AUTHOR RESPONSE TO THE REVIEWS OF "CORMORANT: COVARIANT MOLECULAR NEURAL NETWORKS"

We thank all three reviewers for their insightful comments and positive evaluations of our manuscript. We will update the paper to reflect their suggestions by the camera ready deadline.

We will shortly release a Python library that implements the Cormorant architecture. Currently we are just cleaning up and documenting the code. As for the other points brought up by the reviewers we have the following comments:

1. **Structure and supplement:** As suggested by Reviewer 2, we will move some details of the technical implementation in Section 4.4 to the supplement. This will provide room to more clearly explain some of the "big picture" arguments, as requested by several of the reviewers.
2. **Motivation and physical laws:** Our discussion of electrostatics was only intended to illustrate the algebraic structure of interatomic interactions (of any type) rather than suggest that electrostatics is the *only* type of interaction that we care about. The point of the paper is that we do not need to tell the network what interactions exactly it should learn (it will figure that out by itself), but there are nonetheless physical constraints stemming from symmetries that can be explicitly imposed.
3. **Learning force fields and other vector quantites:** In the present version of the paper we only train on and predict scalar-valued quantities. However, predicting forces in MD-17 would be as simple as taking the gradient of the predicted potential energy. *Learning* from forces requires a loss formulated in terms of the gradient, which can be neatly slotted into modern deep learning frameworks, thanks to automatic differentiation. We just did not reach a point where we could add this by the submission deadline. Regarding predicting vector valued quantities in general, this would only require a slight extension of Cormorant. The reason that in Definition 2 constrain ourselves to scalar outputs is essentially just didactic, to explain the relationship between covariance and invariance.
4. **Citations:** We have cleaned up the bibliography, as requested. We also added the missing references pointed out by the reviewers. Several of these papers we were not familiar with, so we are grateful for the suggestions, especially since they help put our work in a broader context.
5. **Connections with other covariant architectures:** As suggested the reviewers, we will make more explicit the relationship between our work and other covariant architectures, including Tensor Field Networks, SE(3)–covariant networks, and the references suggested by Reviewer 2. Unfortunately, this one page is not enough to properly explain the connections.
6. **"Cormorant is one of the most general architectures":** We can show that Tensor Field Networks for example a special case of a Cormorant-like architecture. However, we agree that without explaining this explicitly our statement sounds a bit boisterous, so we will remove it.
7. **Datasets and experimental results:** We are working on understanding why Cormorant performed relatively poorly on R^2 and μ. We will update the manuscript if we have a satisfactory answer.
8. **Why only nine variables for GDB9?** We found that U, G and H behave very similarly to U_0 so it seemed redundant to include them given that we were squeezed for space (Faber et al. did the same).
9. **Spin:** We do not understand R2's comment about spin. Spin is indeed a vectorial quantity. Line 78 says that the interaction energy between two spins is a scalar, not the spins themselves. Please explain.
10. **Number of parameters:** For MD-17 about 46K, whereas for GDB-9 it is 180K.
11. **Aggregating over all layers on top:** Yes, line 208 implies that at the top of the network we aggregate from all covariant layers. This makes sense for extensive quantities like energy (essentially this is how fast multipole methods work). For other learning targets it is harder to justify, so we are experimenting with the network architecture to see if we can avoid these skip connections.
12. **Minor suggestions and typos:** We found the all suggestions by the reviewers useful, and will incorporate them into the manuscript. We will also fix all the typos.
13. **Reproducibility:** The release of the full Cormorant Pytorch library by the camera ready deadline will ensure that our results are fully reproducible.