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# Efficient Anti-Symmetrization of a Neural Network Layer by Taming the Sign Problem

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**Abstract.** Explicit antisymmetrization of a neural network is a potential candidate for a universal function approximator for generic antisymmetric functions, which are ubiquitous in quantum physics. However, this procedure is a priori factorially costly to implement, making it impractical for large numbers of particles. The strategy also suffers from a sign problem. Namely, due to near-exact cancellation of positive and negative contributions, the magnitude of the antisymmetrized function may be significantly smaller than before anti-symmetrization. We show that the anti-symmetric projection of a two-layer neural network can be evaluated efficiently, opening the door to using a generic antisymmetric layer as a building block in anti-symmetric neural network Ansatzes. This approximation is effective when the sign problem is controlled, and we show that this property depends crucially the choice of activation function under standard Xavier/He initialization methods. As a consequence, using a smooth activation function requires re-scaling of the neural network weights compared to standard initializations.

**Keywords:**
Fermions,
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## 1 Introduction

Simulation of quantum chemistry from first principles depends on the accurate modeling of fermionic system comprised of the electrons. The Pauli exclusion principle dictates that fermionic wavefunctions must be antisymmetric with respect to particle exchange. This antisymmetry poses challenges; for instance, as the number of fermions increases, the effective parameterization of such wavefunctions becomes exceedingly complex for many systems. The antisymmetry condition also results in near-exact cancellation between positive and negative contributions when computing observables. This leads to the so-called fermionic sign problem (FSP), which was originally discovered in quantum Monte Carlo (QMC) simulations [2, 6, 12].

Over the last decade, the scientific community has witnessed a surge in the development of methods employing neural networks (NNs) as universal function approximators. This surge is due to advancements in software tools, hardware capabilities, and algorith-

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mic improvements. These developments have had a significant impact on the modeling of fermionic systems [3–5, 8, 9, 13].

However, constructing a universal NN representation for antisymmetric functions that does not suffer from the curse of dimensionality is still an open question. In the absence of symmetry constraints, even a simple structure such as a two-layer NN can act as a universal function approximator. In theory, one could explicitly antisymmetrize such a two-layer NN to parameterize universal antisymmetric functions. Such an explicitly antisymmetrized NN structure has been recently studied in QMC calculations, which can yield effectively the exact ground state energy for small atoms and molecules [5]. However, the computational cost of this antisymmetrization procedure appears a priori to grow factorially with the system size.

In this paper, we give a procedure to efficiently evaluate the explicit anti-symmetrization of a two-layer neural network using a quadrature procedure. This is surprising due to the factorially many terms in the definition of the anti-symmetrization. For this statement to be meaningful we require that the sign problem is controlled, meaning that the anti-symmetrization does not make the original function vanish due to cancellations. We demonstrate that with the standard Xavier/He initialization, the sign problem is controlled when the activation function in the neural network is rough. Examples of a rough (respectively smooth) activation function in the ReLU (respectively sigmoid). Alternatively, this statement implies that to avoid the sign problem with the sigmoid activation, the weights in the first layer need to be asymptotically larger than the standard Xavier/He initializations.

Among all activation functions, the exponential activation function (real or complex) plays a special role in our analysis. This is because antisymmetrizing a two-layer NN with an exponential activation function gives rise to a determinant (called a Slater determinant), which can be evaluated in polynomial time. By exploring the Fourier representation of a (rough) activation function, we can approximately express the explicitly antisymmetrized two-layer NN as a linear combination of polynomially (with respect to the system size and inverse precision) many Slater determinants. This overcomes the factorial scaling barrier, and gives rise to a polynomial-time algorithm for approximate evaluation of antisymmetrized two-layer neural networks (Theorem 3.3).

## 1.1 Related work

The representation of anti-symmetric functions is extensively studied in physics, where a widely used class of Ansatzes for anti-symmetric functions takes the form of a sum of Slater determinants. Slater determinants can span a dense subset of the anti-symmetric space but the representation is very inefficient. Indeed, even in the case of a finite single-particle state space $|\Omega| = \mathcal{O}(n)$ we would require $\binom{|\Omega|}{n}$ Slater determinants to span the anti-symmetric space. [17] finds certain anti-symmetric functions that cannot be efficiently approximated using a simple sum of Slater determinants, but can be effectively expressed using a more complex Ansatz called the Slater-Jastrow form.

In the machine learning literature there is a rich body of works related to permutation-invariant data, i.e. when the input data is a set [11, 14–16]. But the literature on anti-