

A Study of the Accuracy of Heuristic Functions

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Abstract. From a practical point of view, most problems cannot be optimally solved applying brute-force single-agent search algorithms. Thus, a new class of single-agent search algorithms was devised to find the optimal solution faster and/or consuming less space, heuristic single-agent search algorithms. However, designing accurate heuristic functions is still a major challenge. In this paper, a mathematical model is introduced for characterizing the accuracy of any heuristic function. This is a step ahead in the analysis of heuristic functions since this method could be used to aid other procedures to improve the original heuristic estimations.

1 Introduction

The problem of characterizing accurately the precision of the heuristic function $h(\cdot)$ employed by single-agent search algorithms to reach a goal node t is considered. This is an important issue since it is known that the time complexity of the search algorithms depends upon the accuracy of the heuristic function [15]. Besides, several methods for improving the estimations of an original heuristic function $h(\cdot)$ have been devised so a tool for characterizing the accuracy of the new heuristic function would be helpful for both: spotting where the original heuristic function has to be improved and when to stop. For example, Gaschnig [6] introduced the terms “sub-graph” and “super-graph” with the aim of devising automatically more precise heuristic functions; other ideas follow: criticizing relaxed models [7, 12, 15] of the original heuristic functions; automatic learning methods of new and more accurate heuristic values [1, 2, 8, 9] and even, perimeter search algorithms [3, 14] can be considered as an automatic method for improving the original heuristic estimations of $h(\cdot)$.

As in previous works [4, 5, 6, 15, 16], an abstract model which consists of a tree where every node has exactly b children and is fully expanded up to depth d is considered. The main difference of this research with those works is that cycles are also considered here. An exception to this rule is the work performed by Richard E. Korf and Michael Reid who introduced a tool for analysing heuristic functions in order to estimate accurately the number of nodes generated in practice by any single-agent search algorithm [11, 10]. This work makes use of the so-called α and β distributions introduced by another independent researcher who used them to characterize the performance of the perimeter heuristic functions [13]. The α and β distributions can be derived from the total density function $f(x)$ devised by Korf and Reid.

This paper is arranged as follows: in the following section the mathematical model is introduced from a theoretical point of view;

next, it is discussed how to apply the theoretical model to a real case. Finally, some relevant conclusions are shown.

2 Mathematical model

This section introduces the mathematical model used for modelling the accuracy of the heuristic function $h(\cdot)$. It consists of a probability function of an event named Γ defined below.

2.1 Preconditions

This analysis is restricted to domains which meet the following requirements:

- The state space can be represented as a connected graph, i.e., at least one path $\langle n, n^1, n^2, \dots, t \rangle$ exists from any node n belonging to the state space where t is the target node.
- The cost of all arcs, $c(n, n_i)$, with n_i being a successor of n , is always equal to 1: $c(n, n_i) = c(n_i, n) = 1$.
- The only allowed changes of the heuristic function $h(\cdot)$ from node n to node n_i are $\{-1, +1\}$, when estimating its distance to the same node m : $|h(n, m) - h(n_i, m)| = 1$, where node n_i is a successor of node n , i.e., $n_i \in \text{SCS}(n)$.

Examples are domains like the N-Puzzle [1] when guided by the Manhattan distance, or the problem of finding the shortest path in a maze with obstacles when guided by the sum of the difference of the coordinates x and y [8].

2.2 Characterization of $h(\cdot)$

This mathematical model makes use of the following *domain-dependent* conditional distribution functions:

$$\alpha_i = p(h(n_j, t) = i + 1 | h(n, t) = i), n_j \in \text{SCS}(n)$$

$$\beta_i = p(h(n_j, t) = i - 1 | h(n, t) = i), n_j \in \text{SCS}(n)$$

such that:

$$\alpha_i + \beta_i = 1, \forall i, 0 \leq i \leq h_{max} \quad (1)$$

where h_{max} is the maximum heuristic distance from any node n of the state space to the goal node t . In other words, α_i is the probability that the j th-child of a node n randomly sampled has a heuristic distance to the target node t equal to $i + 1$ where i is the heuristic distance of its parent, n , to the same target node. Conversely, β_i is the probability that the j th-child of a node n randomly sampled has a heuristic distance to the target node t equal to $i - 1$ where i is the heuristic distance of its parent, n , to the same target node.

