Mathematical Modeling and Convergence Analysis of Trail Formation

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Abstract

An ant deposits pheromone along the path that it travels and is more likely to choose a path with a higher concentration of pheromone. The sensing and dropping of pheromone makes it easy to understand the trail forming behavior of ants. The reinforcement tendency of pheromone following behavior ensures selection of the shortest path from a set of paths. The reinforcement tendency of pheromone following behavior also ensures a biased selection of the initially followed paths over a path, which is shorter but discovered through chance at a later point in time. Under what conditions and limits can this *initial bias be reversed*? In this paper, we answer this question based on a theoretical analysis of the trail forming behavior of ants. We believe our results to contribute to the overall area of understanding how to build scalable systems that evolve to solve complex problems (e.g. point covering or the traveling salesman problem) without the necessity of central command-and-control.

Introduction

Ants drop pheromone as they travel and can also sense the concentration of pheromone that may already be present. Given alternative paths, an ant tends to choose the one with a higher concentration of pheromone. A path that happened to be more heavily traveled by the preceding ants has a higher concentration of pheromone and tends to be chosen by the succeeding ones (Deneubourgh *et al.* 1990; Dorigo & Stützle 2004). The sensing of pheromone to choose the travel direction and the dropping of pheromone makes it easy to understand the trail forming behavior of ants.

The reinforcement tendency of pheromone following behavior suggests that the shortest path amongst a set of paths would attract more ants to it further increasing the pheromone concentration (ignoring the evaporation of pheromone). To make this more explicit, consider the situation where ants continuously come out of the nest, choose from one of two paths leading to a food source, collect the food and return using one of the two available paths. Under equal priors, half of the ants coming out of the nest would

choose one path and the other half would choose the other path. Ants traveling along the shorter path would reach the food source quicker and will detect a pheromone trail only on the shorter path for the return journey. That is so because, ants that randomly chose the longer path would not have reached the food source and thus, near the food source, there is no pheromone concentration along the longer path. Therefore the returning ants will choose the shorter path further increasing the pheromone concentration along the shorter path. After a while the ants that took the longer path reach the food source. For their return, they choose the shorter path since it has a higher concentration of pheromone. Similar actions over time ensure that all the ants end up using the shorter path.

The selection of the shortest path is remarkable considering that the optimization is achieved without explicit communication about the merits of one path over another (indeed, an ant having chosen one path has no idea of the length of the other path) or a centralized command-and-control. A more intriguing question however is: can a shorter path discovered at a later point in time become the popular path? The challenge to answering that in the affirmative is that the reinforcement tendency of pheromone following behavior would ensure a biased selection of the initially followed paths over a path, which is shorter though discovered by chance at a later point in time. However, the same argument as above i.e. ants can travel and return on the shorter path more quickly implies that under certain conditions and limits (on the amount of pheromone concentration on the longer paths) it may still be possible to reinforce the shorter path. Under what conditions and limits on the pheromone concentration on the longer paths can this *initial bias be reversed*? In this paper, we provide a theoretical analysis that sheds light on when the *initial bias reversal* can happen.

We have arranged the rest of this paper as follows. Our analysis follows the modeling of the evolutionary process in terms of urn models. We first provide a short background on urn models and then utilize these concepts to analyze the trail forming behavior of ants and provide a rigorous formulation of the conditions under which the initial bias reversal can happen. Finally, we distinguish our work from other theoretical works and conclude with some observations and our future directions.

Urn Models

In this Section, we provide a brief introduction to urn models (for more details, see (Johnson & Kotz 1977; Mahmoud 2003)). In an urn, one assumes balls of a certain number of colors to be present. One draws a ball randomly from the urn and depending on the color of the ball, adds a certain number of balls of that color to the urn. This addition in effect changes the probability of choosing a ball of any specific color. In effect, the preceding choice (drawing a ball of a certain color) changes the probabilities of drawing a specific color in the succeeding draw. This is not unlike how trails are formed in ant colonies where an ant traveling along a certain path, deposits pheromone on it and thus changes the probabilities of a succeeding ant choosing a specific route. We will make the relationship more explicit shortly. For the present, we proceed to describe the urn models.

