Machine Learning Meets Quantum Physics [1]

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Machine Learning

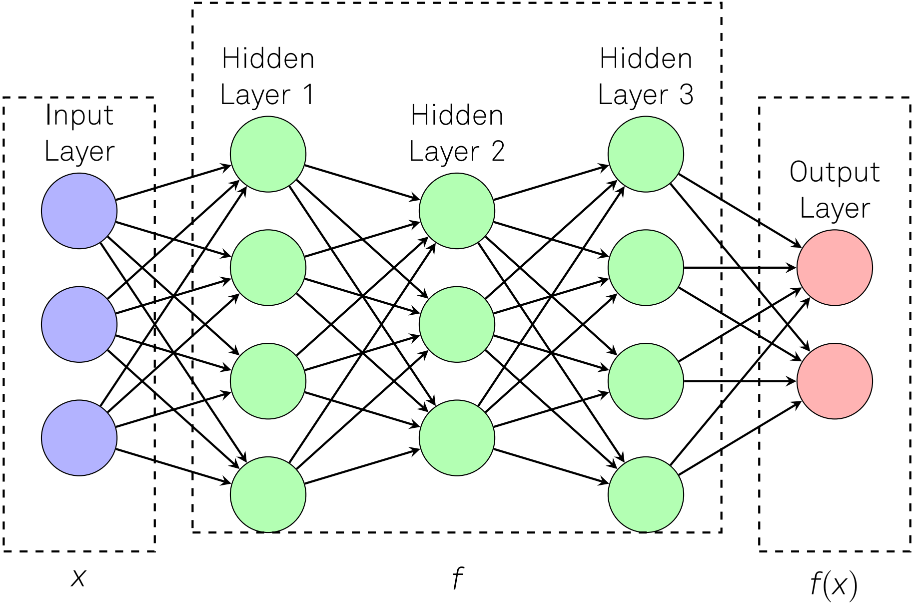
Theoretical Foundations of Machine Learning

Figure: David Hilbert

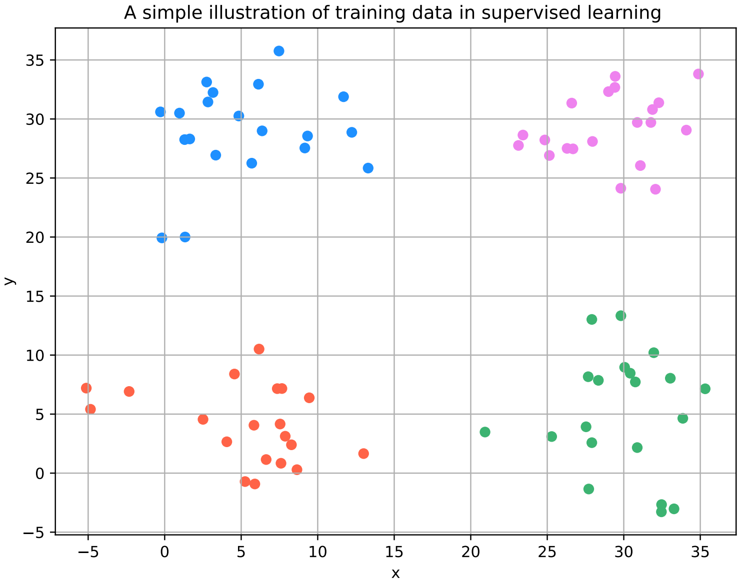
Hilbert's 13th Problem:

- **Question:** Whether a solution of a general seventh-degree equation $x^7 + ax^6 + \cdots + g = 0$ can be expressed as a composition of finite continuous functions of two variables.
- **Kolmogorov's Theorem:** Andrey Kolmogorov proved that any continuous function of n variables can be represented as a finite sum of continuous functions of one variable, combined with addition.
- **Arnold's Contribution:** Vladimir Arnold refined and simplified the result by proving that any multivariable function can be expressed as a finite composition of continuous functions of two variables.

