

Experimenting with machine learning algorithms on quantum computers

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Abstract

A modern számítástechnika jelentős eredményei közé tartozik a gépi tanulás és mesterséges intelligencia alapvető algoritmusainak kifejlesztése és ezek hasznosságának tesztelése különböző feladatokon. Ugyanakkor az elmúlt években a kvantumszámítás is jelentős fejlődésen ment keresztül, olyannyira, hogy 2019-ben a Google kísérleti csapatának sikerült demonstrálnia a kvantumfölényt. A munka során megvizsgáljuk a két terület átfedéséből származó lehetőségeket: klasszikus adatok kvantumozását illetve a klasszikus gépi tanulás segítségével történő kvantumozás hibajavítást.

Gépi tanulási algoritmusok vizsgálata kvantumszámítógépeken

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Kivonat

A modern számítástechnika jelentős eredményei közé tartozik a gépi tanulás és mesterséges intelligencia alapvető algoritmusainak kifejlesztése és ezek hasznosságának tesztelése különböző feladatokon. Ugyanakkor az elmúlt években a kvantumszámítás is jelentős fejlődésen ment keresztül, olyannyira, hogy 2019-ben a Google kísérleti csapatának sikerült demonstrálnia a kvantumfölényt. A munka során megvizsgáljuk a két terület átfedéséből származó lehetőségeket: klasszikus adatok kvantumozását illetve a klasszikus gépi tanulás segítségével történő kvantumozás hibajavítást.

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1 Introduction

Quantum computing is probably the most promising emerging technology with many possible applications across all domains of science and business. The idea of quantum computing was first proposed by Richard P. Feynman as a method to simulate quantum mechanics. Since the size of the Hilbert-space grows exponentially with the complexity of the quantum system, and thus the calculations become intractable on any classical computer, Feynmans idea was to simulate quantum physics on devices that behave themselves according to the rules of quantum physics.

Soon after Feynmans proposal, scientists became to establish the theoretical background of quantum information and quantum computing. Some of the quantum algorithms are proven to have an advantage over any known classical algorithm. One of the first such quantum algorithm is the Deutsch-Jozsa algorithm [1], which decides if a binary function f is balanced or constant. Probably the most notable quantum algorithm was proposed by Peter W. Shor in 1994, which is a polynomial-time quantum algorithm for factoring large integers [2]. This is the first quantum algorithm with a real-life application, because most of the public-key cryptosystems could be broken with an efficient algorithm for integer factoring. Another important quantum algorithm is the Grover's algorithm proposed by Lov K. Grover in 1996 for searching an unordered database [3]. While the best known classical algorithm for searching unordered databases runs in $O(N)$ time, Grover's algorithm solves this problem with $O(\sqrt{N})$ oracle queries. Beyond quantum algorithms, many quantum-inspired algorithms were discovered [4, 5, 6].

2 Quantum Computing with continuous variables

[Dani: cite: Xanadu paper, Photonic Supremacy paper, PsiQuantum Fusion-Based QC]

Continuous variable (CV) systems have infinite degrees of freedom, and therefore the corresponding Hilbert-space is of infinite dimensions. Such systems can be modeled by M harmonic oscillators, which are usually called *modes*. With H_k denoting the Hilbert-space of the k th mode, the Hilbert-space of the full CV system is their direct sum:

$$\mathcal{H} = \bigoplus_{k=1}^M \mathcal{H}_k. \quad (1)$$

The Hamiltonian of mode j can be described by introducing bosonic creation and annihilation operators a_j^\dagger and a_j , obeying the following canonical commutation relations:

$$[\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}, [\hat{a}_j^\dagger, \hat{a}_k^\dagger] = [\hat{a}_j, \hat{a}_k] = 0. \quad (2)$$

The effect of the creation and annihilation operators on the Fock space can be described by the following identities:

$$\begin{aligned} \hat{a}_k^\dagger |n_1, \dots, n_k, \dots\rangle &= \sqrt{1 + n_k} |n_1, \dots, n_k + 1, \dots\rangle \\ \hat{a}_k |n_1, \dots, n_k, \dots\rangle &= \sqrt{n_k} |n_1, \dots, n_k - 1, \dots\rangle \end{aligned} \quad (3)$$

We also introduce the number operator $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$:

$$\hat{a}_k^\dagger \hat{a}_k |n_1, \dots, n_k, \dots\rangle = \hat{n}_k |n_1, \dots, n_k, \dots\rangle = n_k |n_1, \dots, n_k, \dots\rangle \quad (4)$$

Each of the single-mode Hilbert-space \mathcal{H}_k is an infinite-dimensional Fock-space spanned by the eigenvectors of the number operator $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ labeled $\{|n\rangle\}_k$. It is often useful to introduce the canonical position operators X_j and momentum operators P_j which are related to the creation and annihilation operators by the following transformations:

$$\hat{X}_k = \frac{\hat{a}_k + \hat{a}_k^\dagger}{\sqrt{2}} \quad \hat{a}_k = \frac{\hat{X}_k + i\hat{P}_k}{\sqrt{2}} \quad (5)$$

$$\hat{P}_k = \frac{\hat{a}_k - \hat{a}_k^\dagger}{i\sqrt{2}} \quad \hat{a}_k^\dagger = \frac{\hat{X}_k - i\hat{P}_k}{\sqrt{2}} \quad (6)$$

