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Quantum Machine Learning

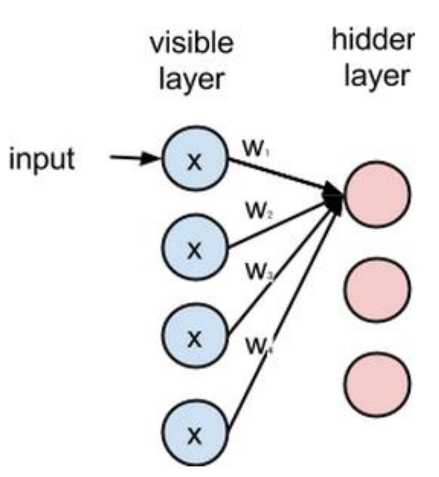
Training Restricted Boltzmann Machines using a Quantum annealer

Vaibhaw Kumar, Gideon Bass, and Joseph Dulny III

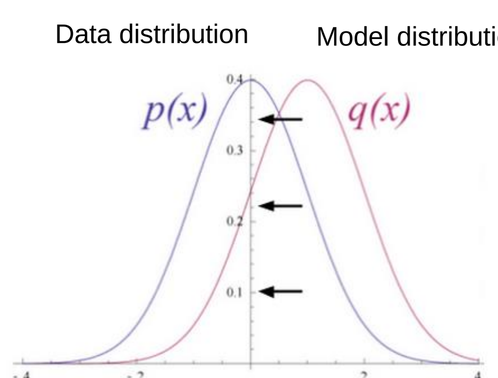
Introduction

Training of Restricted Boltzmann Machines (RBMs) using heuristic techniques on classical hardware may lead to poor learning

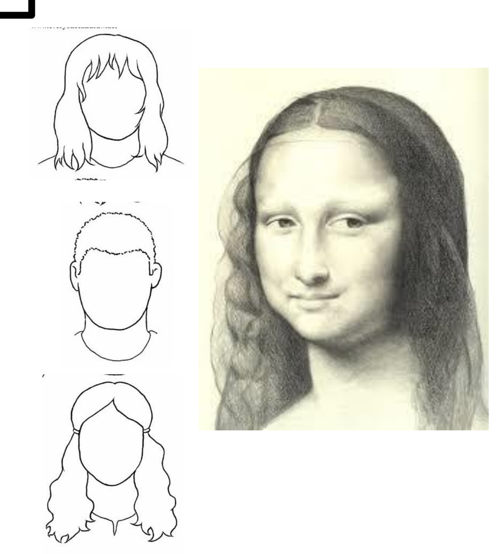
Restricted Boltzmann Machines



A stochastic neural network



Learns data distributions

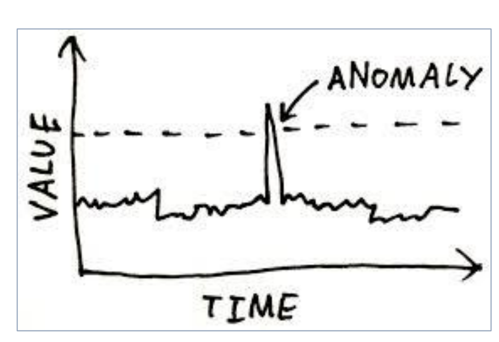


Reconstructs data distribution via feature detection

Applications

Image reconstruction

Collaborative Filtering



Anomaly Detection

Training an RBM

- An RBM consists of a two-layered network where the network units represent binary variables.
- Each visible unit is connected to all the hidden units by network weights.
- The energy of the model closely resembles to the Quadratic Unconstrained Binary Optimization (QUBO), and is given as:

$$E(\boldsymbol{v},\boldsymbol{h}) = \sum_i a_i v_i + \sum_j b_j h_j + \sum_{i,j} w_{ij} v_i h_j$$

