Quantum Technology and Artificial Intelligence

Morten Hjorth-Jensen

Department of Physics and Center for Computing in Science Education, University of Oslo, Norway

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What is this talk about?

The main emphasis is to give you a short and hopefully pedestrian introduction to the whys and hows of machine learning and quantum technologies. And why this could (or should) be of interest.

Thanks to many

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And sponsors

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3. Research Council of Norway (various grants) and my employers University of Oslo and Michigan State University

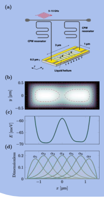
Quantum technology and machine learning/AI

AI for Quantum Technology

- Quantum mechanical many-body theories
- Molecular dynamics
- Density functional theory

Quantum Hardware

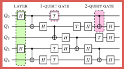
- Quantum control and sensors
- Quantum computers
- Catalysis



Quantum Technology and AI

Quantum Algorithms for AI

- Quantum computing
- Quantum algorithms
- Quantum machine learning
- Quantum inspired classical computing



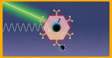
Societal impact and products

New medicines

Better shipping

Financial innovation

Quantum readiness



Quantum sensors and computers

- Drug discovery
- Quantum sensing
- Supply chain optimization
- Financial market modelling and risk analysis
- Material discovery

What is Machine Learning?

Machine Learning (ML) is the study of algorithms that improve through data experience.

Types of Machine Learning:

- **Supervised Learning:** Labeled data for classification or regression.
- **Unsupervised Learning:** No labels; discover hidden patterns.
- **Reinforcement Learning:** Learning through interaction with the environment.

ML Workflow:

$$\text{Data} \rightarrow \text{Model Training} \rightarrow \text{Prediction}$$

What is Quantum Computing?

Quantum computing leverages principles of quantum mechanics to perform computations beyond classical capabilities.

Key Concepts:

- **Superposition:** Qubits can exist in a combination of states.
- **Entanglement:** Correlation between qubits regardless of distance.
- **Quantum Interference:** Probability amplitudes interfere to solve problems.

Qubit Representation:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

What is Quantum Machine Learning?

Quantum Machine Learning (QML) integrates quantum computing with machine learning algorithms to exploit quantum advantages.

Motivation:

- High-dimensional Hilbert spaces for better feature representation.
- Quantum parallelism for faster computation.
- Quantum entanglement for richer data encoding.

Quantum Speedups in ML

Why Quantum?

- **Quantum Parallelism:** Process multiple states simultaneously.
- **Quantum Entanglement:** Correlated states for richer information.
- **Quantum Interference:** Constructive and destructive interference to enhance solutions.

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Example - Grover's Algorithm:

$$\text{Quantum Search Complexity: } O(\sqrt{N}) \text{ vs. } O(N)$$

Advantage: - Speedups in high-dimensional optimization and linear algebra problems.

Challenges and Limitations

1. **Quantum Hardware Limitations:**
   - Noisy Intermediate-Scale Quantum (NISQ) devices.
   - Decoherence and limited qubit coherence times.
2. **Data Encoding:**
   - Efficient embedding of classical data into quantum states.
3. **Scalability:**
   - Difficult to scale circuits to large datasets.

Applications of Quantum Machine Learning

1. **Quantum mechanical many-particle syste,s:**
   - Simulate molecular structures with QML.
2. **Finance:**
   - Quantum optimization for portfolio management.
3. **Image Recognition:**
   - Quantum-enhanced convolutional neural networks.

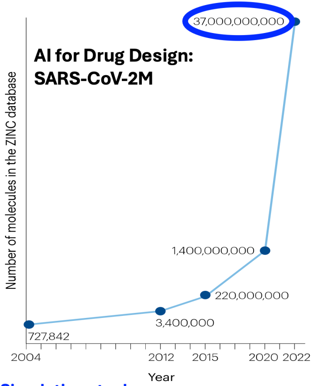
AI/ML and some statements you may have heard (and what do they mean?)