Operators \hat{X}_k and \hat{P}_k are called quadrature operators. Following the notation often used in literature, we group these operators into a vector

$$\boldsymbol{\xi}^\top = (\hat{X}_1, \hat{P}_1, \hat{X}_2, \hat{P}_2, \dots, \hat{X}_k, \hat{P}_k, \dots, \hat{X}_M, \hat{P}_M) \quad (7)$$

We can calculate the commutators $[\boldsymbol{\xi}_k, \boldsymbol{\xi}_l]$ by introducing a symplectic form $\boldsymbol{\Omega}$ as

$$\boldsymbol{\Omega} = \bigoplus_{j=1}^M \boldsymbol{\omega}, \quad \boldsymbol{\omega} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (8)$$

Using this notation, we can write

$$[\boldsymbol{\xi}_k, \boldsymbol{\xi}_l] = i\boldsymbol{\Omega}_{kl} \quad (9)$$

[Dani: Write about homodyne measurements, heterodyne measurements and photon number-resolving measurements] [Dani: Write about different quantum gates.]

3 Machine learning

3.1 Classification and Regression

3.2 Reinforcement learning

3.2.1 Proximal Policy optimization

$$r_t(\theta) = \frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{\text{old}}}(a_t|s_t)} = \log \pi_\theta(a_t|s_t) - \log \pi_{\theta_{\text{old}}}(a_t|s_t) \quad (10)$$

$$\delta_t = r_t + \gamma V^\pi(s_{t+1}) - V^\pi(s_t) \quad (11)$$

$$\hat{A}_t = \sum_{l=0}^{T-t-1} (\gamma\lambda)^l \delta_{t+l} = (\gamma\lambda)^0 \delta_t + (\gamma\lambda) \delta_{t+1} + \dots + (\gamma\lambda)^{T-t-1} \delta_{T-1} \quad (12)$$

$$L^{CLIP}(\theta) = \mathbb{E}_t \left[\min \left(r_t(\theta) \hat{A}_t, \text{clip}(r_t(\theta), 1 - \epsilon, 1 + \epsilon) \hat{A}_t \right) \right] = \mathbb{E}_t \left[\min \left(r_t(\theta) \hat{A}_t, g(\epsilon, \hat{A}_t) \right) \right] \quad (13)$$

$$g(\epsilon, \hat{A}_t) = \begin{cases} (1 + \epsilon) \hat{A}_t, & \hat{A}_t \geq 0 \\ (1 - \epsilon) \hat{A}_t, & \text{otherwise} \end{cases} \quad (14)$$

$$V_{\text{target}}^\pi(s_t) = \sum_{l=0}^{T-t} \gamma^l r_{t+l} \quad (15)$$

$$L^{VF} = \mathbb{E}_t \left[\left(V^\pi(s_t) - V_{\text{target}}^\pi(s_t) \right)^2 \right] \quad (16)$$

$$H[\pi] = \mathbb{E}_t \left[- \sum_{a \in \mathcal{A}} \pi_\theta(a|s_t) \log \pi_\theta(a|s_t) \right] \quad (17)$$

$$L = L^{CLIP} + c_1 L^{VF} + c_2 H[\pi] \quad (18)$$

How to measure the entropy term for a quantum state ρ ? How to measure the KL-divergence of two quantum states ρ_1, ρ_2 ?

Algorithm 1 PPO-Clip

```

1: procedure PPOCLIP( $\epsilon, E, N, T, K$ )
2:   for all  $i \in \{1, \dots, E\}$  do
3:     for all  $n \in \{1, \dots, N\}$  do
4:       Run the old policy  $\pi_{\text{old}}$  in the environment for  $T$  timesteps.
5:       for all  $t \in \{1, \dots, T\}$  do
6:         Calculate the advantage estimate  $\hat{A}_t$ 
7:       end for
8:     end for
9:     for all  $k \in \{1, \dots, K\}$  do
10:      Sample a batch of size  $M \leq NT$  and optimize the surrogate loss  $L$ .
11:    end for
12:  end for
13: end procedure

```

4 Quantum Machine Learning

QSVM paper = [7] HHL paper = [8] Feature Hilbert Spaces = [9] Cv-Qnns -LLoyd = [10] **[Dani: related papers: quantum svm, Kernel methods, HHL algorithm for matrix inversion, quantum-inspired classical algos**

motivation: summary from Lloyd paper, regression, classification, hybrid traning, encoding, inference

General structure: encoding, rotations and beamsplitter = interferometer, squeezing, interferometer, displacement, all = affine transformation + at the end non-linear, e.g., cubic phase operation (numeric instability switch to Kerr gates -> write at the performance test)

