AI & Machine Learning in Physics

PHYS3151 (6 credits)

Time & Place : Tue 13:30-14:20, 14:30-15:20 MB 122
Fri 14:30-15:20 MB 142

Teachers: Zi Yang Meng (zymeng@hku.hk), HOC 231

https://quantummc.xyz/hku-phys3151-machine-learning-in-physics-2023/

Tutor: Ting-Tung Wang (leowdd@connect.hku.hk), HOC 217

AI & Machine Learning in Physics

Teaching Materials:

https://quantummc.xyz/hku-phys3151-machine-learning-in-physics-2023/

Slides / Reading materials

Python notebooks

Assignments

Assessment Methods and Weighting

- Assignments 30%
- Presentation 20%
- Project report 20%
- Exam. 30%

AI & Machine Learning in Physics

Literature: Books

there are many, actually too many

- Ethem Alpaydin, Introduction to Machine Learning, Third Edition, MIT Press 2014
- Simon Haykin, Neural Networks and Learning Machines, Third Edition, Pearson 2009
- Stuart Russell, Peter Norvig, Artificial Intelligence, Third Edition, Pearson 2010

Literature: Online material

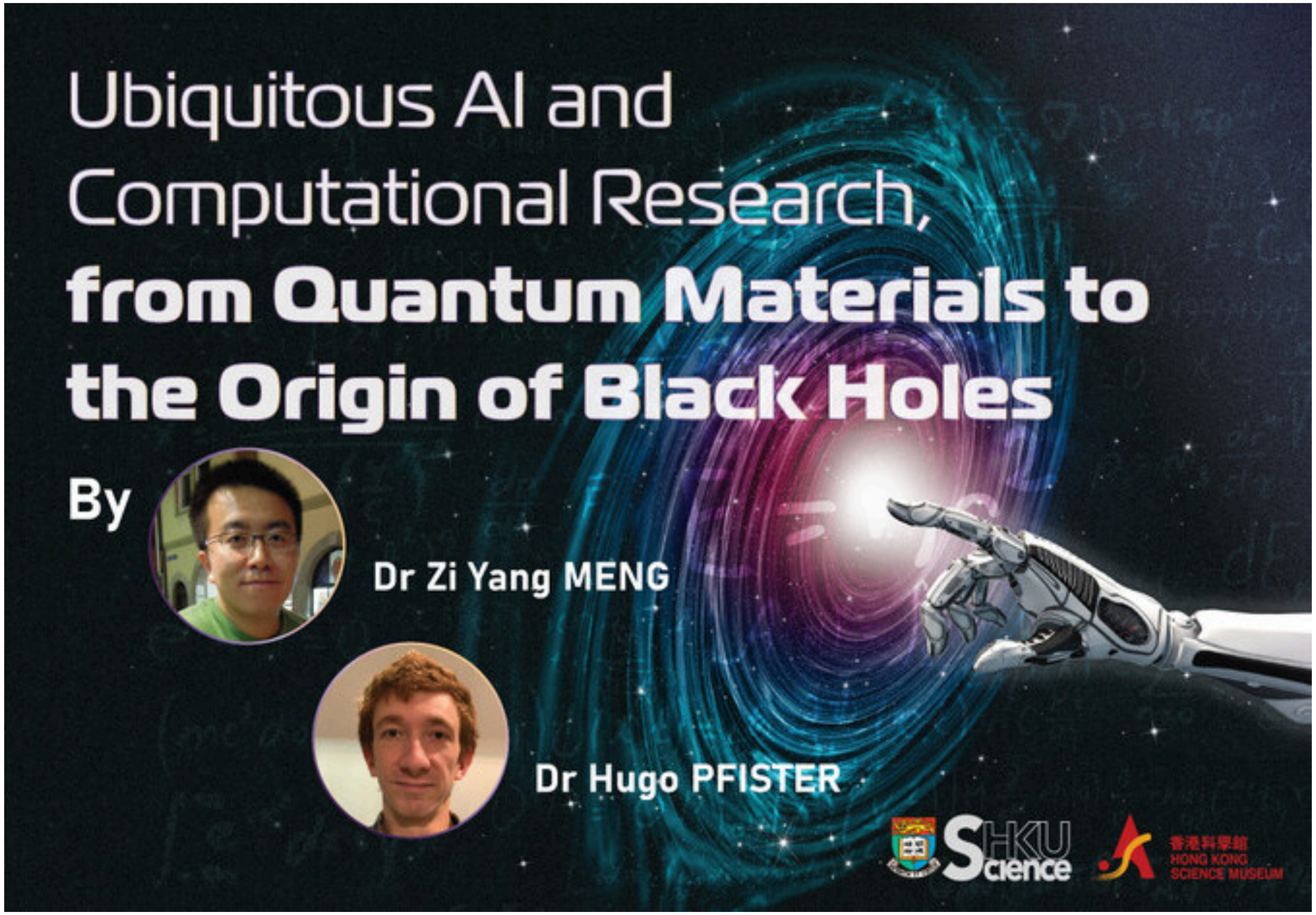
Andrew Ng, Stanford University http://www.holehouse.org/mlclass/

https://www.youtube.com/playlist?list=PLLssT5z_DsK-h9vYZkQkYNWcItqhlRJLN

Neuroscience For Kids http://faculty.washington.edu/chudler/neurok.html

Michael Nielsen, scientist at home, the best reading material for NN

http://neuralnetworksanddeeplearning.com



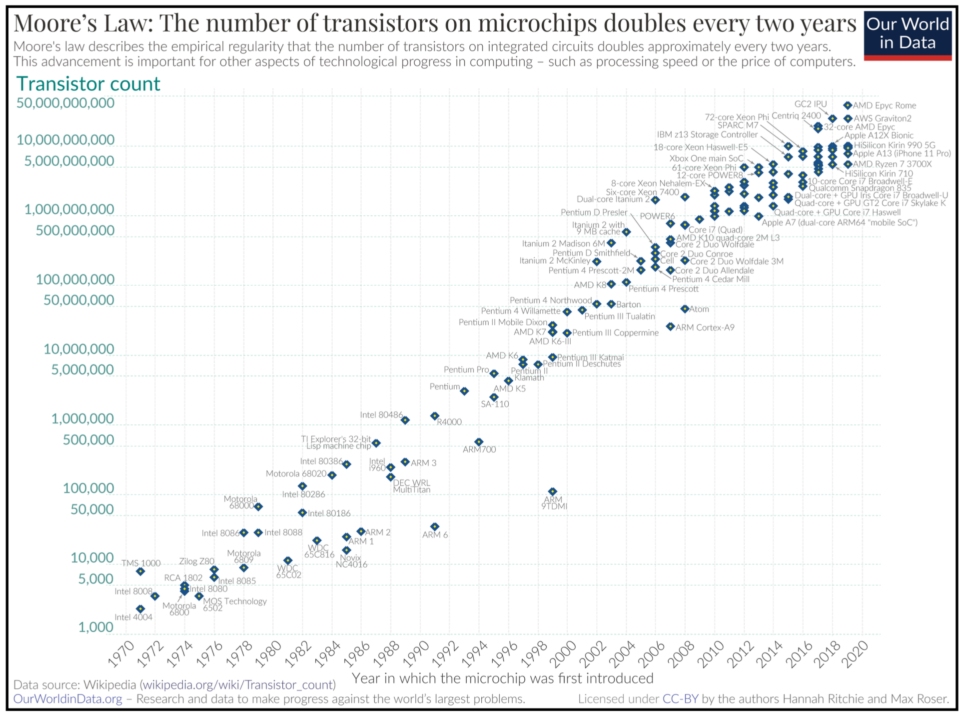
Hong Kong Science Museum 01/15/2022

https://www.scifac.hku.hk/events/ai-computational-research

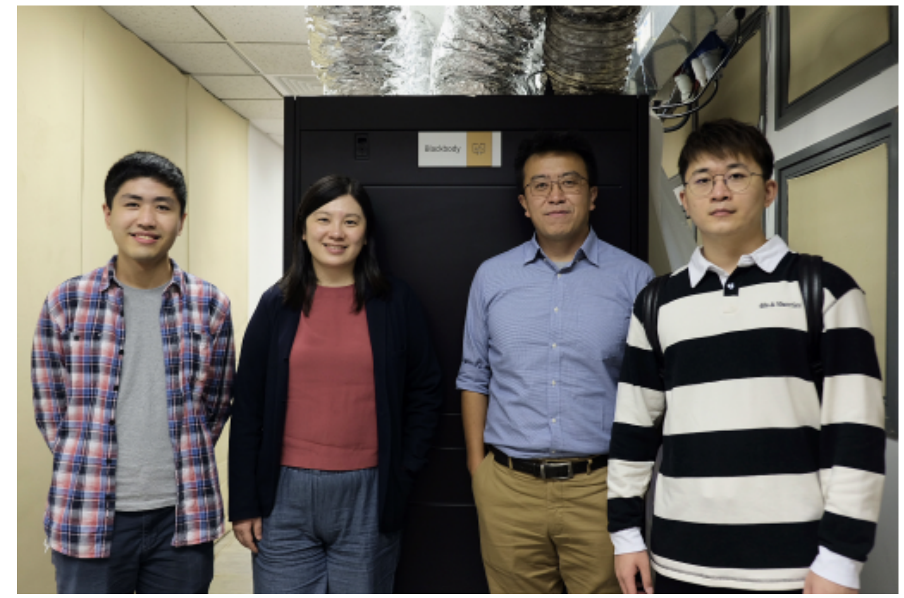
Computation becomes easy

50 years of supercomputer tracks Moore's law

 # transistors doubles every 2 years



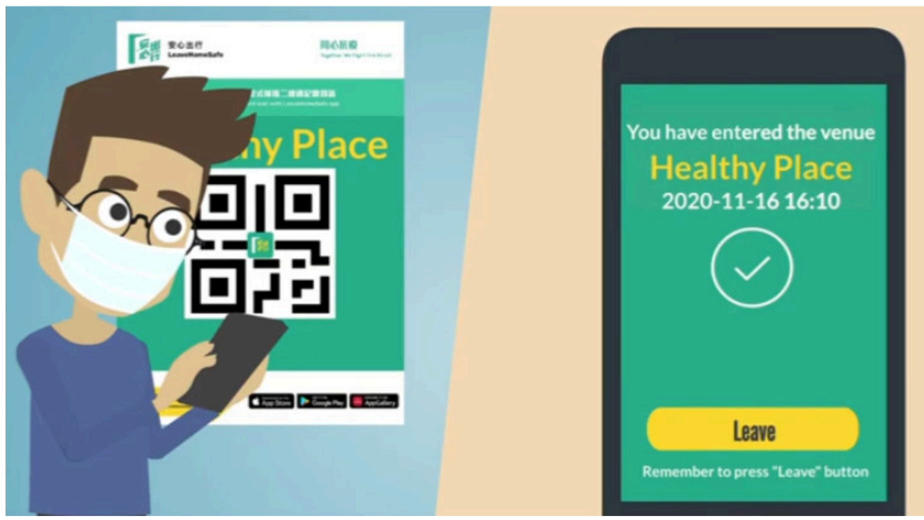
Our own Blackbody



	Supercomputer	Personal Computer	Human Brain
Computational Units	32,000 Xeon CPUs 10^12 transistors	4 CPUs, 10^9 transistors	10^11 neurons
Cycle time	10^-9 sec	10^-9 sec	10^-3 sec
Operations/sec	10^15	10^10	10^17
Memory updates/sec	10^14	10^10	10^14
Weight / Space	150 tons / Basketball court	1 Kg / A4 Paper	1.5 Kg / 1/6 basketball
Power consumption	500 megawatt	100 watt	20 watt

AI & Machine Learning in Physics

In the era of AI & Big data



In April 2017, AlphaGo vs. Jie Ke

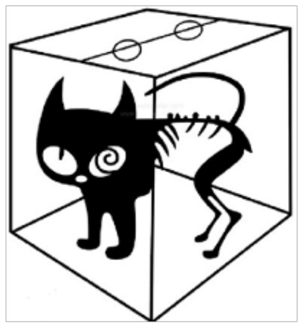
- The machine played perfect…
- I am so behind, unbelievable…
- AlphaGo is not the God, but it is a superior species than human being…

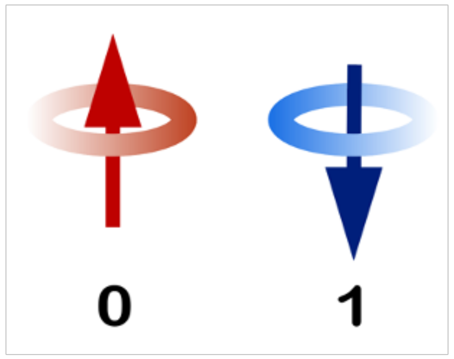
QR / Face Recognition

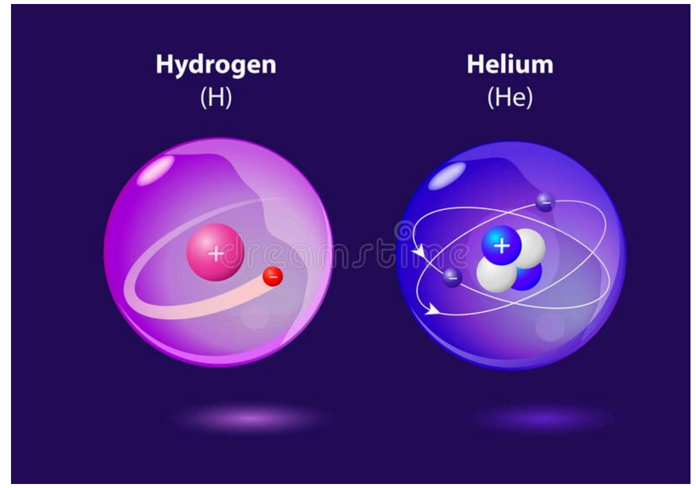
AlphaGo

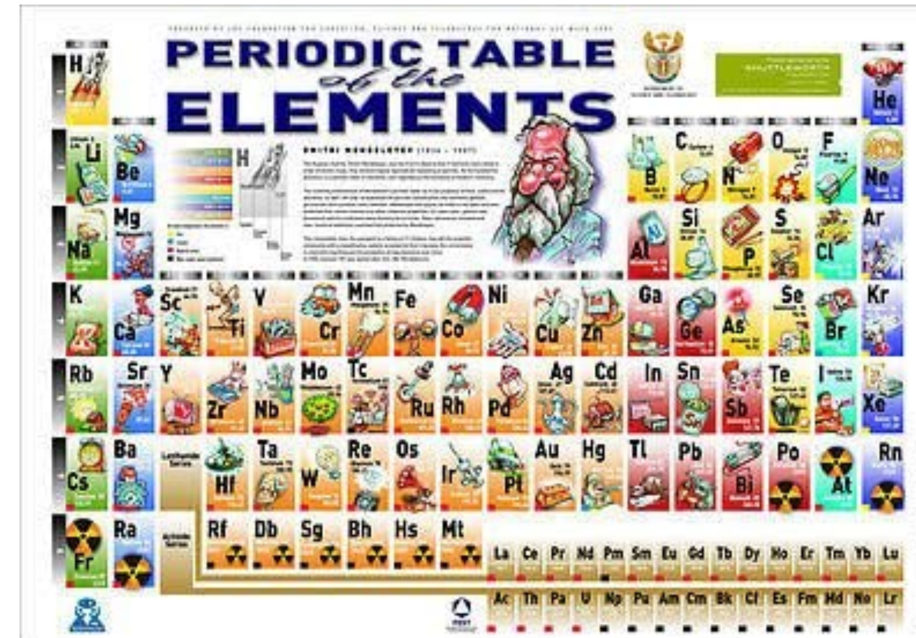
Smart Robots https://www.bostondynamics.com/ **Self-driving Car**

Computation on quantum bit and quantum entanglement









Lead to the famous "exponential wall"

2^N Multi-electron atoms, cannot be solved exactly

Krishna and Radha playing chaturanga

Wheat grains on chessboard — Sissa ibn Dahir, inventor of Chaturanga

$2^{64} - 1$ = 18,446,744,073,709,551,615 grains of wheat, weighing about 1,199,000,000,000 tons.
About 1,645 times the global production of wheat.

