

CAN SCIENCE BE JUST DATA-DRIVEN ?

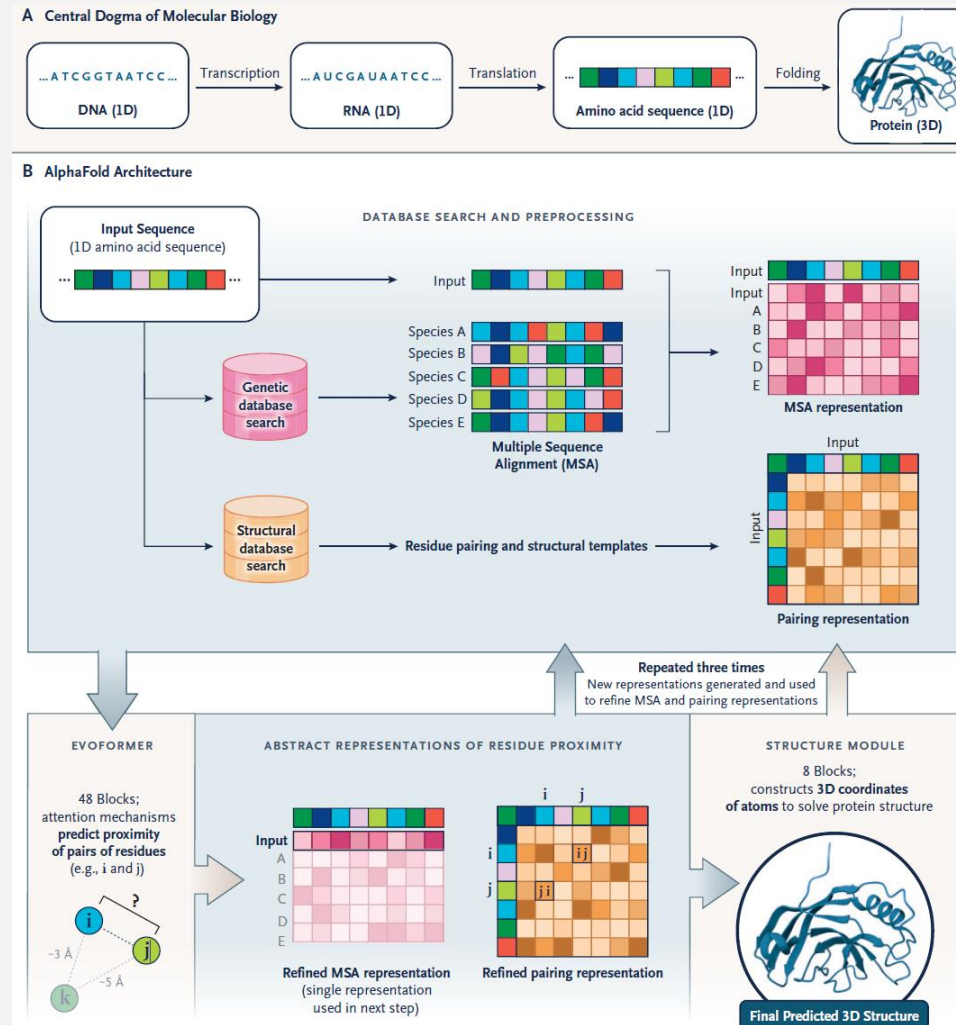
Hugues Bersini
IRIDIA - ULB



2024
A
SPECIAL
YEAR



ALPHAFOLD



MOLECULAR STRUCTURE

Primary (sequence)

Secondary (local folding)

Tertiary (long-range folding)

Quaternary (multimeric organization)

Supramolecular (large-scale assemblies)

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CLINICAL IMPLICATIONS OF BASIC RESEARCH

