Studies of Quantum Dots using Machine Learning

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Outline

Theory

Quantum Mechanics

The mechanics of a quantum system is described by the time-dependent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(\boldsymbol{r},t)\right\rangle = \hat{\mathcal{H}}\left|\Psi(\boldsymbol{r},t)\right\rangle$$

The Time-independent Schrödinger Equation

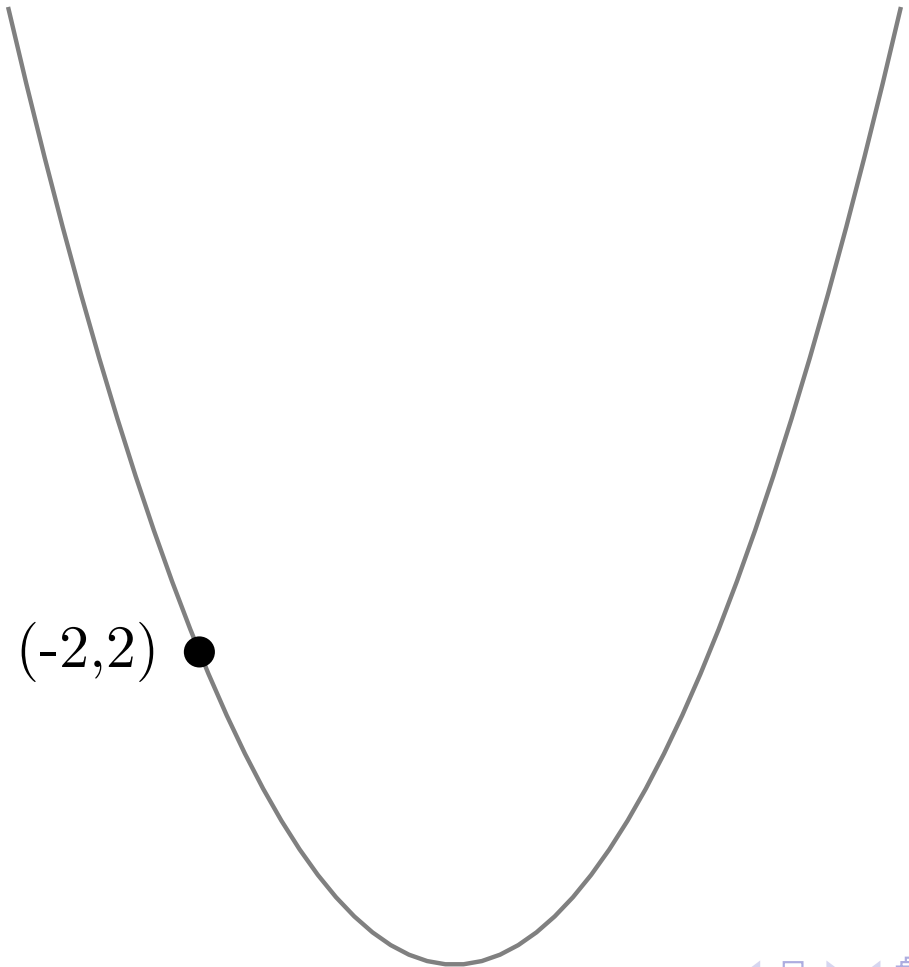
For a stationary system, the Schrödinger equation reduces to

$$E_n = \frac{\int d\boldsymbol{r} \Psi_n^*(\boldsymbol{r}) \hat{\mathcal{H}} \Psi_n(\boldsymbol{r})}{\int d\boldsymbol{r} \Psi_n^*(\boldsymbol{r}) \Psi_n(\boldsymbol{r})}$$

which gives the energy of state n.

