

# Monte Carlo Tree Search driven Falsification

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## Abstract

Simulation-based verification is often the only chance to verify complex hybrid systems and it requires a large amount of time and resources. In particular, the process to find anomalies and faults is called *falsification* because it consists of finding a scenario (a trace of disturbances) that lead the system to falsify the requirements, described as formal specifications.

Many research groups are focusing their effort on techniques for reduction of verification time and recent works adopted search algorithm driven by a heuristic called *robustness*.

In this project, we focused on falsification of Temporal Logic Specification using one of the most promising search algorithm: the Monte Carlo Tree Search, famous for being adopted in AlphaGo. Specifically, we tested this approach on the well-known Automatic Transmission model and analysed the obtained result, describing strenghts and difficulties of MCTS algorithm.

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# 1 Two-Layered Falsification

## 1.1 Introduction

The process of falsification aims to find a counter example to a given specification, such example typically are *hard to find* errors. Typically the search space is huge and the process of verification through simulation is quite expensive, thus a clever strategy to drive the search and properly invest the simulation time is essential.

Following the work done in [3] we decided to use a two layer strategy. On the top level Monte Carlo Tree Search act as a zoomed out view of the search in which, at each control point, the system quantizes the input space in regions and tries to iteratively explore new regions and give to those region an estimation on how promising they are (see section..). On the bottom a generic search algorithm (see section ..) further investigate promising regions at an finer grain coming from the top layer and updates their value of "promisingness" (maybe confidence??).

The MCTS is often used in automated game play (see alphago). This clearly underlines that, in fact, the model we are facing is an adversarial model. As if there was an adversary the error is cleverly placed and the strategy needs to be clever enough to find it.

The MCTS allow to fine tune the balance between exploration and exploitation at a macroscopic level while the choice of the second layer acts in the same way but atomically over points in the search space.

## 1.2 Upper-layer: MCTS

The MCTS aims to iteratively build a tree  $T = (V, E)$  where nodes in  $V$  are labelled with a score  $s$  and a counter  $n$  and edges in  $E$  are labelled with actions. At the start the tree is initialized as a root node with  $s = Inf$  and  $n = 0$ . The execution evolves in different phases.

**Selection:** Starting from the root until reaching a leaf (of the MCTS tree) we move to the node  $n$  maximizing  $UCB(n)$  (see ...). The leaf, say  $L$  will be sampled. If  $L$  is sampled for the first time then  $Rollout(L)$ , else  $Expansion(L)$ .

**Expansion:** For each action  $a$  available from  $L$  we extend  $T$  with a new node  $v$  with  $s = Inf$ ,  $n = 0$  and edge label  $a$ . Then a random child of  $L$ , say  $C_L$ , is chosen to do  $Rollout(C_L)$ .

**Rollout(L)** For each ancestor of  $L$  starting from the root till  $L$  itself, the search algorithm (see section) is run in the region of the selected node. Then starting from  $L$ , the rest of the trace is simulated driven by the search. At the end the trace will have a robustness value of  $v$  which will be used as an estimate for  $L$  and its ancestors by means of  $Backpropagation(L, v)$ .

**Backpropagation(L,v):** From  $L$  till the root, going trough  $L$ 's ancestors say  $L = a_1, a_2, \dots, a_n = root$ , generic  $a_i$  is updated incrementing  $n$  and setting  $s = \max\{n.s, v\}$ .

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**UCB:** In the most general MCTS implementation, given a node  $n$  its UCB value is computed as  $FOO$ , where the idea behind the parameter  $C$  is to fine-tune exploration vs exploitation. When considering the falsification problem thus using robustness as heuristic we face two problem:

- Robustness can have positive yet negative values while classical UCB is designed to work with only positive value.

- Generally, given a specification it is not possible to give an upper bound to the robustness domain.

To overcome both the problems, along the line of CITE, we used  $U_{\cdot}$  defined as BAR.

- tree animation gif

### 1.3 Lower-layer: Search Algorithms

In the very end, the falsification task boils down to a search in the space of the states. We aim to find a falsifying trace of  $k$  disturbances, where  $k$  is the number of desired control points. To do so the MCTS (see Section 1.2) when selects a node at depth  $h$  to rollout from it's basically defining a meta-trace  $\hat{T}$ . The first  $h$  meta-disturb of  $\hat{T}$  ( $\hat{T}$  prefix) are regions of the input space in which to bound the search, and in the suffix the search is allowed in the whole input space. One of the following search algorithm is then used to produce a trace  $T$  accordingly with the semantic of  $\hat{T}$ .

different algo to test the synergy with MCTS and with the falsification in general. also vs overhead brief explanation of the search algorithms.

