Advanced QML algorithms for state preparation

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Qiskit

Motivation

State preparation

Loading data into ***quantum states*** can be difficult.

In the worst case, the data loading is ***exponentially*** expensive and thereby ***impairs*** potential advantage of algorithms such as Quantum Amplitude Estimation.

Approximative data loading schemes can be implemented by using a ***parameterized quantum circuit*** and machine learning techniques.

Quantum Generative Adversarial Networks

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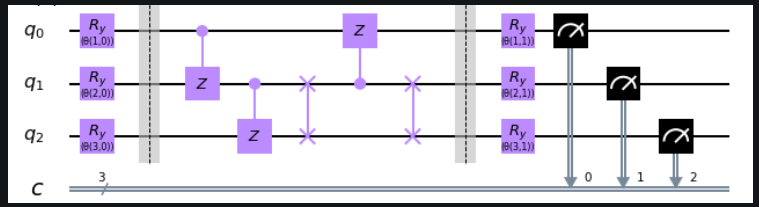
ARTICLE OPEN

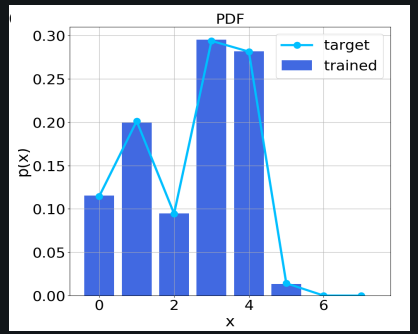
Quantum Generative Adversarial Networks for learning and loading random distributions

Christa Zoufal[1,2*], Aurélien Lucchi[2] and Stefan Woerner[1]

Idea:
Encode probability distribution into a parameterized quantum circuit

Implementation:
Use GAN to learn a probability distribution underlying given data samples





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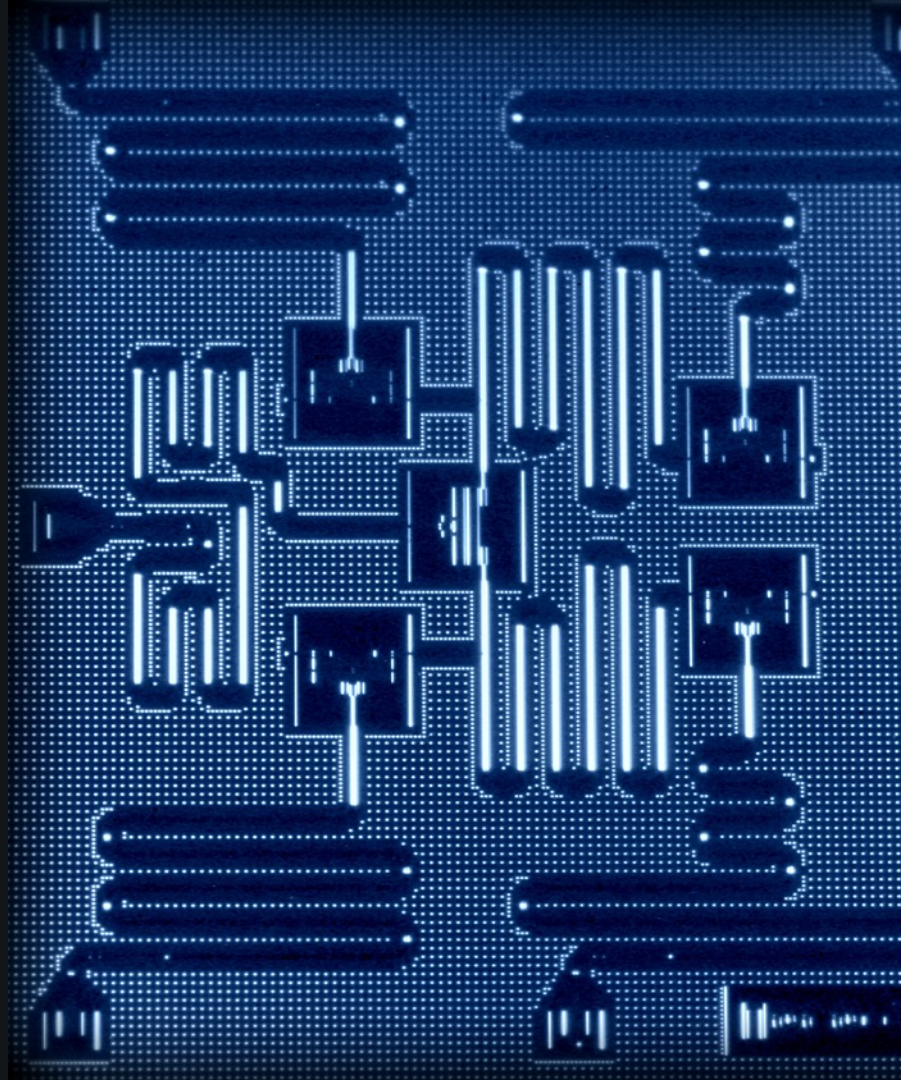
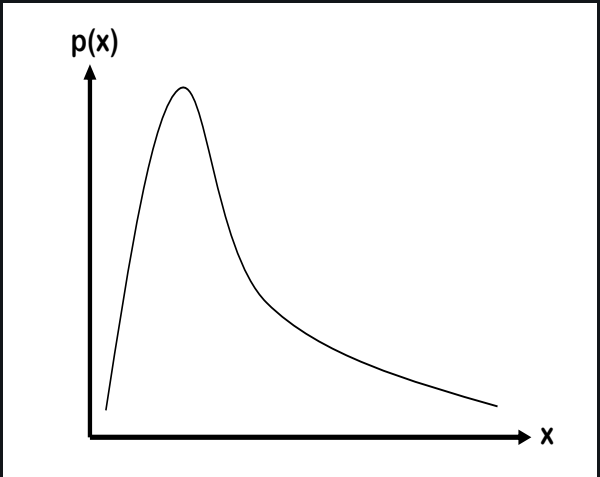
Outlook

- What are (Quantum) Generative Adversarial Networks?
- How do we realize Quantum Generative Adversarial Networks?
- Numerical examples



Distribution Loading



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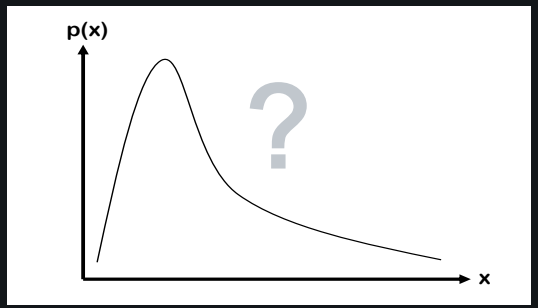
Direct Approach



What about generic distributions?

→best known $O(2^n)$

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Data Loading with qGANs

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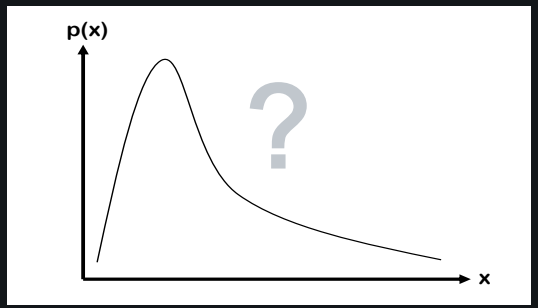

Avoid exponential overhead

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Generative Adversarial Networks

Generated cat images [1]

[1] Mao X., Li Q. (2021) Generative Adversarial Networks for Image Generation. Springer, Singapore.

