Nobel Prizes in 2024

2024 Nobel prizes in physics & chemistry heralded the age of new science, where "computer science becoming embedded in the very fabric of science (Stephen Emmott, Microsoft)"

cf. Creation of the Universe (*PBS*, '85)
"Creation of Universe was sponsored by Microsoft."

Microsoft toward 2020 science (Mar. '06)
https://www.microsoft.com/en-us/research/publication/towards-2020-science-2
Nature special issue on 2020 vision on computing & science (Mar. '06)
http://www.nature.com/nature/journal/v440/n7083

Physics in 100 Years

Computer science will play major roles in physics

- **Increasingly, the development of algorithms will become a central focus of theoretical physics. ... Triumphs of creative understanding such as universality (suppression of irrelevant details), symmetry (informed iteration), and topology (emergence of discrete from continuous) are preadapted to algorithmic thinking.**

- **The work of designing algorithms can be considered as a special form of teaching, aimed at extremely clever but literal-minded and inexperienced students—that is, computers—who cannot deal with vagueness. At present those students are poorly motivated and incurious, but those faults are curable. Within 100 years they will become the colleagues and ultimately the successors of their human teachers, with a distinctive style of thought adapted to their talents.**

- **Two developments will be transformative: naturalized artificial intelligence and expanded sensoria.**

Frank Wilczek (Nobel prize in physics, 2004)

Nobel Prize in Physics(-Computer Science)

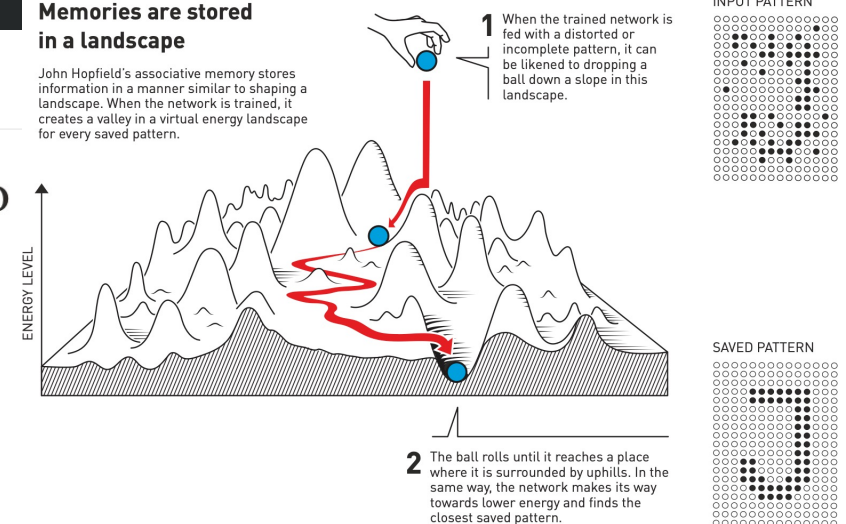## The Nobel Prize in Physics 2024

This year's laureates used tools from physics to construct methods that helped lay the foundation for today's powerful machine learning.

Because physics has contributed tools for the development of machine learning, it is interesting to see how physics, as a research field, is also benefitting from artificial neural networks.

Ill. Niklas Elmehed © Nobel Prize Outreach

John J. Hopfield

Prize share: 1/2

Ill. Niklas Elmehed © Nobel Prize Outreach

Geoffrey E. Hinton

Prize share: 1/2

https://www.nobelprize.org/prizes/physics/2024

The Nobel Prize in Physics 2024 was awarded to John J. Hopfield and Geoffrey E. Hinton "for foundational discoveries and inventions that enable machine learning with artificial neural networks"

"Now what" by John Hopfield (*Princeton*)

Memories are stored in a landscape

John Hopfield's associative memory stores information in a manner similar to shaping a landscape. When the network is trained, it creates a valley in a virtual energy landscape for every saved pattern.

1 When the trained network is fed with a distorted or incomplete pattern, it can be likened to dropping a ball down a slope in this landscape.

ENERGY LEVEL

2 The ball rolls until it reaches a place where it is surrounded by uphills. In the same way, the network makes its way towards lower energy and finds the closest saved pattern.

INPUT PATTERN

SAVED PATTERN

Asynchronous Parallel Processing & Emergent Collective Behavior

Neural networks and physical systems with emergent collective computational abilities

(associative memory/parallel processing/categorization/content-addressable memory/fail-soft devices)

J. J. HOPFIELD

ABSTRACT   Computational properties of use to biological organisms or to the construction of computers can emerge as collective properties of systems having a large number of simple equivalent components (or neurons). The physical meaning of content-addressable memory is described by an appropriate phase space flow of the state of a system. A model of such a system is given, based on aspects of neurobiology but readily adapted to integrated circuits. The collective properties of this model produce a content-addressable memory which correctly yields an entire memory from any subpart of sufficient size. The algorithm for the time evolution of the state of the system is based on asynchronous parallel processing. Additional emergent collective properties include some capacity for generalization, familiarity recognition, categorization, error correction, and time sequence retention. The collective properties are only weakly sensitive to details of the modeling or the failure of individual devices.