Let us assume that an urn of infinite capacity contains balls of k different colors. At each discrete instant, a ball is randomly picked up from the urn and its color is observed. If the color is the ith color, then along with the ball picked, a_{ij} balls, $\forall j = 1, \ldots, k$ are also put back into the urn. For each color picked, it is convenient to represent the number of balls of each color added to the urn, by a matrix. This matrix is usually referred to as a *Replacement Matrix*. For example in the following replacement matrix $\mathbf{A}$,

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{pmatrix}$$

an entry a_{ij} denotes the number of balls of color j added to the urn, if the color of the ball picked is i. The individual entries can be positive, zero or negative[1].

Since a ball is picked from the urn at random, each ball has equal probability of being picked. Therefore the selection of a ball of a particular color is proportional to the proportion of balls of that color in the urn. Once a ball has been selected, the number of balls of each color is updated, therefore the probabilities change according to the previous choice. This is analogous to ant behavior, where the probability of choosing a path is proportional to the amount of pheromone on that path and the probabilities change according to the previous choice on account of pheromone deposited by the ant.

A classic urn model is the *Polya-Eggenberger urn process* (Mahmoud 2003). For a two color problem, the Polya replacement matrix is of the form

$$\begin{pmatrix} s & 0 \\ 0 & s \end{pmatrix}$$

where s is the number of balls of the same color added to the urn. The above replacement scheme is described as the following. Suppose there are white and black balls in the urn. If a black ball is picked, then s additional black balls are put

back into the urn. If a white ball is picked, then s additional white balls are put back into the urn. If there are $k(> 2)$ colors, then the problem is called a *Generalized Polya urn problem* and the corresponding Replacement matrix is $k \times k$ diagonal matrix with the usual constant row sum property.

In the context of the ant problem, the above 2×2 matrix corresponds to the situation where there are two paths. When an ant chooses the first path, pheromone is deposited on that path, corresponding to an increase in the amount of pheromone concentration on that path by s. The entries in the matrix thus capture the amount of pheromone increase when a specific path (row in the matrix) is chosen. In the absence of evaporation, the matrix is a diagonal matrix of positive values corresponding to increase of pheromone when the corresponding path is chosen.

Even slight difference in the entries can lead to a drastic difference in performance obtained. For example, while the evolution process of the Polya urn results in a clear preference of one choice, the *Adverse Campaign model*, given by

$$\begin{pmatrix} 0 & s \\ s & 0 \end{pmatrix}$$

results in a balanced preference.

Thus, one can understand why some ant algorithms that differ only slightly in the update scheme yield very different performance results. In the next section we derive the appropriate replacement matrix for the biological ant model.

Trail Formation as a Polya Process

Suppose ants come out of the nest and move in one direction till a point where they are offered two alternative paths (denoted by A and B). At this point they need to make a decision regarding which path to follow. We assume that in one time instant only one ant makes a decision. This is a reasonable assumption to make because the time instance between consecutive decisions can be arbitrarily small (Bonabeau, Dorigo, & Theraulaz 1999). If the number of ants that make a decision in one time instant is greater than one, then also this analysis is applicable provided the number of ants that make a decision in each time instant is constant. Both of the above possibilities imply that a constant amount of pheromone is added to a path as the result of the decision made. We denote this constant amount of pheromone dropped on account of the decision made by m. The value of m is obtained as the product of number of ants that take a decision in an instant and the amount of pheromone dropped by each ant. If the ant chooses path A, then m amount of pheromone is added to path A, and if the ant chooses path B then m amount of pheromone gets added to path B.

Once an ant chooses a path it keeps dropping constant amount of pheromone along the path that it walks on. The paths are assumed to be independent and once an ant chooses a path it cannot switch between them. Thus, the concentration of pheromone along the complete path is the same as at the decision point. The ants probabilistically choose paths based on the concentration of pheromone at the decision points.

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[1] In the case that some of them are negative, there are additional tenability conditions that must be followed in order to eliminate impossible moves.

In regards to urn models as described in the previous section, for the trail formation process the different paths offered to ants correspond to the different *colors* available in the urn. The picking probability governed by the pheromone concentration in ants corresponds to the *number* of balls in the urn. For ants when a path (color) is picked only the concentration of pheromone (number of balls) of that path (color) is updated by an amount m. Therefore the appropriate replacement matrix for a two path problem will be

$$\left(\begin{array}{cc} m & 0 \\ 0 & m \end{array} \right).$$

The above matrix corresponds to the *Polya-Eggenberger urn model*. Using the above update matrix we derive our results. We start by supposing that the initial concentration of pheromone on paths A and B are C_A and C_B.

