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# Improved understanding of the searching behavior of ant colony optimization algorithms applied to the water distribution design problem

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[1] Evolutionary algorithms (EAs) have been applied successfully to many water resource problems, such as system design, management decision formulation, and model calibration. The performance of an EA with respect to a particular problem type is dependent on how effectively its internal operators balance the exploitation/exploration trade-off to iteratively find solutions of an increasing quality. For a given problem, different algorithms are observed to produce a variety of different final performances, but there have been surprisingly few investigations into characterizing how the different internal mechanisms alter the algorithm's searching behavior, in both the objective and decision space, to arrive at this final performance. This paper presents metrics for analyzing the searching behavior of ant colony optimization algorithms, a particular type of EA, for the optimal water distribution system design problem, which is a classical NP-hard problem in civil engineering. Using the proposed metrics, behavior is characterized in terms of three different attributes: (1) the effectiveness of the search in improving its solution quality and entering into optimal or near-optimal regions of the search space, (2) the extent to which the algorithm explores as it converges to solutions, and (3) the searching behavior with respect to the feasible and infeasible regions. A range of case studies is considered, where a number of ant colony optimization variants are applied to a selection of water distribution system optimization problems. The results demonstrate the utility of the proposed metrics to give greater insight into how the internal operators affect each algorithm's searching behavior.

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## 1. Introduction

[2] Water resources optimization problems can be extremely difficult to solve as they often possess: highly nonlinear objective functions; nonlinear constraints; non-convex objective surfaces; high problem dimensionality; discrete-valued variables; multimodal objective surfaces; and multiple objectives. They also typically involve the execution of computationally expensive deterministic and/or stochastic system simulators. Given these complexities, traditional deterministic optimization methods are often unsatisfactory [Nicklow *et al.*, 2010]. Within the last 20 years, stochastic heuristic optimization approaches, particularly evolutionary algorithms (EAs), have experienced growing popularity, and are now an established component within water resources research. Indeed, EAs, or more

broadly population based metaheuristics, have been applied successfully to a wide range of water resources problems, where applications can be categorized into the following three areas: (1) engineering design problems, for example, water distribution system design [Simpson and Goldberg, 1994; Simpson *et al.*, 1994; Dandy *et al.*, 1996]; design of groundwater remediation systems [Bayer and Finkel, 2007]; design of urban drainage and sewer networks [Cembrowicz, 1994]; design of disinfection stations for potable water [Prasad *et al.*, 2004]; and design of funnel-and-gate systems for groundwater treatment [Bürger *et al.*, 2007]; (2) the development of management strategies, for example, management of ecosystems [Bekele and Nicklow, 2005]; shared aquifer management [Siegfried and Kinzelbach, 2006]; mitigation of drought risk [Kasprzyk *et al.*, 2009]; multipurpose reservoir operation [Baltar and Fontane, 2008]; and design of watershed management processes [Arabi *et al.*, 2006]; and (3) the calibration of models, for example, rainfall-runoff models [Tolson and Shoemaker, 2007; de Vos and Rientjes, 2008]; runoff and erosion models [Laloy and Biolders, 2009]; river water quality models [Wang, 1991]; groundwater models [Zheng, 1997]; and friction factor estimation in distribution systems [Lingireddy and Ormsbee, 1999].

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[3] The appeal of EAs for water resources problems is multifaceted. First, they are global optimizers, able to deal with constrained, nonconvex, multimodal, multiobjective, and high dimensional problems [Deb, 2001]. Second, EAs can be applied to optimization problems with relative ease as they do not require gradient or Hessian information about the objective [Maier et al., 2003]. Third, they can be applied to discrete, or continuous problems [AlRashidi and El-Hawary, 2009]. Finally, the population nature of EAs means that they lend themselves conveniently to parallel computing [Karpouzou et al., 2001], and problems involving stochastic objectives [Smalley et al., 2000].

[4] Many different EAs have been applied to water resources problems, prominent examples of which are genetic algorithms [Holland, 1975], simulated annealing [Kirkpatrick et al., 1983], ant colony optimization (ACO) [Dorigo, 1996], particle swarm optimization [Kennedy and Eberhart, 1995], shuffled complex evolution [Duan et al., 1993], shuffled frog leaping algorithms [Eusuff et al., 2006], differential evolution [Storn and Price, 1997], and genetic programming [Banzhaf et al., 1998]. These algorithms all differ from each other in terms of the conceptual basis and mathematical form of the internal mechanisms they employ to manage the *exploration-exploitation* trade-off, where *exploration* refers to an algorithm's ability to broadly search the decision space in order to avoid premature convergence, and *exploitation* refers to an algorithm's ability to focus on intensive searching in good regions within the search space (note, the terms search space and decision space are used interchangeably within this paper).

[5] Studies on EAs in water resources typically focus on (1) parameter calibration of an algorithm to yield the best performance for a certain problem type [e.g., Duan et al., 1994; Ng and Perera, 2003; Zecchin et al., 2005; Gibbs et al., 2008], (2) the development of additional *exploration* or *exploitation* encouraging mechanisms to improve an algorithm's performance [e.g., Dandy et al., 1996; Afshar, 2006; Jiang et al., 2007; Kollat et al., 2008; Montalvo et al., 2008], or (3) comparative performance of different EA types or EA variants [e.g., Cheung et al., 2003; Elbeltagi et al., 2005; Farmani et al., 2005; Kollat and Reed, 2006; Tang et al., 2006; Zecchin et al., 2007]. Such analyses are typically based only on overall performance indicators using statistics derived from the *best objective value* found within an optimization run, or the *search time* required to find the best solution. Such a framework is adopted within virtually all of the papers cited above, a prominent example of which is the highly cited work of Elbeltagi et al. [2005], who compared GAs, MAs, PSO, ACO, and SFLA applied to a range of continuous and discrete optimization problems. Despite the governing importance of the overall performance statistics, this framework of comparison is somewhat limited, as it fails to give any insight into how an algorithm navigates its way through the decision space in an attempt to find the optimum solution. In other words, it answers the question of which *algorithm variant is best* for a particular problem type, but it does not answer the question of *what it is that drives particular algorithm instances to perform better than others* (for a particular problem). It should be noted that theoretical studies on algorithm convergence and behavior [e.g., Michalewicz, 1996; Clerc and Kennedy, 2002; van den Bergh and Engelbrecht, 2006] have been

excluded from this review, as they usually rely on assumptions that are rarely satisfied in practice.

[6] Understanding why particular algorithm instances perform better than others, for particular problem types, is critical for meaningful future development and application of EAs, as this understanding will serve to inform the development of algorithm operators, and provide guidance for specific algorithm applications. Consequently, there is a need to develop alternative performance metrics that go beyond the measurement of solution quality, i.e., as indicated only by the objective function value.

[7] For both single and multiobjective problems, there has been much work in characterizing an algorithm's performance in a broader sense by considering evolutionary dynamics as manifest by measures based on objective space properties. Notable examples of this work include Hansen et al. [2003], Bayer and Finkel [2004, 2007], and Vrugt et al. [2009] for the optimization of single objective problems, where the best value of the objective function during the evolution, or some related measures (e.g., its statistics in multiple runs, the number of function evaluations required to reach a threshold value, and the algorithm success rate) are used, and Tang et al. [2006], Kollat and Reed [2006, 2007], Vrugt and Robinson [2007], and Kollat et al. [2008] for multiobjective problems, where algorithms are compared using metrics (like convergence, diversity,  $\epsilon$  indicator and hypervolume) that still consider only the mapping of the solutions in the objective space. However, there has been limited work in characterizing an algorithm's performance using measures based on the algorithm's behavior within the decision space. Examples are Chu et al. [2011], who studied population degeneration for specific types of algorithms; Deb and Beyer [2001], who used the Euclidean distance between the best and optimal solutions and the standard deviation of the population; and Kang et al. [2008], who used a measure of the hypervolume covered by the decision variables in the population and the distance of particles from the average position of the swarm to study a variant of PSO. However, in these last two cases, measures were tested only on mathematical functions and it is not clear if the effect of the stochastic search was considered. In addition, the measures used by Kang et al. [2008] can be interpreted with difficulty, making the analysis of algorithm behavior more complicated.

[8] A first step toward addressing the shortcomings of existing EA performance measures outlined above is the development of metrics that can be used to characterize an EA's population dynamics. In this paper, such metrics are developed for ACO algorithms applied to the optimization of the water distribution system problem (WDSP) and it is demonstrated how they serve to provide insight into the manner in which algorithms explore the solution space as they progress in their search.

[9] The WDSP involves determining a feasible, least cost design of a water distribution system subject to hydraulic performance constraints (section 2). The WDSP has been chosen because it is a classical nondeterministic polynomial-time (NP)-hard optimization problem in water resources engineering, and because it has many characteristics in common with other engineering problems (i.e., it is discrete, multimodal, constrained and highly dimensional). As the selected WDSPs are characterized by different properties, the behavioral metrics' ability to highlight the differences in algorithm response is tested.

[10] The paper focuses on four ACO variants: ant system (AS), elitist ant system ( $AS_{elite}$ ), elitist-rank ant system ( $AS_{rank}$ ), and max-min ant system (MMAS) (section 3). As the main evolving principle for the ACO variants is the same, and identical values for the common parameters are employed, a systematic comparison of the algorithms' behaviors as a result of their different operators has been possible.

[11] The proposed metrics measure three types of behavioral characteristics, including (1) the effectiveness of the search in terms of entering into optimal or near optimal regions of the search space and finding solutions of increasing quality, (2) the extent to which the algorithm explores the search space as it converges to solutions, and (3) the amount of the search effort spent in the feasible and infeasible regions of the search space (section 4).

[12] Section 5 describes the case studies to which the proposed behavioral metrics are applied. Section 6 shows and discusses the computational results obtained. Conclusions are given in section 7.

## 2. Optimal Design of Water Distribution Systems

[13] The optimal design of WDSs is an NP-hard combinatorial problem that is nonconvex, typically high dimensional, multimodal and nonlinearly constrained. A WDS is a network of components (e.g., pipes, pumps, valves, tanks) that delivers water from a source to consumers. The optimization of WDSs may be defined as the selection of the lowest cost combination of appropriate component sizes and component settings such that the criteria of demands and other design constraints are satisfied. In practice, the optimization of WDSs can take many forms as WDSs are composed of a number of different components and also have many different performance criteria. Traditionally in the literature, the optimization of WDSs has dealt with a relatively simple and idealized problem, called the water distribution system problem (WDSP) [e.g., *Simpson et al.*, 1994; *Dandy et al.*, 1996; *Savic and Walters*, 1997; *Maier et al.*, 2003; *Montalvo et al.*, 2008].

