Project 2, Quantum Machine Learning. Deadline June 1, Spring 2021

Computational Physics II FYS4411/FYS9411

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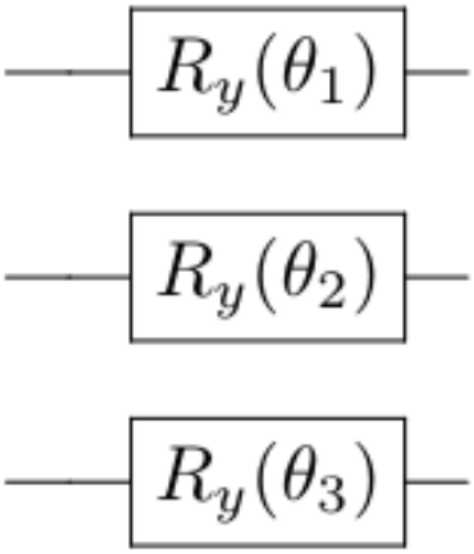
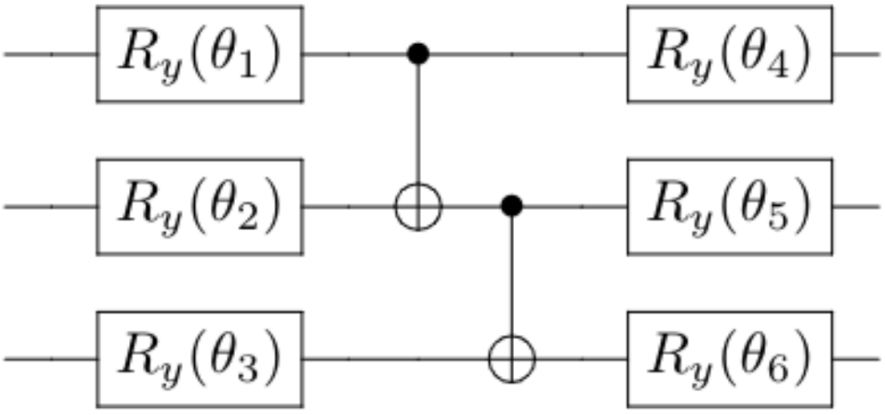
Introduction

Why do people care about "Quantum Machine Learning", or "Quantum Computing" in general? A common observation that motivates quantum computing, although it does not tell the whole story, is the striking fact than quantum information of a quantum system is in a sense larger than the classical information of a comparable classical system. In the case of bits and qubits, n classical bits allows you to store the value of n boolean variables $a \in [0, 1]$, whereas you need 2^n amplitudes $\alpha \in \mathbb{C}$ to describe the state of n quantum bits, or qubits. In other words, the (Hilbert)space in which the qubits live in exponentially bigger than that of the classical counterpart. In the context of parameterized quantum circuits, one may prepare a state in the exponentially large Hilbert space by applying some simple quantum operations to a set qubits that are all initialized in the zero-state.



By varying $\theta_i \in [0, 2\pi]$, one can attain different states. A crucial thing to note is that we are not able to prepare an arbitrary state using this ansatz as it much too constrained and simple: The exponentially large space is not available to us. One might try to remedy this by introducing a more complex ansatz:



We now have an ansatz whose number of operations scales polynomially in the number of qubits(in this case quadratic), and the added complexity enables us to reach a greater part of Hilbert space. Still, it is only a polynomially

large part of it, which is vanishingly small compared to its full size. To have access to the whole space, one would in fact need to perform exponentially many operations, which is practically intractable to do (Nielsen, 4.5.4).

Does this mean that the supposed power of quantum computation is practically inaccessible to us? No. Even though we only reach a very small part of Hilbert space using "cheap" ansatzes, the states we do reach might be very useful for solving a particular problem. Moreover, these states might be classically intractable to compute (source to come), meaning the information they represent is not practical to determine using classical computers. They are however efficiently prepared using quantum computers, as the number of quantum operations needed to be applied is by construction only polynomial.

