

Minimizing decision tree representation of controller strategy

Andreas Holck Høeg-Petersen¹, Kim Guldstrand Larsen¹, Peter Gjøøl Jensen¹,
Andrzej Wasowski²

¹ Aalborg University, Denmark

² IT University of Copenhagen, Denmark

Abstract. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetur id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

1 Introduction

With the tool UPPAAL Stratego [1] it is possible to learn safe and (near-)optimal strategies for controllers of any system that can be modelled as a Markov Decision Process (MDP). This has many important applications, one being the government of cyber-physical systems that often have important safety requirements to avoid real-world catastrophes while also needing to perform at a certain level of expectation to satisfy consumers, citizens or other participants in a network.

For these cases of cyber-physical systems – especially within critical infrastructure such as water management, transport or energy distribution — another important feature of a controller is that it is explainable and understandable by a human expert. A well-established technique for representing machine learning strategies in ways interpretable by humans is with decision trees, where the path from a root node to a leaf node directly specifies how a state of the system is evaluated so that a specific action is decided upon.

In UPPAAL Stratego the strategies learned are represented by a collection of decision trees, one for each action. The leaf nodes of each tree then gives an evaluation of the expected cost of taking that action in the state under evaluation. In Q-learning, the Reinforcement Learning technique powering UPPAAL Stratego, this is called the Q-value and as such, we call the trees Q-trees. While this approach allows for an online discretization of a continuous state space and

improved approximation of the optimal strategy, it does not retain the expressive nature of the decision tree representation of its strategy, as each decision is now an argmin function over the unique evaluation of the expected cost of state-action pairs.

In this paper, we therefore suggest a method for converting a set of Q-trees to a single decision tree representing the same deterministic strategy that the argmin over the set of Q-trees would yield. This makes UPPAAL Stratego able to not only give safe and near-optimal strategies but also to provide them in a fashion that has the benefits of decision tree representation.

However, we often see that the number of paths in these trees grows very large, which again makes them exceedingly hard for humans to actually comprehend. Furthermore, since many controllers of cyber-physical systems will run on embedded hardware with limited space and memory capacity, large strategies might be impossible to even run get running in these systems. Therefore, we also provide an algorithm for minimizing the number of leaf nodes the decision tree by inspecting the Euclidean state space of the system under consideration and the partitions that the strategy entails.

Example 1 As a running example, we consider an artificial strategy σ with a Q-table given by Table 1. The state space $\mathcal{S} \in \mathbb{R}^2$ of the underlying environment is given by $x \in [0, 3]$ and $y \in [0, 3]$ and the set of possible actions is $Act = \{a, b, c\}$. Each entry in the Q-table is a tuple (a, b, c) representing the Q-value (cost) of each of the three actions in that state. The dimensionality of the Q-table is $3 \times 3 \times 3$ and it has 27 Q-entries.

Table 1: Q-table for example strategy. Each entry is a tuple of the Q-values (expected cost) of action a , b and c respectively for some configuration of x and y .

| | $0 < x \leq 1$ | $1 < x \leq 2$ | $2 < x \leq 3$ |
|----------------|----------------|----------------|----------------|
| $0 < y \leq 1$ | (2, 7, 3) | (4, 3, 1) | (6, 8, 1) |
| $1 < y \leq 2$ | (3, 4, 4) | (3, 2, 4) | (3, 5, 9) |
| $2 < y \leq 3$ | (3, 3, 1) | (4, 3, 1) | (2, 7, 3) |

2 Preliminaries

We start by defining some relevant concepts.

Definition 1 (Partitions). A partitioning \mathcal{A} of the state space $\mathcal{S} \in \mathbb{R}^K$ is a set of regions ν that divides \mathcal{S} such that $\bigcup_{\nu \in \mathcal{A}} \nu = \mathcal{S}$ and for any two regions $\nu, \nu' \in \mathcal{A}$ where $\nu \neq \nu'$ it holds that $\nu \cap \nu' = \emptyset$. Each region ν can be expressed in terms of two points, s^{\min} and s^{\max} , so that for each $s = (s_1, \dots, s_K) \in \nu$ it holds that $s_i^{\min} < s_i \leq s_i^{\max}$ for $i = 1, \dots, K$.

Evidently, any discretization of a state space $\mathcal{S} \in \mathbb{R}^K$ is effectively a partitioning. For example, the Q-table in Table 1 corresponds to the partitioning $\mathcal{A} = \{((0,0), (1,1)), ((1,0), (2,1)), \dots, ((1,2), (2,3)), ((2,2), (3,3))\}$.

Definition 2 (Decision tree). A binary decision tree over the domain $\mathcal{S} \in \mathbb{R}^K$ is a tuple $\mathcal{T} = (\eta_0, \mathcal{N}, \mathcal{L})$ where $\eta_0 \in \mathcal{N}$ is the root node of the tree, \mathcal{N} is a set of branching nodes and \mathcal{L} is a set of leaf nodes. Each branch node $\eta \in \mathcal{N}$ consists of two child nodes and a predicate function of the form $\rho(s) = s_i \leq c$ with $s \in \mathcal{S}$ and c being a constant. Each leaf node $\ell \in \mathcal{L}$ is assigned a label from a set of labels \mathcal{U} .

For a decision tree \mathcal{T} , we can obtain a decision $\delta = \mathcal{T}(s)$, $\delta \in \mathcal{U}$ from any state $s \in \mathcal{S}$ by following the *path* from the root node to a leaf by evaluating $\rho(s)$ at every branch node and continuing the path at the left child if the predicate is true and at the right child otherwise. Further, we also allow evaluating a region of \mathcal{S} . Given a region $\nu = (s^{\min}, s^{\max})$, $[\delta]_\nu = \mathcal{T}(\nu)$ is the set of all decisions that can be obtained evaluating configurations of ν , ie. $\mathcal{T}(\nu) = \{\mathcal{T}(s) \mid s \in \nu\}$.