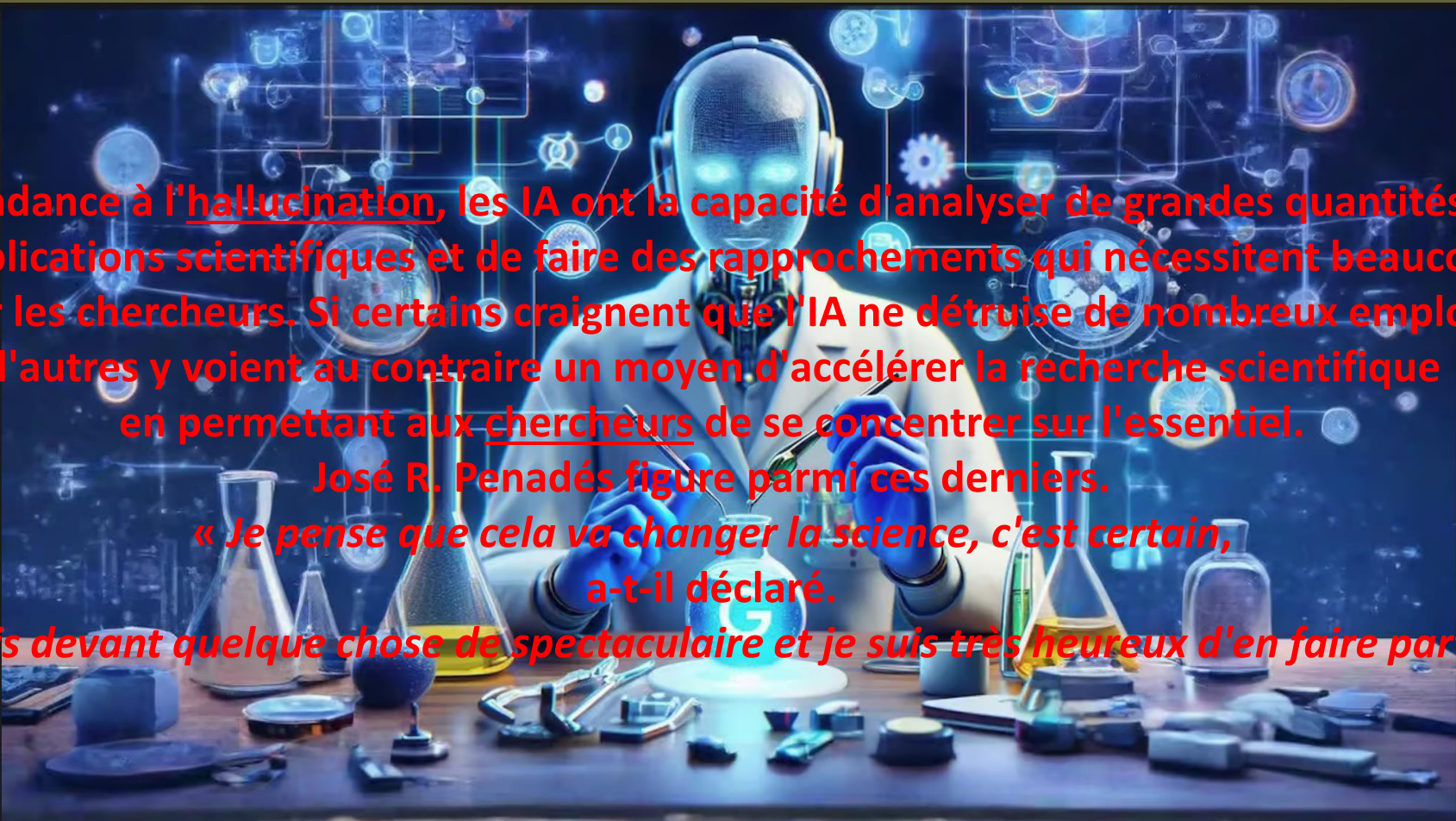
introspectively judge the quality of its outputs.

AI-ML is essentially doing science.

Disclosure forms provided by the author are available with the full text of this article at [NEJM.org](https://nejm.org).

From the Departments of Bioengineering, Genetics, Medicine, and Biomedical Data Science, Stanford University, Stanford, CA.

1. Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. *Nature* 2021;596:583-9.
2. Anfinsen CB, Haber E, Sela M, White FH Jr. The kinetics of formation of native ribonuclease during oxidation of the reduced polypeptide chain. *Proc Natl Acad Sci U S A* 1961;47:1309-14.
3. Lin Z, Akin H, Rao R, et al. Evolutionary-scale prediction of atomic-level protein structure with a language model. *Science* 2023;379:1123-30.



Malgré une tendance à l'hallucination, les IA ont la capacité d'analyser de grandes quantités de données, comme les publications scientifiques et de faire des rapprochements qui nécessitent beaucoup de temps pour les chercheurs. Si certains craignent que l'IA ne détruise de nombreux emplois, d'autres y voient au contraire un moyen d'accélérer la recherche scientifique en permettant aux chercheurs de se concentrer sur l'essentiel.

José R. Penadés figure parmi ces derniers.

« Je pense que cela va changer la science, c'est certain, a-t-il déclaré.

Je suis devant quelque chose de spectaculaire et je suis très heureux d'en faire partie ».

THE GREAT INVASION OF NEURAL NETWORKS AND MACHINE LEARNING



Before we proceed any further, hear me speak.

All:
Speak, speak.

First Citizen:
You are all resolved rather to die than to famish?

All:
Resolved. resolved.

First Citizen:
First, you know Caius Marcius is chief enemy to the people.

All:
We know't, we know't.

First Citizen:
Let us kill him, and we'll have corn at our own price.
Is't a verdict?

All:
No more talking on't; let it be done: away, away!

Second Citizen:
One word, good citizens.

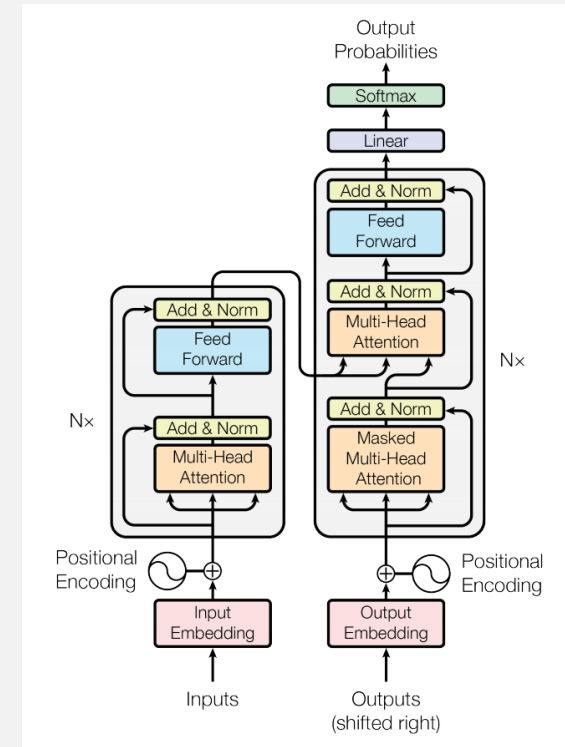
First Citizen:
We are accounted poor citizens, the patricians good.
What authority surfeits on would relieve us: if they
would yield us but the superfluity, while it were
wholesome, we might guess they relieved us humanely;
but they think we are too dear: the leanness that
afflicts us, the object of our misery, is as an
inventory to particularise their abundance; our
sufferance is a gain to them Let us revenge this with
our pikes, ere we become rakes: for the gods know I
speak this in hunger for bread, not in thirst for revenge.