Nobel Prize in Chemistry(-Computer Science)

The Nobel Prize in Chemistry 2024

Google DeepMind

Ill. Niklas Elmehed © Nobel Prize Outreach
David Baker
Prize share: 1/2

Ill. Niklas Elmehed © Nobel Prize Outreach
Demis Hassabis
Prize share: 1/4

Ill. Niklas Elmehed © Nobel Prize Outreach
John M. Jumper
Prize share: 1/4

https://www.nobelprize.org/prizes/chemistry/2024

The Nobel Prize in Chemistry 2024 was divided, one half awarded to David Baker "for computational protein design", the other half jointly to Demis Hassabis and John M. Jumper "for protein structure prediction"

Levinthal paradox (1968): How the Nature folds an amino-acid sequence into a global energy minimum 3D structure (which is known to be NP complete) within microseconds (~ billion molecular-dynamics steps)?

How does AlphaFold2 work?

As part of AlphaFold2's development, the AI model has been trained on all the known amino acid sequences and determined protein structures.
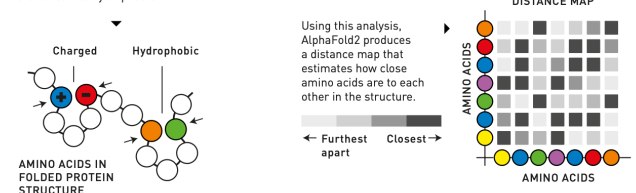
1. DATA ENTRY AND DATABASE SEARCHES

An amino acid sequence with unknown structure is fed into AlphaFold2, which searches databases for similar amino acid sequences and protein structures.

DATABASES

AMINO ACID SEQUENCE

AlphaFold2
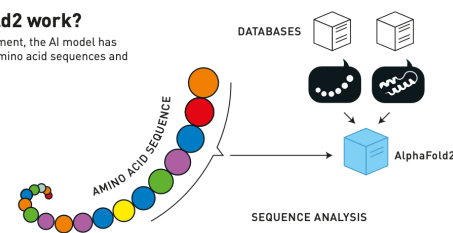
SEQUENCE ANALYSIS

2. SEQUENCE ANALYSIS

The AI model aligns all the similar amino acid sequences – often from different species – and investigates which parts have been preserved during evolution.

In the next step, AlphaFold2 explores which amino acids could interact with each other in the three-dimensional protein structure. Interacting amino acids co-evolve. If one is charged, the other has the opposite charge, so they are attracted to each other. If one is replaced by a water-repellent (hydrophobic) amino acid, the other also becomes hydrophobic.

Have co-evolved   Have co-evolved
UNKNOWN

Charged   Hydrophobic

AMINO ACIDS IN FOLDED PROTEIN STRUCTURE

Using this analysis, AlphaFold2 produces a distance map that estimates how close amino acids are to each other in the structure.

DISTANCE MAP
AMINO ACIDS
← Furthest apart   Closest →
AMINO ACIDS

3. AI ANALYSIS

Using an iterative process, AlphaFold2 refines the sequence analysis and distance map. The AI model uses neural networks called transformers, which have a great capacity to identify important elements to focus on. Data about other protein structures – if they were found in step 1 – is also utilised.

NEURAL NETWORK
CYCLE 1
CYCLE 2
CYCLE 3

4. HYPOTHETICAL STRUCTURE

AlphaFold2 puts together a puzzle of all the amino acids and tests pathways to produce a hypothetical protein structure. This is re-run through step 3. After three cycles, AlphaFold2 arrives at a particular structure. The AI model calculates the probability that different parts of this structure correspond to reality.
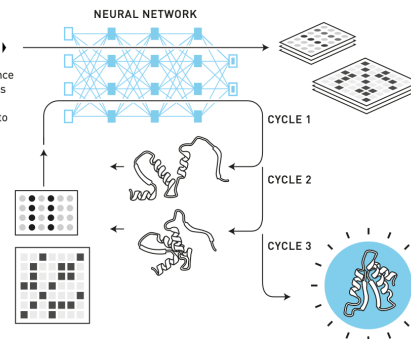
Good News: It's Not the End of the Story

Ultralow-power superbrain?

"I suspect that what is missing (in artificial neural networks) may be a mechanism of **attention**. Attention is likely to be a serial process working on top of the highly parallel distributed processes (PDP)."

Francis Crick (1962 Nobel prize in physiology)

What Mad Pursuit (1988)

https://www.amazon.com/What-Mad-Pursuit-Scientific-Discovery/dp/0465091385

cf. Transformer: Attention is all you need, Ashish Viswani *et al*. ('17)

- Why "deep" neural networks, *c.f.*, a single neuron in the human brain is connected to ~7,000 other neurons *via* synapses — network, "neuromorphic computing"?
- What about "quantum computing" — quantum network?