[14] The decision variables for the WDSP are often the pipe diameters within the system, where more specifically, the decision options are typically the selection of (1) a diameter for a new pipe, or (2) a diameter for a duplicate pipe. The design constraints on the system are the requirement of minimum allowable pressures at each of the nodes. In addition to the design constraints, the hydraulic equations governing fluid flow through a network (e.g., equations of mass and energy conservation for every node and pipe, respectively, of the network)  $S^* = [s_1^* \cdots s_n^*]$ , where

$$S^* = \arg \min_{S \in \mathcal{S}} \sum_{i=1}^n C_i(s_i) \quad (1)$$

$$\mathbf{h}(S^*) \geq \mathbf{0}, \quad (2)$$

where the decision variable space  $\mathcal{S}$  ( $\in \mathbf{N}$  in the following) defines the set of discrete design options for pipe  $i$ ,  $C_i$  is the cost function for pipe  $i$  associated with the choice of the decision variable  $s_i$ ,  $\mathbf{h}$  represents the design performance constraints (e.g., the design pressure being above the minimum allowable pressure), which are determined from a

hydraulic simulation of the network [*Zecchin et al.*, 2007]. In this work, the hydraulic solver used to satisfy the hydraulic equality constraints and to compute the network pressures is EPANET2 [*Rossman*, 2000]. It is important to note that, as EAs are unable to deal directly with constraints, a slightly modified problem (for which the original  $S^*$  is preserved) is typically considered, namely,

$$S^* = \arg \min_{S \in \mathcal{S}} \sum_{i=1}^n C_i(s_i) + p(\mathbf{h}(S)), \quad (3)$$

where  $p$  is a penalty function [*Coello Coello*, 2002], that is only nonzero when the pressure constraints in (2) are not satisfied. Within this work,  $p$  was based on the maximum pressure violation below the required minimum design pressure (for more details, the interested reader is referred to *Zecchin et al.* [2007]).

## 3. Ant Colony Optimization

[15] ACO is an evolutionary algorithmic optimization process based on the analogy of a colony of foraging ants determining the shortest path between a food source and its nest (see *Dorigo et al.* [1996] for examples). The colony is able to *optimize* the excursions of its ants through the process of stigmergy [*Dorigo et al.*, 2000]. Stigmergy refers to the indirect form of communication between the ants that arises from their deposition of pheromone trails. These trails act as sign posts encouraging ants to follow. Gradually, increasingly shorter pheromone trails will be reinforced with greater amounts of pheromone, encouraging more ants to follow them and leaving the longer, and less frequently used, trails to evaporate into nonexistence.

[16] Within the framework of a combinatorial optimization problem, ACOA can be seen as an iterative optimization process where, within each iteration, new information about the search space of the problem is gained and utilized to guide the search in subsequent iterations. It should be noted that the term *iteration* has a meaning equivalent to the term *generation* in genetic algorithms, but it is here preferred because it is consistent with the terminology used by *Maier et al.* [2003], who introduced the application of ACOAs to the WDS problem. The solution generation that occurs within an iteration (i.e., the *searching* of the ants) is a stochastic process governed by a set of probability functions. The mechanism of ACO is to use its gained information to manipulate these functions to increase the probability of the algorithm generating increasingly better, and ultimately optimal (or near-optimal) solutions.

[17] The manipulation of the probability functions is the ACO analogy to the colony of foraging ants modifying their search behavior in response to changes in the detected pheromone trails. ACO deals with a combinatorial optimization problem organized as a graph  $\mathcal{G}(\mathcal{N}, \mathcal{L})$ , where  $\mathcal{N}$  is the set of nodes (decision variables), and  $\mathcal{L}$  is the set of edges linking the nodes (the possible values for each variable). Therefore, a solution to the problem is a feasible tour through  $\mathcal{G}(\mathcal{N}, \mathcal{L})$ . A tour is constructed by an ant by starting at some node, and incrementally selecting edges to follow based on the set of edges that are available to it given its semiconstructed tour. This process is continued until the ant completes its tour. Given a semiconstructed tour  $\tilde{S}$ , the probability that an ant at node  $i$  will select edge  $(i, j)$ , i.e.,

**Table 1.** Summary of Pheromone Update Operations

Algorithm	Parameters <sup>a</sup>	Expression for Pheromone Addition $\Delta\tau_{i,j}(t)$
<i>AS</i>	$\alpha, \beta, \rho, Q, \tau_0, m$	$\Delta\tau_{i,j}(t) = \sum_{k=1}^m I_{S_k(t)}\{(i,j)\} \frac{Q}{f(S_k(t))}$
<i>AS<sub>elite</sub></i>	$\alpha, \beta, \rho, \sigma, Q, \tau_0, m$	$\Delta\tau_{i,j}(t) = I_{S_{g-b}(t)}\{(i,j)\} \sigma \frac{Q}{f(S_{g-b}(t))} + \sum_{k=1}^m I_{S_k(t)}\{(i,j)\} \frac{Q}{f(S_k(t))}$
<i>AS<sub>rank</sub></i>	$\alpha, \beta, \rho, \sigma, Q, \tau_0, m$	$\Delta\tau_{i,j}(t) = I_{S_{g-b}(t)}\{(i,j)\} \sigma \frac{Q}{f(S_{g-b}(t))} + \sum_{k=1}^{\sigma-1} I_{S_{(k)}(t)}\{(i,j)\} k \frac{Q}{f(S_{(k)}(t))}$
<i>MMAS<sup>b</sup></i>	$\alpha, \beta, \rho, P_{best}, \delta, T_{g-b}, Q, \tau_0, m$	$\Delta\tau_{i,j}(t) = I_{S_{(1)}(t)}\{(i,j)\} \frac{Q}{f(S_{(1)}(t))}$

<sup>a</sup>Parameters are as follows:  $\alpha$  = pheromone weighting factor;  $\beta$  = visibility weighting factor;  $\rho$  = pheromone decay factor;  $Q$  = pheromone update coefficient;  $\tau_0$  = initial pheromone;  $m$  = number of ants;  $\sigma$  = number of elitist ants;  $P_{best}$  = coefficient for determining pheromone bounds  $\in (0, 1)$ ;  $\delta$  = pheromone trail smoothing coefficient  $\in [0, 1]$ ; and  $T_{g-b}$  = period of global best pheromone update.  $I_A(a)$  is the indicator function given by 1 if  $a \in A$  and 0 otherwise.

<sup>b</sup>An addition, for *MMAS*, (1) the pheromone on the edges is bounded by  $[\tau_{\max}(t), \tau_{\min}(t)]$ , where  $\tau_{\max}(t) = \frac{Q}{1-\rho} f^{-1}(S_{g-b}(t))$  and  $\tau_{\min}(t) = \tau_{\max}(t) \frac{(1-\sqrt[\rho]{P_{best}})}{(NO_{avg}-1)\sqrt[\rho]{P_{best}}}$ , where  $n$  is the number of decision points and  $NO_{avg}$  is the average number of edges available from each decision point, and (2) each edge undergoes pheromone trail smoothing, which is described by the operation  $\tau_{i,j}(t) \leftarrow \tau_{i,j}(t) + \delta(\tau_{\max}(t) - \tau_{i,j}(t))$ . For more discussion on these mechanisms the reader is referred to *Stützle and Hoos* [2000].

that the value  $j$  is selected for the decision variable  $i$ , is given by the probability function

$$p_{i,j}(t) = \frac{\tau_{i,j}(t)^\alpha \eta_{i,j}^\beta}{\sum_{(i,l) \in \Omega_i(\tilde{S})} \tau_{i,l}(t)^\alpha \eta_{i,l}^\beta}, \quad (4)$$

where  $\Omega_i(\tilde{S})$  is the set of edges available from node  $i$  given the ant's semiconstructed tour  $\tilde{S}$ ,  $\tau_{i,j}(t)$  is the pheromone value on edge  $(i, j)$  in iteration  $t$ ,  $\eta_{i,j}$  is the visibility factor, which indicates local desirability of the edges (e.g., inverse of distance or cost; see *Maier et al.* [2003] and *Zecchin et al.* [2006] for more detail), and  $\alpha$  and  $\beta$  are the relative weighting exponents of pheromone and visibility values, respectively.

[18] The alteration of the pheromone values between iterations is at the heart of ACO learning, as it is by the relative values of these pheromone intensities that the algorithm retains information about good solutions that it has found in its searching history, i.e., learning is achieved through the reinforcement of the pheromone intensities of the edges from good solutions. Between iterations, all pheromone values on each edge decay (evaporate) by a factor of  $1 - \rho$ , where  $0 < \rho < 1$ , and selected edges receive a pheromone addition of  $\Delta\tau_{i,j}(t)$ , that is,

$$\tau_{i,j}(t+1) = \rho\tau_{i,j}(t) + \Delta\tau_{i,j}(t). \quad (5)$$

[19] The pheromone decay occurs to increase the influence of more recent pheromone additions on the actual pheromone intensity of an edge. On an algorithmic level, the decaying mechanism allows for more recent, and better, information to have a greater influence on the probability functions. The pheromone addition is the mechanism whereby the edges of good paths are reinforced with greater amounts of pheromone.

[20] In the main, the mechanism of pheromone addition is the sole attribute that differentiates ACO algorithms from each other. Typically, an ant adds pheromone only to the edges it has traversed, where the value of pheromone is inversely proportional to the "cost" of the solution (for minimization problems). In this way the edges of better solutions receive greater amounts of pheromone. The different formulations of  $\Delta\tau_{i,j}(t)$ , along with a list of each algorithm's

parameters, are given in Table 1. With reference to Table 1, a summary of  $\Delta\tau_{i,j}(t)$  for each algorithm is as follows:

[21] 1. For *AS* [*Dorigo et al.*, 1996], the most simple form of ACO, all ants add pheromone to the paths that they have selected. Exploitation is encouraged through the stronger reinforcement of edges associated with good solutions, and exploration is encouraged by all ants updating their paths.

