
DO-EM: Density Operator Expectation Maximization

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Abstract

Density operators, quantum generalizations of probability distributions, are gaining prominence in machine learning due to their foundational role in quantum computing. Generative modeling based on density operator models (**DOMs**) is an emerging field, but existing training algorithms – such as those for the Quantum Boltzmann Machine – do not scale to real-world data, such as the MNIST dataset. The Expectation-Maximization algorithm has played a fundamental role in enabling scalable training of probabilistic latent variable models on real-world datasets. *In this paper, we develop an Expectation-Maximization framework to learn latent variable models defined through **DOMs** on classical hardware, with resources comparable to those used for probabilistic models, while scaling to real-world data.* However, designing such an algorithm is nontrivial due to the absence of a well-defined quantum analogue to conditional probability, which complicates the Expectation step. To overcome this, we reformulate the Expectation step as a quantum information projection (QIP) problem and show that the Petz Recovery Map provides a solution under sufficient conditions. Using this formulation, we introduce the Density Operator Expectation Maximization (DO-EM) algorithm – an iterative Minorant-Maximization procedure that optimizes a quantum evidence lower bound. We show that the **DO-EM** algorithm ensures non-decreasing log-likelihood across iterations for a broad class of models. Finally, we present Quantum Interleaved Deep Boltzmann Machines (**QiDBMs**), a **DOM** that can be trained with the same resources as a DBM. When trained with **DO-EM** under Contrastive Divergence, a **QiDBM** outperforms larger classical DBMs in image generation on the MNIST dataset, achieving a 40–60% reduction in the Fréchet Inception Distance.

1 Introduction

Recent advances in quantum hardware and hybrid quantum-classical algorithms have fueled a surge of interest in developing learning models that can operate effectively in quantum regimes [1]. Classical models rely on probability distributions; quantum systems generalize these to density operators – positive semi-definite, unit-trace operators on Hilbert spaces—that encode both classical uncertainty and quantum coherence [2]. While there is considerable progress made in quantum supervised learning, there is relatively less progress in unsupervised learning [3].

Latent variable models (LVMs) are a cornerstone of unsupervised learning, offering a principled approach to modeling complex data distributions through the introduction of unobserved or hidden variables [4]. These models facilitate the discovery of underlying structure in data and serve as the foundation for a wide range of tasks, including generative modeling, clustering, and dimensionality reduction. Classical examples such as Gaussian Mixture Models, Factor Analysis, and Hidden Markov Models [5, 6] exemplify the power of latent variable frameworks in capturing dependencies and variability in observed data. In recent years, LVMs have formed the conceptual backbone of

deep generative models including Variational Autoencoders [7], Generative Adversarial Networks [8], and Diffusion-based models [9]. The EM algorithm [10, 11] has been instrumental in deriving procedures for learning latent variables models. These algorithms are often preferred over algorithms which directly maximizes likelihood.

The study of Density Operator-based Latent Variable Models (**DO-LVM**) remains in its early stages, with foundational questions around expressivity, inference, and learning still largely unexplored [12–14]. Leveraging the modeling power of **DO-LVMs** on real-world data remains a significant challenge. Existing approaches rarely scale beyond 12 visible units—limited by restricted access to quantum hardware, the exponential cost of simulating quantum systems, and the memory bottlenecks associated with representing and optimizing **DO-LVMs** on classical devices. As a result, it is currently infeasible to empirically assess whether **DO-LVMs** offer any practical advantage on real-world datasets in terms of modeling power. EM based algorithms can provide a simpler alternative to existing learning algorithms for **DO-LVMs** which directly maximizes the likelihood. However deriving such algorithms in Density operator theoretic setup is extremely challenging for a variety of reasons, most notably there are operator theoretic inequalities, such as Jensen Inequality, which can be directly applied to derive an Evidence lower bound(ELBO) style bound for **DO-LVMs**. Precise characterization of models which are compatible with such bounds and their computational behaviour remains an important area of investigation. In this paper we bridge these research gaps by making the following contributions.

- A Density Operator Expectation-Maximization (**DO-EM**) algorithm is specified using Quantum Information Projection in Algorithm 1. **DO-EM** guarantees log-likelihood ascent in Theorem 4.4 under mild assumptions that retain a rich class of models.
- A Quantum Evidence Lower Bound (QELBO) for the log-likelihood is derived in Lemma 4.1 from a minorant-maximization perspective leveraging the Monotonicity of Relative Entropy.
- **DO-LVMs** are specialized to train on classical data in Section 5 using the **DO-EM** algorithm. This specialization we call **CQ-LVMs**, a class of models with quantum latent variables, can train real world data due to a decomposition proved in Theorem 5.1.
- Quantum-interleaved deep Boltzmann machines (Q_iDBM), a quantum analog of the DBM is defined in Section 5.1. The well known Contrastive Divergence (CD) algorithm for Boltzmann machines is adapted to the Q_iDBM, which when used with **DO-EM** algorithm in Section 5.1, allows Q_iDBMs to be trained on MNIST-scale data.
- First empirical evidence of a modeling advantage when training **DO-LVMs** on standard computers with real-world data is provided in Section 6. Q_iDBMs trained using CD on the MNIST dataset achieve a 40–60% lower Fréchet Inception Distance compared to state-of-the-art deep Boltzmann machines.

2 Preliminaries

Notation The ℓ^2 -norm of a column vector \mathbf{v} in a Hilbert space \mathcal{H} is given by $\|\mathbf{v}\|_2 = \sqrt{\mathbf{v}^\dagger \mathbf{v}}$ where \mathbf{v}^\dagger denotes the conjugate transpose of \mathbf{v} . The set of Hermitian (self-adjoint) operators $\mathcal{O} = \mathcal{O}^\dagger$ on \mathcal{H} is denoted by $\mathfrak{L}(\mathcal{H})$. The positive-definite subset of $\mathfrak{L}(\mathcal{H})$ is denoted by $\mathfrak{L}_+(\mathcal{H})$. The Kronecker product between two operators is denoted $A \otimes B$ and their direct sum is denoted $A \oplus B$ [15]. The identity operator on \mathcal{H} is denoted $I_{\mathcal{H}}$. The null space of an operator $A \in \mathcal{H}$ is denoted by $\ker(A)$.

Latent variable models and EM algorithm Latent Variable Models (LVMs) [4] specify the probability distribution of random variables $V=[V_1, \dots, V_{d_V}]$ through a joint probability model

$$P(V=\mathbf{v} \mid \theta) = \sum_h P(V=\mathbf{v}, H=\mathbf{h} \mid \theta)$$

where $H = [H_1, \dots, H_{d_L}]$ are unobserved random variables. Learning an LVM from data, a problem of great interest in Unsupervised Learning [5], refers to estimating the model parameters θ from a dataset $\mathcal{D} = \{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(N)}\}$ consisting of i.i.d instances drawn from the LVM. Maximum likelihood-based methods aim to maximize $\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \ell_i(\theta)$ where $\ell_i(\theta) = \log P(V=\mathbf{v}^{(i)} \mid \theta)$. The maximization problem is not only intractable in most cases but even gradient-based algorithms, which

can only discover local optima, are difficult to implement because of unwieldy computations in $\ell_i(\theta)$. The EM algorithm [10, 11] is an alternative iterative algorithm with the scheme

$$\theta^{(k+1)} = \underset{\theta}{\operatorname{argmax}} \frac{1}{N} \sum_{i=1}^N Q_i(\theta | \theta^{(k)}), \text{ where } \ell_i(\theta) \geq Q_i(\theta | \theta^{(k)}) \text{ and } \ell_i(\theta^{(k)}) = Q_i(\theta^{(k)} | \theta^{(k)}).$$

Boltzmann machines Boltzmann Machines (BM) are stochastic neural networks that define a probability distribution over binary vectors based on the Ising model in statistical physics [16]. Due to the intractability of learning in fully connected BMs, the Restricted Boltzmann Machine (RBM) was introduced with no intra-layer connections, enabling efficient Gibbs sampling [17–19]. Deep Boltzmann Machines (DBM) [20] stacks RBMs using undirected connections and allow for joint training of all layers. The joint probability of a DBM with L layers, $P(\mathbf{v}, \mathbf{h}^1, \dots, \mathbf{h}^L)$ is defined as

$$P(\mathbf{v}, \mathbf{h}_1, \dots, \mathbf{h}_{d_L}) = \frac{1}{Z} e^{-E(\mathbf{v}, \mathbf{h}_1, \dots, \mathbf{h}_{d_L})} \quad (\text{DBM})$$

where $E(\mathbf{v}, \mathbf{h}^1, \dots, \mathbf{h}^L)$ is called the *Energy Function*, and $Z = \sum_{\mathbf{v}, \mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h}^1, \dots, \mathbf{h}^L)}$ is the *Partition Function* which is typically intractable to compute. Learning in DBMs is difficult due to intractable posterior dependencies. DBMs are usually trained using variants of the Contrastive Divergence algorithm [18, 21, 22]. A detailed discussion on Boltzmann machines and the Contrastive Divergence algorithm is provided in Appendix A.

2.1 Density operators

A density operator on a Hilbert space \mathcal{H} is a Hermitian, positive semi-definite operator with unit trace [2, 23]. The set of Density operators will be denoted by $\mathcal{P}(\mathcal{H})$, and can be regarded as generalizations of probability distributions. A joint density operator $\rho \in \mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ can be *marginalized* to $\rho_A \in \mathcal{P}(\mathcal{H}_A)$ by the partial trace operation $\rho_A = \operatorname{Tr}_B(\rho) = \sum_{i=1}^{d_B} (I_A \otimes \mathbf{x}_i^\dagger) \rho (I_A \otimes \mathbf{x}_i)$ where $\{\mathbf{x}_i\}_{i=1}^{d_B}$ is an orthonormal basis of \mathcal{H}_B . Such a ρ is *separable* if it is a convex combination of *product states* $\rho_A \otimes \rho_B$ with $\rho_A \in \mathcal{P}(\mathcal{H}_A)$ and $\rho_B \in \mathcal{P}(\mathcal{H}_B)$.

Definition 2.1 (Umegaki [24] Relative Entropy). Let ω and ρ be density operators in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ with $\ker(\rho) \subseteq \ker(\omega)$. Their relative entropy is given by $D_U(\omega, \rho) = \operatorname{Tr}(\omega \log \omega) - \operatorname{Tr}(\omega \log \rho)$.

Lindblad [25] showed that the relative entropy does not increase under the action of the partial trace.

