



Zhuojing Huang

Quantum Neural Networks: Libraries and Applications

An example of quantum autoencoder

Newest Trends in High-Performance Data Analytics

01/18/2024

Main Takeaways

Table of contents

- **1** Introduction: Quantum Computing
- 2 Overview: Quantum Neural Network
- 3 Use Case: Quantum Autoencoder
- 4 Getting into the Field
- 5 Main Takeaways

Getting into the Field Main Takeaways

What is Quantum Computing?

Multidisciplinary fields

- Computer science
- Physics
- Mathematics



Essential Concepts in Quantum Computing

Qubits and Supersupposition

- > Utilizes quantum bits, or **qubits**, instead of classical bits.
- Superposition: qubits can exist in multiple states simultaneously.

Entanglement

- The state of one qubit can be dependent on another, even at a distance. "Spooky action at a distance" — Albert Einstein
- > Enables faster information transfer and parallel processing.

Essential Concepts in Quantum Computing

Quantum Gates

Quantum gates act on the qubits in a quantum circuit



- Exploit superposition to process multiple possibilities, allowing for complex operations
- Create entanglement, where the state of two qubits become correlated

Essential Concepts in Quantum Computing



Source: Moreno-Pineda et al., "Molecular Spin Qudits for Quantum Algorithms"

Getting into the Field Main Takeaways

Essential Concepts in Quantum Computing



Source: https://arstechnica.com/science/2015/09/d-wave-unveils-

new-quantum-computing-benchmark-and-its-fast/

:D

Overview: Quantum Neural Network Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Essential Concepts in Quantum Computing



Source: https://arstechnica.com/science/2015/09/d-wave-unveils-

new-quantum-computing-benchmark-and-its-fast/

:D



Source:

https://venturebeat.com/business/ibm-releases-giskit-modules-

that-use-guantum-computers-to-improve-machine-learning/

Why Do We Need Quantum Computers?

Limitations of supercomputers

- Reliant on 20th-century transistor technology
- Slow or unable to solve some complex problems
- What quantum computers can do
 - ► Lead to more efficient computation for certain tasks with parallelism
 - Provide exponential speedup for certain computational tasks:
 - factoring large numbers
 - searching unsorted databases
 - Excel in solving complex optimization problems

Introduction: Quantum Computing Overview: Quantum Neural Network Use Case: Quantum Autoencode October Oscillation (Main Takeaways)

Current stage of Quantum Computing



Source: Berggren, "Quantum Computing with Superconductors"

Current stage of Quantum Computing



Source: Ezratty, "Is there a Moore's law for quantum computing?"

What fields can Quantum Computing be useful?

- Optimization Problems
- Cryptography
- Quantum Simulation
- Machine Learning
- Molecular Modeling
- Integer Factorization

. . .

What is Quantum Neural Network?



Recap on Classical Autoencoder: Basics



Source: Rao, "Learning hard distributions with quantum-enhanced

Encoder and Decoder

- Encoder maps input to a latent space
- Decoder reconstructs data from the latent space

Essential ideas

- Unsupervised
- Reconstruct original data from the compressed data
- Minimize the difference between input and output

Variational Autoencoders"

Recap on Classical Autoencoder: Applications

Data Compression



Source: https://medium.com/edureka/autoencoders-tutorial-cfdcebdefe37

Recap on Classical Autoencoder: Applications

Data Denoising



Source: https://medium.com/analytics-vidhya/reconstruct-corrupted-data-using-denoising-autoencoder-python-code-aeaff4b0958e

Inspired by classical autoencoder

- Inspired by classical autoencoder
- Compress a quantum state onto a smaller amount of qubits, while retaining the initial information
- Can be used for the same purpose, i.e., dimentionality reduction

- Inspired by classical autoencoder
- Compress a quantum state onto a smaller amount of qubits, while retaining the initial information
- Can be used for the same purpose, i.e., dimentionality reduction
- Copy the structure of the classcial autoencoder?