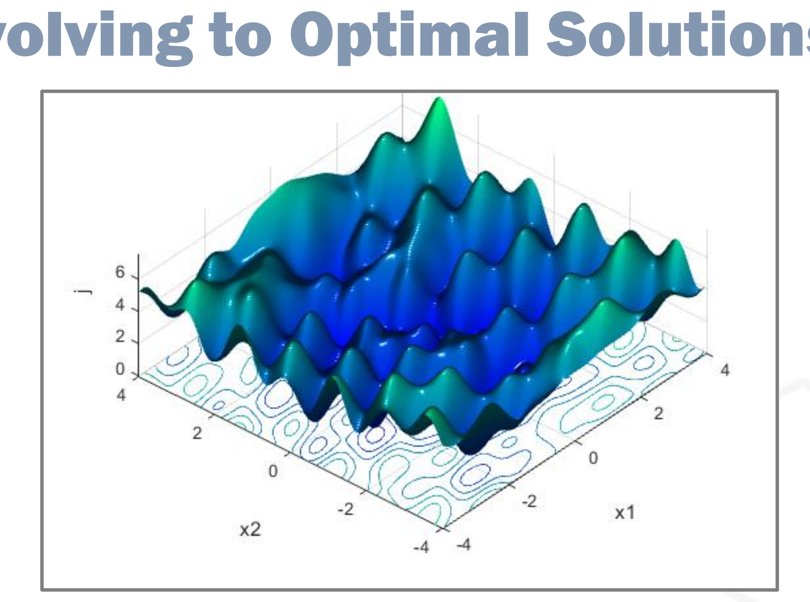
- Training RBMs requires sampling from a distribution

$$P(\boldsymbol{v},\boldsymbol{h}) = \frac{exp(-E(\boldsymbol{v},\boldsymbol{h}))}{\sum exp(-E(\boldsymbol{v},\boldsymbol{h}))} \quad \text{where } \boldsymbol{v},\boldsymbol{h} \text{ are binary valued vectors}$$

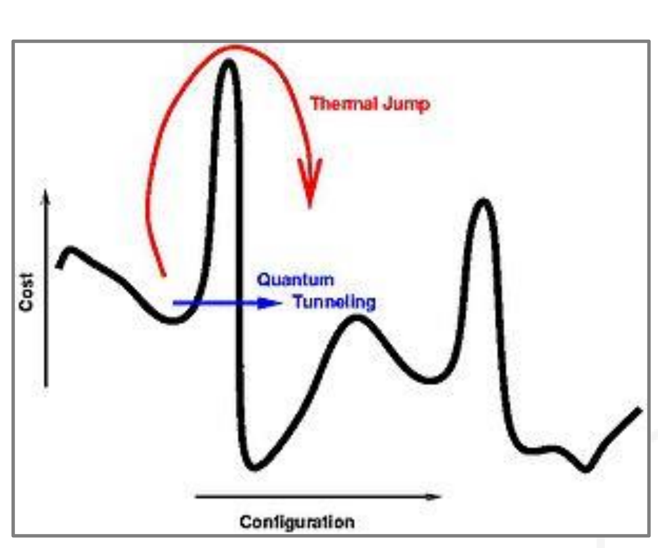
Quantum Computing

Quantum annealing is the only commercially available quantum computing hardware that functions at a large scale. **Quantum annealing offers a new method for solving optimization problems** by taking advantage of the quantum properties of special materials.

Evolving to Optimal Solutions



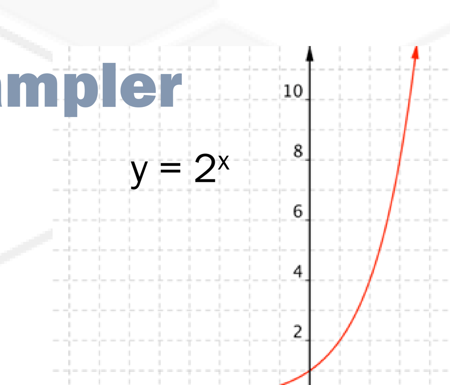
Quantum properties allow the quantum annealer to evolve directly to the optimal solution rather than searching exhaustively for it.



Via a quantum mechanical principle known as the adiabatic theorem, the system should evolve directly into the minimum energy state of the complex mountain range.

Can be used as Boltzmann sampler

Quantum annealers can be run multiple times to generate solutions which follow the Boltzmann distribution.



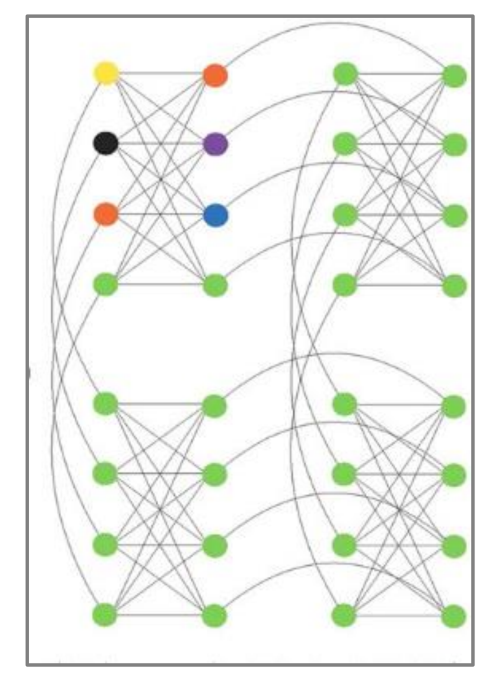
The number of possible states over which computation is needed evolves as 2^x with the dimension of feature space x.