Theorem 2.2 (Monotonicity of Relative Entropy). *For density operators ω and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that $\ker(\omega) \subset \ker(\rho)$, $D_U(\omega, \rho) \geq D_U(\operatorname{Tr}_B \omega, \operatorname{Tr}_B \rho)$.*

Petz [26, 27] showed that Theorem 2.2 is saturated if and only if the Petz Recovery Map reverses the partial trace operation.

Definition 2.3 (Petz Recovery Map). For a density operator ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$, the Petz Recovery Map for the partial trace $\mathcal{R}_\rho : \mathcal{H}_A \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$ is the map

$$\mathcal{R}_\rho(\omega) = \rho^{1/2} \left(\left(\rho_A^{-1/2} \omega \rho_A^{-1/2} \right) \otimes I_B \right) \rho^{1/2}. \quad (\text{PRM})$$

Theorem 2.2 is saturated when $\mathcal{R}_\rho(\omega) = \omega$. Ruskai [28] proved an equivalent condition.

Theorem 2.4 (Ruskai’s condition). *For density operators ω and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that $\ker(\omega) \subset \ker(\rho)$, $D_U(\operatorname{Tr}_B \omega, \operatorname{Tr}_B \rho) = D_U(\omega, \rho)$ if and only if $\log \omega - \log \rho = (\operatorname{Tr}_B \omega - \operatorname{Tr}_B \rho) \otimes I_B$.*

Ruskai’s condition can be interpreted as ω and ρ having the same Conditional Amplitude Operator.

Definition 2.5 (Conditional Amplitude Operator[29]). The conditional amplitude operator of a density operator ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ with respect to \mathcal{H}_A is $\rho_{B|A} = \exp(\log \rho - \log \rho_A \otimes I_B)$.

A detailed discussion on density operators and quantum channels is provided in Appendix B.

3 Density operator latent variable models

In this section, we introduce Density Operator Latent Variable Models (**DO-LVM**) and recover existing models such as the Quantum Boltzmann Machine (QBM) as special cases. We discuss the computational challenges of learning such models from observations.

Definition 3.1 (DO-LVM and the Learning Problem). A Density Operator Latent Variable Model (**DO-LVM**) specifies the density operator $\rho_V \in \mathcal{P}(\mathcal{H}_V)$ on observables in \mathcal{H}_V through a joint density operator $\rho_{VL} \in \mathcal{P}(\mathcal{H}_V \otimes \mathcal{H}_L)$ as $\rho_V = \text{Tr}_L(\rho_{VL}(\theta))$ where the space \mathcal{H}_L is not observed. Learning a **DO-LVM** is the estimation of model parameters θ when a target density operator $\eta_V \in \mathcal{P}(\mathcal{H}_V)$ is specified. This can be achieved by maximizing the log-likelihood

$$\mathcal{L}(\theta) = \text{Tr}(\eta_V \log \rho_V(\theta)). \quad (\text{LP})$$

Remark 3.2. Maximizing the log-likelihood of a **DO-LVM** is equivalent to minimizing $D_U(\eta_V, \rho_V(\theta))$.

We specialize **DO-LVMs** to classical datasets in Section 5.

Hamiltonian-based models The Hamiltonian is a Hermitian operator $H \in \mathcal{L}(\mathcal{H})$ representing the total energy and generalizes the notion of an energy function in classical energy-based models. The model is defined using Gibbs state density matrix analogous to the Boltzmann distribution: $\rho(\theta) = \frac{\exp(H(\theta))}{Z(\theta)}$ with $Z(\theta) = \text{Tr} \exp(H(\theta))$ and $H(\theta) = \sum_r \theta_r H_r$, where $H_r \in \mathcal{L}(\mathcal{H})$ are Hermitian operators and $\theta_r \in \mathbb{R}$ are model parameters. The Quantum Boltzmann Machine is a Hamiltonian-based model inspired by the transverse field Ising model [12]. In this paper, $\text{QBM}_{m,n}$ denotes a model with m visible and n hidden units with

$$H(\theta) = - \sum_{i=1}^{m+n} b_i \sigma_i^z - \sum_{i>j} w_{ij} \sigma_i^z \sigma_j^z - \sum_{i=1}^{m+n} \Gamma_i \sigma_i^x \quad (\text{QBM})$$

where σ_i^z and σ_i^x are $2^{m+n} \times 2^{m+n}$ Pauli matrices defined by $\sigma_i^k = \otimes_{j=1}^{i-1} \mathbf{I} \otimes \sigma^k \otimes_{j=i+1}^{m+n} \mathbf{I}$ where $k \in \{x, z\}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. A QBM is hence a **DO-LVM** with $\rho_V(\theta) = \frac{1}{Z(\theta)} \text{Tr}_L \exp(H(\theta))$.

Setting $\Gamma_i = 0$ recovers the Boltzmann Machine (BM) [12]. However, the density operator representation of these classical models are plagued by their $2^{m+n} \times 2^{m+n}$ dimensionality. The memory requirements for storing and updating models represented by density operators have been prohibitive for QBMs to scale beyond about 12 visible units.

Need for an EM algorithm. As probabilistic LVMs are a special case of **DO-LVMs**, the training challenges they face persist in **DO-LVMs**, which also introduce new operator-theoretic difficulties. Maximizing the log-likelihood of a **DO-LVM** involves operators that do not commute [13]. The direct computation of gradient in Equation (LP) is significantly complicated by the partial trace [30]. Due to the difficulty of working with hidden units, recent work on QBMs have focused on models without hidden units [31, 14, 32, 33]. Demidik et al. [34] studied a Restricted QBM with 12 visible units and 90 hidden units, the largest model studied in literature so far. Refer Appendix B for a detailed survey on QBM literature. Hence, training a QBM, the most popular **DO-LVM** in literature, on real-world data *remains an open challenge*.

Intractability of the gradient of the log-likelihood in probabilistic LVMs is addressed by the EM algorithm. Classical derivations of the EM algorithm fail with density operators since there is no well-defined way to construct conditional density operators [23]. An EM algorithm for density operators using Conditional Amplitude Operators (CAO) was conjectured in Warmuth and Kuzmin [35]. This is insufficient since the CAO does not provide a density operator [29]. In the next section, we appeal to well-known results in quantum information theory to derive an ELBO and EM algorithm for density operators.

4 The DO-EM framework

In this section, we develop an algorithmic framework applicable for learning **DO-LVMs** using a density operator expectation maximization framework.

The classical ELBO is derived for each datapoint using conditional probability and Jensen's inequality. This approach fails for density operators due to the absence well-defined quantum conditional probability [23]. In order to derive an ELBO for **DO-LVMs**, we resort to an approach inspired by the chain rule of KL-divergence [36].

Lemma 4.1 (Quantum ELBO). Let $\mathcal{J}(\eta_V) = \{\eta \mid \eta \in \mathcal{P}(\mathcal{H}_V \otimes \mathcal{H}_L) \ \& \ \text{Tr}_L \eta = \eta_V\}$ be the set of feasible extensions for a target $\eta_V \in \mathcal{P}(\mathcal{H}_V)$. Then for a **DO-LVM** $\rho(\theta)$ and $\eta \in \mathcal{J}(\eta_V)$,

$$\mathcal{L}(\theta) \geq \text{QELBO}(\eta, \theta) = \text{Tr}(\eta \log \rho(\theta)) + S(\eta) - S(\eta_V). \quad (\text{QELBO})$$

Proof sketch: We provide a proof due to Theorem 2.2 in Appendix C.

The classical EM algorithm is a consequence of the ELBO being a minorant of the log-likelihood [37, 38]. However, it is well known that Theorem 2.2 is often not saturated [39–43]. Inspired by an information geometric interpretation of the EM algorithm [44], we study an instance of a quantum information projection problem to saturate QELBO.

4.1 A quantum information projection problem

In this subsection we study the I -projection [36] problem for density operators and show conditions when (PRM) can solve this problem. The problem of Quantum Information Projection (QIP) is stated as follows. Consider a density operator ω in $\mathcal{P}(\mathcal{H}_A)$ and a density operator ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$, find ξ^* in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that

$$\xi^* = \underset{\text{Tr}_B(\xi)=\omega}{\text{argmin}} D_U(\xi, \rho). \quad (\text{QIP})$$

To the best of our knowledge, this problem has not been studied in literature. We know from Theorem 2.2 that the theoretical minimum attained by the objective function in QIP is $D_U(\omega, \text{Tr}_B \rho)$ though it is not always saturated. Inspired by this connection, we explore sufficiency conditions for when PRM solves QIP.

Definition 4.2 (Condition S). Two density operators ω in $\mathcal{P}(\mathcal{H}_A)$ and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ satisfy the sufficiency condition if ρ is full rank, separable, and $[\omega, \text{Tr}_B(\rho)] = 0$ such that $\rho = \sum_{i=1}^{d_A} \alpha_i \mathbf{x}_i \mathbf{x}_i^\dagger \otimes \rho_B^{(i)}$ where $\{\mathbf{x}_i\}_{i=1}^{d_A}$ is an orthonormal basis of \mathcal{H}_A and $\rho_B^{(i)} \in \mathcal{P}(\mathcal{H}_B)$.

Theorem 4.3. Suppose two density operators ω in $\mathcal{P}(\mathcal{H}_A)$ and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that **Condition S** is satisfied, the solution to the information projection problem QIP is PRM.

Proof sketch: The statement holds due to the fact that $[\rho, \mathcal{R}_\rho(\omega)] = 0$ under the conditions in the theorem. Thus, ρ and $\mathcal{R}_\rho(\omega)$ obey Ruskai’s condition. A detailed proof is provided Appendix C.

4.2 DO-EM through the lens of Minorant Maximization

In this section, we present the **Density Operator Expectation Maximization (DO-EM)** algorithm from a Minorant-Maximization perspective and discuss its advantages over direct maximization of the log-likelihood. We prove that the **DO-EM** algorithm can achieve log-likelihood ascent at every iteration under **Condition S**.