1. Fei-Fei Li on ImageNet: **map out the entire world of objects** (The data that transformed AI research)
2. Russell and Norvig in their popular textbook: **relevant to any intellectual task; it is truly a universal field** (Artificial Intelligence, A modern approach)
3. Woody Bledsoe puts it more bluntly: **in the long run, AI is the only science** (quoted in Pamilla McCorduck, Machines who think)

If you wish to have a critical read on AI/ML from a societal point of view, see Kate Crawford's recent text Atlas of AI.

Here: with AI/ML we intend a collection of machine learning methods with an emphasis on statistical learning and data analysis

Machine learning and AI models are computationally expensive



Simulations took:

90 days on **250 GPUs & 640 cpu-core**
1 day on **27000 GPU** Summit supercomputer

Nature Reviews Drug Discovery **23**, 141–155 (2024)

TOP4 Powerful Supercomputers as of Nov 2024

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
		76	1,353.00	2,055.72	24,607
	Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States				
4	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	

Advance nuclear weapon science and scientific discovery.

US$600 million

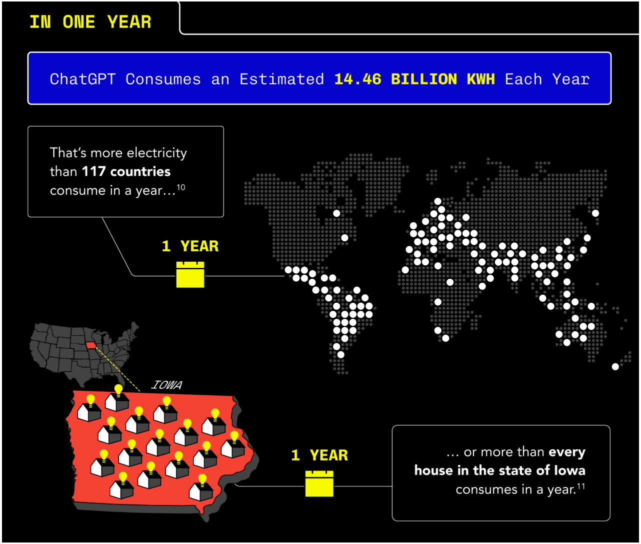
nature reviews drug discovery

Perspective | Published: 08 December 2023

Integrating QSAR modelling and deep learning in drug discovery: the emergence of deep QSAR

4

And power greedy, perhaps quantum computers can reduce the impact?



Taken from https://www.businessenergyuk.com/knowledge-hub/

Main categories of Machine Learning

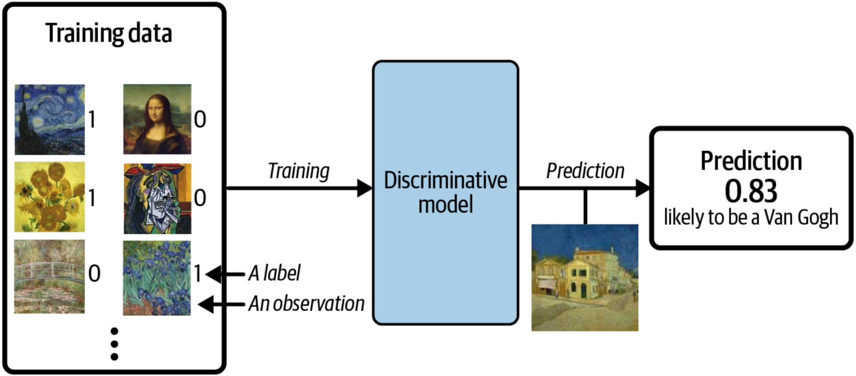
Another way to categorize machine learning tasks is to consider the desired output of a system. Some of the most common tasks are:

- Classification: Outputs are divided into two or more classes. The goal is to produce a model that assigns inputs into one of these classes. An example is to identify digits based on pictures of hand-written ones. Classification is typically supervised learning.
- Regression: Finding a functional relationship between an input data set and a reference data set. The goal is to construct a function that maps input data to continuous output values.
- Clustering: Data are divided into groups with certain common traits, without knowing the different groups beforehand. It is thus a form of unsupervised learning.

