Computational Physics Projects - 2024

MnP Club, IIT Bombay

Quantum Machine Learning

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3 Week 2 - Introduction to VQAs

3.1 A brief note on Variational Quantum Algorithms

Introduced here is a class of quantum algorithms most commonly used to find solutions to problems that involve iterating through a number of points. These involve parameterized quantum circuits that can mimic a desired solution to a desired extent subject to the parameters being rightly chosen. This task of choosing the right parameters for the circuit to be a solution of the problem in hand is offloaded to a classical algorithm that can minimize/maximize or bring close to a desired value a "property" of the quantum circuit. This "property" of the circuit can be the expectation value with respect to a certain operator.
When the task assigned to the classical algorithm is the minimization of the expectation value of the output state of the system with respect to a hamiltonian operator, the quantum-classical loop becomes the **Variational Quantum Eigensolver**. The objective for a VQE is finding the eigenstate of the hamiltonian with the minimum eigenvalue.

3.2 The circuit - Variational Quantum Eigensolver Ansatz

A parameterized quantum circuit operates on an initial state, typically chosen to be $|0\rangle$ ($|000...\rangle$ for a mutli-qubit problem). The output of this circuit operation on the initial state is the output state $|\psi\rangle$ which is desired to be the minimum energy (minimum eigenvalue) eigenstate for the chosen hamiltonian. This parameterized circuit is termed as the **Ansatz** circuit, which forms a foundational element in "quantum machine learning" tasks.
Various kinds of ansatz designs are adopted, the one used here is the **hardware efficient ansatz**, made up of repeating rotation and CNOT operators.
The ansatz can be thought of as a **trial operator** that is the "form" in which the solution is assumed to exist in, and hence the choice of the ansatz structure is crucial.

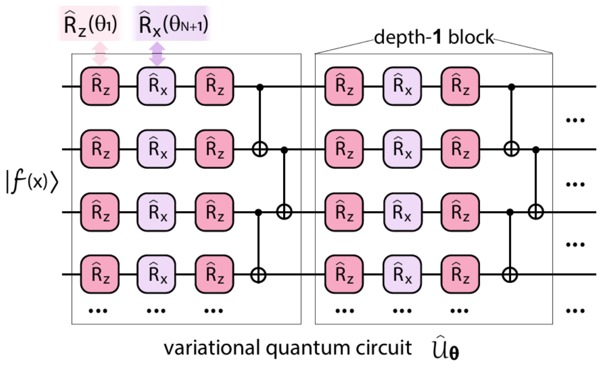

$\hat{R}_z(\theta_1)$
$\hat{R}_x(\theta_{N+1})$
depth-**1** block
$|f(x)\rangle$
$\hat{R}_z$
$\hat{R}_x$
variational quantum circuit $\hat{U}_{\boldsymbol{\theta}}$

Figure 1: Hardware Efficient Ansatz with depth = 2

3.3 Implementation

- A two qubit system with the hamiltonian XX + YY + ZI is chosen.
- A 4 layer HEA with Y and Z rotations is used, leading to 16 iterable parameters.
- The Aer backend is used for the simulations.
- Since this is a VQE, the cost function is the expectation value of the hamiltonian for the output state of the ansatz.
- For the eigennvalue minimization, the minimize function from scipy is used, along with a test for the best minimizer routine.

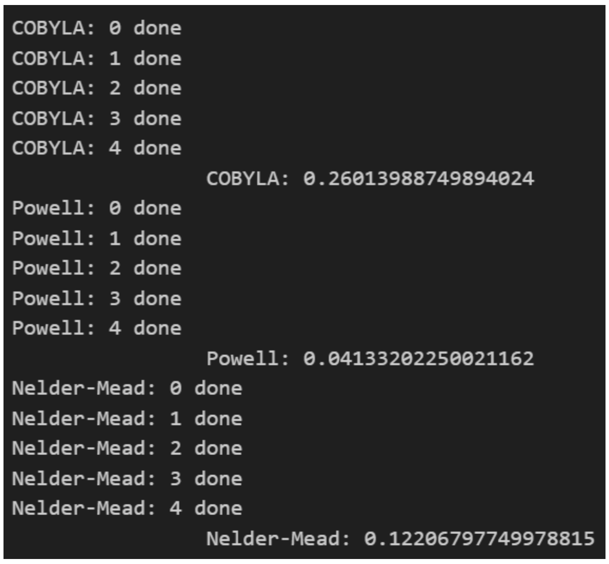
3.4 Results

3.4.1 The best optimizer

After trying the 14 available methods in scipy, the following were deemed useless:

- **Nelder-Mead** - Gradient-free approach - Takes a lot of time - However, it is precise.
- **CG, BFGS** - Desired error not necessarily achieved due to precision loss.
- **Newton-CG, dogleg, trust-ncg, trust-exact, trust-krylov** - More complex, Jacobian computation required
- **L-BFGS-B, TNC** - Couldn't converge - Oscillating series
- **SLSQP, trust-constr** - Incorrect results

After comparing the three most accurate options, the best one was found to be Powel:



```
COBYLA: 0 done
COBYLA: 1 done
COBYLA: 2 done
COBYLA: 3 done
COBYLA: 4 done
                COBYLA: 0.26013988749894024
Powell: 0 done
Powell: 1 done
Powell: 2 done
Powell: 3 done
Powell: 4 done
                Powell: 0.04133202250021162
Nelder-Mead: 0 done
Nelder-Mead: 1 done
Nelder-Mead: 2 done
Nelder-Mead: 3 done
Nelder-Mead: 4 done
                Nelder-Mead: 0.12206797749978815
```