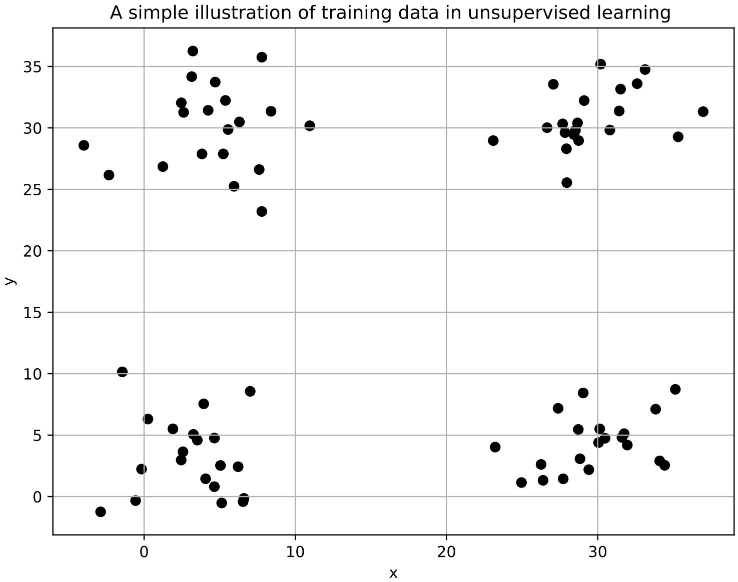
Simple Schematic of Machine Learning



Supervised Learning

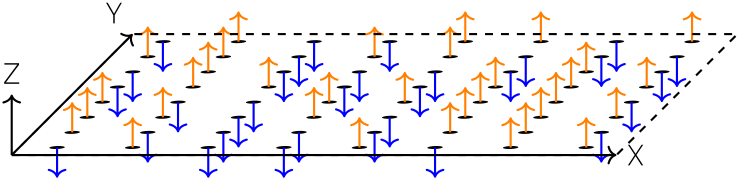


Unsupervised Learning



Uncovering Phases of Matter

Ising Model



$$H = -\sum_{\langle i,j \rangle} J_{ij} s_i s_j - \sum_i h_i s_i$$

Achievement Display

- Juan Carrasquilla: Neural network can be used to encode phases of matter and discriminate phase transitions in correlated many-body systems [2].
- Lei Wang: Unsupervised learning approaches can be used to analyze thermal phase transitions of the classical Ising model [3].
- Evert P. L. van Nieuwenburg: Demonstrate the success of this method on the topological phase transition in the Kitaev chain, the thermal phase transition in the classical Ising model, and the many-body-localization transition in a disordered quantum spin chain [4].

Tensor-Network & Neural-Network

Tensor

Tensor is a general form of number

- 0 rank tensor: Saclar **T**
- 1 rank tensor: Vector $\mathbf{T}_i$
- 2 rank tensor: Matrix $\mathbf{T}_{ij}$

Tensor product

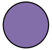
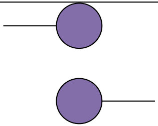
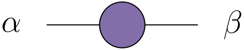
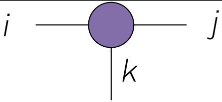
- Kronecker product:

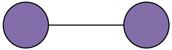
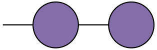
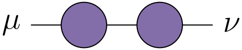
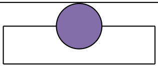
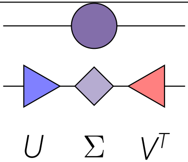
$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

- $|\psi_1\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\psi_2\rangle = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = |\psi_1\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

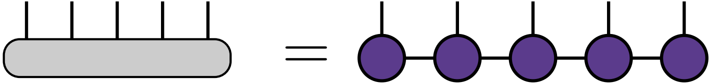
Graphical Representation of Tensor

Diagram	Label
	Scalar a
	Vector $\langle x \vert \& \vert x \rangle$
	Matrix $A_{\alpha\beta}$
	3 rank Tensor B_{ijk}

