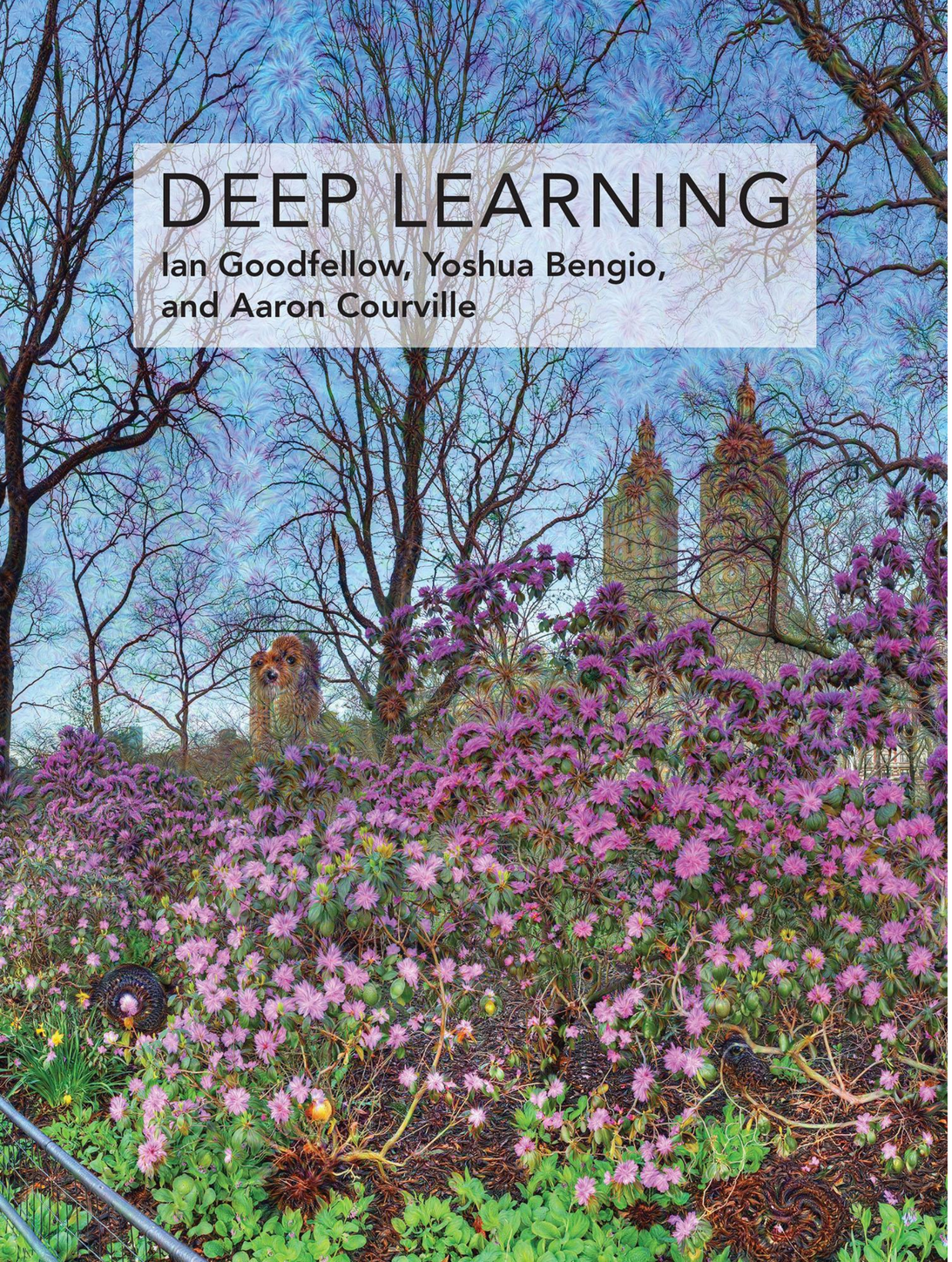


A DEEP LEARNING JOURNEY

YOSHUA BENGIO

New in ML NeurIPS 22 mentorship workshop
November 28th, 2022

Mila

Université de Montréal

IVADO

CIFAR

Falling in Love with a Research Direction

1985-1986:

- finishing my undergrad and wondering what I would do next
- reading lots of papers in various areas
- zoomed in on the neural networks research
- read papers by Geoff Hinton, David Rumelhart and other early connectionists

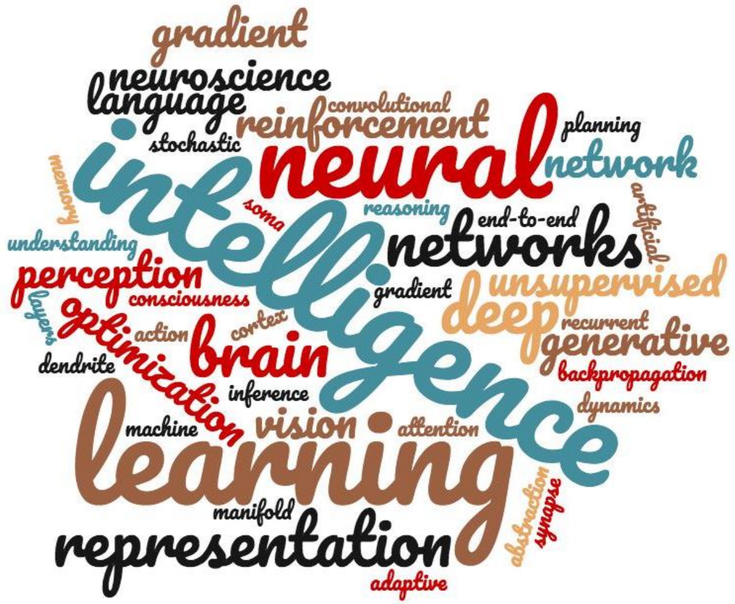
1986-1988:

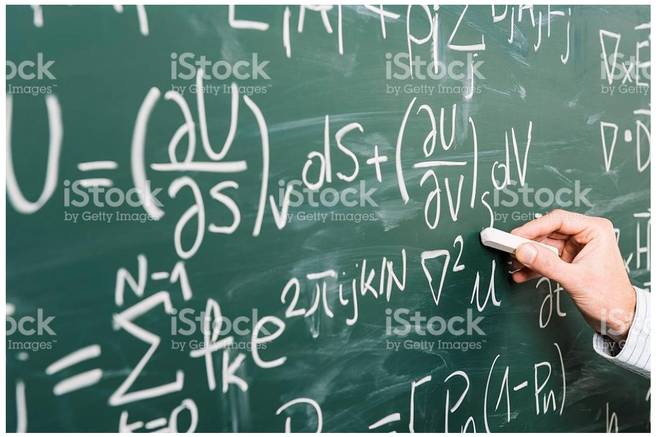
- read about Boltzmann machine, implemented it for phoneme classification
- MSc thesis on Boltzmann machines for speech recognition
- read about backpropagation, got excited about it, started working with it
- when to 1988 Connectionist Summer School and met many other passionate graduate students and researchers

1988-1991: PhD thesis on neural nets (RNNs and ConvNets) and HMMs hybrids

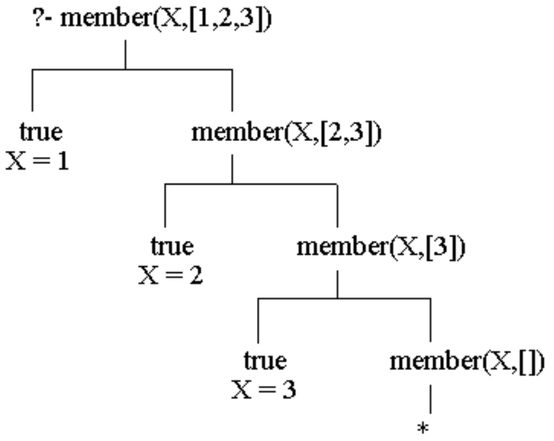
Neural Networks & AI
Extraordinary & Exciting Hypothesis

- There are principles giving rise to intelligence (machine, human or animal) via learning, simple enough that they can be described compactly, similarly to the laws of physics, i.e., our intelligence is not just the result of a huge bag of tricks and pieces of knowledge, but of general mechanisms to acquire knowledge.

