

On the sample complexity of quantum Boltzmann machine learning

L. Coopmans and M. Benedetti [arXiv: 2306.14969]

Presented by:

Luuk Coopmans 21-11-2023

Outline of the Talk

- **.** Introduction: what are QBMs?
- **Main result: polynomial sample complexity**
- **Numerical verification**
- **Discussion and open problems**

Introduction: what are quantum Boltzmann Machines

• A quantum Boltzmann machine (QBM) is a quantum machine learning model that can be used for generatively modelling classical and quantum data.

Introduction: what are quantum Boltzmann Machines

• A quantum Boltzmann machine (QBM) is a quantum machine learning model that can be used for generatively modelling classical and quantum data.

n– qubit parameterised Gibbs state
$$
\rho_{\theta} = \frac{e^{\mathcal{H}_{\theta}}}{\text{Tr}e^{\mathcal{H}_{\theta}}}
$$
,
with ansatz/model Hamiltonian $\mathcal{H}_{\theta} = \sum_{i=1}^{m} \theta_i H_i$.
Any set of (bounded) Hermitian operators $\{H_i\}_{i=1}^{m}$, e.g. Pauli operators.

Introduction: what are quantum Boltzmann Machines

• A quantum Boltzmann machine (QBM) is a quantum machine learning model that can be used for generatively modelling classical and quantum data.

\n- *n*-qubit parameterised Gibbs state
$$
\rho_{\theta} = \frac{e^{\mathcal{H}_{\theta}}}{\text{Tr}e^{\mathcal{H}_{\theta}}}
$$
, with ansatz/model Hamiltonian $\mathcal{H}_{\theta} = \sum_{i=1}^{m} \theta_i H_i$.
\n- Any set of (bounded) Hermitian operators $\{H_i\}_{i=1}^m$, e.g. Pauli operators.
\n- Note: focus here on fully visible QBMs.
\n

Introduction: goal and applications

■ Goal: optimise θ **such that samples taken from the QBM** $s' \sim \rho_{\theta}$ **mimic samples from a** given target dataset $\{s^\mu\}_{\mu=1}^M.$

▪

Introduction: goal and applications

- **Goal: optimise** θ **such that samples taken from the QBM** $s' \sim \rho_{\theta}$ **mimic samples from a** given target dataset $\{s^\mu\}_{\mu=1}^M.$ Si quantum photonic simulator a
- Applications:

▪ …

- **Example 12** Generative modelling of (binarised) classical data *[Amin et al., 1601.02036], [Kappen, 1803.11278]*
- **EXECTE:** Learning physical models from experimental data
- **Example 1 Learning the entanglement Hamiltonian** *[M.K. Joshi et al. arXiv 2306.00057 (2023), C. Kokail et al., PRL 127 (2021)]*
- **Verification of quantum devices** *[J. Wang et al., Nature Physics 13 (2017)]*

Set-up for diamond NV⁻ centre

[J. Wang et al., Nature Physics 13 (2017)]

Introduction: goal and applications

■ Goal: optimise θ **such that samples taken from the QBM** $s' \sim \rho_{\theta}$ **mimic samples from a** given target dataset $\{s^\mu\}_{\mu=1}^M.$ Si quantum photonic simulator

• Relative entropy <u>loss function</u>: $S(\eta \| \rho_{\theta}) = Tr(\eta \log \eta) - Tr(\eta \log \rho_{\theta})$, $\rho_{\theta} =$

$$
\rho_{\theta} = \frac{e^{\mathcal{H}_{\theta}}}{\text{Tr}e^{\mathcal{H}_{\theta}}}
$$

Derivatives:
$$
\frac{\partial S(\eta || \rho_{\theta})}{\partial \theta_k} = \text{Tr}[\rho_{\theta} H_k] - \text{Tr}[\eta H_k].
$$

• Relative entropy <u>loss function</u>: $S(\eta \| \rho_{\theta}) = Tr(\eta \log \eta) - Tr(\eta \log \rho_{\theta})$, $\rho_{\theta} =$

$$
\rho_{\theta} = \frac{e^{\mathcal{H}_{\theta}}}{\text{Tr}e^{\mathcal{H}_{\theta}}}
$$

Derivatives:
$$
\frac{\partial S(\eta || \rho_{\theta})}{\partial \theta_k} = \text{Tr}[\rho_{\theta} H_k] - \text{Tr}[\eta H_k].
$$

- Show that $S(\eta||\rho_{\theta})$ is (strictly) <u>convex.</u>

• Relative entropy <u>loss function</u>: $S(\eta \| \rho_{\theta}) = Tr(\eta \log \eta) - Tr(\eta \log \rho_{\theta})$, $\rho_{\theta} =$

$$
\rho_{\theta} = \frac{e^{\mathcal{H}_{\theta}}}{\text{Tr}e^{\mathcal{H}_{\theta}}}
$$

Derivatives:
$$
\frac{\partial S(\eta || \rho_{\theta})}{\partial \theta_k} = \text{Tr}[\rho_{\theta} H_k] - \text{Tr}[\eta H_k].
$$

- Show that $S(\eta||\rho_{\theta})$ is (strictly) <u>convex.</u>

• Relative entropy <u>loss function</u>: $S(\eta \| \rho_{\theta}) = Tr(\eta \log \eta) - Tr(\eta \log \rho_{\theta})$, $\rho_{\theta} =$

$$
\rho_{\theta} = \frac{e^{\mathcal{H}_{\theta}}}{\text{Tr}e^{\mathcal{H}_{\theta}}}
$$

Derivatives:
$$
\frac{\partial S(\eta || \rho_{\theta})}{\partial \theta_k} = \text{Tr}[\rho_{\theta} H_k] - \text{Tr}[\eta H_k].
$$

- Show that $S(\eta||\rho_{\theta})$ is (strictly) <u>convex.</u>

• Optimize $S(\eta||\rho_{\theta})$ with stochastic gradient descent.

