

# Machine Learning: The Hubbard model

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## **Abstract**

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## 0.1 Theoretical background: Quantumchemical fundamentals

### 0.1.1 Quantumchemical description of molecules

Hartree-Fock method

Full CI method

### 0.1.2 The Hubbard model

The Hubbard Hamiltonian

Overview of the PES of the simplest system

## 0.2 Theoretical background: Neural networks

### 0.2.1 Mathematical foundation of the network

General overview of neural networks

Activation functions

Optimization methods

### 0.2.2 Regularization methods

### 0.2.3 Network analysis

Training analysis

Weight analysis

Activation analysis

## 0.3 Research overview

### 0.3.1 Identification of the roadblocks in modern quantum-chemical research

### 0.3.2 Solutions

### 0.3.3 Overview of planned research topics

## 0.4 Results with regard to predictive power of neural networks

### 0.4.1 Preliminary test: Can a simple network capture the data in a simple well defined system?

### 0.4.2 Simple hyperparameter sweep: Performance vs network complexity

### 0.4.3 Data augmentation <sup>2</sup>

Introduction of permutational symmetries in data

Introduction of noise on the output data

### 0.4.4 Performance of networks trained on less complex systems

### 0.4.5 Performance analysis on networks with simplest architectures

## 0.5 Results with regard to the learned features