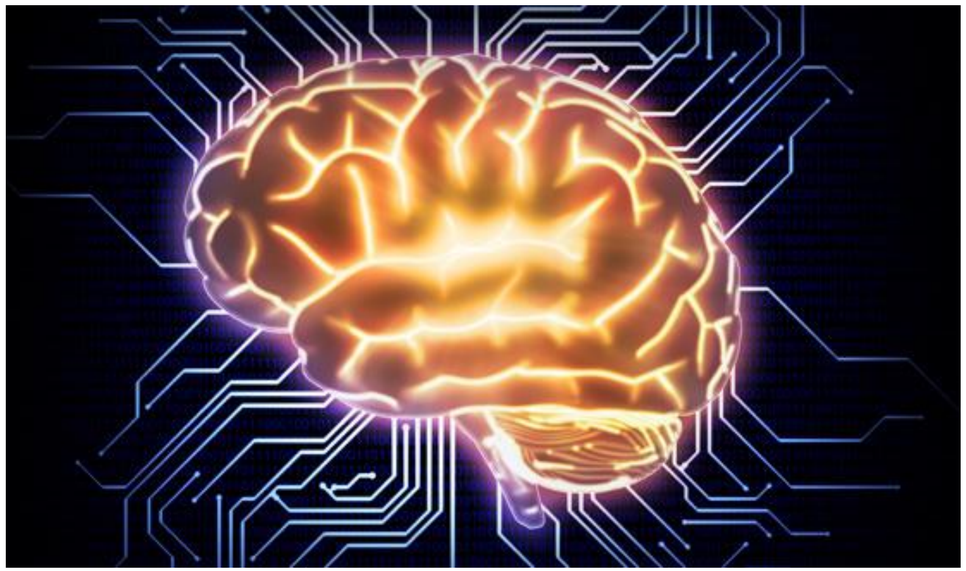




The Machine Learning approach to AI



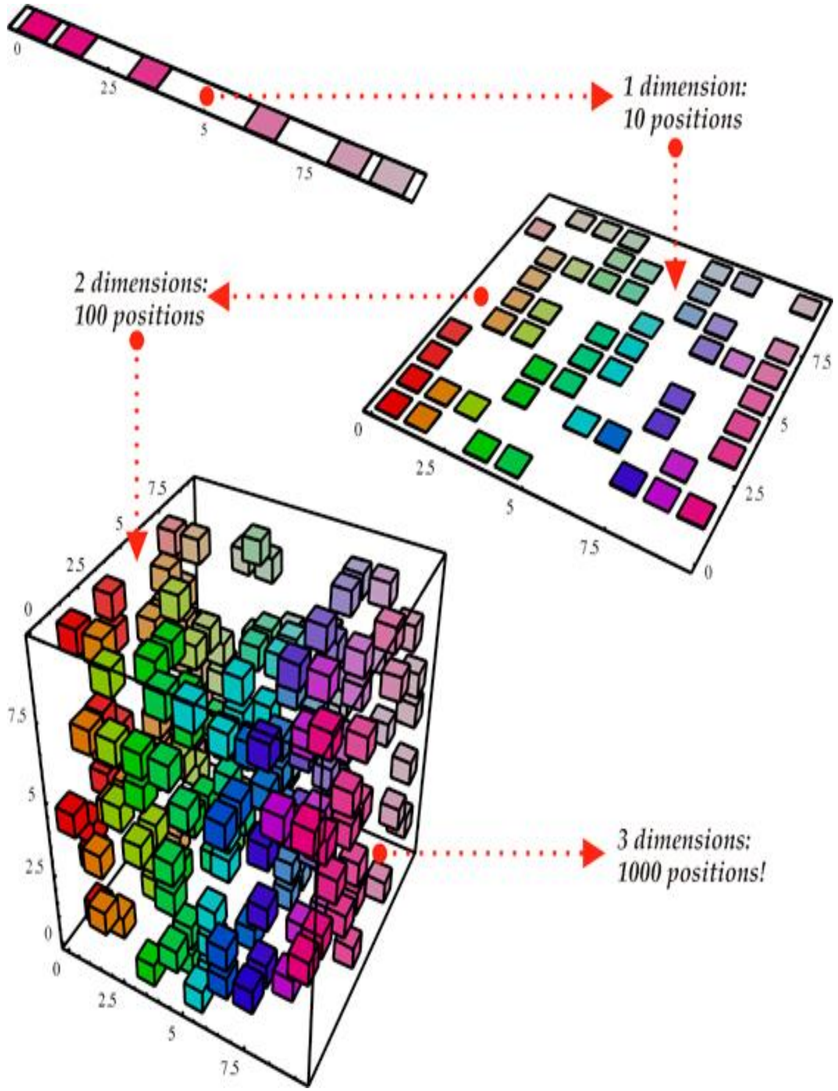
- **Classical AI, rule-based, symbolic**
  - knowledge is provided by humans
    - but intuitive knowledge (e.g. much of common sense) not communicable
  - machines only do inference (using designed alg.)
  - no strong learning, adaptation
  - insufficient handling of uncertainty
  - not grounded in low-level perception and action
- **Machine learning tries to fix these problems**
  - succeeded to a great extent
  - higher-level (conscious) cognition not achieved yet



ML 101. What We Are Fighting Against: The Curse of Dimensionality

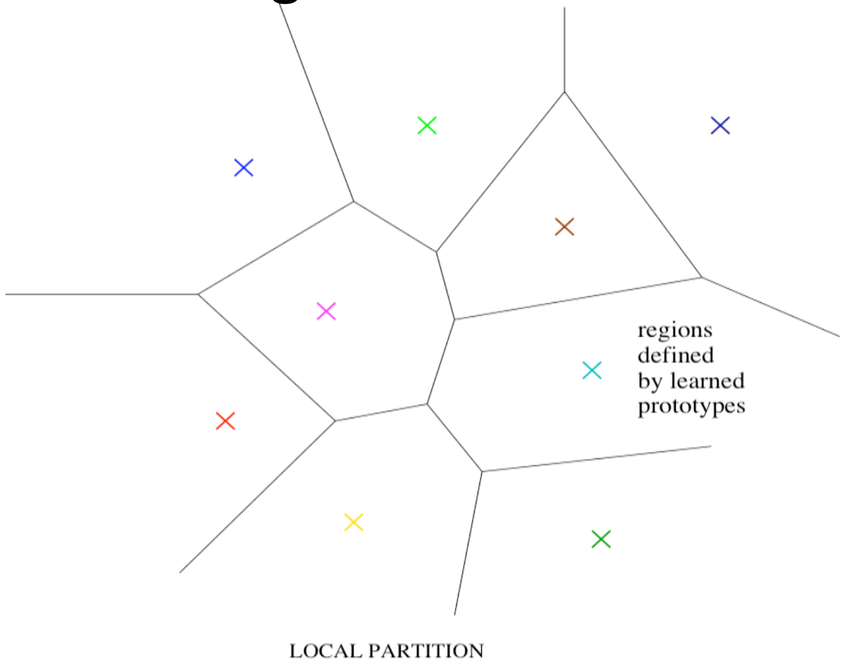
- How can we possibly generalize to settings we have never seen data for?

- Looking at similar examples is not sufficient when dealing with high-dimensional data, like images

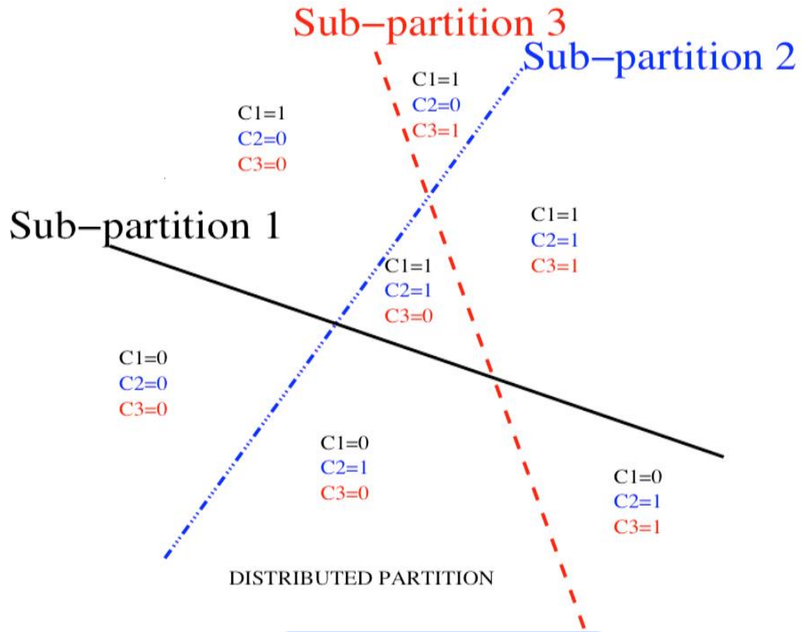


Distributed Representations: The Power of Compositionality

- Distributed (possibly sparse) representations, learned from data, can capture the **meaning** of the data and state
- Parallel composition of features: can be exponentially advantageous



Not Distributed

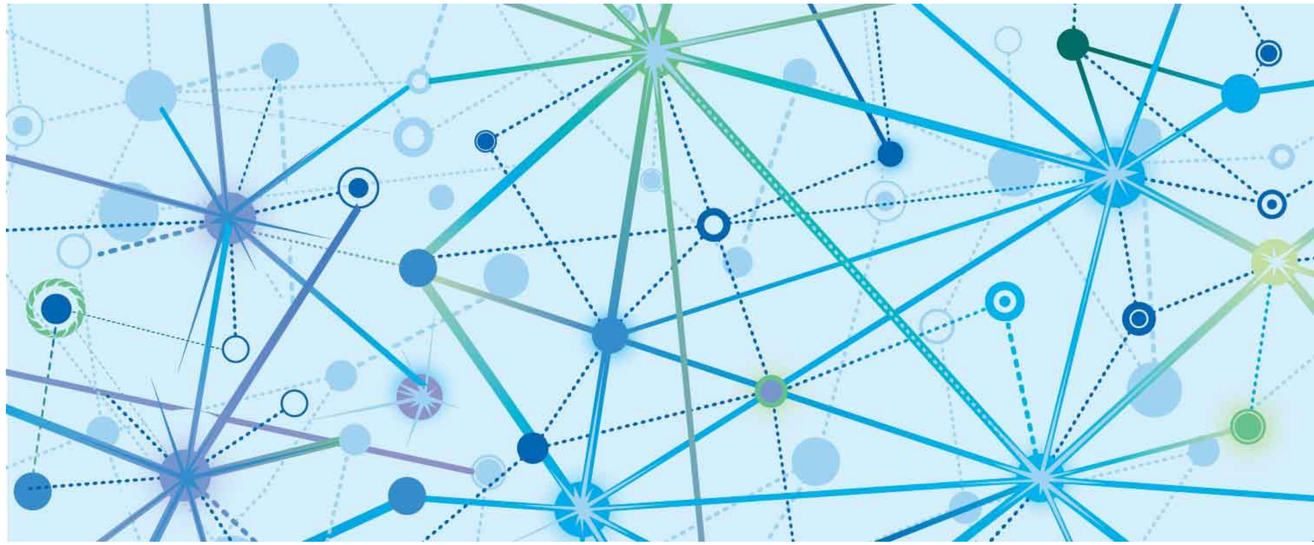


Distributed

Machine Learning & AI → Deep Learning

- Five key ingredients for ML towards AI
  1. Lots & lots of data
  2. Very flexible models
  3. Enough computing power
  4. Computationally efficient inference
  5. **Powerful assumptions that can defeat the curse of dimensionality and achieve strong generalization to new cases**

The Neural Net Approach to AI



- **Brain-inspired**
- Synergy of a large number of simple adaptive computational units
- Focus on **distributed representations**
  - **E.g. word representations** (Bengio et al NIPS'2000)
- View intelligence as arising of combining
  - an objective or reward function
  - an approximate optimizer (learning rule)
  - an initial architecture / parametrization
- End-to-end learning (all the pieces of the puzzle adapt to help each other)

Recap: Machine Learning 101

- Family of functions
- Tunable parameters
- Examples sampled from unknown data generating distribution
- A measure of the error made by the trained function
- Approximate minimization algorithm to search for good choice of parameters, iteratively reducing the average training error