- Inspired by classical autoencoder
- Compress a quantum state onto a smaller amount of qubits, while retaining the initial information
- Can be used for the same purpose, i.e., dimentionality reduction
- Copy the structure of the classcial autoencoder?
 - No

- Inspired by classical autoencoder
- Compress a quantum state onto a smaller amount of qubits, while retaining the initial information
- Can be used for the same purpose, i.e., dimentionality reduction
- Copy the structure of the classcial autoencoder?
 - No
 - Quantum computations follow a unitary evolution
 - Not possible to eliminate or create new qubits during quantum computation

Basic Architecture of QAE



Source: QiskitCommunity, Quantum Autoencoder Tutorial

- Input layer: input $|\psi\rangle$ contrains n qubits
- Bottleneck layer: Reduce the dimensionality to n k qubits
- Output layer: k qubits (all in the state $|0\rangle$) plus the new qubits

Basic Architecture of QAE



Source: QiskitCommunity, Quantum Autoencoder Tutorial

Auxiliary Qubit

- Aid in certain quantum operations
- Entangle quantum state with auxiliary qubits
- Reference State
 - A reference for comparison in quantum algorithms
 - Measure deviations in the quantum system during computation
- Classical Register
 - Store and process classical bits

Current Challenges of QAE

Error Correction

Decoherence

- Limited Qubits
- Qubit Stability

- Motivation: a possible solution to tackle the quantum noise problem
- Goal: reconstruct Greenberger–Horne–Zeilinger (GHZ) states subject to random bit-flips and small unitary noise.
- What are GHZ states?
 - > A certain type of entangled quantum state that involves at least three qubits
 - ► A M-qubit GHZ state can be defined by

$$|\mathrm{GHZ}
angle = rac{|\mathbf{0}
angle^{\otimes M}+|\mathbf{1}
angle^{\otimes M}}{\sqrt{2}}$$

Why do we do this?

- GHZ states are highly entangled quantum states
- ▶ Random bit-flips introduce errors and decoherence in quantum systems
- Crucial for developing effective quantum error correction codes



Architecture

- ▶ A QNN with ℓ layers, denoted as $[m_1, \ldots, m_\ell]$
- Each layer has size m_i , $1 \le i \le \ell$
- The quantum circuit is made up of *Q* qubits, where $Q = 1 + m_1 + w$



$$F(|\phi_i\rangle,\rho) = \langle \phi | \rho | \phi_i \rangle$$

$$\mathsf{p}_0 = \frac{1}{2} (\mathbf{1} + \mathcal{F}(|\phi_i\rangle, \rho))$$

Source: Achache, Horesh, and Smolin, "Denoising quantum states with quantum autoencoders - theory and applications"

Zhuojing Huang

Newest Trends in High-Performance Data Analytics



Reuse the qubits of the precedent layers by resetting themOnly need the qubits representing two consecutive layers

Training

- Unsupervised
- ▶ Train on pairs (x, y); x and y are from the same noisy distribution

• Loss function:
$$C(\kappa) = \frac{1}{N} \sum_{i=1}^{N} F(|\phi_i\rangle, \rho_i^{\kappa})$$

Results





Frameworks support QAE out of the box

Tool	Language
Cirq	Python
Qiskit	Python
Dwave-system	Python
FermiLib	Python
Qbsolv	С
QGL.jl	Julia
Qiskit.js	JavaScript
Qrack	C++
Quirk	JavaScript
Strawberry Fields	Python

Getting into the Field Main Takeaways

Frameworks support QAE out of the box: Qiskit

- Open-source quantum computing framework developed by IBM
- Detailed documentation, tutorials, and examples are available
- Allows users to run quantum circuits on real quantum devices

Building QAE at Home

Import necessary Qiskit libraries

P	ython	
1	from	qiskit import ClassicalRegister, QuantumRegister
2	from	qiskit import QuantumCircuit
3	from	qiskit.circuit.library import RealAmplitudes
4	from	qiskit.quantum_info import Statevector
5	from	qiskit_algorithms.optimizers
6	from	qiskit_algorithms.utils
7	from	<pre>qiskit_machine_learning.circuit.library import RawFeatureVector</pre>
8	from	<pre>qiskit_machine_learning.neural_networks import SamplerQNN</pre>

Source: QiskitCommunity, Quantum Autoencoder Tutorial

Use Case: Quantum Autoencoder

Building QAE at Home





Use Case: Quantum Autoencoder

Building QAE at Home

Define the autoencoder circuit

Source: QiskitCommunity, Quantum Autoencoder Tutorial

Introduction: Quantum Computing

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home



- \blacksquare $q_0 q_3$: Laten space
- \blacksquare $q_4 q_7$: Trash space
- **a** q_8 q_1 1: Reference space
- **q**₁₂: Auxiliary qubit
- c: Classical register

Source: QiskitCommunity, Quantum Autoencoder Tutorial

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home



Source: QiskitCommunity, Quantum Autoencoder Tutorial

Building QAE at home

Maximizing this function corresponds to two states being identical

$$S = 1 - \frac{2}{M} \cdot L \tag{1}$$

Building QAE at Home: Domain Wall

Apply the X gate (bit-flip)