3.4.2 Cost landscape

- **Powell method**

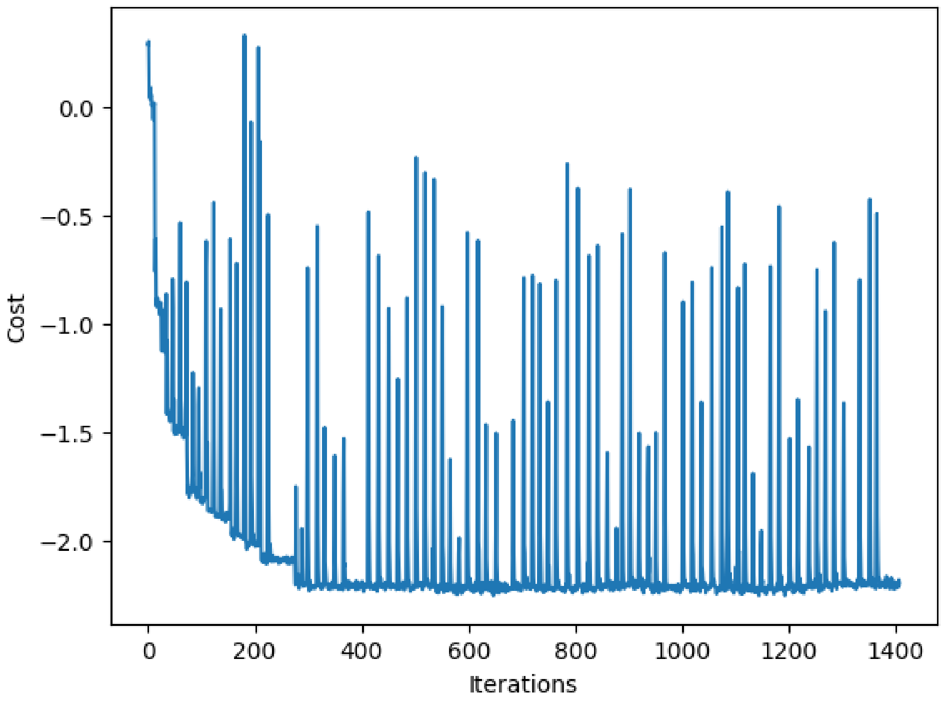


Figure 2: Unstable, ”spikes” in the landscape

- **COBYLA method**

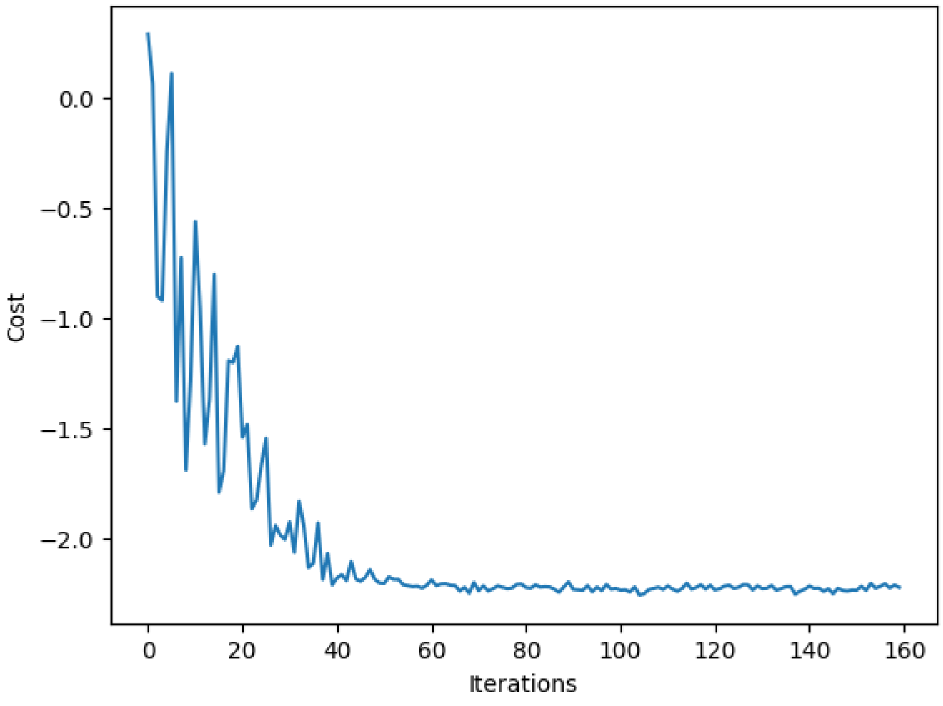
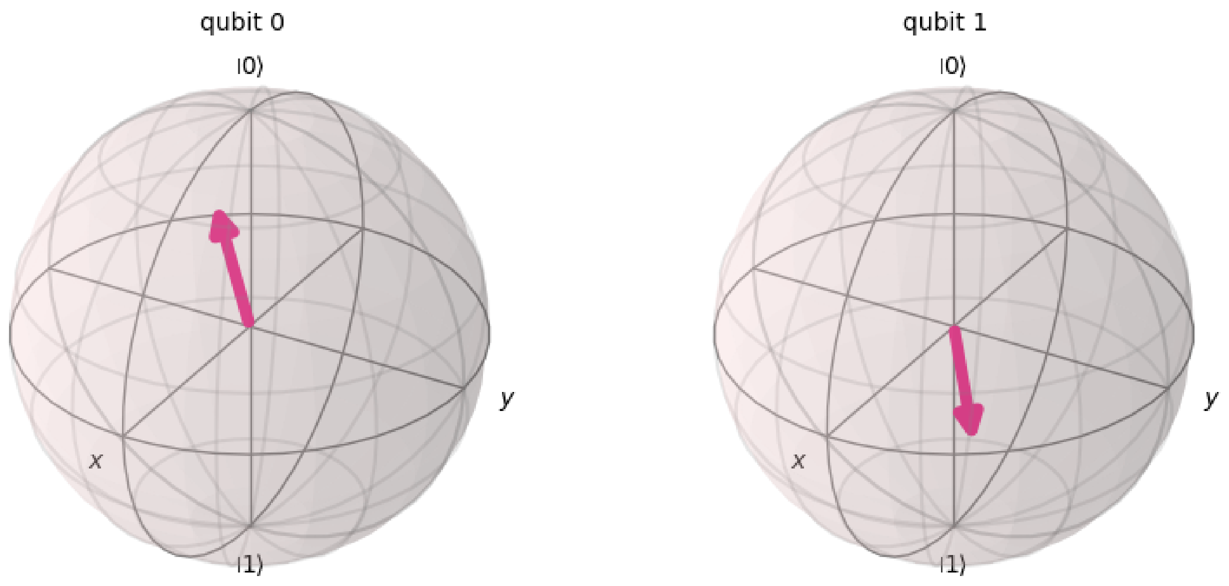