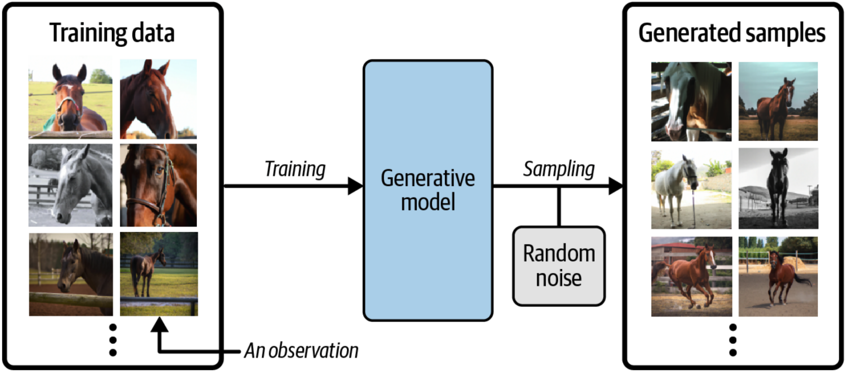
The plethora of machine learning algorithms/methods

1. Deep learning: Neural Networks (NN), Convolutional NN, Recurrent NN, Boltzmann machines, autoencoders and variational autoencoders and generative adversarial networks, stable diffusion and many more generative models
2. Bayesian statistics and Bayesian Machine Learning, Bayesian experimental design, Bayesian Regression models, Bayesian neural networks, Gaussian processes and much more
3. Dimensionality reduction (Principal component analysis), Clustering Methods and more
4. Ensemble Methods, Random forests, bagging and voting methods, gradient boosting approaches
5. Linear and logistic regression, Kernel methods, support vector machines and more
6. Reinforcement Learning; Transfer Learning and more

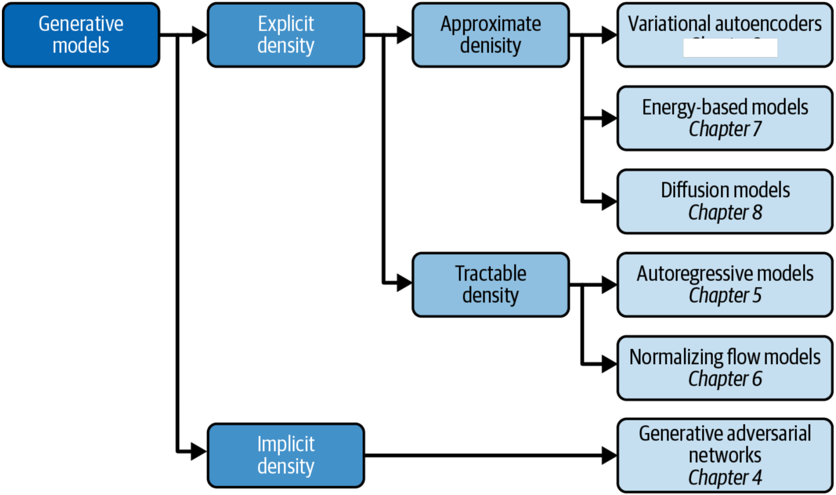
Example of discriminative modeling, taken from Generative Deep Learning by David Foster



Example of generative modeling, taken from Generative Deep Learning by David Foster



Taxonomy of generative deep learning, taken from Generative Deep Learning by David Foster



What are the basic Machine Learning ingredients?

Almost every problem in ML and data science starts with the same ingredients:

- The dataset $\boldsymbol{x}$ (could be some observable quantity of the system we are studying)
- A model which is a function of a set of parameters $\boldsymbol{\alpha}$ that relates to the dataset, say a likelihood function $p(\boldsymbol{x}|\boldsymbol{\alpha})$ or just a simple model $f(\boldsymbol{\alpha})$
- A so-called **loss/cost/risk** function $\mathcal{C}(\boldsymbol{x}, f(\boldsymbol{\alpha}))$ which allows us to decide how well our model represents the dataset.