For a fixed $\theta^{(\text{old})}$, the QELBO is maximized when η is the QIP of $\rho(\theta)$ onto the set of feasible extensions. This allows us to define a potential minorant \mathcal{Q} for the log-likelihood.

$$\begin{aligned} \eta(\theta^{(\text{old})}) &= \underset{\text{Tr}_L \eta = \eta_V}{\text{argmin}} D_U(\eta, \rho(\theta^{(\text{old})})) \\ \mathcal{Q}(\theta; \theta^{(\text{old})}) &= \text{QELBO}(\eta(\theta^{(\text{old})}), \rho(\theta)) \end{aligned}$$

Algorithm 1 DO-EM

- 1: **Input:** Target density operator η_V and $\theta^{(0)}$
 - 2: **while** not converged **do**
 - 3: **E Step:** $\eta^{(t)} = \underset{\eta: \text{Tr}_L \eta = \eta_V}{\text{argmin}} D_U(\eta, \rho(\theta^{(t)}))$
 - 4: **M Step:** $\theta^{(t+1)} = \underset{\theta}{\text{argmax}} \text{Tr}(\eta^{(t)} \log \rho(\theta))$
-

We use \mathcal{Q} to define the **DO-EM** algorithm in Algorithm 1. Models and QIPs that obey Ruskai’s condition provably achieve log-likelihood ascent under the **DO-EM** procedure.

Theorem 4.4 (\mathcal{Q} is a minorant). Let η_V be a target density matrix and $\rho(\theta)$ be a **DO-LVM** trained by the **DO-EM** algorithm. If $\rho(\theta^{(t)})$ and its QIP onto the set of feasible extensions, $\eta^{(t)}$, obey Ruskai’s condition, then \mathcal{Q} is a minorant of the log-likelihood. Then, $\mathcal{L}(\theta^{(t+1)}) \geq \mathcal{L}(\theta^{(t)})$, where $\theta^{(t+1)} = \underset{\theta}{\text{argmax}} \mathcal{Q}(\theta; \theta^{(t)})$.

Proof sketch: Proof using the saturation of Theorem 2.2 is in Appendix C.

Corollary 4.5. For a target density operator η_V and model $\rho(\theta)$ satisfying **Condition S**, the E step is the Petz recovery map $\mathcal{R}_\rho(\eta_V)$. Moreover, such a model trained using the **DO-EM** algorithm achieves provable likelihood ascent at every iteration.

Proof sketch: The proof due to Theorem 4.3 and Theorem 4.4 is given in Appendix C.

The **DO-EM** algorithm can be considered a density operator analog of the classical EM algorithm. We recover the classical EM algorithm from **DO-EM** for discrete models if η_V and $\rho(\theta)$ are diagonal.

The **E Step** in **DO-EM** finds a feasible extension η whose Conditional Amplitude Operator (CAO) is equal to that of the model $\rho(\theta)$. The PRM under **Condition S** is the CAO reweighted by η_V to give a valid density operator. This reduces to classical E step when the CAO reduces to the conditional probability and PRM reduces to Bayes rule. If the model ρ is of the form $\rho_V \otimes \rho_L$, we recover the conjecture in [35].

A log-likelihood involving a partial trace is often intractable. The **M Step** in **DO-EM** algorithm maximizes an expression without the partial trace. The log-likelihood of such expressions may have closed-form expressions for the gradients, for example, using the Lee-Trotter-Suzuki formula [14]. In the classical case, this is equivalent to the EM algorithm maximizing a sum of logarithms instead of a logarithm of sums.

Corollary 4.6. *For a Hamiltonian-based model with E step solution $\eta^{(t)}$, the M step reduces to*

$$\theta^{(t+1)} = \operatorname{argmax}_{\theta} \operatorname{Tr}(\eta^{(t)} H(\theta)) - \log Z(\theta)$$

Proof sketch: The proof due to properties of the matrix logarithm is given in Appendix C.

However, the memory footprint of **DO-LVMs** remain, preventing the application of these models on real-world data. We specialize **DO-LVMs** and **DO-EM** to train on classical data and achieve practical scale.

5 DO-EM for classical data

In this section, we specialize **DO-LVMs** and the **DO-EM** algorithm to classical datasets. We assume, for ease of presentation, that the data $\mathcal{D} = \{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(N)}\}$ is sampled from the set $\mathcal{B} = \{+1, -1\}^{d_V}$. We consider a 2^{d_V} -dimensional Hilbert space \mathcal{H}_V with standard basis $\mathfrak{B} = \{\mathbf{v}_i\}_{i=1}^{2^{d_V}}$. There is a one-to-one mapping between elements of \mathcal{B} and \mathfrak{B} . For any dataset \mathcal{D} , there is an equivalent dataset on \mathcal{H}_V given by $\mathfrak{D} = \{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(N)}\}$. The target density operator is then $\eta_V = \frac{1}{N} \sum_{i=1}^N \mathbf{v}_i \mathbf{v}_i^\dagger$. A **DO-LVM** on d_V -dimensional binary data is therefore a $2^{d_V+d_L} \times 2^{d_V+d_L}$ matrix while the target η_V is a $2^{d_V} \times 2^{d_V}$ matrix.

Specializing **Condition S** to diagonal target density operators, allows the decomposition of a **DO-LVM** into direct sums of smaller subspaces, making the **DO-EM** algorithm computationally easier.

Theorem 5.1. *If ρ_V is diagonal, ρ satisfies **Condition S** if and only if $\rho = \oplus_i \rho_L(i)$ and $P(\mathbf{v}_i) = \operatorname{Tr}(\rho_L(i))$ with $\mathbf{v}_i \in \mathfrak{B}$. The density operator for \mathcal{H}_L for a particular \mathbf{v}_i is then given by $\frac{1}{P(\mathbf{v}_i)} \rho_L(i)$.*

Proof sketch: See Appendix C.

We call models that obey Theorem 5.1 as **CQ-LVMs** since it implies a classical visible probability distribution with a quantum hidden space. QELBO can be specialized to each data point for **CQ-LVMs**.

Lemma 5.2. *For diagonal η_V in $\mathcal{P}(\mathcal{H}_V)$, a **DO-LVM** $\rho(\theta)$ satisfies **Condition S** if and only if it is of the form in Theorem 5.1. The log-likelihood of these models can then expressed as $\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \ell_i(\theta)$ where $\ell_i(\theta) = \log P(\mathbf{v}^{(i)} | \theta)$.*

Proof sketch: The proof is an application of Theorem 5.1 and is given in Appendix C.

The decomposition of the log-likelihood into terms for each datapoint, allows the training of models on real-world data since the target density operator η_V does not have to be initialized. We now show that **CQ-LVMs** are a broad class of models that include several Hamiltonian-based models.

Corollary 5.3. *A Hamiltonian-based model $\rho(\theta) = e^{H(\theta)} / Z(\theta)$ with $H(\theta) = \sum_r \theta_r H_r$ is a **CQ-LVMs** if and only if $H = \oplus_i H_i$ where H_i are Hermitian operators in $\mathcal{L}(\mathcal{H}_L)$ and $i \in [2^{d_V}]$.*

Proof sketch: The proof, due to the properties block diagonal matrices, is given in Appendix C.

We now specialize QELBO and Algorithm 1 to **CQ-LVMs**.

Lemma 5.4. For diagonal η_V in $\mathcal{P}(\mathcal{H}_V)$ and a **CQ-LVM** $\rho(\theta)$, the log-likelihood of a data point $\mathbf{v}^{(i)} \in \mathcal{D}$, $\ell_i(\theta)$ is lower bounded by

$$\ell_i(\theta) \geq \text{Tr} \left(\eta_L \log(P(\mathbf{v}^{(i)}|\theta)\rho_L^{(i)}(\theta)) \right) - \text{Tr}(\sigma_L \log \sigma_L)$$

for any density operator η_L in $\mathcal{P}(\mathcal{H}_L)$ with equality if and only if $\eta_L = \rho_L^{(i)}(\theta)$. Hence, the PRM is given by $\mathcal{R}_\rho(\eta_V) = \oplus_i P_{\mathcal{D}}(V = v_i)\rho_L(i|\theta)$.

Proof sketch: Application of Lemma 5.4 to Lemma 4.1. Proof is given in Appendix C.

This allows us to specialize Algorithm 1 to Algorithm 2, enabling the implementation of **DO-EM** without being restricted by the dimension of η_V . However, models such as the QBM remain intractable for real-world data due to the normalization term, a problem that exists in classical Boltzmann machines as well.

Algorithm 2 DO-EM for CQ-LVM

- 1: **Input:** Data and $\theta^{(0)}$
 - 2: **while** not converged **do**
 - 3: $\mathcal{Q}_i(\theta; \theta^{(k)}) = \text{Tr} \left(\rho_L^{(i)}(\theta^{(k)}) e^{H^{(i)}(\theta)} \right) - \log Z(\theta)$
 - 4: $\theta^{(t+1)} = \text{argmax}_\theta \frac{1}{N} \sum_{i=1}^N \mathcal{Q}_i(\theta; \theta^{(k)})$
-

5.1 Quantum Boltzmann Machine

In this section, we discuss the QBM and define variants which are amenable to implementation on high-dimensional classical data. We first describe QBMs that are **CQ-LVMs**.

Corollary 5.5. A $\text{QBM}_{m,n}$ is a **CQ-LVM** if and only if quantum terms on the visible units are zero.

Proof sketch: The statement is true because of the structure of Pauli matrices which have entries outside the direct sum structure if and only if $i \leq m$. A detailed proof can be found in Appendix C.

The class of semi-quantum models studied in Demidik et al. [34] are **CQ-LVMs**. Training such a QBM is intractable for real-world data since the free energy term, $-\log Z(\theta)$ is intractable even for classical Boltzmann machines. To achieve tractable training of QBMs, we introduce the **Quantum Interleaved Deep Boltzmann Machine (QiDBM)** that can be trained using Contrastive Divergence with a quantum Gibbs sampling step derived here.

