Converting Q-trees to a decision tree

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1 Q-trees

A Q-tree is a binary tree that represents a complete partition of a k-dimensional (state) space according to a learned set of Q-values for a given action in a Reinforcemnt Learning setting. This means, a Q-tree is essentially a replacement for the part of a Q-table that describes one single action. A collection of Q-trees, a Q-forest, that covers all the possible actions is therefore a complete replacement for a Q-table.

The nodes in a Q-tree each give a linear partition of the state space with respect to a certain variable X. The node n_i compares X to some bound b_i and hosts a subtree for states with $X \leq b_i$ and one for $X_i > b_i$. At the leafs, the Q-value for that particular evaluation of the state for a specific action is stored. Each leaf therefore represents not only a Q-value and an action, but also an area of the state space with well-defined bounds.

An example of Q-forest is given in Figure 1. This describes a strategy for a (fictive) setting, where there are three allowed actions, α, β and γ, and two variables to account for, var_1 and var_2.

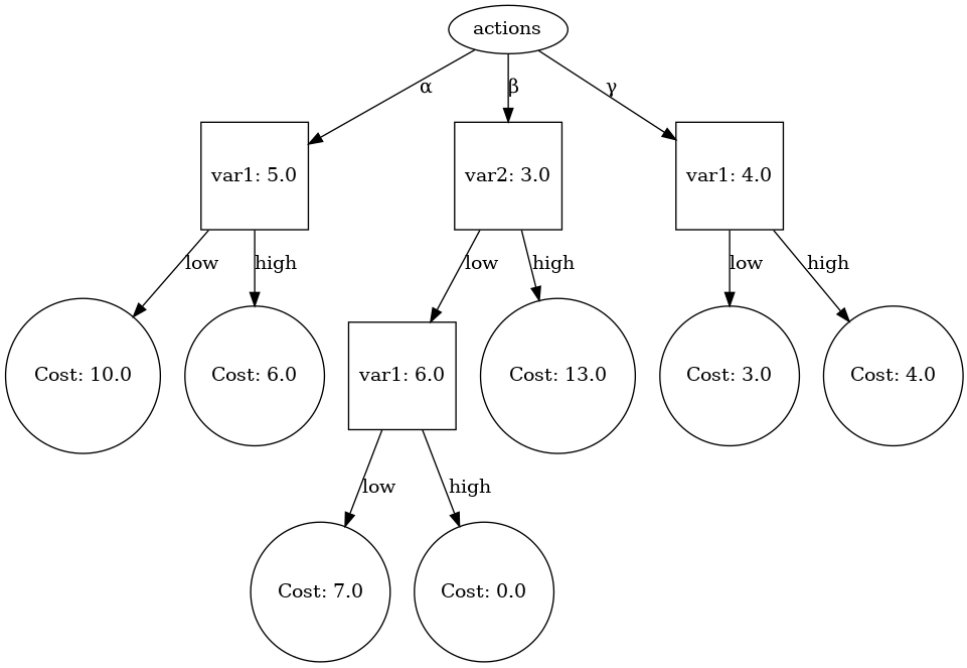


Figure 1: An example of a Q-forest with three actions and two variables.

2 Notation

Let $\mathcal{L} = \{L_1, L_2, \ldots, L_n\}$ be the set of all leaves in a Q-forest, let $\mathcal{A} = \{A_1, A_2, \ldots, A_m\}$ be the set of all possible actions and let $\mathcal{V} = \{V_1, V_2, \ldots, V_k\}$ be the k observable variables in the environment (where $V_i \in \mathbb{R}$ for all $i = 1 \ldots k$). For any $L_i \in \mathcal{L}$, we can define a state partition $S_i = \{(l_{i,1}, u_{i,1}), (l_{i,2}, u_{i,2}), \ldots, (l_{i,k}, u_{i,k})\}$ where $u_{i,j}$ is the *upper* bound for the value of variable V_j at the leaf L_i and $l_{i,j}$ is the *lower* bound. We consider all variables to ultimately be bounded by either positive or negative infinity, meaning that if no smaller bound is given $u_{i,j} = \infty$ and $l_{i,j} = -\infty$.

Now we can define a leaf L_i as a triplet of (a_i, q_i, S_i) where $a_i \in \mathcal{A}$ is the action associated with the Q-tree to which the leaf belongs, $q_i \in \mathbb{R}$ is the expected Q-value and S_i is the state partition that the leaf covers. Notice that we do not actually care about the original trees nor the internal nodes of these trees. All the information relevant to our purpose is contained in $\mathcal{L}$, the complete set of leaves in the forest.

