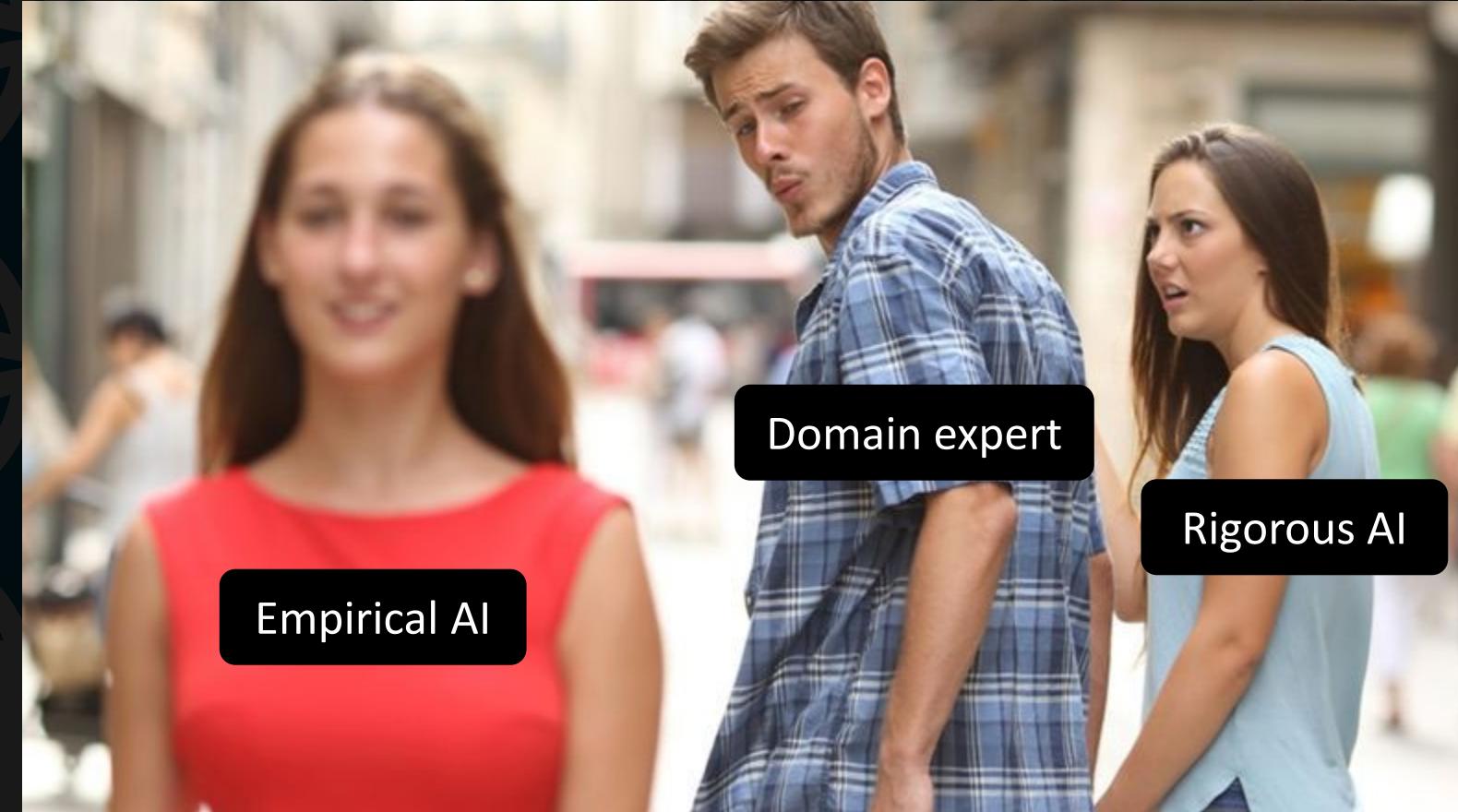
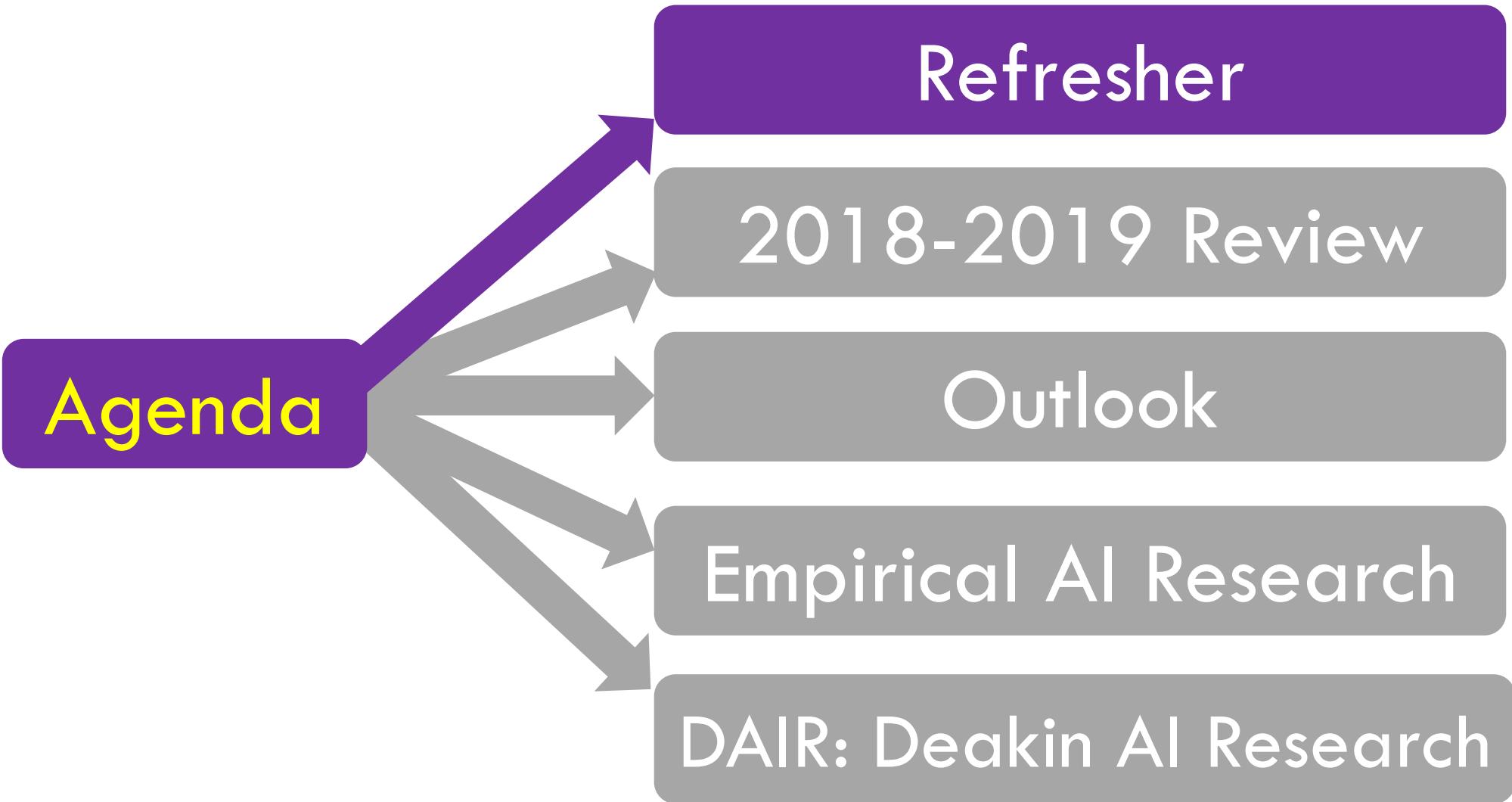


