FUJITSU

Quantum Generative Adversarial Autoencoders: Learning latent representations for quantum data generation

Background

Quantum Autoencoder (QAE)

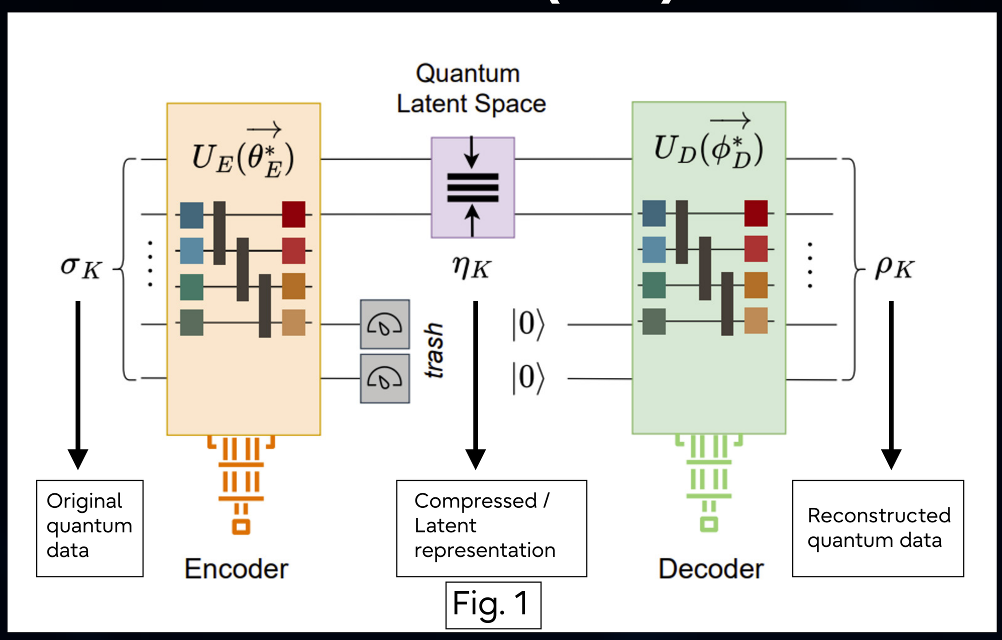


Fig. 1

Quantum Machine Learning (QML) model for compression and reconstruction of quantum states.

Limitations of the QAE

- The QAE lacks generative capabilities.
- Unlike classical ML techniques of latent space regularization, there is no well-defined quantum analogue for the directly accessing a quantum latent space.

Our Proposal

Architecture

The Quantum Generative Adversarial Autoencoder (QGAA) - a novel approach that leverages quantum adversarial learning to model the latent space representation of a trained QAE.

Application

We demonstrate the functioning and the potential utility of the QGAA approach using the following quantum generative tasks:

- Learning the latent representation of a set of 2-qubit entangled states.
- Learning the ground state energy profiles of the parameterized molecular Hamiltonians, of H_2 (4 qubits) and LiH (6 qubits).

The Quantum Generative Adversarial Autoencoder (QGAA)