Second Citizen:
Would you proceed especially against Caius Marcius?

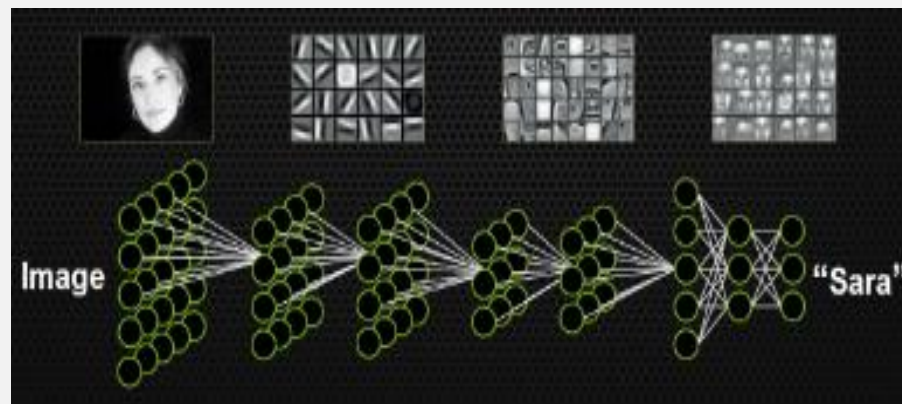
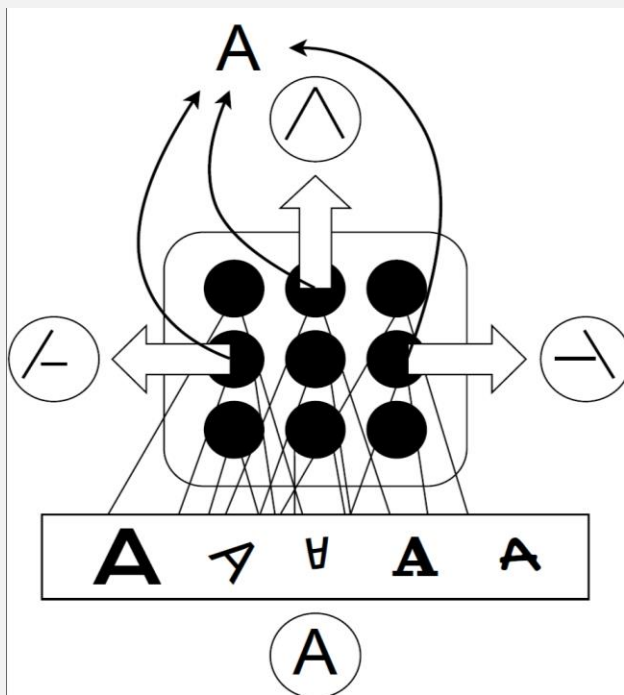
All:
Against him first: he's a very dog to the commonalty.

Second Citizen:
Consider you what services he has done for his country?

First Citizen:
Very well; and could be content to give him good
report fort, but that he pays himself with being proud.



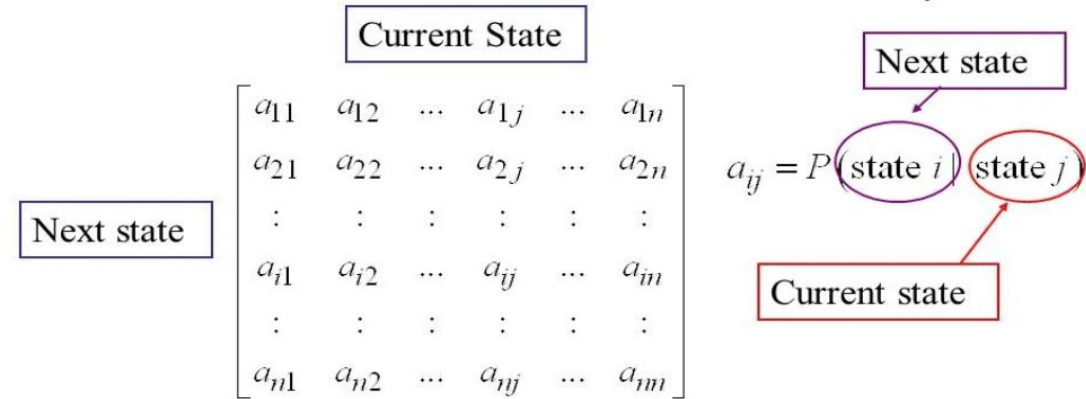
DEEP LEARNING: THE GOING UP IN ABSTRACTION !!