[22] 2. *AS<sub>elite</sub>* [*Bullnheimer et al.*, 1997, 1999] incorporates both updating schemes from *AS* with the exception that the pheromone additions only reinforce the path of the global-best solution,  $S_{g-b}(t)$ , after every iteration. The pheromone addition is scaled up by the additional parameter  $\sigma$  to further encourage elitism, resulting in a more exploitative algorithm.

[23] 3. *AS<sub>rank</sub>* [*Bullnheimer et al.*, 1997, 1999] has a similar updating scheme to *AS<sub>elite</sub>* except that in addition to the elitist solution, only the path elements of the top  $\sigma - 1$  ranked solutions receive a pheromone addition, rather than the solutions from the entire colony. The pheromone additions from the ranked solutions are also scaled up by a factor ranging from 1 to  $\sigma - 1$ , depending on their rank (i.e., the  $k$ th ranked solution  $S_{(k)}(t)$  has a scaling factor of  $\sigma - k$ ). The use of the ranked ants, in addition to the elitist ants, provides a mechanism that encourages exploitation through elitism, but also encourages a degree of exploration through the reinforcement from the ranked ants.

[24] 4. For *MMAS*, [*Stützle and Hoos*, 2000] the  $S_{g-b}(t)$  solution is updated every  $T_{g-b}$  iterations and only the iteration best solution  $S_{(1)}(t)$  receives a pheromone addition every iteration. Moreover, *MMAS* contains two additional mechanisms: (1) pheromone bounding (PB), as a part of which the pheromone values are bounded by  $[\tau_{\min}(t), \tau_{\max}(t)]$  after all edges have been updated and (2) pheromone trail smoothing (PST), which is a global operation aimed at reducing the relative difference between all pheromone trails. Exploration is encouraged by the use of the pheromone bounds (i.e., a smaller  $P_{best}$  (higher  $\tau_{\min}(t)$ ) increases the probability of selection for all edges), as does a large  $\delta$  in the PST process, but this is balanced by *MMAS*'s purely elitist updating policy that encourages exploitation.

[25] Despite the generality of the above framework for representing ACO algorithms, it is important to note that there are variants of ACO that contain mechanisms outside

of its scope, such as ant colony system [Dorigo and Gambardella, 1997].

#### 4. ACO Behavioral Metrics for the Water Distribution System Problem

[26] When studying ACOAs, algorithm operators (e.g., elitism strategies) are often qualitatively described as *exploration* or *exploitation* encouraging [Colorni et al., 1996], implying a certain kind of impact on the searching behavior of an algorithm. However, as discussed in the introduction, quantitative descriptions of behavior are lacking as most studies focus on the objective space characteristics only. Consequently, it is difficult to gain insight as to the actual influence of an operator on an algorithm's searching behavior, largely owing to the lack of definition of the term *behavior*.

[27] Within this paper, the adopted definition of behavior is based on the following two characteristics: (1) an ACOA attempts to optimize an objective by iteratively generating populations of solutions; and (2) ACOAs use information gained from past solutions to influence the nature in which future solutions are generated (in an attempt to increase the probability of finding better solutions, and hence better information with which to continue the generation of improved solutions). It is the nature of ACOAs as systems utilizing experience to guide solution generation that enables them to be viewed as explorative processes, from which a searching behavior is manifest.

[28] The entire information of an ACOA's search is contained within the sequence of sets of the population's solutions generated within each iteration for the entire run time, symbolized by the sequence  $\{\Sigma(t)\}_{t=1}^{I_{\max}}$  where  $\Sigma(t) = \{S_k(t) : k = 1, \dots, m\}$  is the set of the population's solutions in iteration  $t$ ,  $S_k(t)$  is the  $k$ th solution at iteration  $t$ ,  $m$  is the number of solutions in the population and  $I_{\max}$  is the maximum number of iterations. It is the analysis of this sequence of sets that forms the basis of the behavioral analysis presented in this paper. The set of solutions  $\Sigma(t)$  describes the regions of the search space (variable space) that the ACOA is searching, how broad or how narrow the search is, and the quality of the solutions found. If the series of these solution sets are considered in time (iteration number), then the overall dynamic searching behavior of the ACOA can be observed. Therefore, the proposed metrics differ from those used in previous studies on evolutionary algorithms, as they focus on population dynamics and not on objective function values.

[29] In order to be able to interpret the information contained in these sequences, the proposed metrics characterize the following three behavioral attributes: (1) effectiveness, (2) convergence, and (3) percentage of search in the feasible and infeasible regions. The metrics fall into two categories, topological (attributes 1 and 2) and non-topological (attributes 1 and 3). This section describes the metrics in the case of single objective problems. Extensions to multiobjective problems exist but are outside the scope of this paper.

##### 4.1. Topology of the Search Space

[30] Fundamental to the assessment of the searching behavior of ACOAs is the ability to measure the distance of the spread between solutions in a population (e.g., whether

the solution space is being searched widely or whether there is convergence) and is a feature of two of the behavioral metrics used within this paper. A measure of distance for all elements within the set  $\mathcal{S}$  is equivalent to defining a metric  $d$  associated with  $\mathcal{S}$  that defines the distance between any two elements  $S, \tilde{S} \in \mathcal{S}$ . A metric is defined by the map  $\text{dist} : \mathcal{S} \times \mathcal{S} \rightarrow \mathbb{R}_+$ , and satisfies the following properties [Cohen, 2003]:

[31] 1.  $\text{dist}(S, \tilde{S}) = 0$  if and only if  $S = \tilde{S}$ , for all  $S, \tilde{S} \in \mathcal{S}$

[32] 2.  $\text{dist}(S, \tilde{S}) = \text{dist}(\tilde{S}, S)$  for all  $S, \tilde{S} \in \mathcal{S}$

[33] 3.  $\text{dist}(S, \tilde{S}) \leq \text{dist}(S, Z) + \text{dist}(Z, \tilde{S})$ , for all  $S, \tilde{S}, Z \in \mathcal{S}$ .

[34] For a given decision space  $\mathcal{S}$ , there are generally multiple valid distance measures (e.g., Euclidian,  $p$  norm or Hamming), where the choice of which measure to use depends on the needs of the user.

[35] As the WDSP is a combinatorial problem, a simple definition of distance is adopted based on that used by Boese et al. [1994] and Stützle and Hoos [2000] for the traveling salesperson problem (TSP). Within this definition, the distance between  $S$  and  $\tilde{S}$  is taken as the Hamming distance, which basically measures the number of positions at which the corresponding variables of two solutions are different. This is a lucid concept of distance as it indicates the number of decisions that would need to be changed in a solution to make it equal to another solution. Mathematically, the distance between  $S = [s_1 \dots s_n]$  and  $\tilde{S} = [\tilde{s}_1 \dots \tilde{s}_n]$ , by this definition, is described by

$$\text{dist}(S, \tilde{S}) = \sum_{i=1}^n I^C\{s_i, \tilde{s}_i\}, \quad (6)$$

where  $I^C\{a, b\}$  is a complementary indicator function, equal to 1 if  $a \neq b$  and 0 if  $a = b$ . For example, the solution [5 3 7 8] has a distance equal to two from the solution [5 2 7 6] because they differ in the second and the fourth variable.

##### 4.2. Searching Effectiveness Metrics

[36] An effective search is one where the algorithm is able to find optimal or near optimal solutions. In order to quantify this effectiveness, two metrics are proposed, one describing the closeness of the searching to the optimal or known optimal solution  $S^*$ , and the other describing the quality of the solutions generated in terms of their objective function values.

###### 4.2.1. Objective Function Based

[37] The quality of solutions generated in an iteration is given by the set of objective function values of the solutions found within that iteration, i.e.,  $\{f(S_1(t)), \dots, f(S_m(t))\}$ . For single objective optimization problems, the aim of the iteratively generated set of solutions is simply to find better solutions (as opposed to generating an entire population of higher quality solutions). Therefore, a justified metric of searching quality is the minimum value of the objective function found within each iteration, that is,

$$f_{\min}(t) = \min_{S \in \Sigma(t)} \{f(S)\}. \quad (7)$$

This measure is commonly used by researchers [Savic and Walters, 1997; Deb and Beyer, 2001; Hansen et al., 2003]. It should be noted that measures of effectiveness in the objective function space have also been defined and applied

for multiobjective problems [Tang et al., 2006; Kollat et al., 2008].

#### 4.2.2. Topologically Based

[38] Fundamental to ACOs is the generation of solutions that are increasingly close to the optimum. The closeness of an ACOA's searching to the global optimum  $S^*$  can be given as the distance from  $S^*$  to the closest point of the algorithm's searching region, that is, the distance from  $S^*$  to the closest solution within  $\Sigma(t)$ . This property, symbolized by  $\text{dist}_{\min}$ , is given as

$$\text{dist}_{\min} = \min_{S \in \Sigma(t)} \{\text{dist}(S, S^*)\} \quad (8)$$

The variation of  $\text{dist}_{\min}$  with iteration number illustrates the behavior of the algorithm as solutions approach the region that contains the optimum solution, and consequently provides an indication of the effectiveness of an algorithm's searching behavior. For many applications, the global optimum  $S^*$  is not known and so the known least cost solution can be used.

#### 4.3. Convergence Metrics

[39] The term convergence within an ACOA can be used with reference to the objective function space or to the decision variable space. For the first case, it means that the algorithm has reached a phase where objective function improvements are not likely. In the second case, an ACOA has converged when it has a high probability of continually regenerating the same solution. Clearly, convergence in the variable space implies convergence in the objective space.

[40] In this paper, convergence behavior is taken to describe how the spread of solutions evolves up until the point of convergence (assuming that this point has been reached).