For any node η in the tree (branching or leaf) the predicates along the path to this node defines a region ν and we denote this as $\nu = \lambda(\eta)$. In this way, we say that \mathcal{T} induces a partitioning $\mathcal{A}_\mathcal{T} = \{\lambda(\ell) \mid \ell \in \mathcal{L}\}$. For any region ν and a decision tree \mathcal{T} we say, that ν has *singular mapping* in \mathcal{T} if for all $p \in \nu$, $\mathcal{T}(p) = \delta$ for some $\delta \in \mathcal{U}$. Naturally, all regions in $\mathcal{A}_\mathcal{T}$ has singular mapping in \mathcal{T} . For any partitioning \mathcal{B} of the same state space, we say \mathcal{B} *respects* \mathcal{T} if and only if every region $\nu \in \mathcal{B}$ has singular mapping in \mathcal{T} .

3 MaxPartitions algorithm

Since state space discretization for Reinforcement Learning is usually done *before* any learning takes place, the discretization is likely to create adjacent discrete states that are mapped to the same optimal action. The question we would then like to answer is this: if \mathcal{T} is a decision tree representing a trained strategy and $\mathcal{A}_\mathcal{T}$ is its induced partitioning, can we find another partitioning \mathcal{B} which is smaller than $\mathcal{A}_\mathcal{T}$ but still respects \mathcal{T} ?

As an example, we can consider the toy strategy from Example 1. In Figure 1 the strategy is represented as a decision tree (1a) by omitting the specification of cost values of each action and only preserving the optimal action for each discrete state. On the right (1b) is a 2D visualization of the induced partitioning of the state space. It can easily be assessed, that the partitioning has several redundant splits where areas of the same color (meaning they suggests the same optimal action) are split in two. For instance, the region $((0,0), (1,1))$ and the region $((0,1), (1,2))$ both specify a as the optimal action, and we could replace these two regions with a single one given by $((0,0), (1,2))$. Since each region is represented in our decision tree as a leaf node, the fewer regions we have the smaller a tree we need to represent it.

We start by stating the problem of finding maximum sized regions as a problem of local optimization: Given a starting point s^{\min} , find s^{\max} such that

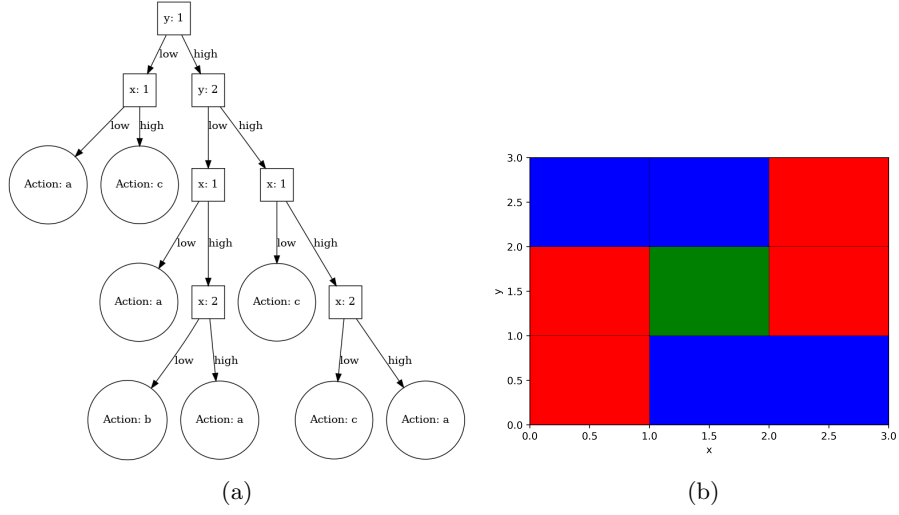


Fig. 1: Two representations of the toy strategy introduced in Example 1. In (a) the Q-table is represented as a decision tree. In (b) a 2D visualization of the state space partitioning is showed, where the colors indicate what the optimal action is in that area of the state space (red for a , green for b and blue for c).

$\nu = (s^{\min}, s^{\max})$ has singular mapping in \mathcal{T} while no other region $\nu' = (s^{\min}, s')$ where $s'_j = s_j^{\max}$ for $j = 1, \dots, i-1, i+1, \dots, K$ and $s'_i > s_i^{\max}$ has this property.

3.1 Details of the algorithm

We introduce a new notation to refer to individual bounds on the dimensions in \mathcal{T} . We denote by \mathcal{T}_i the sorted list of bounds on dimension i and by $\mathcal{T}_{i,j}$ the j th smallest bound on dimension i for each $j = 1, 2, \dots, |\mathcal{T}_i|$. This can be precomputed as a matrix in log-linear time by collecting and sorting the bounds on all branch nodes in \mathcal{T} and allows accessing $\mathcal{T}_{i,j}$ in constant time.

Exploiting this notation, if p is a K -dimensional vector of index pointers to bounds in \mathcal{T} , such that $p_i \in p$ is a pointer to \mathcal{T}_{i,p_i} , then we can define a point at an intersection of bounds in all K dimensions as $s_{\mathcal{T}}^p = (\mathcal{T}_{1,p_1}, \mathcal{T}_{2,p_2}, \dots, \mathcal{T}_{K,p_K})$. We will omit the subscript \mathcal{T} on $s_{\mathcal{T}}^p$ when it is clear from the context.

For the algorithm, we require that the domain of \mathcal{T} is bounded in all K dimensions. This can be achieved by including a minimum and a maximum bound for each dimension i , which is not represented by a branch node in \mathcal{T} . These limit bounds can be negative and positive infinity, in which case we say $\mathcal{T}_{i,1} = -\infty$ and $\mathcal{T}_{i,|\mathcal{T}_i|} = \infty$. Further, in a slight abuse of notation, we define $\mathcal{T}_{i,|\mathcal{T}_i|+1}$ to be some *sentinel* value representing that we are outside the boundaries of dimension i . Correspondingly, we define a sentinel action α , and we say that $\mathcal{T}(s_{\mathcal{T}}^p) = \alpha$ if and only if $\exists p_i \in p, p_i = |\mathcal{T}_i| + 1$.

The algorithm works by maintaining two vectors of index pointers, p^{\min} and p^{\max} , and iteratively increasing p^{\max} until a region $\nu = (s^{p^{\min}}, s^{p^{\max}})$ cannot be expanded further. The regions are stored in a list \mathcal{R} and a list \mathcal{P} is keeping track of the p^{\min} vectors to use as starting points for the region search. Initially, \mathcal{R} is empty and \mathcal{P} contains just a vector of K ones (ie. the vector pointing to the lowest bounds of all K dimensions). The algorithm is given in pseudo-code in Algorithm 1 while the following describes it in more detail.