Figure 3: Comparatively stable

3.4.3 Minimum eigenvalue and the corresponding eigenstate

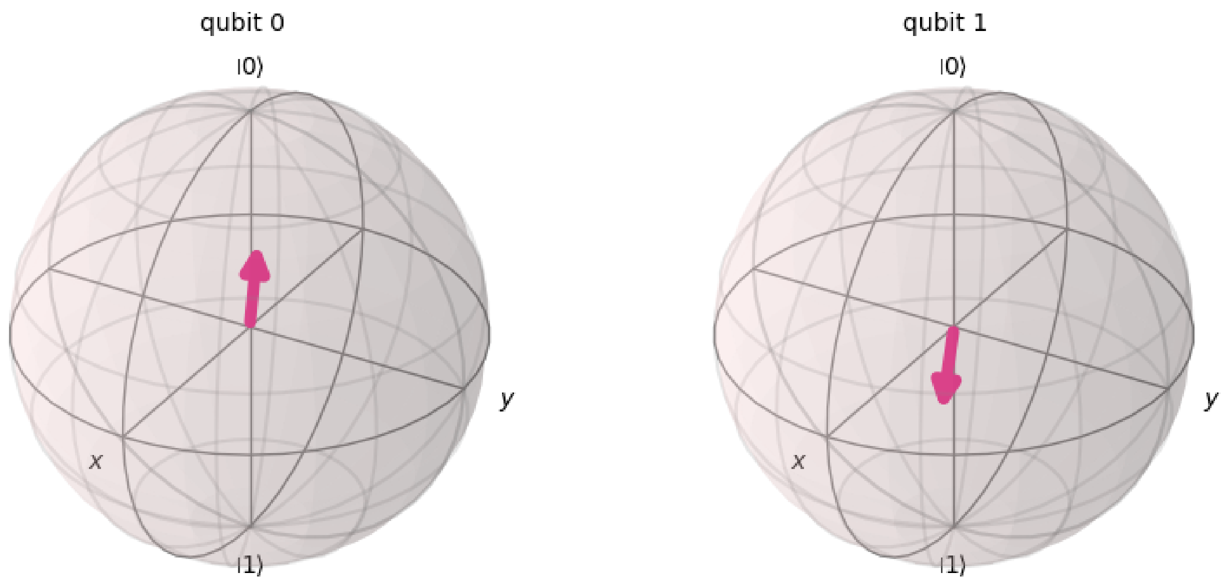
Powell method

Minimum eigenvalue = -2.2250

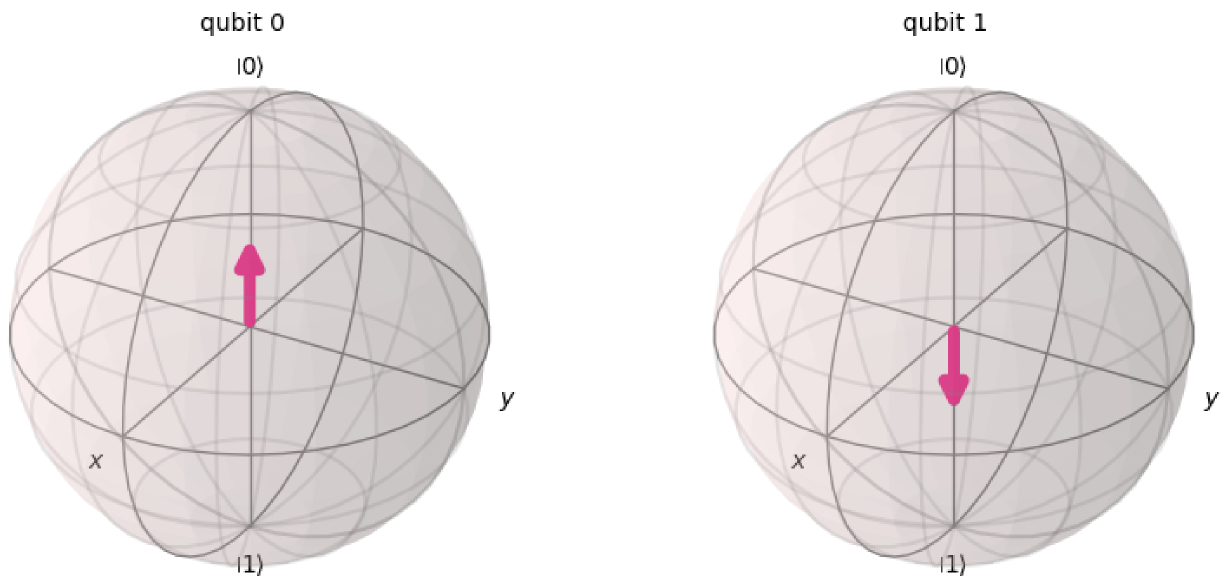


COBYLA method

Minimum eigenvalue = -2.2254



NumpyMinimumEigensolver
Minimum eigenvalue = -2.2361



3.5 Final Conclusions

- In Scipy.optimize, out of the 14 available solver methods, only 2 were suitable for this scenario.
- These were the Powell and COBYLA methods, Nelder-Mead being accurate but slow.
- From an error analysis POV, the results from Powell showed higher similarity to those from the NumPyMinimumEigensolver.
- But, COBYLA outperformed Powell in terms of the monotonicity and stability of the loss landscape.
- The Final minimum Eigenvalues for the two methods do get very close to that obtained from the NumPyMinimumEigensolver.
- After running the experiment multiple times, the final Eigenstate was found to be unstable, sensitive to the initial guess.

4 Week 3 - Solving Differential equations

Here, using objects called ”Differential quantum circuits”, we explore how quantum circuits can represent derivatives and hence try to solve non-linear differential equations.
The differential equation is denoted as $F[d_x f(x), f(x), x] = 0$, with the boundary condition being $f(x_0) = u_0$.
The following article refers to the research paper titled ”Solving nonlinear differential equations with differentiable quantum circuits” by Oleksandr Kyriienko, Annie E. Paine and Vincent E. Elfving.

4.1 A brief introduction to the methodologies used

A ”Quantum Differential Equation Solver”, as we may call it, would need to represent a ”trial solution function” on a quantum circuit, along with a method to compute the required derivatives as per the DE.
The key aspect of the research involves a method called a ”Quantum Feature Map” aided by the parameter-shift rule to represent functions and their derivatives on quantum hardware respectively.