The probability that path A is chosen is given by

$$\frac{C_A}{C_A + C_B} \tag{1}$$

and that of path B is given by

$$\frac{C_B}{C_A + C_B}. \tag{2}$$

If the decision making ant chooses path A, then the concentration of path A is updated to $C_A + m$. The new probability of choosing path A becomes

$$\frac{C_A + m}{C_A + C_B + m}. \tag{3}$$

Since each decision is taken independently of others, the probability that path A is chosen in the second time instant also, is given by

$$\frac{C_A}{C_A + C_B} \times \frac{C_A + m}{C_A + C_B + m}. \tag{4}$$

Similarly at time instant n, the probability that the first x ants choose path A and the successive $(n - x)$ ants choose path B is given by,

$$\frac{C_A}{C_A + C_B} \times \frac{C_A + m}{C_A + C_B + m} \cdots \frac{C_A + (x-1)m}{C_A + C_B + (x-1)m} \times$$
$$\frac{C_B}{C_A + C_B + xm} \times \frac{C_B + m}{C_A + C_B + (x+1)m} \cdots$$
$$\cdots \times \frac{C_B + (n-x-1)m}{C_A + C_B + (n-1)m} \tag{5}$$

To get a succinct expression for the above equation, we first divide the numerator and denominator by m to get,

$$\frac{\frac{C_A}{m}(\frac{C_A}{m} + 1) \dots (\frac{C_A}{m} + x - 1) \frac{C_B}{m}(\frac{C_B}{m} + 1) \dots (\frac{C_B}{m} + n - x - 1)}{(\frac{C_A+C_B}{m})(\frac{C_A+C_B}{m} + 1) \dots (\frac{C_A+C_B}{m} + n - 1)} \tag{6}$$

The multiplicands in the above equation are incomplete expansions for $\Gamma(x + \frac{C_A}{m})$, $\Gamma(x + \frac{C_B}{m})$ and $\Gamma(n + \frac{C_A+C_B}{m})$, where Γ stands for the Gamma function. We multiply and

divide the above equation by $\Gamma(C_A/m)$, to get $\Gamma(x + \frac{C_A}{m})$ in the numerator. Similarly on multiplication with $\Gamma(C_B/m)$ we get $\Gamma(x + \frac{C_B}{m})$, and on multiplication with $\Gamma((C_A + C_B)/m)$, we get $\Gamma(n + \frac{C_A+C_B}{m})$. Combining all the terms we can write the above as

$$\frac{\Gamma(x + \frac{C_A}{m}) \cdot \Gamma(n - x + \frac{C_B}{m}) \cdot \Gamma(\frac{C_A+C_B}{m})}{\Gamma(\frac{C_A}{m}) \cdot \Gamma(\frac{C_B}{m}) \cdot \Gamma(n + \frac{C_A+C_B}{m})} \tag{7}$$

Equation 7 gives an expression for the probability that the *first x* decisions are in favor of path A and the *subsequent $n - x$* in favor of path B. Next we need to derive the probability of choosing path A, x times over all possible sequences of choosing A.

We first note that the sequence of choosing of paths does not alter the above equation. Any sequence of decisions that result in path A being chosen x times and path B being chosen $(n - x)$ times will result in the same equation, only the denominators will be interchanged. Secondly, since there are $\binom{n}{x}$ different sequences of choosing path A, x times, we multiply the above probability by $\binom{n}{x}$ to get the total probability of path A being chosen x times out of n (for all possible sequences).

$$P(x, n) =$$
$$\frac{\Gamma(x + \frac{C_A}{m}) \cdot \Gamma(n - x + \frac{C_B}{m}) \cdot \Gamma(\frac{C_A+C_B}{m}) \cdot \Gamma(n + 1)}{\Gamma(\frac{C_A}{m}) \cdot \Gamma(\frac{C_B}{m}) \cdot \Gamma(n + \frac{C_A+C_B}{m}) \cdot \Gamma(x + 1) \cdot \Gamma(n - x + 1)} \tag{8}$$

$P(x, n)$ denotes the probability of path A being chosen x times out of n decisions. If n and x are large then we can apply Stirling's formula

$$\Gamma(n) = \sqrt{2\pi(n-1)} * \left(\frac{n-1}{e} \right)^{n-1}. \tag{9}$$

On application of Stirling's formula in the terms containing x and n, we get,

$$\frac{(x - 1 + \frac{C_A}{m})^{x - \frac{1}{2} + \frac{C_A}{m}} \cdot (n - x - 1 + \frac{C_B}{m})^{n - x - \frac{1}{2} + \frac{C_B}{m}} \cdot n^{n + \frac{1}{2}}}{(n - 1 + \frac{C_A+C_B}{m})^{n - \frac{1}{2} + \frac{C_A+C_B}{m}} \cdot x^{x + \frac{1}{2}} \cdot (n - x)^{n - x + \frac{1}{2}}} \tag{10}$$

