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

Nobel Prize in Physics(-Computer Science)

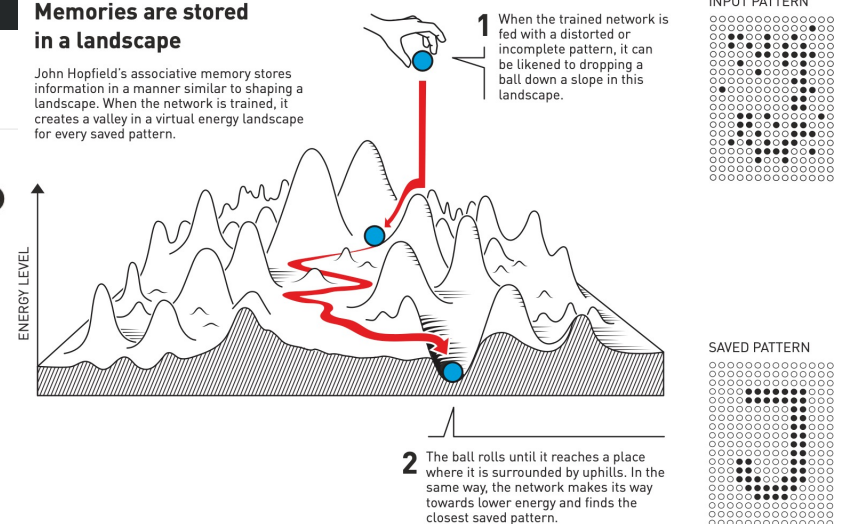## The Nobel Prize in Physics 2024

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

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

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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.

DATABASES

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.
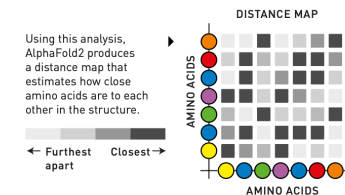
AMINO ACID SEQUENCE → AlphaFold2
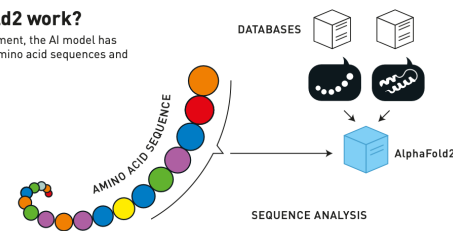
SEQUENCE ANALYSIS

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
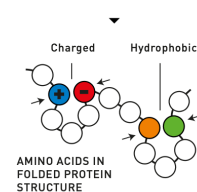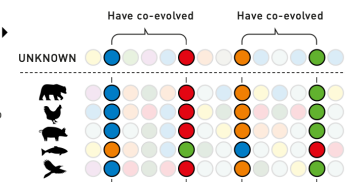
AMINO ACIDS IN FOLDED PROTEIN STRUCTURE

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
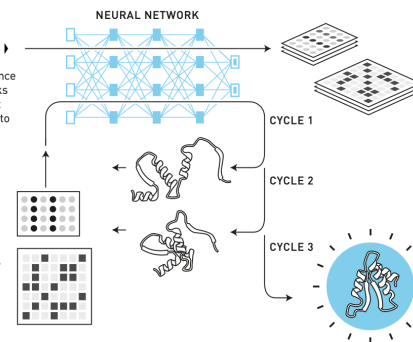
CYCLE 2

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 (USC graduate) *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?**

Final project?