Quantum Technology and Artificial Intelligence

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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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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 Model Example:

$$U(\theta) |x\rangle \implies \text{Quantum Kernel for Classification}$$

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

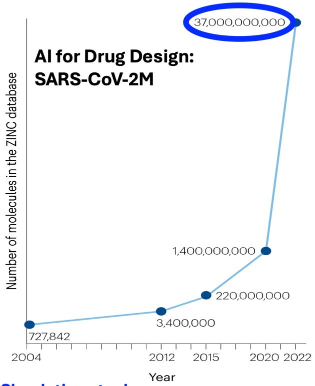
1. Fei-Fei Li on ImageNet: **map out the entire world of objects** (The data that transformed AI research)
2. Russell and Norvig in their popular textbook: **relevant to any intellectual task; it is truly a universal field** (Artificial Intelligence, A modern approach)
3. Woody Bledsoe puts it more bluntly: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

AI for Drug Design: SARS-CoV-2M



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.

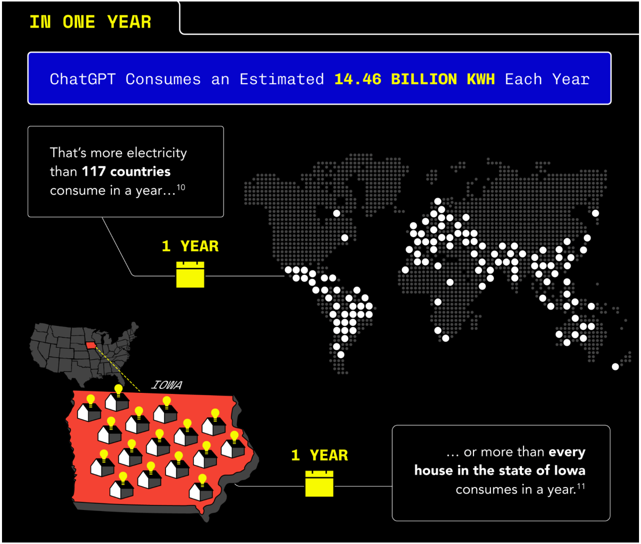
US$600 million

nature reviews drug discovery

Perspective | Published: 08 December 2023

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

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



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

Main categories of Machine Learning

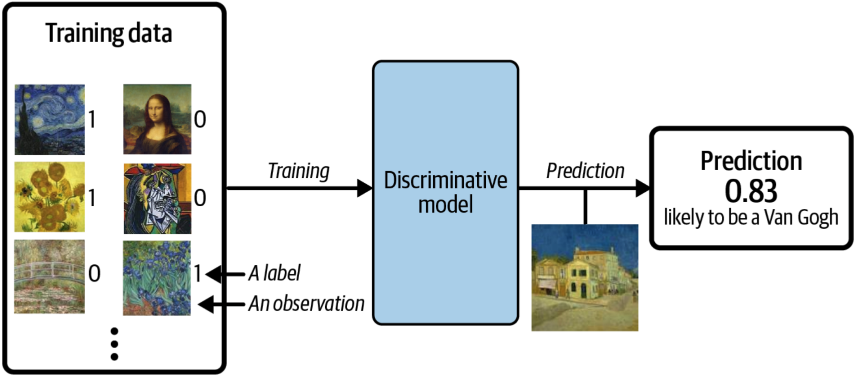
Another way to categorize machine learning tasks is to consider the desired output of a system. Some of the most common tasks are:

- 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.

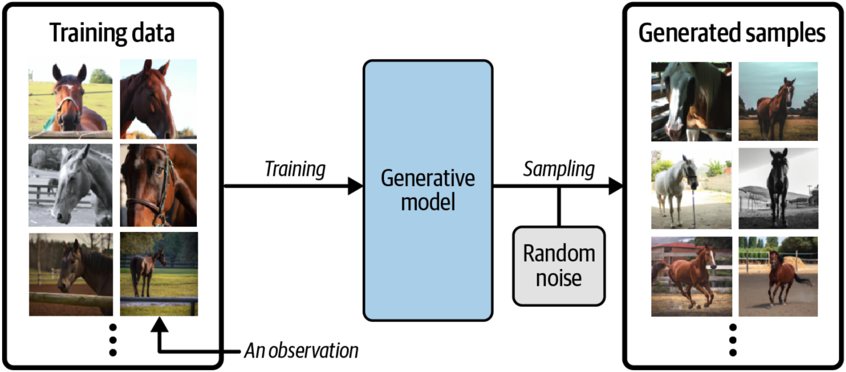
The plethora of machine learning algorithms/methods

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

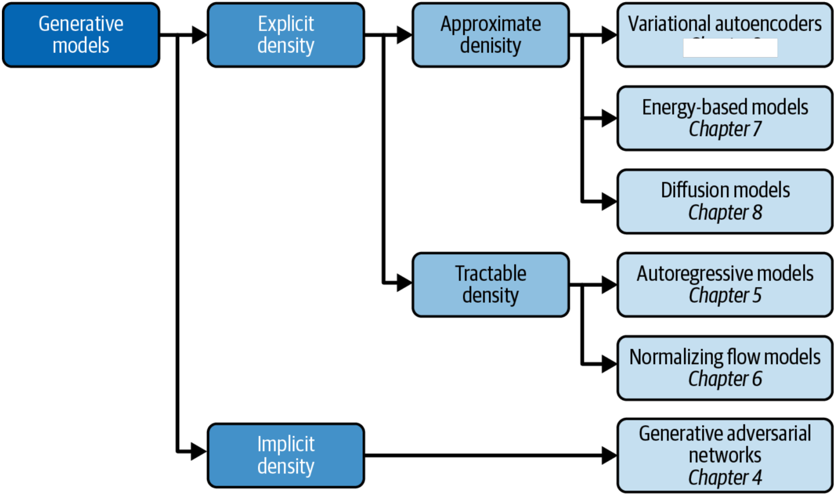
Example of discriminative modeling, taken from Generative Deep Learning by David Foster



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.

Quantum Kernel Estimation:

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

1. Quantum Support Vector Machines (QSVM)

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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.

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 Chemistry:**
   - Simulate molecular structures with QML.
2. **Finance:**
   - Quantum optimization for portfolio management.
3. **Image Recognition:**
   - Quantum-enhanced convolutional neural networks.

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.