IT IS NOT A STATISTICAL PARROT

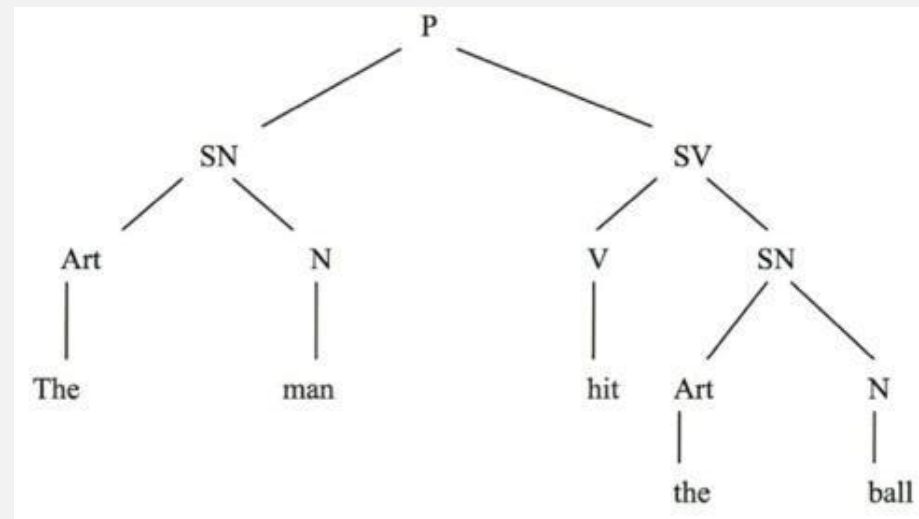
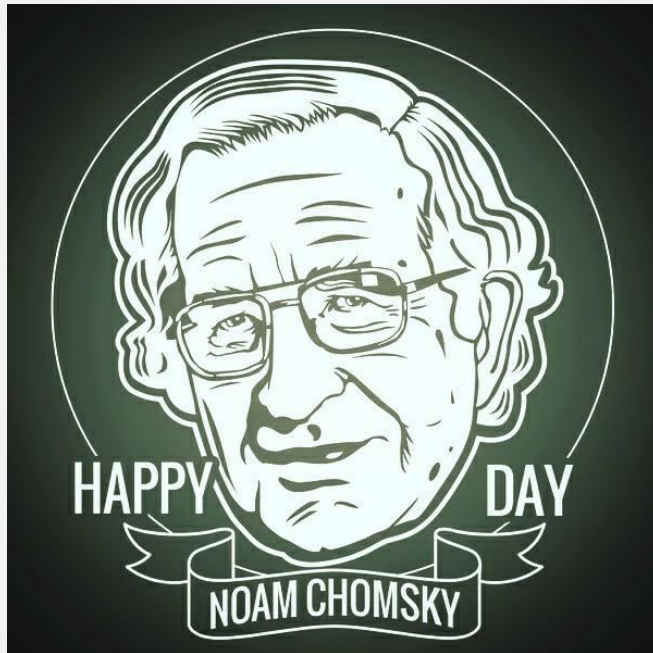
Transition Matrix

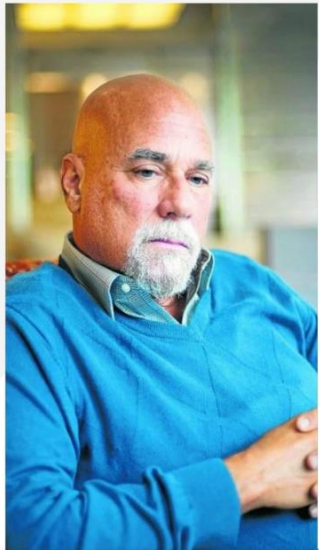
A *transition matrix* associated with a Markov chain with n states is an $n \times n$ matrix T with entries a_{ij}



1. $a_{ij} \geq 0$ for all i and j .
2. The sum of the entries in each column of T is 1.

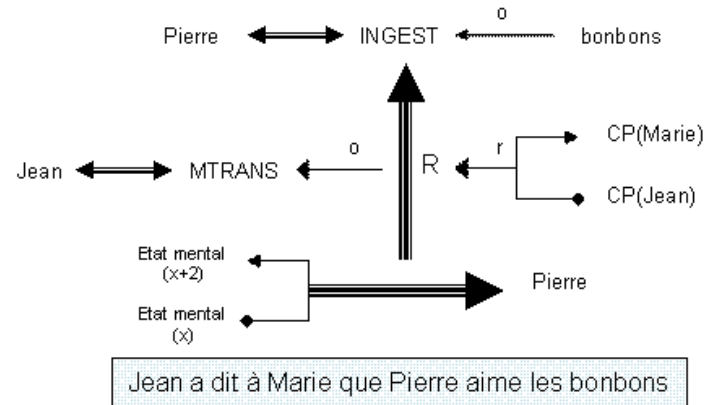
NOAM CHOMSKY





ROGER SCHANK

Dr. Schank is one of the world's leading researchers in the space of Artificial Intelligence. He has spent nearly 50 years working in the field of artificial intelligence and his contributions to this field have been immense. An artificial intelligence theorist, a cognitive psychologist, a scientist, an educational reformer, and an entrepreneur is what portrays Dr. Schank.



- **Nom:** restaurant
- **Objets:** tables
menu
nourriture
addition
argent
pourboire

- **Rôles:** client
serveuse
cuisinier
caissier
patron

- **Conditions d'entrée:**
 - Le client a faim
 - Le client a de l'argent

- **Résultats:**
 - Le client a moins d'argent
 - Le patron a plus d'argent
 - Le client est rassasié
 - Le client est satisfait

- **Scène 1: entrée**
 - Le client entre dans le restaurant
 - Le client cherche une table
 - Le client choisit une place
 - Le client va vers la table
 - Le client s'assoit

- **Scène 3: repas**
 - Le cuisinier donne la nourriture à la serveuse
 - La serveuse apporte la nourriture au client
 - Le client mange la nourriture

- **Scène 2: commande**
 - Le client prend le menu
 - Le client regarde le menu
 - Le client choisit les plats
 - Le client appelle la serveuse
 - La serveuse vient à la table
 - Le client passe la commande
 - La serveuse va à la cuisine
 - La serveuse donne la commande
 - Le cuisinier prépare le plat

- **Scène 4: sortie**
 - La serveuse prépare l'addition
 - La serveuse va vers le client
 - La serveuse donne l'addition au client
 - Le client paie la serveuse
 - Le client donne un pourboire à la serveuse
 - Le client sort du restaurant