# MODERN AI/ML

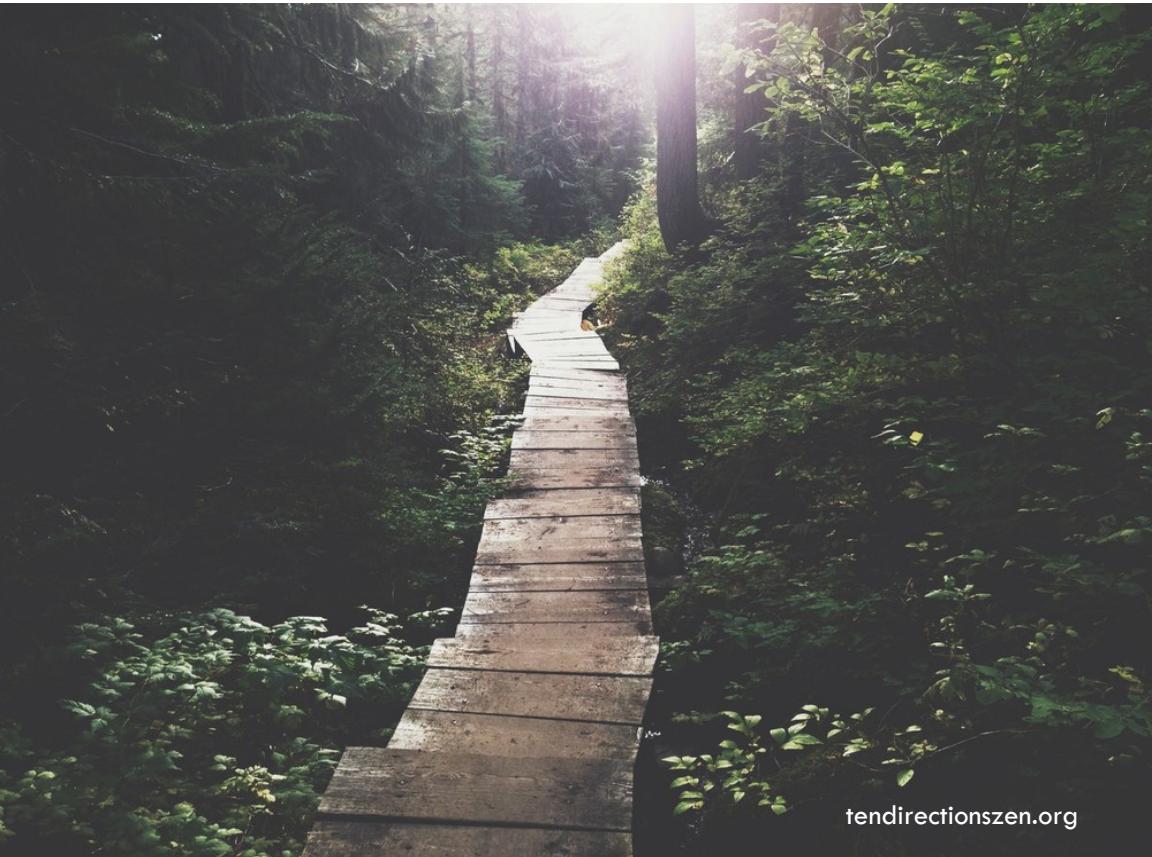
REVIEW • OUTLOOK •  
EMPIRICAL RESEARCH •  
DEAKIN AI RESEARCH

Truyen Tran  
HCMC 05/2019





# AI/ML RESEARCH: DREAM



Among the most challenging scientific questions of our time are the corresponding **analytic** and **synthetic** problems:

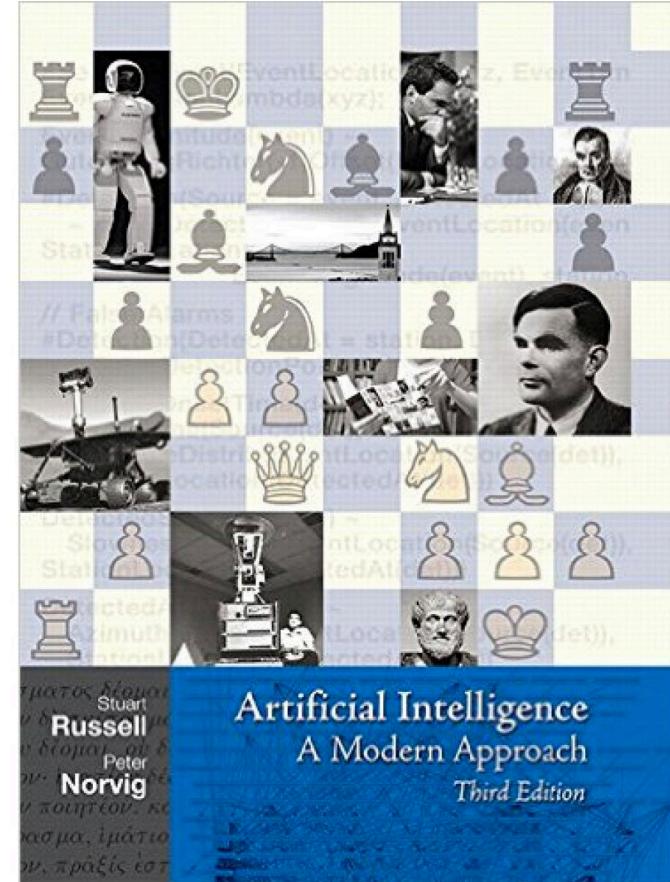
- How does the brain function?
- Can we design a machine which will simulate a brain?

-- *Automata Studies*, 1956.

# WHAT MAKES AI?

Perceiving	Acting
<b>Learning</b>	Robotics
<b>Reasoning</b>	Communicating
Planning	Consciousness
	Automated discovery

*Modern AI is mostly data-driven, as opposed to classic AI, which is mostly expert-driven.*

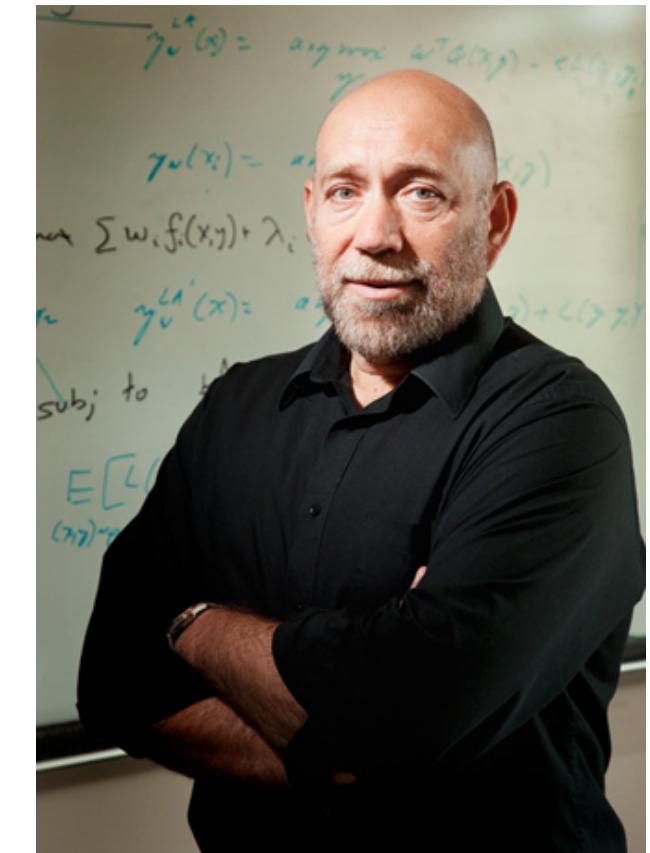


# REASONING

Reasoning is to deduce knowledge from previously acquired knowledge in response to a query (or a cue)

Early theories of intelligence:

- focuses solely on reasoning,
- learning can be added separately and later!  
(Kharden & Roth, 1997).



(Dan Roth; ACM Fellow; IJCAI John McCarthy Award)

Kharden, Roni, and Dan Roth. "Learning to reason." *Journal of the ACM* (JACM) 44.5 (1997): 697-725.

