

Studies of Quantum Dots using Machine Learning

Even Marius Nordhagen

University of Oslo

evenmn@fys.uio.no

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Theory

- Quantum Mechanics

- Machine Learning

Methods

- Variational Monte Carlo

- Restricted Boltzmann Machines

Results

- (Code)

Theory

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

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

The Time-independent Schrödinger Equation



For a stationary system, the Schrödinger equation reduces to

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

which gives the energy of state n .

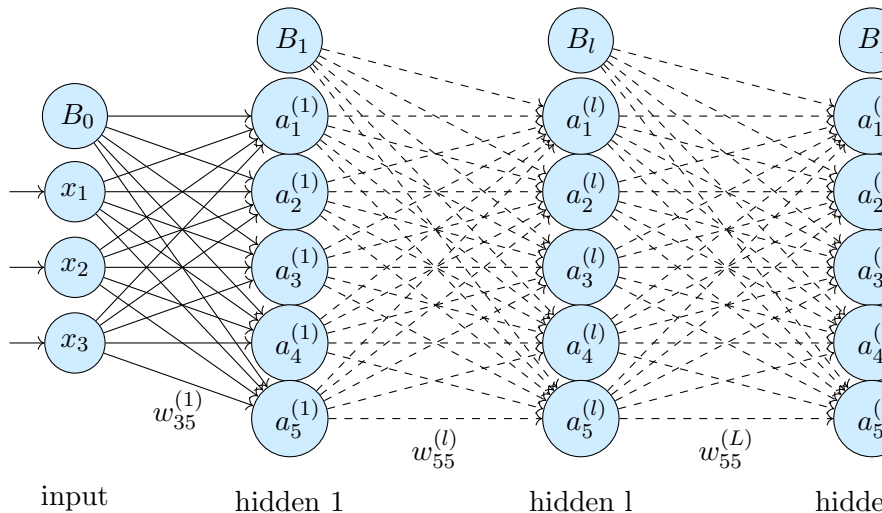
$$\begin{aligned}\hat{\mathcal{H}} &= -\frac{1}{2}\nabla^2 + \frac{1}{2}\omega^2 r^2 \\ &= \langle \hat{T} \rangle + \langle \hat{V} \rangle\end{aligned}$$

Many-body problem

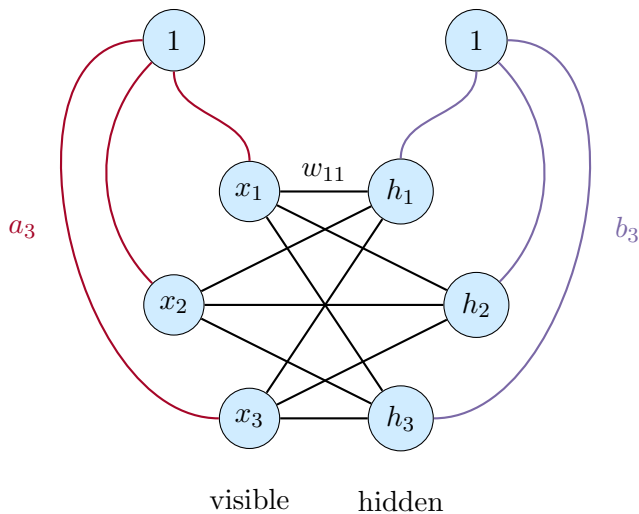
$$\begin{aligned}\hat{\mathcal{H}} &= -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{2}\omega^2 r_1^2 + \frac{1}{2}\omega^2 r_2^2 + \frac{1}{r_{ij}} \\ &= \langle \hat{T}_1 \rangle + \langle \hat{T}_2 \rangle + \langle \hat{V}_1 \rangle + \langle \hat{V}_2 \rangle + \langle \hat{V}_{\text{int}}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

“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

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

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

$$E_{\text{VMC}} = \int d\mathbf{r} E_L(\mathbf{r}) P(\mathbf{r})$$
$$\approx \frac{1}{M} \sum_{i=1}^M E_L(\mathbf{r}_i)$$

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.

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

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.

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

The Jastrow factor is added to account for the correlations

Simple Jastrow factor

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

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



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