How can one leverage this in a machine learning setting? A common approach is to use variants of the previous ansatzes to encode features to qubits by performing rotations, thus embedding the data in a high dimensional quantum state. Subsequent parameterized operations on the qubits then applies powerful transformations to the embedded data in a high dimensional space. Such methods are often described as quantum kernel methods, because of their similarity to classical kernel methods in machine learning.

For this project, you will perform quantum machine learning on the two first targets of Scikit learn iris data set. The data can be obtained the following way

from sklearn import datasets import numpy as np iris = datasets.load$_iris()x = iris.datay = iris.targetidx = np.where(y < 2)weonlytakethefirsttwotargets.$

x = x[idx,:] y = y[idx] x is the feature matrix and y are the targets.

Project 2 a): Encoding the Data Into a Quantum State. For this task you will consider a simple way of encoding a randomly generated data set sample into a quantum state:

import qiskit as qk import numpy as np np.random.seed(42)

p = 2 number of features data$_register = qk.QuantumRegister(p)classical_register = qk.ClassicalRegister(1)$

circuit = qk.QuantumCircuit(data$_register, classical_register)$

sample = np.random.uniform(size=p) target = np.random.uniform(size=1)

for feature$_idxinrange(p) : circuit.h(data_register[feature_idx])circuit.rz(2 * np.pi * sample[feature_idx], data_register[feature_idx])$

print(circuit)

The above code shows how a randomly generated data sample of $p = 2$ features are encoded into a quantum state on two qubits utilizing Qiskit. Each feature is encoded into a respective qubit utilizing a $R_y(\theta)$ gate. The features are scaled with 2π to represent rotation angles (the $R_y(\theta)$ gate performs a rotation). The classical register will be used later for storing the measured value of the circuit. print(circuit) can be utilized at any point to see what the circuit looks like.

Your task is to get familiar with the functionality utilized in the above example and implement your own function to encode the features of the iris data set to a quantum state.

Project 2 b): Processing the Encoded Data with Parameterized Gates. After the quantum state has been encoded with the information of a data set sample, one needs extend the circuit with operations that process the state in a way that allows us to infer the target data. This can be done by introducing quantum gates that are dependant on learnable parameters $\boldsymbol{\theta}$. We will do this in a similar fashion as for the encoding of the features:

n$_p arams = 4theta = 2 * np.pi * np.random.uniform(size = n_p arams)$
circuit.ry(theta[0], data$_r egister[0])circuit.ry(theta[1], data_r egister[1])$
circuit.cx(data$_r egister[0], data_r egister[1])$
circuit.ry(theta[2], data$_r egister[0])circuit.ry(theta[3], data_r egister[1])$
circuit.cx(data$_r egister[0], data_r egister[1])$
print(circuit)

The above parameterization of the quantum state is what we will refer to as the 'ansatz'. Your task is again to familiarize yourself with the functionality utilized in the above example and implement your own ansatz to be utilized together with the features of the iris data set. The number of learnable parameters 'theta' should be arbitrary.

Project 2c):Measuring the Quantum State and Making Inference. The next step is to generate a prediction from our quantum machine learning model. This is done by performing a measurement on the quantum state:

circuit.measure(data$_r egister[-1], classical_r egister[0])shots = 1000$

job = qk.execute(circuit, backend=qk.Aer.get$_b ackend('qasm_s imulator'), shots = shots, seed_s imulator = 42)results = job.result()results = results.get_c ounts(circuit)$

prediction = 0 for key,value in results.items(): if key == '1': prediction += value prediction/=shots print('Prediction:',prediction,'Target:',target[0]) Prediction: 0.285 Target: 0.7319939418114051

In the above example, we are first applying a measurement operation on the final qubit in the circuit, and we are interpreting our prediction as the probability that this qubit is in the 1 state. Make sure all the steps in the example are understood.

Implement your own function that generates a prediction by measuring one of the qubits.