Harmonic Oscillator

$$\begin{aligned}\hat{\mathcal{H}} &= -\frac{1}{2}\nabla^2 + \frac{1}{2}\omega^2 r^2 \\ &= \langle \hat{T} \rangle + \langle \hat{V} \rangle\end{aligned}$$



Circular Quantum Dots

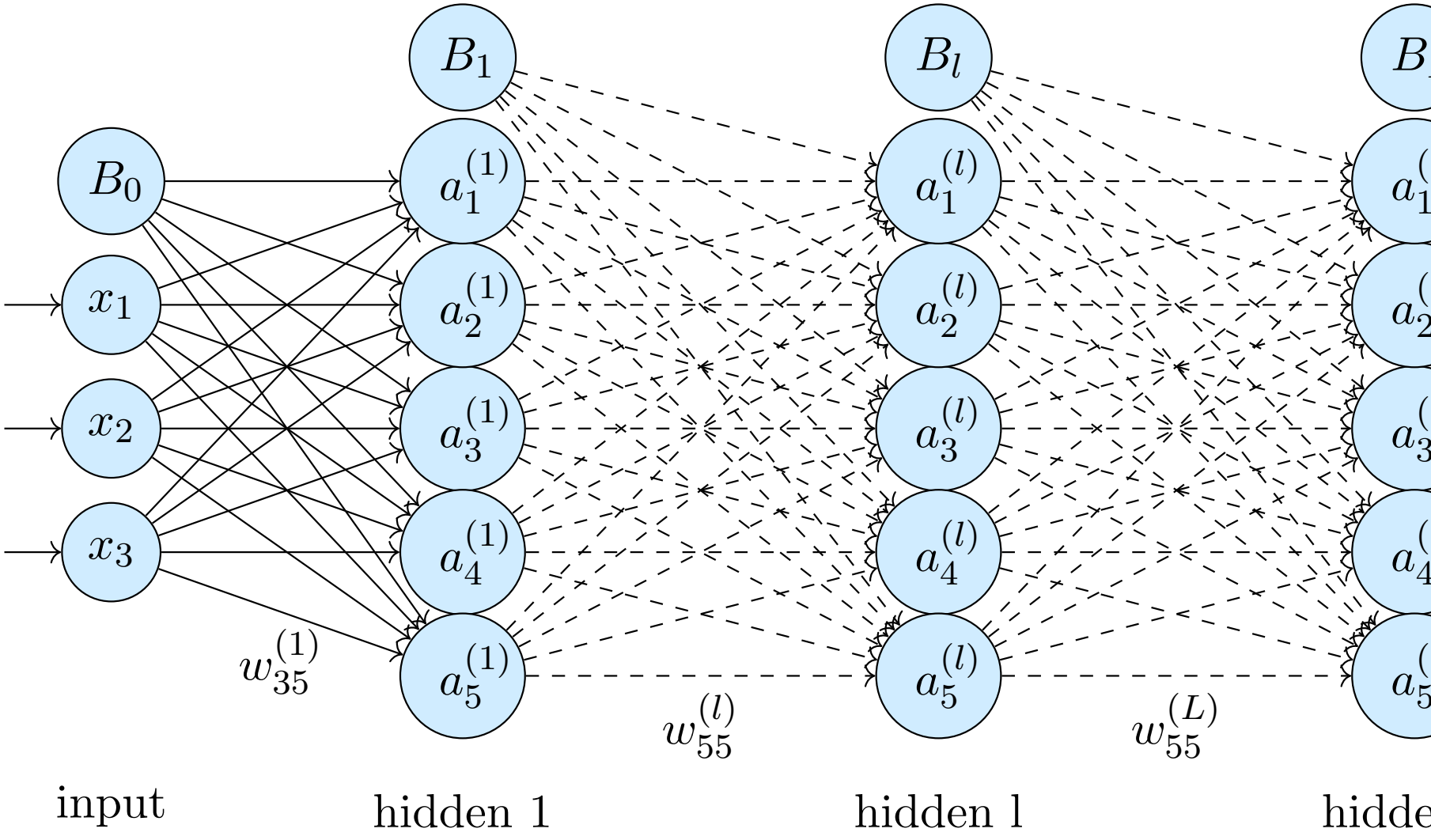
Many-body problem

$$\hat{\mathcal{H}} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{2}\omega^2 r_1^2 + \frac{1}{2}\omega^2 r_2^2 + \frac{1}{r_{ij}}$$
$$= \langle \hat{T}_1 \rangle + \langle \hat{T}_2 \rangle + \langle \hat{V}_1 \rangle + \langle \hat{V}_2 \rangle + \langle \hat{V}_{\text{int}} \rangle$$