As an example of an actual leaf, the 'left-most' leaf in the Q-forest in Figure 1 can be described by the triplet $(\alpha, 10, \{(-\infty, 5), (-\infty, \infty)\})$, assuming that $V_1 = var_1$ and $V_2 = var_2$.

3 The 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 $\mathcal{V}$.

3.1 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 1.

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 leaves 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. An example of this is given in Figure 2, where we have built the root tree from the leaf defined by `Leaf`$(\beta, 7, \{(-\infty, 6), (-\infty, 3)\})$.

Algorithm 1 MakeRoot

```
1: procedure MakeNewNode(var, bound, action, isHigh, prevNode)
2:     node ← Node(var, bound)
3:     if isHigh then
4:         node.high ← Leaf(action, ∞, State(·))
5:     else
6:         node.low ← Leaf(action, ∞, State(·))
7:     if prevNode is not None then
8:         if prevNode.low is None then
9:             prevNode.low ← node
10:        else
11:            prevNode.high ← node
12:    return node

1: function MakeRoot(Leaf(a_0, q_0, S_0))
2:     rootNode ← None
3:     prevNode ← None
4:     for (l_{0,i}, u_{0,i}) in S_0 do
5:         if u_{0,i} < ∞ then
6:             prevNode ← MakeNewNode(V_i, u_{0,i}, a_0, True, prevNode)
7:             if rootNode is None then
8:                 rootNode ← prevNode
9:         if l_{0,i} > −∞ then
10:            prevNode ← MakeNewNode(V_i, l_{0,i}, a_0, False, prevNode)
11:            if rootNode is None then
12:                rootNode ← prevNode
13:    if prevNode.low is None then
14:        prevNode.low ← Leaf(a_0, q_0, S_0)
15:    else
16:        prevNode.high ← Leaf(a_0, q_0, S_0)
17:    return rootNode
```

3.2 Inserting the leaves

To insert the remaining leaves we need a couple of extra helper functions. The task is to identify or construct all the paths in the tree under construction 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 2), 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 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

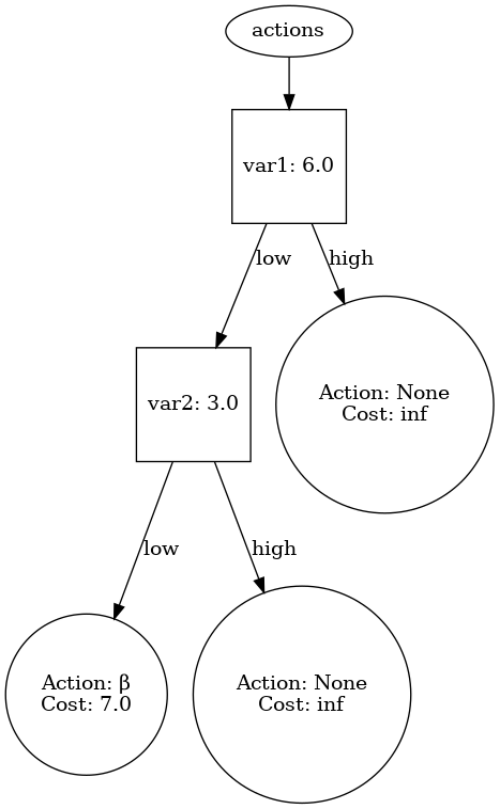


Figure 2: Tree build using `MakeNewNode` and the leaf triplet $(\beta, 7, \{(-\infty, 6), (-\infty, 3)\})$