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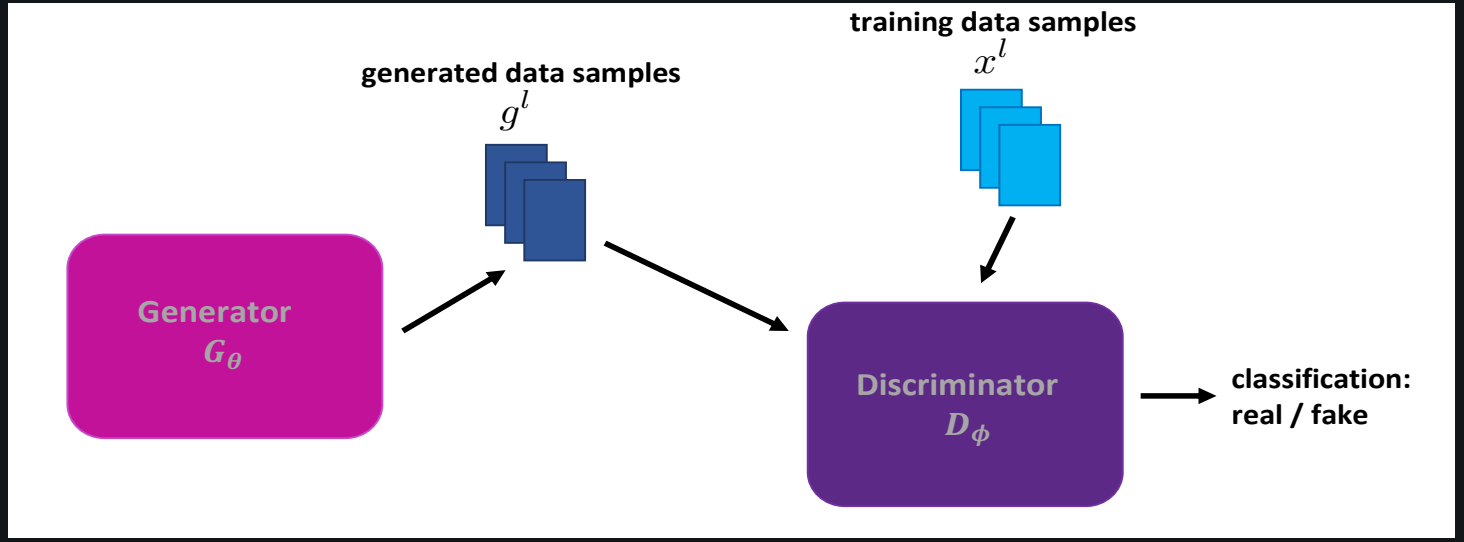
GAN Architecture



Discriminator Network: Distinguish between training data x_i and generated data $G_\theta(z_i)$

Generator Network: Create data $G(z_i)$ that the discriminator cannot distinguish from the **real** data x_i

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Training the discriminator

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$$L_D(\phi) = \frac{1}{m}\sum_{i=1}^{m}\left[\log\left(D_\phi\left(x^{(i)}\right)\right) + \log\left(1 - D_\phi\left(G_\theta\left(z^{(i)}\right)\right)\right)\right]$$

Number of data samples in batch

Training data samples

Random input (prior distribution)

Maximize $L_D(\phi)$ w.r.t ϕ

Goal: Discrimination and labelling of **training data samples** and **generated data samples**

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Training the generator

Qiskit

$$L_G(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\log\left(D_\phi\left(G_\theta\left(z^{(i)}\right)\right)\right)$$

Number of data samples in batch

Random input (prior distribution)

Maximize $L_G(\theta)$ w.r.t. θ

Target: Get the discriminator to label **generated data samples** as **training data samples**

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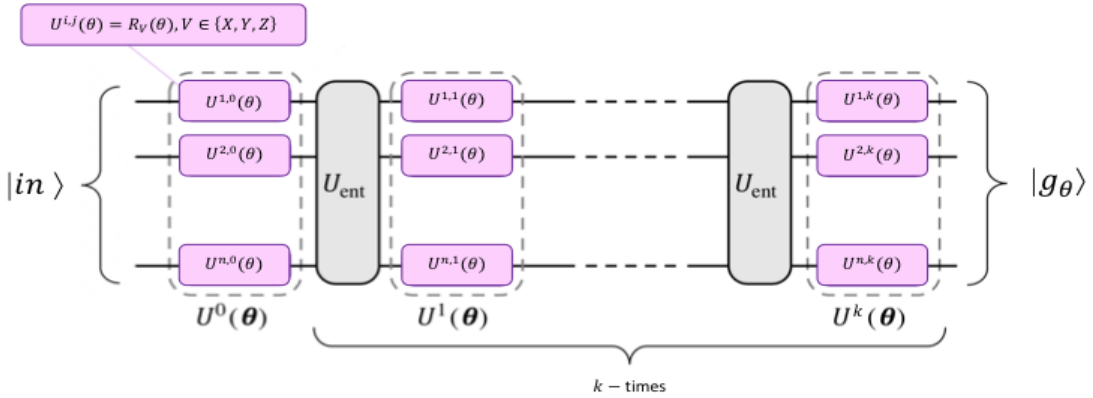
Quantum Generator



$$G_\theta |in\rangle = |g_\theta\rangle \xrightarrow{\text{Measurement: quantum → classical}} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \xrightarrow{\text{Mapping to the training data feature space}} g^l$$

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Training

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$$L_D(\phi, \theta) = \frac{1}{m} \sum_{l=1}^{m} \left[\log D_\phi \left(x^l \right) + \log \left(1 - D_\phi \left(g^l \right) \right) \right]$$

$$G_\theta |in\rangle = |g_\theta\rangle \xrightarrow{\text{measure}} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \xrightarrow{\text{map}} g^l$$

$$L_G(\phi, \theta) = -\frac{1}{m} \sum_{l=1}^{m} \left[\log \left(D_\phi \left(g^l \right) \right) \right]$$

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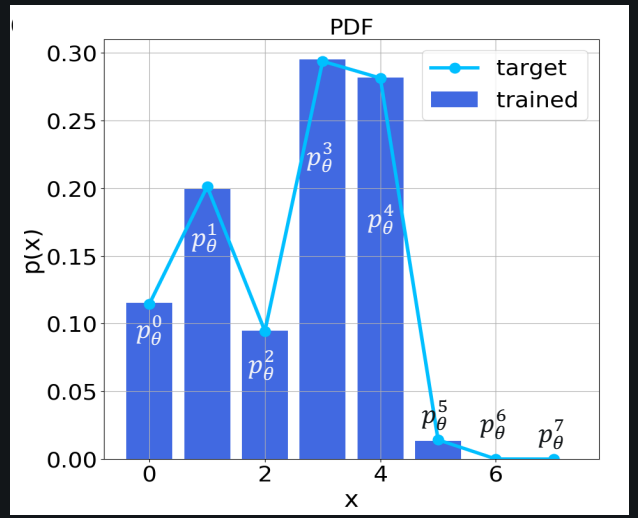
Quantum Generator

$$|g_\theta\rangle = \sum_{i=0}^{2^n-1} \sqrt{p_\theta^i}\,|g^i\rangle$$



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Data Loading with qGANs

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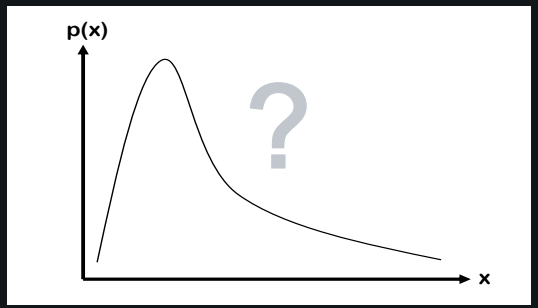

