

Studies of Quantum Dots using Machine Learning



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Outline

- ▶ Motivation
- ▶ Quantum Theory
- ▶ Machine Learning
- ▶ Methods
- ▶ Results
- ▶ Conclusion
- ▶ (Code)



Motivation



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Why quantum dots?

- ▶ Technology¹
- ▶ Theoretically
- ▶ Experimentally (2D)



Why is it challenging?

- ▶ Quantum many-body problem
- ▶ Fermi-Dirac statistics



How to overcome the challenges?

- ▶ Efforts..
- ▶ gh
- ▶ Our approach: Machine Learning^{2,3}



Quantum Theory



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The Time-independent Schrödinger Equation

A stationary quantum mechanical system is described by

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

which gives the energy of state n .



Machine Learning Theory

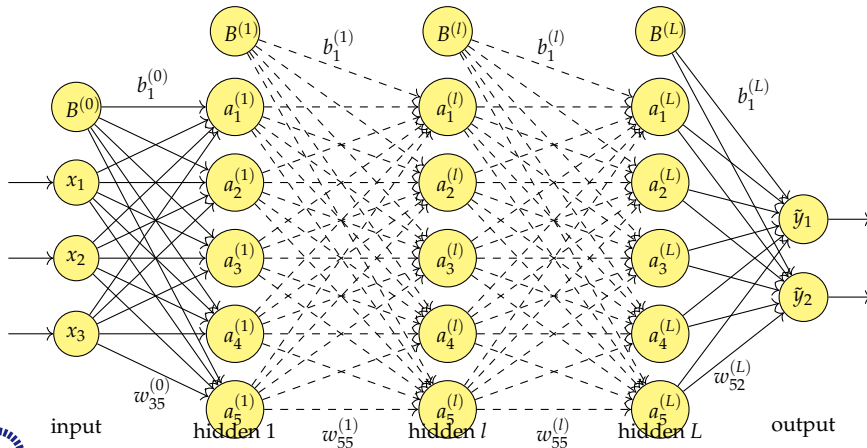


Machine Learning

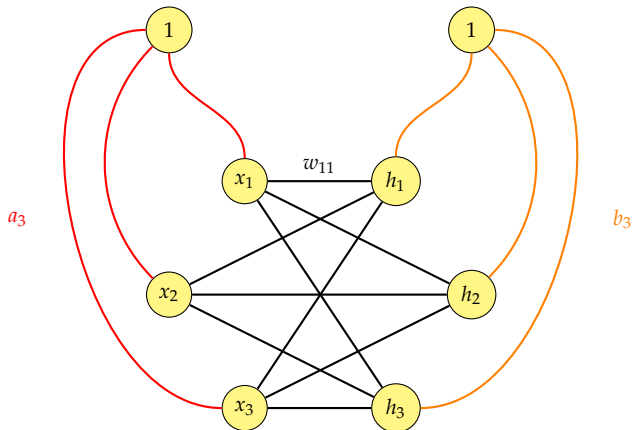
Machine learning is the science of getting computers to act without being explicitly programmed.



Feed-forward Neural Network



Restricted Boltzmann machines



Methods



Variational Monte Carlo (VMC)

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

$$\begin{aligned} E_0 < E_{\text{VMC}} &= \frac{\int d\mathbf{R} \Psi_T(\mathbf{R})^* \hat{\mathcal{H}} \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi_T(\mathbf{R})^* \Psi_T(\mathbf{R})} \\ &= \int d\mathbf{R} \underbrace{\frac{\Psi_T(\mathbf{R})^* \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi_T(\mathbf{R})^* \Psi_T(\mathbf{R})}}_{P(\mathbf{R})} \cdot \underbrace{\frac{1}{\Psi_T(\mathbf{R})} \hat{\mathcal{H}} \Psi_T(\mathbf{R})}_{E_L(\mathbf{R})} \end{aligned}$$

Monte Carlo Integration

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

$$\begin{aligned} E_{\text{VMC}} &= \int d\mathbf{R} E_L(\mathbf{R}) P(\mathbf{R}) \\ &\approx \frac{1}{M} \sum_{i=1}^M E_L(\mathbf{R}_i) \end{aligned}$$

Trial Wave Function

$$P(\mathbf{R}) \propto \Psi_T(\mathbf{R})^* \Psi_T(\mathbf{R})$$

Use the Slater-Jastrow function as our trial wave function

$$\Psi_T(\mathbf{R}) = |\hat{D}(\mathbf{R})|J(\mathbf{R})$$

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

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

Single-particle Functions

The Hermite functions,

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

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

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

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

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

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

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

Jastrow Factor

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

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

Padé-Jastrow factor

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

Results



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Ground State Energy

Number of electrons: $N = 2$. Frequency: ω .

ω	RBM	RBM+SJ	RBM+PJ	VMC	HF *	Exact †
1/6	0.7036(1)	0.67684(7)	0.66715(6)	0.66710(1)	0.768675	2/3
1	3.0803(2)	3.02108(5)	2.999587(5)	2.99936(1)	3.16190	3

*Computation of the Hartree-Fock limit by Mariadason, 2018 [4].

