Algorithm 1 The overall process of CAHAN.

Input: The heterogeneous graph $G = \{V,\ E\}$,
The node feature$\{h_i, \forall i \in V\}$,
The meta-path set $\Phi = \{\Phi_0, \Phi_1, ..., \Phi_m\}$,
The number of attention head K

Output: Drug node representation h_u ,
Disease node representation h_s

for $\Phi_i \in \{\Phi_0, \Phi_1, ..., \Phi_m\}$ **do**
  for $k = 1, 2, ..., K$ **do**
    $h'_i \Leftarrow M_{\phi i} \cdot h_{i0}$
    for $i \in V$ **do**
      Through the meta-path Φ_i wandering to generate metagraphG_i^{mi}
      for $j \in G_i^{mi}$ **do**
        Calculate the importance e_{ij}^{mi} of the context node j to the target node i
      end for
      The Softmax function normalizes e_{ij}^{mi} to obtain α_{ij}^{mi}
      Intra-path aggregation: $h_i^{mi} \Leftarrow \sum_{j \in G_i^{mi}} \alpha_{ij}^{mi} \cdot h'_j$
    end for
  end for
  Concatenate embeddings from K attention heads: $h_i^{mi} \Leftarrow \|_{k=1}^{K} \sigma(\sum_{j \in G_i^{mi}} [\alpha_{ij}^{mi}]_k \cdot h'_j)$
end for
Calculate the average score for each meta-path: $c_{mi} \Leftarrow \frac{1}{|V_A|} \sum_{i \in V_A} \sigma(r^T \cdot (h'_i \| h_i^{mi}))$
Normalization: $\beta_{mi} \Leftarrow softmax(exp(c_{mi}))$
Inter-path aggregation: $h_i^m \Leftarrow \sum_{\Phi_i \in \Phi} \beta_{mi} \cdot h_i^{mi}$
Cross-attention mechanism: $h_u \Leftarrow CrossAttention(h_s^m, h_u^m, h_u^m)$,
$h_s \Leftarrow CrossAttention(h_u^m, h_s^m, h_s^m)$
return h_u, h_s