Qiskit $\otimes$ QCBMs

QAMP 2026 Open House

Issue 64

Quantum Circuit Born Machines in Qiskit

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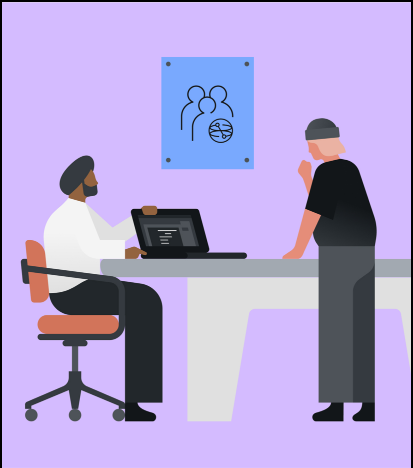
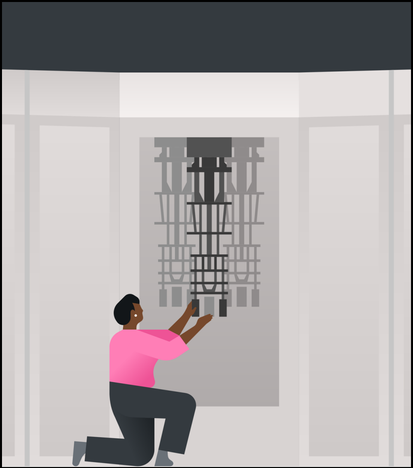


Speakers:
Debshata Choudhury
Jorge Plazas
(mentees)

Mentor:
Natalie Hawkins

Agenda

- Quantum Circuit Born Machines.
- Building blocks and auxiliary functions.
- Experiments.
- QCBMs for molecule generation.



Quantum Circuit Born Machines

$\rightsquigarrow$ Hybrid intrinsic generative models that use quantum circuits to represent probability distributions.

Distribution of data $\rightleftarrows$ Quantum state statistics

$$\pi(X) \quad \sim \quad |\langle X|\psi_\theta\rangle|^2$$

QCBMs - Building blocks

The *circuit* part of a QCBM consist of two kinds of layers:

- Rotation layers.
- Entanglement layers.

This structure can be seen as an instance of the

$$\text{efficient\_su2}$$

ansatz in qiskit.
State statistics are obtained via the

$$\text{Sampler}$$

primitive.

QCBMs - Functions for training

Kernels and similarity measures

In order to train the models various kernels and loss functions were implemented. These were used measure the discrepancy between sampled distributions and target distributions.

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Kernels and similarity measures

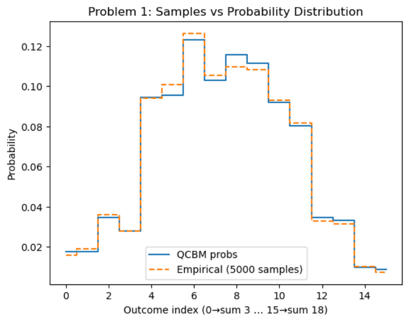
In order to train the models various kernels and loss functions were implemented. These were used measure the discrepancy between sampled distributions and target distributions.

- Radial Basis Function (RBF) Kernel
- Squared Maximum Mean Discrepancy (MMD) Loss.
- Kullback–Leibler (KL) Divergence.

Discrete Gaussian experiment

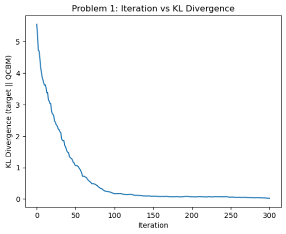
Sum of Three Dice (Discrete Gaussian) Experiment

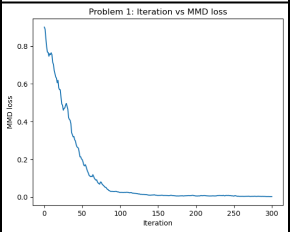
- Fidelity $= 98.7\%$
  Generated distribution closely matches the target distribution.
- Sinkhorn OT $= 0.0925$
  Negligible probability mass movement; near-perfect distribution alignment.



Discrete Gaussian experiment

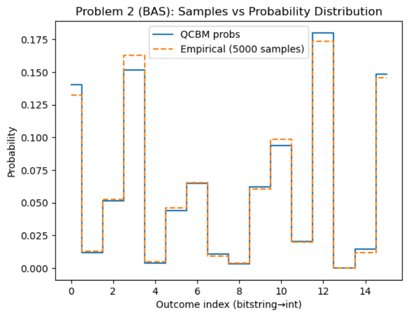
- KL Divergence (low)
  Minimal information loss between true and learned distributions.
- MMD (low)
  Strong sample-level similarity; effective global distribution matching.





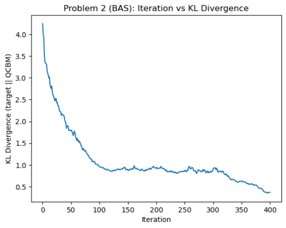
Bars & Stripes (BAS) Experiment

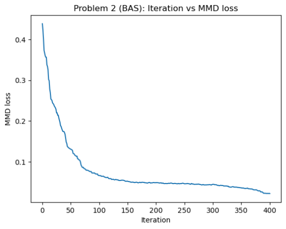
- Fidelity = 72.7%
  Partial match with the target BAS distribution.
- Sinkhorn OT = 0.4456
  Moderate probability mass movement; incomplete alignment with BAS modes.



Bars & Stripes (BAS) Experiment

- KL Divergence (moderate)
  Noticeable divergence due to probability leakage into invalid patterns.
- MMD (moderate)
  Structural similarity present, but mode precision remains imperfect.





Chemical space exploration and molecule generation

Our project was partly inspired by

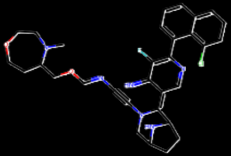
Quantum-computing-enhanced algorithm unveils potential KRAS inhibitors. by Ghazi Vakili, M., Gorgulla, C., Snider, J. et al. [Nature Biotechnology (2025)]

Where QCBMs are used as a component in a hybrid generative model used for the generation of novel KRAS inhibitors[1].

[1] KRAS is a common and hard-to-treat oncogene in many solid cancers.

Chemical space exploration and molecule generation (After [Aspuru-Guzik et al.])

We used STONED-SELFIES in conjunction with QCBMs to learn the probability distribution, within the chemical space, of neighboring KRAS inhibitor molecules.



THANKS

to the QAMP community.

⊕ SPECIAL THANKS

to Astri, Radha and our amazing mentor Natalie Hawkins.

Visit our repo at:
`https://github.com/QCHPC/qiskit_QCBMs`