ROGER SCHANK

PIAGET VS CHOMSKY

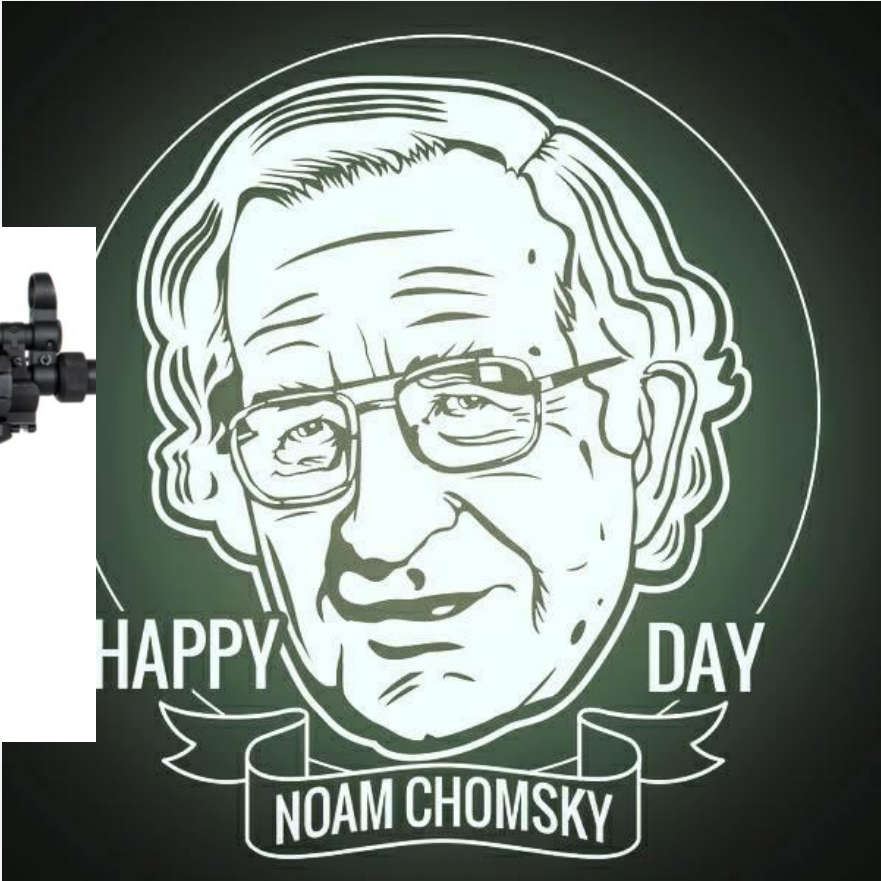
1.2. Les protagonistes



Jean William Fritz Piaget, né le 9 août 1896 à Neuchâtel en Suisse et mort le 16 septembre 1980 à Genève, est un biologiste, psychologue, connu pour ses travaux en psychologie du développement à travers ce qu'il a appelé l'épistémologie génétique (ou structuralisme génétique).



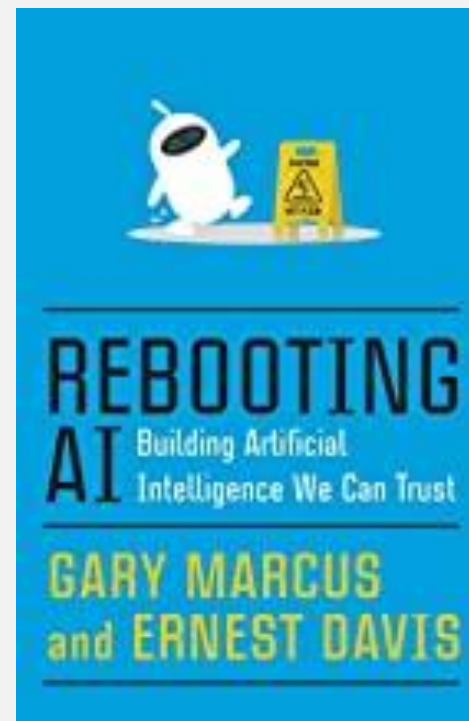
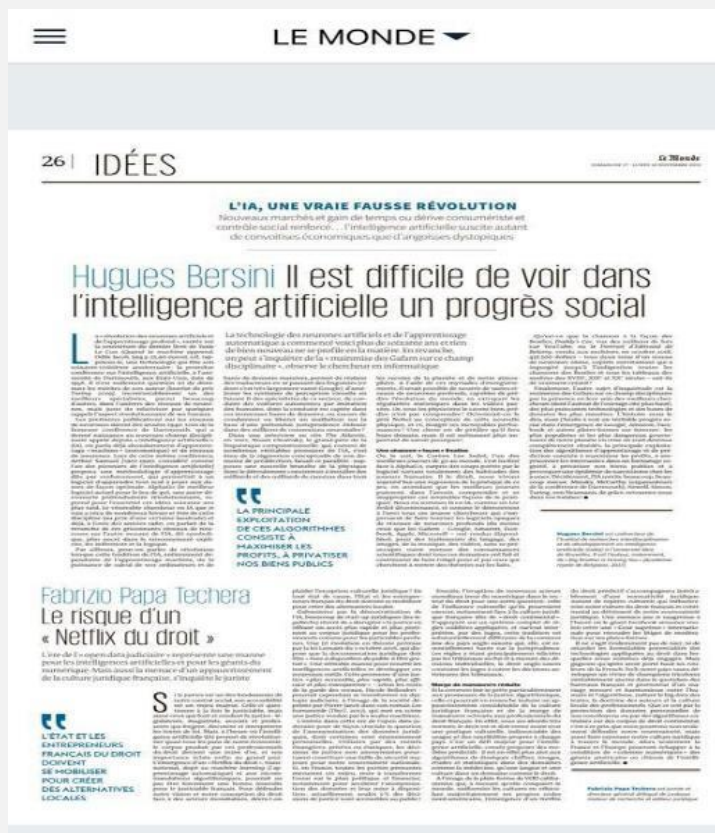
Noam Chomsky né le 7 décembre 1928 à Philadelphie, est un linguiste américain. Professeur émérite de linguistique au Massachusetts Institute of Technology (MIT) de 1955 à 2017, il fonde la linguistique générative.