# WHAT YOU CAN'T DESIGN, LEARN!

## (AKA VARIATIONAL METHOD)

### Filling the slot

- In-domain (interpolation), e.g., an alloy with a given set of characteristics
- Out-domain (extrapolation), e.g., weather/stock forecasting
- Classification, recognition, identification
- Action, e.g., driving
- Mapping space, e.g., translation
- Replacing expensive simulations

Estimating semantics, e.g., concept/relation embedding

Assisting experiment designs

Finding unknown, causal relation, e.g., disease-gene

Predicting experiment results, e.g., alloys  
→ phase diagrams → material characteristics

# MACHINE LEARNING SETTINGS

Supervised learning

(mostly machine  
learning)

A → E

Will be quickly solved for "easy" problems (Andrew Ng)

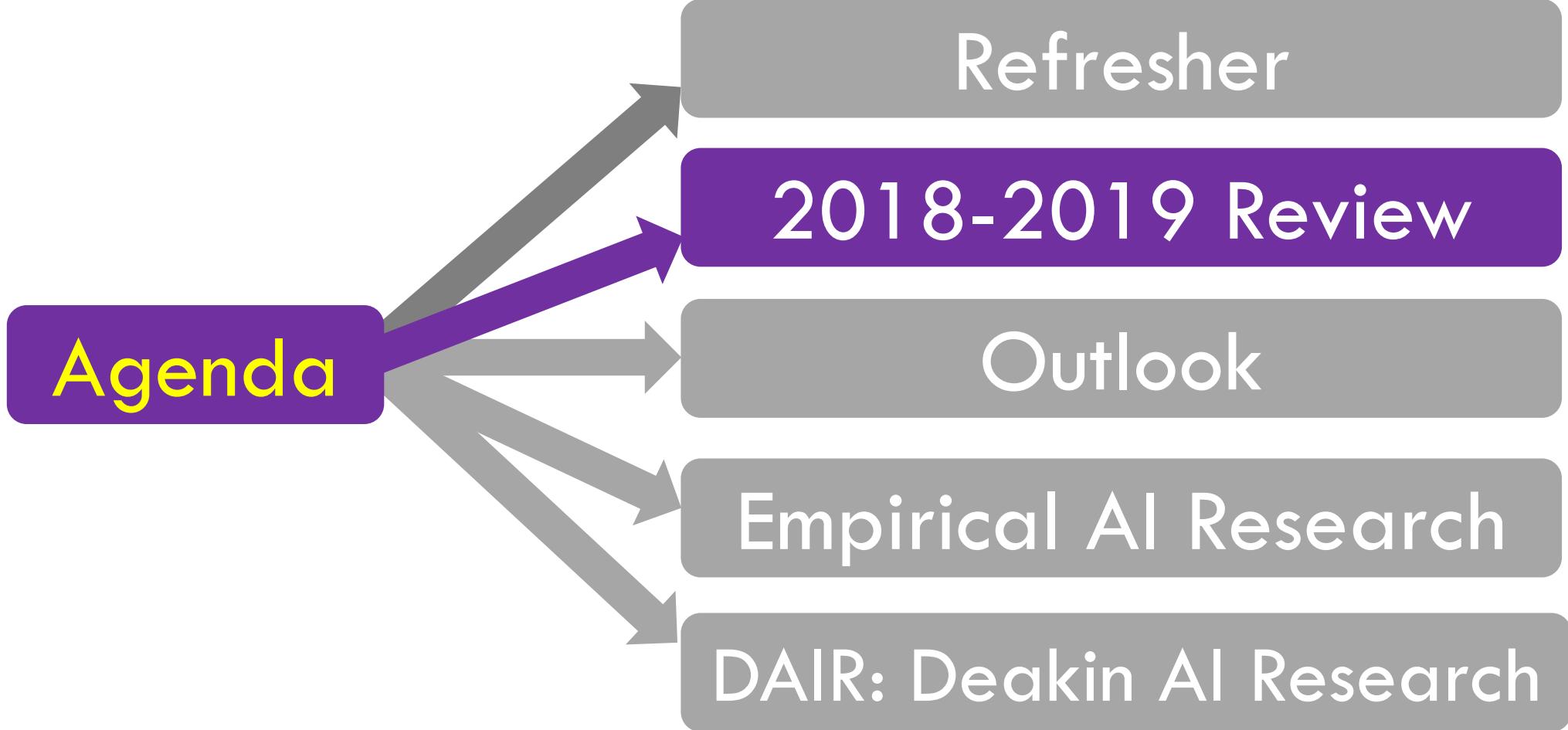
Unsupervised learning

(man)

$$\mathbf{v} \sim P_{model}(\mathbf{v})$$

$$P(\mathbf{v}) \approx P_{data}(\mathbf{v})$$

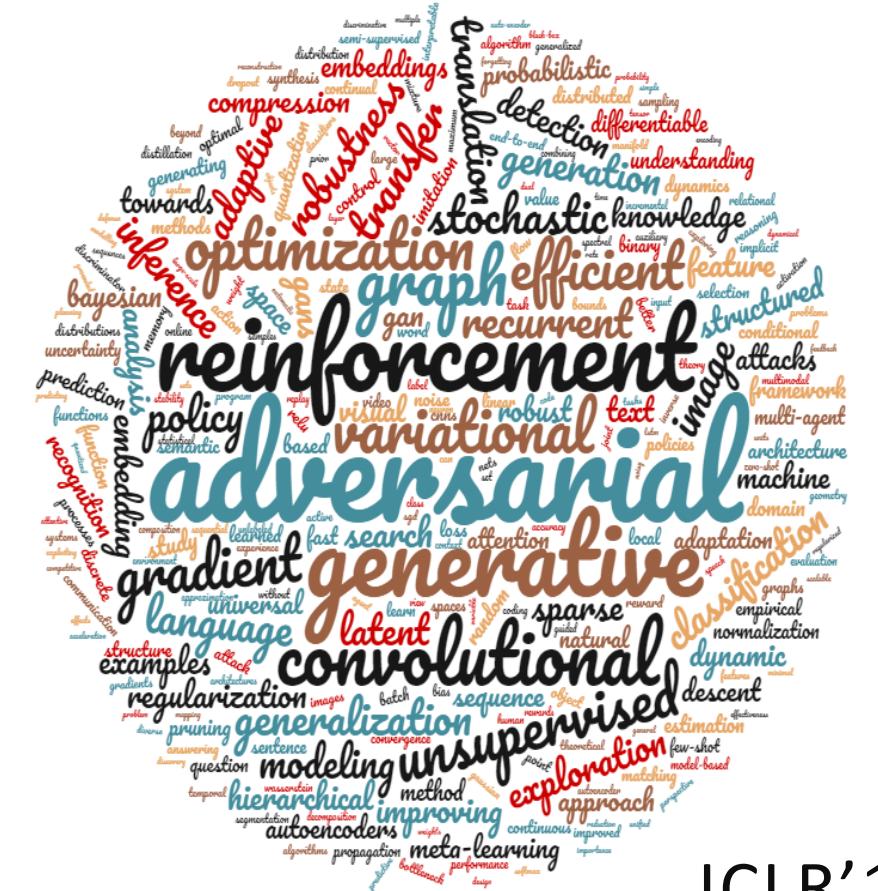
Anywhere in between: semi-supervised learning, reinforcement learning, lifelong learning, meta-learning, few-shot learning, knowledge-based ML