Loss functions: regression, classification

Regularization: keep trace close to zero, non-Gaussian

|

4.1 Parametric quantum circuits

4.2 Variational Quantum Eigensolver

Variational Quantum Eigensolvers [11] are hybrid quantum-classical algorithms designed to find the lowest energy eigenvalue of some Hamiltonian H . VQEs are one of the most studied quantum algorithms because of their expected use cases in quantum chemistry and materials science [12, 13, 14, 15]. The basic idea behind the variational quantum eigensolver is as follows. First we fix the structure of a parametric quantum circuit called the ansatz, defined by a unitary $U(\boldsymbol{\theta})$, where $\boldsymbol{\theta} \in \mathbb{R}^m$ are real parameters. Then we start by some initial state $|\psi_0\rangle$, which is usually $|0\rangle^{\otimes M}$ in the qubit setting. For the continuous variable setting, the initial state can be the vacuum state, a displaced state, a squeezed state, or a photon number eigenstate. After preparing the circuit, we evaluate the expectation value of the Hamiltonian which is eventually the cost, or loss:

$$\mathcal{L}(\boldsymbol{\theta}) = \langle H \rangle = \langle \psi_0 | U^\dagger(\boldsymbol{\theta}) H U(\boldsymbol{\theta}) | \psi_0 \rangle \quad (19)$$

The goal is to minimize the loss \mathcal{L} by iteratively updating the parameters $\boldsymbol{\theta}$ with some update rule. This update rule can be any gradient-free [16] or gradient-based method **[Dani: idezet]**. To use gradient descent optimization in the VQE setting, we need to evaluate the gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}$, which can be challenging, and is described in details in chapter 4.3. Algorithm 2 describes the variational quantum eigensolver with a general gradient-based learning method. Notice that we wrote $\alpha_j^{(t)}$ for the learning rate, since in most modern optimizers like Adam [17], each parameter has its own learning rate and it may depend on the number of iterations already done.

Algorithm 2 VQE

```

1: procedure VQE( $H, K, T, \alpha$ )
2:   for all  $t \in \{1, \dots, T\}$  do
3:     Prepare the ansatz  $U(\boldsymbol{\theta})$ 
4:     Estimate the loss  $\mathcal{L} = \langle \psi_0 | U^\dagger(\boldsymbol{\theta}) H U(\boldsymbol{\theta}) | \psi_0 \rangle$  by averaging  $K$  shots
5:     for all  $\theta_j \in \boldsymbol{\theta}$  do
6:       Calculate the quantum gradient  $\partial_{\theta_j} \mathcal{L}$ 
7:       Update the parameter  $\theta_j \leftarrow \theta_j - \alpha_j^{(t)} \partial_{\theta_j} \mathcal{L}$ 
8:     end for
9:   end for
10: end procedure

```

4.3 Calculating the gradients of the parameters

In this section, we introduce the theory of calculating quantum gradients in the continuous variable setting. We follow the notation of Schuld et. al. [18]. A variational quantum circuit is defined by a unitary $U(\boldsymbol{\theta})$, $\boldsymbol{\theta} \in \mathbb{R}^m$, an initial state $|\psi_0\rangle$ and a measurement operator B . We can understand a variational circuit as $f : \mathbb{R}^m \rightarrow \mathbb{R}$, **[Dani: The Schuld paper writes $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$, maybe a typo???**] which maps the circuit parameters to the expectation value of operator B :

$$f(\boldsymbol{\theta}) = \langle \psi_0 | U^\dagger(\boldsymbol{\theta}) B U(\boldsymbol{\theta}) | \psi_0 \rangle \quad (20)$$

In gradient-based optimizations, we need the gradient $\nabla_{\boldsymbol{\theta}} f$, and this eventually means calculating the partial derivatives $\partial_{\mu} f$, $\mu \in \boldsymbol{\theta}$. In the continuous variable setting, observables are usually polynomials of the quadrature operators X_j and P_j .

5 Results

5.1 Regression

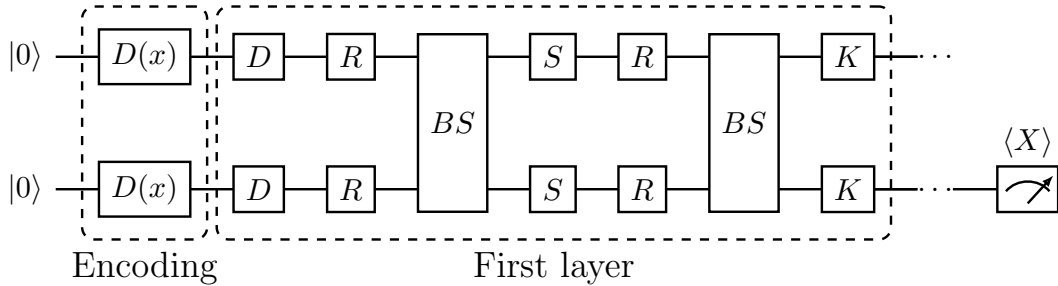


Figure 1.

5.2 Classification

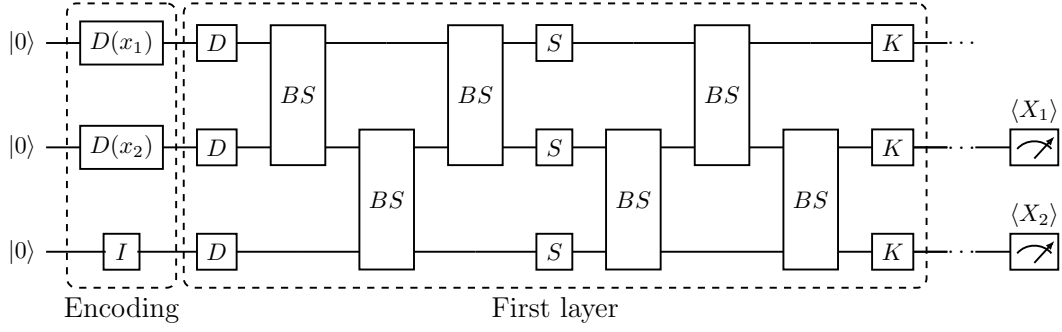


Figure 2.

