Algorithm 1 The algorithm of our proposed SubgraphX.

Input: GNN model $f(\cdot)$, input graph $\mathcal{G}$, MCTS iteration number M, the leaf threshold node number $N_{\min}$, $h(\mathcal{N}_i)$ denotes the associated subgraph of tree node $\mathcal{N}_i$.

Initialization: for each $(\mathcal{N}_i, a_j)$ pair , initialize its C, W, Q, and R variables as 0. The root of search tree is $\mathcal{N}_0$ associated with graph $\mathcal{G}$. The leaf set is set to $S_\ell = \{\}$.

for $i = 1$ to M **do**
  $curNode = \mathcal{N}_0, curPath = [\mathcal{N}_0]$
  while $h(curNode)$ has more node than $N_{\min}$ **do**
    for all possible pruning actions of $h(curNode)$ **do**
      Obtain child node $\mathcal{N}_j$ and its subgraph $\mathcal{G}_j$.
      Compute $R(curNode, a_j) = \text{Score}(f(\cdot), \mathcal{G}, \mathcal{G}_j)$
      with Algorithm 2.
    end for
    Select the child $\mathcal{N}_{next}$ following Eq.(2, 3).
    $curNode = \mathcal{N}_{next}, curPath = curPath + \mathcal{N}_{next}$.
  end while
  $S_\ell = S_\ell \cup \{curNode\}$
  Update nodes in $curPath$ following Eq.(4, 5).
end for
Select subgraph with the highest score from S_ℓ.