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Data Loading with qGANs

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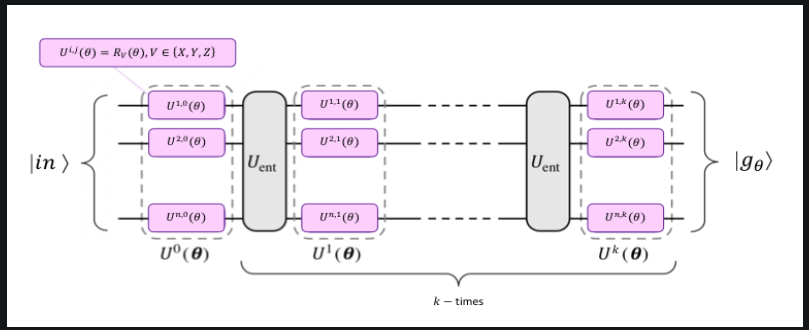

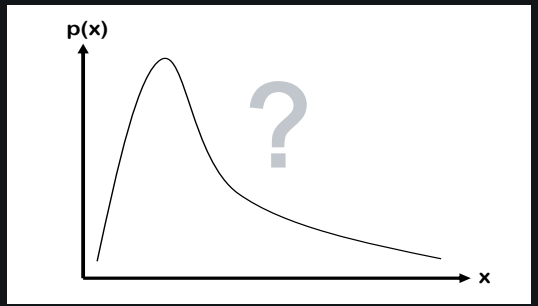

$$|g_\theta\rangle = \sum_{i=0}^{2^n-1} \sqrt{p_\theta^i}\,|g^i\rangle$$

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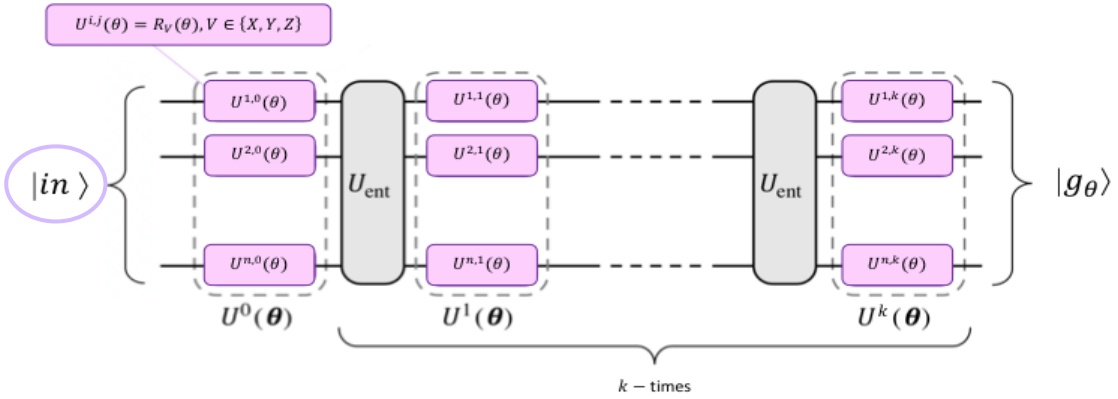
Quantum Generator



What is a good initial state $|in\rangle$?

Investigated candidates: random, uniform, normal according to 1^{st} and 2^{nd} momentum of the training data

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Benchmarking

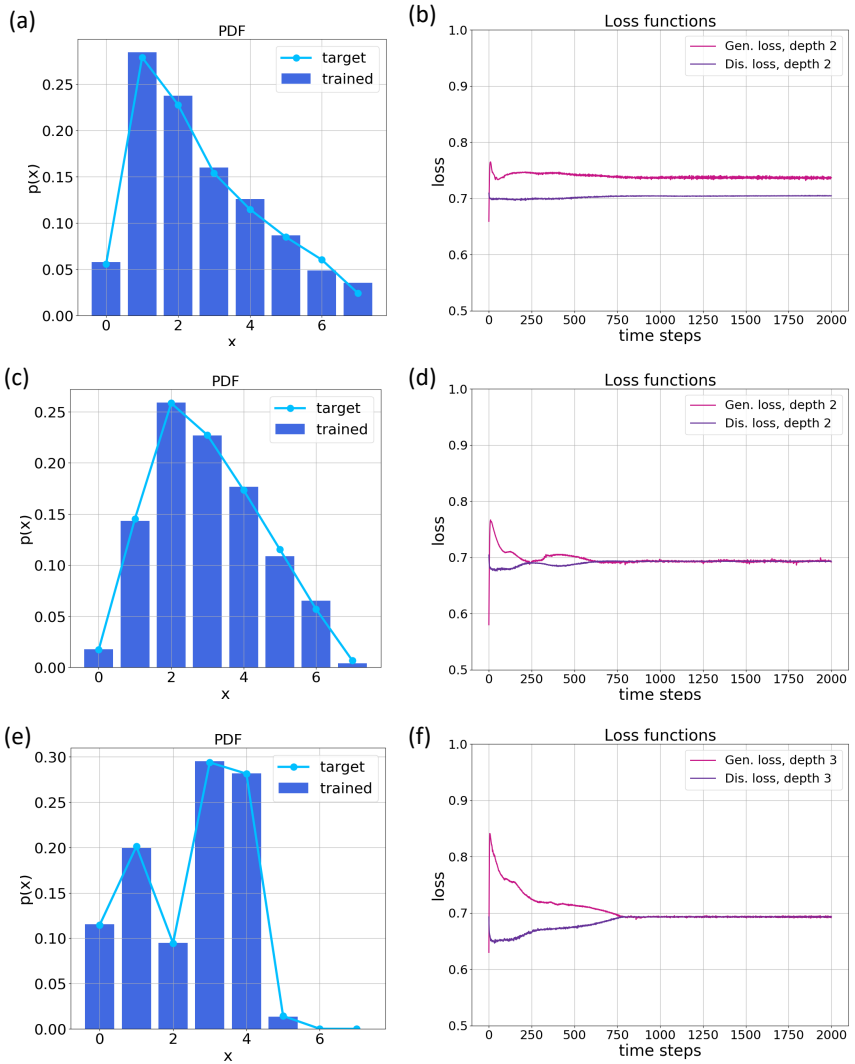
Training Data

Samples from a discretized, & truncated distributions

Generator

Variational form: $RealAmplitudes$

Number qubits: 3



Benchmarking

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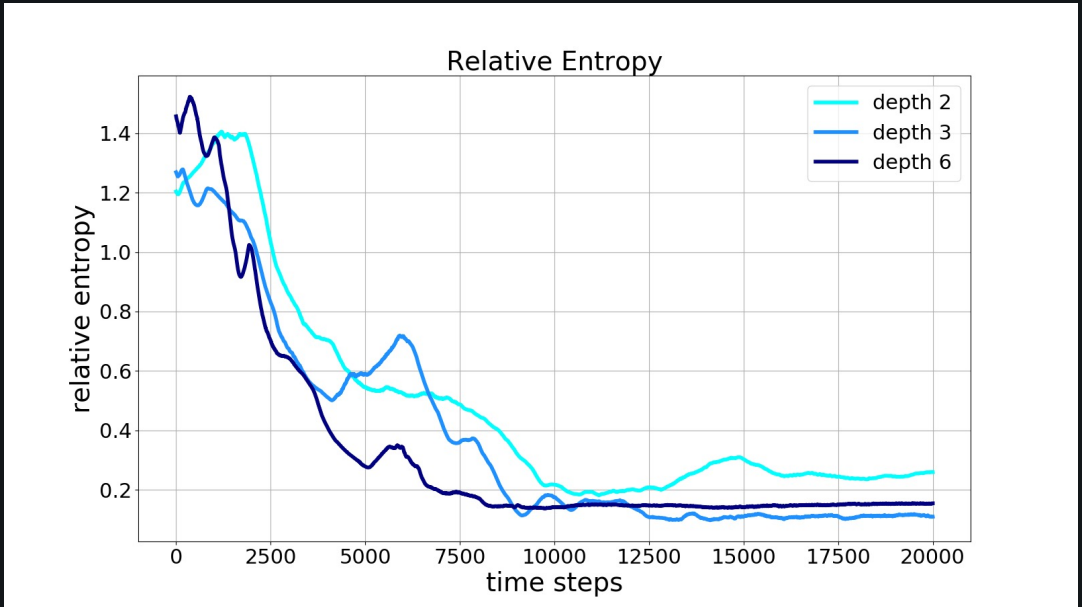
Training Data

