

1 We thank the reviewers for their comments and suggestions. We will incorporate the suggestions in our revised version.
2 Below, we address the main concerns raised in the reviews.

3 **(R1) Contribution with respect to Maron et al. [2019a].** Our work builds upon Maron et al. [2019a]. and extends
4 it in two directions: (i) First, we provide a refined analysis showing that k -order invariant networks are at-least
5 as expressive as k -WL test. This extends the 2-order result discussed in Maron et al. to any k . (ii) We show that
6 incorporating higher order equivariant layers (e.g., matrix multiplication) can strictly increase the expressive power of
7 k -order networks (instead of using higher order tensors). We have used this insight to devise a very simple invariant
8 architecture that empirically outperforms the model suggested in Maron et al. [2019a]. and is theoretically strictly more
9 expressive.

10 **(R1,R3) Contribution with respect to Morris et al. [2019]; “Why does your variant improves over, e.g., 1-2-3
11 GNN?”** The work of Morris et al. [2019] was one of our main inspirations. However, our work does offer two
12 important contributions with respect to this paper. (i) We propose a simple and practical network architecture with
13 provable 3-WL expressive power (section 6, Figure 2). Our 3-WL construction offers two main benefits over the
14 1-2-3-GNN model proposed by Morris et al. [2019]: First, our method requires $O(n^2)$ space per layer compared to
15 $O(n^3)$ required by Morris et al. (see next question for more details). This allowed us to work with a 3-WL expressive
16 model in practice while Morris et al. resorted to a local 3-GNN version, hindering their 3-WL expressive power. Second,
17 from a practical point of view our model is arguably simpler to implement as it only consists of fully connected layers
18 and matrix multiplication (without having to account for all subsets of size 3). (ii) Our first result (section 5), proves that
19 the k -order invariant networks constructed in Maron et al. [2019a] from first principles (i.e., equivariance to permutation
20 action on graphs) surprisingly lead to neural models that can implement k -WL. The k -order invariant networks therefore
21 provide an *alternative* theoretical model to Morris et al. [2019], with provable k -WL expressive power. We believe the
22 community would benefit from exploring different frameworks (although they have the same expressive power). We
23 will add a discussion in the paper.

24 **(R3) "Complexity results on the approach with 3-WL expressive power would be desirable."** We can provide
25 the following complexity analysis for a single layer (i.e., block, see Figure 2). Note that both our method and Morris et
26 al. [2019] use only a few (e.g., 3) layers in the experiments. Assuming a graph with n nodes, dense edge data and a
27 constant feature depth, the layer proposed in Morris et al. has $O(n^3)$ space complexity (number of subsets) and $O(n^4)$
28 time complexity ($O(n^3)$ subsets with $O(n)$ neighbors each). Our layer (block), however, has $O(n^2)$ space complexity
29 as only second order tensors are stored (i.e., linear in the size of the graph data), and time complexity of $O(n^3)$ due to
30 the matrix multiplication. We note that the time complexity of Morris et al. can probably be improved to $O(n^3)$ while
31 our time complexity can be improved to $O(n^{2.5})$ due to more advanced matrix multiplication algorithms.

32 **(R3) Contribution with respect to Xu et al. [2019].** Xu et al. [2019] show that message passing neural networks
33 have limited 1-WL expressive power, and offer a message-passing model that realizes this bound. Our paper extends
34 this result and provides a theoretical connection between a recently suggested method (Maron et al. [2019a]) and
35 higher-order WL tests. Moreover, we propose an architecture that is provably more expressive than the model suggested
36 in Xu et al., with 3-WL expressive power, and compares favorably empirically.

37 **(R1) “Is it really necessary to resort to the "hammer" of the universal approximation theorem?”** This is an
38 interesting question. First of all, it is not clear why using the universal approximation theorem is considered to be a
39 negative thing. Nevertheless, we admit that trying to prove our results without using it is an intriguing question.

40 **(R1) "Are your results tight in terms of shapes of the maps?"** We are not sure we understand the question. If the
41 reviewer asks whether k -order networks cannot implement WL test of degree higher than k , then we did not prove
42 such a result, although it is likely that this statement is correct. One thing that we do discuss at the end of section 6 is
43 a potential way for k -order networks, augmented with an additional polynomial operation, to be as expressive as the
44 $k + 1$ -WL test.

45 **(R2) Code.** We will release code and instructions for reproducing the results in the paper.

46 **(R3) “Why is a different PMP based method introduced by the authors?”** The power sum multisymmetric
47 polynomials (PMP) provide a continuous and differentiable way to encode *vector* multisets. Previous works, e.g.,
48 Zaheer et al. [2017], used the power-sum symmetric polynomials to encode *scalar* multisets, or a delicate and somewhat
49 incomplete exponential encoding scheme. Our approach using PMP provides a much simpler analysis.