$N = 10 \quad 2^{10} = 1{,}024 \sim 10^3$

$N = 20 \quad 2^{20} = 1{,}048{,}576 \sim 10^6$

$N = 30 \quad 2^{30} = 1{,}073{,}741{,}824 \sim 10^9$

$N = 40 \quad 2^{40} = 1{,}099{,}511{,}627{,}776 \sim 10^{12}$

$N = 50 \quad 2^{50} = 1{,}125{,}899{,}906{,}842{,}624 \sim 10^{15}$

Solving exponentially complex problem in polynomial time

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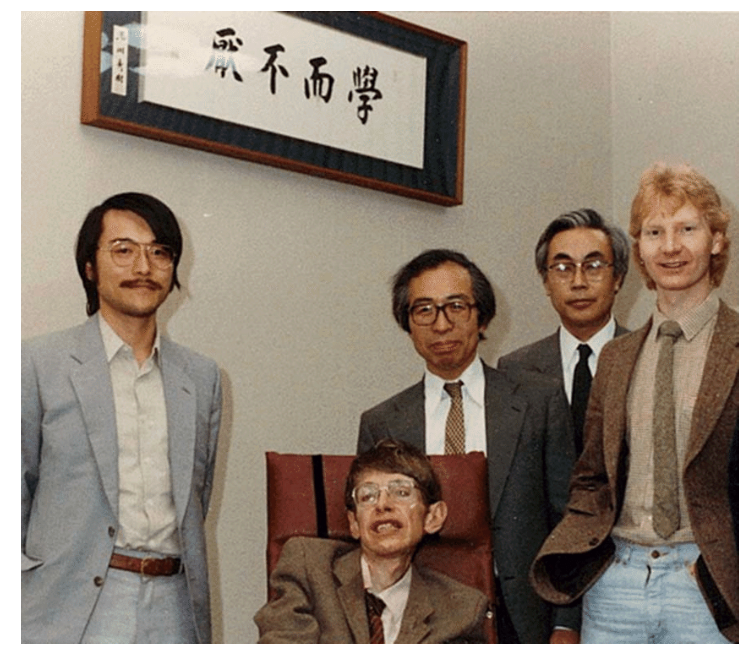
AlphaGo-1

In March 2016, AlphaGo played with Lee Sedol in Seoul.



- its psychological aspects (its relentless concentration) no human can match it···
- The Go skill has improved surprisingly ...

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AlphaGo-2

In April 2017, AlphaGo vs. Jie Ke

- ➢ The machine played perfect…
- ➢ I am so behind, unbelievable…
- ➢ AlphaGo is not the God, but it is a superior species than human being…

AI & Machine Learning in Physics

What happened to AlphaGo?

1. In January 2016, researchers revealed that AlphaGo could play 1 million games in 4 weeks. This means that AlphaGo could play 30,000 games per day. How many games could Lee and Ke play? 10 games/day, 82 years (30,000 days) , only 300,000 games only. AlphaGo has played 300,000,000 games after march 2016!!!→ **Big Data!!!**

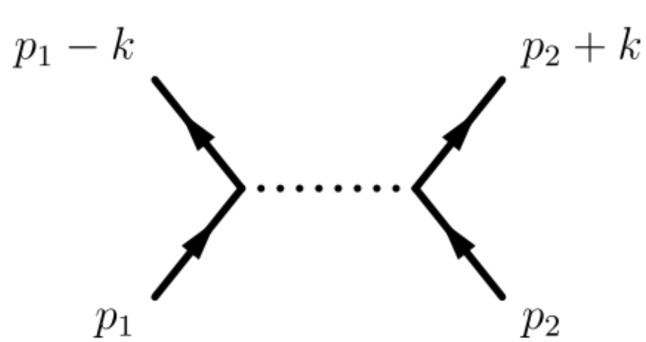
2. Till now, only ~2 million games in total. AlphaGo actually learned from data generated by itself→ **Self learning!!!**

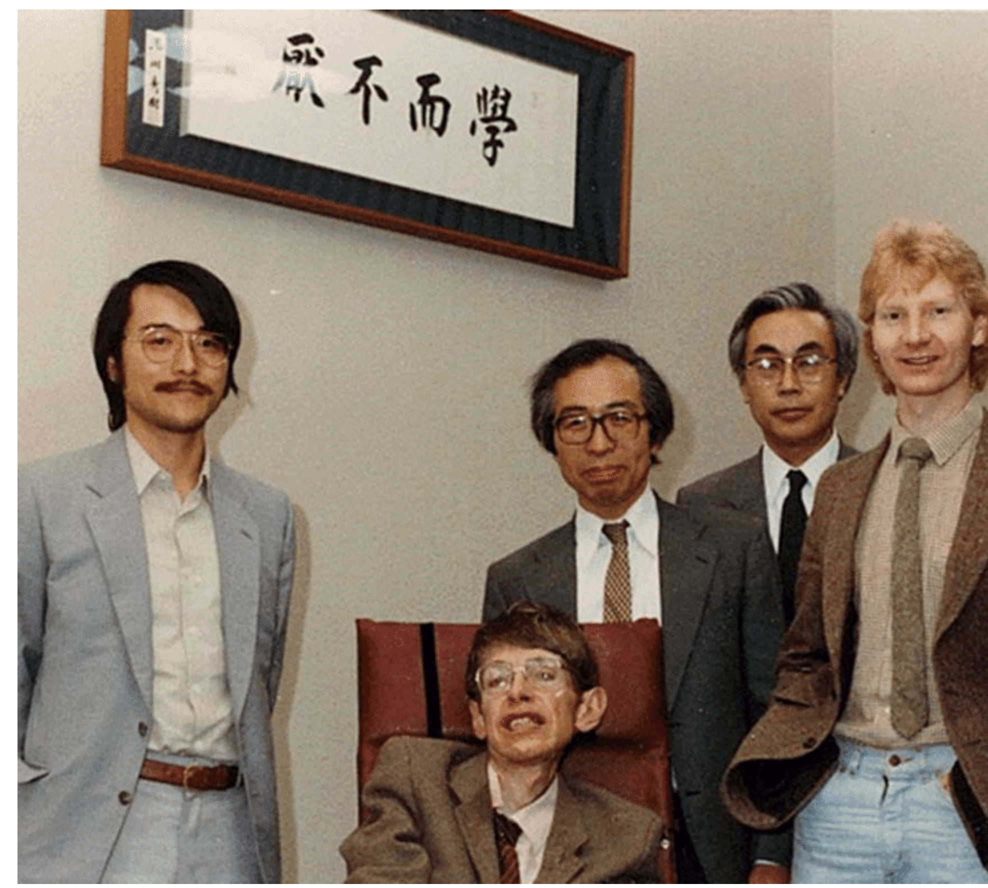
3. Software/Algorithm: 12 layers → 40 layers. **Make it more complicated!!!**

4. Hardware: TPU1 → TPU2. **New Hardware is necessary!!!**

Tensor processing unit (TPU) by google

Hideki Yukawa 汤川秀树





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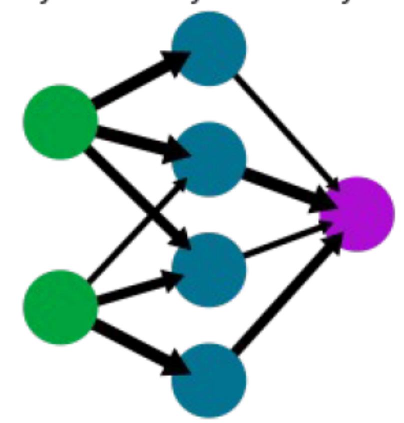
Challenges 1: models are more complicated

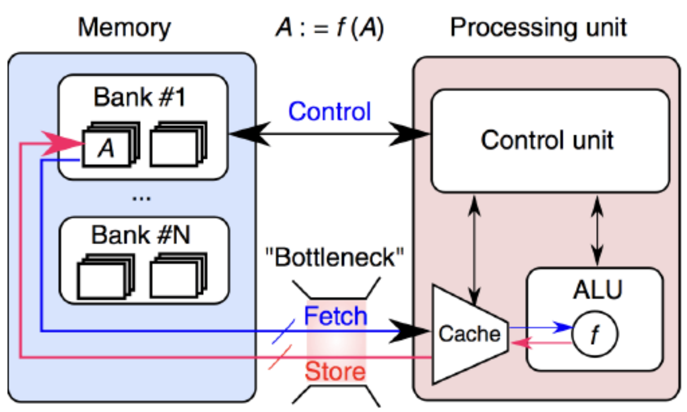
~ 100 layers, ~ 10^6 weights/parameters

A simple neural network



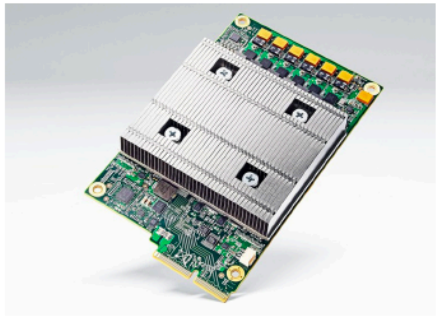
Challenges 2: memory bottleneck

Data fetch is much expensive than data process

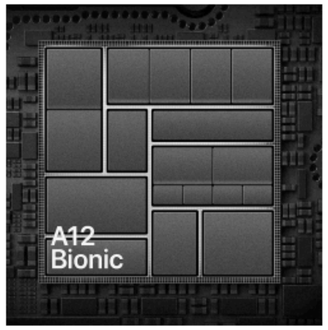


Large on-chip memory, bring computing and memory closer, using low precision computing.

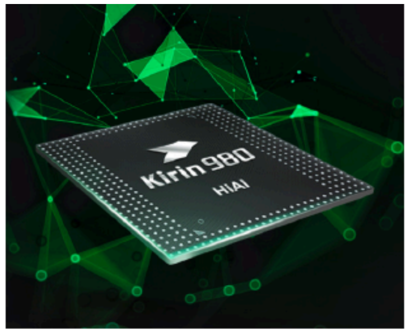
Neural Processing unit (NPU) for AI computing



TPU by Google



A12 Bionic by Apple



Kirin 980 by Huawei

AI & Machine Learning in Physics

Challenges 3: energy consumption

AlphaGo:
- ❑ 176 GPUs, 1202 CPUs
- ❑ 150, 000 Watts

Jie Ke:
- ❑ 1.2L Human Brain
- ❑ ~20 Watts

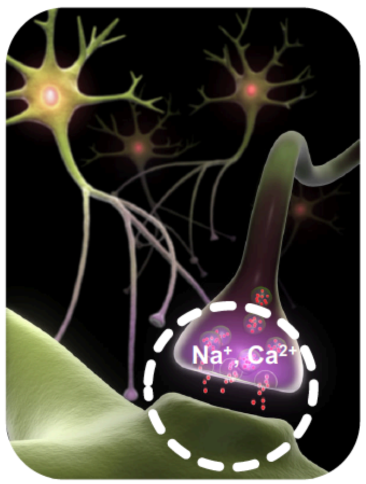
Huge power gap between human brain and CMOS-based AI system

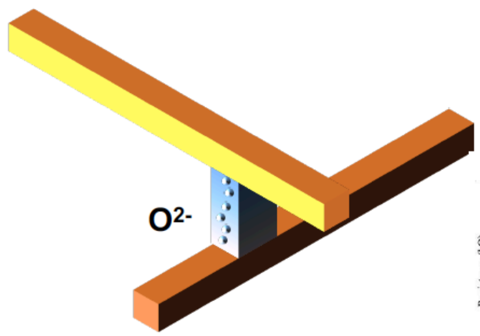
➢ It is much needed to develop **new hardware** with **new device** and **new architecture and new algorithm.**