Algorithm 2 Build decision tree from leaves 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))
```

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 3.

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 $j = 1, 2, \ldots, k$. 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.

Algorithm 3 PUT Q-leaf into an internal node

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

The pseudocode for the function is given in Algorithm 4.

Algorithm 4 Put Q-leaf into a leaf node

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

1: **function** PUTATLEAFNODE($\texttt{Leaf}(a_t, q_t, S_t), \texttt{Leaf}(a_i, q_i, S_i)$)
2: **if** $q_t \leq q_i$ **then**
3: **return** $\texttt{Leaf}(a_t, q_t, S_t)$

4: **for** $(l_{t,j}, u_{t,j})$ in S_t **do**
5: **if** $l_{t,j} < l_{i,j}$ **then**
6: $newNode \leftarrow \text{SPLIT}(a_t, q_t, V_j, l_{i,j})$
7: **return** $\text{PUT}(newNode, \texttt{Leaf}(a_i, q_i, S_i))$

8: **else if** $u_{t,j} > u_{i,j}$ **then**
9: $newNode \leftarrow \text{SPLIT}(a_t, q_t, V_j, u_{i,j})$
10: **return** $\text{PUT}(newNode, \texttt{Leaf}(a_i, q_i, S_i))$

11: **return** $\texttt{Leaf}(a_i, q_i, S_i)$

3.3 Example

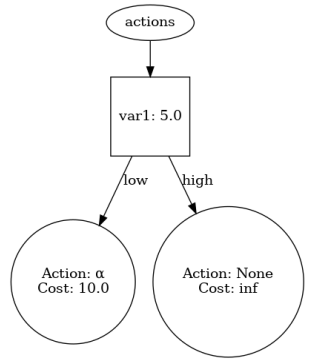
Using this algorithm, we can now construct a decision tree from the Q-forest we saw in Figure 1. For simplicity, we will simply consider the obvious order of the leafs that comes from collecting them from left to right in the figure, that is, we create our root from $\texttt{Leaf}(\alpha, 10, \{(-\infty, 5), (-\infty, \infty)\})$ and the final input to `Put` is $\texttt{Leaf}(\gamma, 4, \{(4, \infty), (-\infty, \infty)\})$. Note that we omit the step where we would insert $\texttt{Leaf}(\beta, 13, \{(\infty, -\infty), (3, \infty)\})$, as this has such a bad Q-value that it is just discarded.

4 Optimization

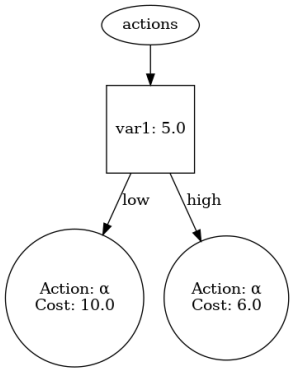
When looking at the final tree in Figure 3, it is obvious that it is not the most compact version of that tree. That is because we have just inserted the leafs in a random order (the order of visual appearance in Figure 1) and there is no attempt at restructuring or balancing the tree during or after construction.

Since the algorithm does not guarantee optimality it is crucial in order to obtain acceptable results that we perform some optimization steps before and after constructing the tree.

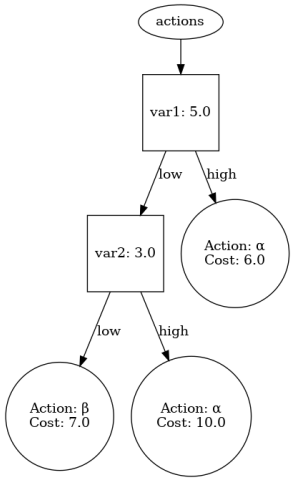
Figure 3: Complete trace of converting the Q-tree in Figure 1 to a single decision tree.



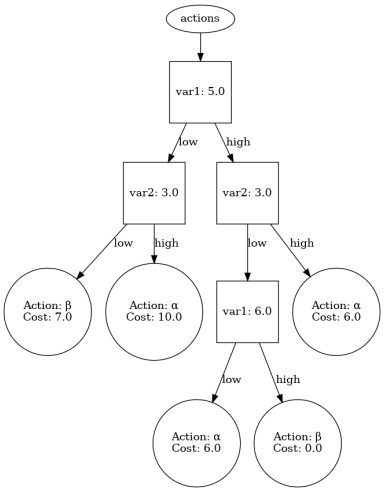
$\texttt{MakeRoot}(\alpha, 10, \{(-\infty, 5), (-\infty, \infty)\})$



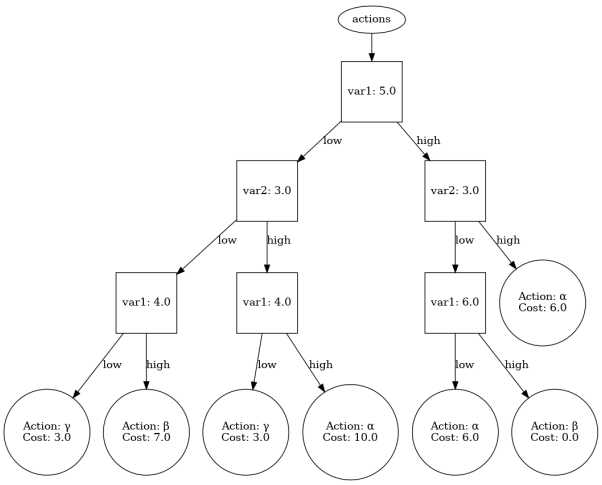
$\texttt{Put}(\alpha, 6, \{(5, \infty), (\infty, -\infty)\})$



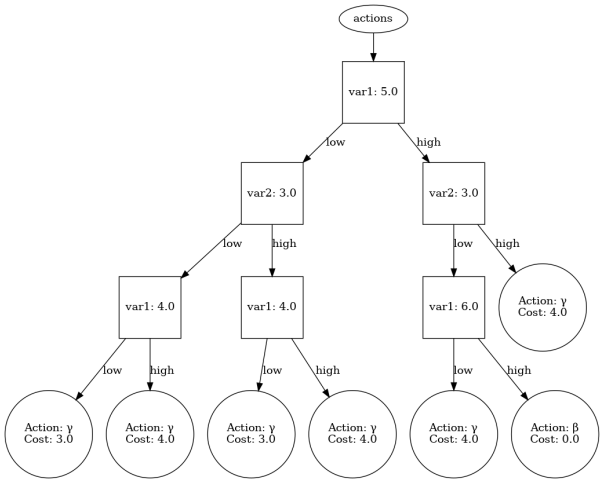
$\texttt{Put}(\beta, 7, \{(-\infty, 6), (3, -\infty)\})$



$\texttt{Put}(\beta, 0, \{(6, \infty), (3, -\infty)\})$