# AI/ML RESEARCH: MODERN REALITY

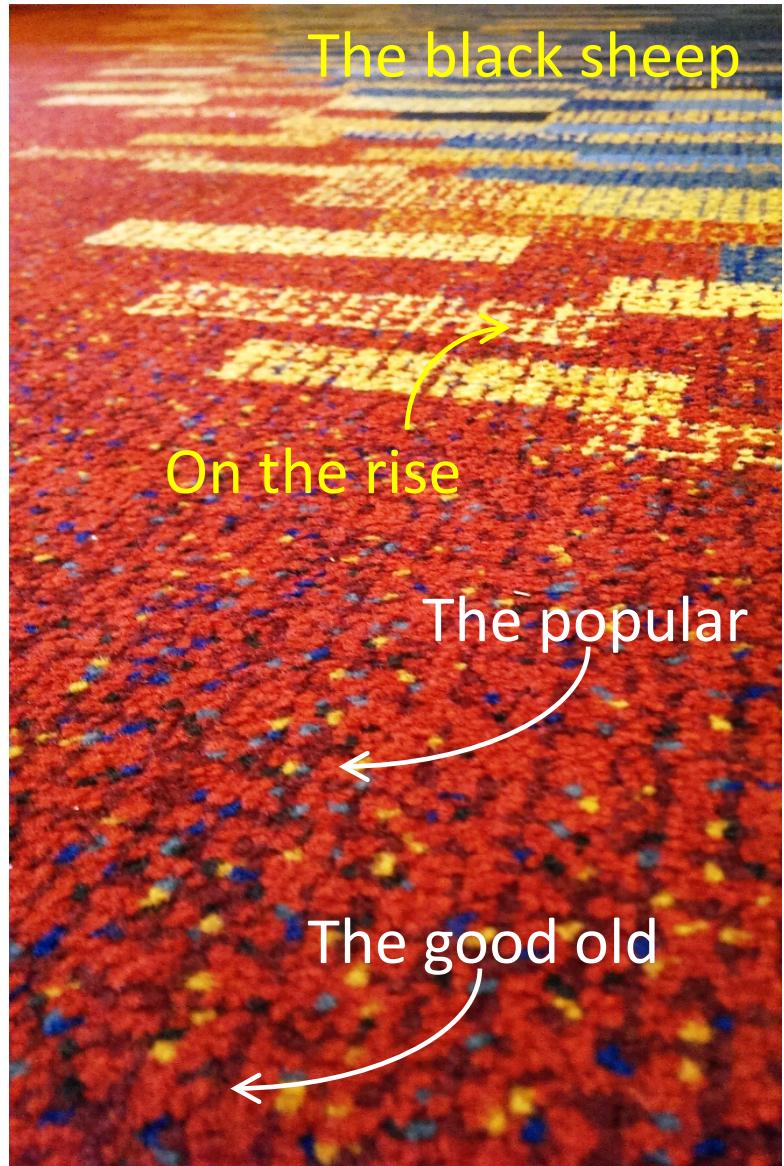


12/05/2019



ICLR'19

9



- Group theory
- Quantum ML/AI
- Theories of consciousness

- Reinforcement learning, imagination & planning
- Deep generative models + Bayesian methods
- **Memory & reasoning**
- Lifelong/meta/continual/few-shot/zero-shot learning
- Universal transformer

- Attention
- Batch-norm
- ReLU & skip-connections
- Highway nets, LSTM/GRU & CNN

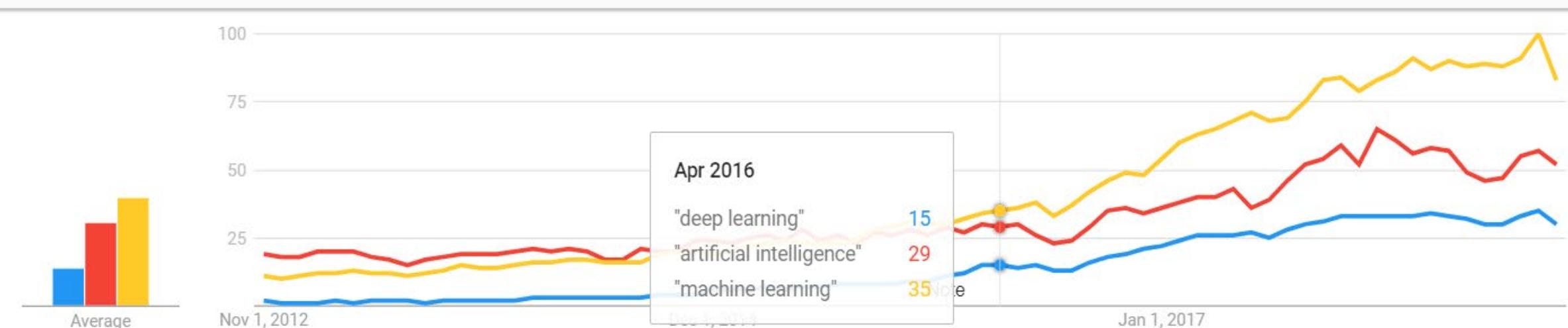
- Representation learning (RBM, DBN, DBM, DDAE)
- Ensemble
- Back-propagation
- Adaptive stochastic gradient

● "deep learning"

● "artificial intelligence"

● "machine learning"

Worldwide, 10/7/12 - 11/7/18



### Compared breakdown by region

● "deep learning" ● "artificial intelligence" ● "machine learning"