• Optimize $S(\eta||\rho_{\theta})$ with stochastic gradient descent.

Theorem 1: after
$$
T = \frac{48\delta_0 m^2(\kappa^2 + \xi^2)}{\epsilon^4}
$$
 iterations, where $\delta_0 = S(\eta || \rho_{\theta^0}) - S(\eta || \rho_{\theta^0},)$, we have solved the QBM learning problem to accuracy ϵ .
Each iteration requires $N \leq \mathcal{O}\left(\frac{1}{\kappa^4} \log \frac{m}{1 - \lambda^{\frac{1}{T}}}\right)$ preparation of the Gibbs state ρ_{θ} .

• Optimize $S(\eta||\rho_{\theta})$ with stochastic gradient descent.

Theorem 1: after
$$
T = \frac{48\delta_0 m^2 (\kappa^2 + \xi^2)}{\epsilon^4}
$$
 iterations, where $\delta_0 = S(\eta || \rho_{\theta^0}) - S(\eta || \rho_{\theta^0 p t})$, we have solved the QBM learning problem to accuracy ϵ .
Each iteration requires $N \leq \mathcal{O}\left(\frac{1}{\kappa^4} \log \frac{m}{1 - \lambda^{\frac{1}{T}}}\right)$ preparation of the Gibbs state ρ_{θ} .

 $m = \text{Poly}(n) \Rightarrow \text{Polynomial sample complexity!}$

• Optimize $S(\eta||\rho_{\theta})$ with stochastic gradient descent.

Theorem 1: after $T = \frac{48\delta_0 m^2(\kappa^2 + \xi^2)}{\epsilon^4}$ iterations, where $\delta_0 = S(\eta \rho_{\theta^0}) - S(\eta \rho_{\theta^0 \text{opt}})$, we have solved the QBM learning problem to accuracy ϵ .	
Each iteration requires $N \leq \mathcal{O}\left(\frac{1}{\kappa^4} \log \frac{m}{1 - \lambda^{\frac{1}{T}}}\right)$ preparation of the Gibbs state ρ_{θ} .	
$m = \text{Poly}(n) \Rightarrow \text{Polynomial sample complexity!}$	

No barren plateaus…

Results: reducing the sample complexity by pretraining

• Sample complexity depends on $\delta_0 = S(\eta || \rho_{\theta^0}) - S(\eta || \rho_{\theta^0}).$

Results: reducing the sample complexity by pretraining

• Sample complexity depends on $\delta_0 = S(\eta || \rho_{\theta^0}) - S(\eta || \rho_{\theta^0}).$

<u>Theorem 2</u>: can reduce δ_0 by <u>pretraining</u> a sub-model defined by a subset of the operators $\{H_i\}_{i=1}^{\tilde{m}}$.

J

Results: reducing the sample complexity by pretraining

• Sample complexity depends on $\delta_0 = S(\eta || \rho_{\theta^0}) - S(\eta || \rho_{\theta^0}).$

<u>Theorem 2</u>: can reduce δ_0 by <u>pretraining</u> a sub-model defined by a subset of the operators $\{H_i\}_{i=1}^{\tilde{m}}$.

- **-** Note δ_0 defined with respect to the larger model
- **Examples: quantum mean-field (MF), Gaussian-Fermionic (GF), geometrically local (GL)**

J

QUANTINUUM

Numerical verification: verifying sampling bound

QUANTINUUM

Summary and discussion

- We have reformulated the QBM learning problem and proved that it can be solved with polynomial sample complexity.
- **Pretraining on a subset of the parameters can only improve the sample complexity.**

Summary and discussion

- We have reformulated the QBM learning problem and proved that it can be solved with polynomial sample complexity.
- **Pretraining on a subset of the parameters can only improve the sample complexity.**
- **Time complexity: combine with Gibbs sampler of your choice (classical or quantum).**

Summary and discussion

- We have reformulated the QBM learning problem and proved that it can be solved with polynomial sample complexity.
- **Pretraining on a subset of the parameters can only improve the sample complexity.**
- Time complexity: combine with Gibbs sampler of your choice (classical or quantum).
- Speedups in quantum Gibbs sampling translate to QBM learning.
	- 1) Generic case: quadratic speedup but possibly exponential time
	- 2) Efficient Gibbs samplers for specific cases??

[O. Watts et al., 2310.07774], [Chen et al., 2311.09207]

3) Resources for experimental demonstration??

Thank you for your attention!

Luuk Coopmans QTML, 21-11-2023

See paper: arXiv: 2306.14969

CUANTINUUM