$\texttt{Put}(\gamma, 3, \{(-\infty, 4), (\infty, -\infty)\})$



$\texttt{Put}(\gamma, 4, \{(4, \infty), (\infty, -\infty)\})$

First of all, the order in which we insert the leafs into the tree has a great influence on the final size of the tree. This comes from the fact, that branch nodes are created whenever the insert operation reaches a leaf that has a worse Q-value than the one that is being inserted and where the state of the leaf is not yet completely determined by the parent nodes. Therefore, if we sort $\mathcal{L}$ in ascending according to the Q-values of the leaves, such that for any two q_i, q_{i+1} it holds that $q_i \leq q_{i+1}$[1] we will increase the likelihood that the tree structure is built in service of the best leaf nodes rather than accommodating for the states of sub-par leaves inserted earlier.

Secondly, as another pre-processing step, we prune any leaves L_i for which there exist a leaf L_j such that $q_j \leq q_i$ and S_j completely contains S_i (in which case, we say that L_j dominates L_i). When $\mathcal{L}$ is sorted, this is simply a matter of traversing $\mathcal{L}$ backwards and comparing each S_i with S_{i-1}. This does not have an effect on the final tree if $\mathcal{L}$ has been sorted before insertion, but it will reduce the size of $\mathcal{L}$ and possibly reduce the build time of the tree.

Lastly, after the tree has been built, we can perform another pruning operation. In this, we search for branch nodes whose two children are both leaf nodes and both have the same action. Since we — for the purpose of using the tree to decide on an *action* given a state — do not care about the actual expected cost of the action, we can merge the two leaf nodes into one and replace their common parent node with it. Doing this iteratively can greatly reduce the size of the tree and not least the complexity of the strategy (when viewed in a RL context). For example, if we look at the final tree of Figure 3, we see that we could actually collapse the entire left subtree into a single leaf nodes telling us to choose action γ. This tells us, that as long as $var_1 \leq 5$ the best action to choose is γ which is a very easily interpretable strategy.

Applying all of these steps can result in significantly smaller trees. In Figure 4 the complete strategy originally shown as a Q-forest in Figure 1 is presented as a decision tree build using all the techniques described in this section.

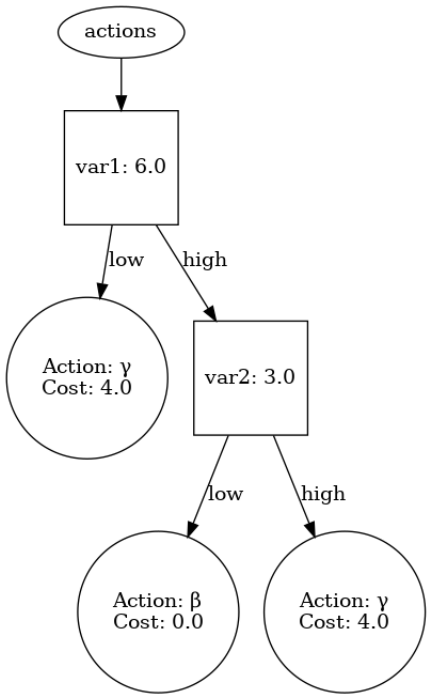


Figure 4: The complete Q-forest of Figure 1 represented as a compact decision tree.

[1]This expects the Q-values to represent *cost* values rather than *rewards*. If the latter is the case, the inequality should be reversed.

4.1 Further optimization

Beyond pre- and post-processing steps, we can also make improvements during construction.

5 Example of HOFOR case

5.1 Test for equivalence

5.2 Safety analysis