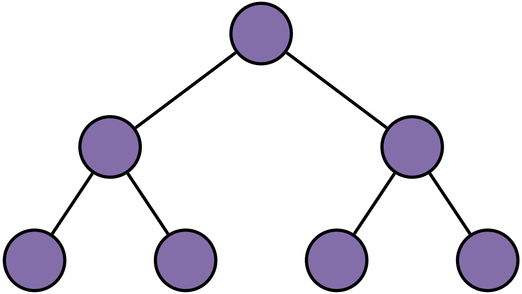
Calculation Diagram	Meaning
	$\langle x \vert x \rangle$
	$A_{\alpha\beta} \vert x \rangle$
	$\vert x \rangle \langle x \vert$
	Trace of matrix
	SVD

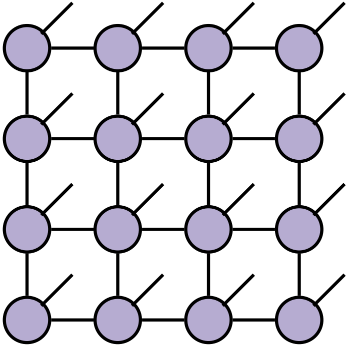
Tensor-Network

- Matrix Product State, MPS:



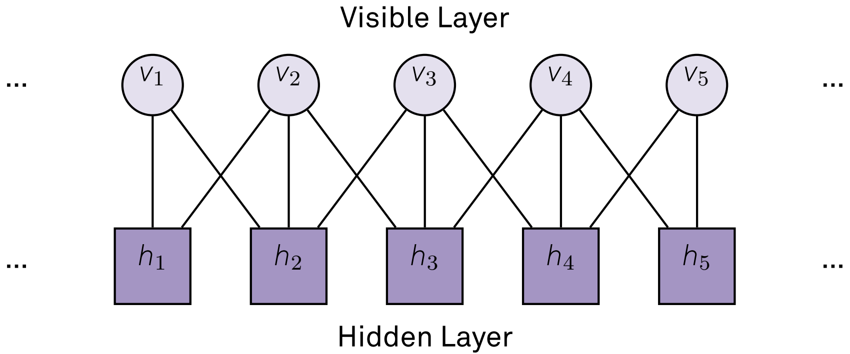
- Tree Tensor Network, TTN:





- Projected Entangled Pair States, PEPS:

Restricted Boltzmann Machine



$$\mathrm{H}(\mathbf{v}, \mathbf{h}) = -\sum_i a_i v_i - \sum_j b_j h_j - \sum_{i,j} v_i W_{ij} h_j,$$

Entanglement in Neural-Network States

Quantum Entanglement

Key Features

- **Non-locality**
- **Indivisibility**
- **Strong Correlation**

Quantum entanglement is a phenomenon in quantum mechanics where two or more particles become correlated in such a way that the state of one particle instantly influences the state of the other, no matter how far apart they are.
Albert Einstein called it "spooky action at a distance."

Concepts in QM & ML

- Tensor Network: Tensor Network, Tensors are multi-dimensional arrays that generalize scalars (0D), vectors (1D), and matrices (2D) to higher dimensions. Tensor Networks are mathematical tools used to represent and analyze complex quantum states and classical data.
- Entanglement Entropy: Entanglement Entropy is a fundamental concept in quantum physics, used to quantify the degree of entanglement in a quantum state. It measures the entanglement between two parts of a quantum system when the system is divided into subsystems. A large Entanglement Entropy indicates stronger entanglement between subsystems A and B.

Entanglement Area Law and Volume law

Feature	Area Law	Volume Law
Entanglement Growth	Scales with boundary area	Scales with volume
Typical Systems	low-energy states, systems with local interactions	high-energy states, systems with long-range interactions
Entanglement Level	lowly entangled quantum states	highly entangled quantum states
Classical Simulation Difficulty	Easier (efficient with tensor networks)	Harder (requires more resources

Short-Range RBM vs. Long-Range RBM

Feature	Short-Range RBM	Long-Range RBM
Interaction Range	Local (connects to nearby units)	Global (connects to any unit)
Number of Parameters	Fewer	More
Computational Complexity	Lower	Higher
Suitable Systems	Local interaction systems (e.g., low-energy states)	Long-range interaction systems (e.g., Coulomb interactions)
Entanglement Behavior	Typically follows area law	follow volume law