The real function evaluation itself can be obtained as the expectation of a predefined Hermitian operator.

4.2 The avenues to achieve the proposed solution

4.2.1 Quantum Feature Maps

These are unitary circuits parameterized by a variable ”x” and a non-linear function ”$\varphi(x)$”, represented as $\hat{U}_\varphi(x)$. These, when applied to the input state $|\emptyset\rangle$ map x to $\hat{U}_\varphi(x)|\emptyset\rangle$. This is called the ”latent space mapping”.
The quantum feature map circuit serves the purpose of closely representing highly non-linear functions and their derivatives. Listed below is one of the possible frameworks for the feature map circuit using sequential Qubit rotations, the ”Product Feature Map”, along with a specific class of it called the Chebyshev feature map.

- **Product Feature Map**: This methodology involves applying a non-linear transformation to x followed by a set of Qubit rotations. It is also allowed to have the circuit made up of multi-layered rotations.
  For an N Qubit system, the mathematical representations can be given as:
  Single layered approach:

  $$\hat{U}_\varphi(x) = \bigotimes_{j=1}^{N} \hat{R}_{\alpha,j}(\varphi[x]), \tag{1}$$

  Multi-Layered approach:

$$\hat{U}_{\varphi}(x) = \prod_{\ell=1}^{L} \bigotimes_{j \in \mathbb{N}_\ell} \hat{R}^{(\ell)}_{\alpha,j}(\varphi_\ell[x]). \tag{2}$$

Where $\hat{R}_{\alpha,j}$ is the Pauli rotation operator acting on Qubit j, involving complex exponentiation of one of the three Pauli matrices, chosen by $\alpha \ \epsilon \ \{x, y, z\}$.

- **Derivative of the Product Feature Map**: Working out the derivative of $\hat{U}_{\varphi}(x)$:

$$\frac{d}{dx}\hat{U}_{\varphi(x)} = \frac{1}{2}\left(\frac{d}{dx}\varphi(x)\right)\left(\sum_{j'=1}^{N}\bigotimes_{j=1}^{N}\hat{R}_{y,j}(\varphi[x] + \frac{\pi}{2}\delta_{j,j'})\right) \tag{3}$$

