# Neural Network Quantum Simulation



SAND2021-10513C

Authors: Conor Smith, Tameem Albash UNM, Dept of Electrical & Computer Engineering, Andrew Baczewski

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## Simulating Quantum Systems with Neural Networks

- The goal is to find the ground state of quantum many body Hamiltonians.
  - This is QMA-Complete and thus we don't expect it to be efficiently solvable even on a quantum computer, without lower bounds on the spectral gap.
- Simulation is difficult because we do not have an efficient representation of the wave function in an exponentially growing Hilbert Space. To see this,

$$\boldsymbol{\psi} = \sum_{spins} \boldsymbol{\psi}_{n_1 \dots n_N} |n_1 \dots n_N >$$

- The coefficients $\boldsymbol{\psi}_{n_1 \dots n_N}$ can, for no entanglement, be broken into:

$$\boldsymbol{\psi}_{n_1 \dots n_N} = C_{n_1} \dots C_{n_N}$$

- With entanglement, this decomposition is not possible, and finding the coefficient values typically becomes exponentially hard with system size.

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## Current Approaches

- Tensor Network Methods
  - Restrict the form of the wavefunction while preserving its "essential" features to focus on a specific corner of Hilbert Space.
    - Examples: MPS (very successful in 1D), PEPs (usually done only on 2d lattices
  - Drawback:
    - Does not generally work well on systems defined on irregular graphs.

- Monte Carlo Methods
  - Sampling based approach that can work with non-sparse wave functions
    - Examples: path integral, projector, variational
  - Drawback:
    - Biased estimators and the sign problem

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## Monte Carlo Approach

- Instead of calculating the coefficients exactly, we can sample from an "ansatz" distribution and optimize the parameters (called "$\theta$" here) of this distribution based on the samples obtained.

$$E(\theta) = \frac{<\boldsymbol{\psi}(\theta)|H|\boldsymbol{\psi}(\theta)>}{<\boldsymbol{\psi}(\theta)|\boldsymbol{\psi}(\theta)>} = \frac{\int |\boldsymbol{\psi}(x,\theta)|^2 \frac{H\boldsymbol{\psi}(x,\theta)}{\boldsymbol{\psi}(x,\theta)} dx}{\int |\boldsymbol{\psi}(x,\theta)|^2 dx}$$

- Where our local energy is defined as $\frac{H\boldsymbol{\psi}(x,\theta)}{\boldsymbol{\psi}(x,\theta)}$

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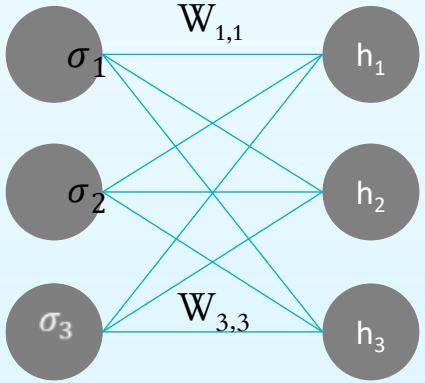
## Restricted Boltzmann Machine

- Idea: Try using various neural networks as ansätze for quantum wave functions.
- Advantages: Agnostic to the Hamiltonian graph, not quite as susceptible to the sign problem, neural networks are very well optimized.
- RBM Energy Example:

$$E = -\sum_j a_j \sigma_j - \sum_i b_i h_i - \sum_{ij} W_{ij} h_i \sigma_j$$




$$\psi(\sigma, \theta) = \sum_{\{h_i\}} e^{-E(\sigma,h)}$$

$\sigma$: Spin Configuration
h: Hidden Spin Configuration {-1,1}
a: Set of weights associated with $\sigma$
b: Set of weights associated h
W: weights connecting the visible and hidden vectors
m: # of hidden units
n: # of visible units

Carleo & Troyer, 2016, https://science.sciencemag.org/content/355/6325/602.abstract

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## Current Status and Why?

Testing on Transverse Field 3-regular 3-XORSAT Hamiltonian:

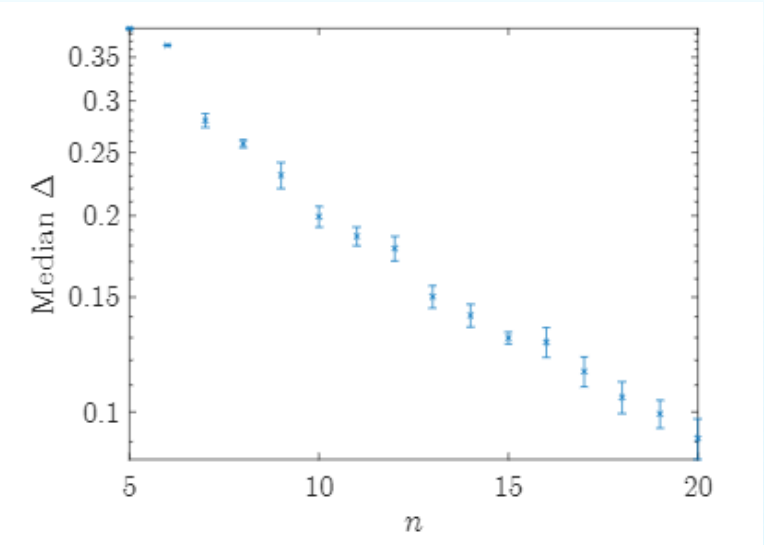
$$H_{XOR} = -(1-s)\sum_i \sigma_i^x - s\sum_{<i,j,k>} J_{ijk}\sigma_i^z \sigma_j^z \sigma_k^z$$

- 3-XORSAT are optimization problems where we have a group of variables (x) which belong to 3 groups and every group satisfies the constraint:

$$x_i \oplus x_j \oplus x_k = b_{ijk} \ (\mathrm{mod}2)$$

$$x_a: \{0,1\}$$

$$b_{ijk} = \{0,1\}$$




- This is a useful system to test this approach on for two reasons:
  - We randomly select the value of $b_{ijk} = \{0, 1\}$ and which triplets the spin sites belong to. This randomness acts a good way to test the neural network generally.
  - When s = ½, the gap between the ground state and first excited state closes exponentially quickly meaning our neural network must become more accurate as the system size grows.