Entanglement in Neural-Network States

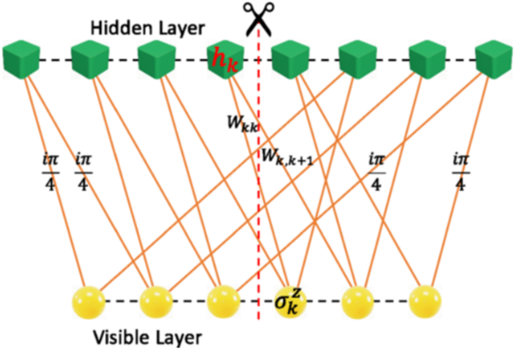


Figure: A Neural-Network Representation [1]

The system is divided into two subsystems, *A* and *B*, the entropy of each subsystem is proportional to its volume. Each visible neuron connects to at most three hidden ones, so the number of parameters needed to describe the subsystem scales linearly with the system size rather than exponentially, as in a conventional tensor-network representation.

Entanglement is not the limiting factor for the efficiency of the neural-network representation!

Quantum Many-Body Problems

Nonlocality, Bell's theorem and Bell's inequalities

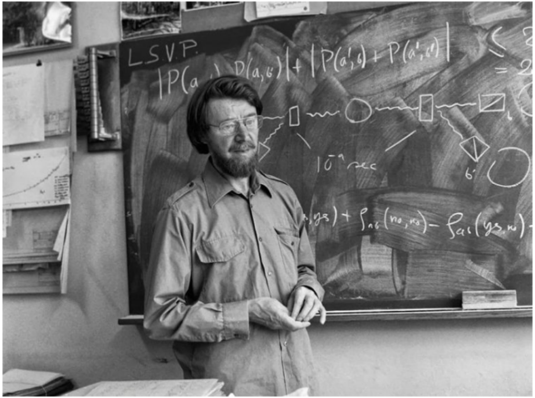


Figure: John Stewart Bell

Nonlocality refers to a phenomenon in quantum systems where there exists a correlation between two or more particles that goes beyond the description of classical locality. Bell’s theorem states that if the predictions of quantum mechanics do not conform to Bell’s inequalities, then quantum nonlocality exists.

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Machine Learning Detection of Bell Nonlocality in Quantum Many-Body Systems

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Phys. Rev. Lett. **120**, 240402 – **Published 14 June, 2018**

DOI: https://doi.org/10.1103/PhysRevLett.120.240402

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Deng [5] et al. used RBM to represent the wave functions of quantum many-body systems. They optimized the internal parameters through reinforcement learning to find the maximum quantum violations of Bell inequalities. RBM successfully detected the violations of multipartite Bell inequalities, demonstrating its advantages in handling complex many-body problems. The RBM method is not limited by the level of entanglement, making it suitable for highly entangled quantum states.

Quantum-Enhanced Machine Learning

Quantum Computing

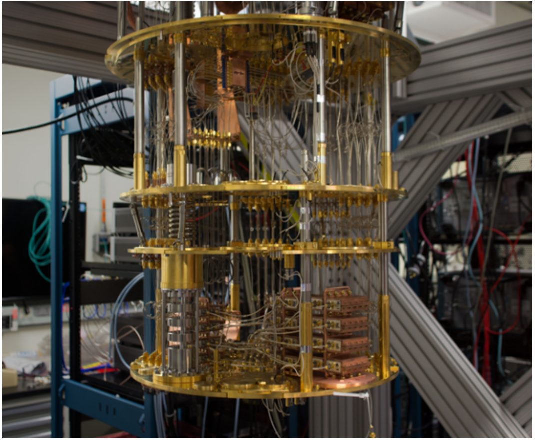


Figure: Quantum Computer

Quantum Computing

The core idea is to use the characteristics of quantum mechanics, such as interference and entanglement, to speed up certain computational tasks.

