Representation of symmetric and anti-symmetric functions

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Totally anti-symmetric functions

For a permutation $\sigma \in \mathfrak{S}_N$ (symmetric group on n symbols):

$$\Psi(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)}) = (-1)^{\sigma} \Psi(x_1, x_2, \ldots, x_N)$$

$\Psi \in \bigwedge^N L^2(\mathbb{R}^d)$ (totally) anti-symmetric, in short:

$$\Psi(\sigma \boldsymbol{x}) = (-1)^{\sigma} \Psi(\boldsymbol{x})$$

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$\Psi \in \Lambda^N L^2(\mathbb{R}^d)$ (totally) anti-symmetric, in short:

$$\Psi(\sigma \boldsymbol{x}) = (-1)^\sigma \Psi(\boldsymbol{x})$$

Why? Identical particles in quantum mechanics

- Bosonic particles: symmetric (also has applications besides quantum);
- Fermionic particles: antisymmetric (Pauli's exclusion principle)

Variational principle for ground state

Given Hamiltonian operator H

$$E_0 = \inf_{\Psi \in \Lambda^N L^2(\mathbb{R}^d)} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

For practical calculations, require to choose an ansatz for antisymmetric functions.

Slater determinants (aka Quantum Chemistry 101)

Let $\{\varphi_i,\ i = 1, 2, \ldots, N\} \subset L^2(\mathbb{R}^d)$ be a set of orthonormal functions

$$\Psi_{\mathsf{SD}}[\{\varphi_i\}](\boldsymbol{x}) = \det \begin{bmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \cdots & \varphi_N(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \cdots & \varphi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(x_N) & \varphi_2(x_N) & \cdots & \varphi_N(x_N) \end{bmatrix}$$

This leads to the Hartree-Fock method, a cornerstone of quantum chemistry.

Going beyond Hartree-Fock

However, for most systems, the ansatz of Slater determinant is too restrictive and leads to huge error (correlation energy).

Many generalizations have been proposed over the years

- Configuration interaction;
- (unitary) Coupled cluster;
- Multi-configurational self-consistent field;
- Slater-Jastrow wavefunctions;
- ...

Remark. An entirely different approach to address anti-symmetry is via second quantization.

Backflow transformation ansatz

Proposed originally by [Feynman-Cohen, Phys Rev 1956] for liquid Helium.

Building blocks: $\varphi \in L^2(\mathbb{R}^d \times \mathbb{R}^{d(N-1)})$ s.t.

$$\varphi(x; \boldsymbol{y}) = \varphi(x; \sigma \boldsymbol{y}), \qquad \forall\, \sigma \in \mathfrak{S}_{N-1}$$

Backflow determinants:

$$\Psi_{\mathsf{BF}}[\{\varphi_i\}](\boldsymbol{x}) = \det \begin{bmatrix} \varphi_1(x_1; \bar{\boldsymbol{x}}_{-1}) & \varphi_2(x_1; \bar{\boldsymbol{x}}_{-1}) & \cdots & \varphi_N(x_1; \bar{\boldsymbol{x}}_{-1}) \\ \varphi_1(x_2; \bar{\boldsymbol{x}}_{-2}) & \varphi_2(x_2; \bar{\boldsymbol{x}}_{-2}) & \cdots & \varphi_N(x_2; \bar{\boldsymbol{x}}_{-2}) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(x_N; \bar{\boldsymbol{x}}_{-N}) & \varphi_2(x_N; \bar{\boldsymbol{x}}_{-N}) & \cdots & \varphi_N(x_N; \bar{\boldsymbol{x}}_{-N}) \end{bmatrix}$$

with the shorthand $\bar{\boldsymbol{x}}_{-i} := (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_N)$

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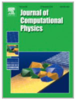

Solving many-electron Schrödinger equation using deep neural networks

Jiequn Han [a], Linfeng Zhang [a], Weinan E [a b c]

RESEARCH

FermiNet: Quantum Physics and Chemistry from First Principles

19 OCTOBER 2020

David Pfau, James Spencer, Alexander Matthews, Matthew Foulkes * (* External authors)

Deep-neural-network solution of the electronic Schrödinger equation

Jan Hermann, Zeno Schätzle & Frank Noé

Nature Chemistry **12**, 891–897 (2020) | Cite this article

No-go result for backflow ansatz?

Theorem (Huang-Landsberg-L.)

For each fixed N, for all total degree D sufficiently large, the algebraic ansatz map Ψ_{BF} is not surjective.

$$\dim(\text{target}) \approx N^{dN-d} \dim(\text{source}),$$

i.e., in general, one needs a linear combination of roughly N^{dN-d} backflow determinants to represent a general antisymmetric polynomial function.

Symmetric functions

Deep Sets [Zaheer et al, NeurIPS 2017], an ansatz for (totally) symmetric function

$$\Psi(\sigma \boldsymbol{x}) = \Psi(\boldsymbol{x}), \qquad \forall\, \sigma \in \mathfrak{S}_N$$

Choose a set of symmetric polynomials $\eta_1, \dots, \eta_m$ and write

$$f(\boldsymbol{x}) = g(\eta_1(\boldsymbol{x}), \eta_2(\boldsymbol{x}), \dots, \eta_m(\boldsymbol{x}))$$

for a general function g.

Deep Sets

Manzil Zaheer[1,2], **Satwik Kottur**[1], **Siamak Ravanbhakhsh**[1],
Barnabás Póczos[1], **Ruslan Salakhutdinov**[1], **Alexander J Smola**[1,2]
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Theorem (Chen-Chen-L.)