A **Quantum Interleaved Deep Boltzmann Machine (QiDBM)** is a DBM with quantum bias terms on **non-contiguous hidden layers**. We describe the Hamiltonian of a three-layered $\text{QiDBM}_{\ell,m,n}$ with ℓ visible units and m and n hidden units respectively in the two hidden layers. For ease of presentation, the quantum bias terms are present in the middle layer.

$$H = - \sum_{i=1}^{\ell+m+n} b_i \sigma_i^z - \sum_{i=1}^{\ell} \sum_{j=1}^m w_{ij}^{(1)} \sigma_i^z \sigma_{\ell+j}^z - \sum_{i=1}^m \sum_{j=1}^n w_{ij}^{(2)} \sigma_{\ell+i}^z \sigma_{\ell+m+j}^z - \sum_{i=1}^m \Gamma_i \sigma_{\ell+i}^x \quad (\text{QiDBM})$$

The quantum interleaving in a QiDBM is necessary to make the Gibbs sampling step tractable. We illustrate the case of the middle layer of $\text{QiDBM}_{\ell,m,n}$. If the non-quantum visible and hidden layers are fixed to \mathbf{v} and $\mathbf{h}^{(2)}$, the hidden units of the quantum layer are conditionally independent. The Hamiltonian of the i^{th} unit of the quantum layer $L^{(1)}$ is given by $H^{L^{(1)}}(i|\mathbf{v}, \mathbf{h}^{(2)}, \theta) = -b_i^{\text{eff}} \sigma_i^z - \Gamma_i \sigma_i^x$. This allows for the tractable sampling from the quantum layer using the expected values

$$\langle \sigma_i^z \rangle_{\mathbf{v}, \mathbf{h}^{(2)}} = \frac{b_i^{\text{eff}}}{D_i} \tanh D_i \text{ and } \langle \sigma_i^x \rangle_{\mathbf{v}, \mathbf{h}^{(2)}} = \frac{\Gamma_i}{D_i} \tanh D_i$$

where $D_i = \sqrt{(b_i^{\text{eff}})^2 + \Gamma_i^2}$ and $b_i^{\text{eff}} = b_i + \sum_{j=1}^{\ell} w_{ij}^{(1)} \mathbf{v}_j + \sum_{j=1}^n w_{ij}^{(2)} \mathbf{h}_j^{(2)}$. The Gibbs step for the non-quantum layers is done as per the classical CD algorithm using the quantum sample from the Z Pauli operator. This closed-form expression for Gibbs sampling without matrices allows CD to run on a QiDBM with the same memory footprint as a DBM. See Appendix C for more details.

6 Empirical evaluation

In this work, we propose a quantum model **CQ-LVM**, and a general EM framework, **DO-EM**, to learn them. In this section, we empirically evaluate our methods through experiments to answer the following questions. Details of the compute used to run all our experiments and baselines are provided in Appendices D and E.

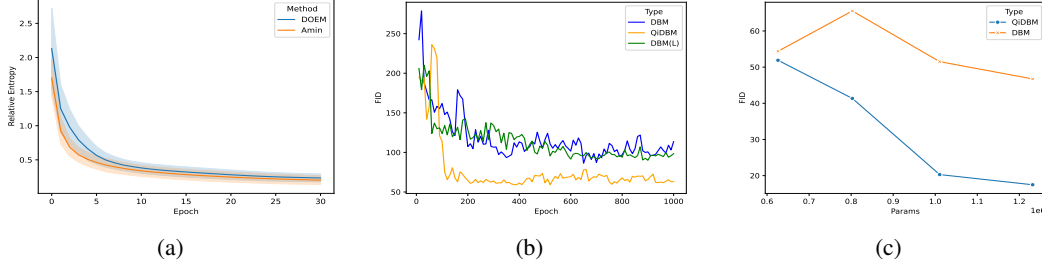


Figure 1: (a) Relative entropy during training with exact computation of a QBM on a mixture of Bernoulli distribution. Showing that DO-EM does lead to decrease in relative entropy. (b) DBM with 6272 hidden units. QiDBM with 6273 hidden units. DBM(L) with 6273 hidden units. (c) FID scores on Binarized MNIST as a function of model parameters of QiDBM and DBM.

- (Q1) **Effectiveness of DO-EM.** Is Algorithm 2, a feasible algorithm for **CQ-LVMs** compared to state of the art algorithms for QBMs ?
- (Q2) **DO-EM on Real World Data.** Does Algorithm 2 scale with the to real world data?
- (Q3) **Performance of DO-EM.** Does Algorithm 2 provide reasonable improvement in performance over classical LVMs?

To answer (Q1), we conduct experiments running exact computation to show that the proposed algorithm is feasible and is practical to implement.

Baselines We compare our method with our implementation of Amin et al. [12] which explores an alternate algorithm for training QBMs.

Dataset and Metrics We use a mixture of Bernoulli dataset introduced in Amin et al. [12] described in Appendix D. We measure the efficacy of our proposed method by measuring the average relative entropy during training.

Results of experiment In Figure 1a, we first observe that the relative entropy of our proposed algorithm does decrease during training, validating our theoretical results and showing, to the best of our knowledge, the first instance of an expectation maximization algorithm with quantum bias. We also observe that the performance is competitive with Amin et al. [12]. We also note that **CQ-LVM** training with DO-EM is faster than Amin et al. [12] and consumes lesser memory.

To answer (Q2) and (Q3), we conduct experiments on DBMs of varying sizes with and without the quantum bias term described in Section 5. We present qualitative results of our experiments in Appendix D.

Baselines. We compare our proposed method with Taniguchi et al. [22], the state of the art for training DBMs. We are unable to reproduce the results in their work and we report the results obtained from their official implementation¹ using the hyper parameters described in their work.

Datasets and Metrics Following prior work [22], we perform our experiments on MNIST and Binarized MNIST dataset [45] which contains 60,000 training images and 10,000 testing images of size 28x28. We measure the FID [46] between 10,000 generated images and the MNIST test set to assess the quality of generation. The Fréchet Inception Distance (FID) is a quantitative metric used to evaluate the quality of images generated by generative models by comparing the statistical distribution of their feature representations to those of real images.

Experiment: Performance of DO-EM To show the superior performance of the proposed method, we compare the FID of our proposed algorithm on Binarized MNIST. We train a QiDBM and DBM with 498, 588, 686, and 784 hidden units with a learning rate of 0.001 for 100 epochs with 2 hidden layers with SGD optimizer with a batch size of 600.

Results of Experiments In Figure 1c, we observe that the proposed algorithm outperforms the DBM in all cases, achieving a minimum FID of 14.77 to the DBM’s 42.61. This experiment shows that simply adding quantum bias terms to a DBM can *improve the quality* of generations by around 65%.

¹https://github.com/iShohei220/unbiased_dbm

Experiment: DO-EM on High Dimensional Data We run CD on 2 DBMs without quantum bias terms according to Taniguchi et al. [22] and CD with quantum bias for a QiDBM on MNIST. Each image corresponds to 6272 visible binary units. The QiDBM has 78.70M parameters with 2 hidden layers with quantum bias added to the second layer with a hidden size of 6272. Both DBMs have 2 hidden layers and have 78.69M and 78.71M parameters and hidden sizes of 6272 and 6273 respectively. We use a learning rate of 0.001 for all experiments and train with a batch size of 600 with SGD optimizer for 1000 epochs. The purpose of this experiment is to show that it is feasible to train large models with quantum bias terms.

Results of Experiments In Figure 1b, we observe that the proposed method outperforms both classical models of similar size with a 45% reduction in FID. We observe that the FID of the model converges to this value in around 400 epochs whereas both DBM models still exhibit instability after 500 epochs. The QiDBM achieves an FID of 62.77 whereas the classical DBMs achieve an FID of 111.73 and 99.17 for the smaller and larger model respectively. This experiment indicates that scaling QiDBMs is feasible and provides a significant improvement in performance. In Appendix D, we show the qualitative differences between generated samples of the DBM and QiDBM. We observe that the generated samples from the QiDBM appear to be better than that of the DBM after only 250 epochs.

Discussion We design **CQ-LVMs** and implement Algorithm 1 to learn different target distributions. We first show that Algorithm 1 is effective in learning **CQ-LVMs** and is competitive with the state of the art in terms of reduction of relative entropy at lower running times for 10 qubits and can be extended to even 20 qubits where others cannot. Next, we see that the addition of quantum bias terms to a DBM when trained using Algorithm 2 shows superior generation quality compared to classical DBMs with a 60% reduction of FID on Binarized MNIST. Next, we show that **QiDBMs** can learn high dimensional datasets like MNIST using Algorithm 2 by scaling models upto 6272 hidden units. We observe that QiDBMs also achieve better performance, with 40% lower FID compared to DBMs of similar sizes. We also observe that QiDBMs converge in about half the amount of time compared to DBMs.

7 Discussion

The paper makes important progress by proposing **DO-EM**, an EM Algorithm for Latent Variable models defined by Density Operators, which provably achieves likelihood ascent. We propose **CQ-LVM**, a large collection of density operator based models, where **DO-EM** applies. We show that QiDBM, an instance of **CQ-LVM**, can easily scale to MNIST dataset which requires working with 6200+ units and outperform DBMs, thus showing that Density Operator models may yield better performance. The specification of **DO-EM** is amenable to implementation on quantum devices.

DO-EM on quantum devices The E Step of the DO-EM algorithm can be implemented on a quantum computer using the method developed by Gilyén et al. [47], where the quantum channel is performing the partial trace operation. The goal is to prepare the Petz recovery map for the partial trace channel $\eta^{(t)} = \mathcal{R}_\rho(\eta_V)$ using PRM. The requirements for this are (1) Quantum access to the input state η_V (2) efficient state preparation of the model’s density matrix $\rho(\theta)$ [48, 49] and (3) Block-encodings for the model’s density matrix and its marginal $\rho_V(\theta) = \text{Tr}_L \rho(\theta)$ [50]. Given these input assumptions, the quantum algorithm implementing PRM consists of three steps [47]: (1) applying $\rho_V^{-1/2}$ on the state η_V , (2) applying the adjoint channel which is straight-forward for the partial trace channel and can be operationally achieved by preparing subsystem L in the maximally mixed state, and (3) applying $\rho^{1/2}$ on the combined system. Both $\rho_V^{-1/2}$ and $\rho^{1/2}$ are implemented using *Quantum Singular Value Transformation (QSVT)* techniques, leveraging block-encodings of the relevant states [50].

The M Step proceeds via gradient descent by the computation of the gradient given by $(\text{Tr}[H_r \eta(\theta^{(t)})] - \text{Tr}[H_r \rho(\theta)])$ for the different terms in the Hamiltonian $H = \sum_r \theta_r H_r$ [14, 33]. The M Step stops when the gradients are small and an updated parameter $\theta^{(t+1)}$ is obtained. This two-step iterative DO-EM procedure continues until convergence. While the gradients can be estimated on existing near-term quantum devices, the E step requires careful design.

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Appendix

In this appendix, we provide the following material.

- In Appendix A, we discuss Boltzmann machines and the Contrastive Divergence algorithm.
- In Appendix B, we provided a discussion on density operators, quantum channels, and related work in training density operator models.
- In Appendix C, we provide the proofs of the theoretical results proposed in the main body.
- In Appendix D, we provide implementation details and additional experiments with the **DO-EM** algorithm.
- In Appendix E, we discuss the computational setup used in our experiments.
- In Appendix F, we discuss the limitations of this work.