First 2 principle components of multivariate, constant maturity treasury rates of US government bonds

Generator

Variational form: $RealAmplitudes$

Number qubits: 6



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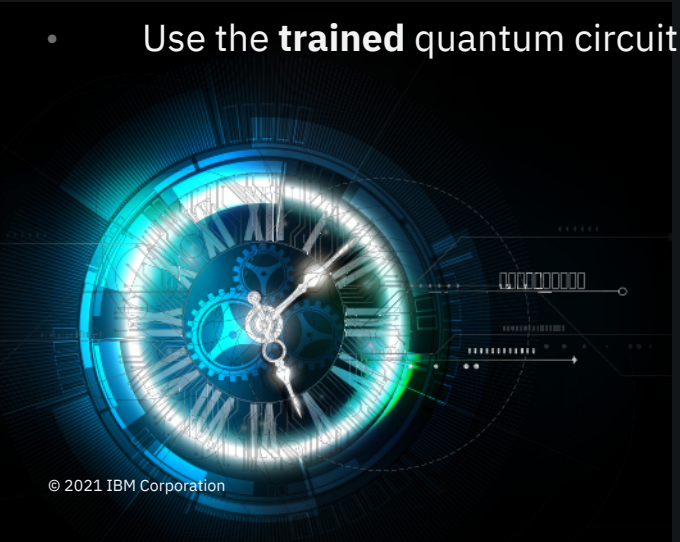
Summary

- **Efficient** loading of approximations to generic probability distributions
- Replace classical neural network with **parameterized** quantum circuit
- Use the **trained** quantum circuit for state preparation in quantum algorithms



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Quantum Boltzmann Machines

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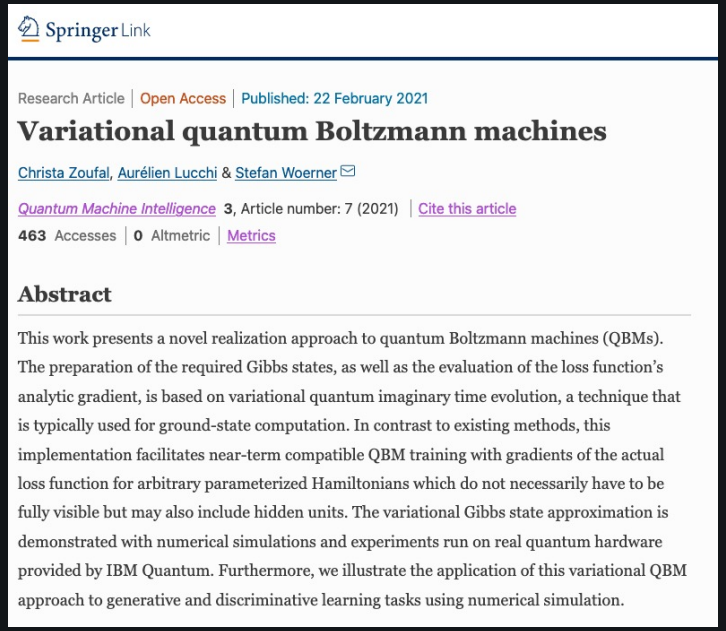

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Variational quantum Boltzmann machines

Christa Zoufal, Aurélien Lucchi & Stefan Woerner

Quantum Machine Intelligence **3**, Article number: 7 (2021) | Cite this article

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Abstract

This work presents a novel realization approach to quantum Boltzmann machines (QBMs). The preparation of the required Gibbs states, as well as the evaluation of the loss function's analytic gradient, is based on variational quantum imaginary time evolution, a technique that is typically used for ground-state computation. In contrast to existing methods, this implementation facilitates near-term compatible QBM training with gradients of the actual loss function for arbitrary parameterized Hamiltonians which do not necessarily have to be fully visible but may also include hidden units. The variational Gibbs state approximation is demonstrated with numerical simulations and experiments run on real quantum hardware provided by IBM Quantum. Furthermore, we illustrate the application of this variational QBM approach to generative and discriminative learning tasks using numerical simulation.

Idea:

Use structural knowledge to define your state preparation problem

Implementation:

Approximate Gibbs State with a constant depth quantum circuit

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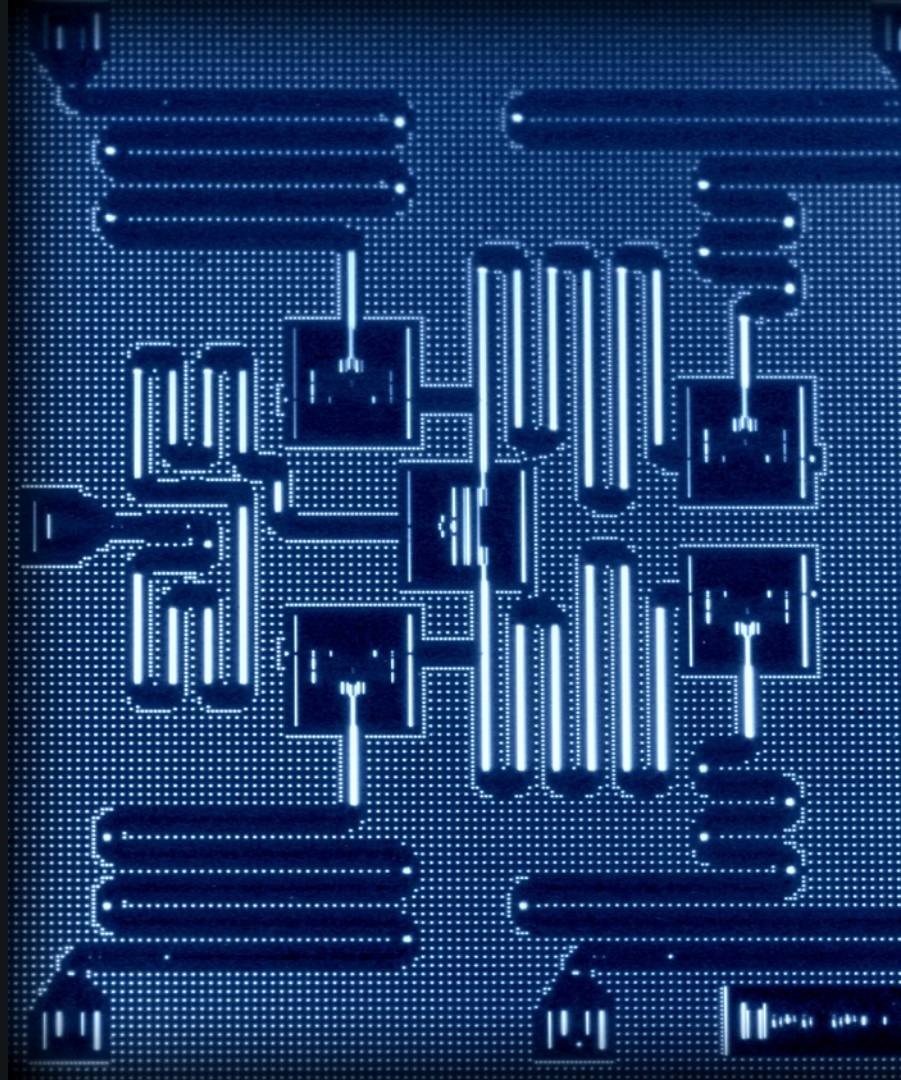
Outlook