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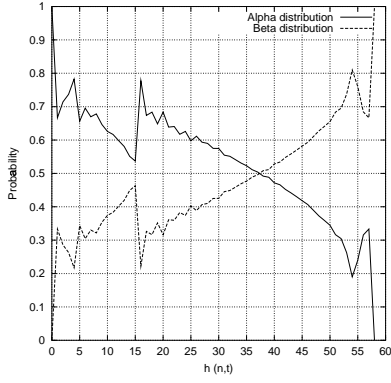


Figure 1. Marginal distributions α and β for the 15-Puzzle

These distributions can either be easily sampled or they can be derived from the total density function introduced by Richard E. Korf and Michael Reid [11, 10], $f(i) = p(h(n, t) = i)$, i.e., the likelihood that the distance from any node n randomly sampled to the goal node t will be exactly equal to i . A method for deriving the distributions α_i and β_i from $f(i)$ is discussed in [13].

Figure 1 shows the distributions α_i and β_i of the Manhattan distance computed with the sampling of 10^6 solvable instances of the 15-Puzzle.

2.3 How the heuristic distances are distributed

Let us denote with $\Gamma^{h_0, \delta}(b, d)$ the number of terminal nodes generated in a uniform tree search, $T(b, d)$, with branching factor b and depth d rooted at a node n whose heuristic distance to the target node t is $h_0 + \delta$. This definition assumes that node n has a heuristic distance to the target node t equal to h_0 .

Figure 2 shows a plausible case where the nodes generated at depth $d = 2$ from the node n have different heuristic distances (shown to the left of internal nodes and below the leaves) to the target node t —somewhere in the state space out of the figure—expressed with different variations of the original heuristic distance $h_0 = h(n, t)$. For example, the number of terminal nodes with a heuristic distance equal to $h_0 + 0 = h_0$ from node n to the target node t is 2 since the first immediate successor of the root has a descendant meeting this property and the second immediate successor of the root adds another one. In other words: $\Gamma^{h_0, 0}(2, 2) = 2$ because for the first successor $\Gamma^{h_0+1, -1}(2, 1) = 1$ and for the second successor $\Gamma^{h_0-1, +1}(2, 1) = 1$. Note how the values δ of the immediate successors of the root have changed their value in order to ensure a final alteration $\delta = 0$ in the root node.

Lemma 1 *The following relationships are always true, i.e., they are axioms of the mathematical model proposed:*

$$\begin{aligned}
 p(\Gamma^{h_0, 0}(b, 0) = 1) &= 1 \\
 p(\Gamma^{h_0, 0}(b, 0) = x) &= 0, \forall x \neq 1 \\
 p(\Gamma^{h_0, \delta}(b, 0) = 0) &= 1, \forall \delta \neq 0 \\
 p(\Gamma^{h_0, \delta}(b, 0) = x) &= 0, \forall \delta \neq 0, \forall x \neq 0 \\
 p(\Gamma^{h_0, \delta}(b, d) = 0) &= 1, \forall \delta, |\delta| > d \\
 p(\Gamma^{h_0, \delta}(b, d) = x) &= 0, \forall \delta, |\delta| > d, \forall x \neq 0
 \end{aligned} \tag{2}$$

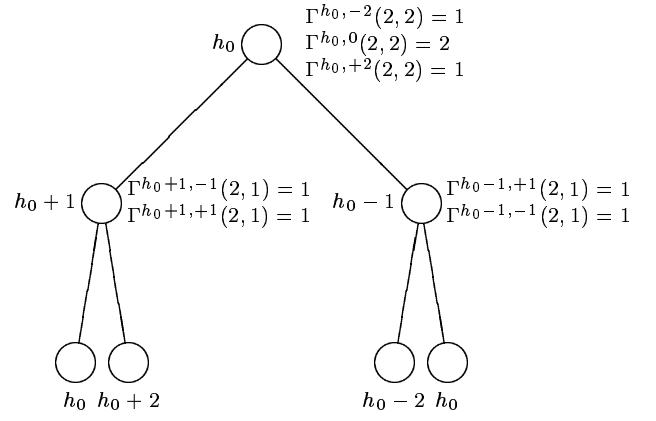


Figure 2. An example of Γ

Proof. They are in fact very easy to understand. They only represent trivial relationships of the cases that have to be taken into account when computing the likelihood of different Γ events. The first four mean that no change δ other than 0 of the original heuristic estimation h_0 can be obtained with a null depth. The last two establish that it is not feasible to alter the original heuristic estimation h_0 in an amount greater than the current depth. \square