We seek to minimize the function $\mathcal{C}(\boldsymbol{x}, f(\boldsymbol{\alpha}))$ by finding the parameter values which minimize $\mathcal{C}$. This leads to various minimization algorithms. It may surprise many, but at the heart of all machine learning algortihms there is an optimization problem.

Low-level machine learning, the family of ordinary least squares methods

Our data which we want to apply a machine learning method on, consist of a set of inputs $\boldsymbol{x}^T = [x_0, x_1, x_2, \dots, x_{n-1}]$ and the outputs we want to model $\boldsymbol{y}^T = [y_0, y_1, y_2, \dots, y_{n-1}]$. We assume that the output data can be represented (for a regression case) by a continuous function f through

$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon.$$

Setting up the equations

In linear regression we approximate the unknown function with another continuous function $\tilde{\boldsymbol{y}}(\boldsymbol{x})$ which depends linearly on some unknown parameters $\boldsymbol{\theta}^T = [\theta_0, \theta_1, \theta_2, \dots, \theta_{p-1}]$.
The input data can be organized in terms of a so-called design matrix with an approximating function $\tilde{\boldsymbol{y}}$

$$\tilde{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\theta},$$

The objective/cost/loss function

The simplest approach is the mean squared error

$$C(\boldsymbol{\Theta})=\frac{1}{n}\sum_{i=0}^{n-1}(y_i-\tilde{y}_i)^2=\frac{1}{n}\left\{(\boldsymbol{y}-\tilde{\boldsymbol{y}})^T(\boldsymbol{y}-\tilde{\boldsymbol{y}})\right\},$$

or using the matrix $\boldsymbol{X}$ and in a more compact matrix-vector notation as

$$C(\boldsymbol{\Theta})=\frac{1}{n}\left\{(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\theta})^T(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\theta})\right\}.$$

This function represents one of many possible ways to define the so-called cost function.

Training solution

Optimizing with respect to the unknown parameters θ_j we get

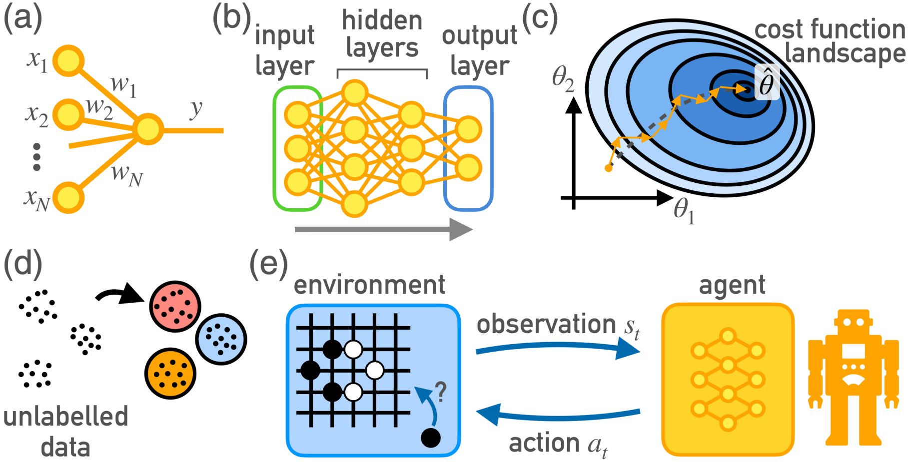
$$\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\theta},$$

and if the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is invertible we have the optimal values

$$\hat{\boldsymbol{\theta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

We say we 'learn' the unknown parameters $\boldsymbol{\theta}$ from the last equation.

