Quantum state reconstruction with RBMs

Consider first a Classical Ising model:

$$H = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$$

With Boltzmann $P(\vec{\sigma}) = \frac{1}{Z} e^{-\beta E(\vec{\sigma})}$

Makes sense that an RBM should be able to reconstruct this.

Positive real wavefunctions

Imagine some quantum system where a basis can be chosen such that

$$|\psi\rangle = \sum_{\sigma} |\sigma\rangle\langle\sigma|\psi\rangle = \sum_{\sigma} \psi(\sigma)|\sigma\rangle$$

and all $\psi(\sigma) \in \mathbb{R}$ and $\psi(\sigma) > 0$

The Born rule states $P(\sigma) = |\psi(\sigma)|^2$

Thus we can construct an RBM such that

$$\psi_\lambda(\sigma) = \sqrt{p_\lambda(\sigma)}$$ (marginalized RBM distrib.)

ie. replace $p_\lambda(\vec{v})$ with $\psi^2_\lambda(\vec{v})$ everywhere & repeat classical RBM training.

Q: - How do you expect the $\#\lambda$ to scale w/ N?
- How will the size of the Trainingset scale?

Measurement of physical observables.

Case 1: a diagonal observable:

$$\hat{O} = O_{\sigma\sigma'}\delta_{\sigma\sigma'} = O_{\sigma\sigma}$$

Simply $\langle \hat{O} \rangle = \langle \psi_\lambda | \hat{O} | \psi_\lambda \rangle$

$$= \sum_\sigma p_\lambda(\sigma)\, O_{\sigma\sigma} \quad (\sigma = \vec{\sigma} \text{ here})$$

Can be approximated by MCMC sampling of the RBM as usual.

(also provide a direct quantification of training accuracy).

Case 2: off-diagonal observables.

$$\langle \hat{O}^{\text{OD}} \rangle = \langle \psi_\lambda | \hat{O}_{\sigma\sigma'} | \psi_\lambda \rangle$$

$$= \sum_{\sigma} \sum_{\sigma'} \psi_\lambda(\sigma') \langle \sigma' | \hat{O}_{\sigma\sigma'} | \sigma \rangle \psi_\lambda(\sigma)$$

$$= \sum_{\sigma} \sum_{\sigma'} \sqrt{p_\lambda(\sigma')} \sqrt{p_\lambda(\sigma)} \, O_{\sigma\sigma'}$$

$$= \sum_{\sigma} p_\lambda(\sigma) \boxed{\sum_{\sigma'} \frac{\sqrt{p_\lambda(\sigma')}}{\sqrt{p_\lambda(\sigma)}} O_{\sigma\sigma'}}$$

"local" estimate of O

As long the $O_{\sigma\sigma'}$ matrix is sufficiently <u>sparse</u> it's expectation value can be estimated by MCMC.

You can see here how sufficient generalization is required.

Q: For which Hamiltonians are wavefunctions always +ve real?

Complex Wavefunctions

More generally $\psi(\vec{\sigma}) = |\psi(\vec{\sigma})| e^{i\phi(\vec{\sigma})}$

Clearly more bases are needed - $P(\vec{\sigma}) = |\psi(\vec{\sigma})|^2$ does not contain fingerprints of the phase ϕ.

Q: How many bases in general? Typically?

How to parameterize a complex wavefunction on an RBM?

- any function approximator (FFNN, CNN)
- Complex weights (Carleo)
- another RBM (say with parameters μ)

e.g. $\psi_{\lambda\mu}(\vec{\sigma}) = \sqrt{p_\lambda(\vec{\sigma})}\, e^{i\phi_\mu(\vec{\sigma})}$, $\phi_\mu(\vec{\sigma}) = \log p_\mu(\vec{\sigma})$

How to train? "Target" (unknown) wavefunction must produce data in different bases (unitary transformation)

$$\psi(\vec{\sigma}^b) = \sum_{\vec{\sigma}} U_{\vec{\sigma}^b, \vec{\sigma}} \psi(\vec{\sigma})$$

where $|\vec{\sigma}^b\rangle = |\sigma_1^{b_1}, \sigma_2^{b_2}, \ldots, \sigma_N^{b_N}\rangle$

ie each spin can be in a different basis.

Phase information is then transmitted via

$$P(\vec{\sigma}^b) = |\psi(\vec{\sigma}^b)|^2$$

Then given a data set $\mathcal{D} = \{\vec{\sigma}^b\}$ we can use a sum of KL divergences in different bases

$$C_{\lambda\mu} = -\frac{1}{\|\mathcal{D}\|} \sum_{\vec{\sigma}^b \in \mathcal{D}} \log |\psi_{\lambda\mu}(\vec{\sigma}^b)|^2$$

$$= -\frac{1}{\|\mathcal{D}\|} \sum_{\vec{\sigma}^b \in \mathcal{D}} \left[\log\left(\sum_{\vec{\sigma}} U_{\vec{\sigma}^b, \vec{\sigma}} \psi_{\lambda\mu}(\sigma)\right) + c.c. \right]$$

etc.

Generally, it is not known how many basis are needed (maximum 2^N), or how many measurements per basis are required...