Learning Long-Term Dependencies with Gradient Descent is Difficult

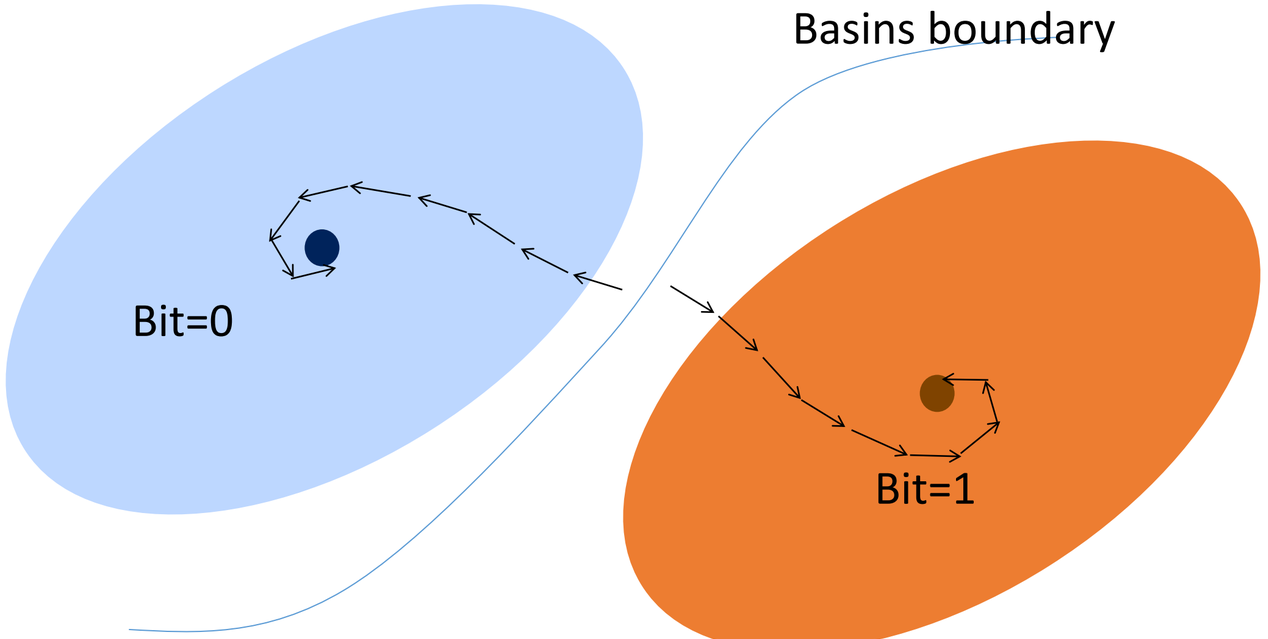


Y. Bengio, P. Simard & P. Frasconi, IEEE Trans. Neural Nets, **1994**

Lesson: negative results can be very important, teach us something that drives much downstream research

How to store 1 bit? Dynamics with multiple basins of attraction in some dimensions

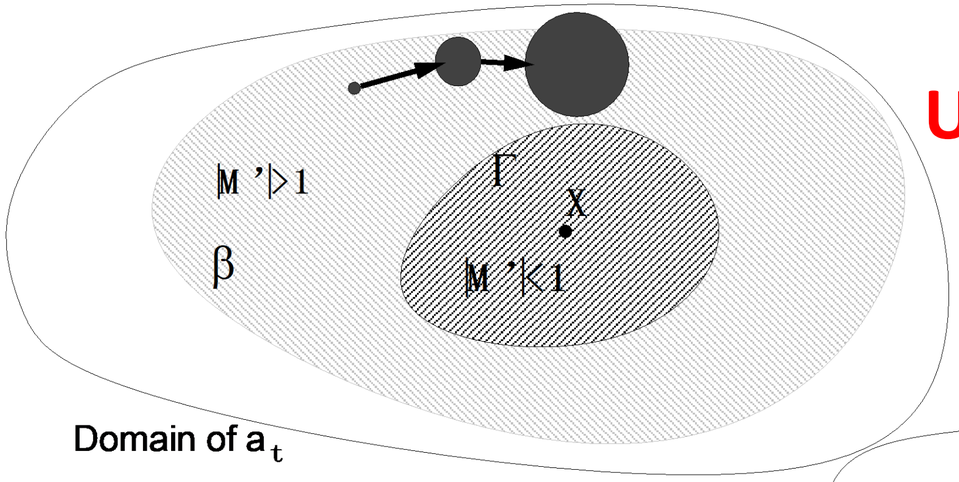
- Some subspace of the state can store 1 or more bits of information if the dynamical system has multiple basins of attraction in some dimensions



Note: gradients MUST be high near the boundary

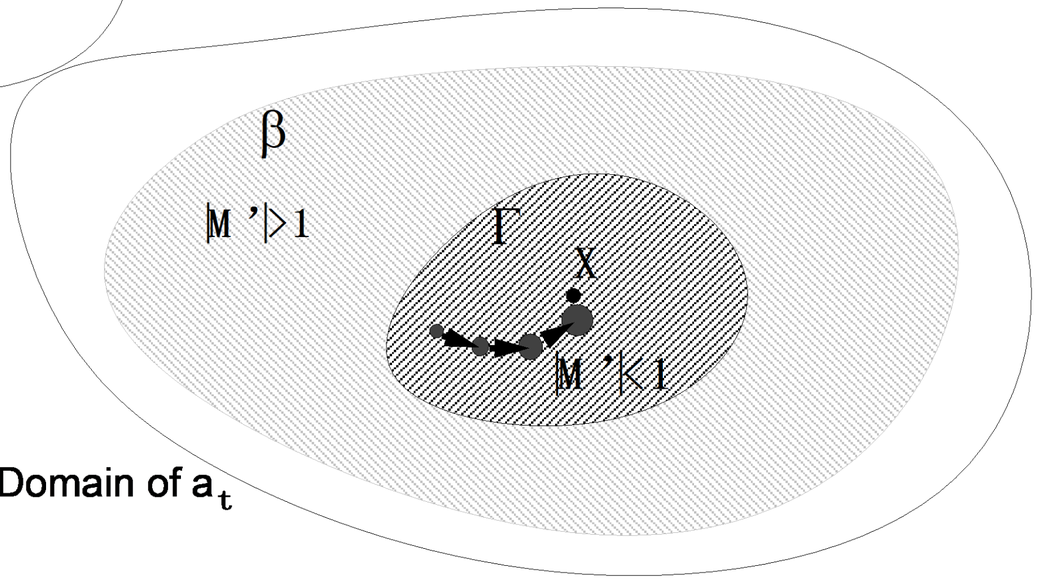
Robustly storing 1 bit in the presence of bounded noise

- With spectral radius > 1, noise can kick state out of attractor



UNSTABLE

- Not so with radius<1



CONTRACTIVE
→ STABLE

Storing Reliably ➔ Vanishing gradients

- Reliably storing bits of information requires spectral radius<1
- The product of T matrices whose spectral radius is < 1 is a matrix whose spectral radius converges to 0 at exponential rate in T

$$L = L(s_T(s_{T-1}(\ldots s_{t+1}(s_t, \ldots))))$$

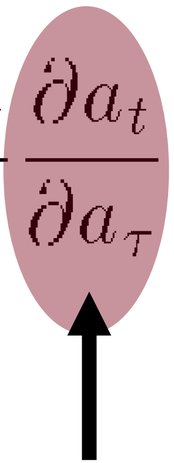
$$\frac{\partial L}{\partial s_t} = \frac{\partial L}{\partial s_T}\frac{\partial s_T}{\partial s_{T-1}}\cdots\frac{\partial s_{t+1}}{\partial s_t}$$

- If spectral radius of Jacobian is < 1 ➔ propagated gradients vanish

Why it hurts gradient-based learning

- Long-term dependencies get a weight that is exponentially smaller (in T) compared to short-term dependencies

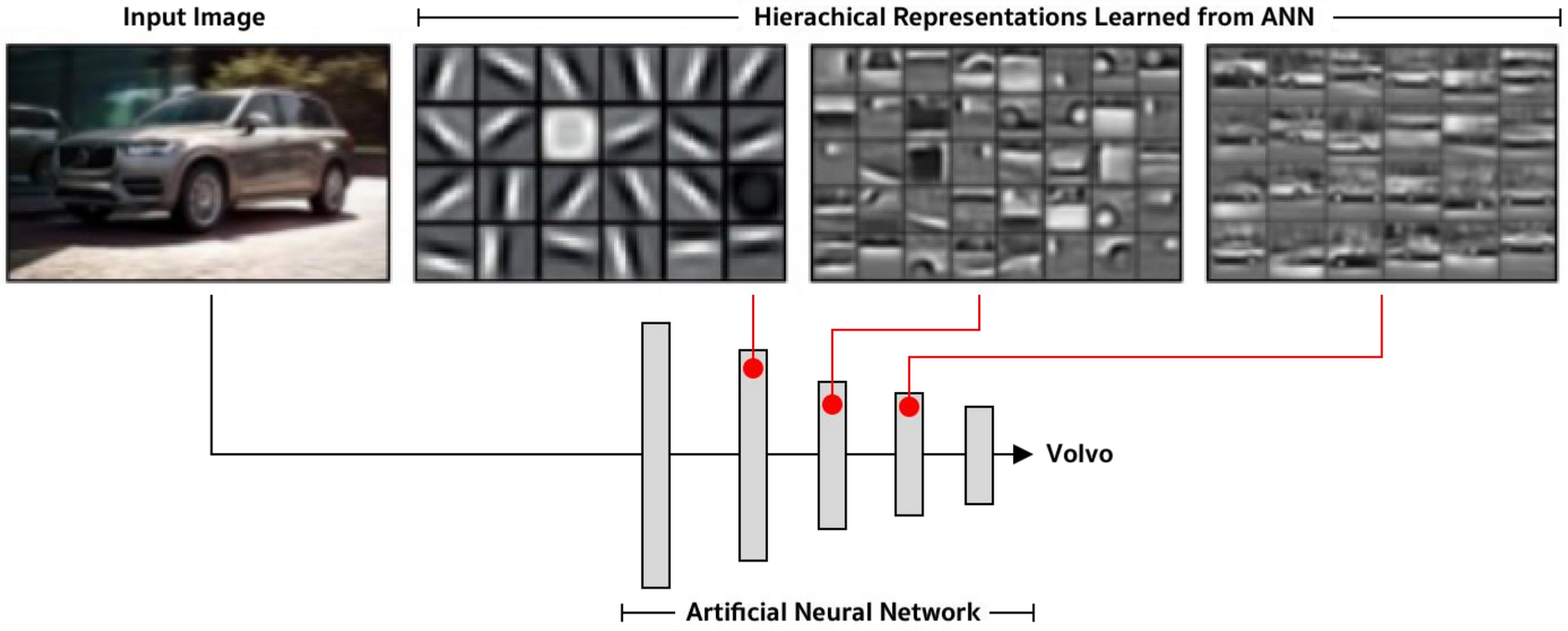
$$\frac{\partial C_t}{\partial W} = \sum_{\tau \leq t} \frac{\partial C_t}{\partial a_\tau} \frac{\partial a_\tau}{\partial W} = \sum_{\tau \leq t} \frac{\partial C_t}{\partial a_t} \frac{\partial a_t}{\partial a_\tau} \frac{\partial a_\tau}{\partial W}$$



Becomes exponentially smaller for longer time differences, when spectral radius < 1

Deep Learning: Learning an Internal Representation

- Unlike other ML methods with either
  - no intermediate representation (linear)
  - or fixed (generally very high-dimensional) intermediate representations (SVMs, kernel machines)
- What is a good representation? Makes other or downstream tasks easier.