Schematic view on Machine Learning approaches



Scientific Machine Learning

An important and emerging field is what has been dubbed as scientific ML, see the article by Deiana et al, Applications and Techniques for Fast Machine Learning in Science, Big Data **5**, 787421 (2022) `https://doi.org/10.3389/fdata.2022.787421`

The authors discuss applications and techniques for fast machine learning (ML) in science – the concept of integrating power ML methods into the real-time experimental data processing loop to accelerate scientific discovery. The report covers three main areas

1. applications for fast ML across a number of scientific domains;
2. techniques for training and implementing performant and resource-efficient ML algorithms;
3. and computing architectures, platforms, and technologies for deploying these algorithms.

ML for detectors

Engineering

Volume 6, Issue 3, March 2020, Pages 264-274

Research Artificial Intelligence—Review

A Survey of Accelerator Architectures for Deep Neural Networks

Yiran Chen [a], Yuan Xie [b], Linghao Song [a], Fan Chen [a], Tianqi Tang [b]

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https://doi.org/10.1016/j.eng.2020.01.007

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Physics driven Machine Learning

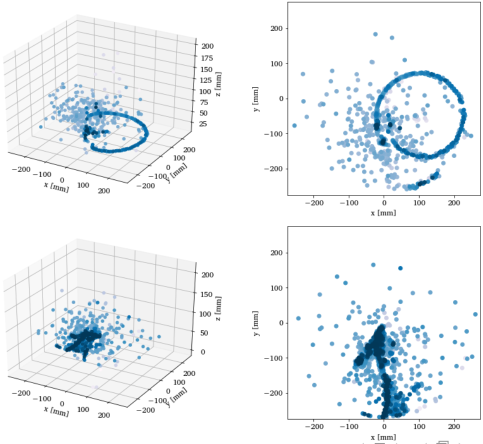
Another hot topic is what has loosely been dubbed **Physics-driven deep learning**. See the recent work on Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators, Nature Machine Learning, vol 3, 218 (2021).

And more

- An important application of AI/ML methods is to improve the estimation of bias or uncertainty due to the introduction of or lack of physical constraints in various theoretical models.
- We expect to use AI/ML algorithms and methods to improve our knowledge about correlations of physical model parameters in data for complex systems. Deep learning methods show great promise in circumventing the exploding dimensionalities encountered in many problems.

Argon-46 by Solli et al., NIMA 1010, 165461 (2021)

Each row is one event in two projections, where the color intensity of each point indicates higher charge values recorded by the detector. The bottom row illustrates a carbon event with a large fraction of noise, while the top row shows a proton event almost free of noise.



Many-body physics, Quantum Monte Carlo and deep learning

Given a hamiltonian H and a trial wave function Ψ_T, the variational principle states that the expectation value of $\langle H \rangle$, defined through

$$\langle E \rangle = \frac{\int d\boldsymbol{R}\Psi^*_T(\boldsymbol{R})H(\boldsymbol{R})\Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R}\Psi^*_T(\boldsymbol{R})\Psi_T(\boldsymbol{R})},$$

is an upper bound to the ground state energy E_0 of the hamiltonian H, that is

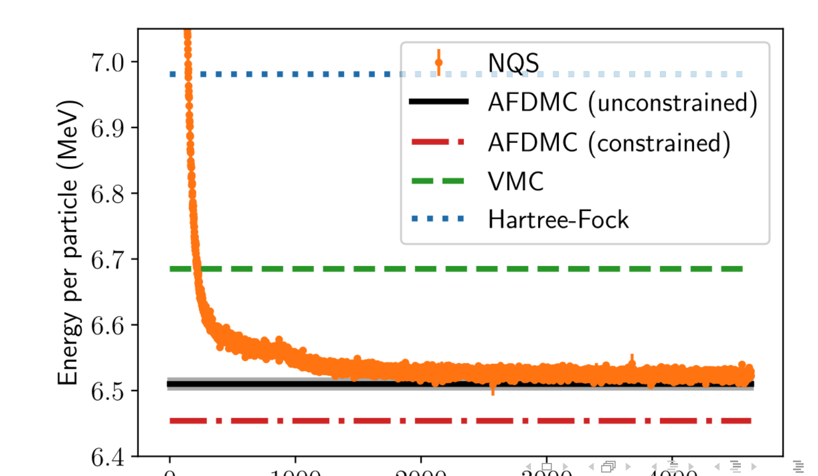
$$E_0 \le \langle E \rangle.$$

In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. Traditional integration methods such as the Gauss-Legendre will not be adequate for say the computation of the energy of a many-body system. **Basic philosophy: Let a neural network find the optimal wave function**