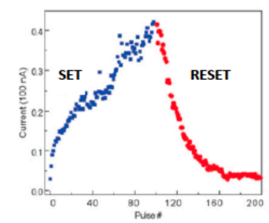
AI & Machine Learning in Physics

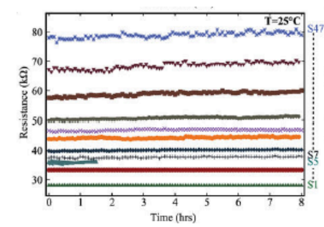
Bio-synapse vs. Electrical synapse

Bio-synapse **Memristor-Electrical synapse**





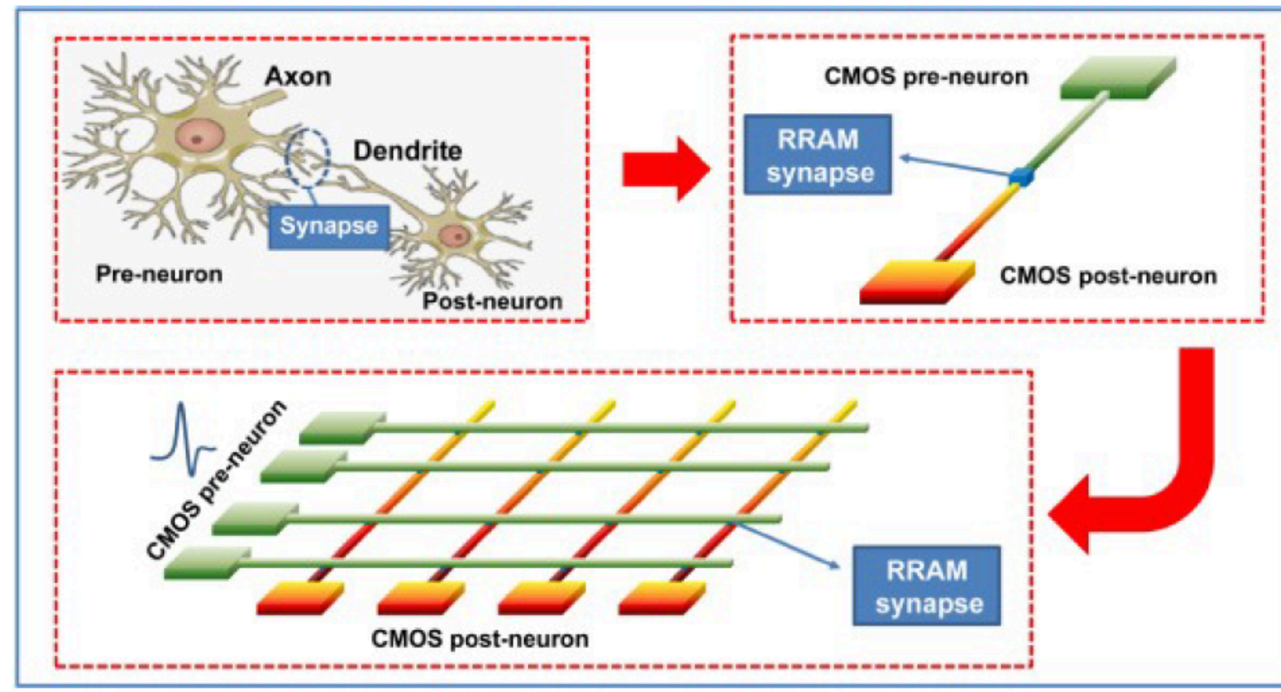




Bio-synapse conductance change through the Na^{+}, CA^{2+} ions movement

Memristor device conductance change through O^{2-} ions movement

Neuromorphic computing



$$\mathbb{R}^{N\times N}$$

$$Ax = b$$

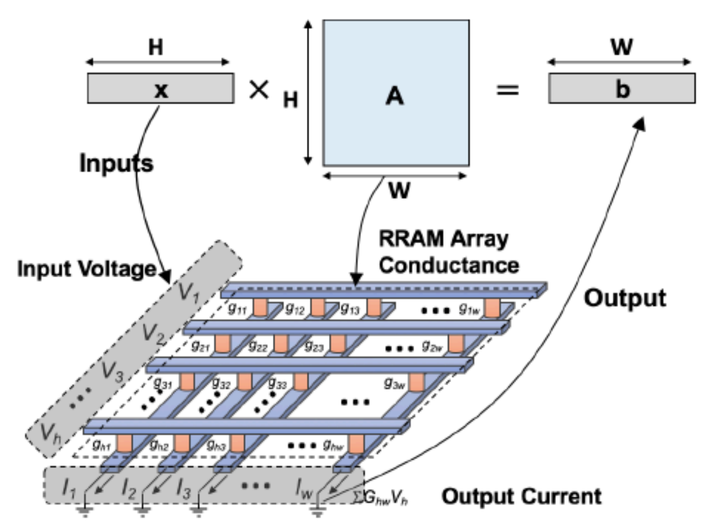
$$O(N^2)$$

$$x = A^{-1}b$$

$$O(N^3)$$

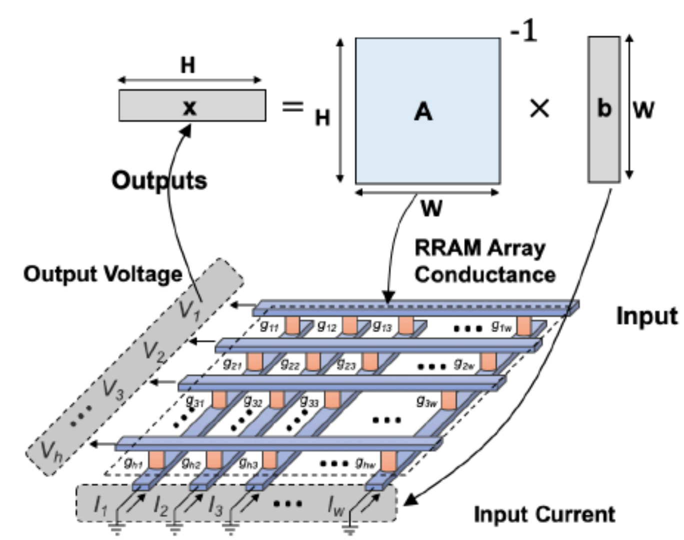
- Vector-Matrix-Multiplication (VMM)

$$\boldsymbol{A}x = b$$



❑ Linear equation solver

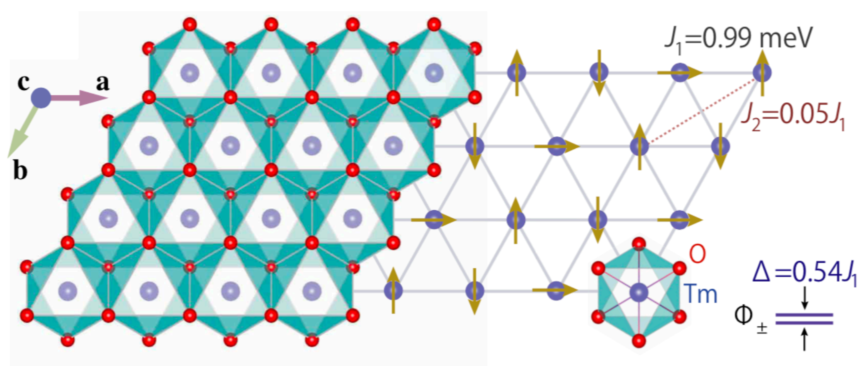
$$\boldsymbol{A}x = b \rightarrow x = \boldsymbol{A}^{-1}b$$



Computing with physical law in memory: Ohm' Law and Kirchhoff' Law

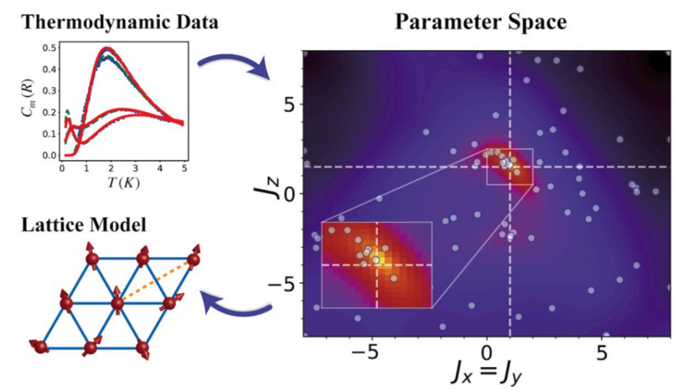
AI & Machine Learning in Physics

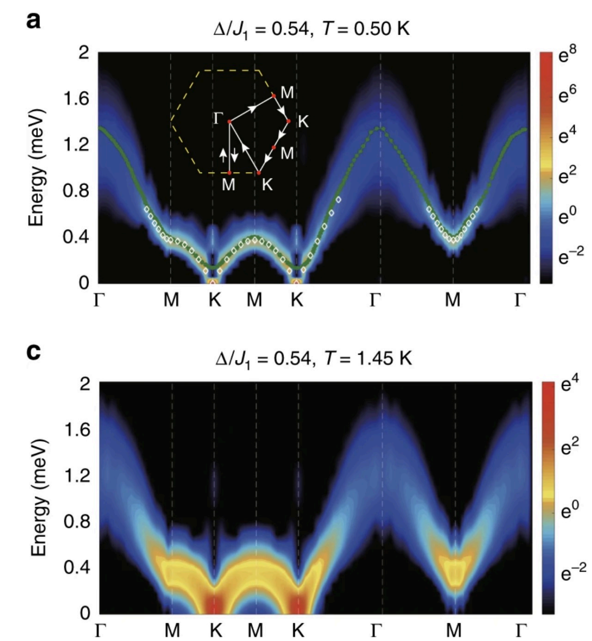
- **Quantum material research connecting physicists in Hong Kong, Beijing and Shanghai**



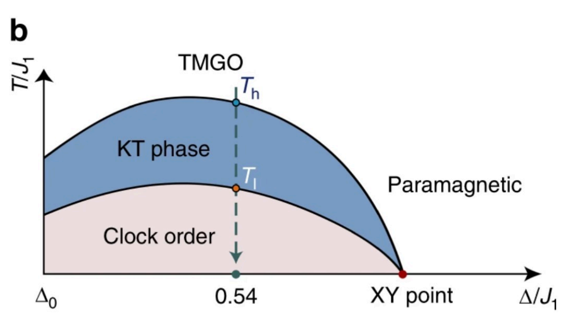
[Nature Communications 11, 1111 (2020)]

auto-gradient, Bayesian optimization

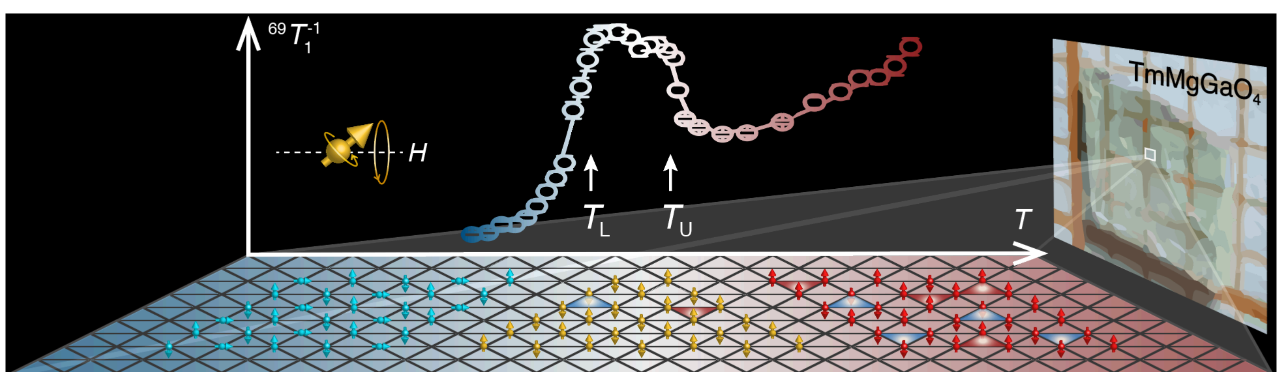




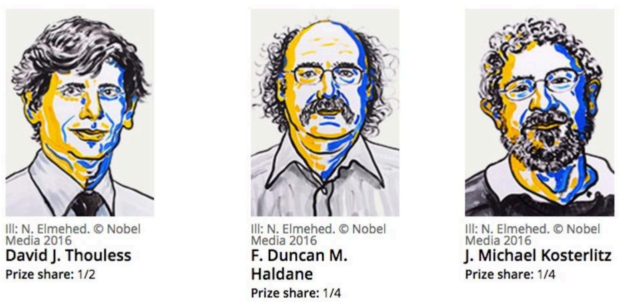
- **Confirming simulated calculations, quantum material research reveals topological KT phase**



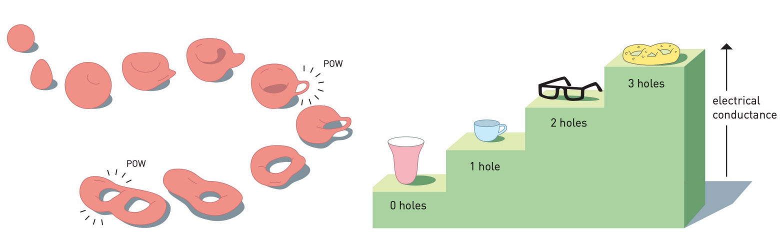
Nuclear magnetic resonance — MRI / CT scans

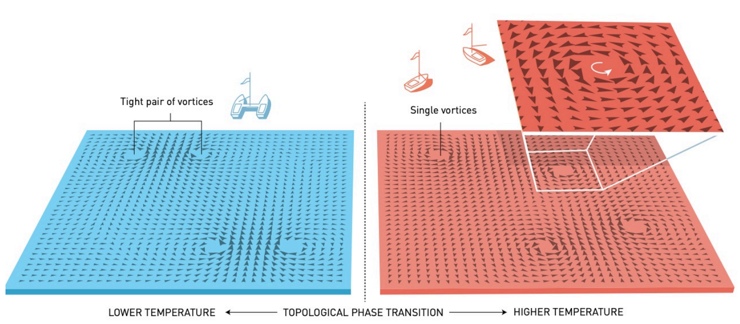


The Nobel Prize in Physics 2016



[Nature Communications 11,5631 (2020)]





Computation and AI could solve the energy crisis

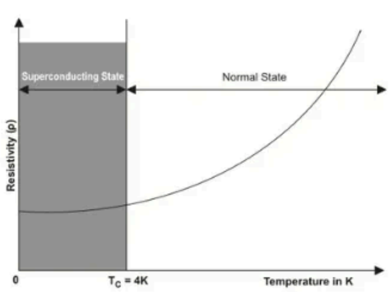
CLP 中電 electric power transmission at high voltage

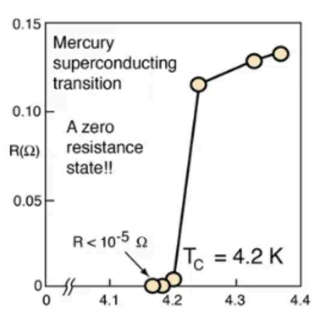
High speed rail

Maglev (magnetic levitation) bullet train with 600 k/h

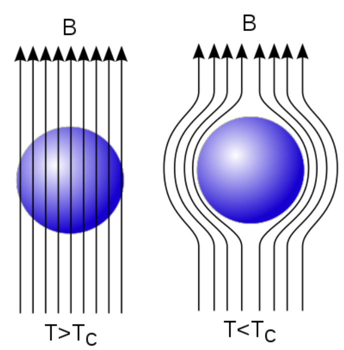
Understanding Quantum Metals

What is Superconductivity?