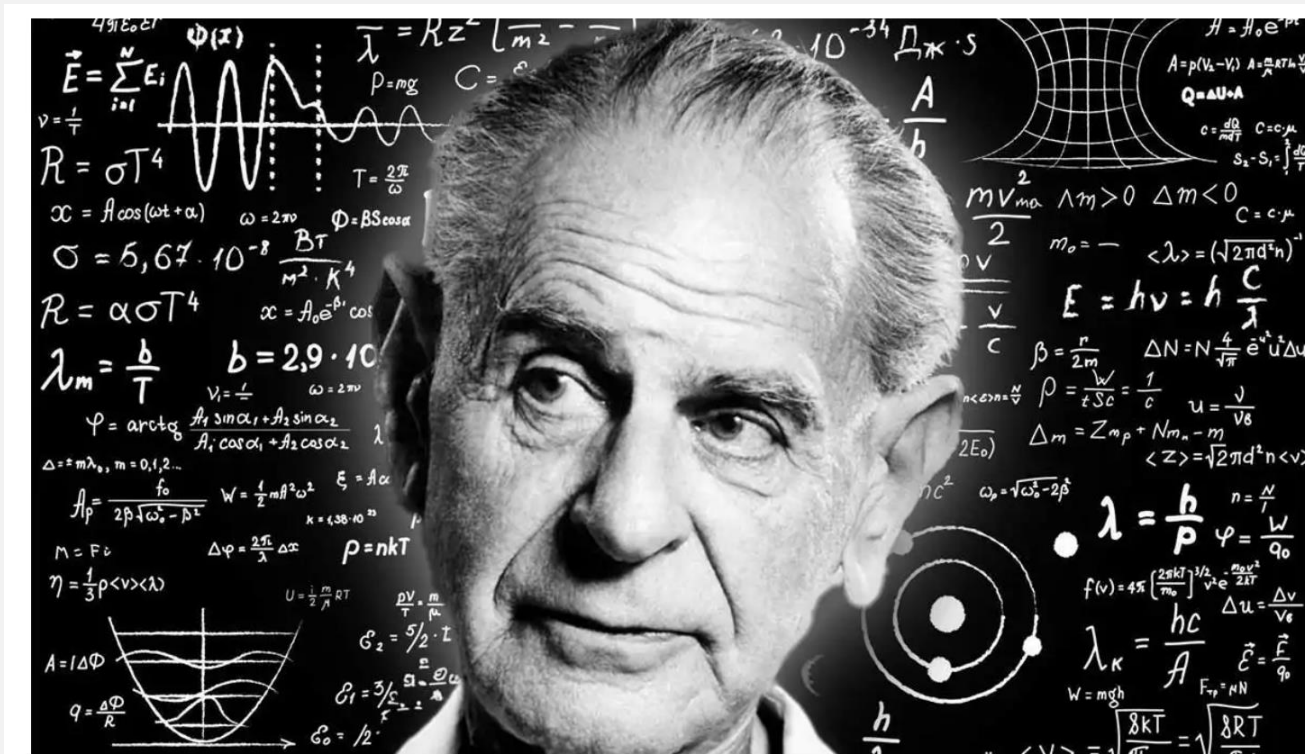
An AI quite creative but in a **virtual, closed and objective world**