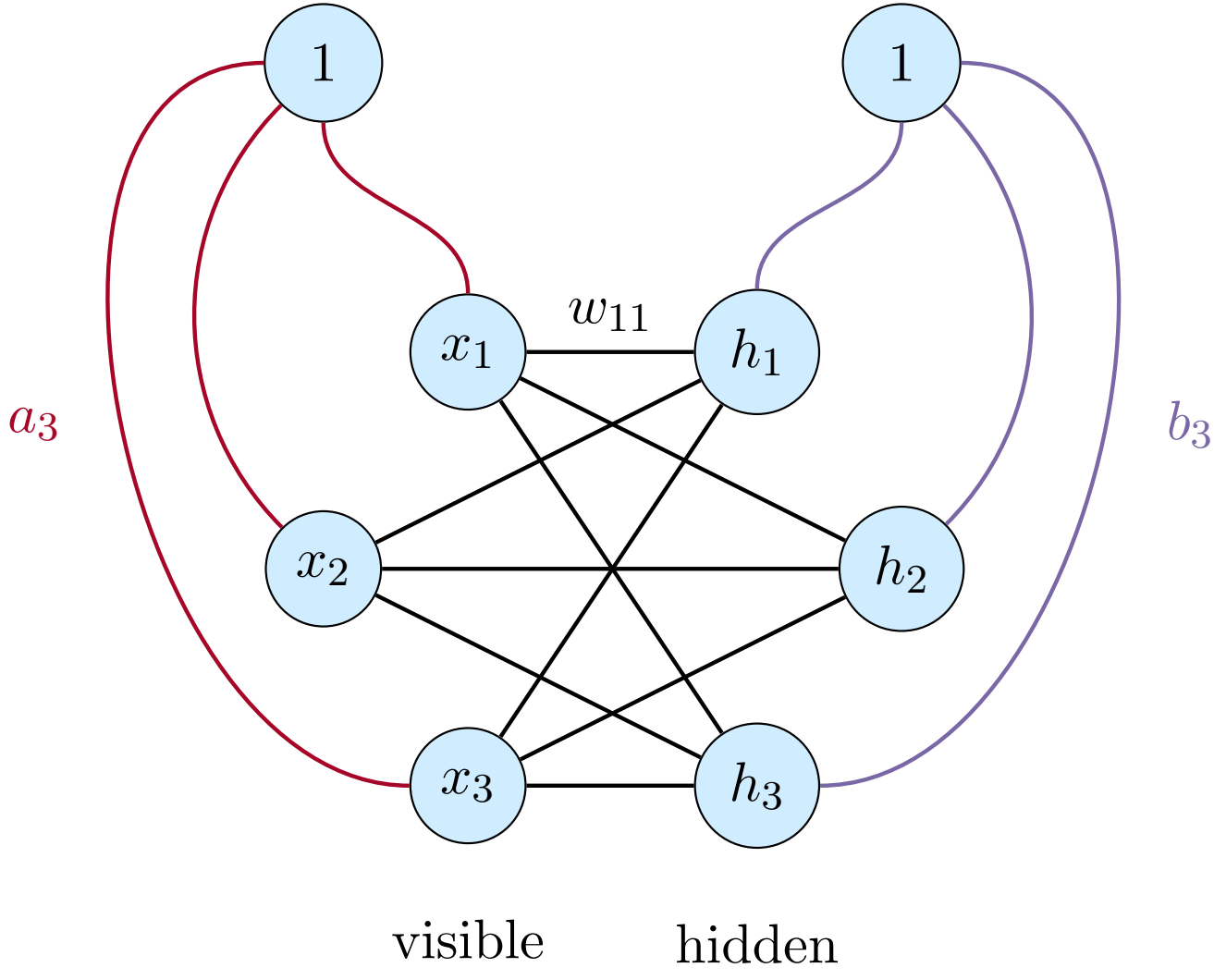
Machine Learning

> *Machine learning is the science of getting computers to act without being explicitly programmed.*

Feed-forward Neural Network



Restricted Boltzmann machines



Methods

Variational Monte Carlo (VMC)