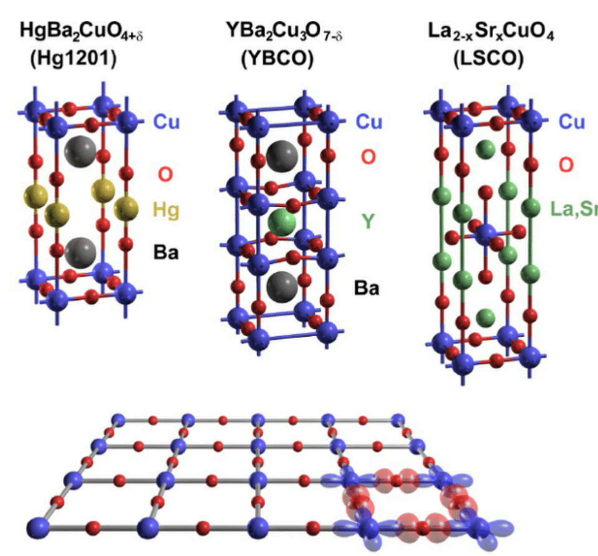


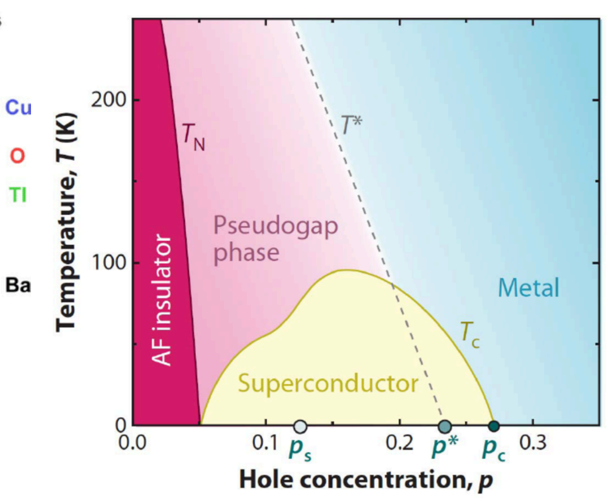
Dutch Physicist
Heike Kamerlingh Onnes
in 1911



superconductors at ~ -270°C

High-temperature superconductors at ~ -100°C





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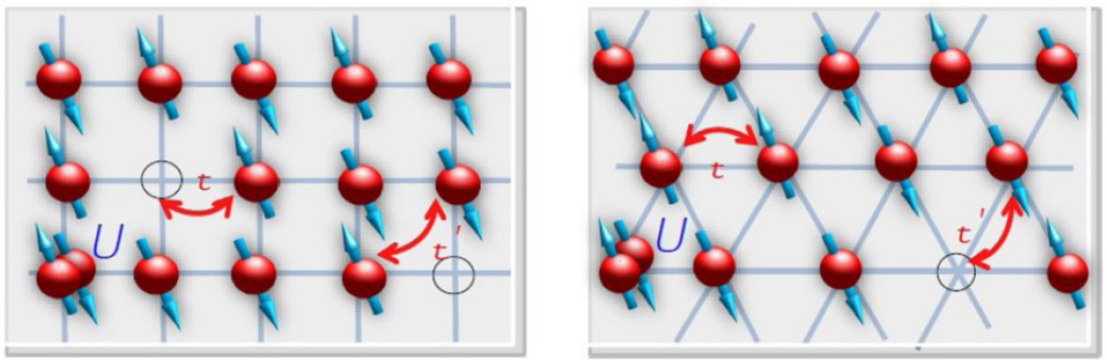
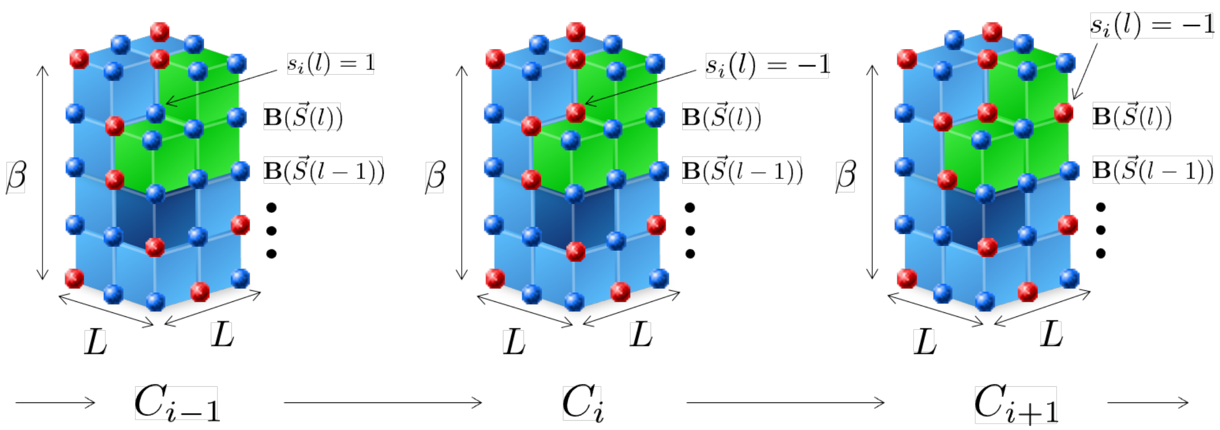


Self-learning Monte Carlo is explainable-AI

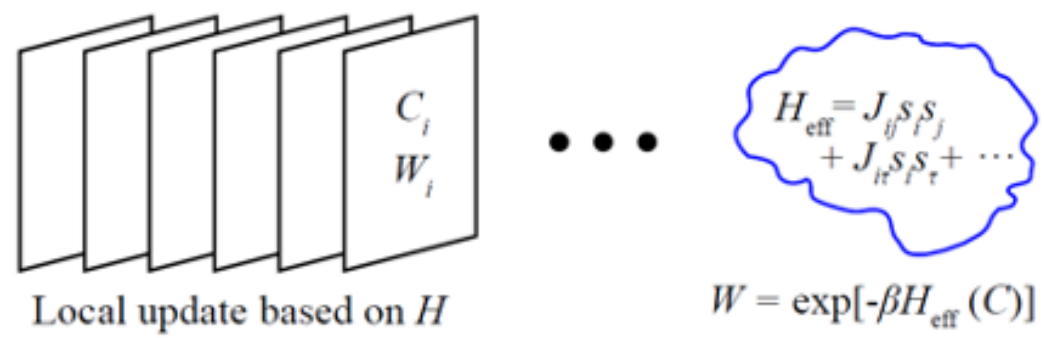


$$Z = \sum_{\{\mathcal{C}\}} e^{-\beta \hat{H}} = \sum_{\{\mathcal{C}\}} \underbrace{\phi[\mathcal{C}] \det\left(\mathbf{1} + \mathbf{B}_\beta \cdots \mathbf{B}_1 \mathbf{B}_0\right)[\mathcal{C}]}_{\omega[\mathcal{C}]} = \sum_{\{\mathcal{C}\}} e^{-\beta H_{eff}[\mathcal{C}]}$$

one of the Delphic maxims and was inscribed in the pronaos (forecourt) of the Temple of Apollo at Delphi

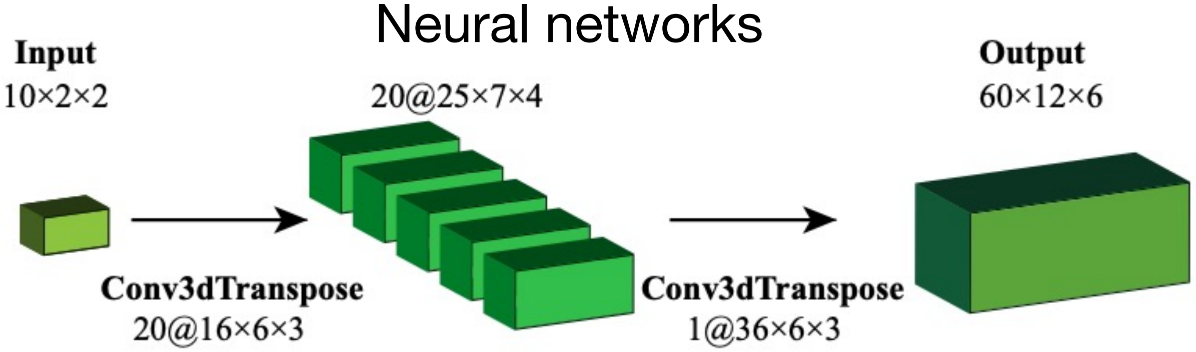
Trilogy of self-learning

[Phys. Rev. B 96, 041119(R) (2017)](#)
[Phys. Rev. B 95, 241104(R) (2017)](#)
[Phys. Rev. B. 95. 041101(R) (2017)](#)



$$H_{\text{eff}}[\mathcal{C}] = E_0 + \sum_{(i,\tau);(j,\tau')} J^{\text{eff}}_{(i,\tau);(j,\tau')} s^z_{i,\tau} s^z_{j,\tau'} + \cdots$$

Neural networks

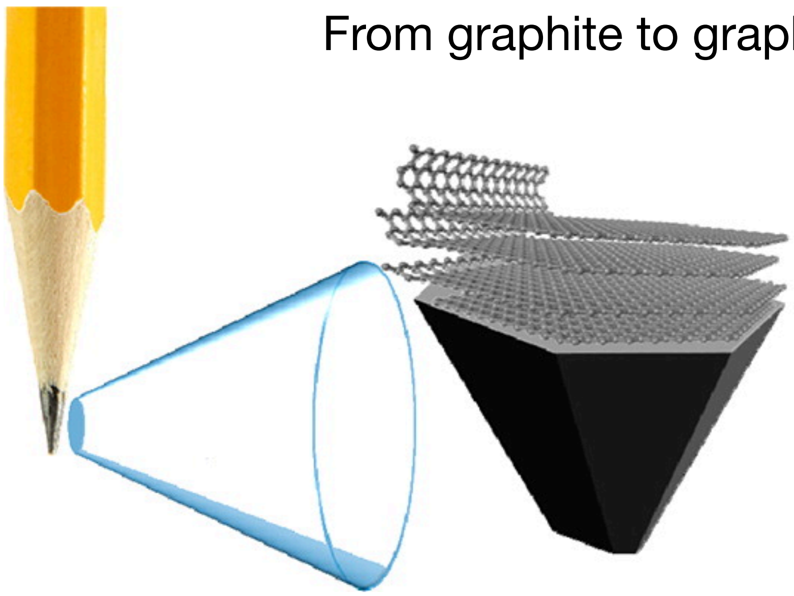


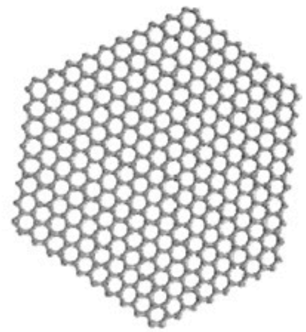
[Chin. Phys. Lett. 39, 050701 (2022)](#)

- Reduce the computation complexity from O(N^4) to O(N^3)
- Increase the acceptance rate of Monte Carlo
- Learn the effective model for quantum materials
- Save the planet

Computation and AI in graphene face masks

From graphite to graphene

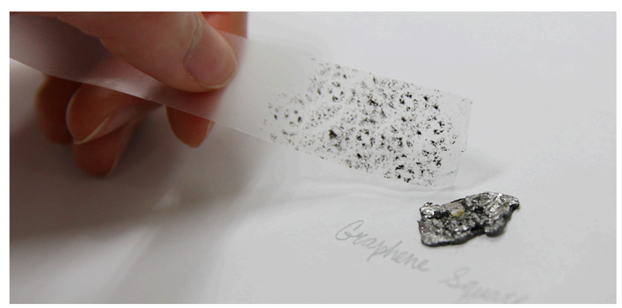




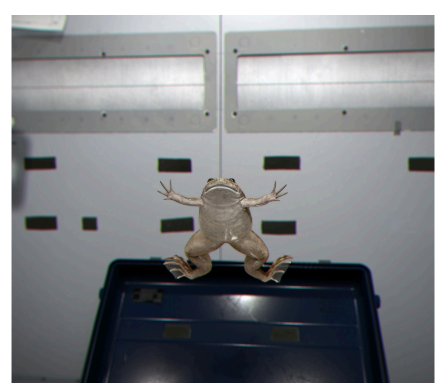
The Nobel Prize in Physics 2010

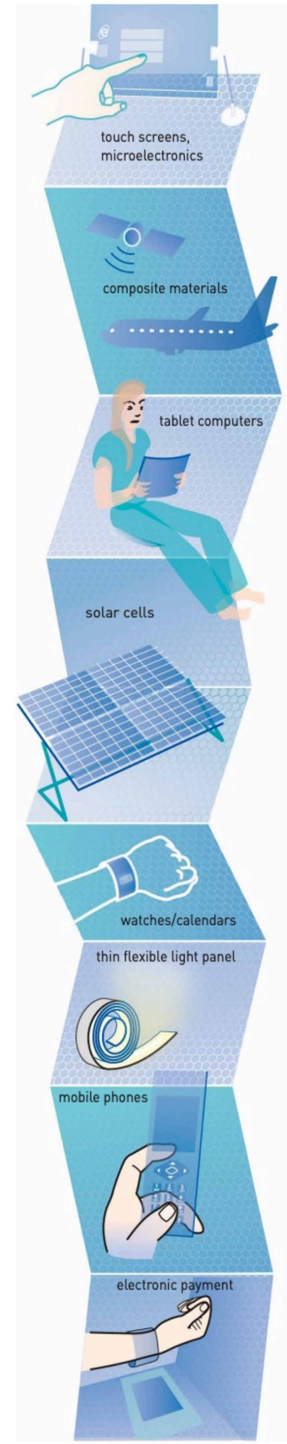
© The Nobel Foundation. Photo: U. Montan
Andre Geim
Prize share: 1/2

© The Nobel Foundation. Photo: U. Montan
Konstantin Novoselov
Prize share: 1/2

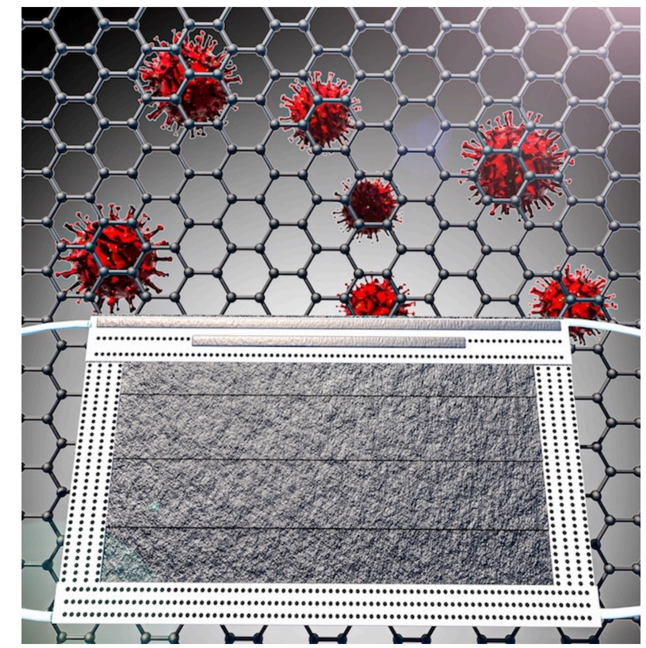


The 2000 Ig Nobel Prize in physics was awarded to Andre Geim, Radboud University Nijmegen, and Michael Berry, University of Bristol, UK, for the magnetic levitation of a live frog.

