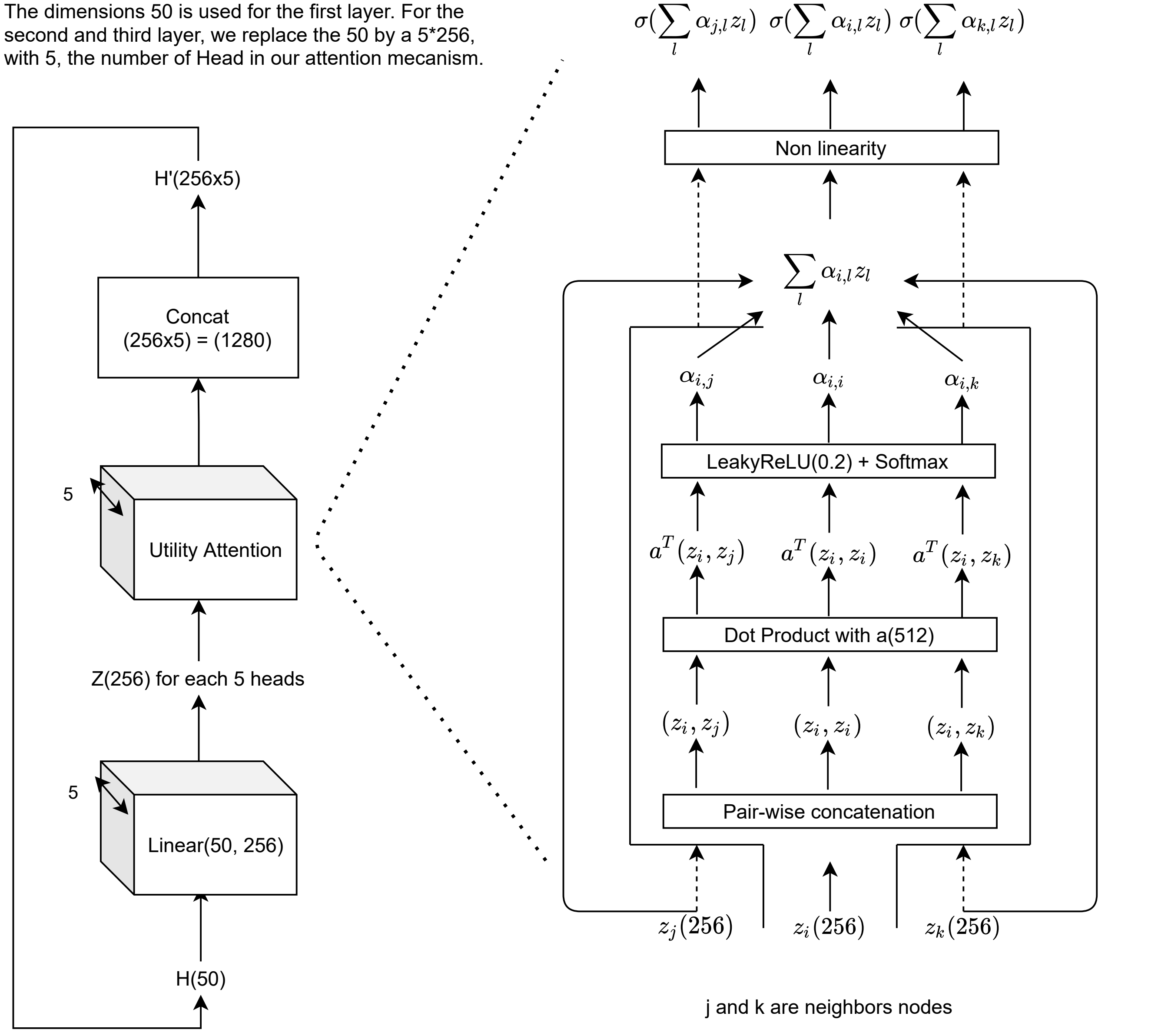
# Utility Attention

The utility attention is used in the Attention graph Network.

The dimensions 50 is used for the first layer. For the second and third layer, we replace the 50 by a 5*256, with 5, the number of Head in our attention mecanism.