Let p^{\min} be the result of popping the lexicographically smallest element of \mathcal{P} . We can then define $s^{\min} = s^{p^{\min}}$ as the ‘lower left’ corner in a region $\nu = (s^{\min}, s^{\max})$ where s^{\max} is the point we want to determine, so that ν has singular mapping in \mathcal{T} . By definition, $s^{\max} = s^{p^{\max}}$ satisfies this requirement for $p^{\max} = (p_1^{\min} + 1, \dots, p_K^{\max} + 1)$, since no branch node in \mathcal{T} splits on a predicate c where $\mathcal{T}_{i, p_i^{\min}} < c < \mathcal{T}_{i, p_i^{\min} + 1}$ for any $i = 1, \dots, K$.

We can now increase p^{\max} by 1 in any dimension i and test for singular mapping in our new region. Additionally, we require that the point $s^{p^{\max}}$ is not already covered by a region in \mathcal{R} , as this would result in overlapping regions. Let \hat{e}_i denote the unit vector parallel to axis i , such that $p + \hat{e}_i = (p_1, \dots, p_i + 1, \dots, p_K)$. Then, the updated region is given by $\nu = (s^{\min}, s^{p^{\max} + \hat{e}_i})$. If $|\mathcal{T}(\nu)| = 1$ and $\forall \nu' \in \mathcal{R}, s^{p^{\max} + \hat{e}_i} \notin \nu'$, then the update did not violate the singular mapping property and we can set $p^{\max} = p^{\max} + \hat{e}_i$. Otherwise, we mark dimension i as *exhausted* so we know not to increase in this dimension again. We then continue, choosing a new dimension not marked as exhausted.

This process is repeated until all dimensions have been exhausted at which point, p^{\max} together with the unchanged p^{\min} defines a region $\nu = (s^{p^{\min}}, s^{p^{\max}})$ that has singular mapping in \mathcal{T} and cannot be expanded further in any dimension. More generally, we can say that given p^{\min} we want to choose $p^\Delta \in \mathbb{Z}^K$ such that $\nu = (s^{p^{\min}}, s^{p^{\min} + p^\Delta})$ has singular mapping in \mathcal{T} and no other $p^{\Delta'} > p^\Delta$ has this property.

Having found ν , we add it to \mathcal{R} . Further, we add to \mathcal{P} all the points we can create from taking p^{\min} and setting $p_i^{\min} = p_i^{\max}$ for all i where $p_i^{\max} < |\mathcal{T}_i|$. These points will later be popped and used as a new p^{\min} for a search for a large region. If \mathcal{P} is not empty, we repeat the entire process, otherwise the algorithm terminates and returns \mathcal{R} which now represents a new partitioning that respects \mathcal{T} .

3.2 Analyzing the algorithm

In the following we provide an upper bound of the running time of MAXPARTITIONS and a proof of correctness.

Running time The first thing to notice is the outer while loop over \mathcal{P} . Points are dynamically added to \mathcal{P} every time a new region is constructed, and in the worst case, K new points (one for each dimension) are added for each region. The number of regions that can be found and constructed is bounded by the size of the original partition $\mathcal{A}_{\mathcal{T}}$, as the worst case is when $\mathcal{A}_{\mathcal{T}}$ is already a minimal

Algorithm 1 MaxPartitions

Require: \mathcal{T} : A binary decision tree over the domain \mathbb{R}^K inducing the partitioning $\mathcal{A}_{\mathcal{T}}$

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1:  $\mathcal{R} \leftarrow \{\}$ 
2:  $\mathcal{P} \leftarrow \{\mathbf{1}^K\}$   $\triangleright \mathbf{1}^K$  is a  $K$ -dimensional vector of ones
3: while  $\mathcal{P}$  is not empty do
4:    $p^{\min} \leftarrow \min \mathcal{P}$   $\triangleright$  Lexicographic min
5:    $\mathcal{P} \leftarrow \mathcal{P} \setminus \{p^{\min}\}$   $\triangleright$  Remove  $p^{\min}$  from  $\mathcal{P}$ 
6:   if  $s_{\mathcal{T}}^{p^{\min}} \notin \mathcal{R}$  then  $\triangleright$  Check  $s_{\mathcal{T}}^{p^{\min}}$  has not been covered yet
7:      $p^{\max} \leftarrow p^{\min} + p^{\Delta}$   $\triangleright$  Select largest  $p^{\Delta}$ 
8:      $\mathcal{R} \leftarrow \mathcal{R} \cup \{(s_{\mathcal{T}}^{p^{\min}}, s_{\mathcal{T}}^{p^{\max}})\}$   $\triangleright$  Add new region to  $\mathcal{R}$ 
9:     for  $i = 1, 2, \dots, K$  do  $\triangleright$  Add points to  $\mathcal{P}$ 
10:      if  $p_i^{\min} \neq p_i^{\max}$  and  $p_i^{\max} < |\mathcal{T}_i|$  then
11:         $\mathcal{P} \leftarrow \mathcal{P} \cup \{(p_1^{\min}, \dots, p_i^{\max}, \dots, p_k^{\min})\}$ 
12: return  $\mathcal{R}$ 

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partitioning that respects \mathcal{T} . In this case, the algorithm will produce $\mathcal{R} = \mathcal{A}_{\mathcal{T}}$ and the number of regions will necessarily be the same. Let $N = |\mathcal{A}_{\mathcal{T}}|$. Then we can state that the outer while loop is bounded by $O(KN)$.

How about finding p^{Δ} ? The procedure is to increment by 1 in any one unexhausted dimension and then check for the validity of that increment. This check has two components: (a) check if the new region still has singular mapping in \mathcal{T} and (b) check if the new region overlaps with any region already in \mathcal{R} . Let $\nu = (s^{\min}, s^{\max})$ be the candidate region for some $p^{\Delta} = \mathbf{1}^K + \hat{\mathbf{e}}_i$ (ie. so $s^{\max} = s^{p^{\min} + p^{\Delta}}$).