Exploit the variational principle in order to obtain the ground state energy

$$E_0 < E_{\mathrm{VMC}} = \frac{\int d\boldsymbol{r} \Psi_T(\boldsymbol{r})^* \hat{\mathcal{H}} \Psi_T(\boldsymbol{r})}{\int d\boldsymbol{r} \Psi_T(\boldsymbol{r})^* \Psi_T(\boldsymbol{r})}$$

$$= \int d\boldsymbol{r} \underbrace{\frac{\Psi_T(\boldsymbol{r})^* \Psi_T(\boldsymbol{r})}{\int d\boldsymbol{r} \Psi_T(\boldsymbol{r})^* \Psi_T(\boldsymbol{r})}}_{P(\boldsymbol{r})} \cdot \underbrace{\frac{1}{\Psi_T(\boldsymbol{r})} \hat{\mathcal{H}} \Psi_T(\boldsymbol{r})}_{E_L(\boldsymbol{r})}$$

Monte Carlo Integration

We attempt to solve the integral by sampling from the probability density function $P(\boldsymbol{r})$

$$E_{\mathrm{VMC}} = \int d\boldsymbol{r} E_L(\boldsymbol{r}) P(\boldsymbol{r})$$

$$\approx \frac{1}{M} \sum_{i=1}^{M} E_L(\boldsymbol{r}_i)$$

Trial Wave Function

$$P(\boldsymbol{r}) \propto \Psi_T(\boldsymbol{r})^* \Psi_T(\boldsymbol{r})$$

Use the Slater-Jastrow function as our trial wave function

$$\Psi_T(\boldsymbol{r}) = |\hat{D}(\boldsymbol{r})| J(\boldsymbol{r})$$

where the Slater matrix, $\hat{D}(\boldsymbol{r})$, contains all the single-particle functions

$$\hat{D}(\boldsymbol{r}) = \begin{pmatrix} \phi_1(\boldsymbol{r}_1) & \phi_2(\boldsymbol{r}_1) & \dots & \phi_N(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_2(\boldsymbol{r}_2) & \dots & \phi_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r}_N) & \phi_2(\boldsymbol{r}_N) & \dots & \phi_N(\boldsymbol{r}_N) \end{pmatrix}$$

Single-particle Functions

The Hermite functions,

$$\phi_n(\boldsymbol{r}) \propto H_n(\boldsymbol{r}) \exp\left(-\frac{1}{2}\alpha\omega|\boldsymbol{r}|^2\right),$$

are used as the single-particle functions for quantum dots in standard VMC. The Gaussian can be factorized out from the Slater determinant.

$$|\hat{D}(\boldsymbol{r};\alpha)| \propto \exp\left(-\frac{1}{2}\alpha\omega|\boldsymbol{r}|^2\right) \begin{vmatrix} H_1(\boldsymbol{r}_1) & H_2(\boldsymbol{r}_1) & \dots & H_N(\boldsymbol{r}_1) \\ H_1(\boldsymbol{r}_2) & H_2(\boldsymbol{r}_2) & \dots & H_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ H_1(\boldsymbol{r}_N) & H_2(\boldsymbol{r}_N) & \dots & H_N(\boldsymbol{r}_N) \end{vmatrix}$$

Restricted Boltzmann Machine

We use the marginal distribution of the visible units as the single-particle functions in the Slater determinant, and see if them can model the correlations

$$\phi_n(\boldsymbol{r}) \propto H_n(\boldsymbol{r}) P(\boldsymbol{r}; \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{W})$$

where $P(\boldsymbol{r})$ is the marginal distribution of the visible units.

$$|\hat{D}(\boldsymbol{r}; \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{W})| \propto P(\boldsymbol{r}; \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{W}) \begin{vmatrix} H_1(\boldsymbol{r}_1) & H_2(\boldsymbol{r}_1) & \dots & H_N(\boldsymbol{r}_1) \\ H_1(\boldsymbol{r}_2) & H_2(\boldsymbol{r}_2) & \dots & H_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ H_1(\boldsymbol{r}_N) & H_2(\boldsymbol{r}_N) & \dots & H_N(\boldsymbol{r}_N) \end{vmatrix}$$

Jastrow Factor

The Jastrow factor is added to account for the correlations
Simple Jastrow factor