In practice, C_A/m and C_B/m are much smaller than n and x, therefore we can write

$$\frac{x^{x - \frac{1}{2} + \frac{C_A}{m}} \cdot (n - x)^{n - x - \frac{1}{2} + \frac{C_B}{m}} \cdot n^{n + \frac{1}{2}}}{n^{n - \frac{1}{2} + \frac{C_A+C_B}{m}} \cdot x^{x + \frac{1}{2}} \cdot (n - x)^{n - x + \frac{1}{2}}} \tag{11}$$

On simplification this results in,

$$\frac{x^{\frac{C_A}{m} - 1} \cdot (n - x)^{\frac{C_B}{m} - 1}}{n^{\frac{C_A+C_B}{m} - 1}} \tag{12}$$

Furthermore, if we represent the proportion x/n as r, then the above can be written as

$$(1/n) * r^{\frac{C_A}{m} - 1} \cdot (1 - r)^{\frac{C_B}{m} - 1} \tag{13}$$

which is the Beta distribution.

Therefore, the total probability of path A being chosen x times out of n decisions, is given by

$$P(A_n = C_A + mx, B_n = C_B + m(n-x))$$
$$= \frac{\Gamma(\frac{C_A+C_B}{m})}{\Gamma(\frac{C_A}{m}) \cdot \Gamma(\frac{C_B}{m})} \cdot \frac{1}{n} \cdot \left(\frac{x}{n}\right)^{\frac{C_A}{m}-1} \cdot \left(1 - \frac{x}{n}\right)^{\frac{C_B}{m}-1} \quad (14)$$

The above probability represents the critical relationship between the initial pheromone concentrations on the paths and the final probability of adoption of each path. The bias on one of the paths (on account of being discovered earlier) can have a significant impact on which path the trail will be formed. If initially one of the paths has a large amount of pheromone on it, then the probability of it being chosen by a large number of ants (given by x) is also large. This explains why if a shorter path is discovered later, it has a low probability of being converged to.

In the next section, we derive the effect of *shortness* of the path on the convergence probability and see what amount of bias on the longer path can be reverted on account of shortness of the other path.

Incorporation of length of paths in the result

Under the assumption that all ants move with the same speed, say one unit distance per unit time, for unequal length paths the ants complete the route on the shorter path earlier in time before the longer path. Therefore the shorter route gets updated (maybe several times in some cases) before the longer one gets updated. This helps in increasing the initial pheromone on the shorter path and adds some amount of bias to the shorter path. This bias on the shorter path, helps it to revert the bias on the longer path.

The value of this bias added to the shorter path on account of its shortness can be incorporated as follows. Assume that the length of the shorter path is $L_A = 1$, and of the longer path is $L_B = ratio$. Then, till the time an ant comes back on the longer path, the expected update on the shorter path on account of faster returns on it is,

$$E[\Delta(C_A)] = P(1, ratio) \cdot m + P(2, ratio) \cdot 2m + \ldots$$
$$+ P(ratio, ratio) \cdot (ratio) \cdot m \quad (15)$$

where $P(.,.)$ is given by equation 8. The expected value is computed by summing the probability that the shorter path will be chosen x times $\times$ the pheromone added on choosing x times. The maximum number of rounds that can be completed on path A before an ant comes back on path B is given by ratio. After the return of the ant on the longer path, the expected update on the longer path will be,

$$E[\Delta(C_B)] = m \cdot P(1,1). \quad (16)$$

To incorporate length, we need to add the above updates to their respective initial pheromone concentrations and then apply equation 8.