For (a), we have to query $\mathcal{T}(\nu)$ which visits all leaves in $l \in \mathcal{T}$ for which $\lambda(l) \cap \nu \neq \emptyset$. Let us denote this set by \mathbf{L}_{ν} and say has size L . The analysis of this operation is complicated. First of all, we have no guarantee that the tree is balanced. If we assume that it is, then the path from the root to a leaf is $O(\log T)$ where $T = (2N) - 1$ is the size of the tree.

Assuming the tree is balanced, the length of the path from the root node to a leaf node is logarithmic in the number size of the tree. However, to query $\mathcal{T}(\nu)$ we do not need to do a $O(L \log N)$ operation. Consider two leaves, $l_j, l_k \in \mathbf{L}_{\nu}$, that share the same path until their common parent node splits them. We only need to follow the path to the parent once and then go to l_j and l_k respectively. In general, if we by $\omega(l)$ denote the set of nodes on the path from the root node to a leaf l , then we need $|\bigcup_{l \in \mathbf{L}_{\nu}} \omega(l)|$ operations to retrieve \mathbf{L}_{ν} .

3.3 From regions to decision tree

The output of the MAXPARTITIONS algorithm is a list of regions with associated actions. For this to be of any use, we need to construct a new decision tree to represent these state-action pairs. To this goal, we face the issue that it is not given (and in fact, very unlikely) that the suggested partitioning can be perfectly represented by a decision tree, as this would require the existence of enough ‘clean splits’ (ie. predicates on some variable that perfectly divides the

regions into two sets with an empty disjunction) to arrange the entire set of regions.

Therefore, we suggest a brute-force algorithm that tries to separate the regions as cleanly as possible. Let \mathbf{R} be a list of regions $\nu \in \mathbf{R}$ with a_ν being the action associated with ν . We iteratively create a branch node that splits \mathbf{R} into two, \mathbf{R}_{low} and \mathbf{R}_{high} , based on a predicate function $\rho(x_i, c) = x_i \leq c$ with $c \in \mathbb{R}$ so that $\mathbf{R}_{low} = \{\nu \in \mathbf{R} \mid \nu_{i,\min} \leq c\}$ and $\mathbf{R}_{high} = \{\nu \in \mathbf{R} \mid \nu_{i,\max} > c\}$. When the list only contains a single element ν , we create a leaf node with action a_ν and return.

The question is how to determine $\rho(x_i, c)$, more specifically which variable x_i to predicate on and at which value c . Ideally, we want to split \mathbf{R} in two equally sized subsets and in a way that no single region would have to occur in both, ie. we would like $\mathbf{R}_{low} \cap \mathbf{R}_{high} = \emptyset$. For this we define an impurity measure $I(\mathbf{R}_{low}, \mathbf{R}_{high})$ that penalises the difference in size between \mathbf{R}_{low} and \mathbf{R}_{high} and the size of the disjunction between the two. Let $abs(a)$ be the absolute value of a and let $|b|$ denote the size of a set b , then

$$I(\mathbf{R}_{low}, \mathbf{R}_{high}) = abs(|\mathbf{R}_{low}| - |\mathbf{R}_{high}|) + |\mathbf{R}_{low} \cap \mathbf{R}_{high}|$$

Our brute-force way of finding the predicate that minimizes I is to iterate over the dimensions in \mathcal{S} and for each dimension i we sort the regions according to their upper bound. Let $\mathbf{R}_i = \{\nu^1, \nu^2, \dots, \nu^n\}$ be the list sorted according to the i th dimension so that for all ν^j, ν^{j+1} it holds that $\nu_{i,\max}^j \leq \nu_{i,\max}^{j+1}$. If we then let $\rho(x_i, c) = x_i \leq c$ with $c = \nu_{i,\max}^j$ we have $|\mathbf{R}_{low}| = j$ and $|\mathbf{R}_{high}| = n - j$. For determining the size of $\mathbf{R}_{low} \cap \mathbf{R}_{high}$ we simply need to count the number of regions ν^{j+m} for $m = 1, 2, \dots, n - j$ whose lower bound is less than our predicate bound c , since these regions will appear both in \mathbf{R}_{low} (because then, by definition, $\rho(x_i, c) = x_i \leq c$ will be true for $x_i = \nu_{i,\min}^{j+m}$ and $c = \nu_{i,\max}^j$) and in \mathbf{R}_{high} (because our sorting ensures that for all ν^j, ν^{j+m} it holds that $\nu_{i,\max}^j \leq \nu_{i,\max}^{j+m}$).

Now we can write our impurity measure in terms of these quantities:

$$I(\mathbf{R}_{low}, \mathbf{R}_{high}) = abs(j - (n - j)) + \sum_{m=1}^n \mathbb{1}(\rho(\nu_{i,\min}^{j+m}, \nu_{i,\max}^j)), \quad \text{for all } \nu^j \in \mathbf{R}$$

where $\mathbb{1}$ is the indicator function, \mathbf{R} is the list of regions sorted according to upper bound and \mathbf{R}_{low} and \mathbf{R}_{high} are the subsets resulting from splitting on the predicate function $\rho(x_i, c) = x_i \leq c$ with $c = \nu_{i,\max}^j$ so that $\mathbf{R}_{low} \subsetneq \mathbf{R}$, $\mathbf{R}_{high} \subsetneq \mathbf{R}$ and $\mathbf{R} \subseteq \mathbf{R}_{low} \cup \mathbf{R}_{high}$.

Finding the best split, ie. the one that minimizes the impurity, is a $O(Kn^2)$ operation, as it requires a nested loop through all the regions for each of the K dimensions (the nested loop being the final summation term over $m = 1, 2, \dots, n - j$ for all $j = 1, 2, \dots, n - 1$). In this work, we have not attempted to find a faster implementation as we found that the size of \mathbf{R} obtained by using our MAXPARTITIONS algorithm did not cause performance issues.

4 From Q-trees to Decision Tree

4.1 Defining Q-trees

In Reinforcement Learning [2] an agent is trying to estimate the expected value (cost or reward) of taking an action A in a state S . This is called the Q-value. Let Act be a finite set of actions and let $\mathcal{S} \in \mathbb{R}^K$ be the state space (a bounded K -dimensional euclidean space) then the goal is to learn the function $Q(s, a) : \mathcal{S}, A \mapsto \mathbb{R}$ that for any $s \in \mathcal{S}$ and $a \in Act$ maps to the Q-value of the state-action pair.