Theorem 1 *Let $T(2, d)$ denote a uniform tree search rooted at node n with a brute branching factor $b = 2$ and depth d . Assuming that node n has a heuristic distance to the target node t equal to h_0 , the probability that $T(2, d)$ has exactly x terminal nodes whose heuristic distance to the target node t is $h_0 + \delta$ is:*

$$p(\Gamma^{h_0, \delta}(b, d) = x) = \sum_{i=0}^x \rho(h_0, \delta, d-1, i) \times \rho(h_0, \delta, d-1, x-i) \tag{3}$$

where ρ is defined as:

$$\rho(h_0, \delta, d, x) = \alpha_{h_0} \cdot p(\Gamma^{h_0+1, \delta-1}(b, d) = x) + \beta_{h_0} \cdot p(\Gamma^{h_0-1, \delta+1}(b, d) = x) \tag{4}$$

Proof. The proof of this theorem can be found in [13]. However, it is worth noting that the formula shown above assumes the heuristic distances of all children of any node n to the target node t are independently distributed. \square

The following theorem generalizes the result of the previous one to an arbitrary branching factor b .

Theorem 2 *Let $T(b, d)$ denote a uniform tree search rooted at node n with a brute branching factor b and depth d . Assuming that node n has a heuristic distance to the target node t equal to h_0 , the probability that $T(b, d)$ has exactly x terminal nodes whose heuristic distance to the target node t is $h_0 + \delta$ is:*

$$p(\Gamma^{h_0, \delta}(b, d) = x) = \sum_{i_1=0}^x \sum_{i_2=0}^{x-i_1} \dots \sum_{i_{(b-1)}=0}^{x-\sum_{j=1}^{b-2} i_j} \left(\rho \left(h_0, \delta, d-1, x - \sum_{j=1}^{b-1} i_j \right) \right) \times$$

$$\prod_{j=1}^{b-1} \rho(h_0, \delta, d-1, i_j) \quad (5)$$

Proof. The proof of this theorem can be found in [13]. As in the previous theorem, it is worth noting that the formula shown above assumes the heuristic distances of all children of any node n to the target node t are independently distributed. \square

2.4 Only-one-optimal-path: A case study

Although the mathematical model introduced herein is not restricted to the case of only-one-optimal-path to the target node t , it will be discussed first for the sake of clarity.

In case there is only one optimal path from any node n to the goal node t , none of the following errors may ever take place if the heuristic function $h(\cdot)$ is perfectly informed [15]:

Alpha error No child of node n , n_i , has a heuristic distance, $h(n_i, t)$, strictly lower than the heuristic distance of the node n , $h(n, t)$.

Since it is assumed there is always just one optimal path $\langle n, n^1, n^2, \dots, t \rangle$ from node n to the target node t , it is clear that $k(n, t) = 1 + k(n^1, t)$ where $k(n, m)$ stands for the cost of the optimal path between the nodes n and m . Thus, if the heuristic function $h(\cdot)$ is perfectly informed: $h(n, t) = 1 + h(n^1, t)$ and, therefore, one child of every node n shall have a heuristic distance strictly lower than the heuristic distance of its parent.

This error prevents the single-agent search algorithm from immediately expanding the node that leads to the optimal path.

Beta error No child of node n , n_i , has a heuristic distance, $h(n_i, t)$, strictly greater than the heuristic distance of the node n , $h(n, t)$.

Since it is assumed there is just one optimal path from any node n to the target node t (and b is reasonably assumed to be at least 2), only one node can have a heuristic value strictly lower than the heuristic distance of its parent so that the rest shall have a value strictly greater than it, if the heuristic function $h(\cdot)$ is perfectly informed.

This error leads the single-agent search algorithm to the expansion of nodes which may or may not lie over the optimal path.

From the previous discussion, the following important result can be drawn since it relates the α and β distributions with the accuracy of the heuristic function. However, before going further the reader is told that in the rest of the paper, α_i is considered equal to a constant value α for the sake of clarity. Though this is clearly an important simplification, it does not necessarily affect the validity of the results to come.

Theorem 3 Assuming there is only one path to the goal node t from any node n whose heuristic distance to t is i , the optimal value of α is $(b-1)/b$.