A Boltzmann machines

The *Contrastive Divergence* (CD) [18, 19] algorithm samples the hidden state for a data point through an iterative sampling scheme to efficiently compute the parameters to model a target distribution by approximating the gradient of the log-likelihood. Building on recent advances in the contrastive divergence method [51], DBMs trained using CD was studied in Taniguchi et al. [22]. We describe the CD Algorithm for a Restricted Boltzmann Machine (RBM), a special case of a DBM with a single layer. Formally, an $\text{RBM}_{m,n}$ is a single layer DBM consisting of a visible layer $\mathbf{v} \in \{0, 1\}^m$ and a hidden layer $\mathbf{h} \in \{0, 1\}^n$, parameterized by weight matrix $\mathbf{W} \in \mathbb{R}^{m \times n}$, bias vectors $\mathbf{a} \in \mathbb{R}^m$ (visible) and $\mathbf{b} \in \mathbb{R}^n$ (hidden). The energy function is given by $E(\mathbf{v}, \mathbf{h}) = -\mathbf{v}^\top \mathbf{W} \mathbf{h} - \mathbf{a}^\top \mathbf{v} - \mathbf{b}^\top \mathbf{h}$. At the t^{th} time step with parameters $\mathbf{W}^{(t)}, \mathbf{a}^{(t)}, \mathbf{b}^{(t)}$, K iterations of sampling is used to sample visible and hidden units. Formally,

$$\begin{aligned} h_j^{(k)} &\sim P(h_j = 1 \mid \mathbf{v}^{(k)}) = \sigma \left(\sum_i W_{ij}^{(t)} v_i^{(k)} + b_j^{(t)} \right) \\ v_i^{(k+1)} &\sim P(v_i = 1 \mid \mathbf{h}^{(k)}) = \sigma \left(\sum_j W_{ij}^{(t)} h_j^{(k)} + a_i^{(t)} \right) \end{aligned}$$

where $\sigma(x) = \frac{1}{1+e^{-x}}$ is the sigmoid function and $\mathbf{v}^{(0)} = \mathbf{v}$ and $k \in [K]$. The parameter updates at the t^{th} step, with learning rate γ is then,

$$\begin{aligned} W_{ij}^{(t+1)} &= W_{ij}^{(t)} + \gamma \left(v_i h_j^{(0)} - v_i^{(K)} h_j^{(K)} \right) \\ a_i^{(t+1)} &= a_i^{(t)} + \gamma \left(v_i - v_i^{(K)} \right) \\ b_j^{(t+1)} &= b_j^{(t)} + \gamma \left(h_j^{(0)} - h_j^{(K)} \right). \end{aligned}$$

B Density operators

Current research explores leveraging quantum mechanics for machine learning either by achieving computational speedups with quantum hardware [52–55], or by capturing more complex data structures through quantum formalisms [56, 57]. The use of density operators, quantum generalizations of classical probability distributions, to model data represents an effort in the latter direction.

A density operator on a Hilbert space \mathcal{H} is a Hermitian, positive semi-definite operator with unit trace [2, 23]. The set of Density operators will be denoted by $\mathcal{P}(\mathcal{H})$, and can be regarded as generalizations of probability distributions. We now define quantum channels that act on density operators.

Let $\mathcal{S}(\mathcal{H})$ denote the set of square linear operators on a finite dimensional Hilbert space \mathcal{H} . A linear map $\mathcal{N} : \mathcal{S}(\mathcal{H}_A) \rightarrow \mathcal{S}(\mathcal{H}_B)$ is *positive* if $\mathcal{N}(X)$ is positive semi-definite for all positive semi-definite operators X in $\mathcal{S}(\mathcal{H})$. Such a map is *completely positive* if $\mathbf{I}_R \otimes \mathcal{N}$ is a positive map for an arbitrary reference system R . A map is *trace preserving* if $\text{Tr}(\mathcal{N}(X)) = \text{Tr}(X)$.

Definition B.1 (Quantum Channel). A quantum channel $\mathcal{N} : \mathcal{S}(\mathcal{H}_A) \rightarrow (\mathcal{H}_B)$ is a linear, completely positive, trace preserving map.

We now define an inner product on operators.

Definition B.2 (Hilbert-Schmidt Inner Product). The Hilbert-Schmidt Inner Product between two operators X, Y in $\mathcal{S}(\mathcal{H})$ is defined as $\langle X, Y \rangle = \text{Tr}(X^\dagger Y)$.

The inner product allows us to define the adjoint of a quantum channel.

Definition B.3. The *adjoint* of a quantum channel $\mathcal{N} : \mathcal{S}(\mathcal{H}_A) \rightarrow (\mathcal{H}_B)$ is the unique linear map $\mathcal{N}^\dagger : \mathcal{S}(\mathcal{H}_B) \rightarrow (\mathcal{H}_A)$ satisfying $\langle Y, \mathcal{N}(X) \rangle = \langle \mathcal{N}^\dagger(Y), X \rangle$ for all X in $\mathcal{S}(\mathcal{H}_A)$ and Y in $\mathcal{S}(\mathcal{H}_B)$.

Lindblad [25] showed that the relative entropy is monotonic under the action of a quantum channel.

Theorem B.4 (Monotonicity of Relative Entropy). *For density operators ω and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that $\ker(\omega) \subset \ker(\rho)$, $D_U(\omega, \rho) \geq D_U(\mathcal{N}(\omega), \mathcal{N}(\rho))$.*

Petz [26, 27] showed that MRE is saturated if and only if the Petz Recovery Map reverses the quantum channel. We provide a resatement of this result from Hayden et al. [58].

Theorem B.5. *For states ω and ρ , $D_U(\omega, \rho) = D_U(\mathcal{N}(\omega), \mathcal{N}(\rho))$ if and only if there exists a quantum channel \mathcal{R} such that $\mathcal{R}(\mathcal{N}(\omega)) = \omega$ and $\mathcal{R}(\mathcal{N}(\rho)) = \rho$. Furthermore, on the support of $\mathcal{N}(\rho)$, \mathcal{R} can be given explicitly by the formula*

$$\mathcal{R}(\alpha) = \rho^{1/2} \mathcal{N}^\dagger \left(\mathcal{N}(\rho)^{-1/2} \alpha \mathcal{N}(\rho)^{-1/2} \right) \rho^{1/2}.$$

This lead to the definition of the Petz Recovery Map.

Definition B.6 (Petz Recovery Map). For a density operator ρ in $\mathcal{P}(\mathcal{H}_A)$, the Petz Recovery Map for a quantum channel $\mathcal{N} : \mathcal{S}(\mathcal{H}_A) \rightarrow \mathcal{S}(\mathcal{H}_B)$ is the map $\mathcal{R}_{\mathcal{N}, \rho} : \mathcal{H}_B \rightarrow \mathcal{H}_A$ defined by

$$\mathcal{R}_{\mathcal{N}, \rho}(\alpha) = \rho^{1/2} \mathcal{N}^\dagger \left(\mathcal{N}(\rho)^{-1/2} \alpha \mathcal{N}(\rho)^{-1/2} \right) \rho^{1/2}.$$

The Petz Recovery Map is a completely positive, trace non-increasing map [23] that does not always map density operators to density operators. Ruskai [28] proved an equivalent condition for the saturation of MRE.

Theorem B.7 (Ruskai's condition). *For density operators ω and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that $\ker(\omega) \subset \ker(\rho)$, $D_U(\mathcal{N}(\omega), \mathcal{N}(\rho)) = D_U(\omega, \rho)$ if and only if $\log \omega - \log \rho = \mathcal{N}^\dagger(\mathcal{N}(\omega) - \mathcal{N}(\rho))$.*

In this work, we focus on the quantum channel defined by the partial trace operation $\mathcal{N}(\rho) = \text{Tr}_B \rho$ and its adjoint $\mathcal{N}^\dagger(\rho_A) = \rho_A \otimes \mathbb{I}_B$. All our results are specialized to this case.

B.1 Related work on Density Operator Models

Most recent works on density operator models (**DOMs**) consider settings without hidden units [14, 32, 59, 31] due to operator-theoretic difficulties brought about by the partial trace operation during gradient evaluation [30]. Other studies considered hidden variable **DOMs**, where the gradient evaluation was accomplished using heuristic methods [12, 60, 61]. As such, these methods rely on the approximate (variational) preparation of the quantum Gibbs state density matrix [48, 49, 62]. Sampling from a Gibbs state distribution can also be performed using a quantum annealer, which may offer advantages even for classical machine learning models [12, 63–65].

These existing approaches rarely scale beyond 12 visible units—limited by restricted access to quantum hardware, the exponential cost of simulating quantum systems, and the memory bottlenecks associated with representing and optimizing **DO-LVMs** on classical devices. EM based algorithms can provide a simpler alternative to existing learning algorithms for **DO-LVMs** which directly maximizes the likelihood. However deriving such algorithms in the density operator theoretic setup is extremely challenging for a variety of reasons. *Most notably operator theoretic analogues of classical inequalities, such as the Jensen Inequality, cannot be directly applied to derive an Evidence lower bound (ELBO) for DO-LVMs.*

C Proofs

Proof of Lemma 4.1

Lemma (Quantum ELBO). *Let $\mathcal{J}(\eta_v) = \{\eta \mid \eta \in \mathcal{P}(\mathcal{H}_V \otimes \mathcal{H}_L) \text{ \& } \text{Tr}_L \eta = \eta_v\}$ be the set of feasible extensions for a target $\eta_v \in \mathcal{P}(\mathcal{H}_V)$. Then for a **DO-LVM** $\rho(\theta)$ and $\eta \in \mathcal{J}(\eta_v)$,*

$$\mathcal{L}(\theta) \geq \text{QELBO}(\eta, \theta) = \text{Tr}(\eta \log \rho(\theta)) + S(\eta) - S(\eta_v).$$

Proof. Since $\eta \in \mathcal{J}(\eta_v)$, $\text{Tr}_L(\eta) = \eta_v$ and $\text{Tr}_L \rho(\theta) = \rho_v(\theta)$. From MRE,

$$\begin{aligned} D_U(\eta, \rho(\theta)) &\geq D_U(\eta_v, \rho_v(\theta)), \\ \text{Tr}(\eta \log \eta) - \text{Tr}(\eta \log \rho(\theta)) &\geq \text{Tr}(\eta_v \log \eta_v) - \text{Tr}(\eta_v \log \rho_v(\theta)), \\ \text{Tr}(\eta_v \log \rho_v(\theta)) &\geq \text{Tr}(\eta \log \rho(\theta)) - \text{Tr}(\eta \log \eta) + \text{Tr}(\eta_v \log \eta_v), \\ \mathcal{L}(\theta) &\geq \text{Tr}(\eta \log \rho(\theta)) + S(\eta) - S(\eta_v). \end{aligned}$$

□

This proof reduces to a proof of the classical ELBO from the chain rule of KL divergence [36] when $\rho(\theta)$ is diagonal.