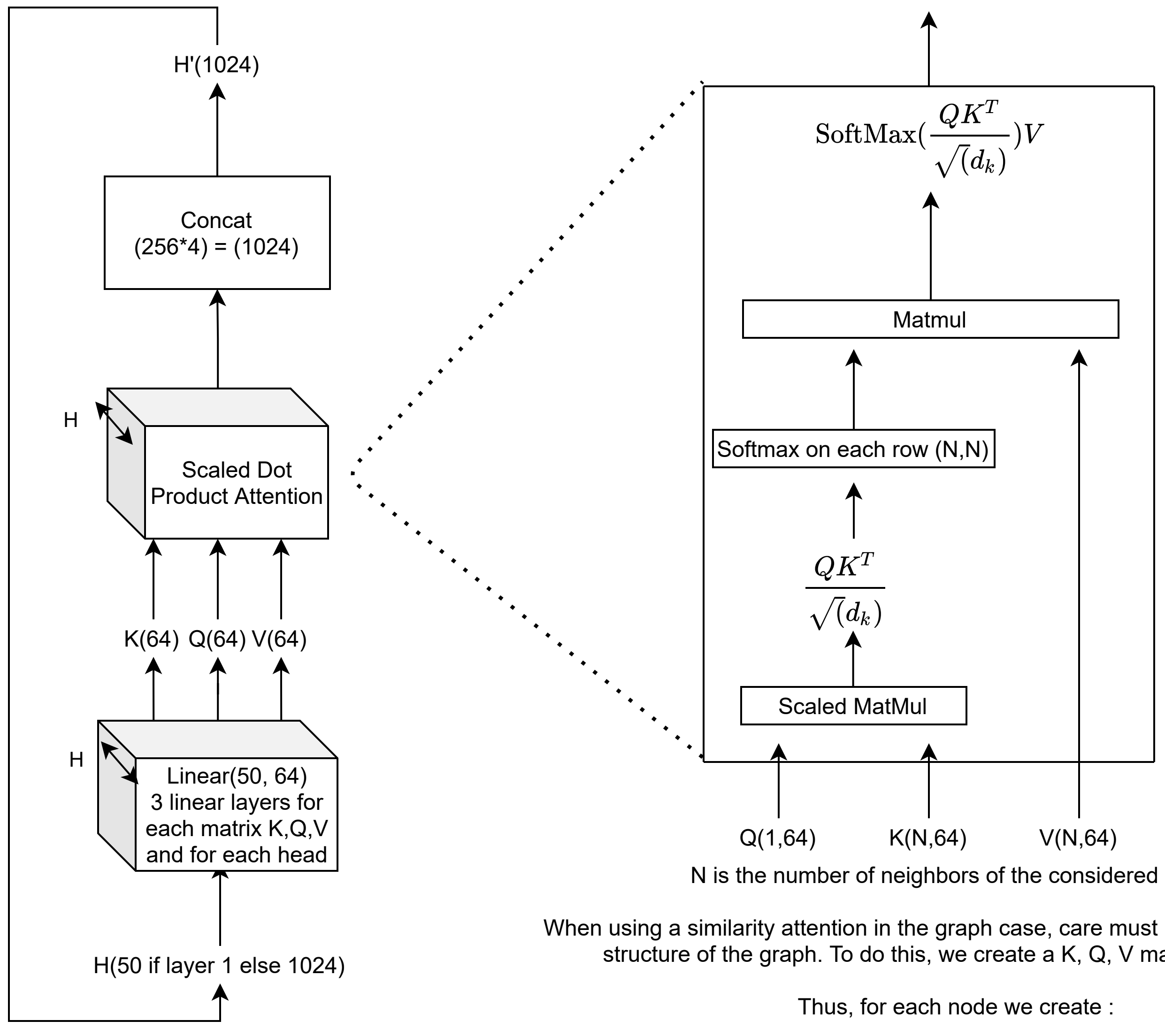
j and k are neighbors nodes

The management of the parallelisation of calculations between the different neighbors is optimised by the DGL library. The embedding of each node is computed before moving to the next layer.

# Similarity Attention

The Similarity Attention was introduced in the paper Attention is all you need.

The dimensions 50 is used for the first layer. For the second and third layer, we replace the 50 by (256*4) = (1024). If we use 64 as the embedding of the Key, Query and value matrix, the number of heads H must verify : H*64=256. So H = 4.


