Semester Project: Variational Monte-Carlo for Continuous Space Many-Body Quantum Physics

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April 22, 2023

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1 Introduction

Multiple areas of physics are nowadays faced with the difficult task of simulating systems obeying the laws of quantum mechanics, the theory that to this day most accurately describes the nature around us. Academic reasearch is in fact exploiting, now more than ever, exotic quantum effects which arise in particular systems. This is why fields such as condensed matter physics, quantum chemistry and quantum optics are in desperate need to explore and analyse a wide variety of systems that could trigger breakthroughs in scientifical developments. However, simulating such systems is a demanding computational task. In general terms, a system of N interacting particles is described by a statevector living in a Hilbert space which scales up exponentially with the number of its constituents. Hence, the complete description of the wavefunction needs exponentially many coefficients, which is normally computationally unfeasible. Nonetheless, in the recent years, new advanced computational techniques along with Machine Learning (ML) methods based on deep learning, have been shown to tackle such systems in a more efficient way. This report sets out to present a statistical-based computational approach to simulating quantum systems, namely *Variational Monte-Carlo* (VMC) approach (mcmillan ground 1965), and how we can combine this with a neural network architecture. VMC is a computational method primarily used to estimate the ground state properties of a quantum system. In particular, the ground-state energy and the corresponding ground-state wavefunction of a system are computed by parametrizing the wavefunction of said system and reducing its energy successively by means of *stochastic gradient descent* (SGD) (ruder overview 2016). Early applications approximated the ground-state of the homogenous electron gas (ceperley ground 1978, ortiz correlation 1994). Later on, the cohesive energies of multiple compounds were estimated (li cohesive 1991, rajagopal variational 1995, malatesta variational 1997).
First efforts of combining VMC with ML culminated in the developement of the so-called Neural Quantum States (NQS). These use neural networks to parameterize the quantum mechanical wavefunction. They have been shown to provide state-of-the-art results on quantum spin-systems such as the one-dimensional transverse field Ising model and antiferromagnetic Heisenberg model (carleo solving 2017). Such models are motivated by the capability of neural networks to approximate an

arbitrary function. The accuracy of such methods has also been shown for systems in continuous space by analysing a variety of atoms and small molecules (hermann deep-neural-network 2020, pfau ab 2020, Pescia 2022).
The work presented here will cover the theoretical backgound which lies behind the idea of VMC for many-body quantum systems in continuous space. Artificial neural networks will also be introduced. We will then move on to consider a system made of N non-interacting bosonic quantum oscillators. Results obtained with the VMC method using simple gaussian and multivariate gaussian ansatze will be presented, and their accuracy analysed. Lastly, we will also show the same results using a NQS-based ansatz. To test the correct functioning of the VMC developed for this project, the NQS model will also be compared to the same ansatz trained using NetKet, an open-source Python library in which every aspect of the work included in this report is already implemented in a more comprehensive way (Vicentini 2022).