THE BLACK HOLE OF DEEP LEARNING

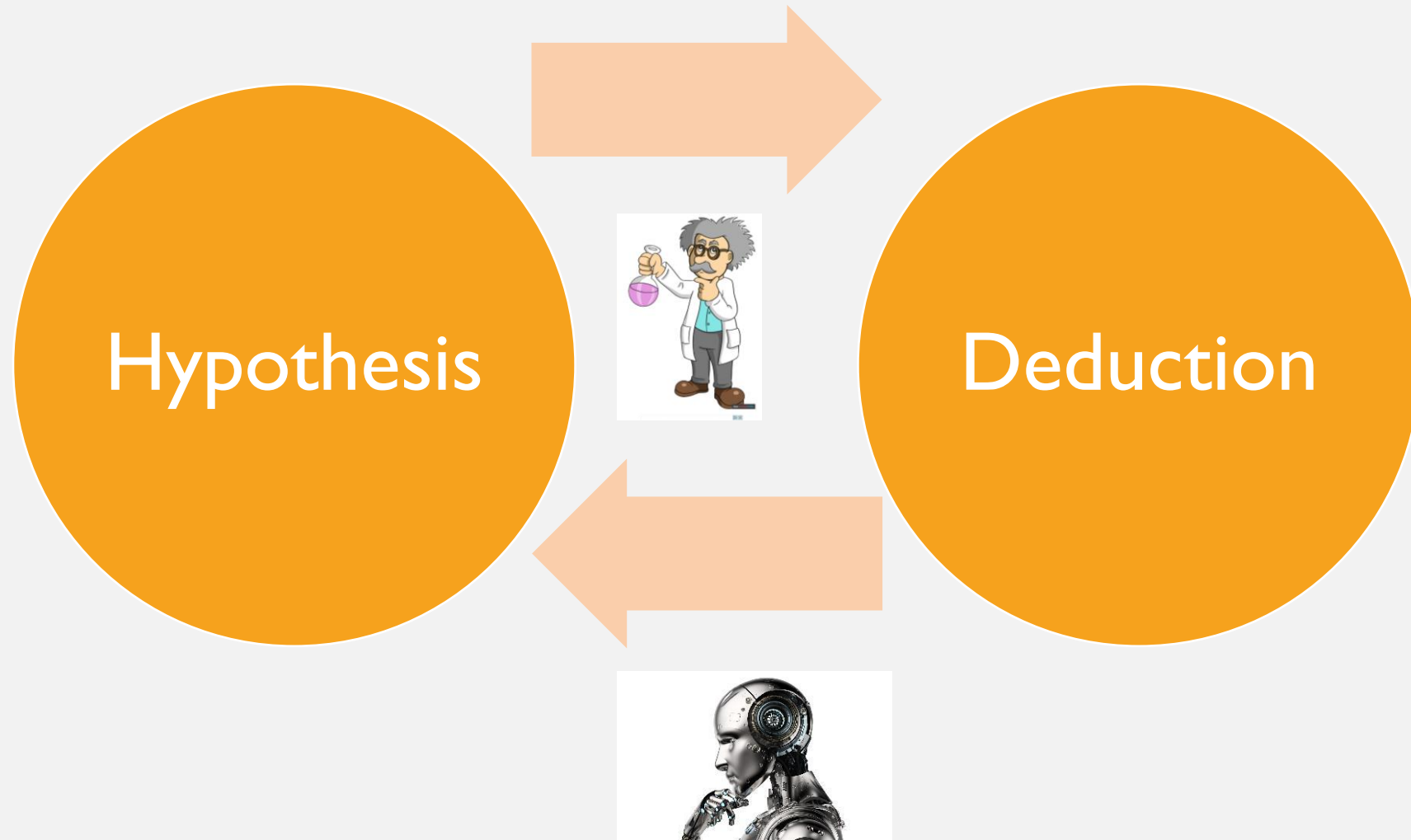


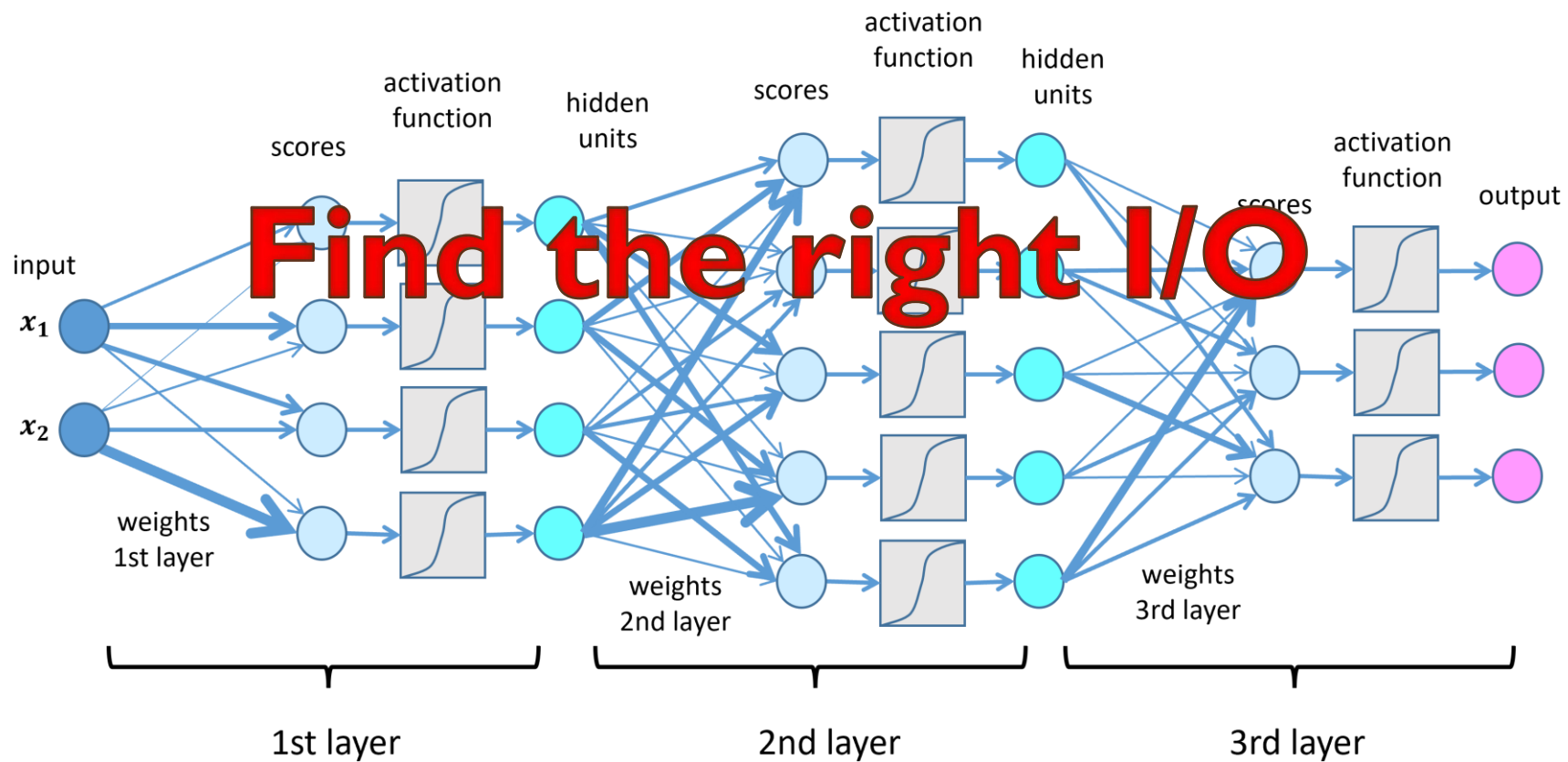
IS KARL POPPER STILL RELEVANT ?