#### 1.3.1 Random Search: MCTS left alone

To have a way to evaluate the contribution purely given by the MCTS layer, we decided to implement a fast yet dumb search strategy. Given a meta-trace  $\hat{T}$ , for each control point  $k$  in  $\hat{T}$ , RS basically samples u.a.r. a disturbance from the appropriate region for such control point. This result in a very fast yet only exploring algorithm.

#### 1.3.2 Hill Climbing: the greedy

Here, the classical Hill Climbing implementation has been used. The only difference is that, since eventually we need a full trace (a trace having a disturbance for each control point), in the case a not worst neighbour is found a random one is selected. To have a stronger falsification power, at the cost of a longer simulation time restart has been implemented. On the other hand to speed up the simulation, at the cost of a weaker falsification power it is possible to limit the number of neighbour tested by the algorithm at each step. Clearly this search strategy is way clever and effective than RS but the simulation time needed to carry on the falsification process whit a non trivial property to falsify is of another order of magnitude.

#### 1.3.3 Simulated Annealing: the impatient

Again, classical search algorithm, basically an HC enriched with a notion of temperature or, as it is in this case, the number of simulated trace. The higher the temperature the hardest is to make a pejorative move. The goal here is to further balance exploration and exploitation and be, in terms of speed and performance in the middle of RS ans HC.

## 2 Experimental phase

focus on experimental details, which model, which specification, which algorithms adopted.

### 2.1 Model and Specifications

The benchmark adopted is the Automatic Transmission by MathWorks, provided in Simulink. It models a vehicle equipped with a transmission controller and allows the user to change two input signals: the throttle and the brake.

There are several specifications defined on this model because it is a common benchmark in verification papers. Starting from the reference paper and [1], we selected two specification:

1. The engine speed never reaches 120.
2. If the vehicle gear is 3 then the speed is always greater than 20.

We selected these two specifications because they are representative of different kind of search. The first one is easier to falsify, compared with the second one.

### 2.2 Implementation of Robustness metric

In order to understand the difficulty of falsification of the second specification, we need to spend a few words on the computation of robustness metric used to drive the search.

According to the definition of Robustness given in[2], this metric gives us a measure of how the state of the model is far from the falsification. In the first specification, the computation of Robustness is simply the difference between the reference speed and the current speed. Conversely, in the second specification the computation is more complex and can be summarized by the following steps:

1. Since the second specification is an implication, we wrote it as an **OR**.
2. The Robustness of the **OR** operator is the max value of the Robustness computed in the two subformulas.
3. The first subformula is the absolute value of the difference between the current gear and the reference gear (3).
4. The second subformula is the difference between the current speed and the reference speed (20).

Notice that the value of the second subformula is positive if the current speed is greater than 20, otherwise is negative. Conversely, the value of the first subformula is a small positive integer.

As a result, when the gear is different from the reference one (3) then the first subformula dominates the Robustness computation. When the gear is the third one, then the value could be dominated by the second subformula only if it is greater than 20 and then positive. Then, the resulting metric space is characterized by long plateau when the current speed is far from 20 and local minima because of the different unit of measurement for gear and speed.

### 2.3 The proposed baseline: URS

The two specifications above have been implemented in an external function in order to maintain a single model file. The Simulink model is characterized by two output blocks, respectively the *speed* and the *gear*. The external function computes the robustness according to the specification, described by a parameter in the configuration file.

The second specification S2 caused too long time to reach falsification and we decided to change its implementation in order to make it suitable to the time and resources that we can use. In particular, one of the main problem of S2 is the different units of measurement that lead to local minima. In fact, whilst speed is between 0 and 100, the gear is an integer value between 1 and 4.

In contrast with the original definition of the Robustness, we proposed to normalize the second subformula of S2 according to the unit scale. Since the speed goes from 0 to 100, we normalize the second subformula dividing by 100. In this way, the Robustness metric is still characterized by long plateau which make the search not trivial but we reduced the number of local minima.