Sort: Interest for "deep learning" ▾

1 Japan



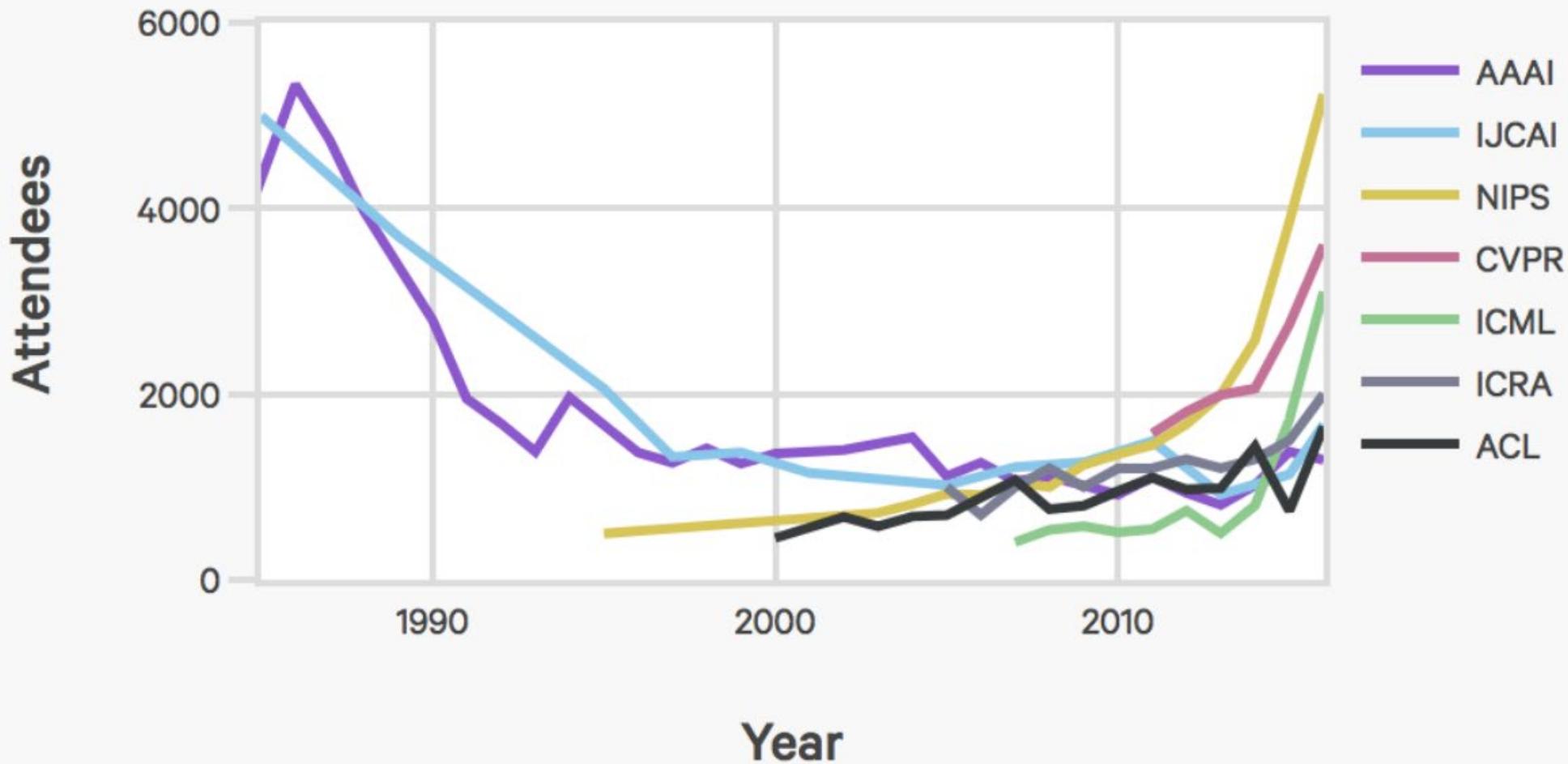
2 South Korea



3 China



# Large Conference Attendance



# MIT TECH REVIEW: 10 BREAKTHROUGHS OF 2018

**3-D Metal Printing** (Markforged, Desktop Metal, GE)

**Artificial Embryos**, aka stem cells (University of Cambridge; University of Michigan; Rockefeller University)

**Sensing City**, aka smart cities (Sidewalk Labs and Waterfront Toronto, 1-2 years)

**AI for Everybody**, aka Cloud AI (Amazon; Google; Microsoft)

**Dueling Neural Networks**, aka GAN (Google Brain, DeepMind, Nvidia)

**Babel-Fish Earbuds**, aka near real time translation (Google and Baidu)

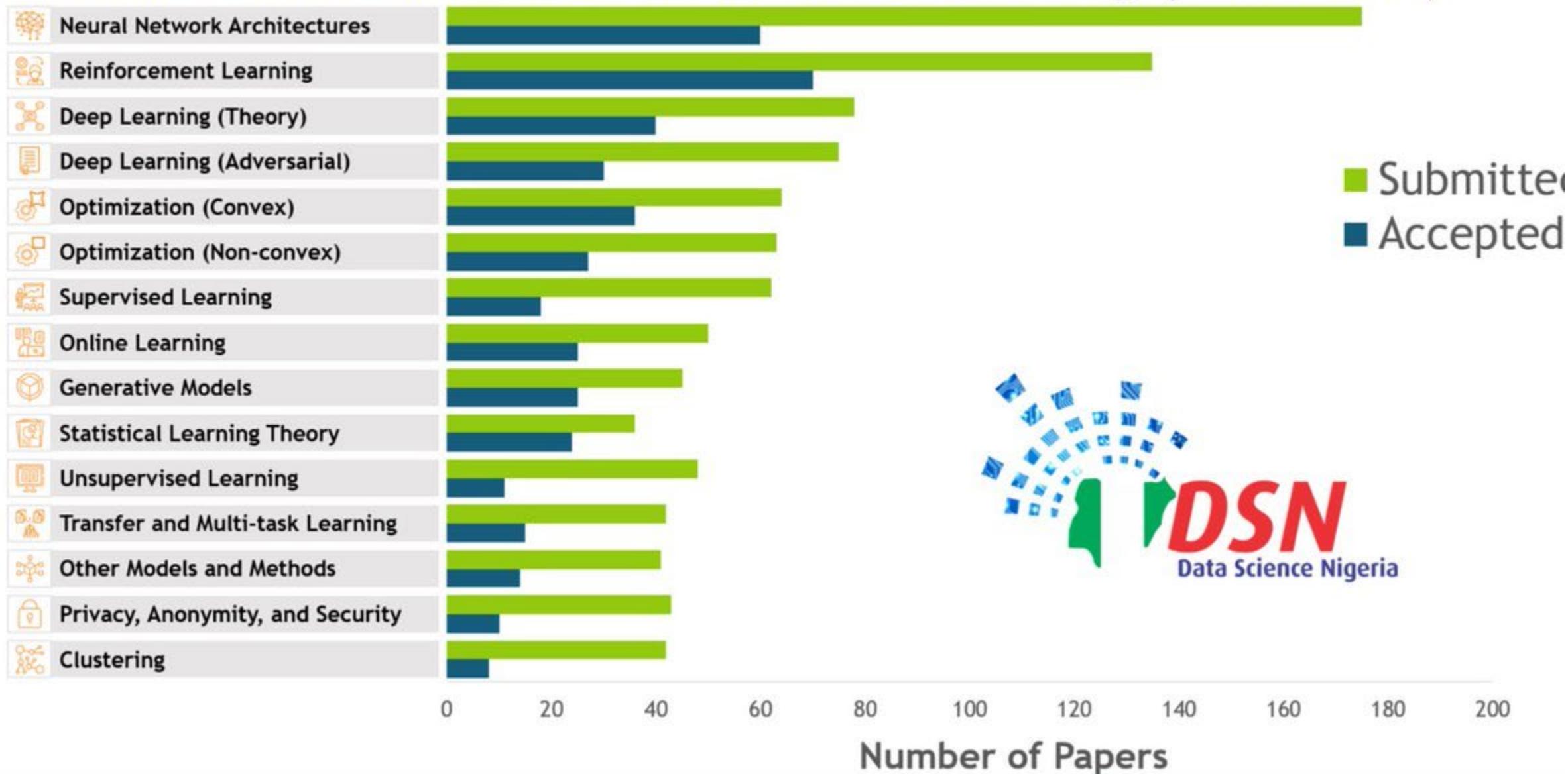
**Zero-Carbon Natural Gas** (8 Rivers Capital; Exelon Generation; CB&I; 3-5 years to come)

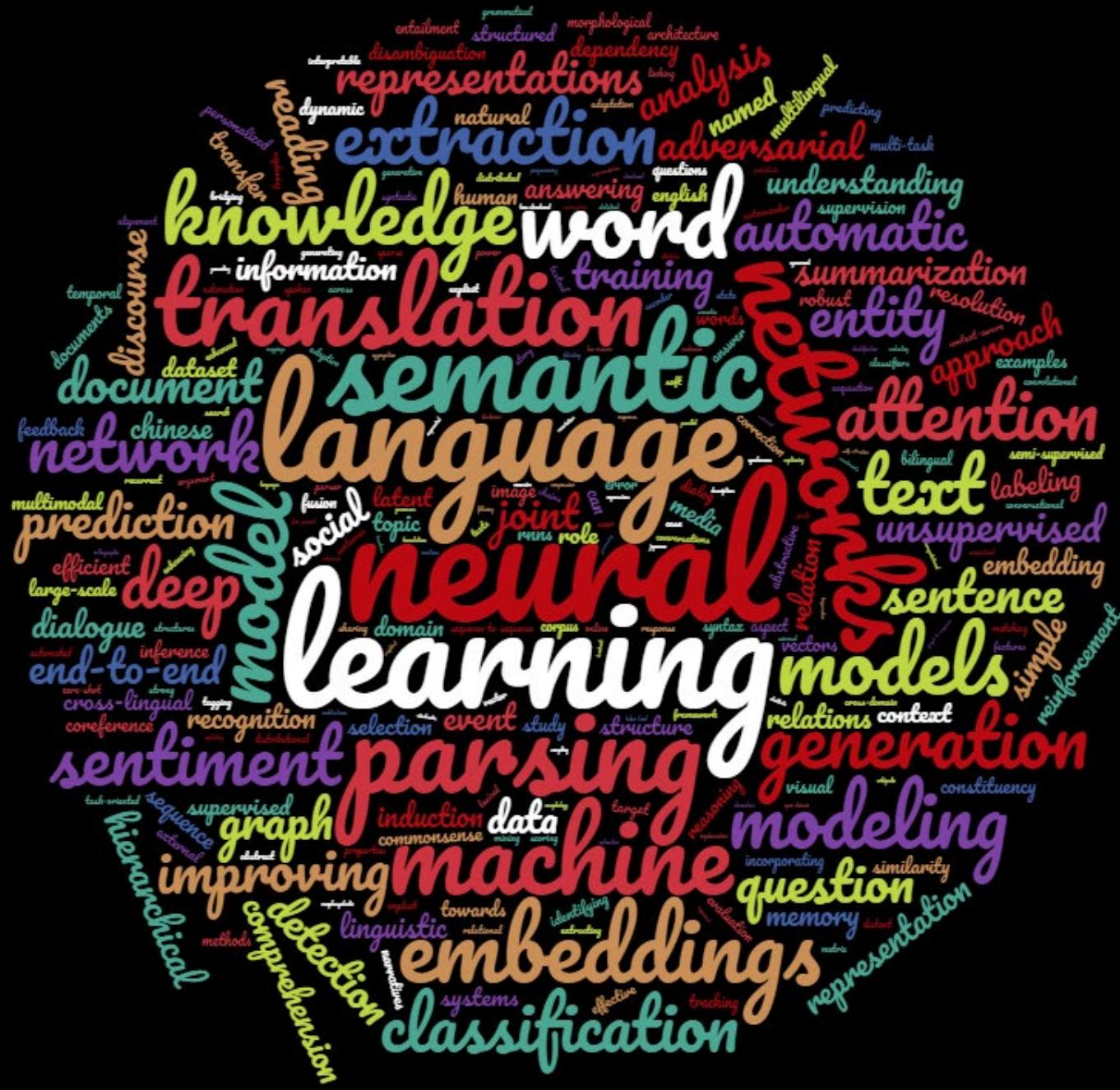
**Perfect Online Privacy** (Zcash; JPMorgan Chase; ING)