Stage 1: Adversarial Learning

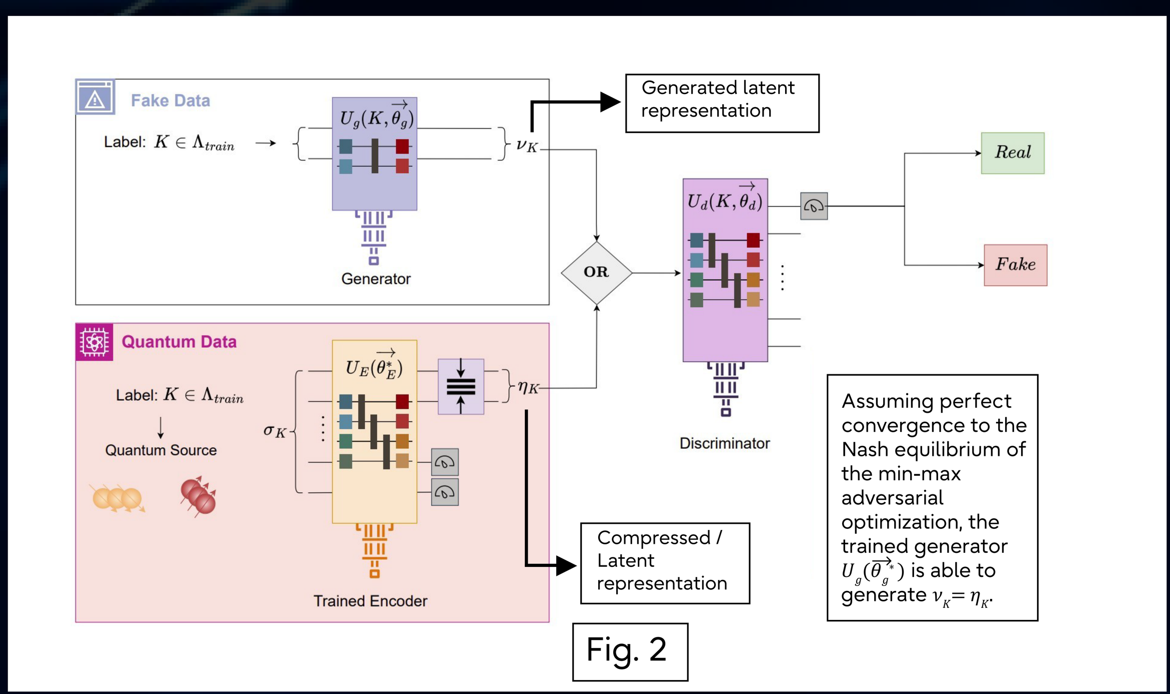


Fig. 2

- **Objective of the generator $U_g(\vec{\theta}_g)$: To optimize $(\vec{\theta}_g)$ to generate ν_K whose likelihood of being classified as fake is minimized.**
- **Objective of the discriminator $U_d(\vec{\theta}_d)$: To optimize $(\vec{\theta}_d)$ such that the likelihood of correct classification, i.e., η_K as real (FIG. 1) and ν_K as fake is maximized based on the quantum state discrimination protocol.**