When \mathcal{S} is continuous, the Q-function either has to be approximated or the state space needs to be discretized. In the latter case, \mathcal{S} can be redefined in terms of well-defined bounded subspaces where each $S \in 2^{\mathbb{R}^K}$ now defines a smaller area of the original state space \mathcal{S} and we by $S_{i,lower}$ and $S_{i,upper}$ respectively denote the lower and upper bound of dimension i in S . Further, we require that $\bigcup_S S = \mathcal{S}$.

For evaluating a particular state s , we say that $S = s$ iff $S_{i,lower} \leq s_i < S_{i,upper}$ for all $i = 1, \dots, K$. This allows for a tabular representation of $Q(s, a)$, where the function is essentially just a lookup-table with $|\mathcal{S}| \times |Act|$ entries. The disadvantage of this approach is that the Q-table quickly grows very large and that many of the discrete states are irrelevant (in the sense that they are never actually visited). This can be remedied if close care is taken to designing the discretization, but this would in itself impose bias onto the learning.

UPPAAL Stratego approaches the task of discretizing the state space in a different way. Instead of schematically discretizing \mathcal{S} *a priori* to the training, discretization is part of the Q-value estimation. What happens is ...

The result is a strategy represented by a set of binary decision trees, each pertaining to a specific action in $a \in Act$, and whose leaf nodes carries the Q-value of taking action a in the state s defined by the constraints in the branch nodes on the path from the root to the leaf. We call these trees *Q-trees* and denote by \mathcal{T}_A the Q-tree for action $A \in Act$ and we define $\mathcal{T}_A(s) = Q(s, a)$ when $A = a$. Given the complete set of Q-trees the matter of choosing the optimal action in a state s can — for a greedy policy π and with the Q-values representing expected cost — be defined as $\pi(s) = \operatorname{argmin}_{a \in Act} \mathcal{T}_A(s)$.

4.2 Converting to decision tree

With Definition ?? we can now consider how to construct a single decision tree \mathcal{T} so that $\pi(s) = \operatorname{argmin}_{a \in Act} \mathcal{T}_A(s) = \mathcal{T}(s)$ for all $s \in \mathcal{S}$. That is, instead of a Q-tree we will construct a decision tree where the leaf nodes carries the action A that satisfies $A = \operatorname{argmin}_{a \in Act} \mathcal{T}_A(\lambda(l))$ for a given leaf l . In the following, we will present the procedure for doing so in general terms while the full specification of the algorithm is available in Appendix A.

First, let \mathcal{L} be the set of every leaf in the set of Q-trees and let each leaf $l \in \mathcal{L}$ be defined as $l = (S^l, a_l, q_l)$ where $S^l = \lambda(l)$ in \mathcal{T}_A , a_l is the action of the Q-tree l originally belonged to and q_l is the Q-value of taking action a_l in state S^l (we

The introduction of a partitioning \mathcal{A} and regions ν which I describe in Section 3 should probably come here instead.

use superscripts in S^l to avoid notational clutter when we later need to index variables and bounds in S^{l_i} and S^{l_j} at the same time). We sort \mathcal{L} in ascending order according to q_l (meaning l_0 has the best Q-value of any leaf) and use the first leaf, l_0 , to build the first path in the tree. This path requires $2 \times K$ branch nodes, one for each lower and upper bound of each dimension in S^l .

The decision about the order in which to predicate the branch nodes on each variable bound can and will greatly affect the size of the tree. However, as determining the optimal ordering of predicates is computationally infeasible [3], we will simply resort to a randomized picking order. For the root node v_0 , we thus pick a variable i and a bound j at random and set $\rho(v_0) = x_i \leq c$ where $c = S_{i,j}^{l_0}$. If j is a lower bound, then we set the left child node to a dummy leaf (we will complete this subtree later) and construct a new branch node for the right child from the remaining pairs of i, j in S^{l_0} and vice-versa if j is an upper bound. We continue this procedure until $S^{l_0} = \lambda(l_0)$ holds true in the tree under construction.

For inserting the another leaf, l_j , we now need to check at each branch node v_m whether we should insert in the left subtree, in the right subtree or in both. In other words, we do two checks: if $\rho(v_m)$ is *true* for $x_i = S_{i,lower}^{l_j}$ we continue the insertion procedure in the left subtree. If $\rho(v_m)$ is *false* for $x_i = S_{i,upper}^{l_j}$ we *also* insert l_j into the right subtree. If both cases evaluates to *false*, we *only* do the insertion in the right subtree. If we encounter a dummy leaf, we either construct a new branch node as we did for the initial path, ie. by randomly picking a still unchecked variable and bound to use for the predicate function, or — in the case that $S^{l_j} = \lambda(l_j)$ already holds true for the tree under construction — simply insert l_j instead of the dummy.

If we encounter a non-dummy leaf we can exploit the fact that the leaf nodes are inserted in a sorted order according to their Q-values. This ensures that if we encounter l_i during insertion of l_j then we know that $q_i \leq q_j$ and we can therefore safely stop the insertion of l_j (in this particular subtree) as we know that for all $s \in S^{l_i} \cap S^{l_j}$ it must hold true that $\pi(s) = a_i$.

When all leaf nodes from the set of Q-trees have been processed the resulting tree \mathcal{T} represents the exact same strategy but now without any notion of Q-values. In the Python library built for this paper, it is possible to export a decision tree representation to a Q-tree representation that can then be imported into UPPAAL **Stratego** in order to test the performance of the strategy. This is done by for each $A \in Act$ creating \mathcal{T}_A as a copy of \mathcal{T} and then for every leaf l setting $q_l = 0$ if $a_l = A$ and $q_l = 999$ if $a_l \neq A$.

5 Minimization techniques

As we can give no guarantees to the minimality of the decision tree created from a set of Q-trees, \mathcal{T} can grow very large and even contain more paths than all the Q-trees combined. This is unwanted, and we therefore present several minimization techniques that can drastically decrease the size of \mathcal{T} .

This subsection and the next (Section 5.1 and 5.2) I am not at all certain about how to actually approach yet. The simple pruning is so simple, that it is almost redundant to describe and the analytical pruning is only partially implemented and not very systematic yet.

5.1 Simple pruning

The algorithm described in Section 4.2 naively inserts leaf nodes without any consideration of optimality (except what little is given from the fact that leaf nodes are inserted in order of Q-value). This yields some obvious cases where branch nodes can be pruned away.