**Genetic Fortune-Telling**, aka DNA-based predictions (Helix; 23andMe; Myriad Genetics; UK Biobank; Broad Institute)

**Materials' Quantum Leap**, aka Quantum computing for molecules (IBM; Google; Harvard's Alán Aspuru-Guzik; 5-10 years to come)

# International Conference on Machine Learning (ICML 2018)





ACL'18



ACL'18

Ignore the obvious





KDD'18

Ignore the obvious



NIPS'18



# NIPS'18

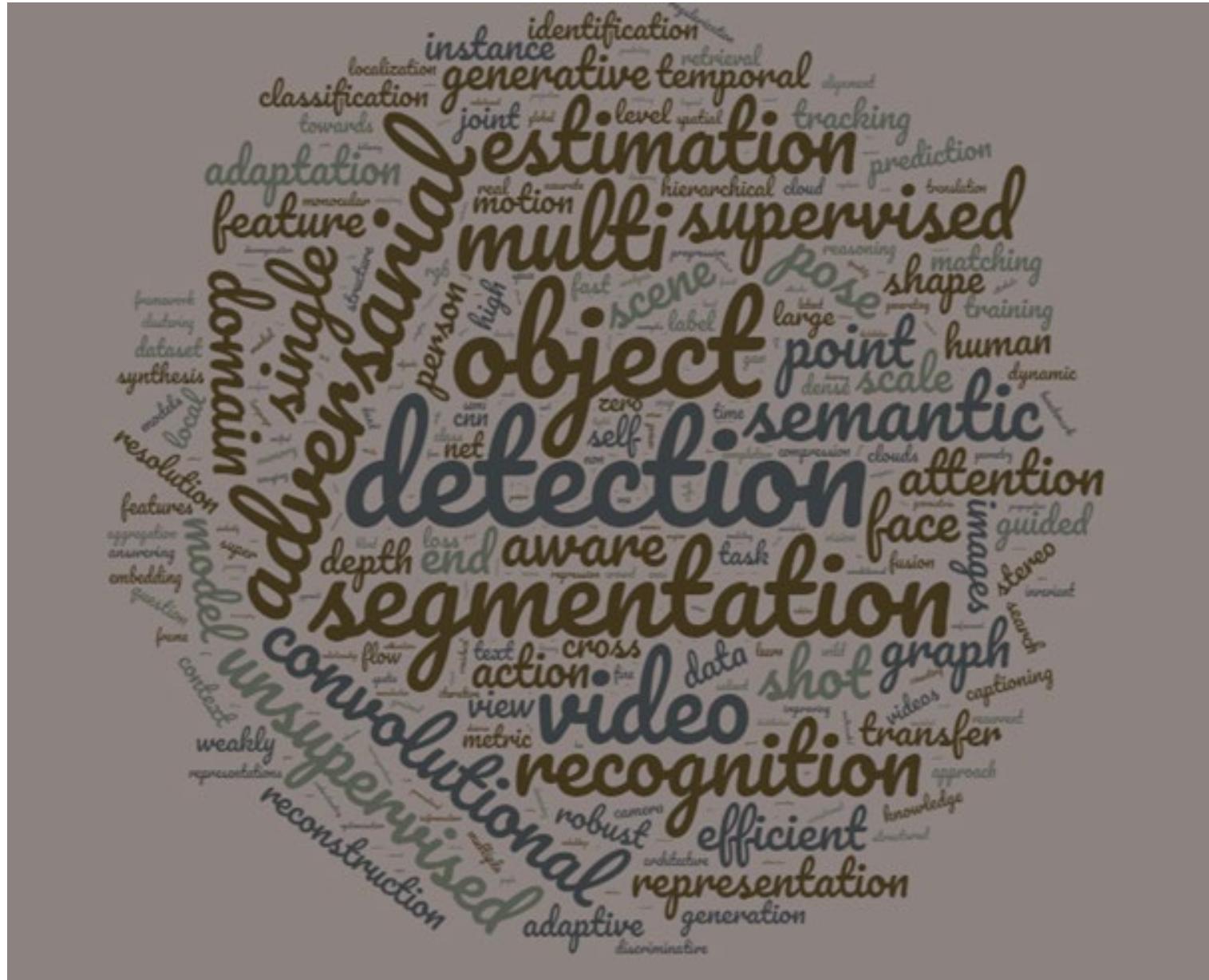
Ignore the obvious



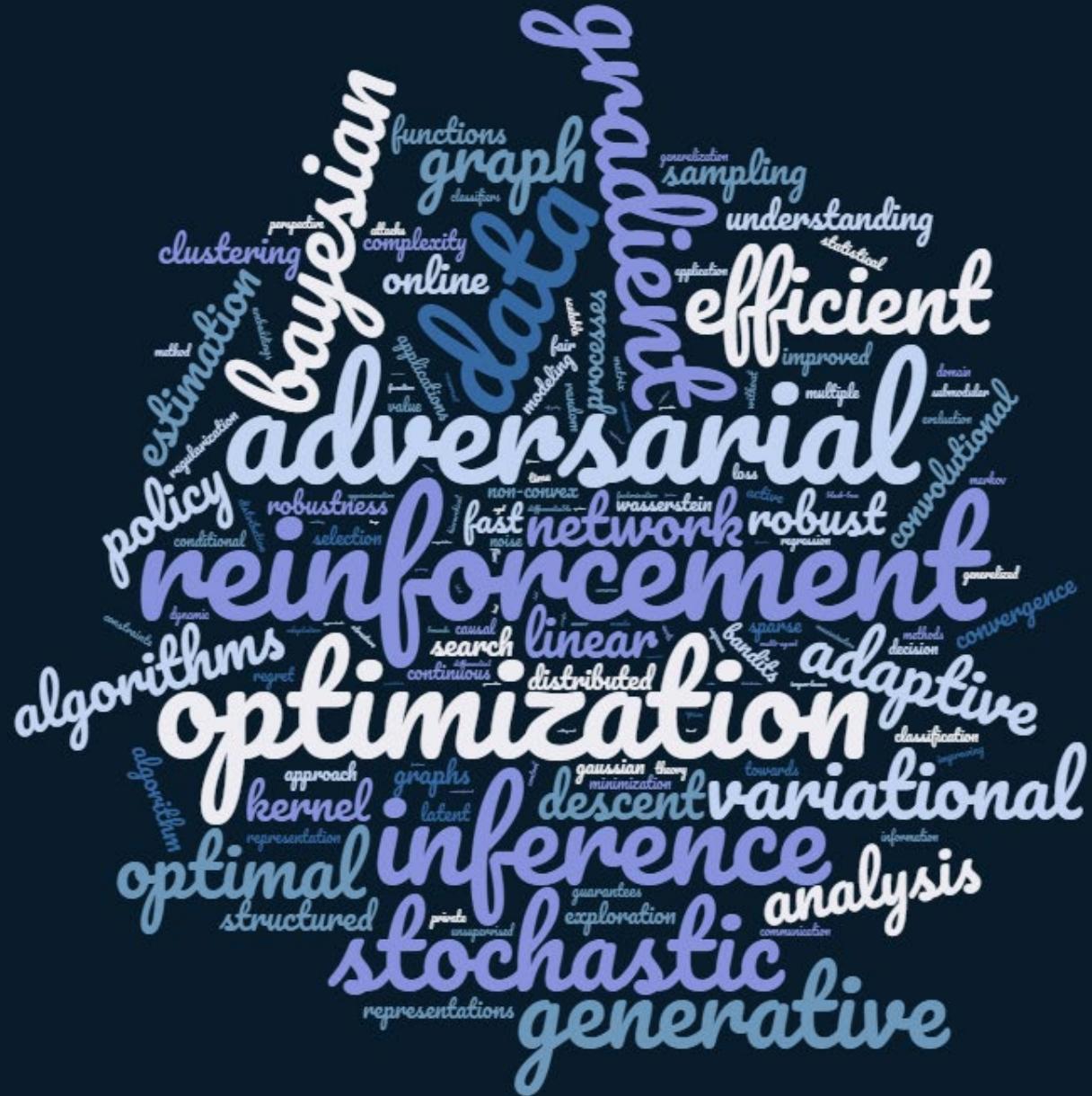
AAAI'19



ICLR'19



CVPR'19



ICML'19  
Ignore the obvious

# A LOOK INTO NIPS'18 WORKSHOPS (1)

## **Uncertainty**

Bayesian Deep Learning

All of Bayesian Nonparametrics  
(Especially the Useful Bits)

## **Data efficiency**

Continual Learning

NIPS 2018 Workshop on Meta-Learning

## **Reinforcement learning**

Deep Reinforcement Learning

Imitation Learning and its Challenges in  
Robotics

Reinforcement Learning under Partial  
Observability

Infer to Control: Probabilistic Reinforcement  
Learning and Structured Control

# A LOOK INTO NIPS'18 WORKSHOPS (2)

## Communication

Learning by Instruction

Emergent Communication Workshop

The second Conversational AI workshop  
– today's practice and tomorrow's potential

Visually grounded interaction and language

## Theories & modelling

Integration of Deep Learning Theories

Relational Representation Learning

Modeling the Physical World: Learning, Perception, and Control

## Impact of AI

Workshop on Ethical, Social and Governance Issues in AI

AI for social good

# RICH SUTTON'S BITTER LESSON

“The biggest lesson that can be read from 70 years of AI research is that general methods that leverage computation are ultimately the most effective, and by a large margin. ”

“The two methods that seem to scale arbitrarily in this way are search and learning.”