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Published: 27 May 2015

Deep learning

Yann LeCun ✉, Yoshua Bengio & Geoffrey Hinton

Nature **521**, 436–444 (2015) | Cite this article

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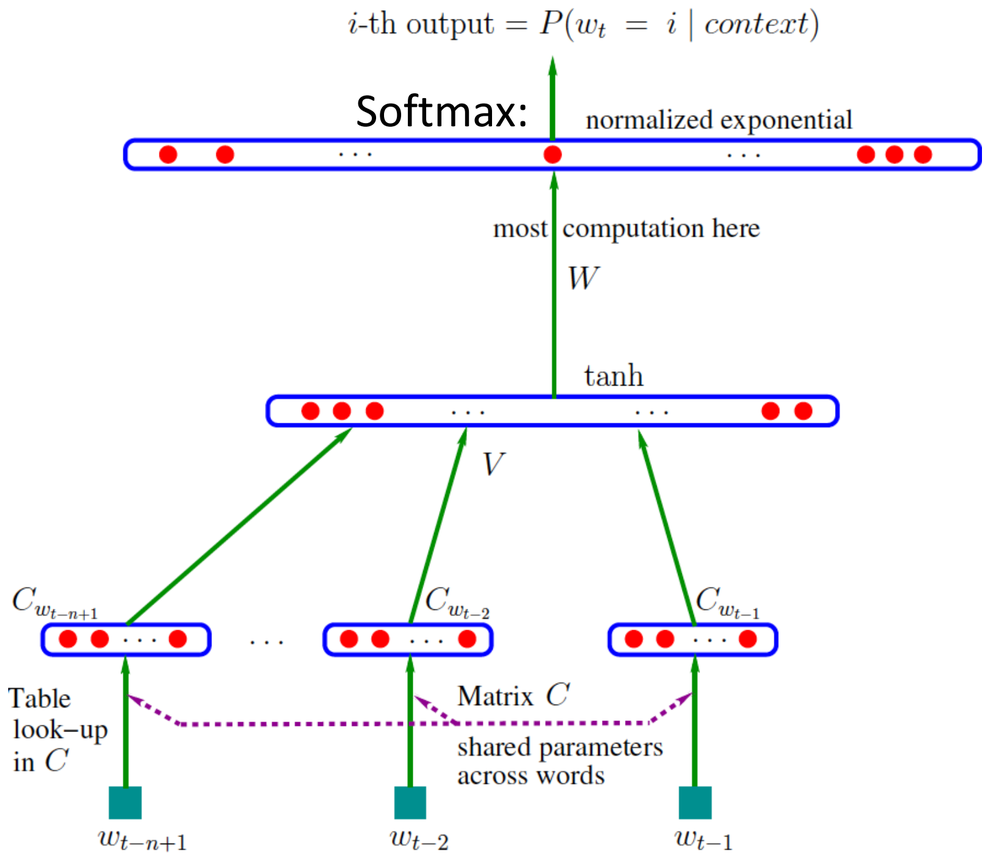
Neural Language Models



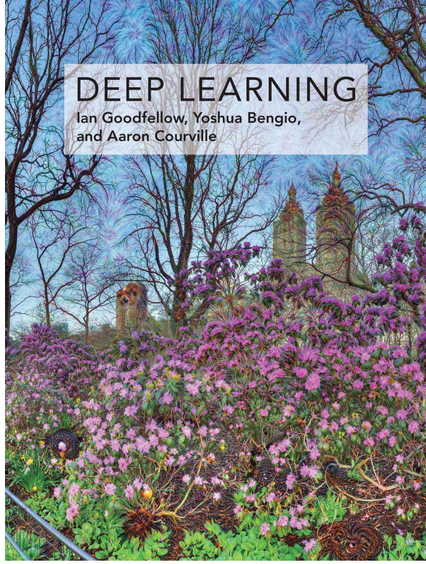
- *Bengio et al NIPS'2000 and JMLR 2003 "A Neural Probabilistic Language Model"*
  - Each word represented by a distributed continuous-valued code vector = embedding
  - Shared across n-grams (tuples of words)
  - Generalizes to sequences of words that are semantically similar to training sequences



$$P(w_1, w_2, w_3, \ldots, w_T) = \prod_t P(w_t | w_{t-1}, w_{t-2}, \ldots, w_1)$$

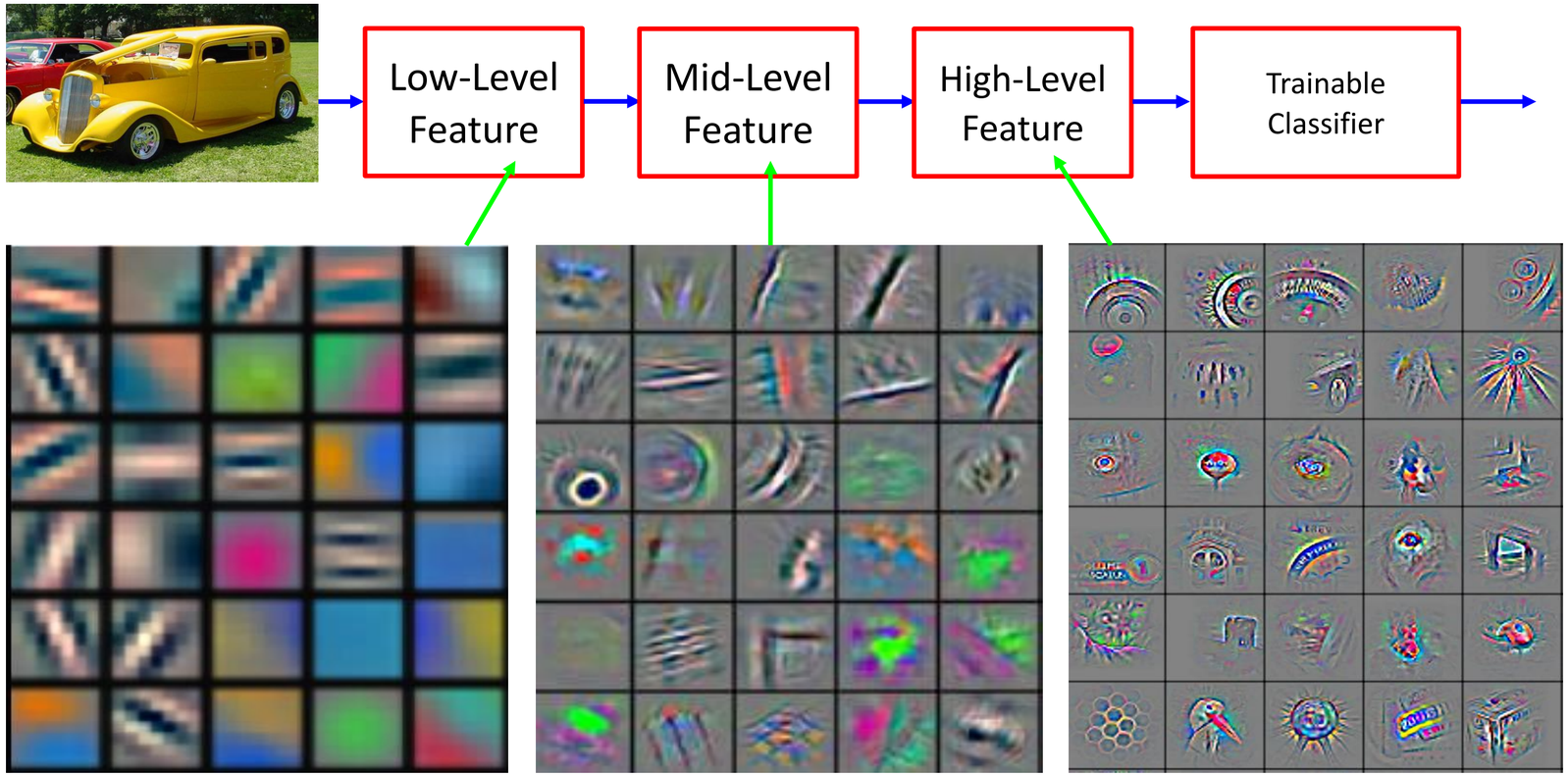
Why Multiple Layers? The World is Compositional

- Hierarchy of representations with increasing level of abstraction
- Each stage is a kind of trainable feature transform
- Image recognition: Pixel → edge → texton → motif → part → object
- Text: Character → word → word group → clause → sentence → story
- Speech: Sample → spectral band → sound → … → phone → phoneme → word

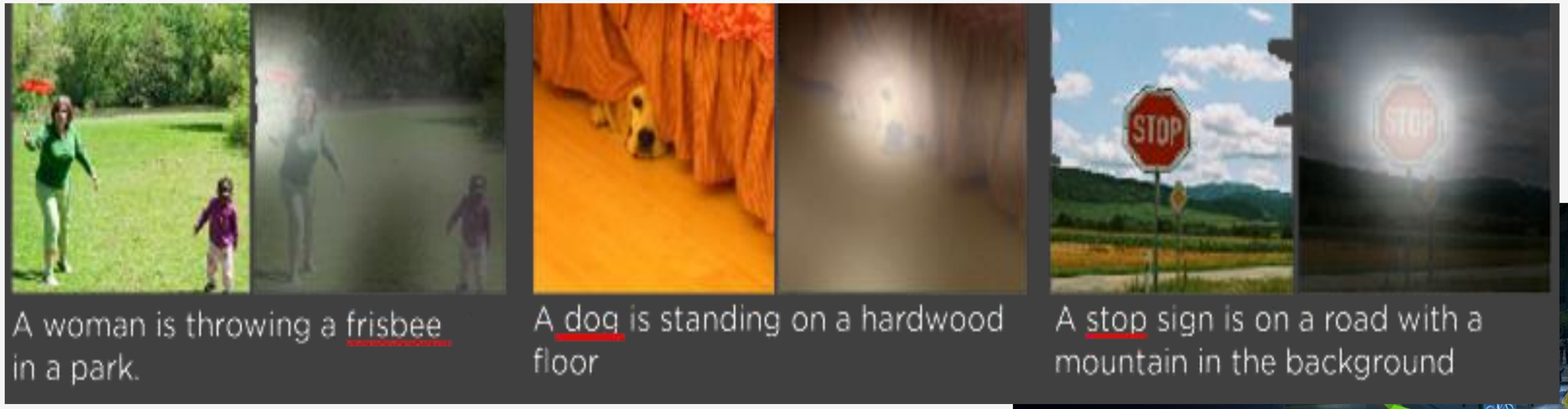


Deep Learning,
MIT Press, 2016

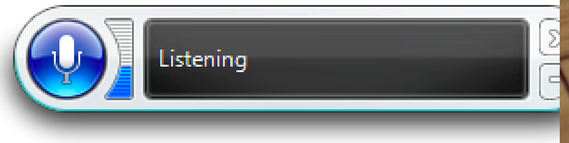
Credits: Yann LeCun



The Deep Learning AI Revolution



Computers have made huge strides in **perception**, manipulating **language**, **generating** images, sounds & molecules, playing **games**, accelerating **science** (3D protein structure from sequence)



