$O(N^2)$ Universal Antisymmetry in Fermionic Neural Networks

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• Slater Determinant

Antisymmetric wavefunction Ansatz:

$$\psi_{\text{single}}(x) = \begin{vmatrix} \phi_1(x_1) & \cdots & \phi_1(x_N) \\ \vdots & & \vdots \\ \phi_N(x_1) & \cdots & \phi_N(x_N) \end{vmatrix} = \det[\phi_i(x_j)].$$

The model family of ψ_{single} is ***not*** universal since ϕ_i only depends on a **single electron**.

• Fermionic Neural Network

Pfau et al. (2020) propose Fermionic neural network (FermiNet) using **multi-electron** functions ϕ_i:

$$\psi_{\text{Fermi}}(x) = \det\left[\phi_i(x_j; \{x_{\backslash j}\})\right].$$

The model family of ψ_{Fermi} is proved to be universal

Lemma 1. *(Universality by Pfau et al. (2020)) For any antisymmetric function $\Psi(x)$, there exist multi-electron functions $\phi_1, \cdots \phi_N$, such that $\forall x$, there is $\psi_{Fermi}(x) = \Psi(x)$.*

• Reducing $O(N^3)$ Computation to $O(N^2)$

To avoid the $O(N^3)$ computation the of determinant, we construct a family of **pairwise Ansatz**:

$$\psi_{\text{pair}}(x) = \prod_{1 \leq i < j \leq N} \mathcal{A} \circ F(x_i, x_j; \{x_{\backslash\{i,j\}}\}),$$

where $\mathcal{A}$ is an antisymmetrizer,

Lemma 2. *(Antisymmetry) $\psi_{pair}(x)$ is antisymmetric under the permutation of any two elements x_m and x_n in x.*

• Instantiation from Han et al. (2019)

Han et al. (2019) propose a special form of pairwise construction using a **two-electron** function:

$$\psi_{\text{Han}}(x) = \phi_C(x) \cdot \prod_{1 \leq i < j \leq N} \left(\phi_B(x_j, x_i) - \phi_B(x_i, x_j)\right).$$

Theorem 1. *(Discontinuity) There exist ground-state wavefunctions $\Psi^g(x)$, such that if there is $\forall x$, $\psi_{Han}(x) = \Psi^g(x)$, then either ϕ_B or ϕ_C must be discontinuous on $\mathbb{R}^{dN}$.*

• Achieving Continuous Universality

The form of ψ_{Han} leads to discontinuity, which is difficult to approximate using neural networks. We provide another instantiation to achieve continuous universality using **multi-electron** functions:

$$\psi'_{\text{pair}}(x) = \prod_{1 \leq i < j \leq N} \left(\phi_B(x_j; \{x_{\backslash j}\}) - \phi_B(x_i; \{x_{\backslash i}\})\right).$$

Theorem 2. *(Continuous universality) For any ground-state wavefunction $\Psi^g(x)$, there exist a continuous multi-electron function ϕ_B, such that $\forall x$, $\psi'_{pair}(x) = \Psi^g(x)$.*

Corollary 1. *(Universality) For any antisymmetric function $\Psi(x)$, there exist a multi-electron function ϕ_B, such that $\forall x$, $\psi'_{pair}(x) = \Psi(x)$.*

• Connection with FermiNet

The form of ψ'_{pair} is actually a special case of ψ_{Fermi}

$$\psi'_{\text{pair}}(x) = \begin{vmatrix} 1 & \cdots & 1 \\ \phi_B(x_1; \{x_{\backslash 1}\}) & \cdots & \phi_B(x_N; \{x_{\backslash N}\}) \\ \phi_B^2(x_1; \{x_{\backslash 1}\}) & \cdots & \phi_B^2(x_N; \{x_{\backslash N}\}) \\ \vdots & \vdots & \vdots \\ \phi_B^{N-1}(x_1; \{x_{\backslash 1}\}) & \cdots & \phi_B^{N-1}(x_N; \{x_{\backslash N}\}) \end{vmatrix},$$

• Extension

We can use more (e.g., two) multi-electron functions

$$\psi''_{\text{pair}}(x) = \prod_{1 \leq i < j \leq N} \begin{vmatrix} \phi_A(x_i; \{x_{\backslash i}\}) & \phi_A(x_j; \{x_{\backslash j}\}) \\ \phi_B(x_i; \{x_{\backslash i}\}) & \phi_B(x_j; \{x_{\backslash j}\}) \end{vmatrix}.$$

Note that ψ''_{pair} becomes ψ'_{pair} when $\phi_A = 1$, thus similar (continuous) universality holds for ψ''_{pair}.

• Initial experiments

Table 1. Ground state energy. The values of 'Exact' column come from Chakravorty et al. (1993). The values of 'ψ'_{pair}' and 'ψ''_{pair}' are averaged on the last 1,000 iterations with sampling stride of 10.

Atom	ψ''_{pair}	ψ'_{pair}	Exact
Li	−7.4782	−7.4781	−7.47806032
Be	−14.6673	−14.6664	−14.66736
B	−24.5602	−24.4475	−24.65391
C	−37.3531	−37.2785	−37.8450
N	−53.1855	−53.0626	−54.5892

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