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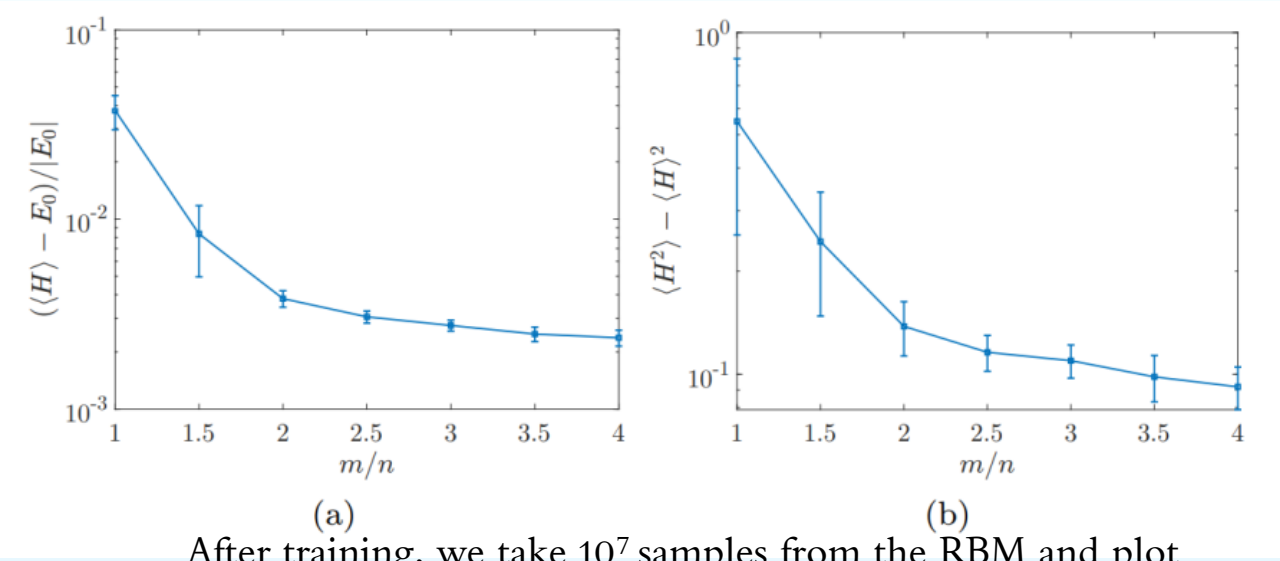
## Preliminary Results




After training, we take $10^7$ samples from the RBM and plot the 95% confidence interval for the hidden unit to visible unit density (m/n) versus the Error and Variance

- We can see here that as we increase the ratio m/n, we obtain smaller Relative Error and Variance.
- There does, however, appear to be a saturation that requires further investigation.

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# Future Work

- We see this project as in the beginning stages with much room for exploration such as:
  - Comparing the complexity of this XORSAT approach to other approaches
  - Benchmarking different Hamiltonians along with different system and parameter sizes
  - Identifying "bottlenecks" in training the networks (complex energy landscapes, unusual probability distributions, etc.)
  - Constructing the networks in different ways, i.e. more layers, convolutional layers, recurrent neural nets, etc.
  - Studying systems unsuitable for tensor methods
  - Studying systems that suffer from the sign problem
  - Time evolution as opposed to a ground state search
  - Comparing performance to quantum algorithms for the same problem

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# References


- Solving the Quantum-Many Body Problem with Artificial Neural Networks, Carleo & Troyer, 2016, https://science.sciencemag.org/content/355/6325/602.abstractQuantum Many-
- Body Dynamics in Two Dimensions with Artificial Neural Networks, Schmitt & Heyl, 2019, https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.125.100503
- The Performance of the Quantum Adiabatic Algorithm on Random Instances of Two Optimization Problems on Regular Hypergraphs, Farhi et al., 2012, https://journals.aps.org/pra/abstract/10.1103/PhysRevA.86.052334 Entropic
- Barriers as a Reason for Hardness in Both Classical and Quantum Algorithms, Bellitti et al., 2021, arxiv:2102.00182


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## Brief Example

$$H_{TFI} = -h\sum_i \sigma_i^x - \sum_{<i,j>} \sigma_i^z \sigma_j^z$$

1. Propose a spin flip and accept the update with probability

$$P = \min(1, |\frac{\psi_{New}}{\psi_{Old}}|^2)$$

2. Sample the Local Energy:

$$E_{Loc} = \frac{H_{TFI}\psi(\sigma,\theta)}{\psi(\sigma,\theta)} = -h\sum_i \frac{\sigma_i^x \psi(\sigma,\theta)}{\psi(\sigma,\theta)} - \sum_{<i,j>} \frac{\sigma_i^z \sigma_j^z \psi(\sigma,\theta)}{\psi(\sigma,\theta)}$$

$$= -h \sum_i \frac{\psi(\sigma_i^x,\theta)}{\psi(\sigma,\theta)} - \sum_{<i,j>} v_i^z v_j^z$$

3. Repeat as many times as necessary to sample the wavefunction distribution

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