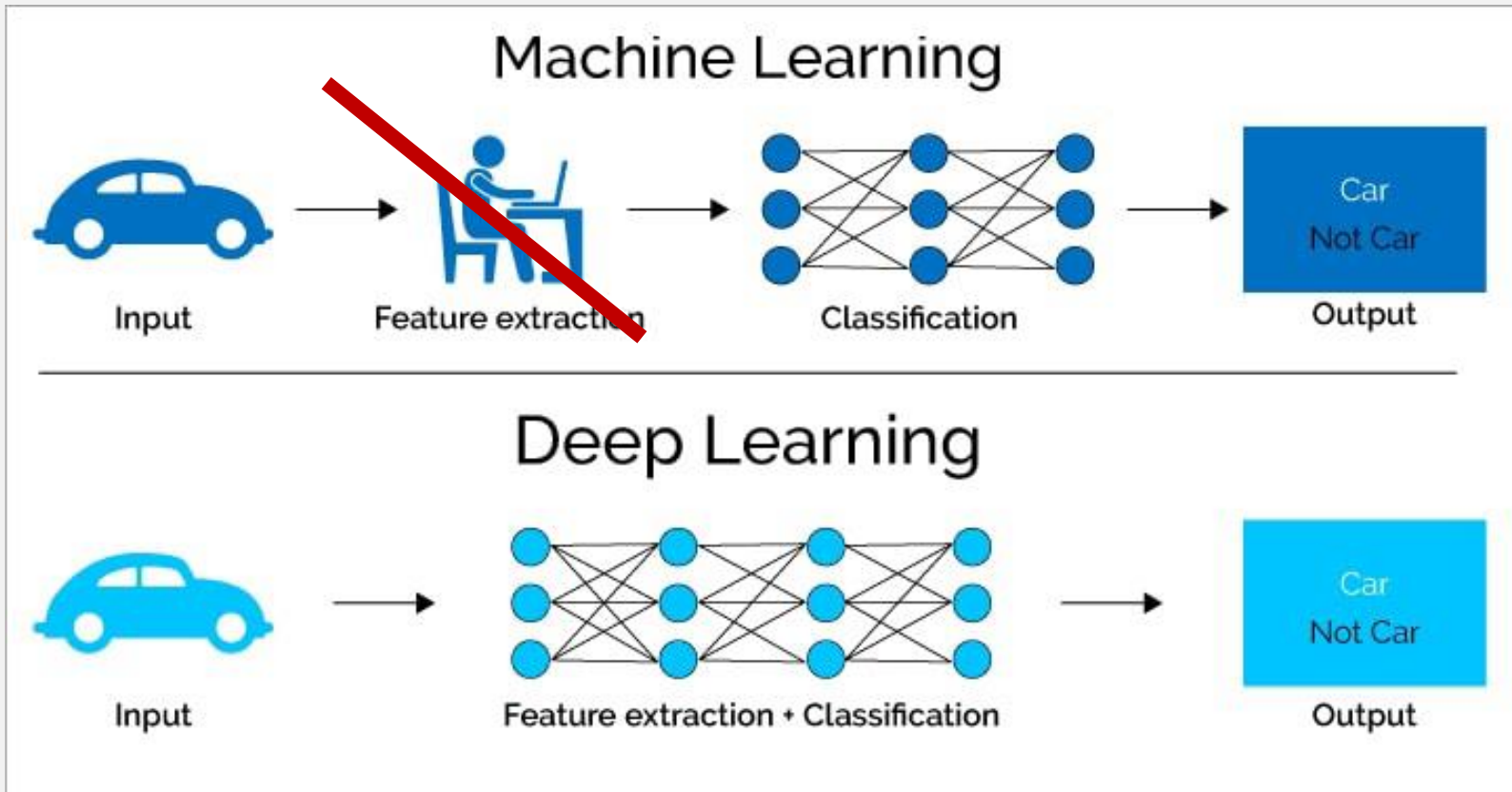


Hypothetico $\longleftrightarrow$ Deduction

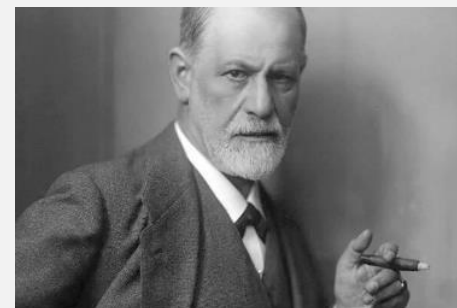
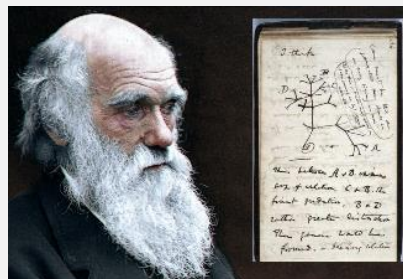
Falsificability







Charleroi-2025



2025