Q&A
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The hyperparameter of optimisation of graph neural networks for molecular property prediction
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Q1: What got you interested in this topic for your PhD?

Things related to our project goal, so I think it's motivated by our EPSRC project which aims to find and develop self-healing materials. We play the computer science role in that group and we build the models to help our colleagues to facilitate their work in materials science, for example, improving experimental strategy. Meanwhile, molecular property prediction is significant task for many research problems, so it means our work could be applied to a wider range of problems.

Q2: Are these able to be applied to other ML networks? How hard are they to implement? Where can I learn to implement them?

I think the core of today's topic includes GNN and Hyperparameter Optimisation. Hyperparameter Optimisation is a quite wide and general topic for most machine learning methods this is not just for the graph neural networks. And I think it's not hard to implement because there are just two parts of work, so you just need to combine them in an iterative way, the model you want to use and a hyperparameter optimisation you select. Probably you need to wait for a relatively long time because hyperparameter tuning is costly. In addition, I think you can find there are quite a lot of python libraries like Optuna and Hyperopt, which provide ready-to-use functions and classes to do Hyperparameter Optimisations.

Q3: Did you initialise the weights from new each iteration?

This is a good question. In our research, we initialise the weights in each new iteration, one iteration denotes a process of searching and evaluating a hyperparameter solution. However, it is possible to fix the weights or partial weights for the next hyperparameter solutions, which is more common in neural architecture search.

Q4: Apart from Optuna, what sort of open python packages are there to use?

Apart from Optuna, do you mean the python packages for GNN or maybe python packages for the Hyperparameter Optimisations? I think Optuna is for Hyperparameter Optimisation. If you want to implement graphing works, you can use TensorFlow, PyTorch and Deep Graph Library. Deepchem is more for deep learning in science