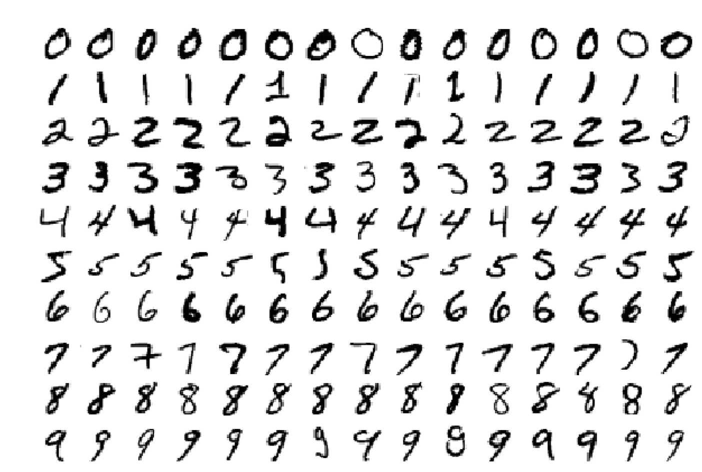
Research

Challenges and ongoing work

Current commercially available quantum annealing hardware has several limitations. We list few below:

- Number of qubits available on the device is limited
- Limited qubit connectivity
- Parameter noise
- Faulty qubits
- Temperature rescaling





Most of the work done so far has looked at implementation details, work on large high-dimensional commercial datasets is missing

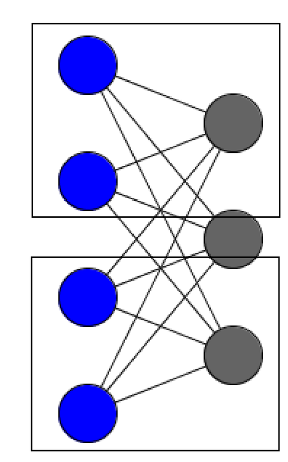
Key Ideas

Enhanced connectivity

We use a different embedding scheme in order to improve the connectivity between the network units. This will be implemented on the quantum annealing chip by creating chains of qubits connected via ferromagnetic coupling.

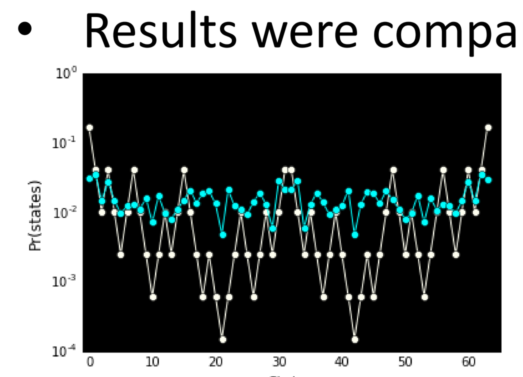
Using a partitioned RBM

We implement a partitioned RBM technique which will allow us to efficiently work with high-dimensional large datasets by dividing the feature space into small subsets. Several small "atomic" RBMs will work on a given subset of the feature space.

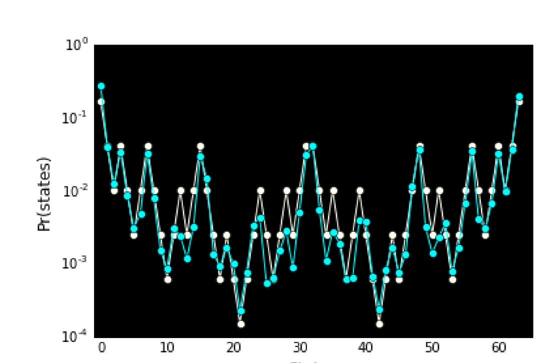


Ising Model Study

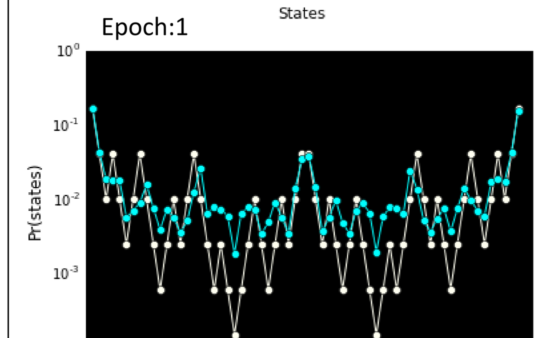
- An Ising model with six spins was modeled using RBMs.
- An artificial training dataset was generated using MCMC simulations.
- Boltzmann samples were obtained by a quantum annealing simulator.
- Results were compared to those obtained using Contrastive Divergence.