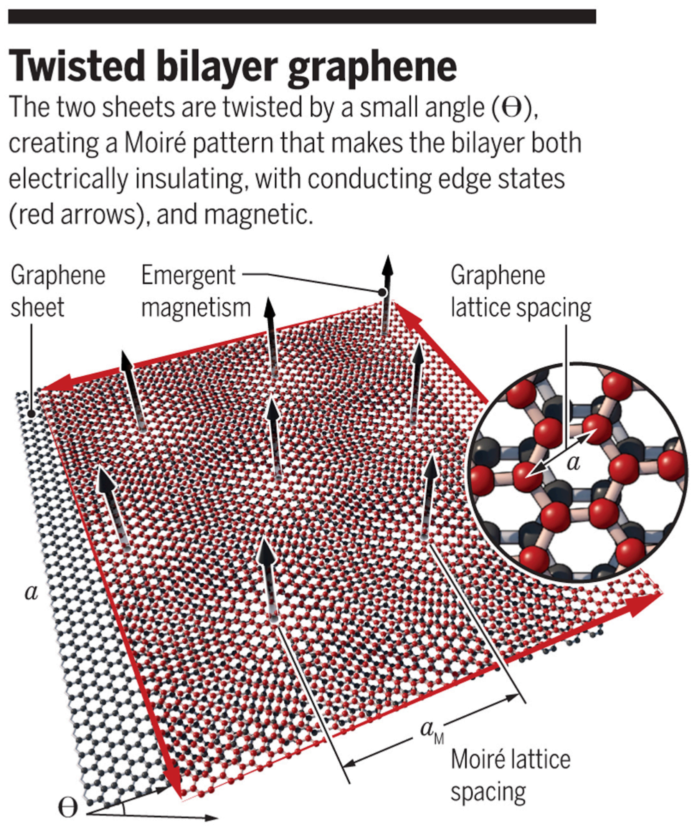


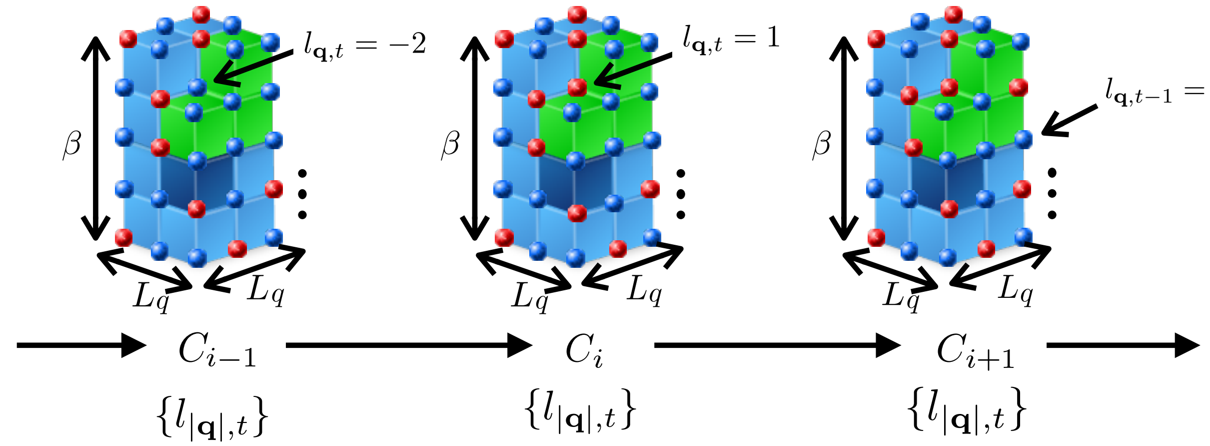


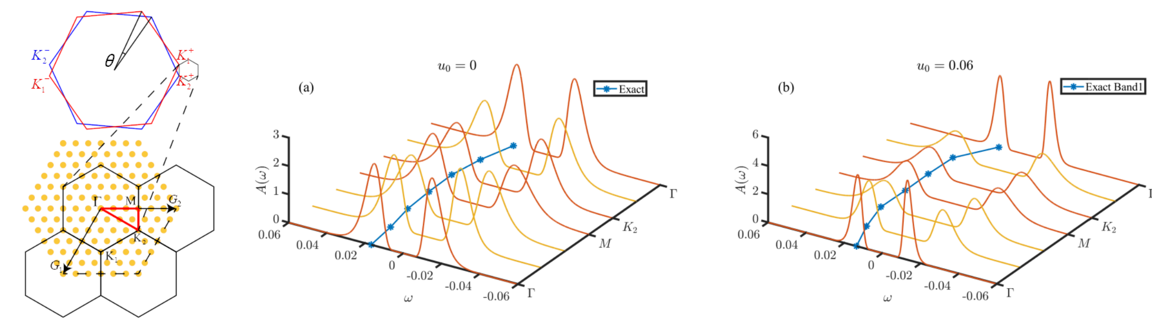
Graphene joins the fight against COVID-19



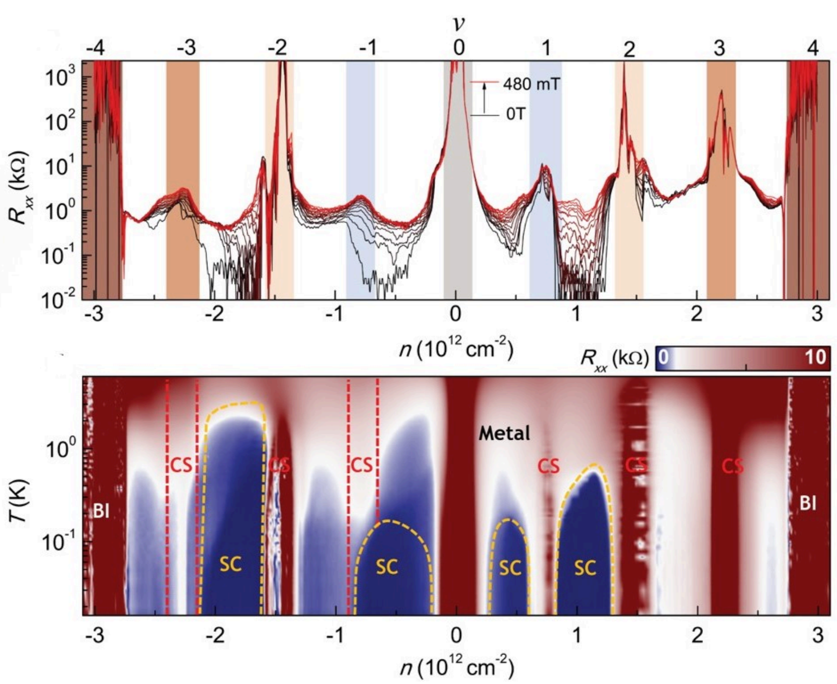
Computation and AI in graphene face masks

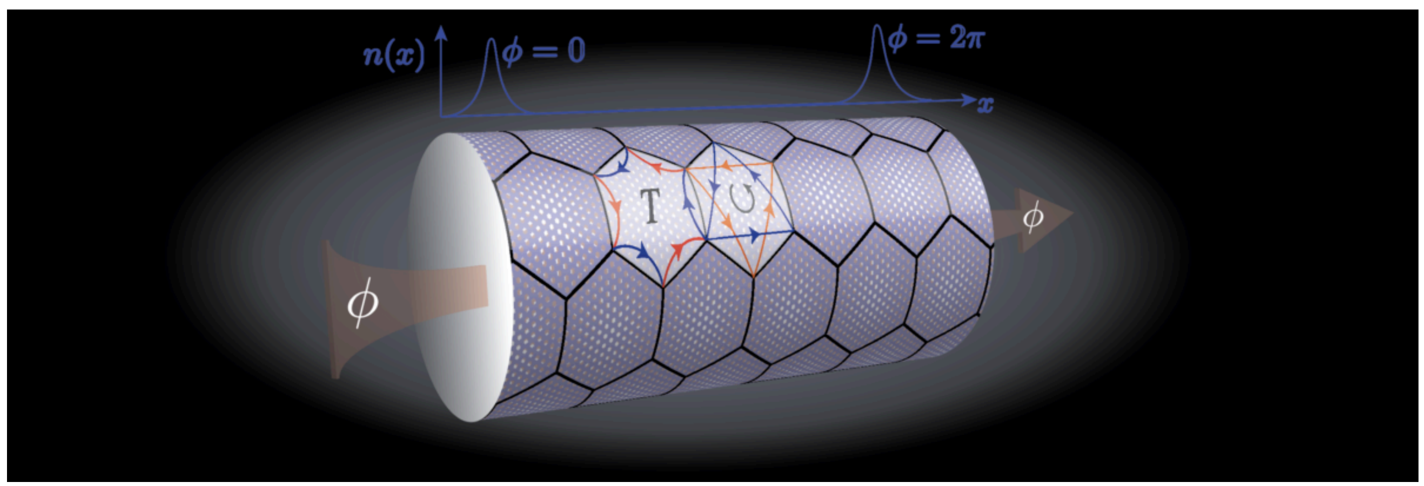






Chin. Phys. Lett. 38, 077305 (2021) Cover story





Nature Communications 12, 5480 (2021)

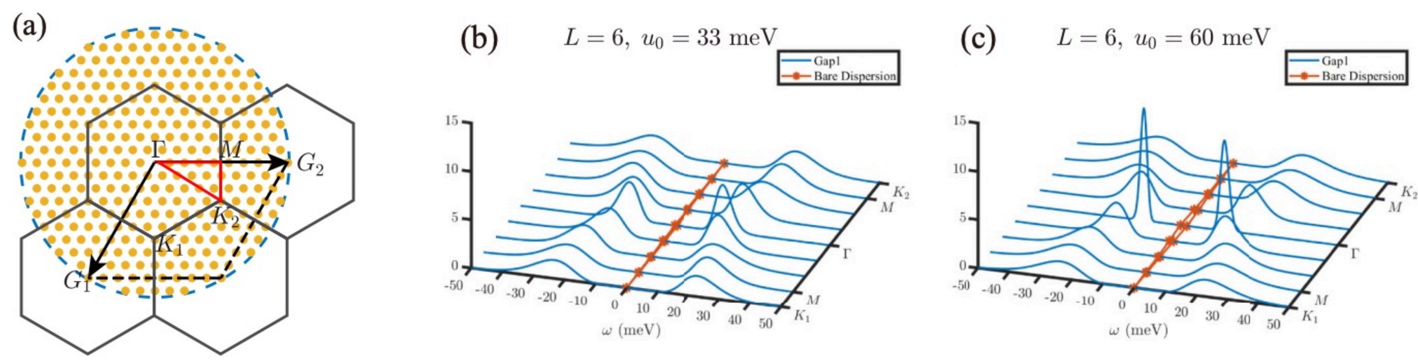
Momentum space quantum Monte Carlo algorithm

Long-range Coulomb + fragile topology

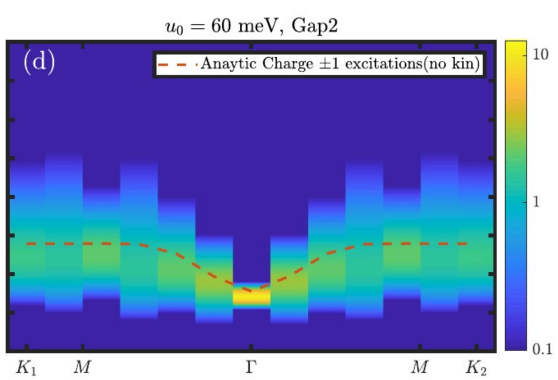
$$H = H_0 + H_{int} \qquad V(q) \sim \frac{1}{q}$$