Proof of Theorem 4.3

We first prove a useful lemma.

Lemma C.1. *The Petz recovery map with respect to a quantum channel \mathcal{N} and density operator ρ is trace preserving if ρ is full rank.*

Proof. This statement is a consequence of the cyclic property of trace and the definition of the adjoint CPTP map \mathcal{N}^\dagger .

$$\begin{aligned} \text{Tr}(\mathcal{P}_{\rho, \mathcal{N}}(\omega)) &= \text{Tr}(\rho^{1/2} \mathcal{N}^\dagger(\mathcal{N}(\rho)^{-1/2} \omega \mathcal{N}(\rho)^{-1/2}) \rho^{1/2}) \\ &= \text{Tr}(\rho \mathcal{N}^\dagger(\mathcal{N}(\rho)^{-1/2} \omega \mathcal{N}(\rho)^{-1/2})) \\ &= \text{Tr}(\mathcal{N}(\rho) \mathcal{N}(\rho)^{-1/2} \omega \mathcal{N}(\rho)^{-1/2}) \\ &= \text{Tr}(\mathcal{N}(\rho)^{1/2} \mathcal{N}(\rho)^{-1/2} \omega \mathcal{N}(\rho)^{-1/2} \mathcal{N}(\rho)^{1/2}) \\ &= \text{Tr}(\mathbf{I} \omega \mathbf{I}) \\ &= \text{Tr}(\omega). \end{aligned}$$

□

This theorem requires ρ to be full rank for $\text{Tr}(\mathcal{N}(\rho)^{1/2} \mathcal{N}(\rho)^{-1/2}) = \mathbf{I}$ since CPTP maps full rank matrices to full rank matrices. We now restate **Condition S** and Theorem 4.3.

Definition 1 (Condition S). Two density operators ω in $\mathcal{P}(\mathcal{H}_A)$ and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ satisfy the sufficiency condition if ρ is full rank, separable, and $[\omega, \text{Tr}_B(\rho)] = 0$ such that

$$\rho = \sum_{i=1}^{d_A} \alpha_i \mathbf{x}_i \mathbf{x}_i^\dagger \otimes \rho_B^{(i)}$$

where $\{\mathbf{x}_i\}_{i=1}^{d_A}$ is an orthonormal basis of \mathcal{H}_A and $\rho_B^{(i)} \in \mathcal{P}(\mathcal{H}_B)$.

Theorem. *Suppose two density operators ω in $\mathcal{P}(\mathcal{H}_A)$ and ρ in $\mathcal{P}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that **Condition S** is satisfied, the solution to the information projection problem QIP is PRM.*

Proof. Since ρ is full rank, the Petz recovery map gives a valid density operator by Lemma C.1. Moreover, **Condition S** guarantees that $[\rho, \rho_A \otimes \mathbf{I}_B] = 0$ and that $\text{Tr}_B \mathcal{R}_{\rho, \text{Tr}_L}(\omega) = \omega$.

As mentioned in the main body of the paper, we prove this theorem by showing that the Petz recovery map commutes with ρ . Since $[\omega, \text{Tr}_B(\rho)] = 0$ and $[\rho, \text{Tr}_B(\rho) \otimes \mathbf{I}_B] = 0$, we know that

$[\rho, \omega \otimes \mathbf{I}_B] = 0$. Note that if two matrices commute, their squareroots also commute because they share the same eigenspace. Since the Petz recovery map with respect to ρ and Tr_B is equal to

$$\mathcal{P}_{\rho, \text{Tr}_B}(\tilde{\sigma}) = \rho^{1/2}((\text{Tr}_B(\rho)^{-1/2} \omega \text{Tr}_B(\rho)^{-1/2}) \otimes \mathbf{I}_B) \rho^{1/2},$$

we know that $[\mathcal{P}_{\rho, \text{Tr}_B}(\omega), \rho] = 0$.

We now show that the Petz recovery map and ρ satisfy the Ruskai condition.

$$\begin{aligned} \log \rho - \log \mathcal{R}_{\rho, \text{Tr}_B}(\omega) &= \log \rho - \log(\rho^{1/2}((\text{Tr}_B(\rho)^{-1/2} \omega \text{Tr}_B(\rho)^{-1/2}) \otimes \mathbf{I}_B) \rho^{1/2}) \\ &= \log \rho - \log(\rho((\text{Tr}_B(\rho)^{-1} \omega) \otimes \mathbf{I}_B)) \\ &= \log \rho - \log \rho - \log(\text{Tr}_B(\rho)^{-1} \omega \otimes \mathbf{I}_B) \\ &= \log(\text{Tr}_B(\rho) \otimes \mathbf{I}_B) - \log(\omega \otimes \mathbf{I}_B) \\ &= (\log(\text{Tr}_B(\rho)) - \log(\omega)) \otimes \mathbf{I}_B. \end{aligned}$$

Hence, PRM attains the minimum possible value in the QIP problem and is the information projection of ρ on to the set of density operators that partial trace to ω . \square

Proof of Theorem 4.4

Theorem (\mathcal{Q} is a minorant). *Let η_v be a target density matrix and $\rho(\theta)$ be a **DO-LVM** trained by the **DO-EM** algorithm. If $\rho(\theta^{(t)})$ and its QIP onto the set of feasible extensions, $\eta^{(t)}$, obey Ruskai's condition, then \mathcal{Q} is a minorant of the log-likelihood. Then, $\mathcal{L}(\theta^{(t+1)}) \geq \mathcal{L}(\theta^{(t)})$, where $\theta^{(t+1)} = \arg\max_{\theta} \mathcal{Q}(\theta; \theta^{(t)})$.*

Proof. From the Ruskai condition, we obtain

$$\mathcal{L}(\theta^{(t)}) = \mathcal{Q}(\theta^{(t)}, \theta^{(t)}). \quad (1)$$

By the definition of $\theta^{(t+1)}$,

$$\mathcal{Q}(\theta^{(t)}, \theta^{(t)}) \leq \mathcal{Q}(\theta^{(t)}, \theta^{(t+1)}). \quad (2)$$

Combining these inequalities with the QELBO, we obtain

$$\begin{aligned} \mathcal{L}(\theta^{(t+1)}) &\geq \mathcal{Q}(\theta^{(t)}, \theta^{(t+1)}); \\ \mathcal{L}(\theta^{(t+1)}) &\geq \mathcal{Q}(\theta^{(t)}, \theta^{(t)}) \quad \text{by (2);} \\ \mathcal{L}(\theta^{(t+1)}) &\geq \mathcal{L}(\theta^{(t)}) \quad \text{by (1).} \end{aligned}$$

\square

Proof of Corollary 4.5

Corollary. *For a target density operator η_v and model $\rho(\theta)$ satisfying **Condition S**, the E step is the Petz recovery map $\mathcal{R}_{\rho}(\eta_v)$. Moreover, such a model trained using the **DO-EM** algorithm achieves provable likelihood ascent at every iteration.*

Proof. We proved in Theorem 4.3 that the Petz Recovery Map satisfies the Ruskai condition under **Condition S**. Hence, the statement is an immediate corollary to Theorem 4.4. \square

Proof of Corollary 4.6

Corollary. *For a Hamiltonian-based model with E step solution $\eta^{(t)}$, the M step reduces to*

$$\theta^{(t+1)} = \arg\max_{\theta} \text{Tr}(\eta^{(t)} \mathbf{H}(\theta)) - \log Z(\theta)$$

Proof. Let $\rho(\theta) = \frac{1}{Z(\theta)} e^{\mathbf{H}(\theta)}$ be a Hamiltonian-based model. For a Hermitian matrix A that is diagonalized as $A = U \Lambda U^\dagger$, the matrix logarithm can be expressed as $\log A = U \log(\Lambda) U^\dagger$.

Applying this to $\rho(\theta)$, we obtain

$$\begin{aligned}\log(\rho(\theta)) &= U \log \left(\frac{1}{Z(\theta)} \Lambda \right) U^\dagger \\ &= U \log(\Lambda) U^\dagger - \log(Z(\theta)) \mathbf{I} \\ &= \mathbf{H}(\theta) - \log(Z(\theta)) \mathbf{I}.\end{aligned}$$

The result follows since $\text{Tr}(\eta^{(t)} \log(Z(\theta)) \mathbf{I}) = \log(Z(\theta)) \text{Tr}(\eta^{(t)} \mathbf{I}) = \log(Z(\theta))$. \square

Proof of Theorem 5.1

Theorem. If ρ_V is diagonal, ρ satisfies **Condition S** if and only if $\rho = \oplus_i \rho_L(i)$ and $P(\mathbf{v}_i) = \text{Tr}(\rho_L(i))$ with $\mathbf{v}_i \in \mathfrak{B}$. The density operator for \mathcal{H}_L for a particular \mathbf{v}_i is then given by $\frac{1}{P(\mathbf{v}_i)} \rho_L(i)$.

Proof. Since ρ satisfies **Condition S**, we know that

$$\rho = \sum_{i=1}^{d_V} \alpha_i \mathbf{x}_i \mathbf{x}_i^\dagger \otimes \rho_L^{(i)}$$

where $\{\mathbf{x}_i\}_{i=1}^{d_V}$ is an orthonormal basis of \mathcal{H}_V and $\rho_L^{(i)} \in \mathcal{P}(\mathcal{H}_L)$. Since ρ_V is diagonal and $\rho_V = \sum_{i=1}^{d_V} \alpha_i \mathbf{x}_i \mathbf{x}_i^\dagger$, we conclude that $\{\mathbf{x}_i\}$ is the standard basis of \mathcal{H}_V ; each \mathbf{x}_i has a 1 at the i^{th} position and zeros elsewhere. Hence, $\rho = \oplus_i \rho_L(i)$. The matrices $\frac{1}{\text{Tr} \rho_L(i)} \rho_L(i)$ are valid conditional density operators since projecting the matrix ρ onto $\mathbf{x}_i \mathbf{x}_i^\dagger \otimes \mathbf{I}_L$ zeroes out all other components. \square

Proof of Lemma 5.2

Lemma. For diagonal η_V in $\mathcal{P}(\mathcal{H}_V)$, a **DO-LVM** $\rho(\theta)$ satisfies **Condition S** if and only if it is of the form in Theorem 5.1. The log-likelihood of these models can then be expressed as $\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \ell_i(\theta)$ where $\ell_i(\theta) = \log P(\mathbf{v}^{(i)} | \theta)$.