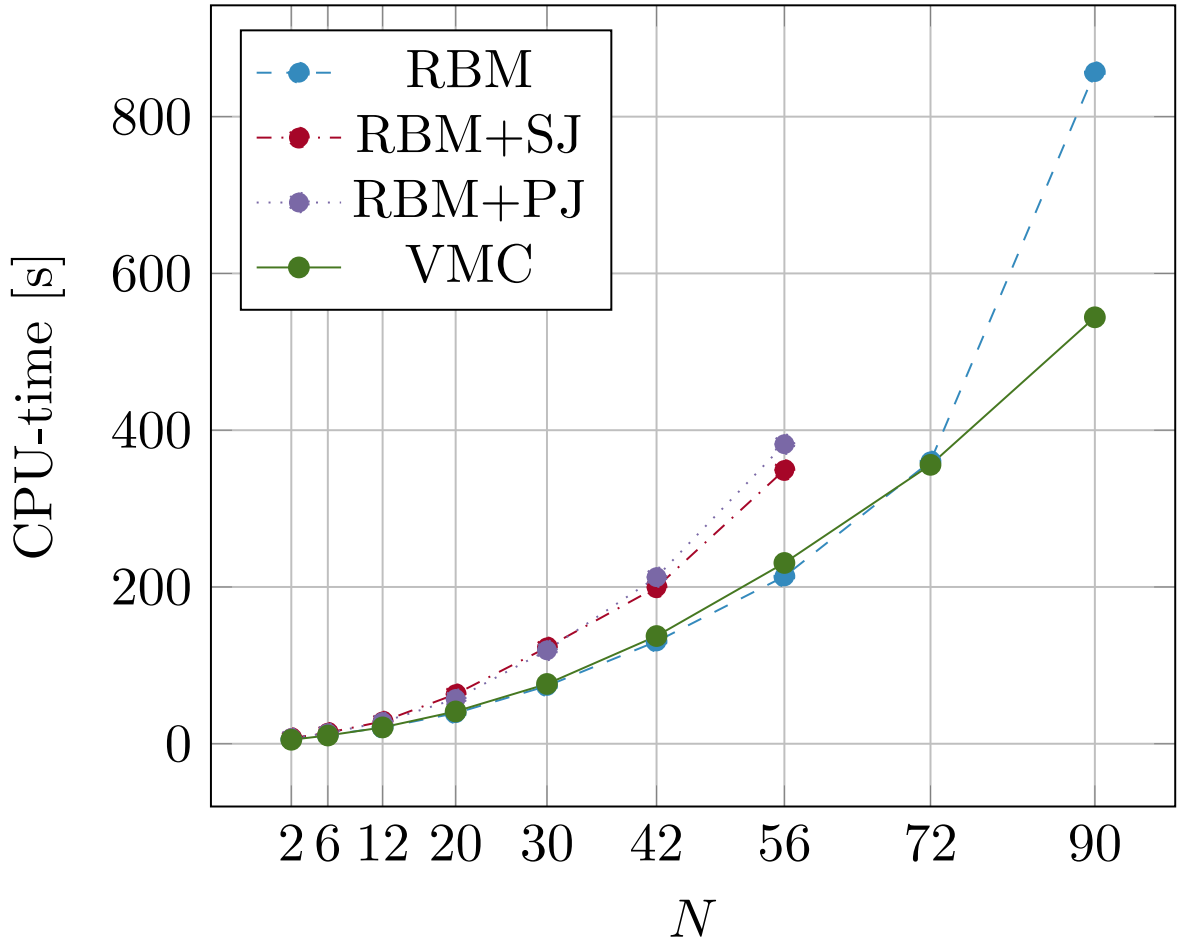
$$J(\boldsymbol{r};\boldsymbol{\beta}) = \exp\left(\sum_{i=1}^{N}\sum_{j>i}^{N}\beta_{ij}r_{ij}\right).$$

Padé-Jastrow factor

$$J(\boldsymbol{r};\beta) = \exp\left(\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right).$$

Results

Computational Cost



Conclusion

Retrospect

RBM is able to account for most of the correlations

RBM+PJ implies to give a lower ground state energy and model the correlations better than a traditional VMC

RBM+SJ is both more expensive and less accurate than its fellow methods, and we see no reason to choose it

Future Work

Repeat the exercise using spherical coordinates - interactions are easier to model in spherical coordinates

Check the ability of modeling the three-body correlations, considering nuclear systems

Reduce the computational cost

Thank you!