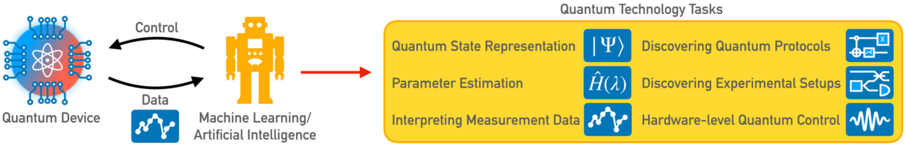
Why Feed Forward Neural Networks (FFNN)?

According to the *Universal approximation theorem*, a feed-forward neural network with just a single hidden layer containing a finite number of neurons can approximate a continuous multidimensional function to arbitrary accuracy, assuming the activation function for the hidden layer is a **non-constant, bounded and monotonically-increasing continuous function**.

Dilute neutron star matter from neural-network quantum states by Fore et al, Physical Review Research 5, 033062 (2023) at density $\rho = 0.04$ fm^{-3}



And then quantum engineering



1. Quantum Support Vector Machines (QSVM)

Quantum Kernel Estimation:

- Maps classical data to a quantum Hilbert space.
- Quantum kernel measures similarity in high-dimensional space.

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Quantum Kernel:

$$K(x, x') = |\left\langle \psi(x)|\psi(x')\middle|\psi(x)|\psi(x')\right\rangle|^2$$

Advantage: - Potentially exponential speedup over classical SVMs.

2. Quantum Neural Networks (QNNs)

Quantum Neural Networks replace classical neurons with parameterized quantum circuits.

Key Concepts:

- Quantum Gates as Activation Functions.
- Variational Quantum Circuits (VQCs) for optimization.

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Parameterized Quantum Circuit:

$$U(\theta) = \prod_i R_y(\theta_i) \cdot CNOT \cdot R_x(\theta_i)$$

Advantage: - Quantum gradients enable exploration of non-convex landscapes.

3. Quantum Boltzmann Machines (QBMs)

Quantum Boltzmann Machines leverage quantum mechanics to sample from a probability distribution.

- Quantum tunneling aids in escaping local minima.
- Quantum annealing for optimization problems.

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Quantum Hamiltonian:

$$H = -\sum_i b_i \sigma_i^z - \sum_{ij} w_{ij} \sigma_i^z \sigma_j^z$$

Advantage: - Efficient sampling in complex probability distributions.

Future Perspectives in QML

1. **Fault-Tolerant Quantum Computing:**
   - Overcoming noise for stable quantum circuits.
2. **Hybrid Quantum-Classical Models:**
   - Combining quantum circuits with classical neural networks.
3. **Quantum Internet:**
   - Distributed quantum machine learning over quantum networks.

Observations (or conclusions if you prefer)

- How do we develop insights, competences, knowledge in statistical learning that can advance a given field?
  - For example: Can we use ML to find out which correlations are relevant and thereby diminish the dimensionality problem in standard many-body theories?
  - Can we use AI/ML in detector analysis, accelerator design, analysis of experimental data and more?
  - Can we use AL/ML to carry out reliable extrapolations by using current experimental knowledge and current theoretical models?
- The community needs to invest in relevant educational efforts and training of scientists with knowledge in AI/ML. These are great challenges to the CS and DS communities
- Quantum computing and quantum machine learning not discussed here
- Most likely tons of things I have forgotten