

1 We would like to thank the reviewers for their constructive comments. Below, we try to respond to their main comments.

2 **R1: Quantitative evaluation.** Indeed, a quantitative evaluation would improve the significance of the empirical results.  
3 Note that each motif exhibits some distinct properties and can be considered as a graph-feature. For instance, a star  
4 graph contains a single node with high degree. The caveman graphs contain many triangles, the ladder graphs consist of  
5 cycles of size 4, etc. For each dataset, we plan to measure how much these properties are satisfied by the learned hidden  
6 graphs and we will report the results in the revised manuscript.

7 **R1: Comparing against  $k$ -step RW.** We have started evaluating the  $k$ -step RW kernel (the implementation contained  
8 in the graphkernels package) on the 10 datasets. We obtained the following average accuracies on MUTAG, ENZYMES  
9 and NCI1: 72.39 ( $\pm$  6.9), 19.00 ( $\pm$  4.4) and 54.06 ( $\pm$  1.6), respectively. We observed that computing the kernel matrix  
10 on the larger datasets (DD, REDDIT-BINARY, REDDIT-MULTI-5K, COLLAB) takes more than 1 day or requires  
11 large amounts of memory (more than 16GB of RAM). Thus, it seems that the  $k$ -step RW kernel is fairly weak and  
12 suffers from time/memory issues. With this in mind, we are not sure if it is worth adding this baseline to the paper.

13 **R1: Large graph datasets.** This is definitely on our agenda for future work. We plan to evaluate the proposed  
14 architecture on the QM9 dataset which contains more than 100k samples.

15 **R2: Fully connected learned graphs.** In our implementation, a hidden graph of order  $n$  is associated with  $n(n-1)/2$   
16 trainable parameters. We do not directly treat these values as the weights of the edges between the different pairs  
17 of nodes, but we first apply the ReLU activation function. Therefore, all the negative values are set equal to 0, and  
18 the corresponding edges are essentially removed. Even though the learned graphs can be complete, we empirically  
19 observed that in most cases, they are fairly sparse. We will make this clear in the revised manuscript.

20 **R2: Feature space of kernels vs. that of proposed model.** Indeed, a graph kernel maps graphs to some Hilbert space  
21 where each dimension typically corresponds to some substructure (e.g., shortest path of specific length, a specific  
22 subtree, etc). This space is different from the one to which our model maps graphs. In our case, each dimension  
23 corresponds to the “similarity” of the input graph and some hidden graph. Furthermore, since the proposed model is  
24 end-to-end trainable, this space is not fixed, but it depends on the structure of the hidden graphs.

25 **R2, R3: Empirical performance.** It is true that the empirical results are not very impressive in general. Even though  
26 the proposed model does not provide a new state-of-the-art in graph classification, still it outperforms the majority of  
27 the GNN baselines on most datasets. We agree that the main strength of the paper is in the novelty of the proposed  
28 architecture, not in the empirical performance (though we believe that it is not that bad).

29 **R2: Papers that first introduced GNNs.** We thank the reviewer for pointing us to these papers. We will rephrase the  
30 sentence and cite the above papers.

31 **R3: Comparing against explainability techniques for GNNs.** We should first mention that our paper is different  
32 from these works in that the main focus of the proposed model is not on providing interpretable explanations for its  
33 predictions, but on dealing with graph-level supervised learning tasks. Note also that the methods proposed in these 3  
34 papers are mainly applied as a post-processing step: they take a trained MPNN and its predictions, and they return an  
35 explanation of these predictions. On the other hand, in the case of the proposed model, these explanations come as a  
36 byproduct of the learning process. Comparing against these methods seems thus to be out of the scope of this paper.

37 Furthermore, note that the explanations generated by the proposed model are similar to those of the method presented in  
38 the third paper (both belong to the family of model-level methods). Note that the third paper has not been published yet  
39 and was posted on arXiv 2 days before the submission deadline of NeurIPS. Therefore, comparing against this method  
40 was also practically infeasible.

41 **R4: MPNNs ignore edge information.** We agree with the reviewer that it is graph-pooling that treats graphs as  
42 sets/multisets of node representations. Since the graph structure (e.g., subtree patterns) is encoded into these repre-  
43 sentations, MPNNs (message passing along with graph-pooling) do not ignore edge information, but they take it into  
44 account. We will rephrase our claim as suggested by the reviewer.

45 **R4: Experiments with different sizes of hidden graphs.** This is mainly due to computational reasons. In our  
46 implementation, the parameters of all hidden graphs are combined into a single trainable matrix. This allows us to  
47 perform operations such as batch matrix multiplications that benefit greatly from GPUs. To employ hidden graphs of  
48 different sizes, we would need to have more than one trainable matrices, and that would slightly increase the running  
49 time of the model.

50 **R4: Comparing against DDGK.** This paper is indeed related to our work. One major difference is that our model is  
51 supervised, while DDGK is unsupervised. We will discuss the difference between this approach and our work in the  
52 related work section, as suggested. The source code of DDGK is also publicly available, and we have started evaluating  
53 it on the 10 graph classification datasets. We will report the results in the revision.