- What are (Quantum) Boltzmann Machines?
- How do we realize Quantum Boltzmann Machines?
- Numerical examples



Boltzmann Machines

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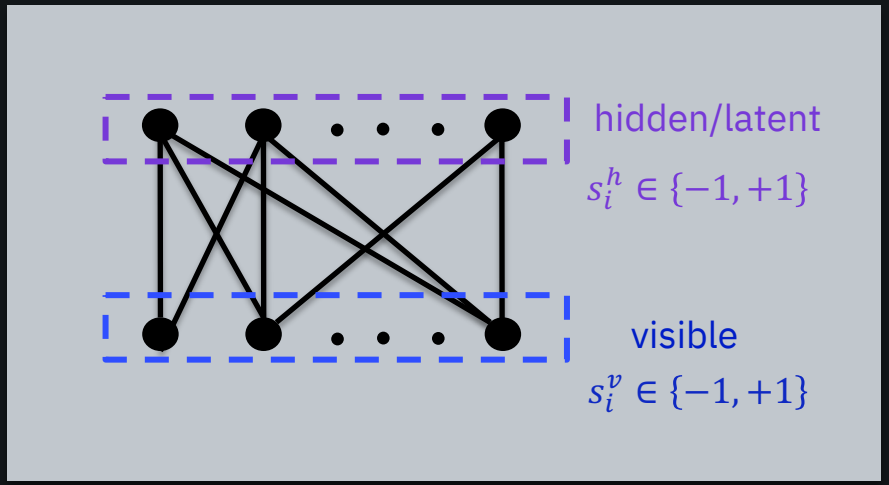
Energy-based Machine Learning Models



Energy function defining the connectivity

$$E_\theta = -\left(\sum_{i<j} \theta_{ij} s_i s_j + \sum_i \tilde{\theta}_i s_i\right)$$

for nodes $\{s_i\}$ and parameters $\{\theta_{ij}\}, \{\tilde{\theta}_i\}$

Probability for a configuration of ***visible nodes***

$$P(v) = e^{-E(v)}/Z$$

Normalization factor

$$Z = \sum_u e^{-E(u)}$$

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Boltzmann Machines

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Aim

Train $\{\theta_{ij}\}, \{\tilde{\theta}_i\}$ s.t. $P(v)$ represents the probability distribution underlying given training data (& training labels)

Loss function

$$\min_{\theta_{ij}, \tilde{\theta}_i} L = -\sum_v P^{data}(v) \log\left(P^{BM}(v)\right)$$

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Quantum Boltzmann Machines

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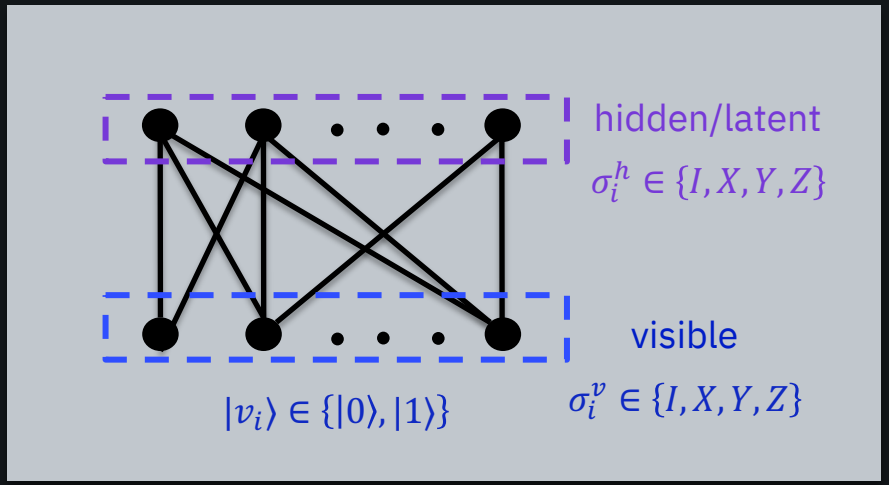
Let's replace bits with qubits.



Hamiltonian defining the connectivity

$$H_\theta = -\left(\sum_{i<j} \theta_{ij}\sigma_i\sigma_j + \sum_i \tilde{\theta}_i\sigma_i\right)$$

for Pauli operators $\{\sigma_i\}$ and parameters $\{\theta_{ij}\}, \{\tilde{\theta}_i\}$

Probability to measure configuration of ***visible qubits*** $|v\rangle$

$$P^{QBM}(v) = Tr\left[\Lambda_v \rho^{Gibbs}\right]$$

Quantum ***Gibbs state***

$$\rho^{Gibbs} = \frac{e^{-H}}{Z}$$

Normalization factor

$$Z = Tr[e^{-H}]$$

Difficult to evaluate classically for some Hamiltonians → sign problem

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Quantum Boltzmann Machines

Qiskit

Aim:
Train $\{\theta_{ij}\}, \{\tilde{\theta}_i\}$ s.t. $P^{QBM}(v) = Tr[\Lambda_v \rho^{Gibbs}]$ represents the probability distribution underlying given training data (& training labels)

Loss function:

1. Classical: $\min_{\theta_{ij}, \tilde{\theta}_i} L = -\sum_v P^{data}(v) \log\left(P^{QBM}(v)\right)$ → Match the sampling probability of a quantum state to the sampling probability of a classical data set

2. Quantum: $\min_{\theta_{ij}, \tilde{\theta}_i} L = -Tr[\rho^{data} \log(\rho^{Gibbs})]$ → Encode the classical probabilities into a rank-1 quantum state

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Quantum Imaginary Time Evolution

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QITE: Given an n-qubit Hamiltonian $H = \sum_i \theta_i h_i$

Wick-rotated Schrödinger equation $\frac{d|\psi(\tau)\rangle}{d\tau} = -(H - E_\tau)|\psi(\tau)\rangle$

$|\psi(\tau)\rangle = \frac{e^{-H\tau}}{C(\tau)}|\psi(0)\rangle$

Normalization $C(\tau) = \sqrt{Tr[e^{-2H\tau}|\psi(0)\rangle\langle\psi(0)|]}$

VarQITE: $\left|\tilde{\psi}\left(\vec{\omega}(\tau)\right)\right\rangle = V\left(\vec{\omega}(\tau)\right)|\psi_{in}\rangle$

parametrized Ansatz input state

Idea:
Approximate state evolution with parameter evolution

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Parameter Evolution

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McLachlan's variational principle for ITE [1]

$$\delta \left\| \left(\frac{d}{d\tau} + H - E_\tau \right) |\tilde{\psi}(\vec{\omega}(\tau))\rangle \right\| = 0$$

gives a system of linear equations

$$A\dot{\vec{\omega}}(\tau) = C$$

$$A_{ij} = Re\left(\frac{\partial \langle \tilde{\psi}(\vec{\omega}(\tau))|}{\partial \omega_i} \frac{\partial |\tilde{\psi}(\vec{\omega}(\tau))\rangle}{\partial \omega_j} \right) \qquad C_i = \frac{1}{2} \frac{\partial \langle \tilde{\psi}(\vec{\omega}(\tau))|H|\tilde{\psi}(\vec{\omega}(\tau))\rangle}{\partial \omega_i}$$

➔Evolve $\vec{\omega}\,(\tau)$ e.g. with explicit Euler

$$\vec{\omega}\,(\tau) \simeq \vec{\omega}\,(\tau - \delta\tau) + \dot{\vec{\omega}}(\tau - \delta\tau)\delta\tau$$

$\mathcal{O}(m(k+m))$
m: # parameters in V
k: # parameters in H

[1] A.D. McLachlan. A variational solution of the time-dependent Schrödinger equation. Molecular Physics, 8(1):39-44, 1964.