To study the interplay of length and bias, we studied the probability of shorter path being more popular at time n. We define a path being more popular at any time, if the probability that it will have more pheromone than the other, is greater than a constant $c < 1$. The probability of proportion

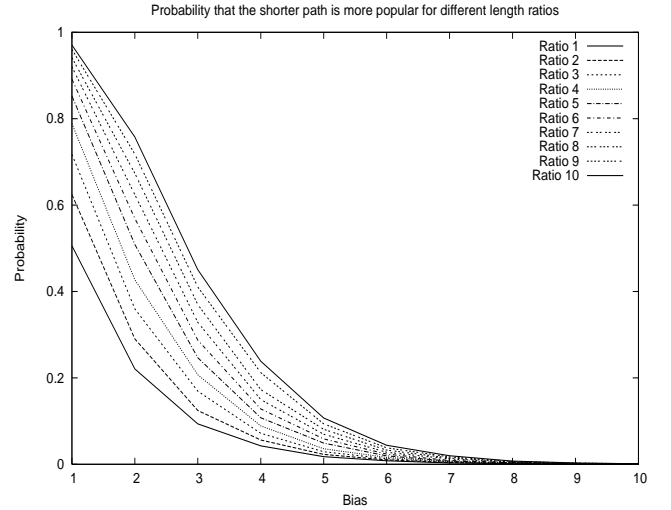Probability that the shorter path is more popular for different length ratios

Figure 1: Each curve indicates the probability of popularity of the shorter path under different initial bias. Bias is the initial amount of pheromone on the longer path when the initial amount of pheromone on the shorter path is 1. The different curves indicate how this probability gets altered for different ratios of length. The lowermost curve is for the case when ratio between the lengths of the longer and shorter path is 1. The probabilities have been obtained for n = 100.

of pheromone on the shorter path greater than any constant c can be obtained as

$$\frac{A_n}{A_n + B_n} = \frac{A_0 + mx}{A_0 + B_0 + mn} > c \quad (17)$$

Manipulating the terms we get

$$x > \frac{A_0(c-1) + B_0 c + nc}{m} \quad (18)$$

Therefore,

$$P\left(\frac{A_n}{B_n} > c\right) = \frac{\Gamma(\frac{A_0+B_0}{m})}{\Gamma(\frac{A_0}{m}) \cdot \Gamma(\frac{B_0}{m})} \cdot \frac{1}{n}$$
$$\times \sum_{x=\lceil \frac{B_0 c + nc + A_0(1-c)}{m} \rceil}^{n} \left(\frac{x}{n}\right)^{\frac{A_0}{m}-1} \cdot \left(1 - \frac{x}{n}\right)^{\frac{B_0}{m}-1} \quad (19)$$

For each ratio of lengths, using $c = 0.5$, [2] we plotted this probability for different bias. Bias is the initial amount of pheromone on the longer path when the initial amount of pheromone on the shorter path is 1. The probabilities have been obtained for n = 100. The figure shows the set of curves, each corresponding to a chosen ratio of lengths. For example the lower most curve, plots the probability for different initial bias, when the $Ratio = L_B/L_A = 1$. Therefore for the case when there is no difference in the initial pheromone concentration, the probability that either will be

[2]The value of c alters the exact probabilities obtained but the nature of the curves remains the same.

more popular is 0.5. Similarly, the other curves represent the change in probability with the bias on the longer path for different ratios of lengths.

With increasing bias on the longer path, the probability that the shorter path will be more popular decreases. With increasing difference in ratios of lengths, this probability increases, i.e. the shorter the optimal path, the more bias it can revert.

This validates the intuitive notion that the shorter that a path is, the more initial bias it can revert. Therefore, one can use the analysis in this section to study the interplay of length and bias, and infer the amount of bias that can be reverted for a particular choice of ratio.

Related Work

Most of the work on ant algorithms focuses on application of foraging in various domains and not on its theory. Though proofs of convergence to the shortest paths exist (Dorigo & Blum 2005), they are very specific to a particular algorithm.

Gutjahr gave convergence results for two ACO algorithms called Graph-Based Ant System (2000) and 1-ANT (2006). Stützle and Dorigo (2002) proved some convergence properties for Ant Colony System and Max-Min ant system. Merkle and Middendorf (2002) propose a deterministic model for ACO algorithms and use it to derive the exact result on permutation problems with a specific structure. Neumann and Witt (Neumann & Witt 2006) give analysis of the 1-ANT algorithm on a symmetric function called ONE-MAX. (Doerr *et al.* 2007) extended the runtime analysis to some other example functions.

These convergence results are very specific to the algorithm used and cannot be extended for other similar algorithms. In many cases they have been tailored to suit the objective function on which analysis is given. In this case the analysis cannot even be extended to other objective functions. Certainly, no convergence results or mathematical analysis for the individual random decision making that leads to the emergence of trail and choosing of the shorter path exist.