Say we have a path $p = \{v_0, v_1, \dots, v_n\}$ where both children of v_n are leaf nodes, l_i and l_j . If $a_i = a_j$ then the predicate at v_n bears no significance and we can replace that node with either l_i or l_j . Now the child of v_{n-1} that used to be v_n is a leaf, which might again result in a situation where v_{n-1} has two leaf children with the same action. Thus, we iteratively check for this condition all the way up through the tree, pruning any such cases.

Something something $\lambda(v_n) = \lambda(l_i) \cup \lambda(l_j) \wedge a_i = a_j \implies \pi(\lambda(v_n)) = a_i = a_j$.

5.2 Analytical pruning

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5.3 Empirical pruning

During training, the partitioning scheme used by UPPAAL Stratego to discretize the state space is explorative in the sense that it is non-deterministic when it creates new partitions. As it goes along, the algorithm discovers areas of interest where the choice of action seem to have greater impact on the overall cost and it then refines its partitioning in these areas.

This leads to somewhat abundance of partitions early on in the training, where more or less random splits turns out to not influence the decision making. These splits are carried on into the final strategy and they are also imported into our converted decision tree where the merging of the different Q-trees actually amplify this abundance.

This has two consequences. One is that the state space will be partitioned in such a way that neighboring partitions actually prescribe the same action, but do not necessarily appear as neighboring leafs in the strategy tree (ie. they do not have the same parent). We will deal with this problem in the Section 3. The other consequence is that we end up with a lot of leaf nodes that in practice will never be visited, as the system that is modeled either never end up in such a

state or because the strategy has the controller behave in such a way, that such a state is always avoided.

To deal with this, we employ a technique we call *empirical pruning*. In contrast to our other effort, this technique is not based on any analysis of the tree structure or state space but instead employs sample data to prune the tree of any leaf nodes that are either never or rarely visited. This has the drawback, that we lose our ability to give guarantees about the strategy, as our sampling *might* just miss an important edge case that our empirically pruned strategy then does not know how to handle. On the other hand, given a large enough sample, this risk is negligible since such a case would most likely have been just as rare during training, meaning the strategy would not even be ready to deal with it properly had it not been pruned from the tree.

The way it works is by gathering a sample of data points $D = \{s_0, s_1, \dots, s_T\}$ representing the state of the system at each time step during a run (or preferably several runs) where the controller acts according to a well trained strategy represented by the tree \mathcal{T} . For each state $s_t \in D$ we increase a counter at the leaf node at the end of the path that came from evaluating $\mathcal{T}(s_t)$.

When this process is done with a sufficiently large D , we can prune all the leaf nodes that were never visited or rarely visited. If we prune the never visited nodes, we call it *zero-pruning*. Pruning nodes visited once is called *one-pruning* and so forth. The pruning is simply done by removing every branch node with a leaf child that is never visited and instead ‘promoting’ the subtree that is its other child.

For example, if we have a path $p = \{\dots, v_{i-1}, v_i, v_{i+1}, \dots\}$ and v_i has a leaf node l for its other child and we see from sampling that l is never visited, then the constraint that v_i represent has no relevance for v_{i+1} . Therefore, we remove v_i and set v_{i+1} as a child of v_{i-1} instead. Doing this iteratively from the ‘left-most’ leaf and all the way through the tree can lead to substantial reductions, as we will show in Section 6, and provided that the sample size is large enough the performance of the pruned strategy stays on par with the original.

This entire intro should possibly be moved to the beginning of this section (Section 5). Also, I would like to be able to describe the ‘issue’ stemming from UPPAAL more precisely but for that, I probably need help from Peter.

6 Experiments

In this section, we will apply the techniques presented in the previous sections to the Bouncing Ball example introduced in [4]. In that example, a ball is given by its position and velocity as it bounces up and down from the floor. A controller is given the choice between two actions — hit or do nothing — and is tasked with keeping the ball bouncing for as long as possible with as few hits as possible.

We perform the following steps:

- Synthesize a strategy in UPPAAL Stratego. This gives us two Q-trees (one for $a = 1$ (hit) and one for $a = 0$ (no hit)) with a combined number of paths 13,405.
- Convert the Q-trees to a single decision tree following the procedure described in Section 4. The conversion is followed by simple pruning (Sec-

tion 5.1). The resulting tree has 84,336 paths and the entailed partitioning can be seen in Figure 2a.

- Run the **MaxPartitions** algorithm on the converted tree. This reduces the number of partitions to only 703.
- Construct a decision tree to represent the new partitioning as described in Section 3.3. This gave a tree with 892 paths. The resulting partitioning is seen in Figure 2b.
- Generate samples from 1000 runs with a maximum of 300 time steps each, logging the state at every 0.5 time step. This gives 600,000 sample data points which we use for empirical pruning, resulting in a tree of just 189 paths.
- *Now maybe something about my analytical pruning that got the tree down to just 164 paths*
- Export all versions of the strategy to UPPAAL Stratego format and compare performance on the system. Results are shown in Table 2.

A couple of things are of notable interest here.

First, converting the strategy from a set of Q-trees to a decision tree vastly increases the total number of paths. Without any minimization effort, it seems that the decision tree of size 84,336 does not yield any particular advantages in terms of explainability and interpretability compared to the two Q-trees with a combined size of 13,405 paths. For cases where there are more variables or possible actions, this would most likely pose an even greater issue.

Table 2: Comparing the performance of controllers for the bouncing ball example over 1000 runs for 120 time steps each before and after various attempts at minimizing the size through either empirical pruning or the **MaxPartitions** algorithm.

| Version | Paths | Expectation (hits) | Deviation |
|--------------------------|--------|--------------------|-----------|
| Q-trees | 13,405 | 38.401 | 0.177 |
| Original DT | 84,336 | 38.431 | 0.178 |
| MaxPartitions | 895 | 38.435 | 0.177 |
| MaxPartitions then Prune | 189 | 38.347 | 0.173 |

Second, the effect of **MaxPartitions** is a drastic reduction in the number of partitions. Even though the list of regions cannot be perfectly represented by a decision tree and the number of paths in the constructed tree thus increases a bit, the tree of size 892 is a decisive improvement from both the original set of Q-trees and the especially the converted tree.