[41] The population of solutions generated by an ACOA within an iteration is spread, in some manner, over the topology of the decision variable space. This spread of solutions gives an indication of how widely, or how tightly, the algorithm is searching (or to use the terminology of Colorni et al. [1996], whether the algorithm is *exploring* broadly through the search space or *exploiting* smaller regions of the search space). In order to quantify this *spread*, the mean of the distances between each of the solutions has been used within this research. This metric is referred to as the mean population searching distance  $\text{dist}_{\text{mean}}$ . Mathematically, this is given as the summation of the distances of each unique pair of solutions divided by the total number of pairs, and is expressed as

$$\text{dist}_{\text{mean}} = \frac{2}{m(m-1)} \sum_{k=1}^m \sum_{l=k+1}^m \text{dist}(S_k(t), S_l(t)), \quad (9)$$

where  $m(m-1)/2$  is the number of unique pairs that exist in a population of size  $m$  and  $S_k(t) \in \Sigma(t)$  is the  $k$ th solution generated in iteration  $t$ . The usefulness of  $\text{dist}_{\text{mean}}$  as a behavioral analysis measure is fully realized when considering its variation as the search progresses. For example, periods of high exploration (i.e., when solutions are spread more evenly throughout the search space) are seen as periods where  $\text{dist}_{\text{mean}}$  is large, the period during which the algorithm converges is characterized by a series of decreasing  $\text{dist}_{\text{mean}}$  values, and the algorithm has converged by iteration

$T$  if  $\text{dist}_{\text{mean}} = 0$  for all  $t \geq T$  (as this indicates that all solutions in  $\Sigma(t)$  are equal). As such,  $\text{dist}_{\text{mean}}$  provides a direct measure of an ACOA's convergence behavior.

#### 4.4. Feasible/Infeasible Region Searching Metric

[42] Many water resource optimization problems are in fact constrained optimization problems. EAs can directly take into account constraints bounding of individual decision variables, however engineering problems have usually additional constraints specifying the design or performance criteria. These are of the form

$$\mathbf{h}(S) \geq \mathbf{0}, \quad (10)$$

where  $\mathbf{h}$  is a vector that usually requires the resolution of nonlinear functions (typically evaluated using a simulation model). The region of feasible solutions is defined as the set of  $S \in \mathcal{S}$  that satisfies (10).

[43] As the optimum solution for constrained problems often lies on the boundary between the feasible and infeasible regions [Simpson and Goldberg, 1994], EAs that are able to search within both of these regions will generally perform better, as they are able to use more information about the area surrounding the optimum than those that are only able to search from within the feasible region [Coello Coello, 2002]. Consequently, a way to observe an algorithm's searching behavior is to consider the proportion of the search that an algorithm dedicates to each region and how this varies throughout the algorithm's total searching time.

[44] In this paper, the metric used to assess searching behavior with respect to feasible and infeasible regions is the percentage of feasible solutions generated within an iteration,  $F\%$ .

### 5. Case Studies

[45] Four different instances of the WDSP problem were optimized using the four different variants of ACO as considered, including ant system (AS), elitist ant system ( $AS_{\text{elite}}$ ), elitist-rank ant system ( $AS_{\text{rank}}$ ), and max-min ant system (MMAS). This enabled a detailed study on the influence of algorithm operators on resultant algorithm behavior, because each variant adopts different operators to manage the exploitation/exploration trade-off.

#### 5.1. WDSP Case Studies

[46] Problem characteristics, as well as the algorithm parameter settings, influence an algorithm's searching performance and behavior [Hansen et al., 2003; Tang et al., 2006; Vrugt and Robinson, 2007; Vrugt et al., 2009; Gibbs et al., 2011]. Therefore, four well-known WDSP instances with different properties are considered to test the applicability and benefit of the behavioral framework: the Two-Reservoir Problem (TRP<sub>8</sub>) [Simpson et al., 1994]; the New York Tunnels Problem (NYTP<sub>21</sub>) [Dandy et al., 1996]; the Hanoi Problem (HP<sub>34</sub>) [Savic and Walters, 1997]; and the Doubled New York Tunnels Problem (2-NYTP<sub>42</sub>) [Zecchin et al., 2005] (note that the subscript in the problem name refers to the number of decision variables).

[47] The TRP<sub>8</sub> involves a rehabilitation and extension design for a 14-pipe network fed by two reservoirs. Three pipes are to be potentially rehabilitated (involving a *do*

**Table 2.** Property of the Case Study Problems<sup>a</sup>

Problem	Size	Feasible Space	Epistasis	Saliency	Structure
TRP <sub>8</sub>	$3.981 \times 10^6$	✓✓✓	✓✓	✓	✓✓✓
NYTP <sub>21</sub>	$1.934 \times 10^{25}$	✓✓✓	✓✓	✓✓✓	✓✓
HP <sub>34</sub>	$2.865 \times 10^{26}$	✓	✓✓✓	✓✓✓	✓✓
2-NYTP <sub>42</sub>	$3.741 \times 10^{50}$	✓✓	✓✓	✓✓	✓✓

<sup>a</sup>A larger number of ticks indicates a larger degree of the specific characteristic.

*nothing* option, a cleaning option, or replacement with a pipe with one of six diameter options) and five pipes are to be designed (selection of a diameter from six options), creating a total solution space of  $3.981 \times 10^6$  designs. The NYTP<sub>21</sub> involves the design of a system upgrade for a 21 pipe network fed by a single reservoir. For each pipe, there are 16 design options (the *do nothing* option, or the selection of a parallel pipe with one of 15 diameter options) creating a solution space of  $1.934 \times 10^{25}$  designs. The HP<sub>34</sub> involves the design of a new 34-pipe network fed by a single reservoir. For each pipe there are six diameter options, creating a total search space of  $2.865 \times 10^{26}$  designs. The 2-NYTP<sub>42</sub>, is essentially a combination of two NYTP<sub>21</sub>, problems connected via the single reservoir. The search space for the 2-NYTP<sub>42</sub> has  $3.741 \times 10^{50}$  designs.

[48] As mentioned above, an algorithm's behavior for a certain problem instance is influenced by not only the algorithm's internal mechanisms, but also the search space properties. Important properties for constrained problems are [after Gibbs *et al.*, 2011]: problem size (the size of the search space); the relative size of the feasible space; variable epistasis (an indicator of the nonlinear interaction between decision variables); variable saliency (an indicator of the relative influence of decision variables on the objective); and problem structure (an indicator of how structured a problem is in terms of the number of local optima, and the size of the regions of attraction for these optima). In realistic problems, assessment of these properties is complicated by the size of the search space and the resulting difficulty in obtaining representative results, and by the presence of constraints. As the quantification of these properties is still largely an open question [Gibbs *et al.*, 2011], a qualitative description is given in Table 2. The justification for the rankings provided in Table 2 is given below.

[49] *Size of feasible space.* An estimate of the size of the feasible space was made by computing the number of feasible solutions from a random sample, leading to the ranking given in Table 2. The HP<sub>34</sub> is notoriously difficult in terms of finding the feasible region [Savic and Walters, 1997; Zecchin *et al.*, 2007], which was confirmed by the fact that no feasible solutions were generally found by random sampling.

[50] *Epistasis.* In WDSP problems, the objective function is composed of two terms: the pipe cost and the penalty cost for infeasible solutions. As the pipe cost is a linear function of the pipe cost per unit of length and the pipe length, the variables (diameter sizes) are separable and the cost of  $C(s_1 + s_2, s_1 + s_2) = C(s_1, s_2) + C(s_2, s_1)$ , where  $C()$  is the cost of a solution with two variables and  $s_1$  and  $s_2$  are two diameter sizes. However, the objective function contains also the penalty for infeasible solutions. This penalty is related to the diameter sizes by the hydraulic equations. If the hydraulic solution is infeasible, the objective function will no longer have linear properties, e.g.,  $S(s_1 + s_2, s_1 + s_2)$

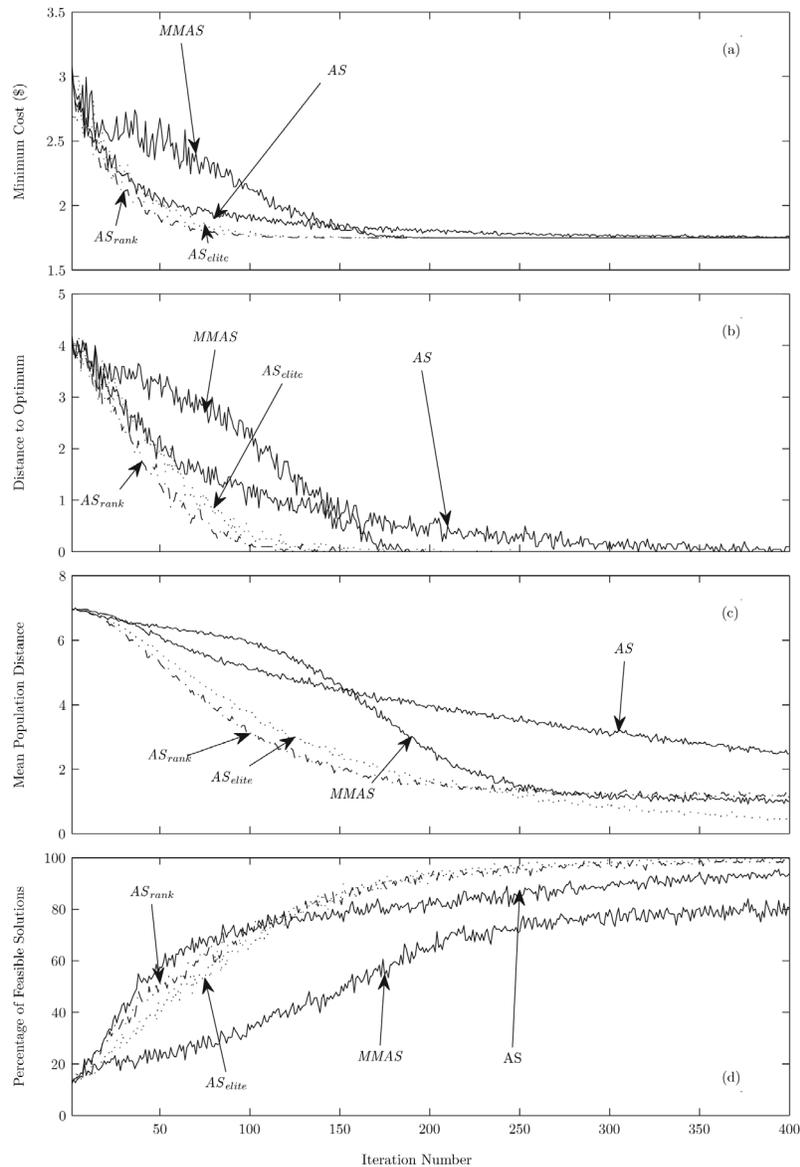
can be a feasible solution, while  $S(s_1, s_2)$  and/or  $S(s_2, s_1)$  can be infeasible with a much larger objective function value  $S()$ . Loops in the network configuration decrease the separability of the variables, meaning that there is a high coupling between the variables and their influence on the objective function for infeasible solutions. Epistasis is, therefore, related to the size of the feasible space and the network configuration. Consequently, as can be seen in Table 2, the HP<sub>34</sub> problem has high epistatic variable interaction because of its small feasible space and large number of loops, while, in comparison, the NYTP<sub>21</sub> is a low epistasis problem.