Individual ant's random decisions are difficult to model because of their inherent randomness and the dependence of one ant's decision on the past random decisions of other ants. In this paper we modeled the individual random decision making as the ball picking process in an urn model. The dependence on past decisions was incorporated as the addition of balls in the urn because of the previous decisions.

Discussion

Algorithms inspired by the trail formation behavior of ants have been used to solve complex problems such as the point covering problem (Hua *et al.* 2004), the traveling salesman problem (Gambardella & Dorigo 1995), the multi label classification problem (Chan & Freitas 2006) to name a few.

The probability of solving a specific problem can be better understood using the analysis presented in this paper and possible algorithmic adjustments can be made to increase the probability of success. For example, all ant algorithms discover new paths (or solutions) with some exploration probability. Usually long paths (or bad optima) are discovered before shorter ones are discovered. Since many longer paths will be discovered before the optimal one, they develop a "bias" that motivates ants to pursue them and not the shorter path. Therefore there is no guarantee that even if the shorter path is discovered later, ants will continue pursing it. In the context of biological ants this means that even if an ant discovers the optimal path to the food source, it is not necessary that this information will be successfully delivered to the rest of the colony and the trail may not form on the optimal path.

Analogously, in the case of artificial ants that are used to solve complex problems like scheduling, routing etc., this means that even if a shorter route is discovered later, it may be ignored by the agents who may continue using a previously discovered longer route. Therefore, it is an important to know how much bias can be tolerated by the system. Not only does it give the probability of convergence to the shortest path but is also crucial in setting the exploration probability. We describe this utility with a specific example. The Traveling Salesperson Problem (TSP) requires finding the shortest possible trip through a set of cities (or nodes), visiting each node exactly once before finally returning home. The TSP can be represented as a complete graph $G = (N, A)$ with N being the set of of $n = |N|$ nodes and A the set of paths connecting the nodes. Each path is assigned a weight d_{ij} which represents the distance between cities i and j. The pheromone trails τ_{ij} in the TSP refers to the desirability of visiting city j directly after i (Dorigo & Stützle 2004). Ant Colony System (ACS), (Dorigo & Gambardella 1997) one of the best performing ant algorithms for TSP, constructs tours by initially placing ants on random nodes. Then an ant k, located at city i moves to a city j according to the following proportion rule,

$$ j = \left\{ \begin{array}{ll} \operatorname{argmax}_{l \epsilon N_i^k} \{\tau_{il}[\eta]^\beta\}, & \text{if } q \leq q_0 \\ J, & \text{otherwise} \end{array} \right. \quad (20) $$

where, η is heuristic information usually set to $1/d_{ij}$, β is a parameter, q is a random variable uniformly distributed in $[0, 1]$, $q_0 (0 \leq q_0 \leq 1)$ is a parameter and J is a random variable.

This implies that with probability q_0 the ant exploits the information about the paths that has been collected by choosing the paths according to their pheromone concentrations and with $(1 - q_0)$ it performs a biased exploration of the paths. The parameter q_0 allows modulation of the degree of the exploration and the choice of whether to concentrate the search of the system around the best solution so far (exploitation). To obtain good results, tuning of this parameter is required (Dorigo & Stützle 2004). There is no mathematical analysis that guides the choice of this parameter.

The analysis in this paper provides a criterion on how to choose q_0. For a given exploration probability q_0, it is possible to determine how much bias can accumulate on a path under worst case. For this bias one can use the analysis to calculate the probability of degree of closeness to the optimal solution.

Conclusion

Ants are known to self organize and form trails between their nest and a food source. The reasons behind this behavior are known; however, the mathematical model and the interrelationship between parameters like pheromone increment at every step, initial pheromone deposits at a path, and the number of ants that choose a path etc were not known. Specifically, it was not clear whether the effect of the initial bias gained on a longer path can be reversed, and emergence of a trail can occur on a shorter path discovered later.

In this paper we proposed the use of urn models to analyze the individual random decisions of ants. Since urn models capture the evolving probabilities after every decision, they can be used to analyze various ant algorithms. It is easy to extend this analysis to other ant algorithms, which is not possible for previously proposed methods of analysis.

When ants select a path with probability linearly proportional to the concentration of pheromone on it and drop constant amount of pheromone on the path chosen, we showed that at any given time the ratio of choices between paths follow a Beta distribution. In future, we plan to incorporate evaporation of pheromone on paths and extend the analysis to multiple paths.

Acknowledgement

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