Given $d \geq 1$, $N \geq 1$, and a compact subset $\Omega \subset \mathbb{R}^d$. Let $\eta_1, \ldots, \eta_m$ generate $\mathcal{P}^{d,N}_{sym}(\mathbb{R})$ as $\mathbb{R}$-algebra.
For any $f : \Omega^N \to \mathbb{R}$ totally symmetric and continuous, there exists a unique continuous function $g : \boldsymbol{\eta}(\Omega^N) \to \mathbb{R}$ such that

$$f(\boldsymbol{x}) = g(\boldsymbol{\eta}(\boldsymbol{x}))$$

where $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots, \eta_m)$.

The generation condition can be relaxed [Wang et al, ICLR 2024].

Orbit distinguishing property: Given $\boldsymbol{x}$, $\boldsymbol{x}'$, if $\eta_k(\boldsymbol{x}) = \eta_k(\boldsymbol{x}')$ for all $k = 1, \ldots, m$, then $\exists \sigma \in \mathfrak{S}_N$, s.t., $\sigma \boldsymbol{x} = \boldsymbol{x}'$.

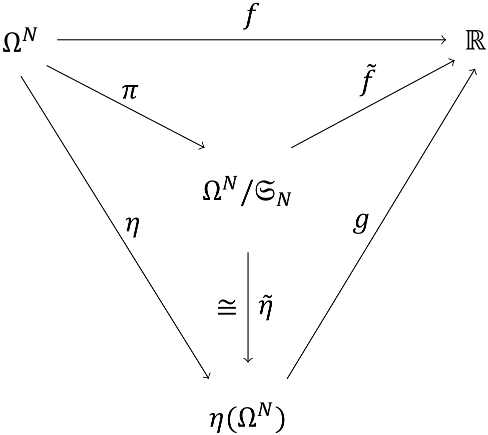

Figure: Commutative diagram for the proof of Theorem.

Symmetry to antisymmetry

Perhaps we can "borrow" results from symmetric case?

An old attempt:

$$\Psi(\boldsymbol{x}) = \Psi_0(\boldsymbol{x})\Phi_{\mathrm{sym}}(\boldsymbol{x})$$

for a specific anti-symmetric function Ψ_0.

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Works well for $d = 1$ [Cauchy, J. Ecole Polytech. 1815] by choosing

$$\Psi_0(\boldsymbol{x}) = \det \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{N-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^{N-1} \end{bmatrix} = \sum_{i<j} (x_j - x_i)$$

Vandemonde determinant (aka Slater det. w/ $\varphi_k(x) = x^{k-1}$)

However does not work in higher dimension (known in the physics / chemistry literature as the nodal surface difficulty)

From symmetry to antisymmetry

A new attempt to change the ansatz, inspired by Deep Sets:

$$\Psi(\boldsymbol{x}) = g(\eta_1(\boldsymbol{x}), \eta_2(\boldsymbol{x}), \dots, \eta_m(\boldsymbol{x}))$$

where $(\eta_1, \dots, \eta_m)$ sastify

- η_k is anti-symmetric and continuous;
- $\eta_k(\boldsymbol{x}) = 0$ if and only if $x_i = x_j$ for some $i \neq j$;
- orbit distinguishing for $\mathfrak{S}_N$.

Take-home summary of ansatz:

Linear combination of dets $\longrightarrow$ general odd function g of dets

Theorem (Chen-L.)

Given $d \geq 1$, $N \geq 1$, *and a compact subset* $\Omega \subset \mathbb{R}^d$, *let* $(\eta_1, \dots, \eta_m) : \Omega^N \to \mathbb{R}^m$ *satisfy the assumption.*
For any $f : \Omega^N \to \mathbb{R}$ *totally antisymmetric and continuous, there exits a unique continuous and odd function* $g : \boldsymbol{\eta}(\Omega^N) \to \mathbb{R}$ *such that*

$$f(\boldsymbol{x}) = g(\boldsymbol{\eta}(\boldsymbol{x}))$$

where $\boldsymbol{\eta} = (\eta_1, \eta_2, \dots, \eta_m)$.

Question: How large m needs to be?

Explicit construction for $\boldsymbol{\eta}$ (and an upper bound for m):

Key idea: Projecting points to $1D$.

- Set $m = \frac{N(N-1)}{2} \cdot (d-1) + 1$;
- Choose random vectors $\{w_i\}, i = 1, \cdots, m \subset \mathbb{S}^{d-1}$;
- Take η_k to be a Vandermonde determinant

$$\eta_k(\boldsymbol{x}) = \det \begin{bmatrix} 1 & w_k^\top x_1 & (w_k^\top x_1)^2 & \cdots & (w_k^\top x_1)^{N-1} \\ 1 & w_k^\top x_2 & (w_k^\top x_2)^2 & \cdots & (w_k^\top x_2)^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & w_k^\top x_N & (w_k^\top x_N)^2 & \cdots & (w_k^\top x_N)^{N-1} \end{bmatrix} = \sum_{i<j} w_k^\top (x_j - x_i)$$

$(\eta_1, \dots, \eta_m)$ satisfy the assumption with high probability (suffices to make sure that the $1D$ projections can distinguish points).

Conclusion

$$\Psi(\boldsymbol{x}) = g(\eta_1(\boldsymbol{x}), \ldots, \eta_m(\boldsymbol{x}))$$

- Ansatz for symmetric and antisymmetric functions;
- Exact representation for continuous functions;
- Efficiency: m depends mildly on d and N;

Some interesting directions:

- Regularity / singularity for wave-functions (in terms of g and $\boldsymbol{\eta}$);
- Training schemes for variational Monte Carlo;
- Applications to quantum systems.

Thank you for your attention

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Reference:

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- with Chongyao Chen and Ziang Chen, Representation theorem for multivariable totally symmetric functions, Commun. Math. Sci. [arXiv:2211.15958]
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