  The parameter-shift rule form becomes visible when the expectation with respect to an operator $\hat{C}$ is written out:

$$\frac{d}{dx}\langle\emptyset|\hat{U}_{\varphi}(x)^{\dagger}\hat{C}\hat{U}_{\varphi}(x)|\emptyset\rangle = \frac{1}{4}\left(\frac{d}{dx}\varphi(x)\right)\left(\langle\hat{C}\rangle^{+} - \langle\hat{C}\rangle^{-}\right) \tag{4}$$

  where:

$$\langle\hat{C}\rangle^{\pm} = \sum_{j'=1}^{N}\bigotimes_{j=1}^{N}\langle\varnothing|\hat{R}^{\dagger}_{y,j}(\varphi[x] \pm \frac{\pi}{2}\delta_{j,j'})\hat{C}\hat{R}_{y,j}(\varphi[x] \pm \frac{\pi}{2}\delta_{j,j'})|\varnothing\rangle \tag{5}$$

- **Chebyshev Feature Map**: This is a sub-class of the product feature map, obtained by choosing $\varphi(x)$ as $2n\cos^{-1}x$ for some integer n.
  The reason for this choice becomes evident as the true form of the rotation operator is revealed as being made up of two Chebyshev functions by the Euler's identity.

  A short note on Chebyshev functions and their utility here: Chebyshev functions are simple polynomial functions aided by trigonometric relations:

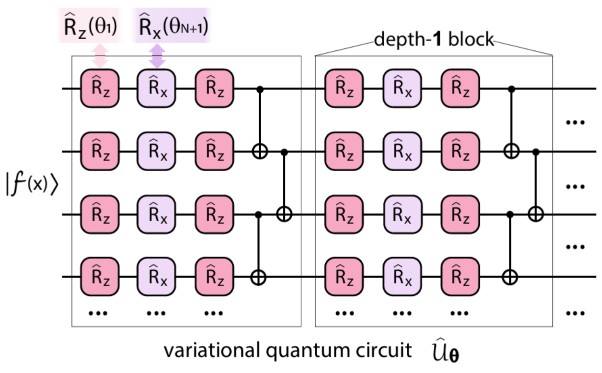
$$T_n(cos(\theta)) = cos(n\theta)$$
$$U_n(cos(\theta))sin(\theta) = sin((n+1)\theta)$$

  These are powerful in that when used as basis, two functions can be multiplied (called "**chaining**") to give rise to another two functions orthogonal to the initial two functions, and hence can provide a rich representation of functions.
  The chaining property enables to grow the basis set through state concatenation.

4.2.2 Variational Quantum Circuit - Ansatzes

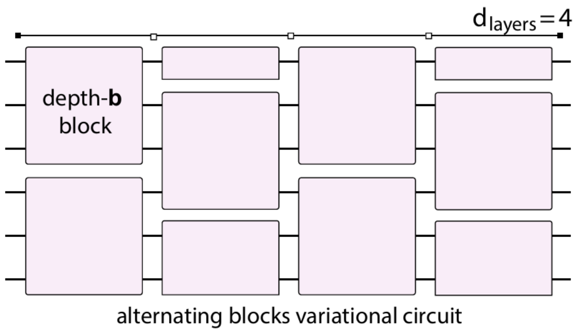
The ansatz manipulates the latent space basis function and brings the derivatives and the function to the required form.
A difference from the approach used in the Variational Quantum Eigensolver is that here the gradient is computed by the quantum circuit itself and fed to a classical optimizer such as GD, Adam, SGD, etc. whereas the VQE approach just uses the quantum circuit as an oracle to compute the ansatz state followed by Hamiltonian expectation computation.

- **Hardware efficient ansatz**: Rotations followed by CNOT gates for entanglement.



$\hat{R}_z(\theta_1)$
$\hat{R}_x(\theta_{N+1})$
depth-**1** block
$|f(x)\rangle$
$\hat{R}_z$
$\hat{R}_x$
variational quantum circuit $\hat{\mathcal{U}}_{\boldsymbol{\theta}}$

- **Alternating blocks ansatz**:



4.2.3 Cost Operator

- **A predefined hermitian operator**: A hermitian operator $\hat{C}$ is used for which the expectation value, parameterized by a non-linear dependence on x and the variational angles can be used to evaluate the real value of the function.
  The function can be evaluated as:

$$f(x) = \langle f_{\varphi,\theta}(x)|\hat{C}|f_{\varphi,\theta}(x)\rangle \tag{6}$$

4.2.4 Loss Function

- **Quantifying "distance"**: The purpose of any loss function in optimization problems is to measure how far the solution is to the desired value in some vector space relevant to the problem case. Here, a "distance" metric is needed to evaluate how far the $F[d_x f(x), f(x), x]$ form is from 0, the desired value.
  A standard choice for the distance measure is the MSE, while MAE and KL Divergence are also beneficial for specific problems.

4.2.5 Boundary Handling

Unlike an analytical pen and paper approach to solving differential equations where we first obtain a general form of the solution and then adjust parameters of the general form to fit the boundary conditions, here the DQC takes a numerical approach, and hence the need of including the boundary condition somewhere in the loss arises.

- **Pinned handling**: Adds a boundary term to the overall loss function:
$$\mathcal{L}_\theta[d_x f, f, x] = \mathcal{L}_\theta^{(\text{diff})}[d_x f, f, x] + \mathcal{L}_\theta^{(\text{boundary})}[f, x] \tag{7}$$
- **Floating handling**: Boundary term is added in the function evaluation:
$$f(x) = f_b + \langle f_{\varphi,\theta}(x)|\hat{C}|f_{\varphi,\theta}(x)\rangle \tag{8}$$
f_b is updated at each iteration:
$$f_b \leftarrow u_0 - \langle f_{\varphi,\theta}(x_0)|\hat{C}|f_{\varphi,\theta}(x_0)\rangle \tag{9}$$
- **Optimized handling**: This is the standard "offload tasks to the optimizer" approach, where we just expect the optimizer to come up with a "good" solution, here the function is computed from the mapping as:
$$f(x) = f_c + \langle f_{\varphi,\theta}(x)|\hat{C}|f_{\varphi,\theta}(x)\rangle, \tag{10}$$
The f_c term adjusts the function to satisfy the boundary, and itself is a parameter for the optimizer to adjust.