H'(1024)
Concat
(256*4) = (1024)
H
Scaled Dot Product Attention
K(64) Q(64) V(64)
H
Linear(50, 64)
3 linear layers for each matrix K,Q,V and for each head
H(50 if layer 1 else 1024)
$\mathrm{SoftMax}(\frac{QK^T}{\sqrt(d_k)})V$
Matmul
Softmax on each row (N,N)
$\frac{QK^T}{\sqrt(d_k)}$
Scaled MatMul
Q(1,64)
K(N,64)
V(N,64)

N is the number of neighbors of the considered node.

When using a similarity attention in the graph case, care must be taken to keep the structure of the graph. To do this, we create a K, Q, V matrix per node.

Thus, for each node we create :

- The matrix K which contains the embedding of the keys of all the neighboring nodes.
- the Q matrix which contains the embedding of the query of the considered node
- the V matrix which contains the embedding of the values of the neighboring nodes

# Architecture

Here is a schema of the architecture used in our implementation of the Attention Graph Network.

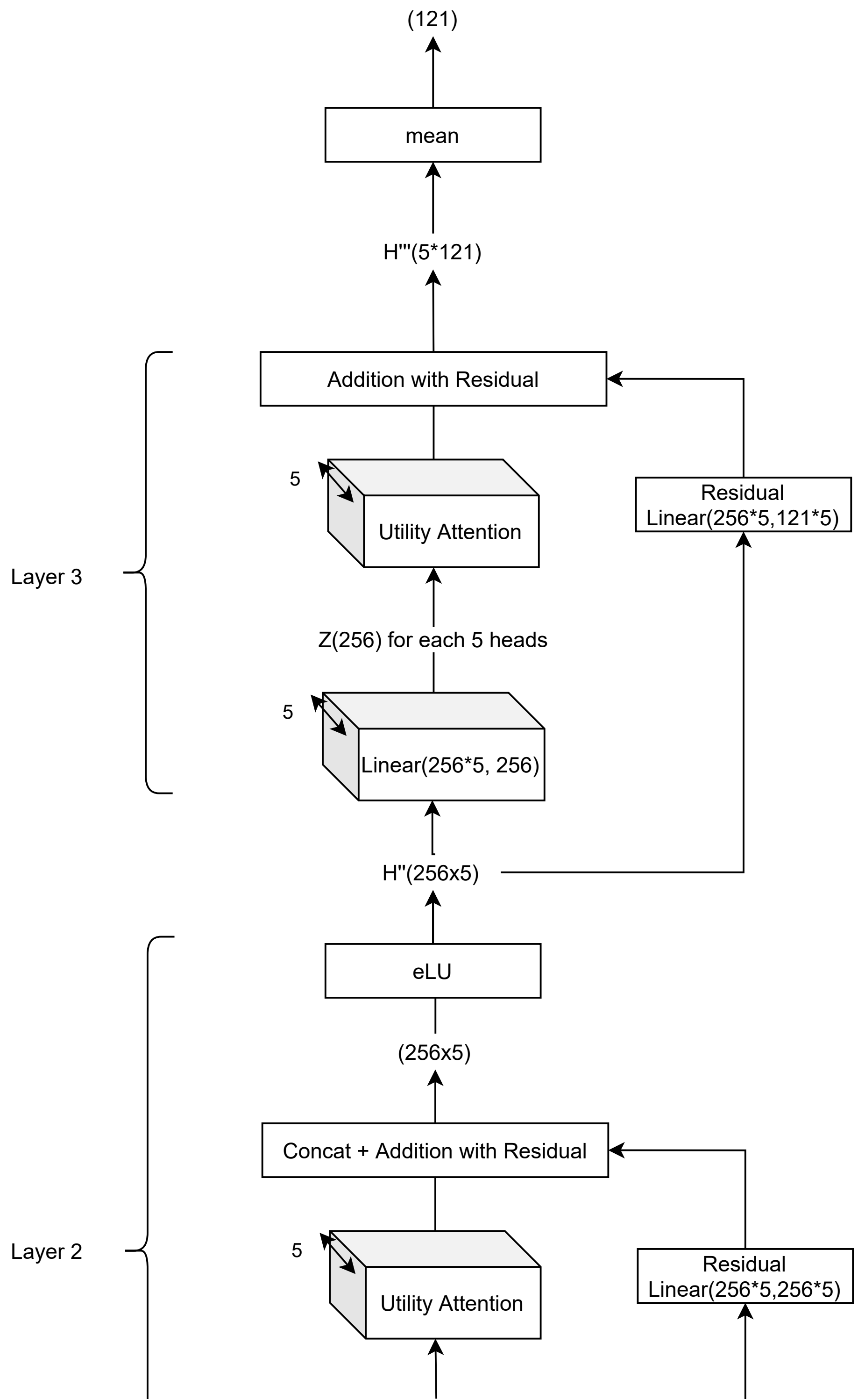
Our architecture is a slight modification of the one proposed in the paper for the Inductive Learning on the PPI dataset. The paper proposes a number of heads of 4, 4, 6 for layers 1, 2 and  3. But we take 5 heads for each layer in order to simplify a bit. As in the paper, we do not use dropout nor do we use regularization or data augmentation.