[51] *Variable saliency.* If only the pipe cost is considered in the objective function, the saliency is defined by the homogeneity of pipe lengths: if there are pipes that are much longer than others, they will have a larger influence on the total cost of the network and therefore a larger saliency. Hence, for feasible solutions, saliency depends only on pipe length. However, for infeasible solutions, it depends also on the network configuration (through the nonzero penalty cost). For example, for networks with only one reservoir and one feeder pipe (as in HP<sub>34</sub>), the saliency of that pipe will be greater than in the case of numerous feeder pipes (as in NYTP<sub>21</sub> and 2-NYTP<sub>42</sub>). For problems with multiple reservoirs (as in TRP<sub>8</sub>), the variable saliency is expected to be more homogeneous, as the alternate flow paths in the network mean that no single pipe will dominate hydraulic behavior. As feasibility has a large impact on the objective function value, saliency is strongly related to the hydraulic importance of the pipe: the wrong size of the only feeder pipe to the water system can compromise the network feasibility, regardless of the other pipe diameters, while in the case of more feeder pipes, this effect is mitigated.

[52] *Structure.* Given the linear dependence on the variables for feasible solutions, the smoothness of the search space is clearly related to the size of the feasible space and the distribution of the feasible solutions in the space. The infeasible space can contribute to the degree of isolation of the optima, and can therefore affect algorithm performance [Vassilev *et al.*, 2000]. Given this, HP<sub>34</sub> is considered to be the hardest instance among the WDSPs analyzed as, for many pipe variables, a slight change in one variable can make a feasible solution infeasible. In contrast, the TRP<sub>8</sub> is considered the problem with the most structure, as the hydraulic characteristics, i.e., network configuration, node demands, and diameters, allow a greater flexibility in the diameter setting.

## 5.2. Outline of Computational Experiments

[53] The behavioral metrics (7)–(10) from section 4 were used to analyze the behavior of the four ACO variants applied to each WDSP. The parameter settings used for each algorithm were taken from Zecchin *et al.* [2007]: the fundamental parameters  $\alpha$ ,  $\beta$ ,  $\rho$ ,  $\tau_0$  and  $m$  were obtained from the parameter heuristics developed by Zecchin *et al.* [2005], and the other parameters for the additional operators in  $AS_{elite}$ ,  $AS_{rank}$ , and  $MMAS$ , were determined from an extensive parameter sensitivity analysis. For brevity, they are not mentioned in their entirety here, but it should be noted that  $m = 25, 90, 170$  and  $80$  for the TRP<sub>8</sub>, NYTP<sub>21</sub>, 2-NYTP<sub>42</sub>, and the HP<sub>34</sub>, respectively, resulting in a total of  $m \times I_{max} = 10^4, 4.5 \times 10^4, 5.1 \times 10^5$  and  $1.2 \times 10^5$  hydraulic network simulations for each case study. As in Zecchin *et al.* [2007], all results were averaged over 20 runs, each



**Figure 1.** Behavioral metrics for  $AS$ ,  $AS_{elite}$ ,  $AS_{rank}$ , and  $MMAS$  applied to  $TRP_8$  problem: (a)  $f_{min}$ , (b)  $dist_{min}$ , (c)  $dist_{mean}$ , and (d)  $F_{\%}$ . Results are averaged over 20 runs.

executed with a different random seed, with the aim of obtaining statistically meaningful results. An analysis of the individual runs confirmed that the variation between metrics at each time point for different runs was small, indicating that the averages are a good indication of the expected behavior.

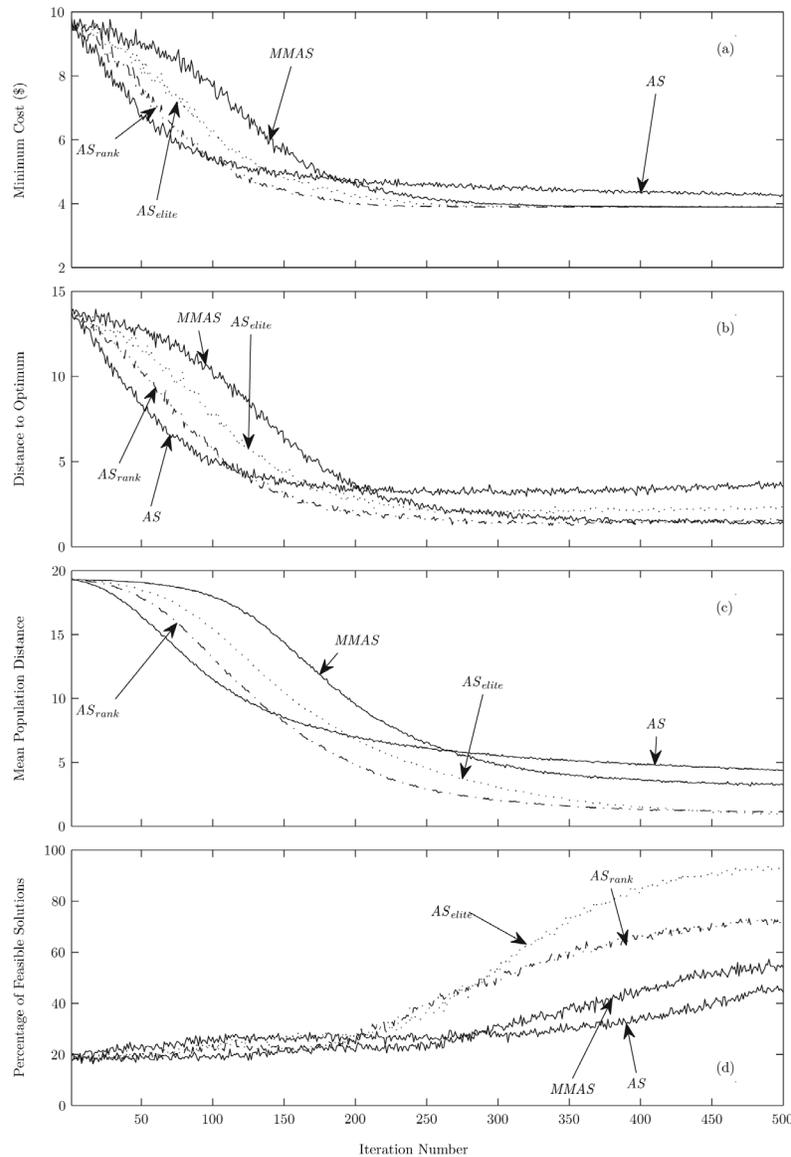
[54] Among the four behavioral metrics, only  $dist_{min}$  requires a priori knowledge of the optimal solution to be computed. From a complete enumeration of the  $TRP_8$ , *Simpson and Goldberg* [1994] found that there were two different optimum solutions, therefore, in this analysis, the minimum distance was taken from the closest optimum. For all other case studies, the optimum is not known, as complete enumeration is not possible. As such, the known lowest cost solutions are used in place of  $S^*$ . Details of these solutions are given by *Zecchin et al.* [2005] for the  $NYTP_{21}$  and the  $2-NYTP_{42}$ , and *Zecchin et al.* [2006] for the  $HP_{34}$ .

For ease of discussion, it is assumed that these known optimum solutions lie in a region close to the actual optimum.

## 6. Results and Discussion

[55] The results for the case studies are presented in Figures 1, 2, 3 and 4 for the  $TRP_8$ , the  $NYTP_{21}$ , the  $2-NYTP_{42}$  and the  $HP_{34}$ , respectively, where the following are given for each the iteration values for the metrics: the minimum objective value function found,  $f_{min}$  (Figures 1a–4a); the minimum distance from the optimum,  $dist_{min}$  (Figures 1b–4b); the mean population distance,  $dist_{mean}$  (Figures 1c–4c); and the percentage of feasible solutions in the population,  $F_{\%}$  (Figures 1d–4d).

[56] The results discussed below demonstrate the descriptive power of the metrics, and their ability to provide insight into the workings of the algorithms and their interactions with different types of water distribution system problems. Section 6.1 highlights common behavioral trends observed



**Figure 2.** Behavioral metrics for *AS*, *AS<sub>elite</sub>*, *AS<sub>rank</sub>*, and *MMAS* applied to NYTP<sub>21</sub> problem: (a)  $f_{\min}$ , (b)  $\text{dist}_{\min}$ , (c)  $\text{dist}_{\text{mean}}$ , and (d)  $F_{\%}$ . Results are averaged over 20 runs.