#### Uniform Random Sampling - Robustness Distribution

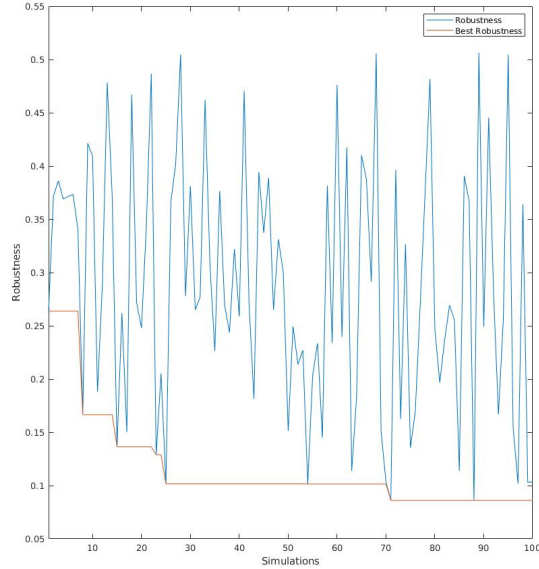


Figure 1: Robustness distribution over 100 simulation of URS search. This random distribution highlights that there is no learning in URS. Moreover, all the values are in  $[0,1]$  because we are using the normalized version of specific S2 and is rather likely to reach the third gear at least once during the simulation with random values.

## 2.4 Experiments

In order to evaluate the effectiveness of the proposed falsification framework, we executed a bunch of experiments on the Automatic Transmission model considering several search algorithms: Uniform Random Sampling (URS), MCTS with Random Search (MCTS+RS), MCTS with Hill Climbing (MCTS+HC), MCTS with Simulated Annealing (MCTS+SA).

Since the execution of experiments is based on randomness, we repeated the same experiment 10 times to ensure more confident results.

First of all, we observed that the effectiveness of MCTS is based on its capacity to build the complete tree. In fact, the MCTS algorithm is characterized by a inherent phase of exploration which allows to have a general view of the space (tree width) and the time (tree height). Only when the tree is complete, the MCTS algorithm results effective and specializes the search. As a consequence, if the branching factor of the nodes is too high, the number of simulation required to build the entire tree is huge and the MCTS doesn't result effective, compared with the URS.

Thus, in order to exploit the power of MCTS, we tuned the split parameters for the input signals. The Speed signal has been split into 2 regions and the Brake signal has been split into 3 regions, then the branching factor of the tree is 6. In the original paper [3], they adopted a different tuning but we observed that such tuning is not effective compared with the URS algorithm. Moreover, for reason of time and resources, the experiments below have been configured with budget parameter equal to 100, it means that the maximum number of iterations of MCTS is 100 and then this is an upperbound in the number of simulations.

The tables below show the obtained results varying the parameter  $C$  which balance the value of exploration and exploitation in the UCB formula. The tables contain the following fields:

- Algo: Search algorithm adopted.
- C: Value of parameter  $C$ .
- Avg Trace Falsification: Number of trace before falsification, considering only the tests which falsify the specification.
- Success Rate: Number of tests which falsify the specification.
- Robustness: statistics on robustness value.
- Time: statistics on elapsed time, both time are considered as average of the all number of experiments.

Finally, the results varying the input space partitioning are reported in the Table 3 in order to emphasize the influence of hyperparameter tuning.

Experiments on specification S1

Algo	C	Avg Trace Falsification	Success Rate	Robustness			Time (sec)	
				min	avg	std dev	tot	trace
URS	- - -	40.0	2/10	-4.07960	4.91882	5.514537	178.014	2.010
MCTS+RS	0.500	- - -	0/10	5.30248	8.34921	2.400517	559.916	5.599
MCTS+HC	0.500	94.0	1/10	-1.93401	5.07959	4.386757	1034.225	10.405
MCTS+SA	0.500	24.0	1/10	-0.68394	7.71311	4.152730	891.788	9.781
MCTS+RS	0.250	62.0	4/10	-4.52952	2.80386	4.995340	355.163	4.198
MCTS+HC	0.250	74.4	5/10	-3.63763	2.02058	4.289398	676.262	7.774
MCTS+SA	0.250	74.6	7/10	-10.29078	-2.38069	3.744391	597.866	7.297
MCTS+RS	0.125	46.5	8/10	-6.27352	-1.28520	3.320830	170.078	2.996
MCTS+HC	0.125	68.1	8/10	-4.61933	-0.07330	4.719893	380.664	5.127
MCTS+SA	0.125	48.5	8/10	-6.43350	-0.69363	5.875865	304.758	5.225
MCTS+RS	0.000	64.5	2/10	-4.20689	6.83323	7.070816	325.054	3.510
MCTS+HC	0.000	41.0	4/10	-2.64884	1.95654	3.712926	430.037	5.589
MCTS+SA	0.000	78.0	2/10	-1.51834	4.81908	6.613282	558.383	5.834

Table 1: Comparison between MCTS and URS, given a budget of 100 simulations and varying the parameter  $C$  in order to balance exploration and exploitation in the search. The input signals have been split into 2 and 3 region.