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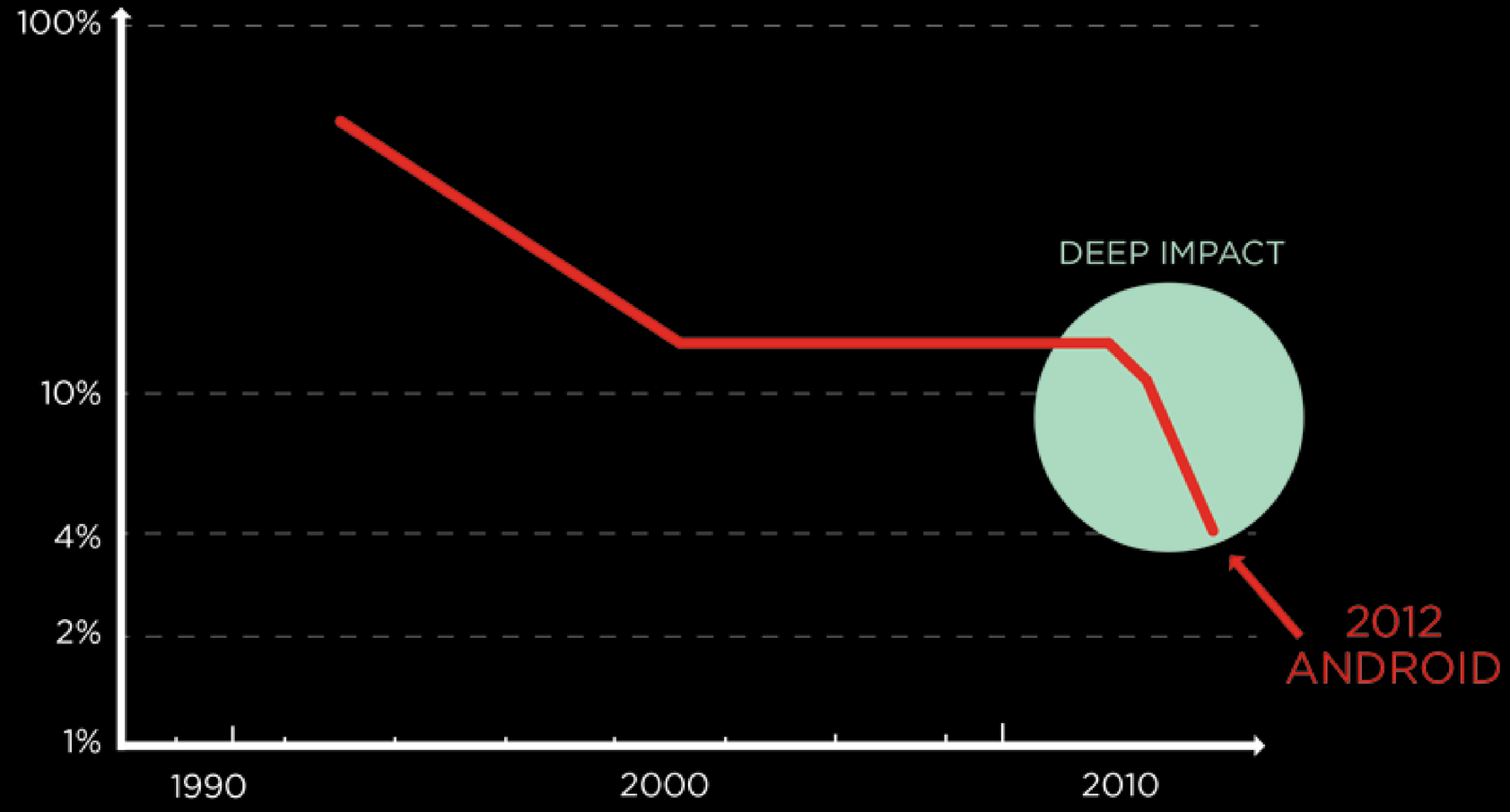
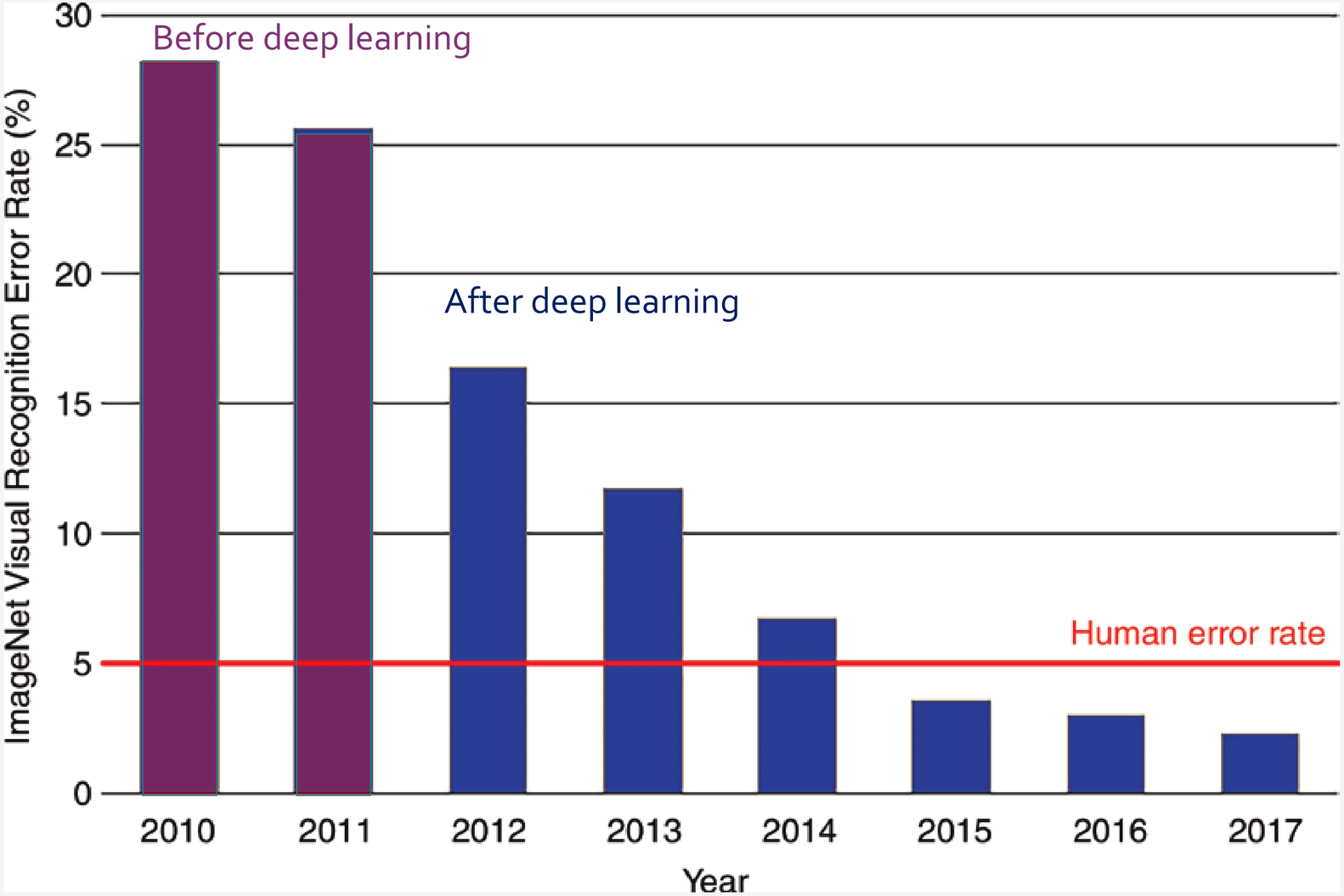
2010-2012: breakthrough in speech recognition



Source: Microsoft

ImageNet Breakthrough in 2012



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Persist and Pull the Threads

1996-2012 neural net winter:

- AI research loses its ambition to reach human-level intelligence
- focus on "simpler" (easier to analyze) ML
- difficult to convince grad students to work on neural nets

Persist, but ask the hard questions:

- Following our intuitions
- But try to validate experimentally or mathematically
- Pull the threads to clarify them, ask WHY questions, try to UNDERSTAND
- Importance of support group (CIFAR program)

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Generative Adversarial Networks

Goodfellow et al & Bengio NIPS 2014

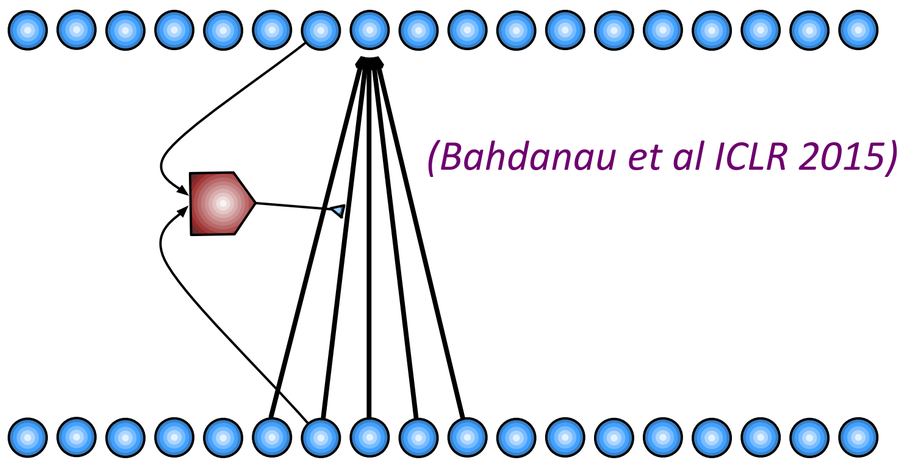
2014 2015 2016 2017 2018

this bird is red with white and has a very short beak

Xu et al 2018, AttnGAN

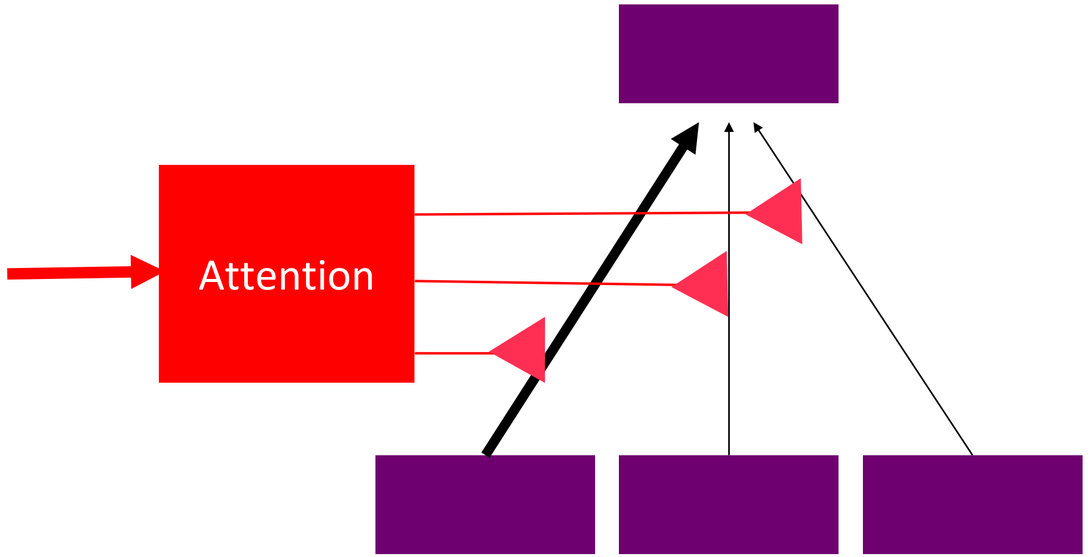
THE ATTENTION REVOLUTION

- **Focus** on a one or a few elements at a time
- *Learn where to attend, depending on context*