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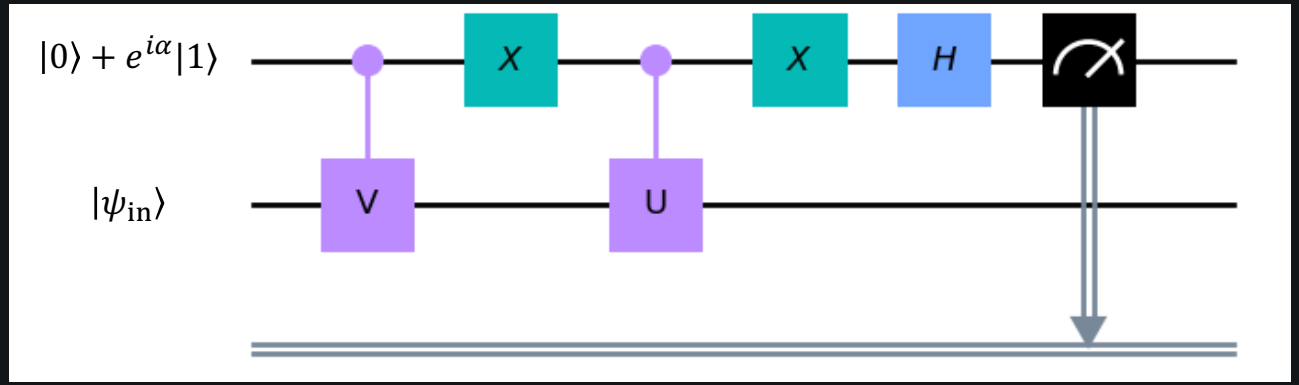
SLE Components



[1]

$$\text{Re}(e^{i\alpha}\text{Tr}[U^{\dagger}V|\psi_{in}\rangle\langle\psi_{in}|])$$

$$A_{ij} = Re\left(\frac{\partial\langle\tilde{\psi}(\vec{\omega}(\tau))|}{\partial\omega_i}\frac{\partial|\tilde{\psi}(\vec{\omega}(\tau))\rangle}{\partial\omega_j}\right)$$

$$C_i = Re\left(\frac{\partial\langle\tilde{\psi}(\vec{\omega}(\tau))|}{\partial\omega_i}H|\tilde{\psi}(\vec{\omega}(\tau))\rangle\right)$$

[1] Simulating physical phenomena by quantum networks- R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme,Phys. Rev. A 65, 042323 – 2002.

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VarQITE for Gibbs State Preparation

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Target state

$$\rho_{Gibbs} = \frac{e^{-H_A/k_BT}}{Z}$$

Normalization factor $Z = Tr\left[e^{-H_A/k_BT}\right]$

Method

- $\tau = \frac{1}{2k_BT}$
- $H_{AB} = H_A \otimes I_B$
- $\left|\widetilde{\psi}(0)\right\rangle_{AB} = (|00\rangle + |11\rangle)^{\otimes n} \Rightarrow \quad Tr_B\left[\left|\widetilde{\psi}(0)\right\rangle\left\langle\widetilde{\psi}(0)\right|_{AB}\right] = I\,\frac{1}{2^n}$

$\left|\widetilde{\psi}(\tau)\right\rangle = \frac{e^{-H_{AB}\tau}}{C(\tau)}\left|\widetilde{\psi}(\omega(0))\right\rangle$

$\tilde{\rho}_{Gibbs} = Tr_B[\left|\widetilde{\psi}(\tau)\right\rangle\left\langle\widetilde{\psi}(\tau)\right|]$

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Gibbs State Preparation Example

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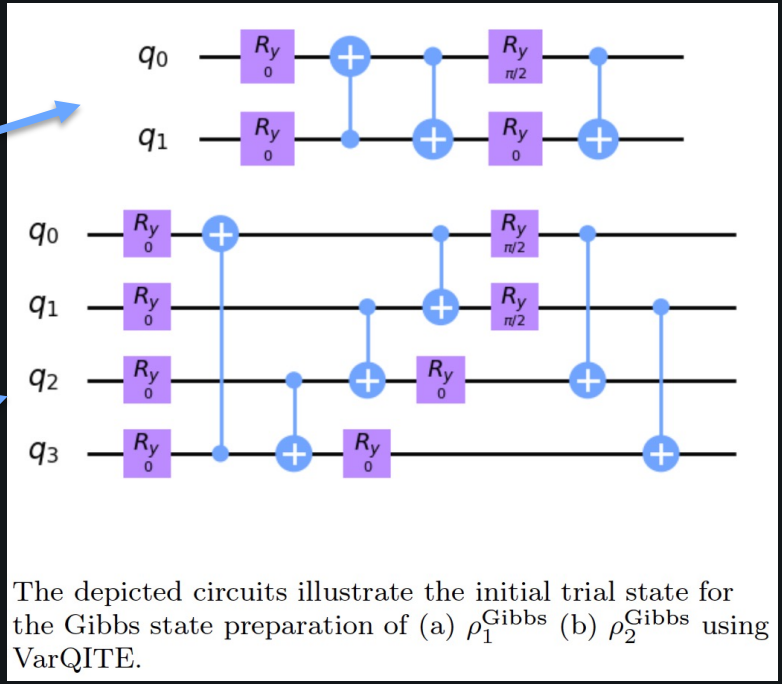
$$H_1 = 1.0Z,$$

$$H_2 = 1.0ZZ - 0.2ZI - 0.2IZ + 0.3XI + 0.3IX.$$

$$\rho_1^{\text{Gibbs}} = \begin{pmatrix} 0.12 & 0. \\ 0. & 0.88 \end{pmatrix},$$

$$\rho_2^{\text{Gibbs}} = \begin{pmatrix} 0.10 & -0.06 & -0.06 & 0.01 \\ -0.06 & 0.43 & 0.02 & -0.05 \\ -0.06 & 0.02 & 0.43 & -0.05 \\ 0.01 & -0.05 & -0.05 & 0.05 \end{pmatrix}.$$



The depicted circuits illustrate the initial trial state for the Gibbs state preparation of (a) ρ_1^{Gibbs} (b) ρ_2^{Gibbs} using VarQITE.