Third, the decrease in the number of paths after empirically pruning the tree indicates that many areas of the state space are never visited in practice. It is also remarkable, that by utilizing this sample data we can further reduce the already minimized tree by a factor of 4 without sacrificing performance.

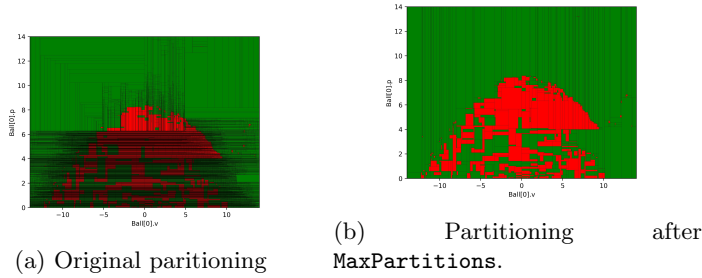


Fig. 2: A 2D visualization of the partitioning (dotted lines) of the state space before and after `MaxPartitions`. The x-axis is velocity and the y-axis is the balls position. Green areas represents the action ‘no hit’, red areas represents ‘hit’.

6.1 dtControl

The tool `dtControl` [5] has the ability to take a synthesized strategy represented as a look-up table and convert the representation to a decision tree that respects the safety requirements but compresses the size immensely. This is naturally of great interest for our case, but both the Q-tree representation and our own decision tree conversion alters the setup somewhat.

However, even though the tool actually supports directly working with the output format of UPPAAL Stratego, this is only the case for strategies learned using the `control[]` directive, which controls for certain defined safety parameters to always be respected. In our case of the bouncing ball example, the controller is trained with the `minE[]` directive, which minimizes a given parameter (in this case, the number of times the controller hits the ball).

Instead, we had to create our own output files to use as input for `dtControl`. According to the documentation, a controller strategy can be specified in a simple CSV format where each line contains an allowed state/action pair, that is, N values representing a state where the following M values constitutes an allowed action. For example, in the case of the bouncing ball, we have two state variables (position and velocity) and one action variable (hit or not hit), meaning each line would have three values.

We have attempted two experiments with different ways of specifying our original controller.

In the first experiment, we used the trained controller to generate 30,000 samples of state/action pairs. That is, the UPPAAL model was run for 300 time steps with the trained controller deciding what action to take in each encountered state and then the state/action pairs were logged at each 0.01 time step.

In the second experiment, we converted the strategy a set of Q-trees (the initial UPPAAL format) to a DT as described in Section 4. This DT had a partition size (number of leaves/paths) of 91,054. We used these partitions as the input data to `dtControl` by taking the maximum value of each variable in each individual partition together with the optimal action of that state. That

This is very experimental

is, we effectively specified the discretization of the state space by defining the bounds of each state paired with the allowed/optimal action.

Table 3: Comparing the performance of controllers for the bouncing ball example over 1000 runs for 120 time steps each before and after various attempts at minimizing the size through `dtControl`.

| Version | Paths | Construction time | Expectation (hits) |
|--------------|--------|-------------------|--------------------|
| Original DT | 91,054 | — | 38.431 |
| Samples | 27,234 | 8:14 | 318.411 |
| State bounds | 521 | 0:41 | 315.769 |

The results when applying the generated strategies to the model in UPPAAL are given in Table 3 together with the baseline original decision tree directly converted from the Q-tree set. As is seen, when we used samples, we still got a somewhat large DT that took more than 8 minutes to generate. And the performance (expected number of hits) is substantially worse than the baseline version. For the version based on state bounds, we got a much smaller tree with only 521 paths, but the performance was still very far from the original.

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Appendices

A Converting Q-trees to Decision Tree — Algorithm

The goal is to take all the leafs of a Q-forest and from these build a single binary decision tree, that through evaluation of a state arrives at a leaf node indicating the best action to take. The general idea of the algorithm is to repeatedly take the next leaf L_i in \mathcal{L} , which we (because of our sorting) know to have the best Q-value, and insert its action into the decision tree we are building so that it respects S_i . This means, that the internal nodes of the tree will still be checks on variables in \mathcal{V} .

A.1 Creating the root

We initialise the tree from the lowest valued leaf in \mathcal{L} which we will denote L_0 . The operation of inserting L_0 into the at this point empty tree requires special attention, since we have to create split nodes for all the variable bounds $(l_{0,i}, u_{0,i})$ in S_0 . We denote this operation **MakeRoot** and its pseudocode is given in Algorithm 2.

The operation iterates through all tuples $(u_{0,i}, l_{0,i})$ in S_0 and whenever it encounters a bound that is different from the limit (which we here assume to be infinity) it has to insert a new node into the tree. This is done via the **MakeNewNode** procedure, which we define as a helper function to avoid repetitions in the algorithm. This function takes the variable V_i that the encountered bound relates to, the value of the bound and the action of the leaf, we are inserting. It then creates a new internal node, that represents the partition according to the inequality $V_i \leq b$ where $b \in (u_{0,i}, l_{0,i})$.

Now, **MakeNewNode** also takes two additional arguments, one boolean to indicate if the bound is an upper bound or not and the current parent node (which might be **None**). If the bound is an upper bound, then we know that $Q(a_0) = q_0$ only holds if $V_i \leq u_{0,i}$. This means, that L_0 should be inserted somewhere in the left ('low') subtree of the newly created node, while the right ('high') subtree should for now just be set to some random leaf with a very poor Q-score (we will find better values for these subtrees when we process the remaining leaf nodes of \mathcal{L}).

Lastly, if the current parent node is not **None**, then we know it has one subtree that is set (like above) and one that itself is **None** as it is reserved for our newly created node. We therefore set the undefined child of the parent node to our new node and returns this new node, which is then marked as being the new parent node. If this our first new, we also mark it as our root node.

When we have processed all the bounds in S_0 , we insert L_0 at the 'free' spot in the parent node and return the root node. With this approach, we end up with an initial tree that is very shallow and basically only has one interesting leaf at the maximum depth of the tree.