- Operating on unordered SETS

- SOTA in NLP, gave rise to Transformers



Deep Reinforcement Learning Breakthrough (2016)

- AlphaGo beat world champion Lee Sedol 4-1
- Not expected by AI and Go experts
- Combines deep learning with reinforcement learning

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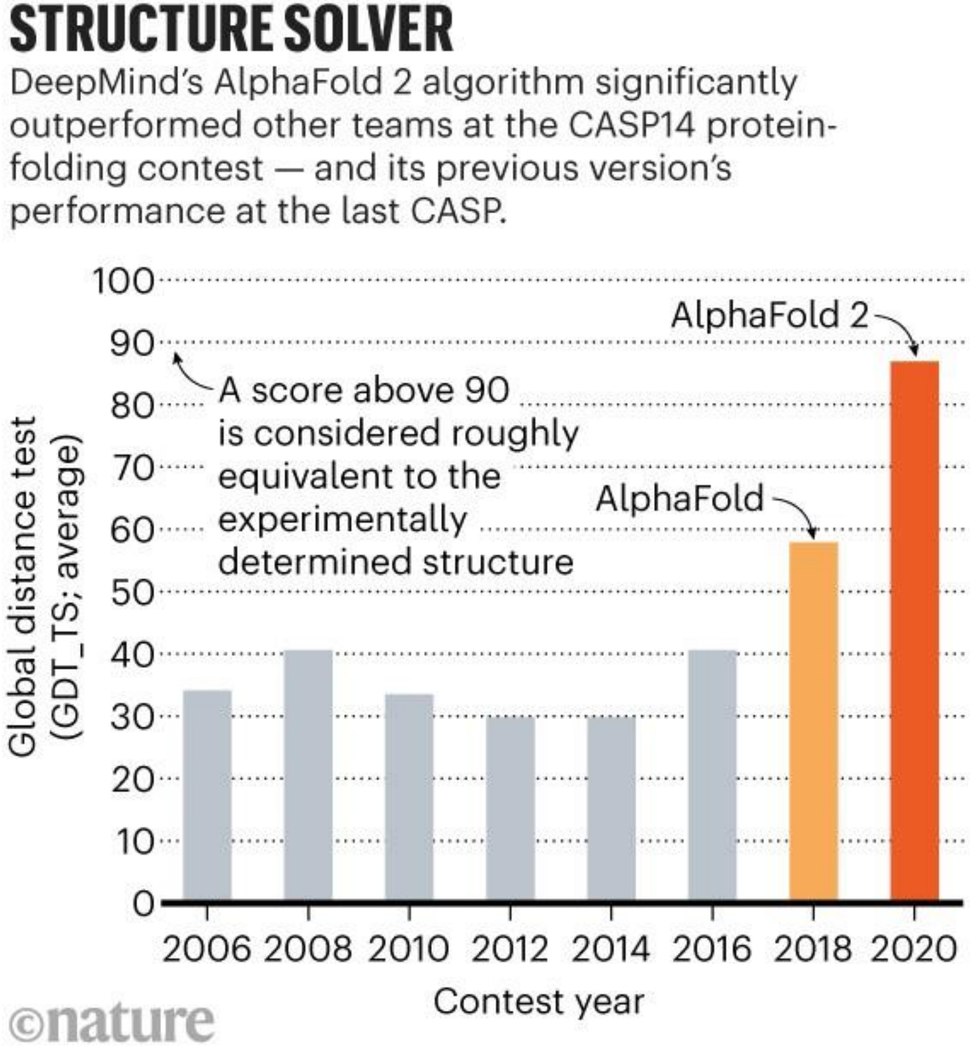
Biological Breakthrough: Protein Structure from Sequence with AlphaFold 2 (2021)

Using attention graph neural networks



Staying Humble

- Better not even think about awards, prizes, recognition: dangerous distractions!
- Ego can blind us, make us overconfident, is the enemy of scientific discoveries
- Hurts our ability to be flexible in our ideas, question what we took for granted, listen to others who disagree with us
- I changed my mind several times: supervised vs unsupervised in 2005, frequentist vs Bayesian in 2022.

2018 Turing Award, announced in the Spring of 2019

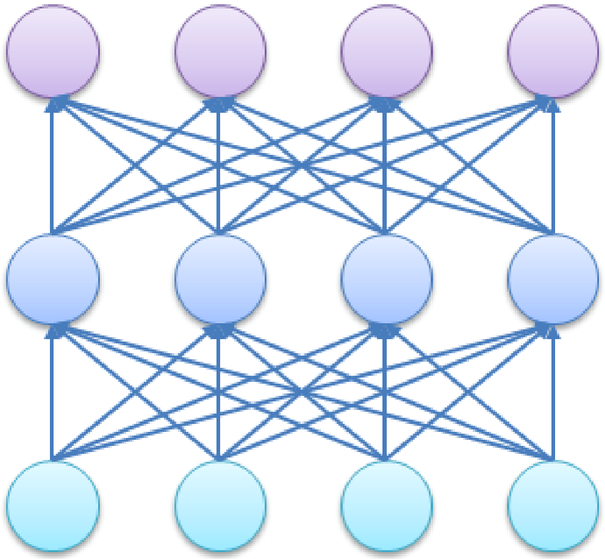
Learning Higher Levels of Abstraction

(Bengio & LeCun 2007)

- The big payoff of deep learning is to allow learning higher levels of abstraction
- Higher-level abstractions **disentangle the explanatory variables and their causal mechanisms**, which would allow much easier generalization and transfer to new tasks

How to Discover Good Disentangled Representations

- How to discover abstractions?
- What is a good representation? ***(Bengio et al 2013)***
- Need clues (= inductive biases) to help **disentangle** underlying factors **and their dependencies**, e.g.
  - Spatial & temporal scales
  - Simple & sparse dependencies between factors
    - *Consciousness prior*
  - Causal / mechanism independence
    - *Controllable variables = interventions*
  - Multiple spatial and temporal scales
    - *Coarse high-level factors explain lower-level details*



Bypassing the curse of dimensionality

We need to build compositionality into our ML models

Just as human languages exploit compositionality to give representations and meanings to complex ideas

Exploiting compositionality: **exponential** gain in representational power

Distributed representations / embeddings: feature learning

Current deep architectures: multiple levels of feature learning

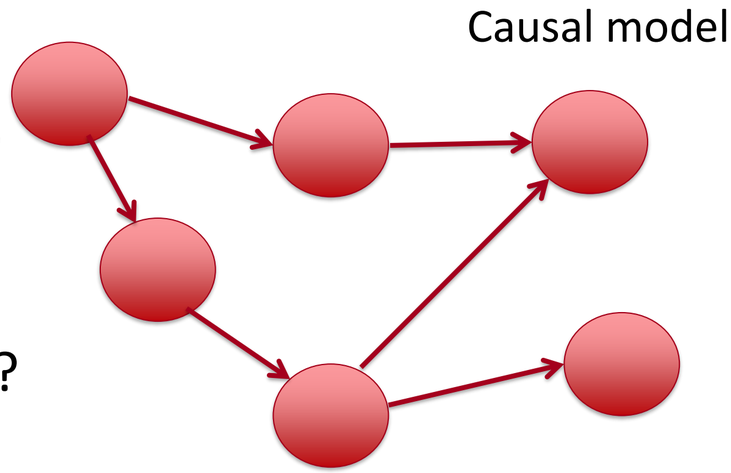
System 2 deep learning: compose a few concepts at a time

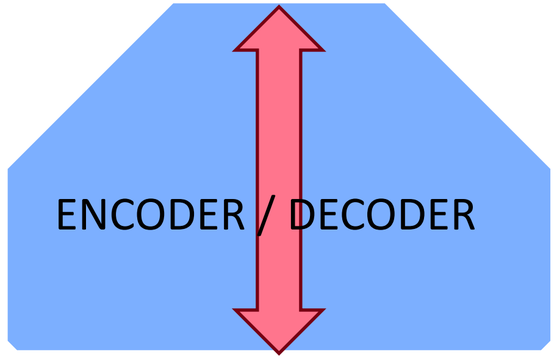
Prior assumption:

compositionality useful to describe the world around us efficiently

Deep Learning Objective: discover causal representation

- What are the right representations? Causal variables explaining the data
- How to discover them (as a function of observed data)?
- How to discover their causal relationship, the causal graph?
- How are actions corresponding to causal interventions?
- How is raw sensory data related to high-level causal variables and how do high-level causal variables turn into low-level actions and partial observations?
- **Need additional biases: causality is about changes in distribution**





Raw input/output

Missing from Current ML: Understanding & Generalization Beyond the Training Distribution

- Learning theory only deals with generalization within the same distribution
- Models learn but do not generalize well (or have high sample complexity when adapting) to modified distributions, non-stationarities, etc.
- Poor reuse, poor modularization of knowledge

Generalization Beyond the Training **Distribution**

- **Current industrial-strength ML suffers from robustness issues due to poor performance OOD**
- If not **iid**, need alternative assumptions, otherwise no reason to expect generalization
  - How do distributions change?
  - Humans do a lot better!
  - Inductive biases inspired from brains?
  - ***How do humans re-use knowledge***?