4.3 Algorithm Workflow

With the components in hand, the workflow can now be described.

- The first step involves choosing the feature map circuit, the non linear function $\varphi(x)$, the VQC, the cost operator, the loss function, classical optimizer and regularization, if any.
- The parameters for the optimizer to update are the ansatz parameters θ, whereas the x variable used in the feature map circuit is the variable for function evaluation.
- A grid of points $\mathbb{X}$ to be used to evaluate the solution of the method at each iteration, are initialized.
- Also, the variational parameters θ are randomly initialized.
- The Derivative Quantum Circuits are constructed based on the differentials involved in the DE.
- The loss function is computed for the entire grid of points.
- The gradient of the loss function with respect to θ is computed for the optimizer.
- The algorithm is a quantum-classical loop, where a classical optimizer algorithm, say, Adam, calls the trial function and its derivatives as quantum oracles to compute the parameter update term from the loss gradient.
- When the loss converges, the algorithm returns $\theta_{optimal}$ for which:
$$f(x) = \langle\emptyset|\hat{U}_\varphi(x)\hat{U}_\theta|\hat{C}|\hat{U}_\theta\hat{U}_\varphi(x)|\emptyset\rangle$$

4.4 Implementation

4.4.1 Linear differential equation

The following linear DE is solved here:

$$\frac{dy}{dx} + \lambda y \left(\kappa + \tan(\lambda x)\right) = 0, \quad y(0) = 1 \tag{11}$$

- **Feature Map:** 6 Qubit Chebyshev feature map, without a tower-type rescaling.
- **Ansatz:** 20 layer Hardware Efficient Ansatz.
- **Cost operator:** Total magnetization.
- **Loss function:** Sum of Mean-squared ODE, boundary and regularization errors.
- **Optimizer:** Adam.
- **Regularization:** Error with respect to the actual solution at points [-1, -0.75, -0.5, -0.25, 0, 0.25, 0.5, 0.75, 1].
- λ: 1
- κ: varied in the range [0.1, 0.5, 1, 2]

4.4.2 Differential equation with highly nontrivial dynamics

The following linear DE is solved here:

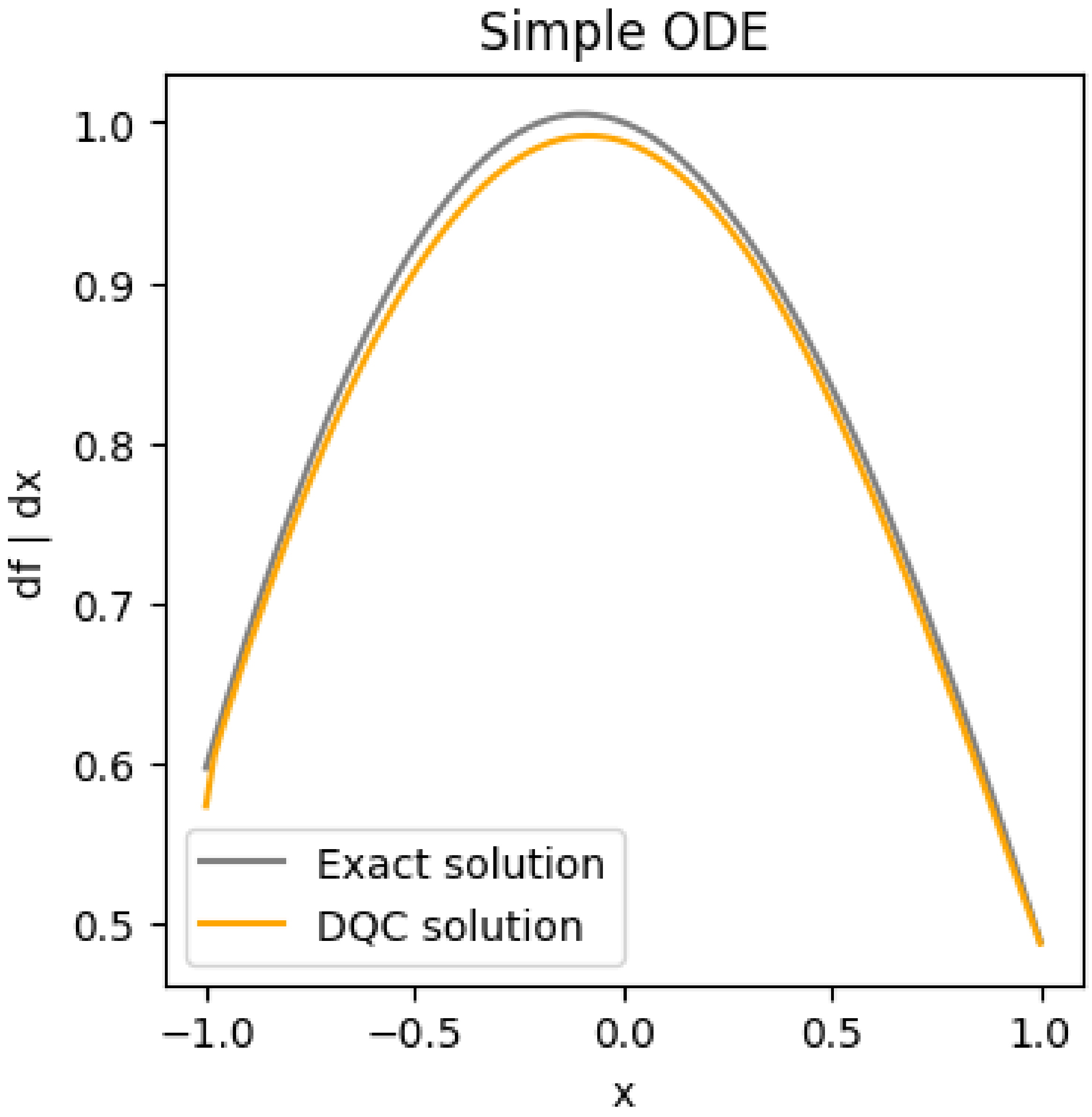
$$\frac{dy}{dx} - 4y + 6y^2 - \sin 50x - y\cos 25x + 0.5 = 0, \quad y(0) = 0.75 \tag{12}$$