A.2 Inserting the leaf nodes

To insert the remaining leaf nodes we need a couple of extra helper functions. The task is to identify or construct all the paths in the tree under construction

Algorithm 2 MakeRoot

```

1: procedure MAKENEWNODE(var, bound, action, isHigh, prevNode)
2:   node  $\leftarrow$  Node(var, bound)
3:   if isHigh then
4:     node.high  $\leftarrow$  Leaf(action,  $\infty$ , State( $\cdot$ ))
5:   else
6:     node.low  $\leftarrow$  Leaf(action,  $\infty$ , State( $\cdot$ ))
7:   if prevNode is not None then
8:     if prevNode.low is None then
9:       prevNode.low  $\leftarrow$  node
10:    else
11:      prevNode.high  $\leftarrow$  node
12:   return node

1: function MAKEROOT(Leaf(a0, q0, S0))
2:   rootNode  $\leftarrow$  None
3:   prevNode  $\leftarrow$  None
4:   for (l0,i, u0,i) in S0 do
5:     if u0,i <  $\infty$  then
6:       prevNode  $\leftarrow$  MAKENEWNODE(Vi, u0,i, a0, True, prevNode)
7:       if rootNode is None then
8:         rootNode  $\leftarrow$  prevNode
9:     if l0,i >  $-\infty$  then
10:      prevNode  $\leftarrow$  MAKENEWNODE(Vi, l0,i, a0, False, prevNode)
11:      if rootNode is None then
12:        rootNode  $\leftarrow$  prevNode
13:   if prevNode.low is None then
14:     prevNode.low  $\leftarrow$  Leaf(a0, q0, S0)
15:   else
16:     prevNode.high  $\leftarrow$  Leaf(a0, q0, S0)
17:   return rootNode

```

that leads to leaf nodes where the action of the leaf that are being inserted is to be preferred.

When we insert $L_i = (a_i, q_i, S_i)$, we will always either encounter an internal branch node that defines a split on a variable and has two subtrees, or we encounter a leaf node storing an action, a Q-value and a state partition. We therefore define a general Put function (Algorithm 3), that takes a root node and a leaf triplet to be inserted and decides what to do based on the type of the root node (either a branch node or a leaf node).

We will first deal with situation where we encounter an internal node, N_j , which splits on variable V_k at bound b . We now need to check on what side of this split S_i falls (it might be both). So we test on both $u_{i,k} > b$ and $l_{i,k} < b$. If the first check is true, then we know that S_i defines an area for V_k that can be larger than b , why we have to visit the right ('high') subtree of N_j . Likewise

Algorithm 3 Build decision tree from leaf nodes of Q-tree

```

1: function PUT(root, Leaf(a, q, S) )
2:   if root is Node then
3:     return PUTATBRANCHNODE(root, Leaf(a, q, S))
4:   else ▷ root is a Leaf
5:     return PUTATLEAFNODE(root, Leaf(a, q, S))

```

for the latter test, only then we have to continue our insertion in the left (‘low’) subtree. Note that both tests can be true.

We do, however, need to keep track of the implicit limitations we put on S_i as we go along. When continuing our insertion of L_i in the subtree of N_j defined by $V_k > b$, then we should reflect in S_i that now V_k has a lower bound b , that is, we should set $l_{i,k} = b$. We do this in the algorithm through an implicit helper function **SetLower**(*state*, *var*, *bound*) (and likewise **SetUpper** for updating the upper bound). The pseudocode for this is given in Algorithm 4.

Algorithm 4 PUT Q-leaf into an internal node

```

1: function PUTATBRANCHNODE(Node(Vk, b, low, high), Leaf(ai, qi, Si) )
2:   if  $l_{i,k} < b$  then
3:      $S'_i \leftarrow \text{SETUPPER}(S_i, V_k, b)$ 
4:      $low \leftarrow \text{PUT}(low, \text{Leaf}(a_i, q_i, S'_i))$ 
5:   if  $u_{i,k} > b$  then
6:      $S'_i \leftarrow \text{SETLOWER}(S_i, V_k, b)$ 
7:      $high \leftarrow \text{PUT}(high, \text{Leaf}(a_i, q_i, S'_i))$ 
8:   return Node(Vk, b, low, high)

```

The second case is when we encounter a leaf node during the insertion operation. We denote this node as L_t to indicate that it is a leaf already present in the tree under construction. First, we check if the Q-value of L_t is better than that of L_i , in which case we do nothing and abort the insert operation. If q_i on the other hand is the better option, then we need to insert L_i but in a way that respects S_i .

It is guaranteed at this stage, that S_t contains S_i , that is $u_{t,j} \geq u_{i,j}$ and $l_{t,j} \leq l_{i,j}$ for all $j = 1, 2, \dots, k$. But this also means that in the cases where the bounds on S_t are strictly larger or smaller than those of S_i then we need to insert a new internal node to ensure this partition before we can insert L_i . In other words, if $u_{t,j} > u_{i,j}$, then we need to create a branch node that splits on V_j at bound $b = u_{i,j}$ and whose right (‘high’) subtree is the original leaf L_t but with an updated state S_t where $l_{t,j} = u_{i,j}$. The left (‘low’) subtree should also, for a start, be set to L_t but then we continue the insert operation on this side, either creating more branch nodes or eventually inserting a_i and q_i in place of a_t and q_t .

The pseudocode for the function is given in Algorithm 5.

Algorithm 5 Put Q-leaf into a leaf node

```

1: procedure SPLIT(action, q, var, bound, state)
2:   highState  $\leftarrow$  SETLOWER(state, var, bound)
3:   lowState  $\leftarrow$  SETUPPER(state, var, bound)
4:   high  $\leftarrow$  Leaf(action, q, highState)
5:   low  $\leftarrow$  Leaf(action, q, lowState)
6:   return Node(var, bound, low, high)

2: function PUTATLEAFNODE(Leaf(at, qt, St), Leaf(ai, qi, Si))
3:   if qt  $\leq$  qi then
4:     return Leaf(at, qt, St)

4:   for (lt,j, ut,j) in St do
5:     if lt,j < li,j then
6:       newNode  $\leftarrow$  SPLIT(at, qt, Vj, li,j)
7:       return PUT(newNode, Leaf(ai, qi, Si))

8:     else if ut,j > ui,j then
9:       newNode  $\leftarrow$  SPLIT(at, qt, Vj, ui,j)
10:      return PUT(newNode, Leaf(ai, qi, Si))

11:  return Leaf(ai, qi, Si)

```