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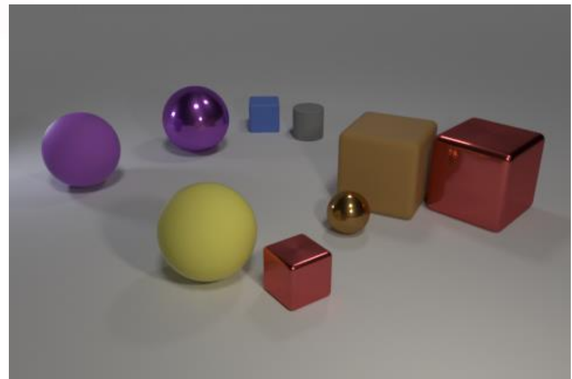
SYSTEMATIC GENERALIZATION

- Studied in linguistics
- **Dynamically recombine existing concepts**
- <u>Even when new combinations have 0 probability under training distribution</u>
  - E.g. Science fiction scenarios
  - E.g. Driving in an unknown city

- Not very successful with current DL, which can ”overfit” the training **distribution**
  (Lake & Baroni 2017)
  (Bahdanau et al & Courville ICLR 2019)
  CLOSURE: (Bahdanau et al & Courville arXiv:1912.05783) on CLEVR

(Lake et al 2015)



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THE GAP FROM SOTA AI & HUMAN-LEVEL INTELLIGENCE

- Sample complexity: number of examples needed to learn a task
- Out-of-distribution generalization
- Out-of-distribution speed of adaptation (transfer learning)
- Causal discovery and reasoning
- Compositional knowledge representation & inference

UNIQUE CAUSE FOR THE GAP: CONSCIOUS PROCESSING?

Hypothesis:

This gap originates from a type of computation, knowledge representation and inference associated with conscious processing in humans, not yet mastered in AI

CONSCIOUS PROCESSING HELPS HUMANS DEAL WITH OOD SETTINGS

Faced with novel or rare situations, humans call upon conscious attention to combine on-the-fly the appropriate pieces of knowledge, to reason with them and imagine solutions.

→ we do not follow our habitual routines, use conscious thinking in novel settings.

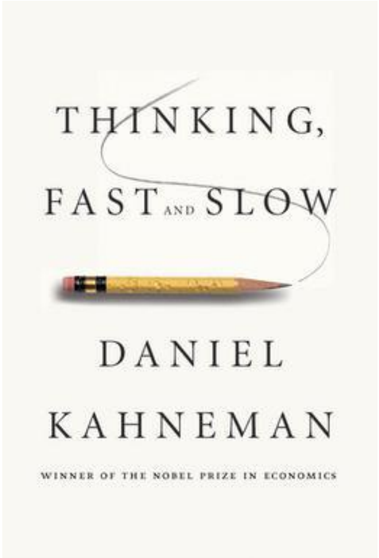
SYSTEM 1 VS. SYSTEM 2 COGNITION

2 systems (and categories of cognitive tasks):

Manipulates high-level / semantic concepts, which can be recombined combinatorially

System 1

- Intuitive, fast, **UNCONSCIOUS**, 1-step parallel, non-linguistic, habitual
- Implicit knowledge
- Current DL



System 2

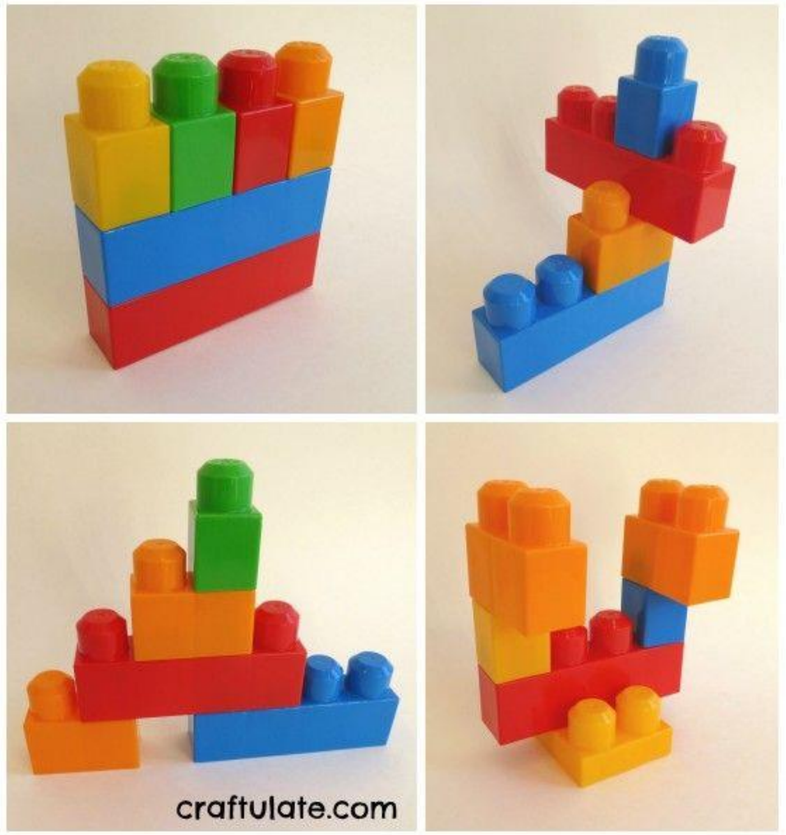
- Slow, logical, **sequential**, **CONSCIOUS**, linguistic, algorithmic, planning, **reasoning**
- Explicit knowledge
- DL 2.0

FROM REASONING TO OOD GENERALIZATION?

- **Current industrial-strength ML (including in NLP) suffers from robustness issues due to poor performance OOD**
- Humans use higher-level cognition (system 2) for out-of-distribution generalization
- Why and how does it help?
- How is that related with agency? causality?
- How do we incorporate these principles in deep learning to obtain both system 1 and system 2 deep learning?

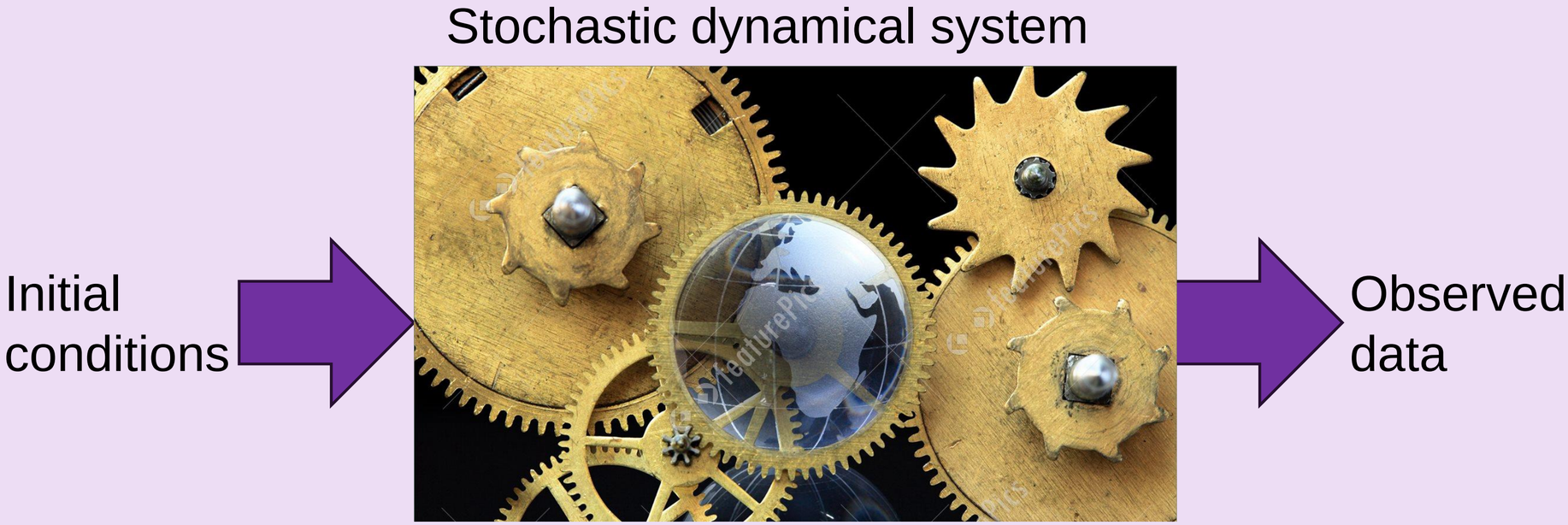
FACTORIZING KNOWLEDGE INTO COMPOSABLE PIECES FOR REASONING

- **Current deep learning**: homogenous architectures, **knowledge is not localized**, completely distributed
- **Transfer learning**: reuse just the relevant pieces of knowledge; minimizes interference; maximizes reuse
- **System 2 reasoning selects and combines nameable pieces of knowledge to form thoughts** (imagined futures, counterfactual past, solutions to problems, interpretations of inputs, etc).
- How to **factorize knowledge** into the right recomposable pieces?



Transfer to modified distribution: Beyond the iid assumption

- iid assumption too strong → poor out-of-distribution generalization
- relaxed assumptions: **same causal dynamics**, different state/intervention



Causality as a framework for OOD generalization, transfer learning, continual learning, etc

- Factor **stationary knowledge** (causal mechanisms) from **non-stationary knowledge** (the values of variables)
- **Intervention** = change in variables that is not just due to the default cause-effect links, but due to an agent
- **Causal model = family of distributions** (which includes tasks)
- The index over these distributions is the choice of interventions (or initial state)
- Stationary knowledge is factorized into **recomposable causal mechanisms**

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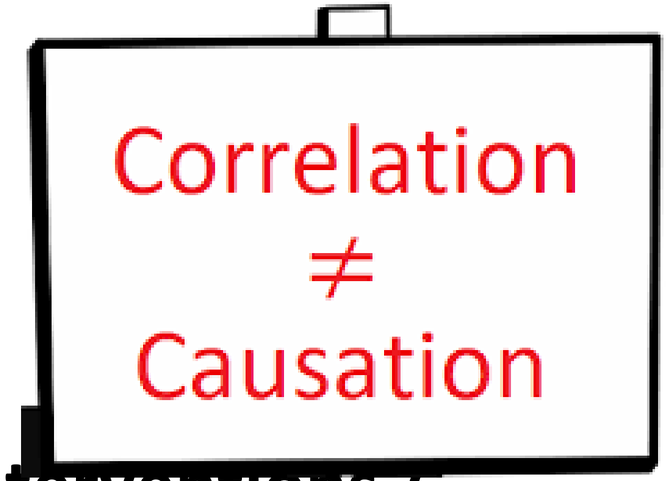
Why Causal?