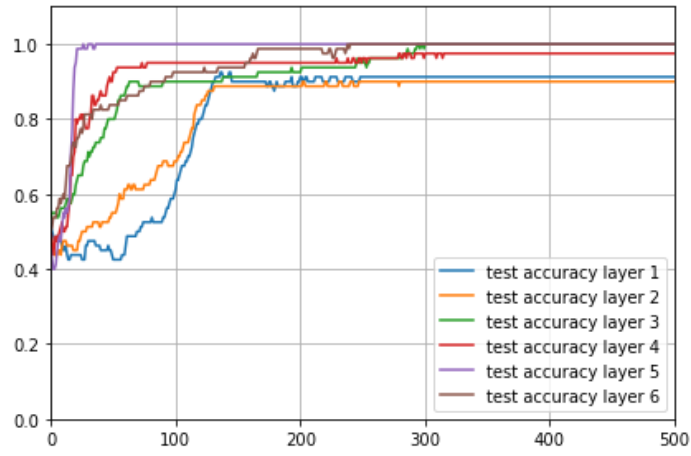


Figure 3.



Figure 4.

5.3 CV-VQE for the Bose-Hubbard model

The Bose-Hubbard model introduced first by Gersch and Knollman in 1963 for the description of interacting spinless bosons on a lattice, such as ultracold bosonic atoms on an optical lattice [19, 20].

This model has also gained popularity because it is found to be an adequate model for the description of the Superfluidity-Mott insulator (SF-MI) transition, which has been experimentally demonstrated [21, 22]. We chose this model, because an exact diagonalization of the Bose-Hubbard Hamiltonian with respect to a finite dimensional Fock-basis is possible and thus the model is numerically solvable. This enables the verification of the correctness of the results given by our variational quantum solver for small problem instances.

The Bose Hubbard model which we used in our simulations is defined by the following Hamiltonian expressed with the bosonic creation and annihilation operators:

$$H = -t \sum_{i=1}^{M-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2} \sum_{i=1}^M n_i^2, \quad (21)$$

where M is the number of bosonic modes in the system. If we restrict the total number of bosons in the system to be N , the dimension of the restricted Fock-space is

$$D = \frac{(N + M - 1)!}{N!(M - 1)!}, \quad (22)$$

which explosively grows with the system size. Therefore finding the groundstate of the Bose-Hubbard Hamiltonian for larger systems can be intractable even on classical supercomputers, making quantum computers, especially continuous-variable quantum computers a potential candidate for solving these problems in the future. Compared to the original definition of the Bose-Hubbard Hamiltonian, we omitted the term $-\mu \sum_i n_i$, because it is not relevant in our particular experiments.

5.3.1 Solving the model by exact diagonalization

[Dani: Analytic solution by diagonalization] If we want to calculate the groundstate of a Bose-Hubbard model, then we need to solve the eigenvalue-problem of Hamiltonian 21. Of course a general Fock-space corresponding to a bosonic system is infinite-dimensional, therefore we have to restrict the system so that a maximum of N particles are allowed in each mode:

$$|0, 0, \dots, 0\rangle, |0, 0, \dots, N\rangle, |0, 0, \dots, 1, N\rangle, \dots |N, N, \dots, N\rangle.$$

Then, we can relabel the Fock-states so that each Fock basis has its own unique label j :

$$|n_{M-1}, n_{M-2}, \dots, n_1, n_0\rangle = \left| \sum_{k=0}^{M-1} n_k (N+1)^k \right\rangle. \quad (23)$$

This is useful, because with these relabeled states we can calculate the matrix elements of the new Hamiltonian:

$$H_{jj'} = \langle j | H | j' \rangle = \langle n_{M-1}, n_{M-2}, \dots, n_1, n_0 | H | n'_{M-1}, n'_{M-2}, \dots, n'_1, n'_0 \rangle \quad (24)$$

We can further reduce the dimension of the Hilbert space if we prescribe that the total number of photons must be N :

$$\sum_k n_k = N.$$

In this case for example if the number of modes is $M = 4$ and the total number of particles is $N = 4$, the dimension of the restricted Hilbert-space is only 35.

The resulting matrix $H_{jj'}$ is usually a sparse matrix (see fig. 5), and can be diagonalized using existing software.