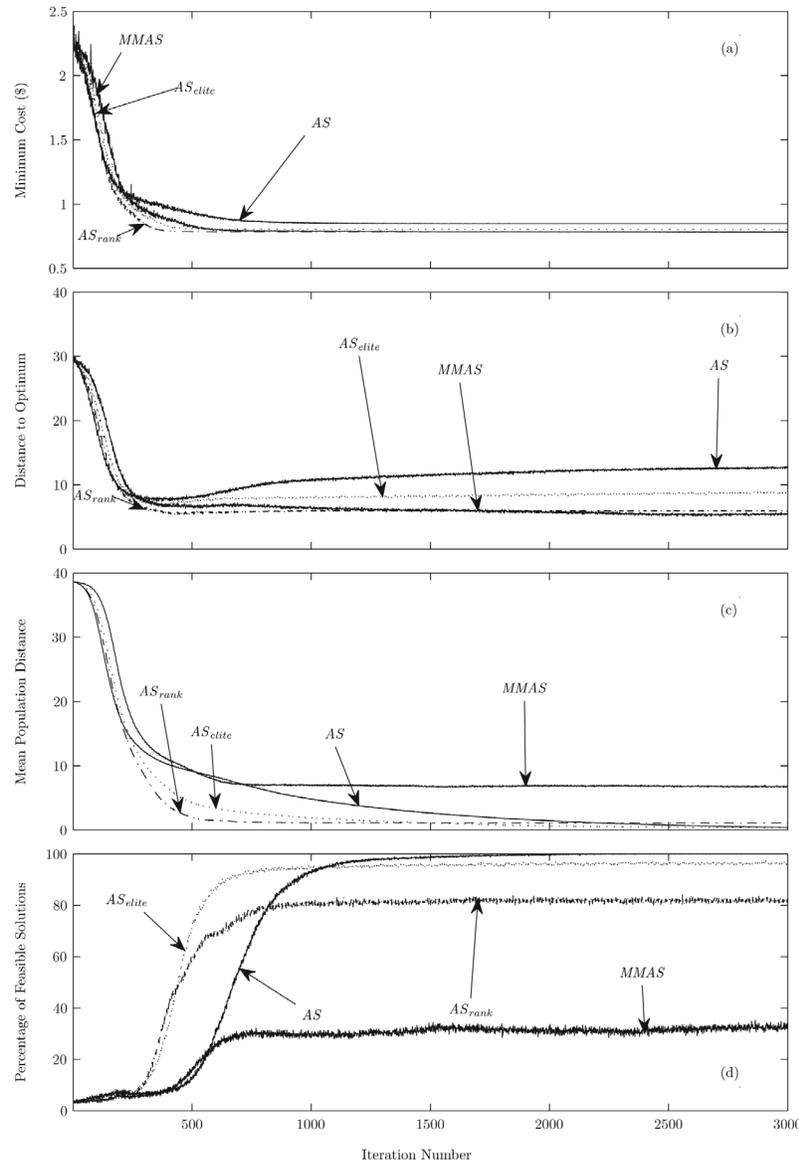
from the metrics, and section 6.2 focuses on how the different exploitative and explorative mechanisms of the algorithms can be understood by analyzing the metrics.

### 6.1. General Behavior

[57] Considering Figures 1c–4c, the convergence behavior for all of the ACO variants tended to fall into three distinct phases: initially the algorithms started with a broad search throughout the search space (i.e., high  $\text{dist}_{\text{mean}}$  values); this was followed by a period of fast convergence for all case studies except *AS* in TRP<sub>8</sub>, where the majority of the algorithms' convergence occurred (i.e., the main phase of reduction in  $\text{dist}_{\text{mean}}$ ); and the final phase, which was characterized by a period of slower convergence, during which the reduction in  $\text{dist}_{\text{mean}}$  tended to plateau, meaning that each algorithm tended to focus its search on a smaller region of the search space. The degree of prominence of the

presence of each of these phases is dependent on both algorithm and problem type.

[58] These three phases of searching can also be observed with the other metrics. Considering the effectiveness of the search, as demonstrated through Figures 1a–4a and 1b–4b, for all cases, the broad searching within the initial phase is coupled with the generation of low-quality solutions (high  $f_{\min}$  and high  $\text{dist}_{\min}$ ). However, it can be seen that the fast convergence of the second phase was generally indicative of effective searching (except for *AS* applied to the HP<sub>34</sub>), as this convergence corresponded to a decreased distance from the optimum region for most instances (as seen by the decreasing series of  $\text{dist}_{\min}$ ), implying convergence to the near-optimal regions of the search space. As expected, the descent into regions closer to the optimum was accompanied by an increase in solution quality (as seen by the decreasing series of  $f_{\min}$  in Figures 1a–4a), because for the WDSP problem, local optimal solutions generally contain a subset

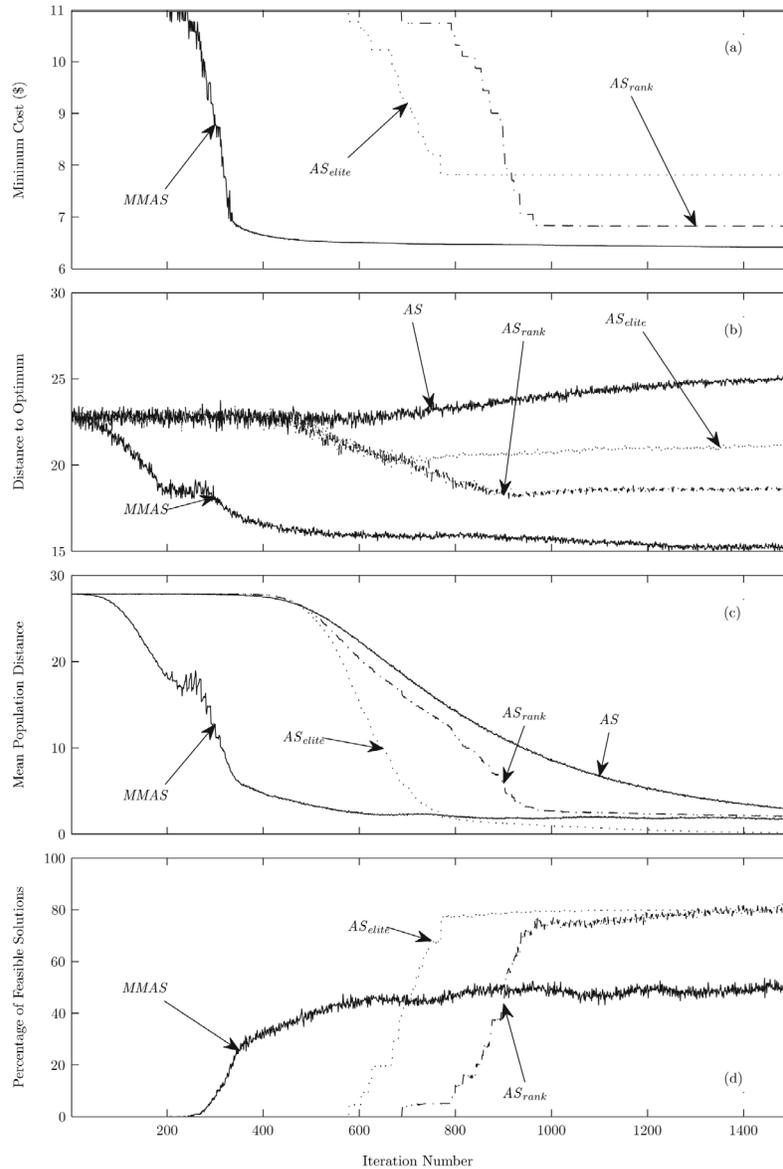


**Figure 3.** Behavioral metrics for  $AS$ ,  $AS_{elite}$ ,  $AS_{rank}$ , and  $MMAS$  applied to 2-NYTP<sub>42</sub> problem: (a)  $f_{min}$ , (b)  $dist_{min}$ , (c)  $dist_{mean}$ , and (d)  $F_{\%}$ . Results are averaged over 20 runs.

of the globally optimal solution. It should be noted that ACOAs depend on this correlation for successful searching behavior [Stützle and Hoos, 2000]. In the third phase, the algorithms tended to all behave differently, with some variants deviating on some problem types ( $AS$  and  $AS_{elite}$  applied to the larger three case studies) and others descending closer to the optimum. However, for all algorithms, the rate of change of  $dist_{min}$  in the third phase was much reduced from that exhibited during the earlier phases. The same behavior can be seen in the convergence metric,  $dist_{mean}$ .

[59] For all algorithms, the percentage of the search spent in the feasible region,  $F_{\%}$ , can also be considered to have three distinct phases. However, the transition point of these phases tended to lag that of the other metrics for the larger case studies. Within its initial phase,  $F_{\%}$  tended to start very low (0% for the HP<sub>34</sub>, and less than 20% for the other case studies). For the algorithms applied to the three larger case studies (NYTP<sub>21</sub>, HP<sub>34</sub>, and 2-NYTP<sub>42</sub>),  $F_{\%}$  did not increase

dramatically (i.e., the second phase for  $F_{\%}$ ) until the point at which the algorithms had concluded their rapid convergence phase (see  $dist_{mean}$  in Figures 2c–4c). In the final phase of  $F_{\%}$ , the searching intensified in the feasible region, tending to reach an equilibrium ratio of feasible to infeasible solutions. The fact that  $F_{\%}$  increased dramatically only after the rapid convergence phase has the following interesting implication: the algorithms were able to find the near-optimal region based on the few feasible solutions they initially found, and upon finding the feasible region, the algorithms converged, and increased their searching in the feasible region around the optimal solution. For the two largest case studies (HP<sub>3</sub>, and 2-NYTP<sub>42</sub>),  $MMAS$ , and to a lesser extent  $AS_{rank}$ , kept a reasonable percentage of their search in the infeasible region. Due to the low value of  $dist_{mean}$ , it can be deduced that these algorithms were searching close to the boundaries between the feasible and infeasible regions. As shown by  $dist_{min}$ , the effectiveness of this searching resulted



**Figure 4.** Behavioral metrics for  $AS$ ,  $AS_{elite}$ ,  $AS_{rank}$ , and  $MMAS$  applied to  $HP_{34}$ , problem: (a)  $f_{min}$ , (b)  $dist_{min}$ , (c)  $dist_{mean}$ , and (d)  $F_{\%}$ . Results are averaged over 20 runs.

in these algorithms descending closer to the known optimum than the other algorithms.

[60] In comparing the properties of the problems from Table 2 with the behavioral measures in Figures 1–4, some common observations can be made. Most notably, as the problem difficulty increased (greater problem size, smaller feasible space and less structure), so did the algorithms' time spent in the first broad searching convergence phase (sustained high  $dist_{mean}$ ,  $dist_{min}$  and  $f_{min}$ ). This is particularly clear for  $AS_{rank}$  and  $AS_{elite}$  applied to the  $HP_{34}$ . This observation of the behavioral measures can be understood to result from the increased searching time required by the algorithms to find solutions of a quality that is sufficiently high to cause the search to converge.