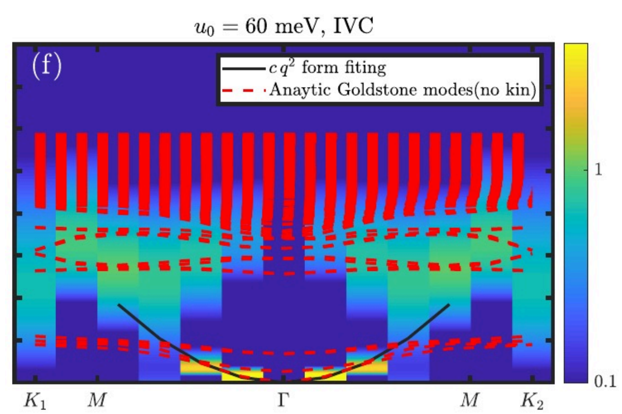
$$\delta\rho_{\mathbf{q}+\mathbf{G}} \sim \sum_{\mathbf{k}\in mBZ, m_1, m_2, \tau, s} \lambda_{m_1,m_2,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})\, d^\dagger_{\mathbf{k},m_1,\tau,s} d_{\mathbf{k}+\mathbf{q},m_2,\tau,s}$$

$$H_0 = \sum_m \sum_{\mathbf{k},\tau,s} \epsilon(\mathbf{k}) d^\dagger_{\mathbf{k},m,\tau,s} d_{\mathbf{k},m,\tau,s} \qquad H_{int} = \frac{1}{2\Omega}\sum_{\mathbf{q},\mathbf{G}} V(\mathbf{q}+\mathbf{G})\, \delta\rho_{\mathbf{q}+\mathbf{G}}\, \delta_{-\mathbf{q}-\mathbf{G}}$$

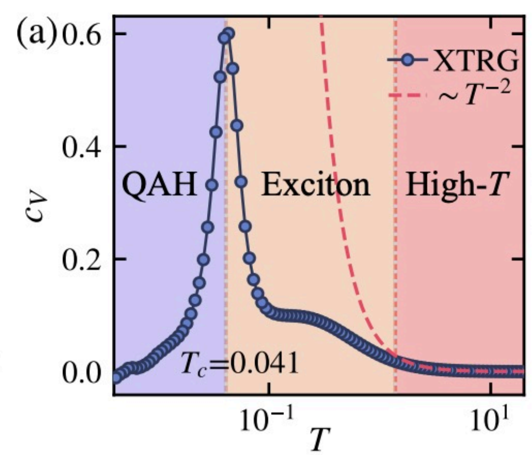


Collective excitations





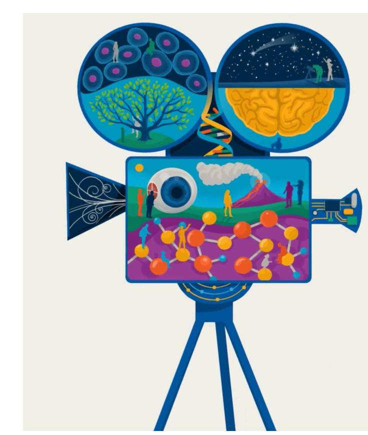
Tensor-network, thermodynamic computation



nature awards science in shorts

Science in Shorts playlist 2022

Watch and share the best Shorts from 2022. Which is your favourite?



Phys. Rev. Lett. 130, 016401 (2023)
Phys. Rev. Lett. 128, 157201 (2022)
Phys. Rev. B 105, L121110 (2022)
Nature Communications 12, 5480 (2021)

https://youtu.be/c5-bFYELO28

The quantum teleportation pencil

Are you sitting comfortably? And concentrating hard? We're entering the realms of superfast computing based on quantum teleportation via twisted graphene lattices. But don't worry, you'll be fine as long as you have a pencil handy.

Bin Bin Chen & Zi Yang Meng

The University of Hong Kong

AI & Machine Learning Basics

Tradition: Task —> algorithm (algorithm for loop, sorting)

Big data era: Don’t have algorithm —> lack in knowledge, make up for in data

Approximation detect certain patterns or regularities, Data Mining

- Model with some parameters, model can be predictive or descriptive.
- Learning is the execution of a computer program to optimise the parameters of the model using the training data or past experience.
- Using theory of statistics, math and physics: building mathematical models, making inference from a sample
- Using computer science: efficient algorithm to solve the optimisation problem, store and process big data; representation and algorithmic solution for inference needs to be efficient
- The computational efficiency may be as important as predictive accuracy

AI & Machine Learning Basics

Infer hidden association rule from observed data
In the era of "big data"

Basket analysis

- In retail, associations between products bought by the customers
- People do not buy at random
- There are certain patterns (association rule) in the data, machine extract them

Conditional probability P(Y|X), Y is the product one would like to condition on X,

P(chips | beer) = 0.8   P(bread | milk) = 0.71

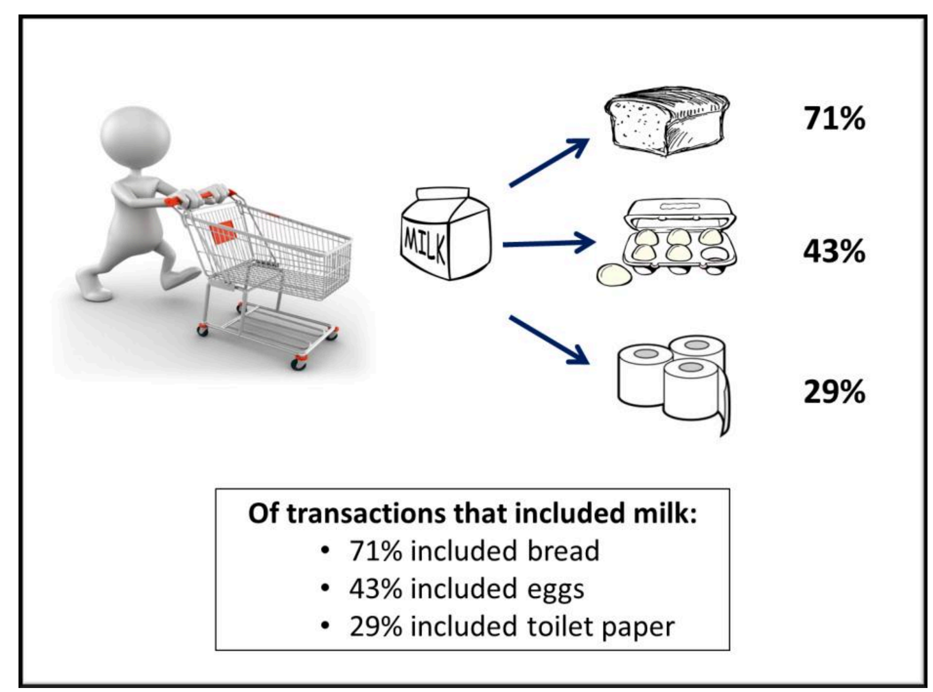
P(Y|X, D) where D is the set of customs attributes, gender, age, martial …

Books / Music / Shows :
P (Game of Thrones | Fantasy, male) =
P (The daily show | Comedy, layman) =
P (Last Week Tonight with John Oliver | Comedy, sophisticated) =
P (Late-night with Seth Meyers | Comedy, politics) = …

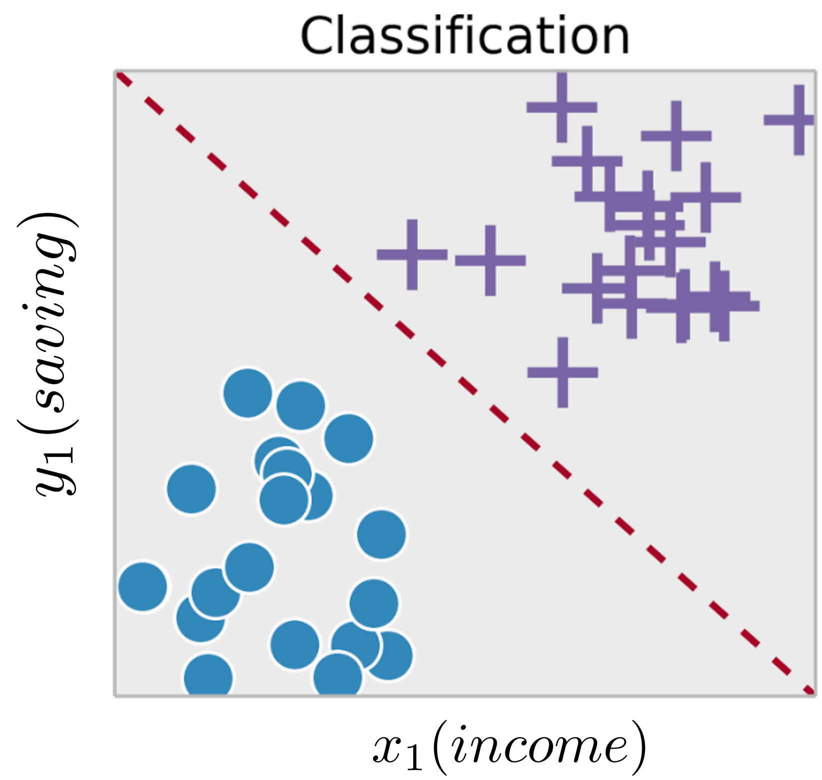
Webpages:

Social medias:

In spam email detection
In Fintech, credit application, stock market
In medical diagnosis, COVID-19
In Science, physics, astronomy, biology, …



AI & Machine Learning Basics



Classification: input —> classifier —> output

Discriminant (two classes):

Banks classify credit for low-risk and high-risk customers

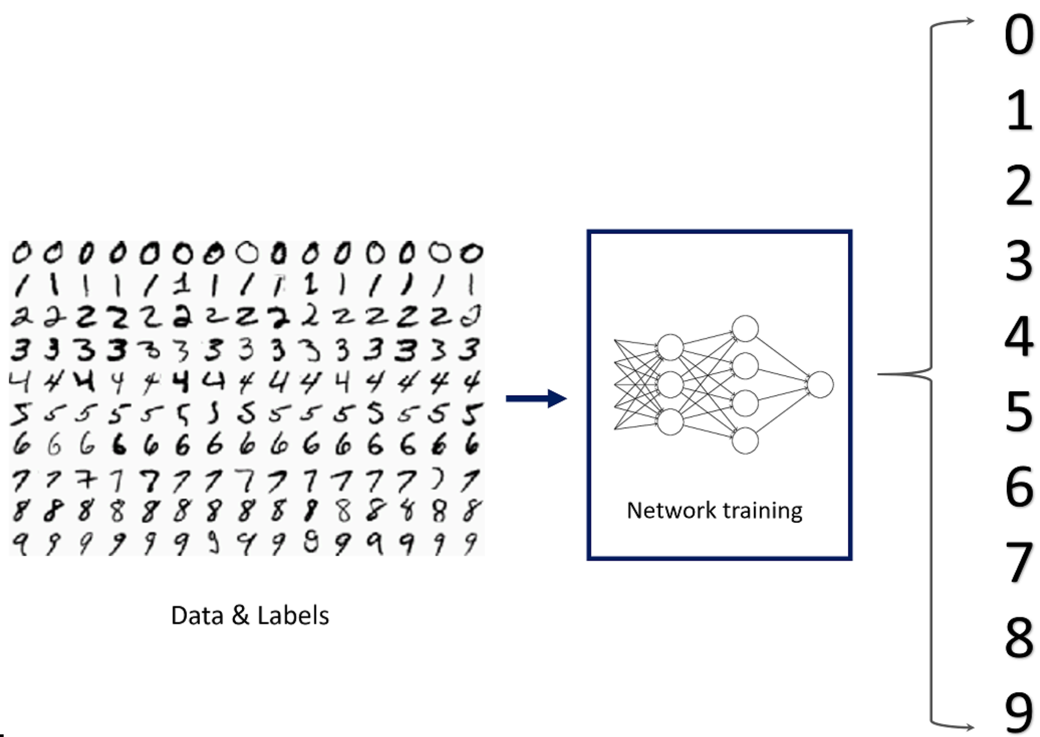
income, saving, profession, age, past financial history, …

Machine learning fits a model to the past data,
calculate the risk for a new application,
decide to accept or refuse
We have a rule that fits the past data, if the future is similar to the past

Predictions: decide new customer is low-risk and high-risk

Pattern recognition (multiple classes):

Handwritten character recognition, MNIST database
Face recognition, medical diagnosis,
Speech recognition, time series, machine translation,
natural language processing



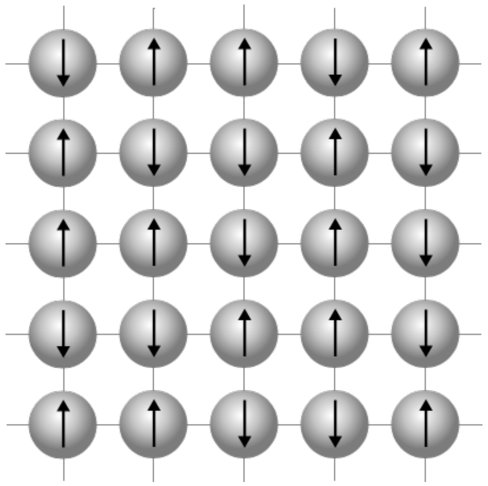
Knowledge extraction: rule is simpler than data

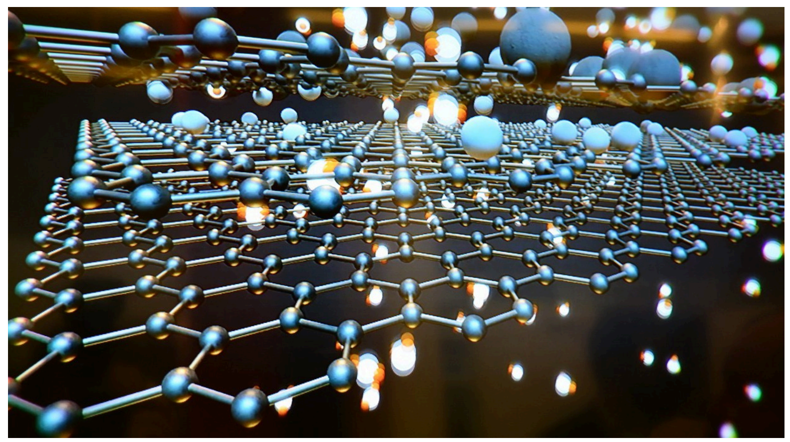
Phase transition, Landau-Ginzburg paradigm, order parameters