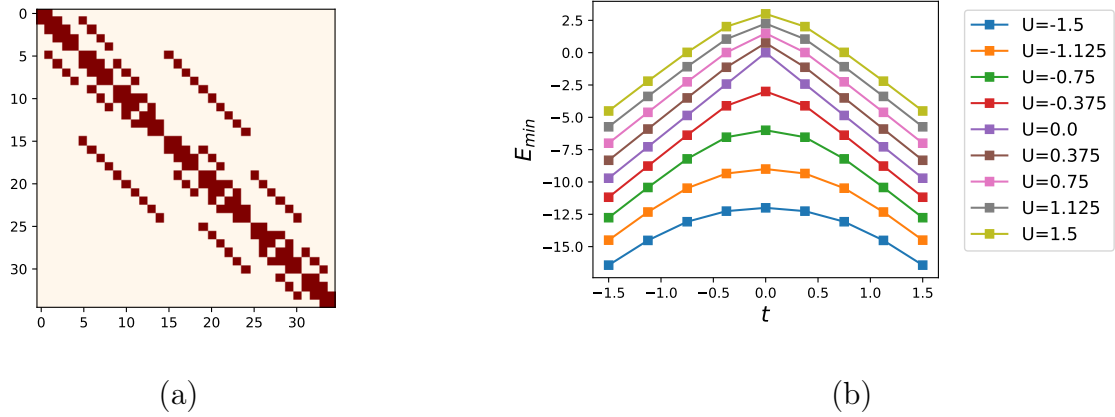


Figure 5. (a) Visual representation of a sparse Hamiltonian matrix $H_{jj'}$ for a Bose-Hubbard model with $\dim(\mathcal{H}) = 35$. Darker points show the non-zero elements in the matrix (b) Numerical solutions of the ground-state energy for different U and t values.

5.3.2 Variational solutions

VQEs introduced in section 4.2 are shown to be effective for simulating different fermionic quantum systems, like molecules or metals [12, 13, 14, 15]. In this chapter we demonstrate a photonic VQE for finding the ground-state energy of a Bose-Hubbard model. Furthermore, we show that stochastic gradient descent methods can be applied to the VQE to reduce the number of shots required, and thus reduce the overall cost of finding the ground state energy on a quantum hardware.

The variational circuit $U(\theta)$ can be realized with sequences of quantum gates, in our case photonic quantum gates. Since we want the total number of particles in the system to be preserved during the simulations, we must use photon-number preserving gates only. We composed each quantum layer from Beamsplitters, Kerr-gates and Cross-Kerr-gates (see fig. 7).

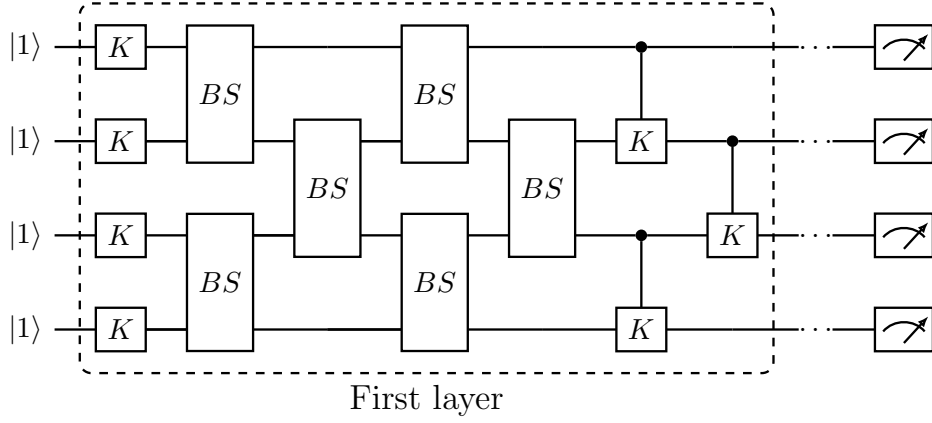


Figure 6. Illustration of a variational ansatz circuit with its first layer. Initially, each of the four qumodes contain a single photon. The layer is built up from Kerr-gates, CrossKerr gates and Beamsplitters, which are passive optical gates, so the total number of photons is preserved.

Throughout the numerical experiments, we set initially one single photon in each of the four qumodes i.e. $|\psi_0\rangle = |1\rangle^{\otimes M}$, and applied a number of identical quantum layers followed by quadrature measurements.