[61] Also, for the problems of increased difficulty, the algorithms' effectiveness decreased. The metric  $f_{min}$  shows that only for the  $TRP_8$  problem did all the algorithms reach the optimal solution (Figure 1a), while, for the other case

studies, they reached different average results. This is particularly clear for  $HP_{34}$  (Figure 4), where the  $AS$  results are not plotted for  $f_{min}$  and  $F_{\%}$ , as the algorithm was unable to locate feasible solutions for any of the runs. Similarly, the  $dist_{min}$  metric gives some insight into the influence of the increased problem size and the contemporaneous decrease in problem structure for the WDSP instances. For example,  $AS$  diverged slightly for  $NYTP_{21}$  and markedly for  $2-NYTP_{42}$  and  $HP_{34}$ ;  $AS_{elite}$  diverged slightly only for the larger two problems. However, the solution quality for these algorithms continued to increase (except  $AS$  applied to  $HP_{34}$ ).

[62] The implications of the behavior outlined in the preceding paragraph, coupled with the continued convergence shown by the  $dist_{mean}$  metric, are that these algorithms were converging to suboptimal solutions. A hypothesis based on these observations is outlined as follows. There exists a big valley structure in the fitness landscape (which is the space formed by mapping all the possible values of the objective

function in (3)), as demonstrated by the fact that, during the rapid descent phase, the behavior of  $\text{dist}_{\min}$  was well correlated with that of  $f_{\min}$ . The ACO algorithms were able to effectively converge to good regions of the solution space during this phase, as displayed by decreasing  $\text{dist}_{\text{mean}}$  being matched by a decreasing series of  $\text{dist}_{\min}$ . However, the landscape was observed to possess a much more complicated microstructure in the near-optimal regions, as demonstrated by  $\text{dist}_{\min}$ , indicating a deviation from the optimum (for some algorithms) but  $f_{\min}$  continuing to decrease. Some algorithms were less successful within this region, as observed by the continued convergence where  $\text{dist}_{\text{mean}}$  was not matched by a decreasing series of  $\text{dist}_{\min}$ . Therefore, the behavioral metrics can give insight into the problem characteristics, although in a qualitative way. In particular, one of the advantages of the proposed metrics is that they can relate the peculiarities of the problem to those of the algorithm. As the problem difficulty is also a function of the algorithm used, the metrics can be usefully applied to improve the algorithm's search.

## 6.2. Exploitative and Explorative Mechanisms and Algorithm Behavior

[63] The results obtained also illustrate the usefulness of the proposed behavioral metrics in highlighting the differences in the way the investigated ACO variants manage the exploitation/exploration trade-off through operators encouraging elitism (exploitation) or population diversity (exploration). For example, the results obtained highlight the value of the proposed metrics in terms of gaining an insight into the reasons behind the relatively poor performance of *AS*. While  $f_{\min}$  is able to indicate that *AS* performs poorly, only the proposed metric of convergence,  $\text{dist}_{\text{mean}}$ , provides an insight into why this might be the case. As can be seen from Figures 1–4, the  $\text{dist}_{\text{mean}}$  metric for *AS* is typically larger than that for the other algorithms within the final phase of the search, indicating that the algorithm was unable to exploit good information to achieve a tighter and more focused search within the near optimal region, which was a characteristic of the other algorithms. Therefore, the additional exploitative mechanisms of  $AS_{\text{elite}}$ ,  $AS_{\text{rank}}$ , and *MMAS* improved their performance for all case studies, particularly the  $HP_{34}$ , where exploitation appeared to play a crucial role in locating the feasible region.

[64] The results obtained indicate that the effectiveness metrics,  $f_{\min}$  and  $\text{dist}_{\min}$ , are able to show the superiority of the quasi-elitist strategy employed by  $AS_{\text{rank}}$  compared to the elitist strategy employed by  $AS_{\text{elite}}$ , as  $AS_{\text{rank}}$  was, on average, able to find solutions closer to the optimum than  $AS_{\text{elite}}$  for every case study considered (Figures 2a–4a and 2b–4b). In considering the convergence behavior of these algorithms, it is interesting to note that, although  $AS_{\text{rank}}$  tended to converge faster than  $AS_{\text{elite}}$  within the second search phase,  $AS_{\text{elite}}$  converged to a smaller region in the search space than  $AS_{\text{rank}}$  in the final phase.

[65] On an operator level, the difference between  $AS_{\text{elite}}$  and  $AS_{\text{rank}}$  is that  $AS_{\text{rank}}$  reinforces information of a number of the top unique solutions found within an iteration, whereas  $AS_{\text{elite}}$  reinforces information from all solutions, in addition to that from the elite solution. The quasi-elitist strategy employed by  $AS_{\text{rank}}$  was observed to exploit good information from the range of top solutions in the early stages of the search, while allowing for sufficient exploration in the later

stages of the search when it had converged to a near optimal region. This behavior can be observed for two of the larger problems in Figures 2c and 3c, where  $AS_{\text{rank}}$  has a smaller  $\text{dist}_{\text{mean}}$ , also associated with a smaller  $\text{dist}_{\min}$  (plot (b)), than  $AS_{\text{elite}}$  for the first part of the evolution, and has a larger  $\text{dist}_{\text{mean}}$  toward the end. In contrast, the strategy employed by  $AS_{\text{elite}}$  tended to slow convergence in the initial stages (due to the reinforcing of information from all solutions), and resulted in too much of an emphasis on exploitation in the later stages (due to the elitism), which led to the divergence of the search away from the optimum region for some of the case studies. This is clearly shown in Figure 4c after the 600th iteration. Note also that, in this case study, the initial phase of smaller  $\text{dist}_{\text{mean}}$  for  $AS_{\text{rank}}$  is absent. This is likely caused by the difficulty in finding feasible solutions. It is clear from this discussion that the topological metrics have enabled a more detailed characterization of the effects of the different algorithm operators than would otherwise be possible.

[66] The two metrics of effectiveness,  $f_{\min}$  and  $\text{dist}_{\min}$ , show that *MMAS* was able to find equal or better solutions for every case study. The  $\text{dist}_{\text{mean}}$  and  $F\%$  metrics highlight that *MMAS* is a highly explorative algorithm, but still maintains the ability to exploit the good information it finds. The explorative nature of *MMAS* is evidenced by the longer exploration phase in the initial part of the search (for all case studies except  $HP_{34}$ ), as demonstrated by the larger  $\text{dist}_{\text{mean}}$  in Figures 1, 2 and 3 and the broader exploration in the final convergence phase. The theoretical proof of the longer exploration phase of *MMAS* is given in Appendix A.

[67] *MMAS*'s ability to effectively exploit good information is evident from  $\text{dist}_{\min}$ , as despite its slower descent to the optimum region, it was able to find solutions closer to the optimum than all other algorithms, for all case studies but  $TRP_8$ , where  $AS_{\text{elite}}$  and  $AS_{\text{rank}}$  also reached the optimal solution. *MMAS* also maintained a relatively high percentage of its search within the infeasible region (Figures 1, 3 and 4). This, combined with the fact that it maintained a confined exploration in the latter stages, demonstrates that *MMAS* was searching closely on the boundary between the feasible and infeasible regions, which is where the optimum lies for the WDSP [Simpson et al., 1994]. As evidenced from the results obtained, this ability to maintain a relatively compact exploration (through the exploration encouraging pheromone bounding mechanism), combined with an elitist mechanism to guide the search (through the elitist update strategy), provides an extremely effective overall strategy.

[68] The superiority of *MMAS*'s performance for the notoriously difficult  $HP_{34}$  is worth some further analysis. All other algorithms struggled to find the feasible region (if at all), and upon finding this region, they tended to converge prematurely to some distance from the optimal region (as demonstrated by the plateauing of  $\text{dist}_{\min}$  for  $AS_{\text{elite}}$  and  $AS_{\text{rank}}$  in Figure 4b), which is a common issue for highly constrained problems [Coello Coello, 2002]. In contrast, *MMAS* was able to effectively explore through the infeasible region to find the feasible region, and then effectively explore within the feasible region and avoid premature convergence. The reason behind this can be explained by *MMAS*'s pheromone bounding mechanism, which provides a continual encouragement for mild exploration, and inhibits dominating exploitative forces.

[69] A general conclusion from this is that exploitation is important for finding the feasible region, however, once the

feasible region has been found, exploitation must be balanced with mild exploration to prevent premature convergence.

## 7. Conclusions

[70] The sheer size and complexity of water resources optimization problems has led to the extensive use of evolutionary algorithms within the water resources research community. The comparative analysis of different EA variants has typically been limited to considering the final performance statistics, consequently ignoring the algorithms' searching behavior. In this paper, metrics for comparing the searching behavior of ACOs applied to the water distribution design optimization problem have been presented. ACOA searching behavior was quantified in terms of population dynamics and, in particular, (1) the effectiveness of the search to locate the optimal regions and improve on solution quality, (2) convergence behavior, and (3) searching behavior with respect to the percentage of the search spent in the feasible and infeasible regions of the solution space. To quantify the effectiveness of the search, two metrics have been used. These described the quality of the solutions generated in terms of the objective function and the topological closeness of the search to the known optimal solution. To consider the convergence behavior, a metric was used that considered the topological spread of solutions in the solution space. To relate the search to the regions of feasible and infeasible solutions, the relative percentage of the solutions found in either region was considered.

[71] The results of the four ACO variants applied to four different WDSP instances indicate that the use of these metrics serves to provide greater insight into the operational behavior of the algorithms than has previously been achieved by only considering the final performance statistics. In particular, the metrics have been able to identify the different stages in an algorithm's search, and the roles of exploration-exploitation in these stages. An interesting general insight provided by the metrics was that the most effective algorithms: (1) contained elitist operators that facilitated the identification of the feasible region, resulting in convergence to near optimal regions relatively early on in the search; and (2) contained mechanisms that ensured that these elitist operators did not result in premature convergence, but facilitate a focused exploration later on in the search in the near-optimal region.

[72] The proposed behavioral metrics also have the potential for facilitating a deeper understanding of the behavior of other population based EAs (e.g., genetic algorithms, particle swarm optimization, and differential evolution) applied to a broader class of water resources problems, and indeed, optimization problems generally, as the only properties the metrics require are (1) an algorithm that iteratively generates populations of solutions; (2) an objective function; (3) a defined topology within the variable space of the optimization problem; and (4) a feasible region within the variable space.