### 3 Analysis of the results

In this section, a contextual analysis of the experimental results and of what are the factors which caused such results. Before analysing the results, we enforce that many problem was overcome in order to obtain and evaluate the proposed approach.

For example, randomness in Matlab is not always random as one would expect. In fact, at every startup the seed which generate the random sequence is the same, thus we had to further tweak the environment in order to avoid the risk to select a favorable configuration. Moreover, the object orientation in poorly handled in Matlab, especially when you decide to use a Simulink model. In fact, we faced with problems and poor performances caused by scope overloading. To solve these problems, we had to rewrite the all code avoiding object-orientation and only using scripts and global scopes. We did all our best to give structure and cleanliness to the code using packages and structs.

#### 3.1 Comments

The first experiments presented consider a fixed input space partitioning (2x3) and have been tested on both specifications S1 and S2, varying the parameter  $C$ .

**S1** *The engine speed never reaches 120.* Clearly the robustness function resulting by S1 is proportional to the brake signal and inversely proportional to throttle, *i.e.* high value of throttle and low value of brake lead to low robustness. As a consequence, minimizing the robustness should be quite straightforward, even using a greedy search, such as Hill Climbing.

According to this intuition, the best performing experiments are those with a reasonably small value for  $C = 0.125$ , as you can see in Table 1. Recall that a small  $C$  means give a bias towards exploitation rather than exploration. Thus, encouraging the exploitation reflects the monotonic



Experiments on specification S2

Algo	C	Avg Trace Falsification	Success Rate	Robustness			Time (sec)	
				min	avg	std dev	tot	trace
URS	- - -	- - -	0/10	0.02080	0.06130	0.03130	408.585	4.086
MCTS+RS	0.500	90.0	2/10	0.00000	0.05430	0.04420	397.635	4.056
MCTS+HC	0.500	53.0	7/10	0.00000	0.00490	0.00840	1039.426	15.517
MCTS+SA	0.500	- - -	0/10	0.00071	0.04930	0.04330	681.465	6.815
MCTS+RS	0.250	- - -	0/10	0.00661	0.03571	0.02372	572.351	5.723
MCTS+HC	0.250	29.1	9/10	0.00000	0.00023	0.00073	914.175	26.076
MCTS+SA	0.250	46.0	1/10	0.00000	0.06933	0.09205	941.542	9.977
MCTS+RS	0.125	42.7	3/10	0.00000	0.04101	0.03548	275.017	3.325
MCTS+HC	0.125	31.6	8/10	0.00000	0.00388	0.00843	497.749	11.466
MCTS+SA	0.125	76.3	4/10	0.00000	0.05349	0.11098	506.049	5.577
MCTS+RS	0.000	32.0	1/10	0.00000	0.14757	0.16817	473.518	5.113
MCTS+HC	0.000	36.6	5/10	0.00000	0.01148	0.01682	1322.240	19.317
MCTS+SA	0.000	- - -	0/10	0.00834	0.16304	0.14714	873.488	8.734

Table 2: Comparison between MCTS and URS, given a budget of 100 simulations and varying the parameter C in order to balance exploration and exploitation in the search. The input signals have been split into 2 and 3 region.

nature of the robustness of S1 and then exploiting promising regions gives back promising results.

The results obtained by MCTS and Hill Climbing (MCTS+HC) represent another evidence of this intuition. Furthermore, the computational overhead due to the Hill Climbing search is almost negligible. The reason is that the search proceeds almost straight, following the steepest hill of the robustness curve and then Hill Climbing easily finds not pejorative neighbour.

Conversely, favouring exploration (*e.g.*  $C = 0.5$ ) results in extremely poor results. In fact, the falsification rate is even worst than URS and the reason is that most of the budget is wasted in the exploration of the huge state space. Moreover, the overhead of Hill Climbing (MCTS+HC) and Simulated Annealing (MCTS+SA) is quite relevant because exploration of less promising regions leads to difficulties in finding not pejorative neighbours (MCTS+HC presents a net 2x overhead).

**S2** *If the vehicle gear is 3 then the speed is always greater than 20.* As already said in the Section 2.1, this specification is not trivial at all and a clever strategy is needed in order to do any falsification. Evidence of this is the fact that Uniform Random Sampling (URS) is never able to falsify such requirement, as can be observed from Table 2.

The best performing strategy here is again MCTS and Hill Climbing (MCTS+HC), which is able to falsify S2 specification 9 times out of 10 with  $C = 0.25$ .

Note that:

- The  $C$  hyper-parameter balances two factors, exploitation and exploration.
- The exploration factor is not normalized, typically is  $\in [0, 2.5]$ .
- The exploitation is normalized  $\in [0, 1]$ .

