Algorithm 2 The algorithm of subgraph Shapley value.

Input: GNN model $f(\cdot)$ with L layers, input graph $\mathcal{G}$ with nodes $V = \{v_1, \ldots, v_m\}$, subgraph $\mathcal{G}_i$ with k nodes $\{v_1, \ldots, v_k\}$, Monte-Carlo sampling steps T.

Initialization: Obtain the L-hop neighboring nodes of $\mathcal{G}_i$, denoted as $\{v_{k+1}, \cdots, v_r\}$. Then the set of players is $P' = \{\mathcal{G}_i, v_{k+1}, \cdots, v_r\}$.

for $i = 1$ **to** T **do**

  Sampling a coalition set S_i from $P' \setminus \{\mathcal{G}_i\}$.

  Set nodes from $V \setminus (S_i \cup \{\mathcal{G}_i\})$ with zero features and feed to the GNNs $f(\cdot)$ to obtain $f(S_i \cup \{\mathcal{G}_i\})$.

  Set nodes from $V \setminus S_i$ with zero features and feed to the GNNs $f(\cdot)$ to obtain $f(S_i)$.

  Then $m(S_i, \mathcal{G}_i) = f(S_i \cup \{\mathcal{G}_i\}) - f(S_i)$.

end for

Return: $\text{Score}(f(\cdot), \mathcal{G}, \mathcal{G}_i) = \frac{1}{T} \sum_{t=1}^{T} m(S_i, \mathcal{G}_i)$.