## Appendix A: Proof of Residual Exploration for MMAS

[73] The prolonged residual exploration of MMAS can be explained by considering the influence of the pheromone bounding on the decision point probability functions. For the MMAS algorithm, under some mild assumptions, the

probability of selecting the global best path  $S_{g-b}(t)$  as  $t \rightarrow \infty$  is  $P_{best}$  [Stützle and Hoos, 2000]. Given the multigraph structure of the WDSP, the probability of selecting  $(i, j) \in S_{g-b}(t)$  at decision point  $i$  is  $\sqrt[NO_i]{P_{best}}$ . Within the MMAS formulation, as  $t \rightarrow \infty$ ,  $\tau_{i,j}(t) \rightarrow \tau_{min}(t)$  for all  $(i, j) \notin S_{g-b}(t)$ . Consequently, the remaining probability is evenly distributed among these  $NO_i - 1$  edges and the resulting probability of selecting  $(i, j) \notin S_{g-b}(t)$  is

$$\frac{1 - \sqrt[NO_i]{P_{best}}}{NO_i - 1},$$

Expressing the sample variance of the probability weights,  $\sigma_{p_i}^2(t)$ , using these probability values, the asymptotic form of  $\sigma_{p_i}^2(t)$  for MMAS, can be expressed as

$$\lim_{t \rightarrow \infty} \sigma_{p_i}^2(t) = \frac{1}{NO_i} \left( \frac{NO_i \sqrt[NO_i]{P_{best}} - 1}{NO_i - 1} \right)^2. \quad (A1)$$

Assuming homogeneity in the probability distributions and  $NO_i = NO_{avg}$  for  $i = 1, \dots, n$ , an estimate of the limiting mean colony distance can be derived by substituting (A1) into the expected value of the mean population searching distance,  $E[\text{dist}_{mean}(t)]$ .

[74] To express  $E[\text{dist}_{mean}(t)]$  in term of the variance of the probability weights  $\sigma_{p_i}^2(t)$ , the mean population distance is rewritten by substituting equation (6) into (9):

$$\text{dist}_{mean} = \frac{2}{m(m-1)} \sum_{k=1}^m \sum_{l=k+1}^m \sum_{i=1}^n I\{s_{k,i}(t), s_{l,i}(t)\}, \quad (A2)$$

where  $s_{k,i}(t)$  is the selection made at decision point  $i$  by ant  $k$  in iteration  $t$ . The quantity  $\text{dist}_{mean}$  can be viewed as a random variable as the solutions  $S_k(t)$  are random vectors of stochastically generated decisions  $s_{k,i}(t)$ ,  $i = 1, \dots, n$  by each ant. For all algorithms with no local procedures that alter the pheromone levels, for each  $i$ , the  $s_{k,i}$ ,  $k = 1, \dots, m$  are independent identically distributed with the distribution

$$\Pr\{s_{k,i}(t) = s\} = \begin{cases} p_{i,j}(t) & \text{for } s = j \in \Omega_i \\ 0 & \text{otherwise,} \end{cases}$$

where the subsets  $\Omega_i$  consist of  $NO_i$  possible values for the decision variable  $s_{k,i}(t)$ .

[75] The function of the random variables  $I\{s_{k,i}(t), s_{l,i}(t)\}$  is also a random variable but with state-space  $\{0, 1\}$ . To determine the distribution of  $I\{s_{k,i}(t), s_{l,i}(t)\}$ , we first consider  $\Pr\{I\{s_{k,i}(t), s_{l,i}(t)\} = 0\}$ . Now, the event  $I\{s_{k,i}(t), s_{l,i}(t)\} = 0$  is equivalent to the event  $s_{k,i}(t) = s_{l,i}(t)$ . Considering all the values that  $s_{k,i}(t)$  and  $s_{l,i}(t)$  can take, it is seen that the two events are also equivalent

$$\Pr\{s_{k,i}(t) = s_{l,i}(t)\} = \bigcup_{j=1}^{NO_i} \{s_{k,i}(t) = j\} \cap \{s_{l,i}(t) = j\},$$

and therefore

$$\Pr\{I\{s_{k,i}(t), s_{l,i}(t)\} = 0\} = \Pr\left\{\bigcup_{j=1}^{NO_i} \{s_{k,i}(t) = j\} \cap \{s_{l,i}(t) = j\}\right\}.$$

The events  $\{s_{k,i}(t) = j\} \cap \{s_{l,i}(t) = j\}$  for  $j = 1, \dots, NO_i$  are disjoint, therefore, applying the law of total probability gives

$$\Pr\{I\{s_{k,i}(t), s_{l,i}(t)\} = 0\} = \sum_{j=1}^{NO_i} \Pr\{\{s_{k,i}(t) = j\} \cap \{s_{l,i}(t) = j\}\}.$$

The events  $\{s_{k,i}(t) = j\}$  and  $\{s_{l,i}(t) = j\}$  are independent, each with probability  $p_{i,j}(t)$  and therefore

$$\Pr\{I\{s_{k,i}(t), s_{l,i}(t)\} = 0\} = \sum_{j=1}^{NO_i} p_{i,j}^2(t).$$

The distribution of  $I\{s_{k,i}(t), s_{l,i}(t)\}$  is then given by

$$\Pr\{I\{s_{k,i}(t), s_{l,i}(t)\} = x\} = \begin{cases} 1 - \sum_{j=1}^{NO_i} p_{i,j}^2(t) & \text{for } x = 1 \\ \sum_{j=1}^{NO_i} p_{i,j}^2(t) & \text{for } x = 0 \\ 0 & \text{otherwise.} \end{cases}$$

Taking expectations of (A2) and utilizing the linear nature of the expectation function we get

$$\begin{aligned} E[\text{dist}_{mean}] &= \frac{2}{m(m-1)} \sum_{k=1}^m \sum_{l=k+1}^m \sum_{i=1}^n E[I\{s_{k,i}(t), s_{l,i}(t)\}] \\ &= \frac{2}{m(m-1)} \sum_{k=1}^m \sum_{l=k+1}^m \sum_{i=1}^n \left(1 - \sum_{j=1}^{NO_i} p_{i,j}^2(t)\right) \\ &= \sum_{i=1}^n \left(1 - \sum_{j=1}^{NO_i} p_{i,j}^2(t)\right). \end{aligned} \quad (\text{A3})$$

Equation (A3) states that the expected mean distance between the colony's solutions is equal to the summation over all decision points of the probability that two randomly generated decisions select different options. The probability  $p_{i,j}^2(t)$  is related to the sample variance of the probability weights  $\sigma_{p,i}^2(t)$  by

$$\sigma_{p,i}^2(t) = \frac{1}{NO_i - 1} \left( \sum_{j=1}^{NO_i} p_{i,j}^2(t) - \frac{1}{NO_i} \right). \quad (\text{A4})$$

[76] The values of  $\sigma_{p,i}(t)$  are bounded below by 0, when all probability weights are the same, and above by  $1/\sqrt{NO_i}$ , when all probability weights are zero except for one edge which has a probability weight of 1. Combining (A3) and (A4) to remove the summation term the desired expression that relates the expected average distance between a colony's solutions to the variance of the probability weights is achieved:

$$E[\text{dist}_{mean}(t)] = \sum_{i=1}^n (NO_i - 1) \left( \frac{1}{NO_i} - \sigma_{p,i}^2(t) \right). \quad (\text{A5})$$

If it can be assumed that the number of edges is the same for all decision points, i.e.,  $NO_i = NO_{avg}$ ,  $i = 1, \dots, n$  (this is generally true for WDSPs), then  $E[\text{dist}_{mean}(t)]$  can be approximated as a function of the mean of the probability variance,  $\bar{\sigma}_p^2(t)$ . That is,

$$E[\text{dist}_{mean}(t)] \approx n(NO_{avg} - 1) \left( \frac{1}{NO_{avg}} - \bar{\sigma}_p^2(t) \right). \quad (\text{A6})$$

where  $n$  is the number of decision points and  $NO_{avg}$  is the average number of options per decision point. Equation (A6) can be verified by noticing that (1)  $E[\text{dist}_{mean}(t)]$  is at a maximum when  $\bar{\sigma}_p^2(t) = 0$  (intuitively, it would be expected that the search is at its broadest when all options have equal probability of being selected, which occurs when the standard deviation is zero); and (2)  $E[\text{dist}_{mean}(t)] = 0$  when  $\bar{\sigma}_p^2(t)$  is at its theoretical upper limit of  $1/NO_{avg}$ , which occurs only when one option per decision point has a probability of 1 of being selected (clearly, for this situation it would be expected that  $E[\text{dist}_{mean}(t)] = 0$ , as only one solution would be continually selected). An interesting point about Equation (A6) is that  $E[\text{dist}_{mean}(t)]$  is independent of the colony size  $m$ , and that it is only dependent on the search space properties  $n$  and  $NO_{avg}$  and the probability distributions through their sample variance of the probability weightings. However, clearly, for larger  $m$ , there would be a greater density of solutions distributed within the ball of radius  $E[\text{dist}_{mean}(t)]$ .

[77] Therefore by substituting (A1) into the expected value of the mean population searching distance (A6) the following result is obtained:

$$\lim_{t \rightarrow \infty} E[\text{dist}_{mean}(t)] = \left(1 - \sqrt[n]{P_{best}}\right) \sum_{i=1}^n \frac{NO_i(1 + \sqrt[n]{P_{best}}) - 2}{NO_i - 1}. \quad (\text{A7})$$

Equation (A7) effectively shows that *MMAS* does not converge, in the sense that  $E[\text{dist}_{mean}(t)] \rightarrow 0$  as  $t \rightarrow \infty$ , therefore, there will always be some residual exploration even as  $t \rightarrow \infty$ . It is important to note that this result is not in conflict with that of *Gutjahr* [2002] (who proved the convergence of an algorithm similar to *MMAS*), as this paper assumed a lower bound of pheromone that decayed to zero as  $t \rightarrow \infty$ . In this situation,  $P_{best}$  would be a function of the lower bound and would tend to unity as  $t \rightarrow \infty$ , which would clearly satisfy the convergence requirement that  $\sigma_{p,i}^2(t) \rightarrow 1/NO_i$  and  $E[\text{dist}_{mean}(t)] \rightarrow 0$  as  $t \rightarrow \infty$ . Preliminary investigations have shown that estimates of the theoretical limits from (A1) and (A7) are close to the actual observed values at the final iteration  $I_{max}$ , with the differences being attributed to the variation in the options visibility values of the available options.

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