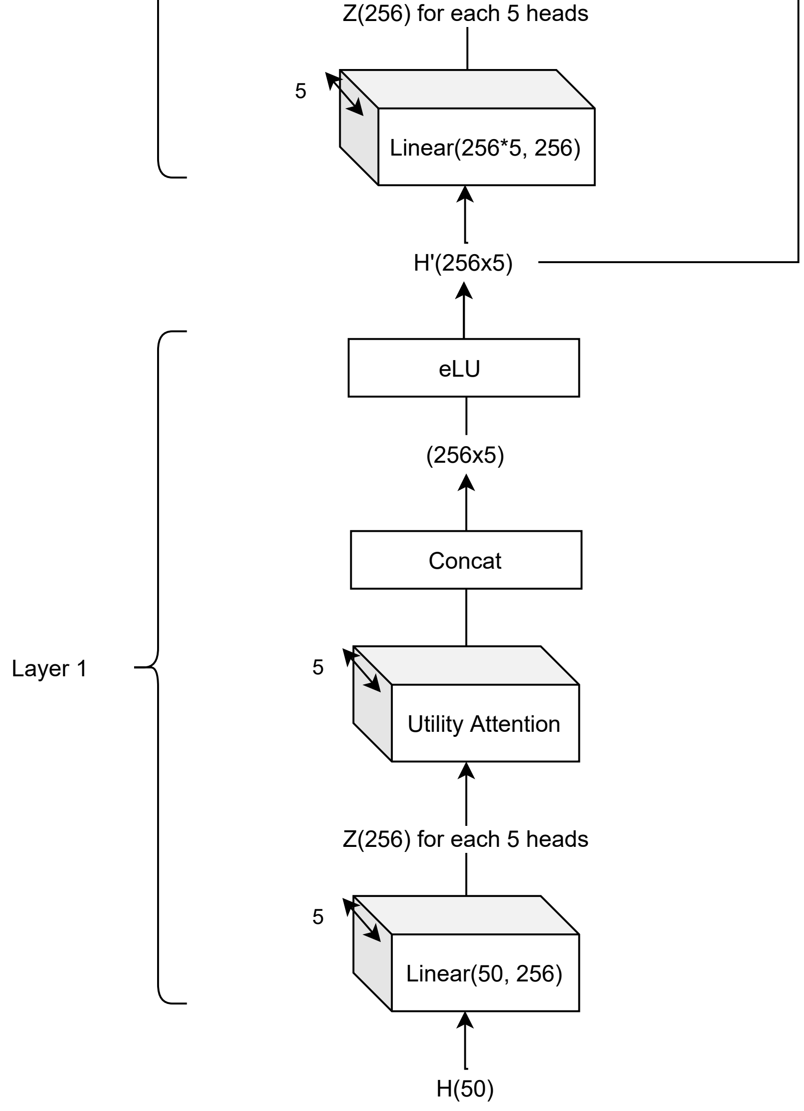
The notation Linear(Entry dim, Output Dim) gives the size of the embeddings passing through it as in PyTorch.

The Layer 3 is identical to the layer 2 with just three differences:

- We do not concatenate, but we mean on the head dimension.
- There is no non-linearity such as the eLU in layer 2.
- The embedding used in the attention is not of size 256 but of size 121 which is the number of classes.

At the end of our neural network, there is no need to add a sigmoid because nn.BCEWithLogitsLoss will apply it internally.





We begin with a graph with an embedding on each node containing 50 features.
We do not write the number of node here because it varies from graph to graph. But we make the calculation in parallel on each node before going to the next layer.