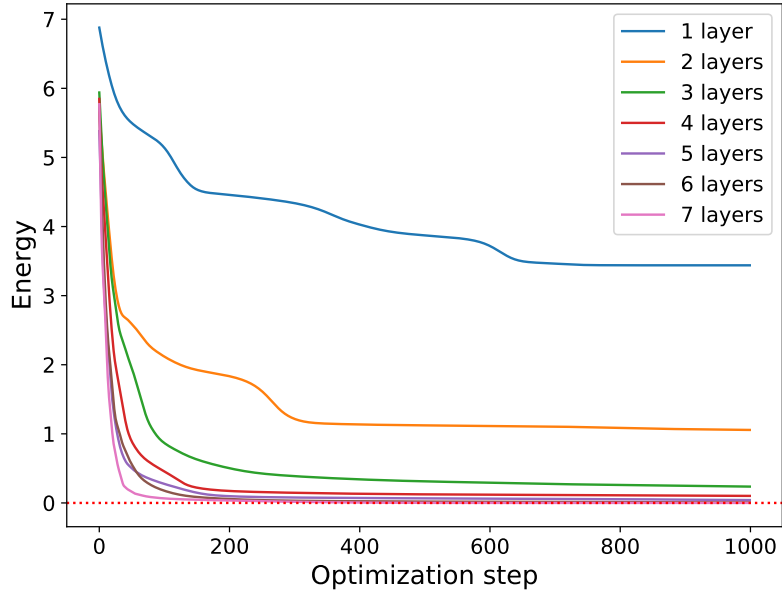
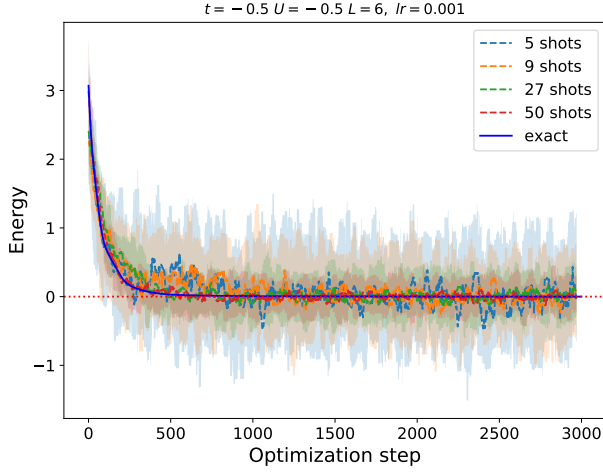
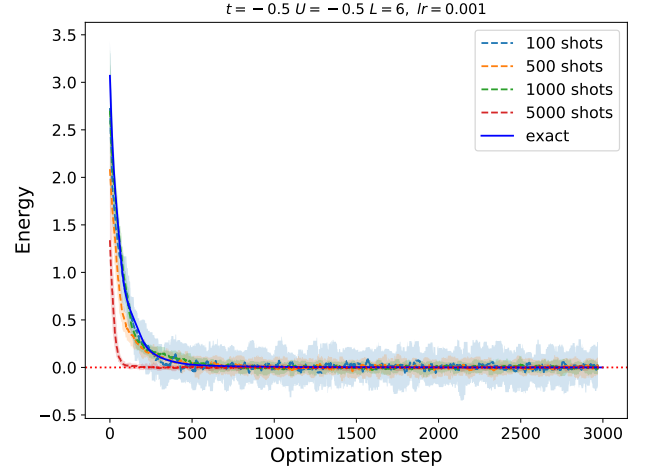


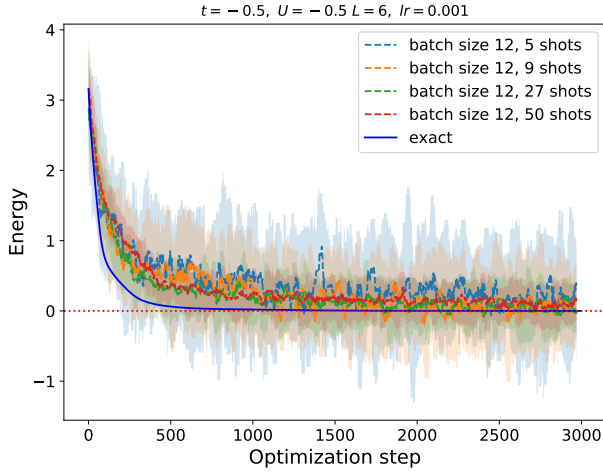
Figure 7.



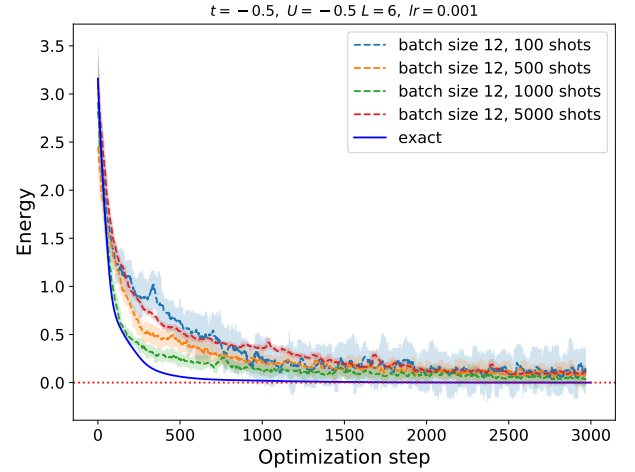
(a) first



(b) second



(c) third



(d) fourth

Figure 8. caption

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A Mathematical preliminaries

A.1 Hilbert spaces

Definition 1. *Hilbert-space*

Given a field T (real or complex), a vector space \mathcal{H} endowed with an inner product, is called a Hilbert-space, if it is a complete metric space with respect to the distance function induced by the inner product. The inner product is a map $\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow T$, for which $\forall x, y, z \in \mathcal{H}$:

- $\langle x | x \rangle \geq 0$
- $\langle x | x \rangle = 0 \iff x = \mathbf{0} \in \mathcal{H}$
- $\langle x | y \rangle = \langle y | x \rangle^*$, where $*$ denotes complex conjugation.
- $\langle x | \alpha y + \beta z \rangle = \alpha \langle x | y \rangle + \beta \langle x | z \rangle$, where $\alpha, \beta \in T$

