Title: Machine learning in physics

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Categories: Category:Machine learning, Category:Quantum information science, Category:Quantum programming, Category:Theoretical computer science

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Introduction

Glossary

History

Classical mechanics

Old quantum theory

Bra–ket notation

Hamiltonian

Interference

Complementarity

Decoherence

Entanglement

Energy level

Measurement

Nonlocality

Quantum number

State

Superposition

Symmetry

Tunnelling

Uncertainty

Wave function Collapse

Collapse

Bell's inequality

CHSH inequality

Davisson–Germer

Double-slit

Elitzur–Vaidman

Franck–Hertz

Leggett inequality

Leggett–Garg inequality

Mach–Zehnder

Popper
Quantum eraser Delayed-choice
Delayed-choice
Schrödinger's cat
Stern–Gerlach
Wheeler's delayed-choice
Overview
Heisenberg
Interaction
Matrix
Phase-space
Schrödinger
Sum-over-histories (path integral)
Dirac
Klein–Gordon
Pauli
Rydberg
Schrödinger
Bayesian
Consciousness causes collapse
Consistent histories
Copenhagen
de Broglie–Bohm
Ensemble
Hidden-variable
Many-worlds
Objective-collapse
Quantum logic
Superdeterminism
Relational
Transactional
Relativistic quantum mechanics
Quantum field theory
Quantum information science
Quantum computing
Quantum chaos
EPR paradox
Density matrix

Scattering theory

Quantum statistical mechanics

Quantum machine learning

Aharonov

Bell

Bethe

Blackett

Bloch

Bohm

Bohr

Born

Bose

de Broglie

Compton

Dirac

Davisson

Debye

Ehrenfest

Einstein

Everett

Fock

Fermi

Feynman

Glauber

Gutzwiller

Heisenberg

Hilbert

Jordan

Kramers

Lamb

Landau

Laue

Moseley

Millikan

Onnes

Pauli

Planck

Rabi

Raman

Rydberg

Schrödinger

Simmons

Sommerfeld

von Neumann

Weyl

Wien

Wigner

Zeeman

Zeilinger

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Applying machine learning (ML) (including deep learning) methods to the study of quantum systems is an emergent area of physics research. A basic example of this is quantum state tomography , where a quantum state is learned from measurement. [1] Other examples include learning Hamiltonians, [2] [3] learning quantum phase transitions , [4] [5] and automatically generating new quantum experiments. [6] [7] [8] [9] ML is effective at processing large amounts of experimental or calculated data in order to characterize an unknown quantum system, making its application useful in contexts including quantum information theory , quantum technology development, and computational materials design. In this context, for example, it can be used as a tool to interpolate pre-calculated interatomic potentials , [10] or directly solving the Schrödinger equation with a variational method . [11]

Applications of machine learning to physics

Noisy data

The ability to experimentally control and prepare increasingly complex quantum systems brings with it a growing need to turn large and noisy data sets into meaningful information. This is a problem that has already been studied extensively in the classical setting, and consequently, many existing machine learning techniques can be naturally adapted to more efficiently address experimentally relevant problems. For example, Bayesian methods and concepts of algorithmic learning can be fruitfully applied to tackle quantum state classification, [12] Hamiltonian learning, [13] and the characterization of an unknown unitary transformation . [14] [15] Other problems that have been addressed with this approach are given in the following list:

Identifying an accurate model for the dynamics of a quantum system, through the reconstruction of the Hamiltonian ; [16] [17] [18]

Extracting information on unknown states; [19] [20] [21] [12] [22] [1]

Learning unknown unitary transformations and measurements; [14] [15]

Engineering of quantum gates from qubit networks with pairwise interactions, using time dependent [23] or independent [24] Hamiltonians.

Improving the extraction accuracy of physical observables from absorption images of ultracold atoms (degenerate Fermi gas), by the generation of an ideal reference frame. [25]

Calculated and noise-free data

Quantum machine learning can also be applied to dramatically accelerate the prediction of quantum properties of molecules and materials. [26] This can be helpful for the computational design of new molecules or materials. Some examples include

Interpolating interatomic potentials; [27]

Inferring molecular atomization energies throughout chemical compound space ; [28]

Accurate potential energy surfaces with restricted Boltzmann machines; [29]

Automatic generation of new quantum experiments; [6] [7]

Solving the many-body, static and time-dependent Schrödinger equation; [11]

Identifying phase transitions from entanglement spectra; [30]

Generating adaptive feedback schemes for quantum metrology and quantum tomography . [31] [32]

Variational circuits

Variational circuits are a family of algorithms which utilize training based on circuit parameters and an objective function. [33] Variational circuits are generally composed of a classical device communicating input parameters (random or pre-trained parameters) into a quantum device, along with a classical Mathematical optimization function. These circuits are very heavily dependent on the architecture of the proposed quantum device because parameter adjustments are adjusted based solely on the classical components within the device. [34] Though the application is considerably infantile in the field of quantum machine learning, it has incredibly high promise for more efficiently generating efficient optimization functions.