This result is very easy to demonstrate. Instead, other evidence is given to support this assertion. Considering a node n whose heuristic distance to the target node is h_0 , the probability that n has exactly one immediate successor with a heuristic distance to t equal to $h_0 - 1$ can be computed from equation (5) as follows:

$$p(\Gamma^{h_0, -1}(b, 1) = 1) = b\rho(h_0, -1, 0, 1) \rho^{b-1}(h_0, -1, 0, 0) =$$

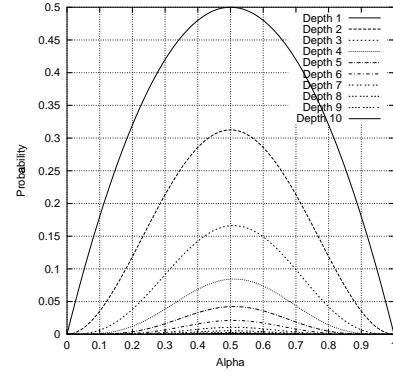


Figure 3. Observing different depths with $b = 2$

$$\begin{aligned} & b \left(\alpha p(\Gamma^{h_0+1, -2}(b, 0) = 1) + \beta p(\Gamma^{h_0-1, 0}(b, 0) = 1) \right) \times \\ & \left(\alpha p(\Gamma^{h_0+1, -2}(b, 0) = 0) + \beta p(\Gamma^{h_0-1, 0}(b, 0) = 0) \right)^{b-1} = \\ & b\beta\alpha^{b-1} \end{aligned} \quad (6)$$

where all the probabilities can be immediately derived from the axioms shown in (2). This result can be generalized. Let us consider a node n whose heuristic distance to the target node is h_0 . The probability that n has exactly one child at depth d with a heuristic value to the target node equal to $h_0 - d$ can be computed also from equation (5):

$$\begin{aligned} & p(\Gamma^{h_0, -d}(b, d) = 1) = \\ & b\rho(h_0, -d, d-1, 1) \rho^{b-1}(h_0, -d, d-1, 0) = \\ & b \left(\alpha p(\Gamma^{h_0+1, -(d+1)}(b, d-1) = 1) + \right. \\ & \left. \beta p(\Gamma^{h_0-1, 1-d}(b, d-1) = 1) \right) \times \\ & \left(\alpha p(\Gamma^{h_0+1, -(d+1)}(b, d-1) = 0) + \right. \\ & \left. \beta p(\Gamma^{h_0-1, 1-d}(b, d-1) = 0) \right)^{b-1} = \\ & b \left(\beta p(\Gamma^{h_0-1, 1-d}(b, d-1) = 1) \right) \left(\alpha + \beta\alpha^{b(d-1)} \right)^{b-1} \end{aligned} \quad (7)$$

since $p(\Gamma^{h_0+1, -(d+1)}(b, d-1) = 0) = 1$ and $p(\Gamma^{h_0+1, -(d+1)}(b, d-1) = 1) = 0$ according to the axioms shown in (2). On the other hand:

$$p(\Gamma^{h_0, 1-d}(b, d-1) = 0) = \rho^b(h_0, 1-d, d-2, 0) = \alpha^{b(d-1)} \quad (8)$$

Finally, it is worth noting that $p(\Gamma^{h_0-1, 1-d}(b, d-1) = 1)$ has been left unsolved in equation (7) since it relates to the same Γ event than the original one but with depth decreased in one unit. Therefore, the original probability is recursively defined in terms of the probability of shorter depths.

Figure 3 shows the probability of having exactly one terminal node with a heuristic distance equal to h_0 minus different depths ranging from 1 (top) to 10 (bottom) which is assumed to be the target node t when traversing a tree with $b = 2$. As it can be seen, the probability reaches a maximum when α equals $(b-1)/b = 1/2$ for all depths.

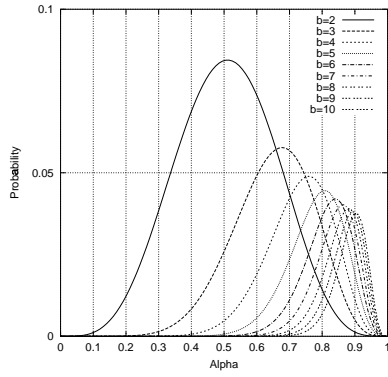


Figure 4. Different values of b for $d = 4$

Indeed, theorem 3 does not relate the optimal value of α to the depth of the search tree, d , but the branching factor, b .