Stage 1: Adversarial Learning

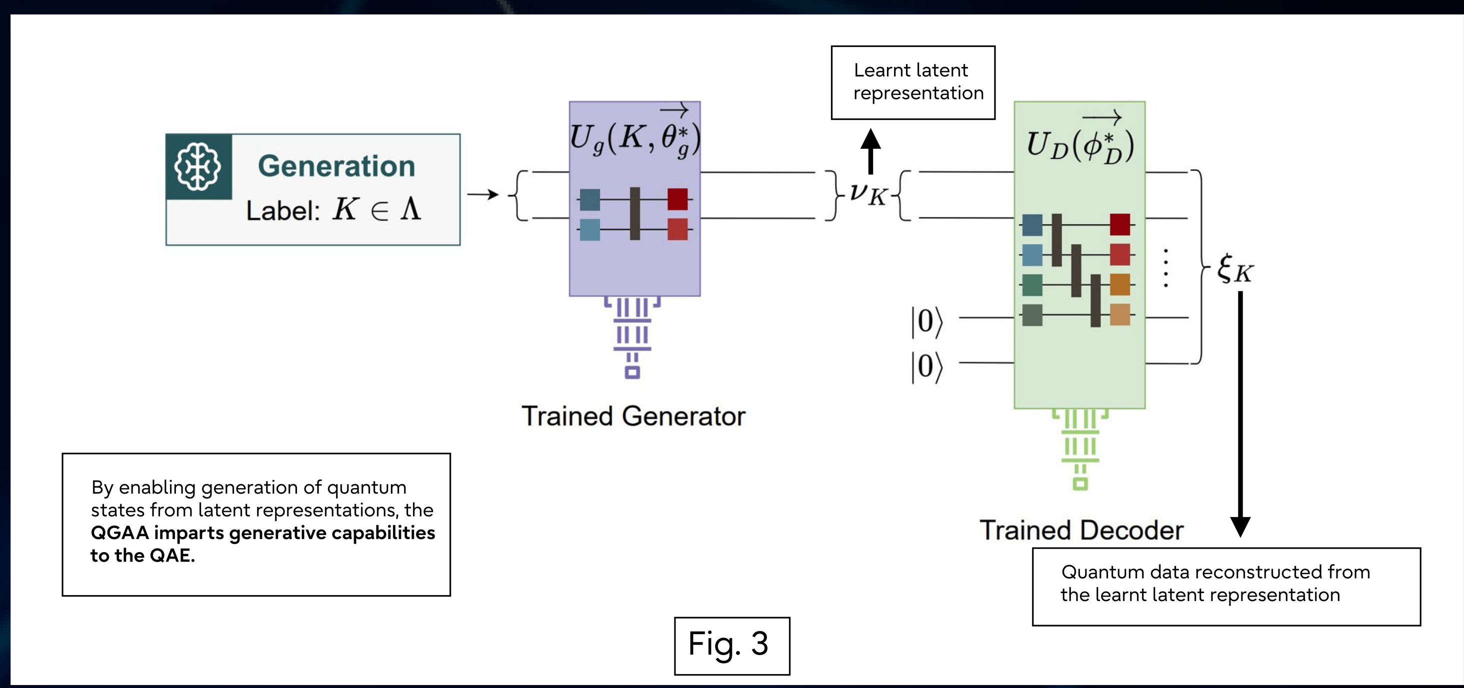


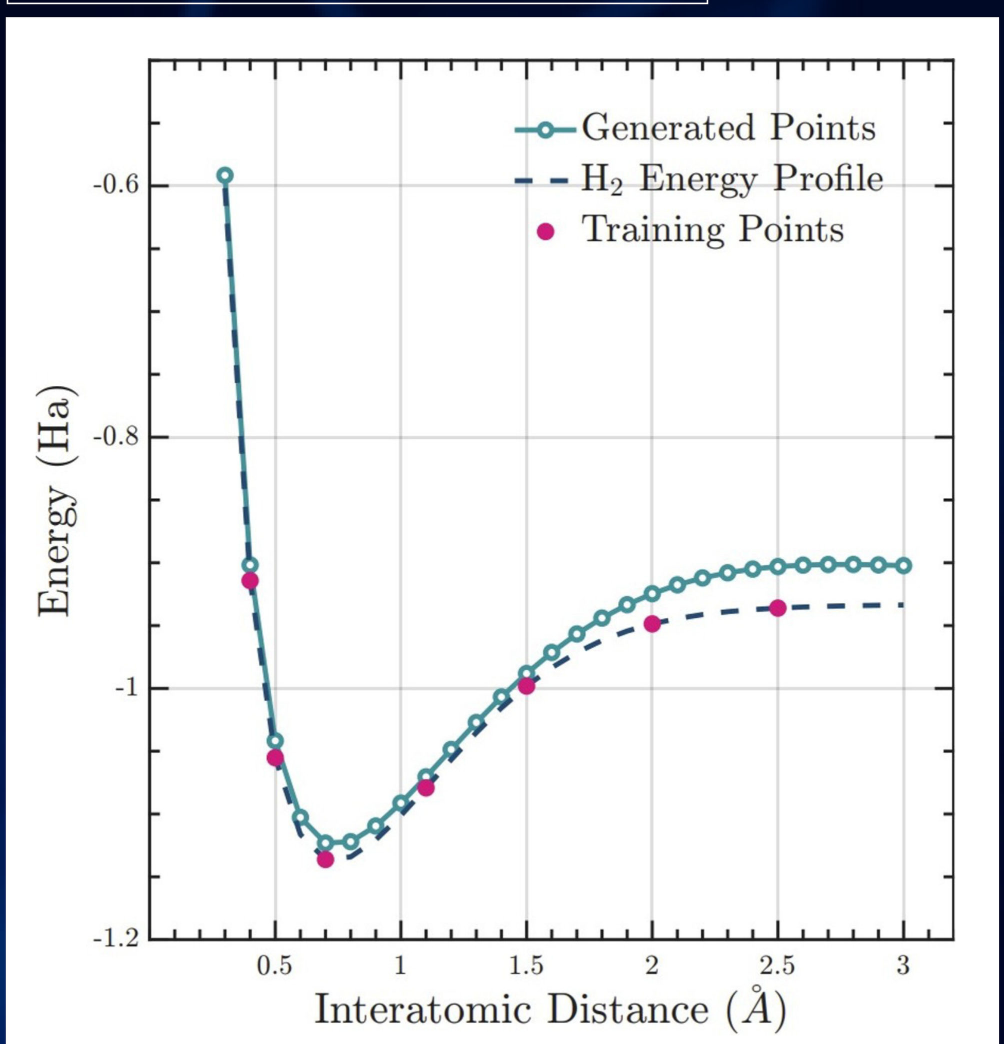
Fig. 3

- **The generated latent state $\nu_K = \eta_K$ (assuming perfect learning of the latent representation) is fed into the trained decoder $U_D(\vec{\theta}_D^*)$ (FIG. 1), to reconstruct $\xi_K = \rho_K$.**
- **Assuming that the trained QAE performs perfect reconstruction, i.e., $\rho_K = \sigma_K$, then $\xi_K = \sigma_K$.**

Application: Generation of the ground state energy profile of molecular Hamiltonians of H_2

- A QAE is trained on a subset of molecular ground states, $\{\sigma_r\}$ of the Hamiltonian $\mathcal{H}(r)$, to compress them to a quantum latent space $\{\eta_r\}$.
- Upon executing the two stages of the QGAA, the trained generator is able to directly generate latent states $\{\nu_K\}$, such that $E_{true} \approx E_{gen}$, upon reconstructing $\{\zeta_r\}$.
- Average Error over different values of r, $\langle|\Delta E|\rangle = \langle|E_{true} - E_{gen}|\rangle$ is 0.02 ± 0.01 Ha for the case of H_2.
- For similar experiments using LiH data, $\langle|\Delta E|\rangle$=0.06± 0.02 Ha.

$E_{true} = \mathrm{Tr}\{\mathcal{H}(r)\sigma_r\} \mid E_{gen} = \mathrm{Tr}\{\mathcal{H}(r)\zeta_r\}$



(Plot is based on experiments on a quantum simulator.)

Conclusion and Outlook

- Our novel approach enables direct access to the latent space of a trained QAE.
- Compared to training the QGAN on the original data, our approach demonstrates a more resource efficient implementation of the QGAN by enabling adversarial training in a lower dimensional quantum latent space.
- Even learning approximate latent representations has utility for warm starting in QML applications such as initial state preparation for a Variational Quantum Eigensolver (VQE).

Naipunnya Raj*, Rajiv Sangle*, Avinash Singh, Krishna Kumar Sabapathy
Quantum Lab, Fujitsu Research of India Pvt. Ltd.

* These authors contributed equally to this work.