Aim
Evaluate fidelity $\mathrm{F}(\rho_{QBM}, \rho_{target})$ throughout VarQITE

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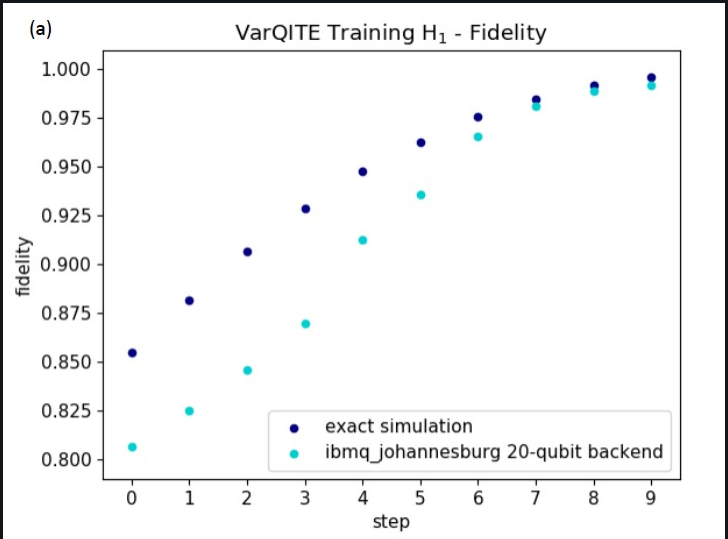
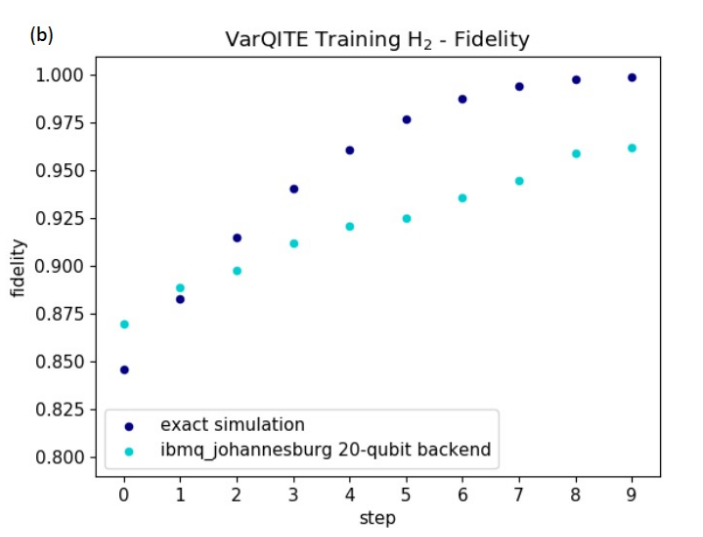
Gibbs State Preparation Example





Backend: IBM Q Johannesburg

VarQITE: 10 steps/Gibbs state preparation

Convergence Measure: $\mathrm{F}(\rho_{QBM}, \rho_{target})$

Fidelity between trained and target Gibbs state with VarQITE for (a) ρ_1^{Gibbs} (b) ρ_2^{Gibbs} trained with an ideal simulator and real quantum hardware, i.e., the *ibmq_johannesburg* 20-*qubit* backend. Each simulation used 10 time steps.

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QBM Training

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Loss function

$$L = -\sum_v P^{data}(v)\log\left(P^{QBM}(v)\right) = -\sum_v P^{data}(v)\log\left(Tr\left[\Lambda_v \rho^{Gibbs}\right]\right)$$

Gradient loss function

$$\frac{\partial L}{\partial \theta_i} = -\sum_v P_v^{data}\frac{\frac{\partial Tr\left[\Lambda_v \rho^{Gibbs}\right]}{\partial \theta_i}}{Tr[\Lambda_v \rho^{Gibbs}]}$$

$$\frac{\frac{\partial Tr\left[\Lambda_v \rho^{Gibbs}\right]}{\partial \theta_i}}{Tr[\Lambda_v \rho^{Gibbs}]} = \frac{Tr\left[\Lambda_v \, \partial e^{-H} / \partial \theta_i\right]}{Tr[\Lambda_v e^{-H}]} - \frac{Tr\left[\partial e^{-H} / \partial \theta_i\right]}{Tr[e^{-H}]} \quad -\left\langle \frac{\partial H}{\partial \theta_i} \right\rangle$$

➔ **Golden-Thompson**

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QBM Training

Qiskit

Loss function

$$L = -\sum_v P^{data}(v)\log\left(P^{QBM}(v)\right) = -\sum_v P^{data}(v)\log\left(Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}(\vec{\omega}(\tau))\right]\right)$$

Gradient loss function

$$\frac{\partial L}{\partial \theta_i} = -\sum_v P_v^{data}\frac{\frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \theta_i}}{Tr[\Lambda_v \tilde{\rho}^{Gibbs}]}$$

➔ **But with VarQITE**

$$\frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \theta_i} = \frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \vec{\omega}(\tau)}\frac{\partial \vec{\omega}(\tau)}{\partial \theta_i}$$

Automatic differentiation

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QBM Training

Qiskit

Gradient w.r.t. trial state parameters

$$\frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \vec{\omega}(\tau)} = \frac{\partial \langle \psi(\tau)|\Lambda_v|\psi(\tau)\rangle}{\partial \vec{\omega}(\tau)}$$

First order gradient of an expectation value w.r.t. a quantum state

Gradient w.r.t. the Hamiltonian parameters

$$\partial\theta_i \left(A\dot{\vec{\omega}}(\tau)\right) = \partial\theta_i C$$

Compute the derivative of the SLE resulting from McLachlan

$$A\frac{\partial\dot{\vec{\omega}}(\tau)}{\partial\theta_i} = \frac{\partial C}{\partial\theta_i} - \frac{\partial A}{\partial\theta_i}\dot{\vec{\omega}}(\tau)$$

System of linear equations that involves higher order gradients

Evolve $\dot{\vec{\omega}}(\tau)$ with explicit Euler

$$\frac{\partial\vec{\omega}(\tau)}{\partial\theta_i} \simeq \frac{\partial\vec{\omega}(\tau-\delta\tau)}{\partial\theta_i} + \frac{\partial\dot{\vec{\omega}}(\tau-\delta\tau)}{\partial\theta_i}\delta\tau$$

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QBM Training

Qiskit

Loss function

$$L = -\sum_v P^{data}(v)\log\left(P^{QBM}(v)\right) = -\sum_v P^{data}(v)\log\left(Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}(\vec{\omega}(\tau))\right]\right)$$

Gradient loss function

$$\frac{\partial L}{\partial \theta_i} = -\sum_v P_v^{data} \frac{\frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \theta_i}}{Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}$$

➔ **But with VarQITE**

$$\frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \theta_i} = \frac{\partial Tr\left[\Lambda_v \tilde{\rho}^{Gibbs}\right]}{\partial \vec{\omega}(\tau)} \frac{\partial \vec{\omega}(\tau)}{\partial \theta_i}$$

Automatic differentiation

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Implementation

Qiskit

$A\dot{\vec{\omega}}(\tau) = C$

Training procedure

$H = \sum_i \theta_i h_i$ $\quad A\frac{\partial\dot{\vec{\omega}}(\tau)}{\partial\theta_i} = \frac{\partial C}{\partial\theta_i} - \frac{\partial A}{\partial\theta_i}\dot{\vec{\omega}}(\tau)$x