†Semi-analytical ground state energy calculated by Taut, 1993 [5].

Ground State Energy

Number of electrons: $N = 20$. Frequency: ω .

ω	RBM	RBM+SJ	RBM+PJ	VMC	HF [‡]	DMC [§]
0.1	30.824(2)	30.567(3)	30.1553(9)	30.0403(2)	31.1902	29.9779(1)
1.0	159.428(3)	156.816(4)	156.104(1)	155.8900(4)	158.004	155.8822(1)

[‡]Computation of the Hartree-Fock limit by Mariadason, 2018 [4].

[§]Ground state energy estimate using the diffusion Monte Carlo method.
By Høgberget, 2013 [6].

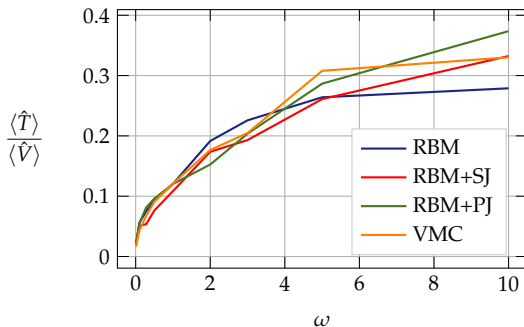


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Energy distribution

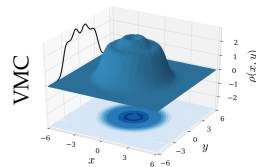
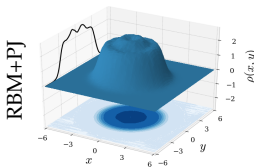
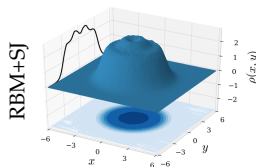
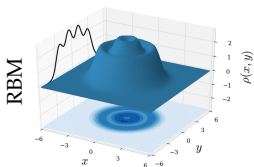
Number of electrons: $N = 20$. Frequency: ω .

Ratio between the kinetic energy, $\langle \hat{T} \rangle$, and the total potential energy, $\langle \hat{V} \rangle$.



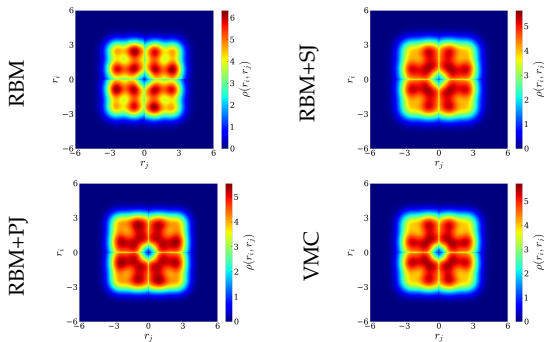
One-body density

Number of electrons: $N = 20$. Frequency: $\omega = 1.0$.



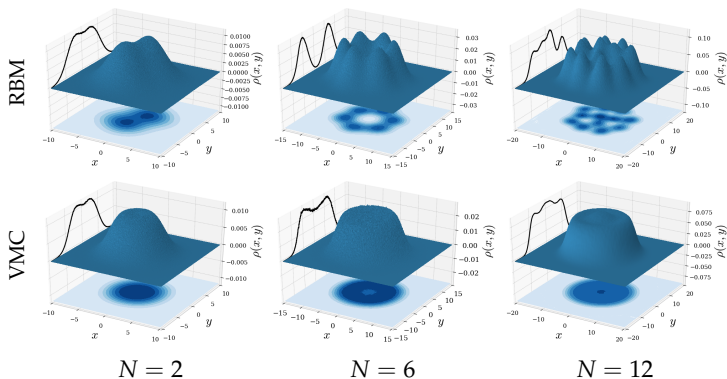
Two-body density

Number of electrons: $N = 20$. Frequency: $\omega = 1.0$.



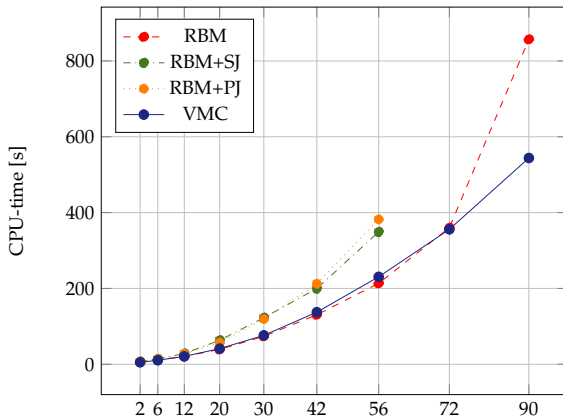
Low-frequency dots

Number of electrons: N . Frequency: $\omega = 0.1$.



Computational Cost

Number of electrons: N .



Conclusion



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Conclusions

- ▶ 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!



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