Sign problem

Machine learning techniques can be used to find a better manifold of integration for path integrals in order to avoid the sign problem. [35]

Fluid dynamics

Physics discovery and prediction

A deep learning system was reported to learn intuitive physics from visual data (of virtual 3D environments) based on an unpublished approach inspired by studies of visual cognition in infants. [40] [39] Other researchers have developed a machine learning algorithm that could discover sets of basic variables of various physical systems and predict the systems' future dynamics from video recordings of their behavior. [41] [42] In the future, it may be possible that such can be used to automate the discovery of physical laws of complex systems. [41] Beyond discovery and prediction, "blank slate"-type of learning of fundamental aspects of the physical world may have further applications such as improving adaptive and broad artificial general intelligence . [additional citation(s) needed] In specific, prior machine learning models were "highly specialised and lack a general understanding of the world". [40]

See also

Quantum computing

Quantum machine learning

Quantum annealing

Quantum neural network

HHL Algorithm

References

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Differentiable programming
Information geometry
Statistical manifold
Automatic differentiation
Neuromorphic computing
Pattern recognition
Ricci calculus
Computational learning theory
Inductive bias
IPU
TPU
VPU
Memristor
SpiNNaker
TensorFlow
PyTorch
Keras
scikit-learn
Theano
JAX
Flux.jl
MindSpore
Portals Computer programming Technology
Computer programming
Technology
v
t
e
DiVincenzo's criteria
NISQ era
Quantum computing timeline
timeline
Quantum information
Quantum programming
Quantum simulation
Qubit physical vs. logical
physical vs. logical
Quantum processors cloud-based

cloud-based
Bell's
Eastin–Knill
Gleason's
Gottesman–Knill
Holevo's
No-broadcasting
No-cloning
No-communication
No-deleting
No-hiding
No-teleportation
PBR
Quantum speed limit
Threshold
Solovay–Kitaev
Schrödinger-HJW
Classical capacity entanglement-assisted quantum capacity
entanglement-assisted
quantum capacity
Entanglement distillation
Entanglement swapping
Monogamy of entanglement
LOCC
Quantum channel quantum network
quantum network
State purification
Quantum teleportation quantum energy teleportation quantum gate teleportation
quantum energy teleportation
quantum gate teleportation
Superdense coding
Post-quantum cryptography
Quantum coin flipping
Quantum money
Quantum key distribution BB84 SARG04 other protocols
BB84
SARG04
other protocols

Quantum secret sharing
Algorithmic cooling
Amplitude amplification
Bernstein–Vazirani
BHT
Boson sampling
Deutsch–Jozsa
Grover's
HHL
Hidden subgroup
Magic state distillation
Quantum annealing
Quantum counting
Quantum Fourier transform
Quantum optimization
Quantum phase estimation
Shor's
Simon's
VQE
BQP
DQC1
EQP
QIP
QMA
PostBQP
Quantum supremacy
Quantum volume
QC scaling laws
Randomized benchmarking XEB
XEB
Relaxation times T 1 T 2
T 1
T 2
Adiabatic quantum computation
Continuous-variable quantum information
One-way quantum computer cluster state
cluster state
Quantum circuit quantum logic gate

quantum logic gate

Quantum machine learning quantum neural network

quantum neural network

Quantum Turing machine

Topological quantum computer

Hamiltonian quantum computation

Codes 5 qubit CSS GKP quantum convolutional stabilizer Shor Bacon–Shor Steane Toric gnu

5 qubit

CSS

GKP

quantum convolutional

stabilizer

Shor

Bacon–Shor

Steane

Toric

gnu

Entanglement-assisted

Cavity QED

Circuit QED

Linear optical QC

KLM protocol

Neutral atom QC

Trapped-ion QC

Kane QC

Spin qubit QC

NV center

NMR QC

Charge qubit

Flux qubit

Phase qubit

Transmon

OpenQASM – Qiskit – IBM QX

Quil – Forest/Rigetti QCS

Cirq

Q#

libquantum

many others...

Quantum information science

Quantum mechanics topics