AI & Machine Learning Basics

Ising model, continuous phase transition
workhorse for statistical physics

https://mattbierbaum.github.io/ising.js/

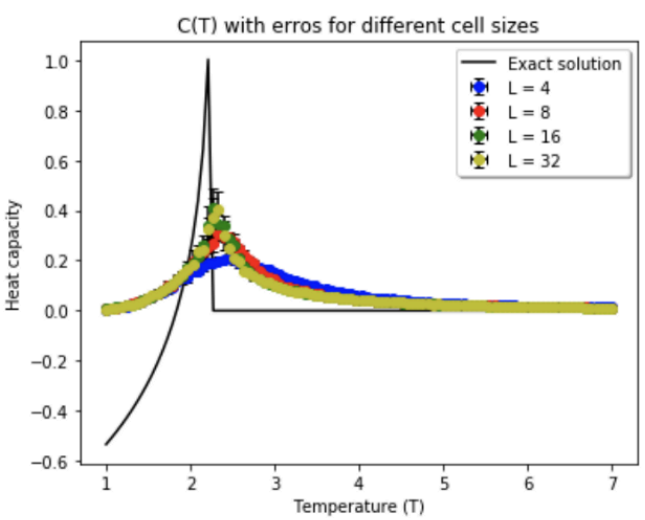


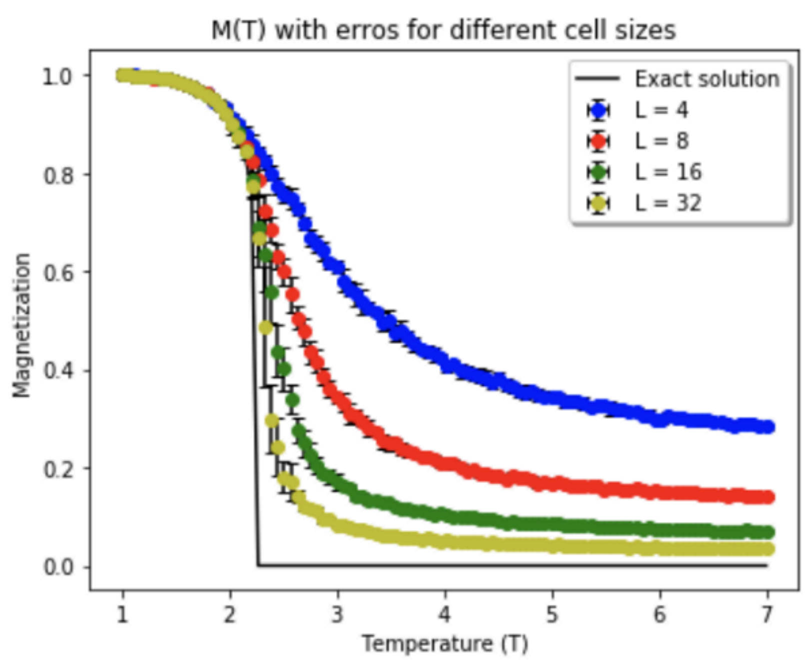


$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z \qquad S_i^z = \pm 1$$

Configuration space: 2^N

https://en.wikipedia.org/wiki/Ising_model#/media/File:Ising_quench_b10.gif





$$m = \frac{1}{N} \left| \sum_{i=1}^{N} S_i^z \right|$$

$$m(T) = |T - T_c|^\beta \text{ with } \beta = 1/8 \text{ in 2D}$$

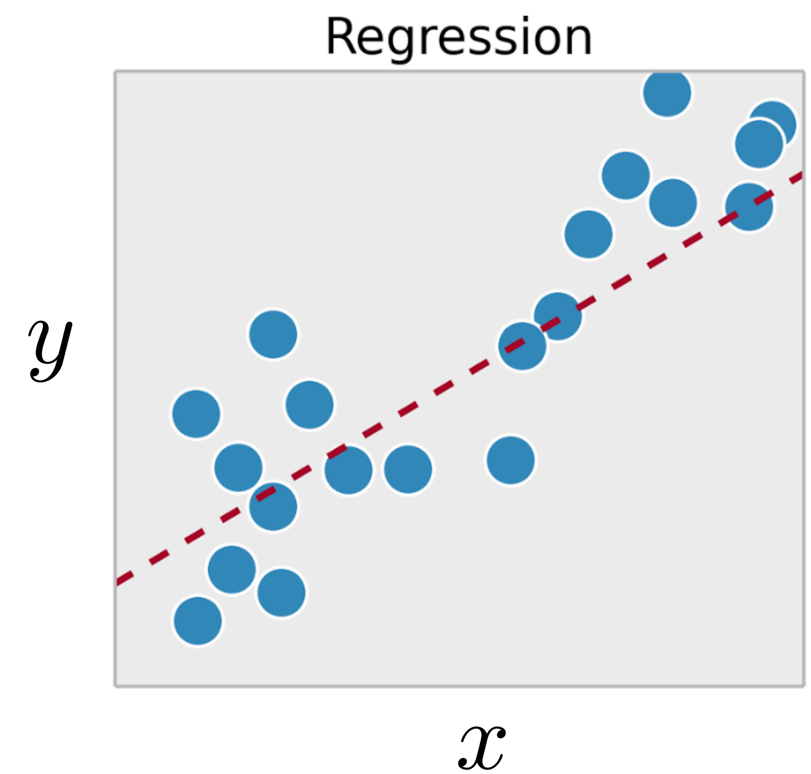
AI & Machine Learning Basics

Regression: $$y = h_\Theta(x) = \Theta \cdot x$$

$$\{(x_j^{(i)}, y^{(i)}), \theta_j\};\ j = 1, 2, \cdots, N;\ i = 1, 2, \cdots, M; N < M$$

$$y^{(i)} = \theta_0 + \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)} + \cdots + \theta_N x_N^{(i)}$$

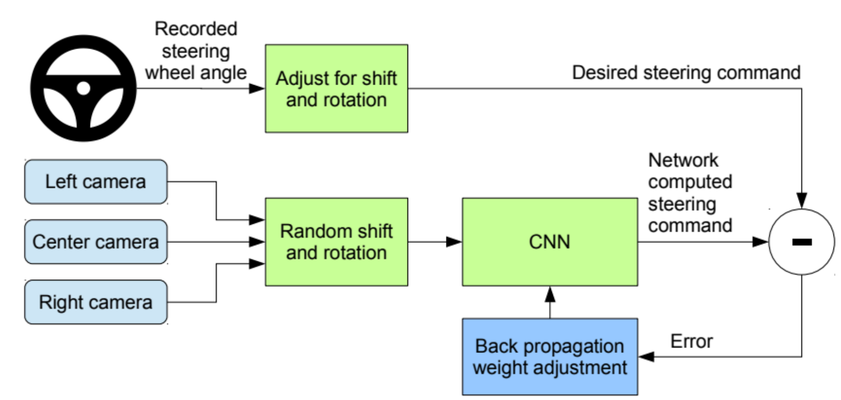
$$\begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_N^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \cdots & x_N^{(2)} \\ & \vdots & & \vdots & \\ 1 & x_1^{(M)} & x_2^{(M)} & \cdots & x_N^{(M)} \end{bmatrix} \cdot \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_N \end{bmatrix} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(M)} \end{bmatrix}$$



Prediction & forecasting: $$\underline{\underline{X}} \cdot \underline{\Theta} = \underline{Y}$$

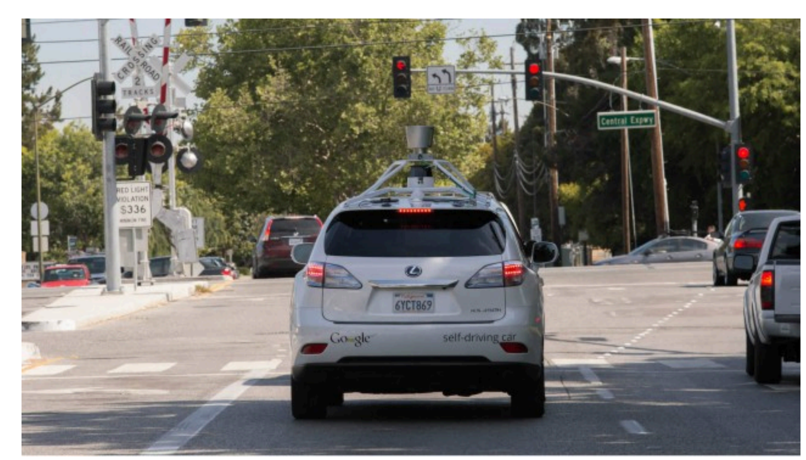
Least squares by Legendre 1805 and Gauss 1809
normal equation, Gradient descent and Conjugate Gradients, Lagrange multiplier

- Model / hypothesis $$h_\Theta(x)$$
- Loss / cost function $$\mathcal{L}(\Theta|X) = \sum_{i=1}^{M} L(y^{(i)}, h_\Theta(x^{(i)}))$$
- Optimisation procedure $$\Theta^* = \arg\min_\Theta \mathcal{L}(\Theta|X)$$

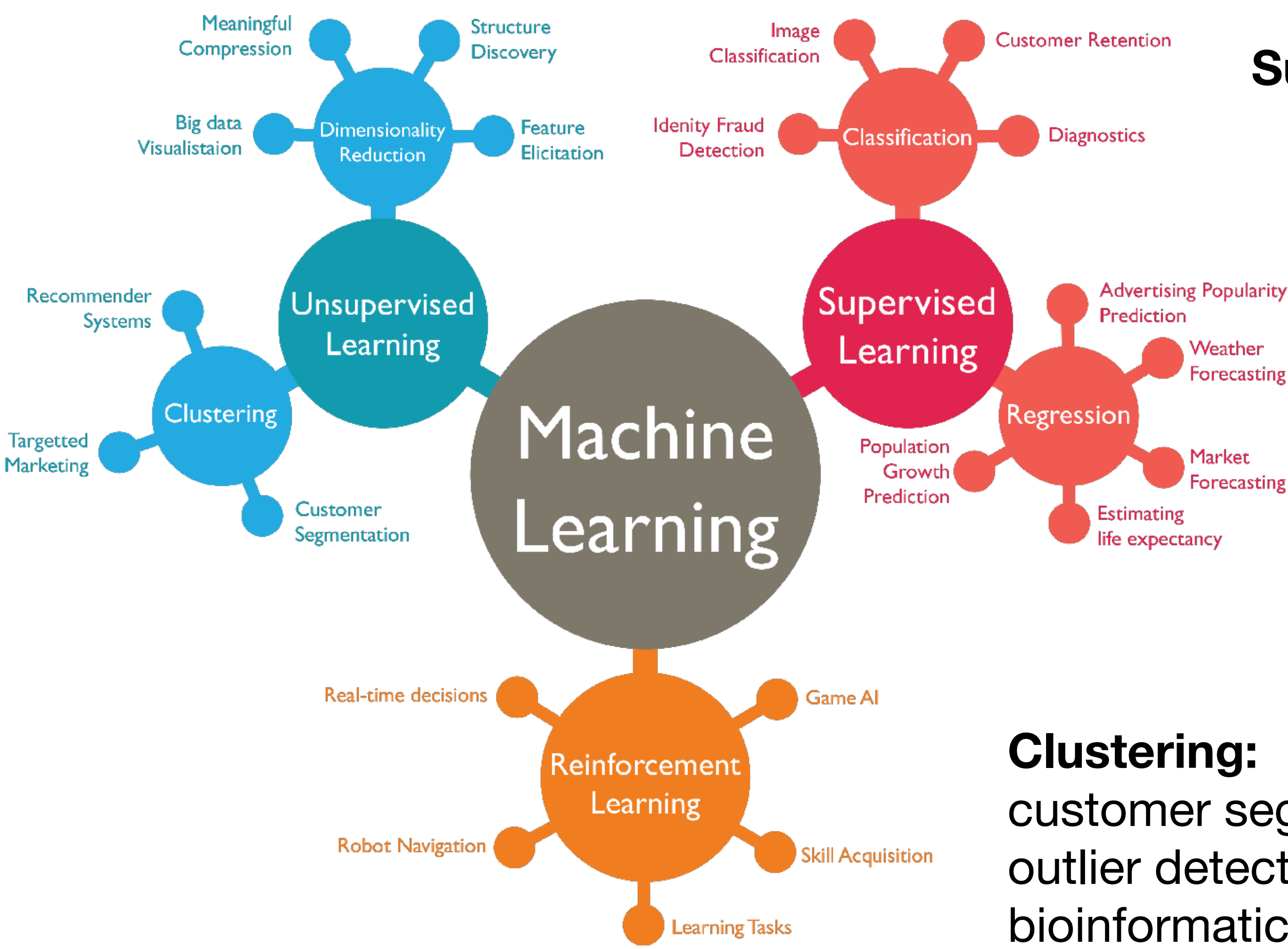


Example: Self-Driving car

Input: sensors on the car, video caramel, GPS, …;
Output: steering wheel;
Training data: monitoring and recording the action of human driver



AI & Machine Learning Basics



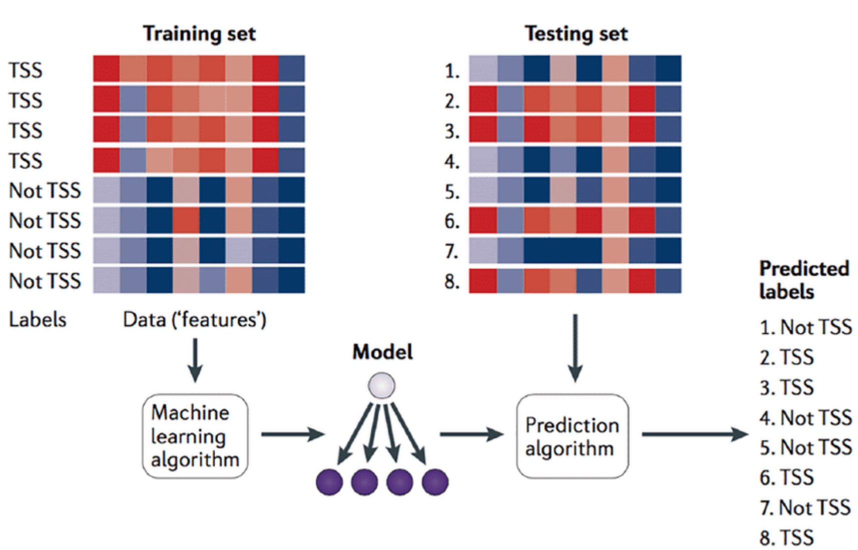
Supervised Learning: Classification & Regression