Figure 4 shows the probability functions that result from applying equation (7) to different branching factors b ranging from 2 (the leftmost) to 10 (the rightmost) for the same depth $d = 4$. In all cases, the probability function reaches a peak when $\alpha = (b-1)/b$ as theorem 3 predicted.

2.5 Searching in grids: A practical case

Let us consider a grid with $N \times N$ cells where it is only permitted to move to the horizontally or vertically adjacent cells —i.e., diagonal moves are strictly forbidden. Let us consider the problem of finding the shortest path between $(n-1, n-1)$ and (n, n) such that $n \leq N$. Obviously, the branching factor b will approach 4 for larger values of N . According to theorem 3, a perfectly informed heuristic should show an α value equal to $3/4$.

For this problem it is well known that the sum of the difference of the coordinates x and y is a perfect heuristic which avoids the expansion of sub-optimal nodes. In other words, the class of admissible single-agent search algorithms are able to find the optimal solution with a linear time complexity [15]. However, when considering this heuristic it turns out that $\alpha \simeq 2/4 = 1/2$ since, in most cases, two out of four children get closer to the target node whereas the other two get a unit further. Thus, it seems a divergence has arisen between the theoretical model and these empirical observations.

The problem lies in the fact that our grid has no obstacles in between such that there are different paths for reaching the same target node t from the same node s , i.e., there are transpositions. For the sake of clarity, let us consider the easiest case: finding an optimal path of length $d = 2$ as illustrated in figure 5(a) which shows only a portion of a very large grid. In this case, there are two solutions, namely: $\langle East, South \rangle$ and $\langle South, East \rangle$, so that our previous analysis does not apply directly.

If we remove the transpositions by inserting obstacles between cells appropriately, figure 5(b) results where obstacles are highlighted with thick segments. In this case, there is only one optimal path: $\langle South, East \rangle$. Before turning our attention to the case of figure 5(a), let us see how the accuracy of the selected heuristic function in the case shown in figure 5(b) can be predicted. In this case the branching factor is close to $b = 3$ though it is slightly larger. There-

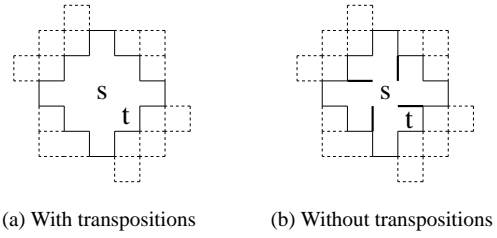


Figure 5. Searching in a maze at depth $d = 2$

fore, a perfect heuristic function $h(\cdot)$ is expected to have $\alpha \simeq 2/3$ and the current value of α is $\frac{25}{36} \simeq \frac{2}{3}$.

This value results from the computation of the mean number of descendants that increment the heuristic distance of its parent to the target node t . For example, the node two steps over t and the node to the left of t have two descendants out of three which lead to nodes further from the target node; the node two steps to the left of t and the node immediately over t have three children and all of them increment the heuristic distance of its parent; and so on. The resulting summation is divided by 12, the total number of nodes which have a heuristic distance to the target node t equal to either 1 or 2. The small difference between the expected value and the real value is explained because: firstly, the heuristic branching factor is not exactly $b = 3$ but slightly larger and secondly, because $\alpha = 2/3$ cannot be achieved exactly when considering the geometry of the problem, i.e., there is no way to get exactly $\alpha = 2/3$. Moreover, the real value obtained is the closest we can get. Thus, the heuristic employed is said to be perfect.

Even in the more complex case of domains with transpositions, as the one shown in figure 5(a), it is still feasible to use the mathematical model introduced herein to derive the optimal value of α which characterizes a perfect heuristic function $h(\cdot)$. As mentioned above, there are two different paths in this case to the target node t . Therefore, the probability that two children at depth $d = 2$ (equal to the optimal cost) have a heuristic value equal to $h_0 - 2$ where h_0 is the heuristic distance from the start node s to the target node t follows $\Gamma^{h_0, -2}(4, 2)$ that can be computed using equation (5):

$$\begin{aligned}
 p(\Gamma^{h_0, -2}(4, 2) = 2) &= \\
 \sum_{i_1=0}^2 \sum_{i_2=0}^{2-i_1} \sum_{i_3=0}^{2-i_1-i_2} \rho \left(h_0, -2, 1, 2 - \sum_{j=1}^3 i_j \right) &= \\
 \prod_{j=1}^3 \rho(h_0, -2, 1, i_j) &= \\
 4\rho(h_0, -2, 1, 2)\rho^3(h_0, -2, 1, 0) + & \\
 6\rho^2(h_0, -2, 1, 1)\rho^2(h_0, -2, 1, 0) & \quad (9)
 \end{aligned}$$

and:

$$\begin{aligned}
 \rho(h_0, -2, 1, 0) &= \\
 \alpha p(\Gamma^{h_0+1, -3}(4, 1) = 0) + \beta p(\Gamma^{h_0-1, -1}(4, 1) = 0) &=
 \end{aligned}$$