The norm induced by this inner product is a map $\| \cdot \| : \mathcal{H} \rightarrow T$ defined as

$$\|x\| = \sqrt{\langle x | x \rangle},$$

And the metric induced by this norm is defined as

$$d(x, y) = \|x - y\| = \sqrt{\langle x - y | x - y \rangle}.$$

The space \mathcal{H} is said to be complete if every Cauchy-sequence is convergent with respect to the norm, and the limit is in \mathcal{H} . That is, each sequence x_1, x_2, \dots , for which

$$\forall \varepsilon > 0 \exists N(\varepsilon) \text{ so, that } n > m > N(\varepsilon) \implies \|x_n - x_m\| < \varepsilon.$$

Definition 2. *Linear functional*

Let \mathcal{H} be a Hilbert-space over the field T . Then, the map $\varphi : \mathcal{H} \rightarrow T$ is called a linear functional, if

$$\varphi(\alpha x + \beta y) = \alpha \varphi(x) + \beta \varphi(y), \quad \forall \alpha, \beta \in T, x, y \in \mathcal{H}.$$

Definition 3. *Dual space*

Given a Hilbert-space \mathcal{H} , its dual space, \mathcal{H}^* is the space of all continuous linear functionals from the space \mathcal{H} into the base field. The norm of an element in \mathcal{H}^* is

$$\|\varphi\|_{\mathcal{H}^*} \stackrel{\text{def}}{=} \sup_{\|x\|=1, x \in \mathcal{H}} |\varphi(x)|.$$

Theorem 1. *Riesz representation theorem*

For every element $y \in \mathcal{H}$, there exists a unique element $\varphi_y \in \mathcal{H}^*$, defined by

$$\varphi_y(x) = \langle y|x \rangle, \quad \forall x \in \mathcal{H}.$$

The mapping $y \mapsto \varphi_y$ is an antilinear mapping i.e. $\alpha y_1 + \beta y_2 \mapsto \alpha^* \varphi_{y_1} + \beta^* \varphi_{y_2}$, and the Riesz-representation theorem states that this mapping is an antilinear isomorphism. The inner product in \mathcal{H}^* satisfies

$$\langle \varphi_x | \varphi_y \rangle = \langle x | y \rangle^* = \langle y | x \rangle.$$

Moreover, $\|y\|_{\mathcal{H}} = \|\varphi_y\|_{\mathcal{H}^*}$.

Definition 4. Dirac-notation

From now on, the elements in \mathcal{H} will be denoted by $|x\rangle$ and their corresponding element in \mathcal{H}^* as $\langle x|$.

A.2 Linear operators on Hilbert spaces

Definition 5. Linear operators

A map $\hat{A} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ is a linear operator, if

$$\hat{A}(\alpha |x\rangle + \beta |y\rangle) = \alpha(\hat{A}|x\rangle) + \beta(\hat{A}|y\rangle).$$

Remark 1. If not stated otherwise, we will assume that $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$.

Remark 2. Operators will be denoted with a hat ($\hat{\cdot}$).

Definition 6. Bounded linear operators

A linear operator $\hat{A} : \mathcal{H} \rightarrow \mathcal{H}$ is bounded, if

$$\exists m \in \mathbb{R} : |\langle v | \hat{A} | v \rangle| \leq m \langle v | v \rangle, \quad \forall |v\rangle \in \mathcal{H}$$

Remark 3. The set of all bounded operators on \mathcal{H} is denoted $\mathcal{B}(\mathcal{H})$.

Definition 7. Commutators and anticommutators

Since operators usually do not commute, its useful to define their commutator and anticommutator:

$$\begin{aligned} [\hat{A}, \hat{B}] &= \hat{A}\hat{B} - \hat{B}\hat{A} \\ \{\hat{A}, \hat{B}\} &= \hat{A}\hat{B} + \hat{B}\hat{A} \end{aligned}$$

Definition 8. Operator norm

The operator norm of an operator \hat{A} is defined as

$$\|\hat{A}\| \stackrel{\text{def}}{=} \inf\{c \geq 0 : \|\hat{A}|v\rangle\| \leq c\| |v\rangle \|, \quad \forall |v\rangle \in \mathcal{H}\}$$

Definition 9. Trace-class operators

An operator \hat{A} is called trace-class if it admits a well defined and finite trace $\text{Tr} [\hat{A}] = \sum_j \langle j | \hat{A} | j \rangle$

Definition 10. Positive operators

An operator \hat{A} is called positive if $\langle v|\hat{A}|v\rangle \geq 0, \forall |v\rangle \in \mathcal{H}$. If $\hat{A} = \sum_j \lambda_j |j\rangle\langle j|$ then \hat{A} is positive if $\lambda_j \geq 0$.

Definition 11. Projections An operator $\Pi : \mathcal{H} \rightarrow \mathcal{H}$ is a projection if $\Pi^2 = \Pi$.