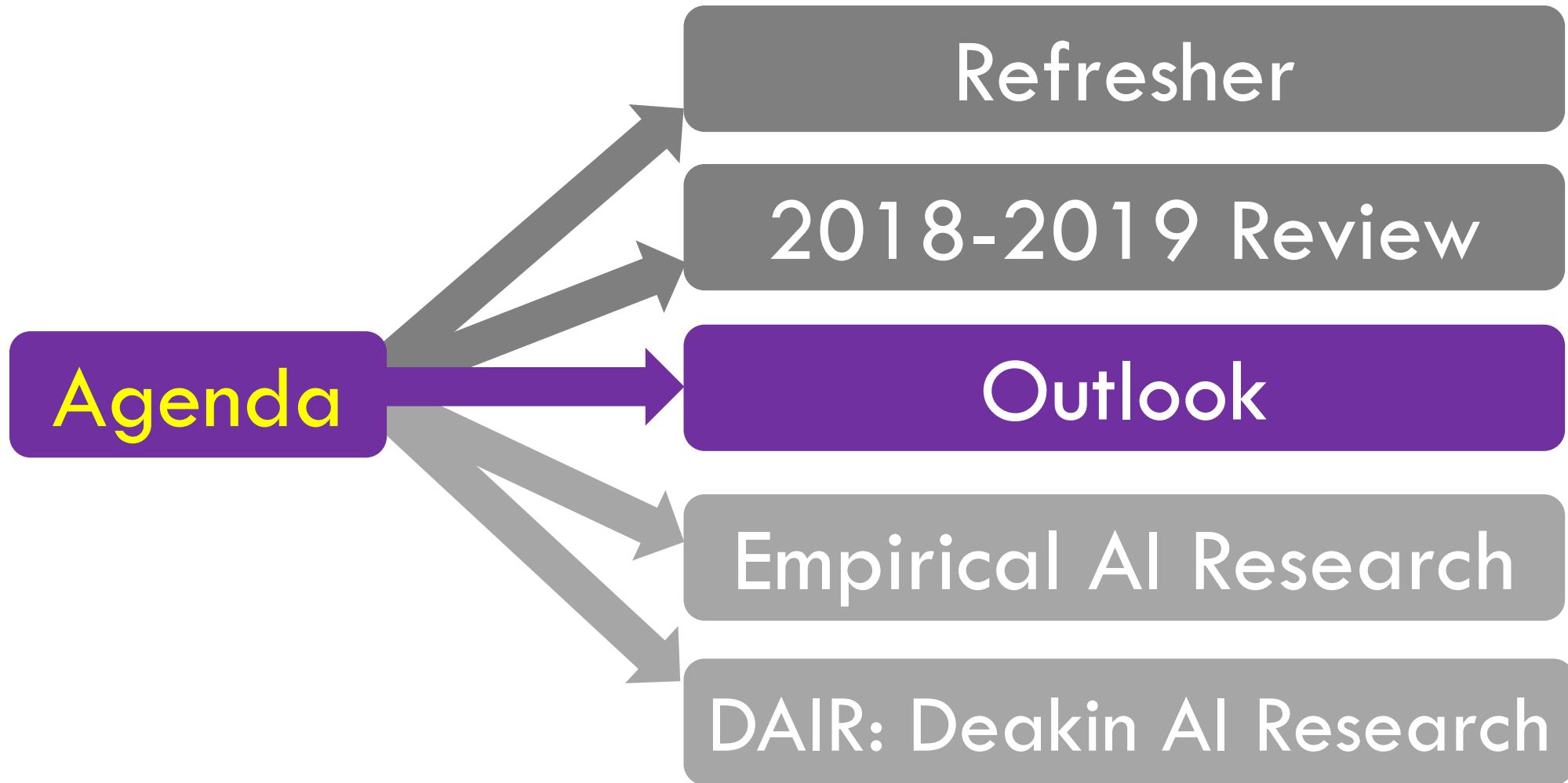
Andrej Karpathy

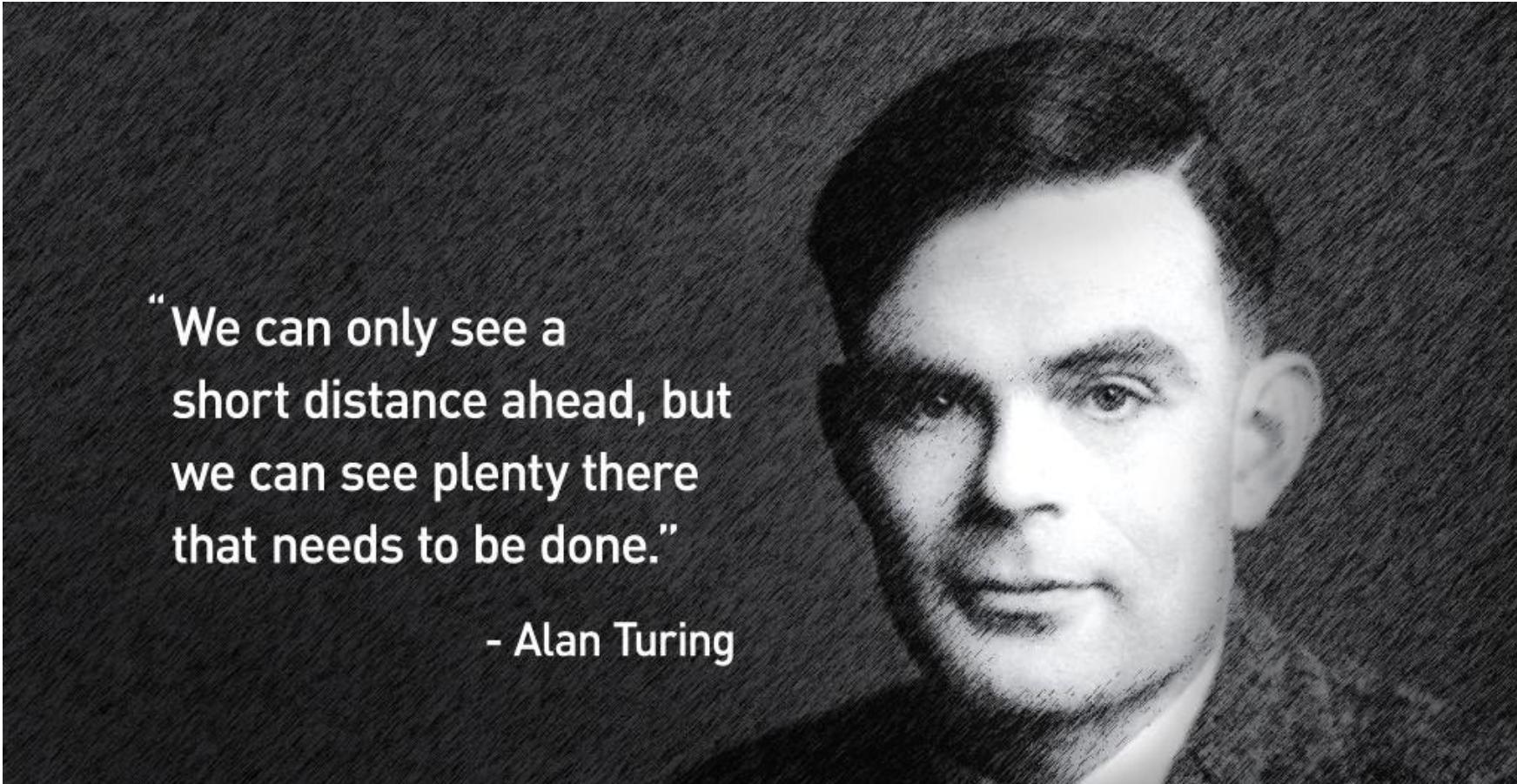
@karpathy

Following

“The Bitter Lesson” by Sutton, on the longevity of domain knowledge in algorithms. Also apparent if you skim through old AI journals. [incompleteideas.net/Incldeas/BitterLesson.html](http://www.incompleteideas.net/Incldeas/BitterLesson.html) ...

9:12 AM - 15 Mar 2019





**“We can only see a  
short distance ahead, but  
we can see plenty there  
that needs to be done.”**

**- Alan Turing**

<https://twitter.com/nvidia/status/1010545517405835264>

# G. MARCUS' CRITICISM OF DL (JAN 2018)

1. Data hungry
2. No “deep” abstraction, sensitive to noise, hard to transfer
3. No natural way to deal with hierarchy
4. Struggles with open-ended inference (e.g., answer not in the data)
5. Black-box
6. Uses little prior knowledge
7. Correlation, not causation
8. Assumes stable world
9. Sensitive to adversarial examples
10. Difficult to engineer

# WHEN IN DOUBT, ASK WHAT DOES BRAIN DO?

Perceive the world  
Conceptualize  
Reason about things  
Imagine the future  
Plan what to do  
Act  
Learn

Think about self  
Have emotion  
**Be conscious**  
Love  
Be happy and pursue happiness  
Be ethical  
Socialize

Then ask what computer can do.

Which ones are Turing computational?

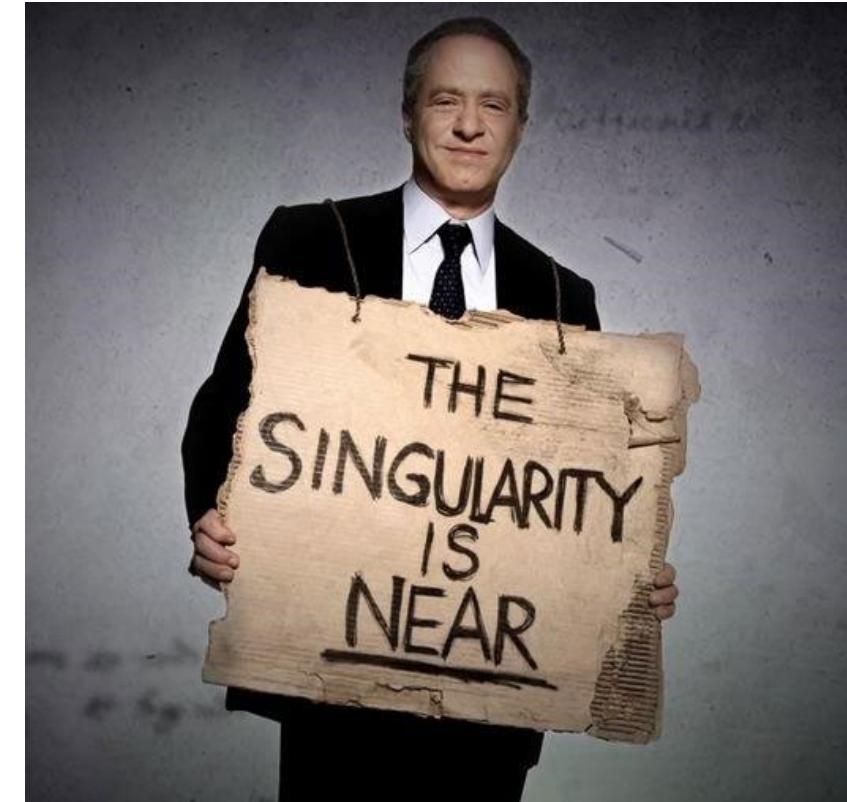
# RECURSION | BOOTSTRAPPING

The entire history of human's invention: Tool that produces tools