The ratio among the two factors is in the order of 2.5. Then, using  $C = 0.25$ , this ratio is mapped into a more reasonable and performing 0.6 factor which favours exploitation and maintains exploration.

Experiments on different partitioning

Algo	Part	Avg Trace Falsification	Success Rate	Robustness			Time (sec)	
				min	avg	std dev	tot	trace
URS	- - -	- - -	0/10	0.02080	0.06130	0.03130	408.585	4.086
MCTS+RS	2x3	90.0	2/10	0.00000	0.05430	0.04420	397.635	4.056
MCTS+HC	2x3	53.0	7/10	0.00000	0.00490	0.00840	1039.426	15.517
MCTS+SA	2x3	- - -	0/10	0.00071	0.04930	0.04330	681.465	6.815
MCTS+RS	2x2	70.0	3/10	0.00000	0.06517	0.06197	631.963	6.804
MCTS+HC	2x2	48.7	7/10	0.00000	0.00099	0.00163	1479.660	22.530
MCTS+SA	2x2	- - -	0/10	0.00561	0.05776	0.02567	1393.552	13.936

Table 3: Comparison of search algo with fixed  $C=0.5$  and varying the input space partitioning. Test on spec S2.

Finally, in the experiments which falsify the specification, the number of simulated trace is surprisingly small, as reported by the column *Avg Trace Falsification*. This is due the effectiveness of the search algorithm and highlights their performance.

**Execution Times** In conclusion, a brief consideration of the execution time is worth to be made. However, even if the performances for Hill Climbing are quite good even for this non-trivial specification, they come with a higher cost. The *Time* column of Table 2 highlights that the time needed to simulated a single trace with MCTS+HC is 26.076 seconds, compared with 5.723 seconds needed for MCTS+RS and 9.977 seconds for MCTS+SA. Having a cluster of multiple machines would allow to test multiple configuration of the same experiment and exploit *a posteriori* those configurations which expand the tree, pruning those configurations which waste time on not relevant regions.

Comparing the times of the several MCTS implementations with the Uniform Random Sampling (URS), one can notice that the overhead of MCTS layer is minimal. In fact, the difference between the overall times for URS and MCTS+RS is not relevant and then, we can conclude that the upper layer is performed with a little overhead. Unfortunately, this is only true when using Random Sampling as search algorithm. Any other search algorithm ends up in a more consistent overhead, after all *there is no free lunch*.

**State Space Partitioning** Table 3 show another direction of tests we investigated on. In such experiment, the state space is partitioned in a different way: the throttle and the brake has been divided into two regions (2x2) or in two and three regions respectively (2x3), as in the previous experiments. This may sound as a pointless modification but it opens up the scenario described till now to a new perspective. This new partitioning induces a MCTS tree with a smaller branching factor (4 vs 6). Direct consequence is that:

1. The space partitioning is coarse grained.
2. MCTS has an higher view of the search space.
3. Lower branching factor allow the MCTS to finish earlier the tree building.
4. The effort is moved to the search algorithm in the rollout phase.

The experiments done are only a few and still far to a conclusion. However, they produce a slight improvement in Falsification Rate as well as Avg Trace Falsification. This fact sheds the light on the importance of hyper-parameter tuning because it could lead to a relevant boost in performances (see Section 3.2).

### 3.2 Hyperparameters

As already remarked, the role of hyper-parameters and the importance of a proper tuning of those is crucial for effectiveness of search algorithm. Having the computational power to do so, a proper grid search in the space of hyper-parameter should be performed to fine-tune the system and fully exploit its potentiality. The hyper-parameters that should be investigated are the following:

1.  $C$ : in order to balance exploration and exploitation and to better combine MCTS with a given search strategy.
2. Space partitioning: in order to control MCTS branching factor.
3. Disturbance quantization: in order to control the search space and to avoid its explosion.
4. Control Points: in order to define the degree of freedom of the simulation itself.

Clearly a full search is prohibitive thus a clever approach should be devised in order to performs hyper-parameters optimization.

## 4 Conclusion

To conclude the work presented, we decided to briefly propose some future develops that may enchant the system implemented.

- A learning model can be used to learn  $C$  and adjust it at run time adaptively in a reinforcement learning fashion.
- A non agnostic version of the system can be produced by using the specification to falsify to infer an ordering over MCTS nodes to bias toward know-to-be-good regions.
- An adaptive UCB normalization over the exploration parameter can be made at a given point in the simulation by catching the max value found up till that moment and using such value as a scaling factor for the original exploration factor.

The system presented, which eventually obtains good performances, could largely benefits form all this tree new directions.

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