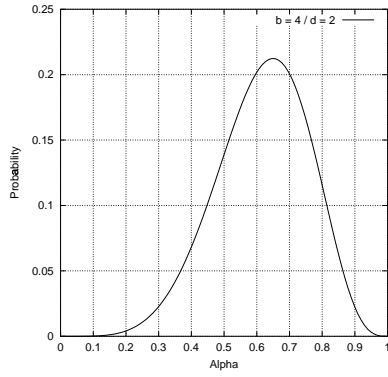


Figure 6. $p(\Gamma^{h_0, -2}(4, 2) = 2)$

$$\begin{aligned} \alpha \times 1 + \beta \times \alpha^4 &= \alpha(1 + \beta\alpha^3) \\ \rho(h_0, -2, 1, 1) &= \\ \alpha p(\Gamma^{h_0+1, -3}(4, 1) = 1) + \beta p(\Gamma^{h_0-1, -1}(4, 1) = 1) &= \\ \alpha \times 0 + \beta \times 4\beta\alpha^3 &= 4\alpha^3\beta^2 \\ \rho(h_0, -2, 1, 2) &= \\ \alpha p(\Gamma^{h_0+1, -3}(4, 1) = 2) + \beta p(\Gamma^{h_0-1, -1}(4, 1) = 2) &= \\ \alpha \times 0 + \beta \times 6\beta^2\alpha^2 &= 6\alpha^2\beta^3 \end{aligned} \quad (10)$$

such that expression (9) yields:

$$\begin{aligned} p(\Gamma^{h_0, -2}(4, 2) = 2) &= \\ 4(6\alpha^2\beta^3)(\alpha(1 + \beta\alpha^3))^3 + 6(4\alpha^3\beta^2)^2(\alpha(1 + \beta\alpha^3))^2 & \end{aligned} \quad (11)$$

Figure 6 shows the shape of $p(\Gamma^{h_0, -2}(4, 2) = 2)$. This function has a maximum in the interval $[0, 1]$ in $\alpha = 0.65$, very close (hence, different) to the optimal value of α when there is only one path to the goal state, $\alpha = 2/3$. Therefore, perfect heuristics are characterized with $\alpha = 0.65$ in this case. The real value of α is:

$$\alpha = \frac{1}{12} \left(4 \times \frac{1}{2} + 8 \times \frac{3}{4} \right) = \frac{1}{12} \times 8 = \frac{2}{3} \quad (12)$$

The slight difference between the expected value ($\alpha = 0.65$) and the real value ($\alpha = 2/3$) is explained once again with the geometry of the problem. As a matter of fact, there is no way to achieve exactly the value $\alpha = 0.65$ and the closest we can get is $\alpha = 2/3$ so that the heuristic is termed as perfect again for the case of two paths to the target node t , i.e., when considering transpositions.

3 Conclusions

A mathematical model for the characterization of the accuracy of heuristic functions has been introduced:

- Heuristic errors have been classified in two categories: alpha and beta errors. Both types of errors can be successfully explained with the α and β distributions so that when no error happens an optimal value of α has been derived for the special case of only one optimal path to the goal node t .

- Moreover, the mathematical tool introduced herein allows the computation of optimal values of α for problems with transpositions or, in a broad sense, with problems that have more than one optimal path to the target node t .
- The most relevant conclusion is that the performance of $h(\cdot)$ is explained in terms of the α and β distributions. Though these functions are very *domain-dependent*, they can be computed for every domain.

It should be noted, however, that slight differences shall always be expected between the optimal values of α derived by this method and the real values of α . These slight differences are attributed to the fact that the branching factor is not expected to be uniform and/or that the geometry of the problem may impose the impossibility to get the optimal value. If these issues would be properly addressed, an accurate method for improving the heuristic estimations of $h(\cdot)$ would become possible.

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