Ρ	ython
1	<pre>def domain_wall(circuit, a, b):</pre>
2	# Here we place the Domain Wall to qubits a - b in our circuit
3	<pre>for i in np.arange(int(b / 2), int(b)):</pre>
4	circuit.x(i)
5	return circuit
6	
7	ae = auto_encoder_circuit(num_latent, num_trash)
8	<pre>qc = QuantumCircuit(num_latent + 2 * num_trash + 1, 1)</pre>
9	<pre>qc = qc.compose(domain_wall_circuit, range(num_latent + num_trash))</pre>
10	<pre>qc = qc.compose(ae)</pre>
11	<pre>qc.draw("mpl")</pre>

Source: QiskitCommunity, Quantum Autoencoder Tutorial

Building QAE at Home: Domain Wall

Initialize Qubits

- > Start with 8 qubits, initially set to the $|0\rangle$ state.
- Apply X-Gates
 - > Apply an X-gate (bit-flip) operation on qubits 1 through 4.
 - > This flips the states to $|1\rangle$, representing the "domain wall."

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home: Domain Wall



Source: QiskitCommunity, Quantum Autoencoder Tutorial

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home: Domain Wall

Define loss function

Python	
1 def 2 3 4	<pre>cost_func_domain(params_values): probabilities = qnn.forward([], params_values) # we pick a probability of getting 1 as the output of the network cost = np.sum(probabilities[:, 1])</pre>

Source: QiskitCommunity, Quantum Autoencoder Tutorial

Introduction: Quantum Computing

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home: Domain Wall



Zhuojing Huang

Newest Trends in High-Performance Data Analytics

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home: Domain Wall





Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Building QAE at Home: Domain Wall

Compare final fidelity between input and output

Python

3

- 1 domain_wall_state = Statevector(domain_wall_circuit).data
- 2 output_state = Statevector(test_qc).data
- 4 fidelity = np.sqrt(np.dot(domain_wall_state.conj(), output_state) ** 2)

▶ Fidelity of our Output State with our Input State: 0.9740570467513804

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways







Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways



Introduction: Quantum Computing

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways



Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Mai

Main Takeaways





Introduction: Quantum Computing

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Ma

Main Takeaways

Building QAE at Home: Image Compression



Results with smaller images

- ▶ Image size: 4 × 8
- Number of qubits: 5
- Laten space: 3
- Trash space: 2

Source: QiskitCommunity, Quantum Autoencoder Tutorial

Main Takeaways

- Push the boundaries of machine learning capabilities
- Applications: optimization, data compression, and data denoising
- Integrate into industry: the key to the full power of quantum computing
- Ongoing research promises enhanced efficiency and scalability
- Out-of-the-box frameworks like Qiskit facilitate experimentation

Introduction: Quantum Computing

Overview: Quantum Neural Network

Use Case: Quantum Autoencoder

Getting into the Field Main Takeaways

Conclusion

"Nature isn't classical, and if you want to make a simulation of Nature, you'd better make it quantum mechanical"

—- Richard Feynman

References

Achache, Tomer, Lior Horesh, and John Smolin. "Denoising quantum states with quantum autoencoders – theory and applications". In: (Dec. 2020). arXiv: 2012.14714 [guant-ph]. URL:

https://arxiv.org/abs/2012.14714.

- Ayoade, O., P. Rivas, and J. Orduz. "Artificial Intelligence Computing at the Quantum Level". In: *Data* 7 (2022), p. 28. URL: http://link.aip.org/link/?RSI/72/4477/1.
- Berggren, Karl. "Quantum Computing with Superconductors". In: *Proceedings of the IEEE* 92 (2004), pp. 1630–1638. DOI: 10.1109/JPR0C.2004.833672.

Ezratty, Olivier. "Is there a Moore's law for quantum computing?" In: (2023).

Moreno-Pineda, Eufemio et al. "Molecular Spin Qudits for Quantum Algorithms". In: *Chemical Society Reviews* 47 (2017). DOI: 10.1039/C5CS00933B.

QiskitCommunity. Quantum Autoencoder Tutorial. Qiskit Machine Learning Repository. 2023. URL: https://github.com/qiskit-community/qiskit-machine-

learning/blob/stable/0.7/docs/tutorials/12_quantum_autoencoder.ipynb.

Rao, A. "Learning hard distributions with quantum-enhanced Variational Autoencoders". In: (May 2023). arXiv: 2305.01592 [quant-ph].