A.3 Hermitian Operators, Unitary Operators, Spectral theorem, Hadamard-lemma

Definition 12. Hermitian adjoint

Consider a **bounded** linear operator $\hat{A} : \mathcal{H} \rightarrow \mathcal{H}$. The hermitian adjoint of \hat{A} is a bounded linear operator $\hat{A}^\dagger : \mathcal{H} \rightarrow \mathcal{H}$ which satisfies

$$\langle y|\hat{A}|x\rangle = \left(\langle x|\hat{A}^\dagger|y\rangle\right)^*, \quad \forall |x\rangle, |y\rangle \in \mathcal{H}. \quad (25)$$

Definition 13. Hermitian operators

A bounded linear operator $\hat{H} : \mathcal{H} \rightarrow \mathcal{H}$ is Hermitian if

$$\hat{H} = \hat{H}^\dagger, \quad \text{i.e. } \hat{H}|x\rangle = \hat{H}^\dagger|x\rangle, \quad \forall |x\rangle \in \mathcal{H}. \quad (26)$$

Definition 14. Unitary operator

A bounded linear operator $\hat{U} : \mathcal{H} \rightarrow \mathcal{H}$ is unitary if

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = 1, \quad \text{in other words, } \hat{U}^\dagger = \hat{U}^{-1}. \quad (27)$$

Definition 15. Eigenvalues and eigenvectors

Consider bounded linear operator \hat{A} . If exist a vectors $|k\rangle \in \mathcal{H}$ such that

$$\hat{A}|k\rangle = \lambda_k |k\rangle, \quad (28)$$

then $|k\rangle$ is called an eigenvector of \hat{A} and λ_k is the corresponding eigenvalue.

An important property of Hermitian operators is that they can be diagonalized with real eigenvalues. This is formally stated by the spectral theorem:

Theorem 2. The Spectral theorem

Let \hat{A} be a bounded Hermitian operator on some Hilbert-space \mathcal{H} . Then there exists an orthonormal basis in \mathcal{H} which consists of the eigenvectors of \hat{A} and each eigenvalue of \hat{A} is real.

This means that any bounded Hermitian operator \hat{H} can be decomposed as

$$\hat{H} = \sum_k \lambda_k \hat{P}_k = \sum_k \lambda_k |k\rangle\langle k| \quad (29)$$

where λ_k and $|k\rangle$ are the eigenvalues and eigenvectors of \hat{H} .

Definition 16. Exponential of operators If X is a linear operator, we can define the exponential of X :

$$e^X = \sum_{n=0}^{\infty} \frac{X^n}{n!}$$

Important: The product of exponentials of operators generally isn't equal to the exponential of their sum:

$$e^X e^Y = e^{Z(X,Y)} \neq e^{X+Y},$$

where $Z(X, Y)$ is given by the Baker-Campbell-Hausdorff formula:

$$\begin{aligned} Z(X, Y) = & X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}[X, [X, Y]] - \frac{1}{12}[Y, [X, Y]] - \frac{1}{24}[Y, [X, [X, Y]]] \\ & - \frac{1}{720}([[[[X, Y], Y], Y], Y] + [[[Y, X], X], X], X) + \dots \end{aligned}$$

It is however equal if $[X, Y] = 0$:

$$\text{if } [X, Y] = 0 \implies e^X e^Y = e^{X+Y}$$

There are 2 important special cases:

Theorem 3. The Hadamard-lemma

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \dots$$

Theorem 4. If X and Y commute with their commutator, i.e. $[X, [X, Y]] = [Y, [X, Y]] = 0$, then:

$$e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]}$$

Theorem 5. If $[X, Y] = sY$ with $s \in \mathbb{C}, s \neq 2i\pi n, n \in \mathbb{Z}$ then:

$$e^X e^Y = \exp\left(X + \frac{s}{1 - e^{-s}}Y\right)$$

A.4 Pure and mixed quantum states

Definition 17. Quantum states

A quantum state of a quantum system is a mathematical entity that provides a probability distribution for the outcomes of each possible measurement on the system.

Definition 18. Pure quantum states

Pure quantum states are quantum states that can be described by a vector $|\psi\rangle$ of norm 1.

If one multiplies a pure quantum state by a complex scalar $e^{i\alpha}$, then the new state is physically equivalent to the former, thus $|\psi\rangle$ and $e^{i\alpha}|\psi\rangle$ are the same pure state. The transformation $|\psi\rangle \rightarrow e^{i\alpha}|\psi\rangle$

does not change the outcomes of measurements on the state, however the phase α is important in quantum algorithms.

Example. For example, the states $\frac{1}{\sqrt{2}}(|0\rangle + e^{i\pi} |1\rangle)$ and $\frac{1}{\sqrt{2}}(|0\rangle + e^{i\frac{\pi}{2}} |1\rangle)$ are not the same quantum state, but in both states there is 50-50 percent probability of measuring $|0\rangle$ and $|1\rangle$.

Definition 19. Density Matrix

A quantum state $\hat{\rho}$ is a trace-1, self-adjoint, positive semidefinite operator. The set of quantum states is

$$\mathcal{S}(\mathcal{H}) = \{\hat{\rho} : \hat{\rho} \geq 0, \hat{\rho} = \hat{\rho}^\dagger, \text{Tr} [\hat{\rho}] = 1\}$$

A quantum state is pure if and only if $\hat{\rho}^2 = \hat{\rho}$. Also, if ρ is a pure state, then it can be written as $\hat{\rho} = |\psi\rangle\langle\psi|$. The operator ρ is called the density operator or density matrix.