

# Studies of Quantum Dots using Machine Learning



Even Marius Nordhagen

University of Oslo

*evenmn@fys.uio.no*

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# Outline

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



# Motivation



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# Why quantum dots?

- ▶ Technology<sup>1</sup>
- ▶ 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<sup>2,3</sup>



# 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

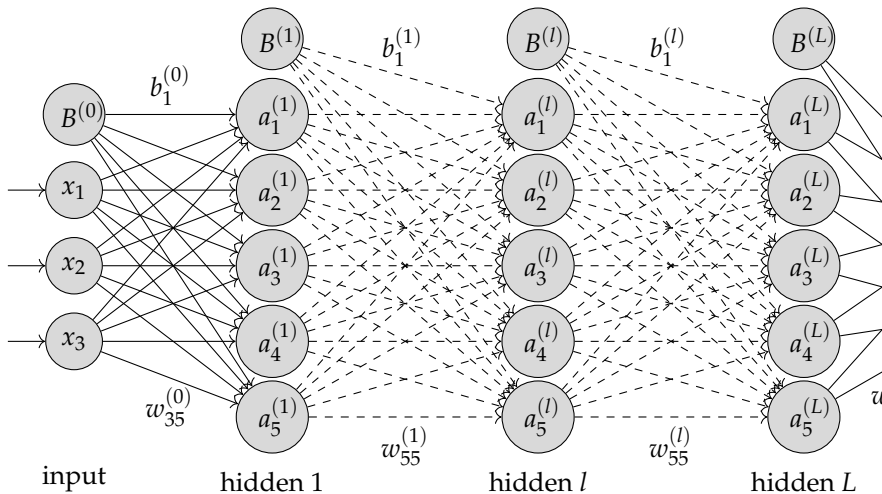


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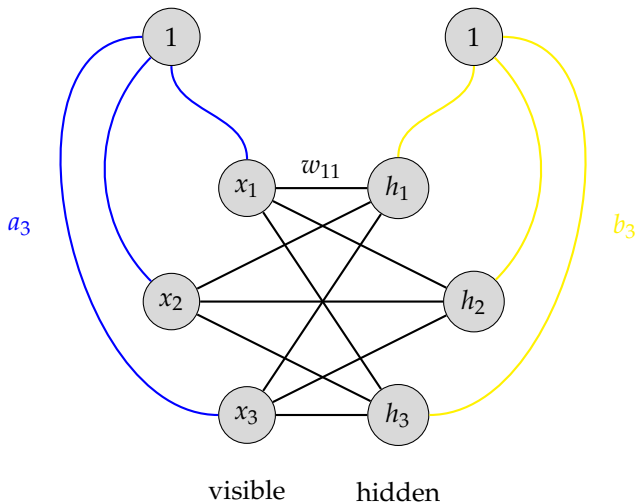
# Machine Learning

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

# Feed-forward Neural Network



# Restricted Boltzmann machines



# Methods



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# 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 they 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



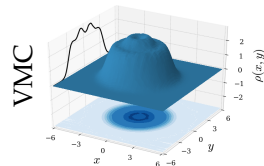
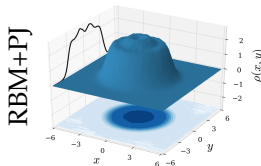
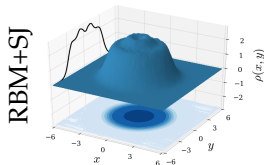
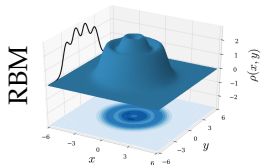
# Ground State Energy

**Table:** Ground state energy of two-dimensional quantum dot with  $N = 2$  electrons and frequency  $\omega = 1.0$ .

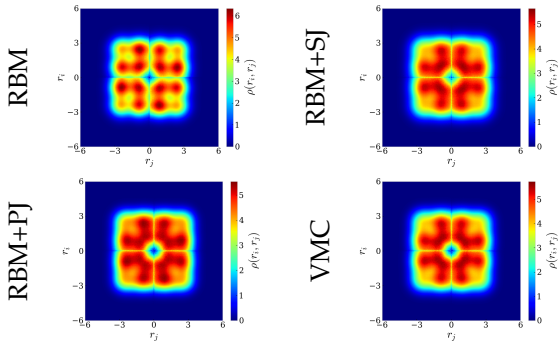
$\omega$	RBM	RBM+SJ	RBM+PJ	HF <sup>†</sup>	Exact <sup>††</sup>
1/6	0.7036(1)	0.67684(7)	0.66715(6)	0.768675	2/3
1	3.0803(2)	3.02108(5)	2.999587(5)	3.1690	3



# One-body density



# Two-body density



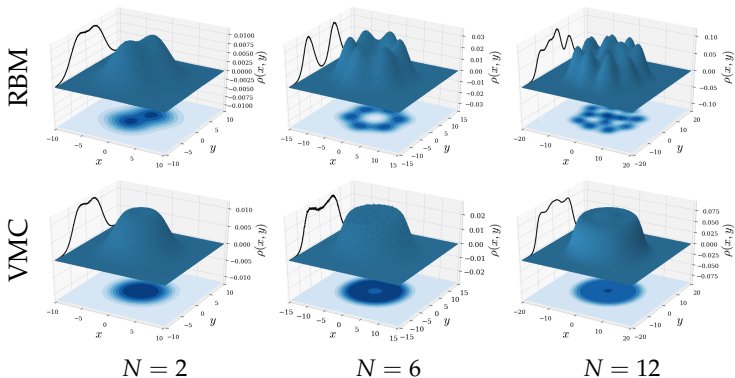
# Energy distribution

Distribution between various energy sources

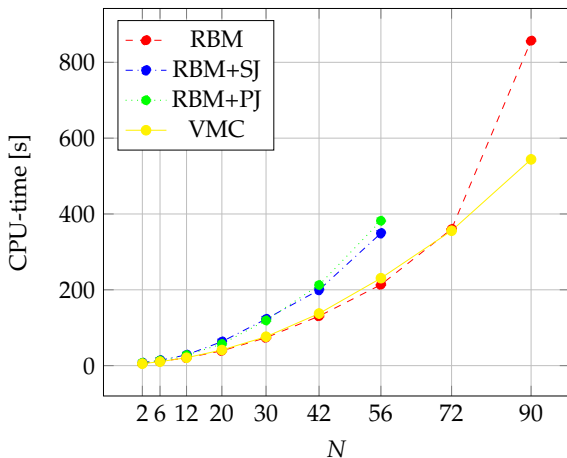




# Low-frequency dots



# Computational Cost



# 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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