- Qubit
- Superposition
- Entanglement
- Quantum Gates
- Quantum Measurement

The HHL Algorithm [6]

$$\mathbf{A}\vec{x} = \vec{b}$$

$\mathbf{A}$ is an $N \times N$ matrix, and $\vec{x}$ and $\vec{b}$ are N-dimensional vectors.
The time complexity of classical algorithms, such as Gaussian elimination, for solving a system of linear equations is $\mathbf{O}(N^3)$.
The core idea of the HHL algorithm is to leverage the parallelism of quantum computing and quantum superposition to accelerate the solution of systems of linear equations.
Encode the vector b as a quantum state $|b\rangle$, and use Quantum Phase Estimation (QPE) to estimate the eigenvalues of matrix $\mathbf{A}$. Ultimately, the algorithm outputs a quantum state $|x\rangle$. The time complexity of the algorithm is about $\mathbf{O}(log(N))$.

END

In conclusion, although quantum machine learning still faces many challenges. marriage of machine learning and quantum physics is a promising field. Their mutual enhancement will drive scientific and technological progress.

Reference

[1] Sankar Das Sarma et al. "Machine learning meets quantum physics". en. In: *Physics Today* 72.3 (Mar. 2019), pp. 48–54.

[2] Juan Carrasquilla and Roger G. Melko. "Machine learning phases of matter". en. In: *Nature Phys* 13.5 (May 2017), pp. 431–434.

[3] Lei Wang. "Discovering phase transitions with unsupervised learning". en. In: *Phys. Rev. B* 94.19 (Nov. 2016), p. 195105.

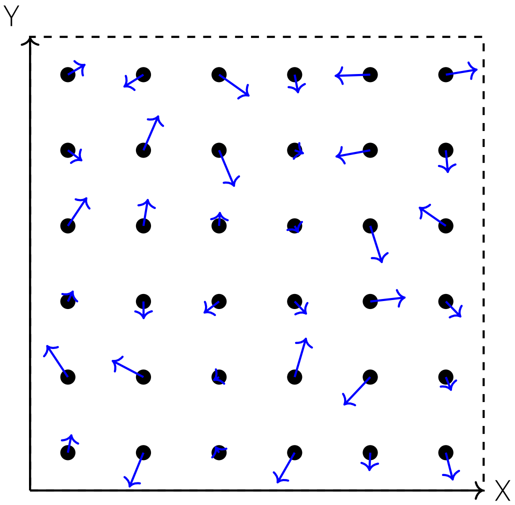
[4] Evert P. L. Van Nieuwenburg et al. "Learning phase transitions by confusion". en. In: *Nature Phys* 13.5 (May 2017), pp. 435–439.

[5] Dong-Ling Deng. "Machine Learning Detection of Bell Nonlocality in Quantum Many-Body Systems". en. In: *Phys. Rev. Lett.* 120.24 (June 2018), p. 240402.

[6] X. Gao et al. "A quantum machine learning algorithm based on generative models". en. In: *Sci. Adv.* 4.12 (Dec. 2018), eaat9004.

Q & A

Heisenberg Model



$$H = -\sum_{\langle i,j \rangle} J\mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{h}_i \cdot \mathbf{S}_i$$

Contraction

- $A_i^j = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$

  Contraction of A_i^j is

  $A_i^i = \sum a_{ii} = \mathrm{Tr}(A_i^j)$

- $A_i^j = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}, \quad B_j^k = \begin{pmatrix} 7 & 8 \\ 9 & 10 \\ 11 & 12 \end{pmatrix}$

  $A_i^j B_j^k = C_i^k = \begin{pmatrix} 58 & 64 \\ 139 & 154 \end{pmatrix}$

- $A_{ijk}^{xy} B_{lmn}^{jk} C_{xyz}^{mn} = D_{ilz}$

Input and output of A_{ijk}^{xy}

Input	Output
B^{ijk}	B'^{xy}
C_{xy}	C'_{ijk}
D_{xy}^{ij}	D'_k
E_x^{ijk}	E'^y
F_x^{jk}	$F_i'^y$
G_x^k	$G_{ij}'^y$
O_{xy}^{ijk}	O'

$$|00\rangle \xrightarrow{\textit{Hadamard Gate}} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle \xrightarrow{\textit{CNOT Gate}} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$