Proof. The log-likelihood is given by $\mathcal{L}(\theta) = \text{Tr}(\eta_V \log \rho_V(\theta))$. Since η_V is diagonal and $[\eta_V, \rho_V] = 0$, ρ_V is diagonal. Hence, Theorem 5.1 applies.

Since η_V and ρ_V are diagonal, we expand the log-likelihood into a sum across the dataset \mathfrak{D}

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \log P(\mathbf{v}^{(i)} | \theta)$$

giving the required expression. \square

Proof of Corollary 5.3

Corollary. A Hamiltonian-based model $\rho(\theta) = e^{\mathbf{H}(\theta)} / Z(\theta)$ with $\mathbf{H}(\theta) = \sum_r \theta_r \mathbf{H}_r$ is a **CQ-LVM** if and only if $\mathbf{H} = \oplus_i \mathbf{H}_i$ where \mathbf{H}_i are Hermitian operators in $\mathfrak{L}(\mathcal{H}_L)$ and $i \in [2^{d_V}]$.

Proof. The Taylor series of the matrix exponential is given by $e^X = \sum_{k=0}^{\infty} \frac{1}{k!} X^k$. Since \mathcal{H} is a block diagonal matrix, the powers of \mathcal{H} are also block diagonal. Therefore ρ is also a block diagonal matrix as required.

Similarly, the Taylor series of the matrix logarithm is given by $\log X = -\sum_{k=1}^{\infty} \frac{1}{k} (I - X)^k$. If $(\log Z)\rho = e^{\mathcal{H}}$ is a block diagonal matrix, then its logarithm \mathcal{H} is also a block diagonal matrix as required. \square

Proof of Lemma 5.4

Lemma. For diagonal η_V in $\mathcal{P}(\mathcal{H}_V)$ and a **CQ-LVM** $\rho(\theta)$, the log-likelihood of a data point $\mathbf{v}^{(i)} \in \mathfrak{D}$, $\ell_i(\theta)$ is lower bounded by

$$\ell_i(\theta) \geq \text{Tr} \left(\eta_L \log(P(\mathbf{v}^{(i)}|\theta) \rho_L^{(i)}(\theta)) \right) - \text{Tr}(\eta_L \log \eta_L)$$

for any density operator η_L in $\mathcal{P}(\mathcal{H}_L)$ with equality if and only if $\eta_L = \rho_L^{(i)}(\theta)$. Hence, the PRM is given by $\mathcal{R}_\rho(\eta_V) = \oplus_i P_{\mathcal{D}}(V = \mathbf{v}_i) \rho_L(i | \theta)$.

Proof. We first note that $\rho(\mathbf{v}|\theta)$ is full rank for all \mathbf{v} and θ . Let η_L be an arbitrary density operator on $\mathcal{P}(\mathcal{H}_L)$. The Umegaki relative entropy between two density operators is always non-negative when defined.

$$\begin{aligned} D_U(\eta_L, \rho(\mathbf{v}^{(i)}|\theta)) &\geq 0 \\ -S(\eta_L) - \text{Tr}(\eta_L \log(\rho(\mathbf{v}^{(i)}|\theta))) &\geq 0 \\ -\text{Tr} \left(\eta_L \log \left(\frac{P(\mathbf{v}^{(i)}|\theta)}{P(\mathbf{v}^{(i)}|\theta)} \rho(\mathbf{v}^{(i)}|\theta) \right) \right) &\geq S(\eta_L) \\ \text{Tr} \left(\log \left(P(\mathbf{v}^{(i)}|\theta) \right) I_L \right) - \text{Tr} \left(\eta_L \log \left(P(\mathbf{v}^{(i)}|\theta) \rho(\mathbf{v}^{(i)}|\theta) \right) \right) &\geq S(\eta_L) \\ \log \left(P(\mathbf{v}^{(i)}|\theta) \right) &\geq \text{Tr} \left(\eta_L \log \left(P(\mathbf{v}^{(i)}|\theta) \rho(\mathbf{v}^{(i)}|\theta) \right) \right) + S(\eta_L) \\ \ell_{(i)}(\theta) &\geq \text{Tr} \left(\eta_L \log \left(P(\mathbf{v}^{(i)}|\theta) \rho(\mathbf{v}^{(i)}|\theta) \right) \right) + S(\eta_L). \end{aligned}$$

The equality condition is direct since $D_U(\eta_L, \rho(\mathbf{v}^{(i)}|\theta)) = 0$ if and only if $\eta_L = \rho(\mathbf{v}^{(i)}|\theta)$.

The Petz Recovery Map, is immediately obtained by applying **Condition S** to Lemma 5.2. \square

Proof of Corollary 5.5

Corollary. A $\text{QBM}_{m,n}$ is a **CQ-LVM** if and only if quantum terms on the visible units are zero.

Proof. We recall the Hamiltonian of a $\text{QBM}_{m,n}$.

$$H = - \sum_{i=1}^{m+n} b_i \sigma_i^z - \sum_{i>j} w_{ij} \sigma_i^z \sigma_j^z - \sum_{i=1}^{m+n} \Gamma_i \sigma_i^x$$

We first note that Corollary 5.3 implies that the Hamiltonian is CQ if and only if it is a direct sum of 2^m matrices of size $2^n \times 2^n$.

The only off-diagonal entries of the Hamiltonian are from the quantum bias terms Γ_i . Recall that σ_i^x are defined as

$$\sigma_i^k = \otimes_{j=1}^{i-1} I \otimes \sigma^k \otimes_{j=i+1}^{m+n} I$$

where $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. It is easy to see that $\sigma_i^x = \oplus_{j=1}^i (\sigma^k \otimes_{j=i+1}^{m+n} I)$ for $i > m$ which satisfies the condition in Corollary 5.3.

To prove the other direction, we observe that the Kronecker product $\sigma^x \otimes M = \begin{pmatrix} 0 & M \\ M & 0 \end{pmatrix}$ for any square matrix M . When $i \leq m$, this results in matrices larger than $2^n \times 2^n$ with non-zero entries which cannot then be represented as a direct sum of $2^n \times 2^n$ matrices. Hence, $\Gamma_i = 0$ if $i \leq m$. \square

Justification for Gibbs sampling step

In this subsection, we denote vectors in Hilbert space $|x\rangle \in \mathcal{H}$, their adjoint in the dual space $\langle y| \in \mathcal{H}^*$, and their inner product $\langle y|x\rangle \in \mathbb{C}$. The Z and X basis is the eigenbasis of the σ_i^z and σ_i^x operators respectively. We consider the Ising model with a transverse field only in the hidden layer and establish elementary properties of the Hamiltonian. Below, $|v\rangle$ is in the Z basis and each component $|v_i\rangle$, $i \in [m]$ is labeled by its eigenvalue $v_i = \pm 1$ of the single-spin Pauli operator σ_i^z .

Thus, it corresponds to $\mathbf{v} \in \{-1, 1\}^m$ in the main text. State vectors in other layers also follow this convention. The index $k \in [2^m]$ below and $k = 0$ corresponds to all the spins $v_i = -1$.

$$H = \sum_{i,j} w_{ij} \sigma_i^z \sigma_j^z + \sum_i b_i \sigma_i^z + \sum_{j \in L} \Gamma_j \sigma_j^x \quad (3)$$

The data density operator is defined over the visible Hilbert space and is assumed to be diagonal in the Z-basis.

$$\eta_V = \sum_k \alpha_k |v^{(k)}\rangle \langle v^{(k)}| = \sum_{k=1}^{2^m} \alpha_k \Lambda_k \text{ where } \alpha_k \geq 0 \text{ and } \sum_{k \in V} \alpha_k = 1.$$

Proposition C.2 (Commutation with the Hamiltonian). *Let $\Lambda_k = |v^{(k)}\rangle \langle v^{(k)}|$ denote a projection operator in the Z-basis of the visible Hilbert space. If the transverse field only appears on the hidden qubits, the following holds*

$$[H, \Lambda_k \otimes I_L] = 0.$$

The Hamiltonian (3) may then be written as

$$H = \sum_k \Lambda_k \otimes \hat{H}_k, \text{ with } \hat{H}_k = \text{Tr}_V[(\Lambda_k \otimes I_L)H].$$

Definition C.3 (QRBM Model). A model with Hamiltonian of the form 3 is called Quantum Restricted Boltzmann machine if there are no hidden-hidden qubit interactions i.e., $w_{ij} = 0$ for all $i, j \in L$, and no visible-visible interactions $w_{ij} = 0$ for all $i, j \in V$.