- **Feature Map:** 10 Qubit Tower Chebyshev feature map.
- **Ansatz:** 25 layer Hardware Efficient Ansatz.
- **Cost operator:** Total magnetization.
- **Loss function:** Sum of Mean-squared ODE, boundary and regularization errors.
- **Optimizer:** Adam.
- **Regularization:** Error with respect to the actual solution at points [0, 0.2, 0.4, 0.6, 0.8, 1].

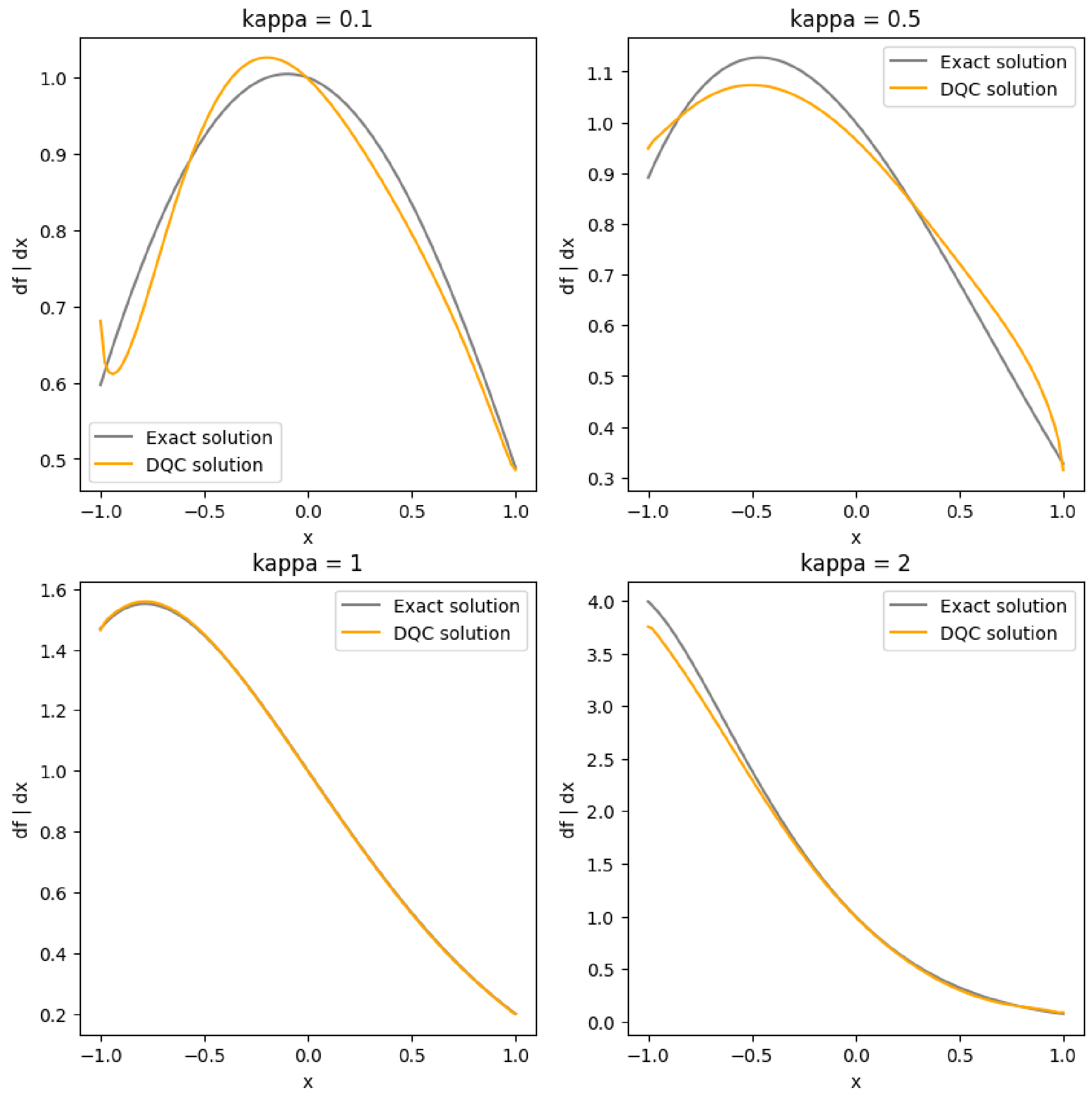
4.5 Results

4.5.1 Linear differential equation

Solution for $\kappa = 0.1,\ \lambda = 1$



Varying κ, keeping λ fixed at 1
S



4.5.2 Differential equation with highly nontrivial dynamics

References

- Quantum Computation and Quantum Information by Michael A. Nielsen and Isaac L. Chuang
- Variational Quantum Algorithms: `https://arxiv.org/abs/2012.09265`
- Solving nonlinear differential equations with differentiable quantum circuits: `https://arxiv.org/abs/2011.10395`