Epoch:1

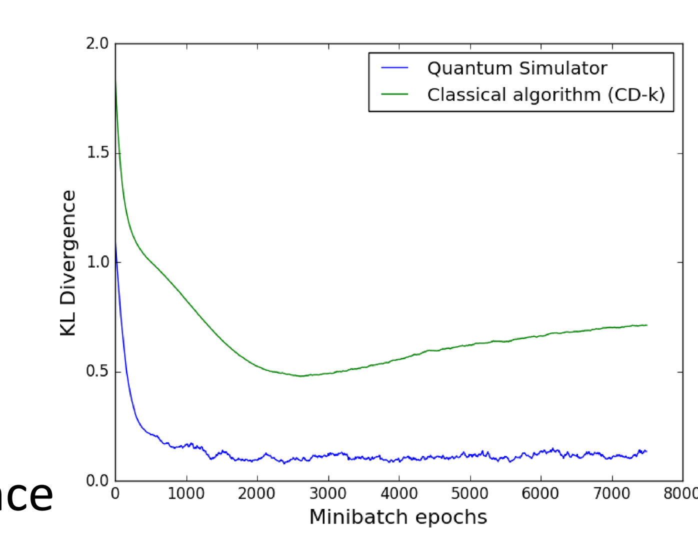


Epoch:800

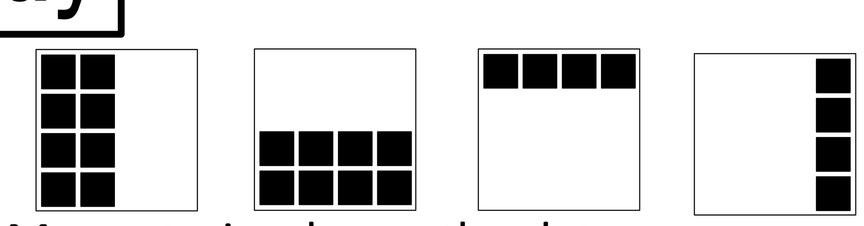


Epoch:400

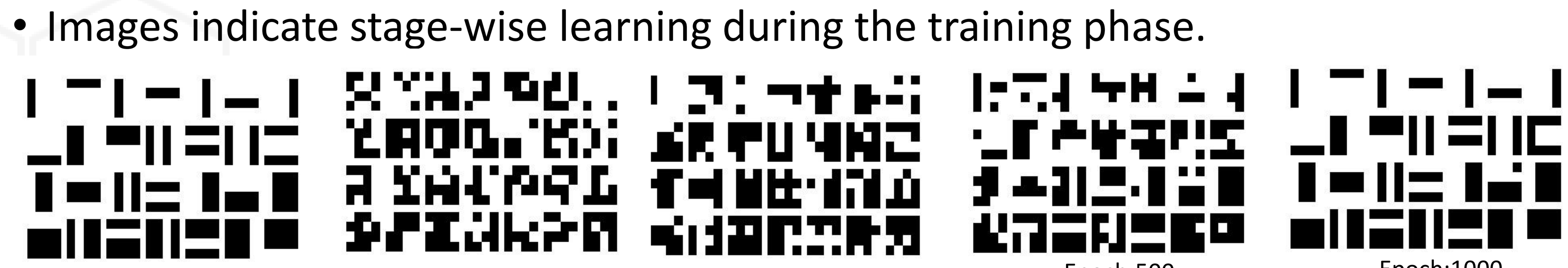
KL Divergence is a metric which indicates the difference between actual data distribution and the model distribution



Bars and Stripes Study



- Bars and Stripes Model data was used.
- Dataset contained 28 4x4 pixel images.
- A 16 visible and 16 hidden unit single RBM was trained over the data.
- Training was carried out by generating samples from a quantum annealed
- simulator.
- Images indicate stage-wise learning during the training phase.



Training set Epoch:1 Epoch:250 Epoch:500 Epoch:1000

Conclusions

- Working with small tractable datasets we have demonstrated that quantum annealing based training outperforms learning based on classical heuristics.
- Currently we are implementing these ideas to train an RBM on a large commercial dataset using quantum hardware.