For this model, \hat{H}_k is

$$\hat{H}_k = E^{(k)} I_L + \sum_{j \in L} b_j^{(k)} \sigma_j^z + \Gamma_j \sigma_j^x. \quad (4)$$

Here $E^{(k)} = \sum_{i \in V} b_i v_i^{(k)}$ and $b_j^{(k)} = \sum_{i \in V} w_{ij} v_i^{(k)} + b_j$. The Hamiltonian 4 is thus non-interacting and is readily diagonalizable. These become independent qubit systems in an external magnetic field given by $\mathbf{D}_j^{(k)} = (\Gamma_j, 0, b_j^{(k)})$. We shall denote the magnitude of the field by $|\mathbf{D}_j^{(k)}| = \sqrt{(b_j^{(k)})^2 + \Gamma_j^2}$. Each qubit system has eigenvalues $E^{(k)} \pm |\mathbf{D}_j^{(k)}|$. Dropping the constant $E^{(k)}$, expected values can be calculated using the partition function $Z_j = 2 \cosh |\mathbf{D}_j^{(k)}|$. If we have the visible layer clamped to a vector $|\mathbf{v}\rangle = |v^{(k)}\rangle$, the expected values of the spins $j \in L$ in the hidden layer are

$$\begin{aligned} \langle \sigma_j^z \rangle &= \frac{b_j^{(k)}}{|\mathbf{D}_j^{(k)}|} \tanh |\mathbf{D}_j^{(k)}| \\ \langle \sigma_j^x \rangle &= \frac{\Gamma_j}{|\mathbf{D}_j^{(k)}|} \tanh |\mathbf{D}_j^{(k)}| \end{aligned} \quad (5)$$

Similarly, in a QiDBM, the total Hamiltonian $[H, \Lambda_{k,V} \otimes I_{L^{(1)}} \otimes \Lambda_{k',L^{(2)}}] = 0$ for projection operators taken in the Z basis. If we clamp the visible layer to $\mathbf{v} = \mathbf{v}^{(k)}$ and the second hidden layer to $\mathbf{h}^{(2)} = \mathbf{h}^{(2)(k')}$, the resulting Hamiltonian

$$\hat{H}_{k,k'} = E^{(k,k')} I_{L^{(1)}} + \sum_{j \in L^{(1)}} b_j^{(k,k')} \sigma_j^z + \Gamma_j \sigma_j^x,$$

which is again non-interacting and readily diagonalizable. $E^{(k,k')} = \sum_{i \in V} b_i v_i^{(k)} + \sum_{i' \in L^{(2)}} b_{i'} h_{i'}^{(2)(k')}$ and the biases in the first hidden layer $j \in L^{(1)}$ are $b_j^{(k,k')} = \sum_{i \in V} w_{ij}^{(1)} v_i^{(k)} + \sum_{i' \in L^{(2)}} w_{ij}^{(2)} h_{i'}^{(2)(k')} + b_j$. With these, the external fields are now $\mathbf{D}^{(k,k')} = (\Gamma_j, 0, b_j^{(k,k')})$ and the expected values are again given by (5). The conditional probabilities for sampling in the Z and X basis are again given by

$$\begin{aligned} P(h_j^{(1)z} = 1 | \mathbf{v} = \mathbf{v}^{(k)}, \mathbf{h}^{(2)} = \mathbf{h}^{(2)(k')}) &= \frac{1 + \langle \sigma_j^z \rangle}{2}, \\ P(h_j^{(1)x} = 1 | \mathbf{v} = \mathbf{v}^{(k)}, \mathbf{h}^{(2)} = \mathbf{h}^{(2)(k')}) &= \frac{1 + \langle \sigma_j^x \rangle}{2}. \end{aligned}$$

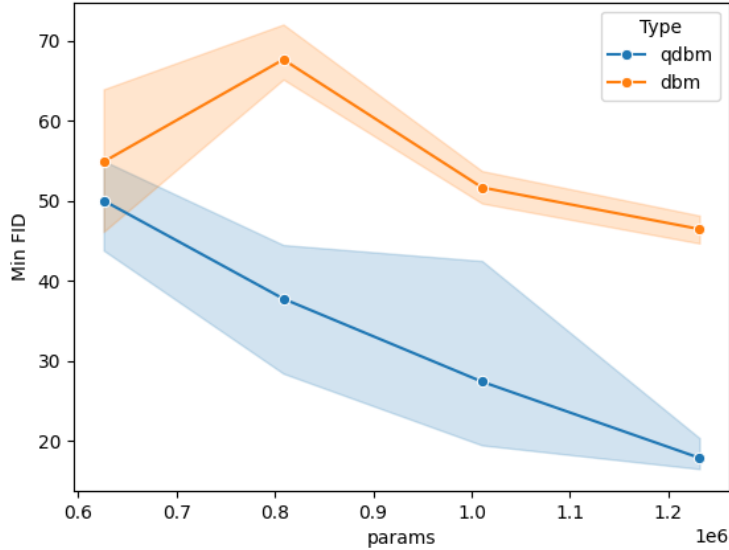


Figure 2: FID vs Parameters of QiDBM and DBM on Binarized MNIST with error bars.

D Experimental details and Additional Experiments

D.1 Additional Experiments

In this section, we restate key details of our experiments presented in the main body of this work. In the interest of keeping this section self-contained, we restate our experimental setup. Following the implementation of [22], we use $\{0, 1\}$ encoding instead of $\{-1, 1\}$.

To compare the effect of the addition of quantum bias, we compare the performance of trained models with and without quantum bias across different sizes. We train a QiDBM and DBM on 1 bit MNIST with hidden sizes 498, 588, 686, and 784 for 100 epochs with 2 hidden layers with SGD optimized to perform Contrastive Divergence with a batch size of 600. In Figure 1 (c), we plot the number of parameters with the minimum FID obtained over 100 epochs. We observe that the model with quantum bias clearly outperforms the models without quantum bias. We also observe that the QiDBM obtains similar FID scores with much fewer parameters than the DBM. In Figure 2, we provide the same plot with 3 different random seeds. We continue to observe that the QiDBM outperforms the DBM.

In Figure 3, we show generated images from different stages of training between QiDBMs and DBMs trained on 8 bit MNIST at randomly selected checkpoints. We observe that the QiDBM produces better quality images in earlier stages of training.

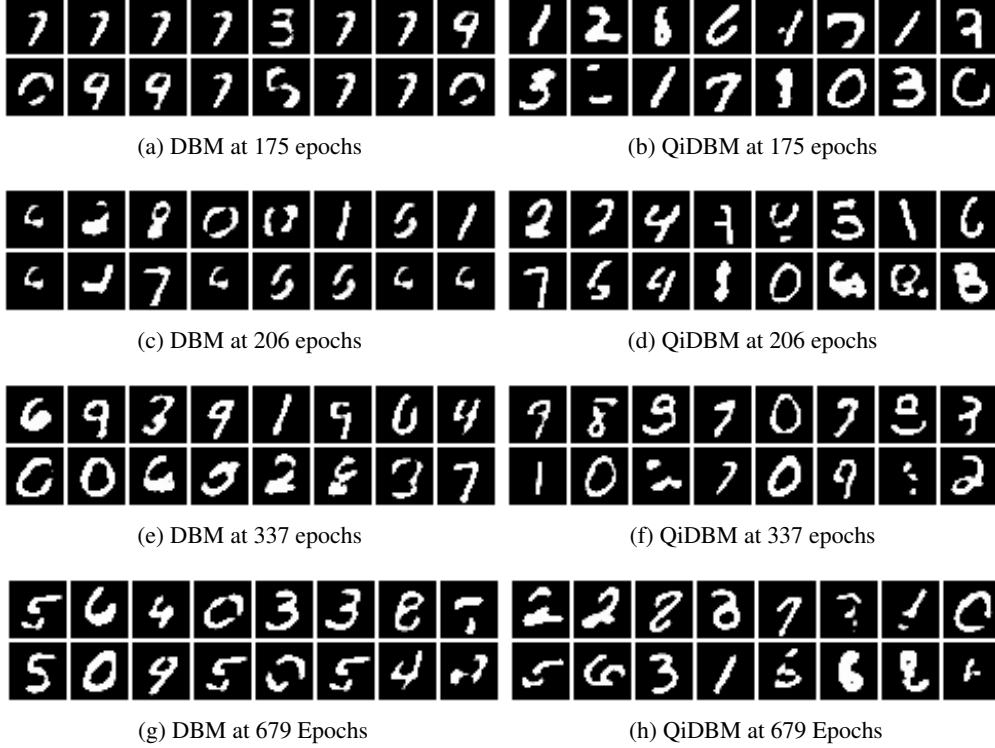


Figure 3: Generated samples during training. DBM generated images on the Left and QiDBM generated images on the Right

D.2 Mixture of Bernoulli Dataset

We describe the dataset from Amin et al. [12] used in our experiments to showcase the practicality of our proposed method. A Bernoulli distribution is built on a randomly selected mode and the average probability distribution over M such modes determines the mixture of Bernoulli distribution. The distribution can be written as

$$P_v^{\text{data}} = \frac{1}{M} \sum_{k=1}^M p^{N-d_v^k} (1-p)^{d_v^k} \quad (6)$$

where N is the dimension of data, p is the probability of success, and d_v^k is the Hamming distance between v and the randomly selected mode. We use 100 randomly sampled datasets of 1000 samples each with $N = 1000$, $M = 8$, $N = 8$, and $p = 0.9$.

E Compute Platform

Implementation Details We implement our proposed methods in PyTorch 2.5.1.

Hardware Tables 1 and 2 details the hardware we use to conduct our experiments. Values in (*) indicated reported values obtained from <https://www.amd.com/en/products/accelerators/instinct/mi200/mi210.html>. Machine 1 runs Ubuntu 22.04.3 LTS with kernel 6.8.0-40-generic with the hardware in Table 1. Machine 2 runs Ubuntu 22.04.1 LTS with kernel 5.15.0-127-generic with the hardware in Table 2. Our software stack comprises of 3.12.8, PyTorch 2.5.1, torchvision version 0.20.1.

Table 1: Machine 1: Specifications of GPU hardware used for computation

CPU Model Name	AMD EPYC 9654 96-Core Processor
CPU(s)	192
Thread(s) per core	1
Core(s) per socket	96
Socket(s)	2
NUMA node(s)	2
CPU MHz(Max)	3707.8120
L1d & L1i cache	6 MiB
L2 cache	192 MiB
L3 cache	768 MiB
RAM	1.48 TiB (DDR5, 4800 MT/s)
GPU Model name	Instinct MI210
GPU(s)	4
GPU Architecture	AMD Aldebaran
Dedicated Memory Size(per GPU)	64 GB
ROCm Version	6.0.2
Peak FP32 Performance*	22.6 TFLOPs
Peak FP64 Performance*	22.6 TFLOPs
Memory Clock*	1.6 GHz
Peak Memory Bandwidth*	1.6 TB/s

Table 2: Machine 2: Specifications of GPU hardware used for computation

CPU Model Name	Intel(R) Core(TM) i9-10980XE
CPU(s)	36
Thread(s) per core	2
Core(s) per socket	18
Socket(s)	1
NUMA node(s)	1
CPU MHz(Max)	4800.0000
L1d & L1i cache	576 KiB
L2 cache	18 MiB
L3 cache	24.8 MiB
RAM	125GiB
GPU Model name	NVIDIA GeForce RTX 3090
GPU(s)	2
Dedicated Memory Size(per GPU)	24 GB
CUDA Version	12.2

F Limitations

This work only addresses finite dimensional Hilbert spaces, analogues of discrete probability spaces. While most of the results in this work generalize to the continuous case, we leave their analysis for future work. Although the DO EM algorithm is amenable to implementation on a quantum computer, as discussed in Section 7, its precise design and analysis needs further research.