopted algorithms belonging to the ant colony optimization family appear to be invariant to transformation of units. In this paper, we have formally proved that ant system, $\mathcal{MAX}$–$\mathcal{MIN}$ ant system, and ant colony system are indeed *weekly-invariant*. In other words, the sequence of solutions they produce does not depend on the scale of the problem instance at hand. The technique adopted for proving the theorems is basically the same for the three algorithms. In the three cases, the proof is of an inductive nature: We prove that if some conditions are fulfilled at the beginning of iteration h, then the solutions produced at iteration h are the same whenever solving any two instances that are equivalent up to a linear transformation of units. Moreover, the same conditions hold also at the following iteration $h + 1$. The prove is concluded by showing that the conditions are fulfilled at the beginning of the first iteration. The same technique can be adopted for formally showing the invariance of other algorithms belonging to the ant colony optimization family. It is worth noticing here that the initialization of the pheromone plays a critical role: In order for the algorithm to be invariant, the pheromone should be initialized in an invariant way. Definitions 9, 16, and 25 guarantee the invariance of the initialization. A similar remark holds for what concerns the heuristic information. In order to obtain an invariant algorithm, the heuristic information should meet Condition 1 as given in the statement of Theorems 1, 4, and 7.

As a second contribution, the paper introduces three algorithms: *si*AS, *si*$\mathcal{MM}$AS, and *si*ACS. These algorithms are *functionally equivalent* to AS, $\mathcal{MM}$AS, and ACS, respectively, but they enjoy the further property of being *strongly invariant*. In other words, besides producing the same sequence of solutions irrespective of any linear transformation of units, these algorithms are such that the *pheromone* and the *heuristic information* do not change with the units adopted.

Blum and Dorigo [1] were the first to draw attention to the property that in this paper we call *strong invariance*. This property is definitely desirable for at least two main reasons: first, it reduces possible numerical problems in the implementations and contributes therefore to enhance the stability of the algorithm; second, it greatly improves the readability of the solution process. In order to achieve the strong invariance, Blum and Dorigo [1] have defined a new framework they named *hyper-cube*. An *hyper-cube* version of AS, $\mathcal{MM}$AS, or ACS is effectively a new algorithm which shares with its originating (non-*hyper-cube*) version much of the underlying ideas but that is not functionally equivalent to the latter. The main advantage of the strongly-invariant algorithms we have proposed in the paper is indeed that they are proved to be functionally equivalent to their respective original counterpart. The properties of these algorithms do not need therefore to be studied from scratch: The results reported in the existing literature on ant colony optimization, which are rather substantial, directly extend to these new algorithms. In particular, AS, $\mathcal{MM}$AS, and ACS have been successfully applied to a variety of problems and therefore an assessment of the performance of *si*AS, *si*$\mathcal{MM}$AS, and *si*ACS under a large number of experimental conditions is already available.

Anyway, the significance of the introduction of *si*AS, *si*$\mathcal{MM}$AS, and *si*ACS is mostly theoretical and speculative. Indeed, the very possibility of defining a strongly invariant algorithm that is functionally equivalent to a give ACO algorithm sheds new light on ant colony optimization.

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