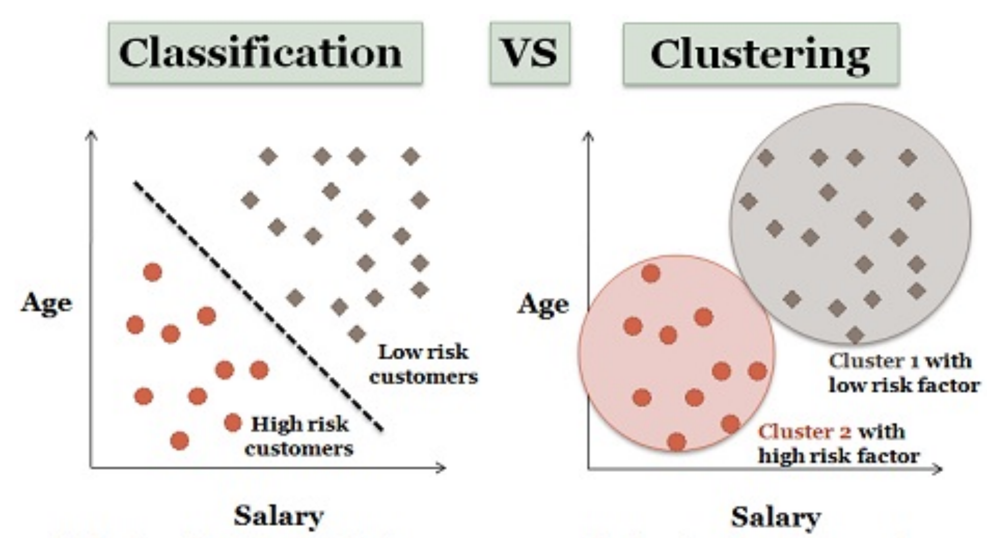
Input —> machine/model —> Output
Correct outputs are provided by the supervisor

Unsupervised Learning: only have input data

Find regularities from the input

Clustering:
customer segmentation, customer relationship management, outlier detection; Image compression
bioinformatics: DNA, RNA, amino acids, Motif, Proteins, sequence alignments





Risk classification for the loan payees on the basis of customer salary

AI & Machine Learning Basics

Reinforcement learning (policy generation):
Single action is not important, good policy is the sequence of correct actions.

Game playing:

AlphaGo is CNN with 12 convolution layers

Robot navigation:

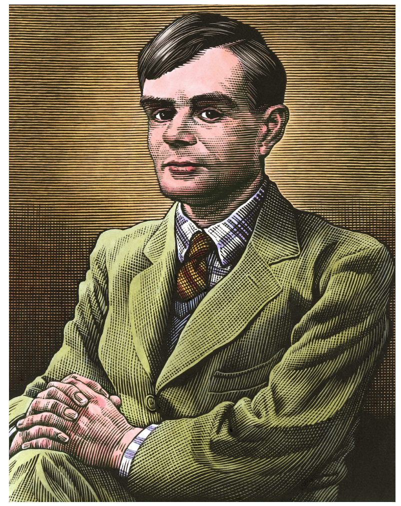
Correct sequence of action to reach the goal state from an initial state

Watch this!

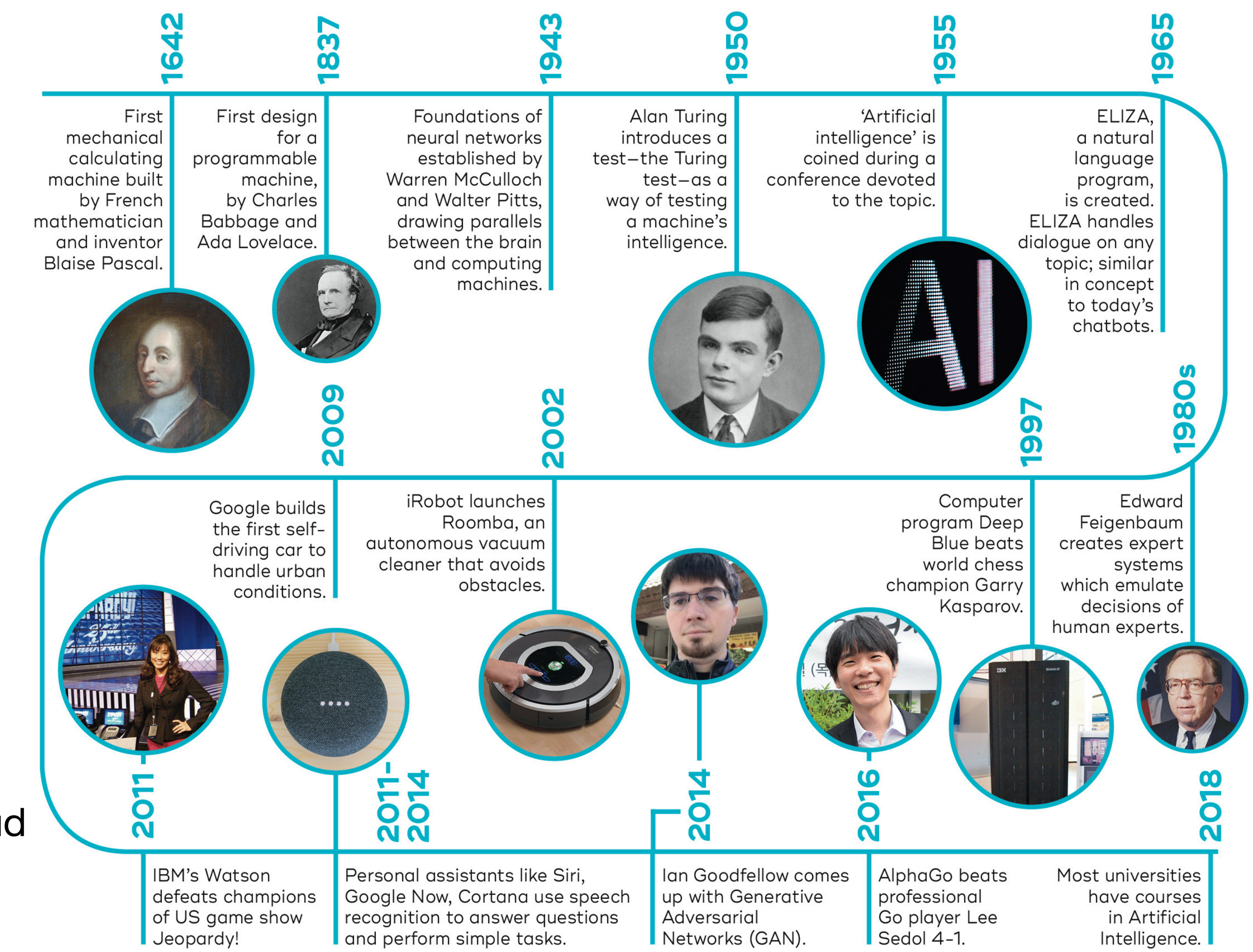
https://www.bostondynamics.com/spot

AI & Machine Learning Basics

A bit of history



Church-Turing thesis:
If a human could not distinguish between responses from a machine and a human, the machine could be considered “intelligent”.



1943, McCullouch and Pitts, artificial neutrons
1955, workshop at Dartmouth College, Allen Newell (CMU), Herbert Simon (CMU), John McCarthy (MIT), Marvin Minsky (MIT), …
1958, Rosenblatt, perceptron
1974, first AI winter
1987, second AI winter
1997, IBM Deepblue vs Kasparov, logistics, data mining, medical diagnosis, …
2016, Alpha Go vs Lee Sedol
2017, Alpha Go vs Ke Jie
Xbox, Smartphone, affordable neural networks, cloud computing, internet of things …
2020, COVID-19

Content

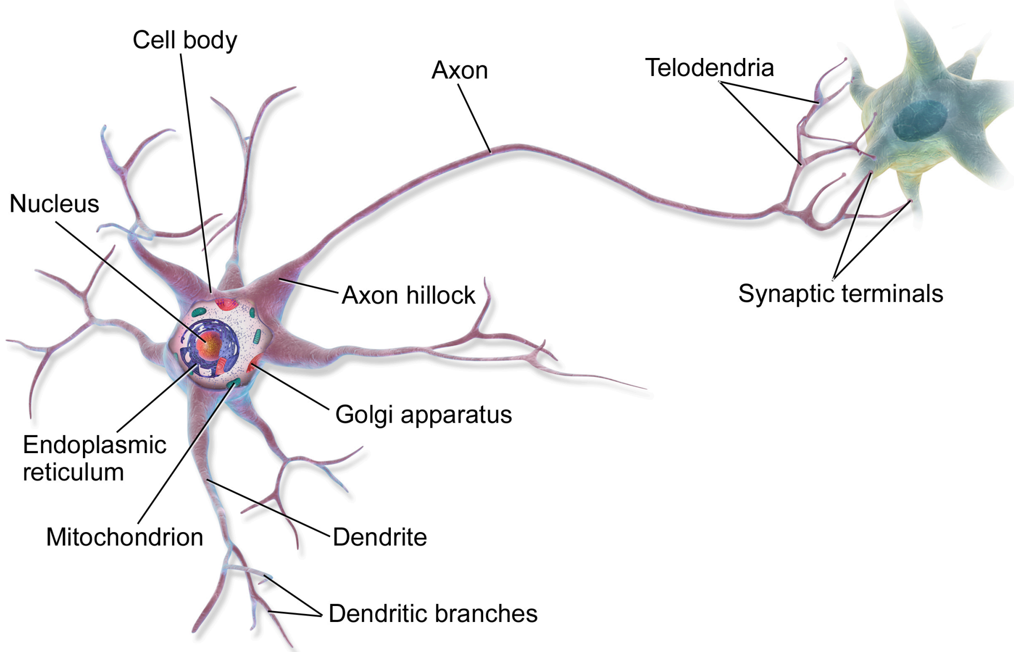
0. Introduction

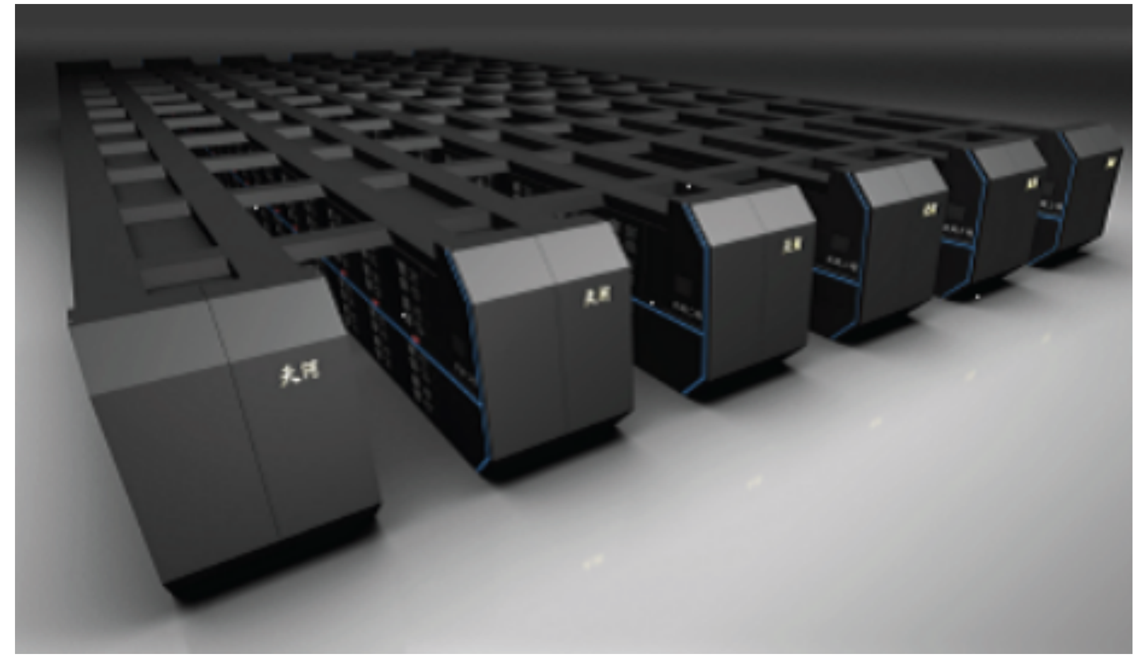
1. Regression
   1.1 Multivariate Linear Regression (curve fitting)
   1.2 Regularization (Lagrange multiplier)
   1.3 Logistic Regression (Fermi-Dirac distribution)
   1.4 Support Vector Machine (high-school geometry)

2. Dimensionality Reduction/feature extraction
   2.1 Principal Component Analysis (order parameters)
   2.2 Recommender Systems
   2.3 Clustering (phase transition)

Content

AI & Machine Learning Basics





	Supercomputer	Personal Computer	Human Brain
Computational Units	32,000 Xeon CPUs 10^12 transistors	4 CPUs, 10^9 transistors	10^11 neurons
Storage units	10^14 bits RAM 10^15 bits Storage	10^11 bit RAM 10^13 bit Storage	10^11 neurons 10^14 synapses
Cycle time	10^-9 sec	10^-9 sec	10^-3 sec
Operations/sec	10^15	10^10	10^17
Memory updates/sec	10^14	10^10	10^14
Weight / Space	150 tons / Basketball court	1 Kg / A4 Paper	1.5 Kg / 1/6 basketball
Power consumption	500 megawatt	100 watt	20 watt

AI & Machine Learning Basics

Evolution gives human a large brain and a mechanism to learn, such that we could update ourselves with experience and adapt to different environments.

All sciences are fitting models to data.

Induction is a process of extracting general rules from a set of particular cases.

But we are at the point such analysis can no longer done by people, we need computer (machine) to learn for us.
AI is multidisciplinary
Physics, mathematics, chemistry, …
Cognitive science
Statistics: association is inference, learning is estimation, classification is discriminate analysis.
Engineering: classification is pattern recognition

Vision, speech and robotics, learnt from sample data
Signal processing in vision and speech recognition

Neural networks, kernel-based algorithms (SVMs) in bioinformatics and language processing

Generative models, explain data through interaction of hidden factors

Lots of example data and sufficient computing power, reduced cost of storage, larger dataset over internet and cheaper computation, COVID19
Made possible now but not in the 1950s and 60s

Intelligence seems not to originate from outlandish formula, but rather from patient, sometimes brute-force use of a simple, straightforward algorithm.