PHYS4041 (2022-2023)
An introduction to practical quantum computing
PROJECTS
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As the assessment for the module, you are required to write a short paper in the format of a 2-column scientific journal article. You should write the paper using latex and the revtex package for formatting that follows the style of APS journals. Your project will be undertaken as part of a group and your paper should have 2-3 pages. Make sure to divide the work evenly! You should write a single paper as a group, but all members of the group should submit the paper, any accompanying code, and a statement on their involvement in the project.

As a guide, the paper should have (but is not restricted to) the following elements / structure:

1. Title
2. Author list
3. Abstract
4. Introduction
5. Setup of the problem
6. Results and discussion
7. Conclusion and outlook
8. Bibliography

Below are several possible projects for you to choose from, which you will be able to submit on Moodle. Based on your choices you will be put into groups. I will arrange group meetings with you to happen in our normal 9am slot on Fridays. All of the projects include the same steps but in different settings. Whatever project you choose, you will be tested on the same skills, but you may find a particular setting more interesting.

Note: it would be great to have something run on the real IBM devices. However, I am aware that running on the quantum computers takes a significant amount of time and can be a bit problematic. Since it amounts to a change of a few lines of code you will not be marked down if this can't be achieved during the project. With that said, performing such experiments provides a natural chance to discuss the realities of working with current noisy quantum computers (but you could introduce this anyway), which can lead to a stronger discussion in your paper.

PROJECT 1: VQE for molecules.

In this project we will implement and test the Variational Quantum Eigensolver (VQE) algorithm. The VQE algorithm was first demonstrated in the context of quantum chemistry by finding the ground state of simple molecules [1, 2]. This is the case we will also focus on. We will expand on the example given in the lecture notes by finding the ground state for different molecular separations to find the lowest energy separation.

Main tasks

1. Solve the H-He+ molecule from lecture notes but with different separation values R (corresponding to different coefficients in the Hamiltonian)

2. Perform and compare VQE optimisation with the different methods for computing (or approximating) gradients

3. Investigate changing the depth of the VQE ansatz

Further investigation

1. Consider different VQE ansatz circuits and compare

2. Perform VQE for different (more complicated) molecules

3. Run optimised circuits on IBM devices

4. Perform optimisation process on IBM device

PROJECT 2: Quantum machine learning classification.

In this project we will perform and test quantum machine learning on the task of classification. This will build on the code on Moodle for the MNIST handwritten digit classification.

Main tasks

1. Modify code to perform binary classification on different pairs of digits.
2. Implement different methods for encoding the image data (using simulator)
3. Test and compare different depths for the ansatz circuit
4. Compare different methods for computing (or approximating) gradients

Further investigation

1. Perform binary classification using fashion MNIST
2. Implement multi-class classification
3. Run an optimised circuit on IBM device

PROJECT 3: Quantum generative adversarial network.

In this project we will create a quantum circuit to generate handwritten digits, trained using the MNIST dataset. The approach for generating these images will be to use Generative Adversarial Networks consisting of a quantum generator and a classical discriminator.

Main tasks

1. Write code to implement Quantum GAN, based on `https://pennylane.ai/qml/demos/tutorial_quantum_gans/`
2. Investigate generating different digits
3. Investigate different methods for patching
4. Investigate different circuit structures
5. Compare different methods for computing (or approximating) gradients

Further investigation

1. Generate Fashion MNIST instead of MNIST handwritten digits.
2. Run an optimised circuit on IBM device

PROJECT 4: Quantum Convolutional Neural Networks

In this project we classify MNIST handwritten digits using a quantum version of convolutional neural networks. This consists of a quantum convolutional layer, followed by a classical dense neural network

Main tasks

1. Write code to implement Quantum Convolutional Network, based on `https://pennylane.ai/qml/demos/tutorial_quanvolution/`
2. Test with multi-class classification
3. Compare against comparable classical neural network
4. Compare different methods for computing (or approximating) gradients

Further investigation

1. Classify Fashion MNIST instead of MNIST handwritten digits.
2. Run an optimised circuit on IBM device

References

[1] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, "A variational eigenvalue solver on a photonic quantum processor," *Nature Communications*, vol. 5, p. 4213, sep 2014.

[2] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, and J. M. Gambetta, "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets," *Nature*, vol. 549, pp. 242–246, sep 2017.