Project 2d): Putting it all together. Now it is time to put together all of the above steps. Ideally, you should make a class or a function that given a feature matrix of n samples and an arbitrary number of model parameters, returns a vector of n outputs. For example:

n = 100 number of samples p = 4 number of features theta = np.random.uniform(size=20) array of model parameters X = np.random.uniform(size=(n,p)) design matrix y$_p red = model(X, theta)prediction, shape(n)$

We will now deal with how to train the model:

Project 2e): Parameter Shift-Rule and Calculating the Analytical Gradient. Since the model with random initial parameters is no good for

inference, we need to optimize the parameters in order to yield good results, as is the usual with machine learning.

Since we are dealing with classification, we will use cross-entropy as the loss function

$$L = -\sum_{i=1}^{n} y_i \ln f(x_i; \boldsymbol{\theta}),$$

where y_i are the target labels, and $f(\boldsymbol{x}_i; \boldsymbol{\theta})$ is the output of our model for a given sample $\boldsymbol{x}_i$ and parameterization $\boldsymbol{\theta}$). We calculate the gradiant by taking the derivative of the loss with respect to the parameters

$$\frac{\partial}{\partial \boldsymbol{\theta}_k} L = \sum_{i=1}^{n} \frac{f_i - y_i}{f_i(1-f_i)} \frac{\partial}{\partial \boldsymbol{\theta}_k} f_i,$$

where $f_i = f(x_i; \boldsymbol{\theta})$ for clarity. The only term we do not know how to calculate is $\frac{\partial}{\partial \boldsymbol{\theta}_k} f(x_i; \boldsymbol{\theta})$, but it turns out there is a simple trick to do this, the so-called parameter shift-rule
citeParameterShift. To calculate the derivative of the model output, we need to evaluate the model twice with the respective parameter shifted by a value $\frac{\pi}{2}$ up and down. The two resulting outputs are then put together to yield the derivative

$$\frac{\partial f(x_i; \theta_1, \theta_2, \ldots, \theta_k)}{\partial \theta_j} = \frac{f(x_i; \theta_1, \theta_2, \ldots, \theta_j + \pi/2, \ldots, \theta_k) - f(x_i; \theta_1, \theta_2, \ldots, \theta_j - \pi/2, \ldots, \theta_k)}{2}$$

Train your model by utilizing the Parameter Shift-Rule and some gradient descent algorithm. Compare your results with for example logistic regression.

Regular gradient descent does the job, but it is often outperformed by momentum based optimizers like Adam.

Project 2f): Adding Variations on the Data Encoding and Ansatz. Change/add more gates to the encoder and the parameterized ansatz to produce a more complex model (See for example figure 4 and figure 5 in https://arxiv.org/abs/2011.00027 for inspiration). Train these new models on the iris data set. How do they compare? As a more challenging problem, you may train on the first few features of the Breast Cancer Data as well to see how the more powerful model performs.

from sklearn.datasets import load$_b reast_c ancer$

data = load$_b reast_c ancer()x = data.datafeaturesy = data.targettargets$

Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.
- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.
- Include the source code of your program. Comment your program properly.
- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.
- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.
- Try to evaluate the reliabilty and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.
- Try to give an interpretation of you results in your answers to the problems.
- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.
- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.

Format for electronic delivery of report and programs

The preferred format for the report is a PDF file. You can also use DOC or postscript formats or as an ipython notebook file. As programming language we prefer that you choose between C/C++, Fortran2008 or Python. The following prescription should be followed when preparing the report:

- Use canvas to hand in your projects, log in at `http://canvas.uio.no` with your normal UiO username and password.
- Upload **only** the report file! For the source code file(s) you have developed please provide us with your link to your github domain. The report file should include all of your discussions and a list of the codes you have developed. The full version of the codes should be in your github repository.

- In your github repository, please include a folder which contains selected results. These can be in the form of output from your code for a selected set of runs and input parameters.
- Still in your github make a folder where you place your codes.
- In this and all later projects, you should include tests (for example unit tests) of your code(s).
- Comments from us on your projects, approval or not, corrections to be made etc can be found under your Devilry domain and are only visible to you and the teachers of the course.

Finally, we encourage you to work two and two together. Optimal working groups consist of 2-3 students. You can then hand in a common report.