- **Causal model = family of distributions indexed by interventions / environments / initial states** etc **with shared parameters (mechanisms)**
- Learner must predict the effect of interventions, needs to generalize **Out-Of-Distribution = to new interventions**
- Intervention = perfectly realized **abstract actions** of an agent
  - more realistic: intentions to achieve a change in abstract variable **= goal**
- Unlike multi-task and meta- learning, instead of learning task- or environment specific parameters, perform inference on interventions

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MAIN SYSTEM 2 INDUCTIVE BIASES

Modularity (millions of "experts" in cortex), reusable modules

- dynamic selection of composition of which modules are relevant at any time

Working memory bottleneck (handful of items at a time)

- Past content of WM is available to all expert modules
- Competition between modules and cooperation to select (discrete?) content

Sparsity of high-level dependencies (few variables at a time interact)

- same variable may be involved in several dependencies, multiple modules
- dependencies (energy fn) operate conditionally on correctly typed args

Sequential selection of "thoughts", each involving just 1 or few modules

Causal semantics of variables, localized intervention=high-level intention

RECENT EVIDENCE OF OOD GAINS WITH SYSTEM 2 INDUCTIVE BIASES

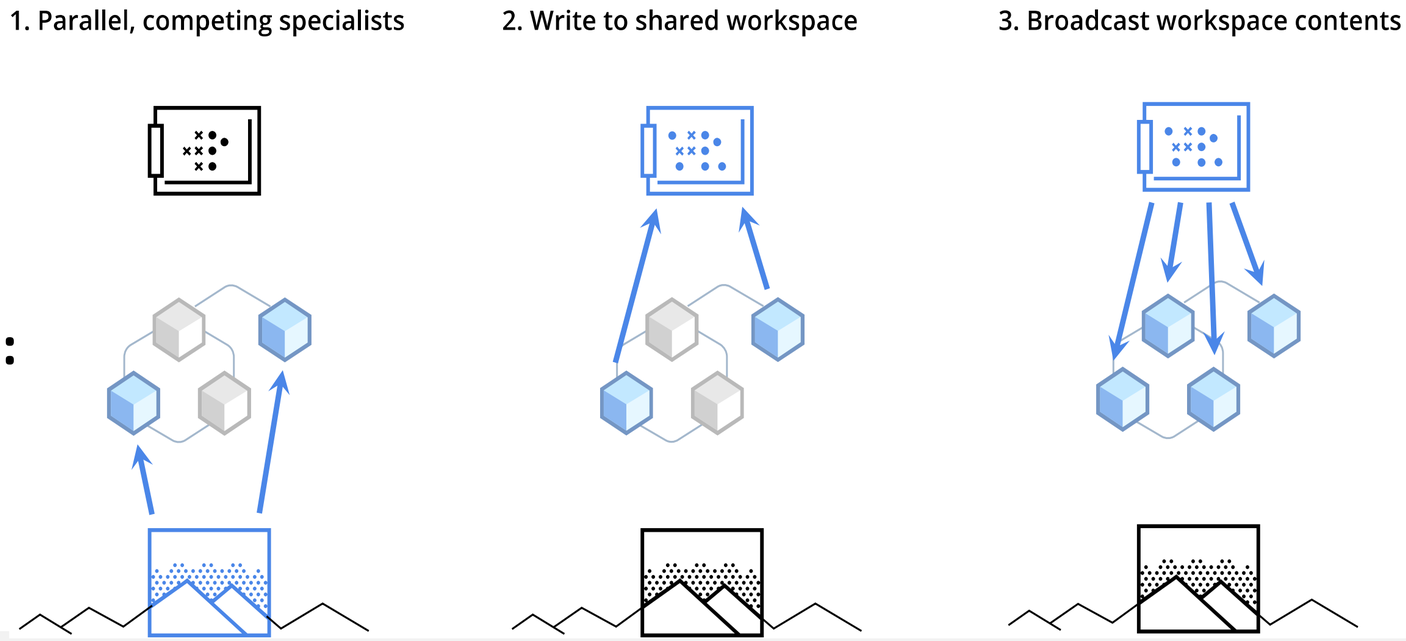
- **Recurrent Independent Mechanisms:** *Goyal et al 2019, arXiv:1909.10893, ICLR 2021*
- **Coordination Among Neural Modules Through a Shared Global Workspace:** *Goyal et al 2021, arXiv:2103.01197, ICLR 2022*
- **Neural Production Systems:**

  Goyal et al 2021, arXiv:2103.0193,

  NeurIPS 2021
- **Discrete-Valued Neural Communication:**

  Liu et al 2021, arXiv:2107.02367,

  NeurIPS 2021



Large deep nets as probabilistic inference and probabilistic reasoning machines:

BAYESIAN STRUCTURE LEARNING WITH GENERATIVE FLOW NETWORKS

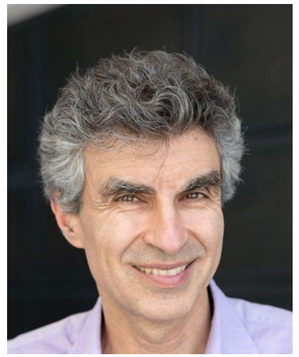
UAI'2022, arXiv:2202.13903

Tristan Deleu, António Góis, Chris Emezue, Mansi Rankawat, Simon Lacoste-Julien, Stefan Bauer, Yoshua Bengio









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GFLOWNET TUTORIAL

https://tinyurl.com/gflownet-tutorial

Papers at NeurIPS 2021, ICML 2022, UAI 2022, NeurIPS 2022, +ArXiv

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ML going out of labs, into society

- ML is not just a research question anymore
- ML-based products are being designed and deployed

➔ **new responsibility for AI scientists, engineers, entrepreneurs, governments**

AI is a Powerful Tool

- AI = **tool**
- Dual-use
- **Wisdom race**: advances in technology vs advances in wisdom
- **How to maximize its beneficial use and minimize its misuse?**

Montreal Declaration (2017)

1- **WELL-BEING** PRINCIPLE

2- **RESPECT FOR AUTONOMY** PRINCIPLE

3- **PROTECTION OF PRIVACY AND INTIMACY** PRINCIPLE

4- **SOLIDARITY** PRINCIPLE

5- **DEMOCRATIC PARTICIPATION** PRINCIPLE

6- **EQUITY** PRINCIPLE

7- **DIVERSITY INCLUSION** PRINCIPLE

8- **PRUDENCE** PRINCIPLE

9- **RESPONSABILITY** PRINCIPLE

10- **SUSTAINABLE DEVELOPMENT** PRINCIPLE

https://www.montrealdeclaration-responsibleai.com/the-declaration

Dangers and Concerns with AI

- Big Brother and killer robots
- Misery for jobless people, at least in transition
- Manipulation from advertising and social media
- Reinforcement of social biases and discrimination
- Increased inequality and power concentration in few people, companies & countries

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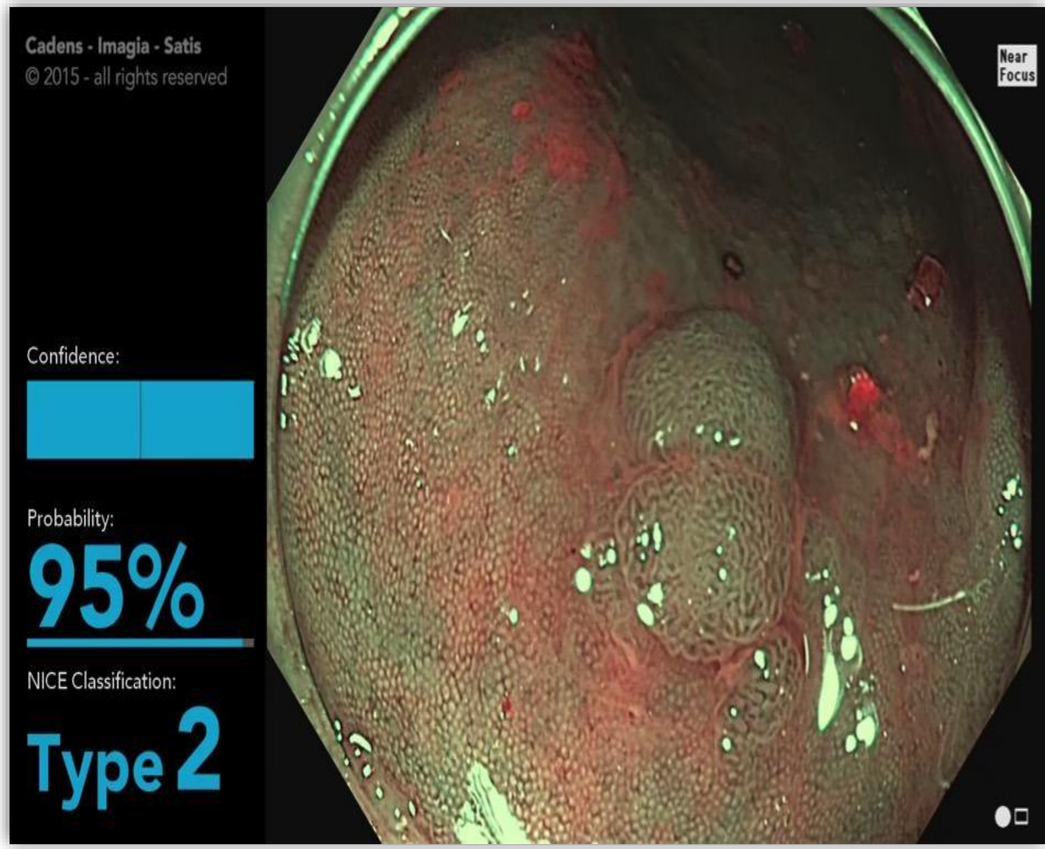
Beneficial AI Potential

- Medical applications
- Environmental applications
- Educational applications
- Democratizing justice
- Humanitarian applications

Etc.



Imagia detects cancer cells, helps doctors

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Market Failure:
Societal vs Commercial Value of Innovations

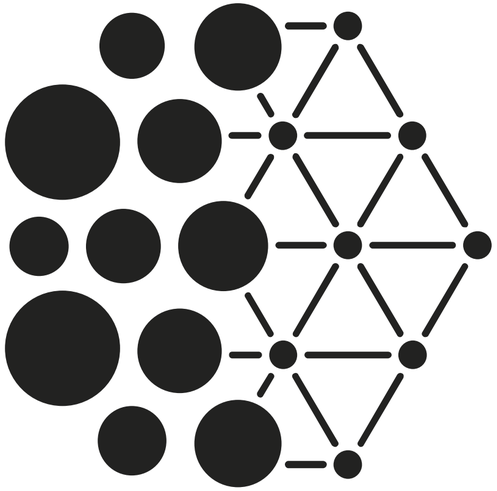
Some innovations would be greatly beneficial to society but do not have enough commercial value (or too much risk) for current markets

e.g. involve **PUBLIC GOODS**

- **AI for discovering new antibiotics: needed to prevent next pandemic**
- AI for discovering new carbon capture materials
- AI to fight climate change, AI to bring better education worldwide

➔ Governments should invest $ and academics should invest efforts to fill the gap

THANK YOU!



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Université de Montréal

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