Initialize H_θ and choose a set of initial θ

1. Use VarQITE to prepare ρ_ω^{Gibbs}

   & to compute $\frac{\partial\omega}{\partial\theta}$ for H_θ

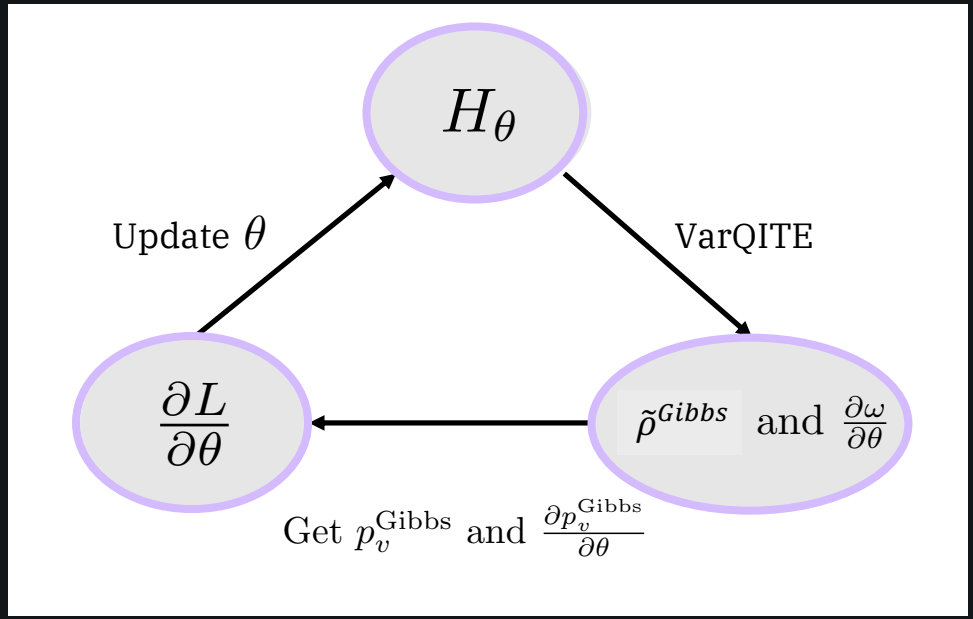
2. Sample to get p_v^{Gibbs}

   & apply the chain rule to get $\frac{\partial p_v^{Gibbs}}{\partial\theta}$

3. Compute the resulting $\frac{\partial L}{\partial\theta}$

4. Update θ with a classical optimizer

Repeat steps 1.-4.



$$\frac{\partial L}{\partial\theta_i} = -\sum_v P_v^{data}\frac{\frac{\partial Tr[\Lambda_v\tilde{\rho}^{Gibbs}]}{\partial\theta_i}}{Tr[\Lambda_v\tilde{\rho}^{Gibbs}]}$$

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Generative QBM Example

Target

Bell state

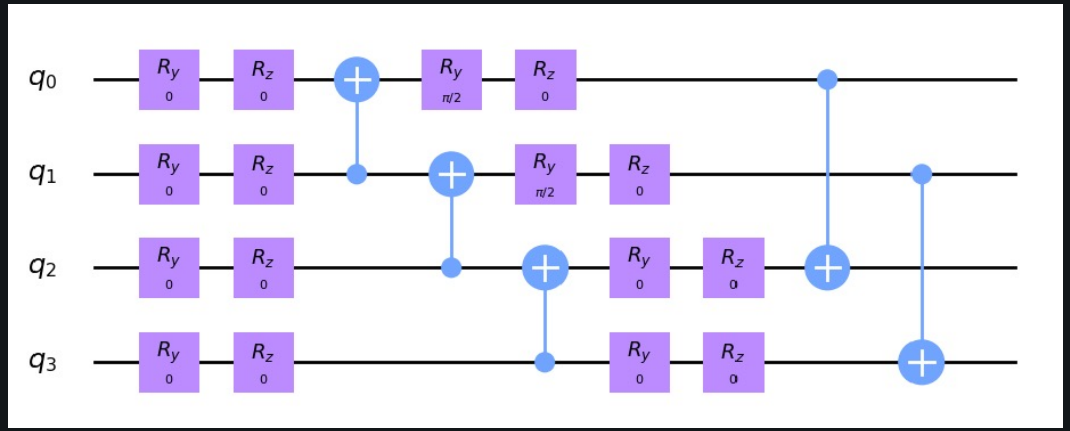
sampling probabilities ground state: $\mathrm{p}^{data} = [0.5, 0, 0, 0.5]$

Specify Model

$H_{QBM} = \alpha \cdot ZZ + \beta \cdot IZ + \gamma \cdot ZI$

$\mathrm{p}_{QBM} = Tr[|i\rangle\langle i|\rho_{QBM}]$

Starting state $|\tilde{\psi}(\vec{\omega}(0))\rangle =$



Aim
Train α, β, γ

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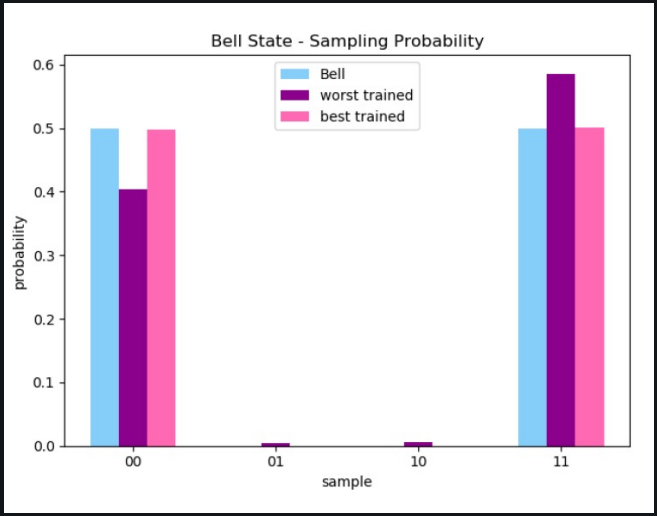
Generative QBM Example

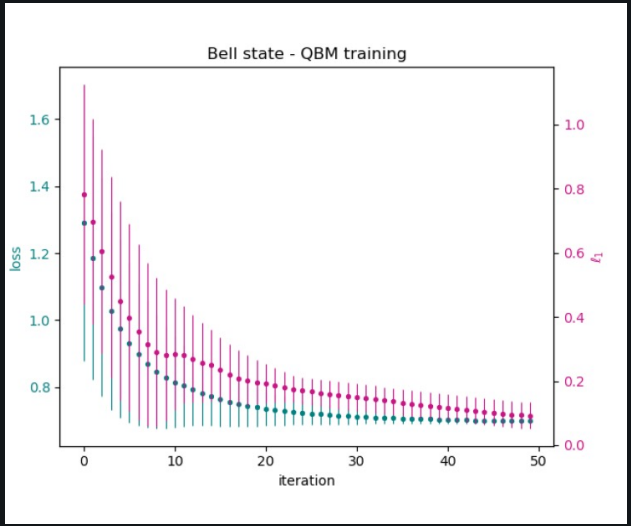
Initialization: $\alpha, \beta, \gamma \sim \mathrm{U}[-1, 1]$

VarQITE: 10 steps/Gibbs preparation

Optimization: Amsgrad

Convergence Measure: loss, $\|p_{ground} - p_{QBM}\|_1$





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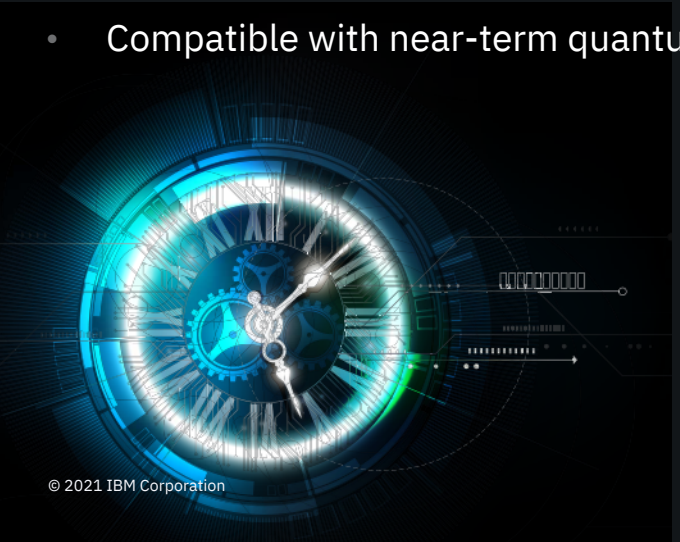
Summary

- Explore **data structure** to construct suitable Hamiltonians
- Use **automatic differentiation** for the QBM training
- Compatible with near-term quantum computers due to **constant-depth** quantum circuits



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Key messages

- To explore quantum algorithms for **data processing** we need to load the data into a quantum state
- Data loading can be **difficult** or even exponentially expensive
- QML can be used to implement approximate but **efficient** data loading schemes

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