5 Week 4 - Pasqal Challenge - ETH Quantum Hackathon 2024

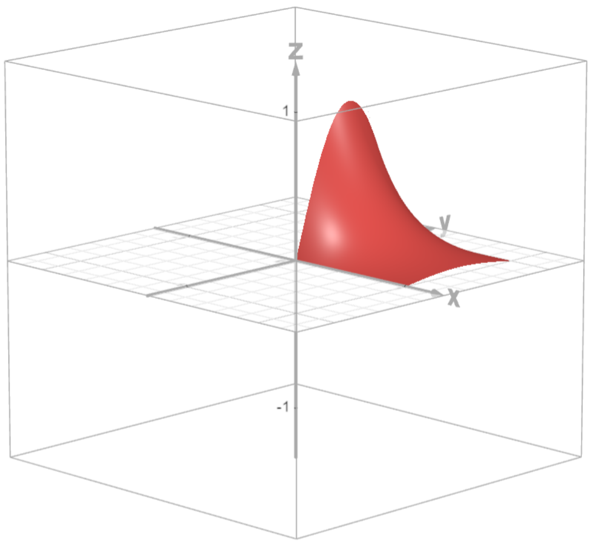
5.1 The Task - Solving a Partial Differential Equation in 2D

The 2D Laplace equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{13}$$

Over the domain (x,y) $\epsilon[0, 1]^2$ with the 4 boundary conditions:
- u(0, y) = $sin(\pi y)$
- u(x, 0) = 0
- u(1, y) = $e^{-\pi} sin(\pi y)$
- u(x, 1) = 0

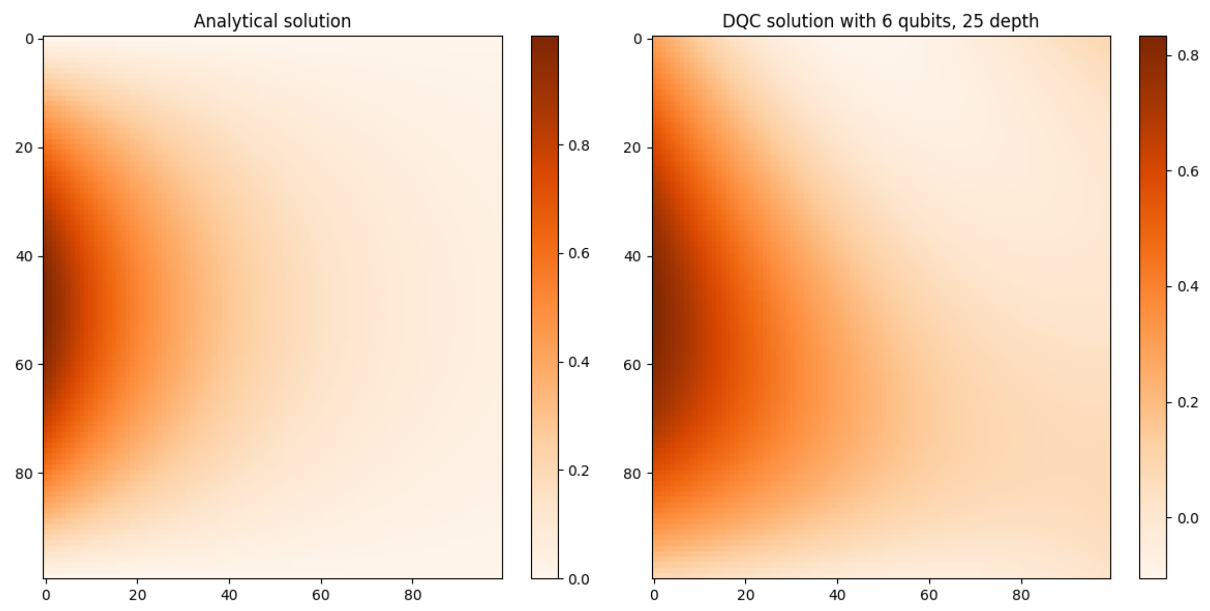
The analytical solution of this problem is: $e^{-\pi x} sin(\pi y)$, as plotted below:



5.2 Implementation

- **Feature Map:** 6 Qubit Fourier feature map.
- **Ansatz:** 25 layer Hardware Efficient Ansatz.
- **Cost operator:** Ising Hamiltonian
- **Loss function:** Sum of Mean-squared ODE and boundary errors.
- **Optimizer:** Adam.
- **Regularization:** None

5.3 Results


Analytical solution
DQC solution with 6 qubits, 25 depth