For past 50 years: Software that writes software

Basis for the prediction of Singularity in 2045 by Ray Kurzweil

- The Law of Accelerating Returns



# DARPA: 3 WAVES OF AI

First wave (1960s-1990s): hand-crafting rules, domain-specific, logic-based

- Can't scale.
- Fail on unseen cases.

Second wave (1990s-2010s): machine learning, general purpose, statistics-based

- Needs lots of data
- Less adaptive
- Little explanation

Third wave (2010s-2030s): learning + reasoning, general purpose, human-like

- Requires less data
- Adapt to change
- Has contextual and common-sense reasoning
- Explainable

# RODNEY BROOKS' PREDICTION

**2020:** The popular press starts ... **the era of Deep Learning is over.**

**2022:** Driverless "taxi" service in a major US city, restricted settings.

**2023:** **A conversational agent** for **long term context**, and without recognizable and repeated patterns.

**2030:** An AI system with an **ongoing existence** at the level of a mouse.

**2048:** A robot that seems as intelligent, as attentive, and as faithful, as a dog.



# BY FRANCOIS CHOLLET (JULY 2017)

**Models closer to general-purpose computer programs**, built on top of rich primitives—this is how we will get to **reasoning and abstraction**.

**Non-backprop**: Move away from just differentiable transforms.

**AutoML**: Models that require less involvement from human engineers.

**Meta-learning** systems based on reusable and modular program subroutines.

<https://blog.keras.io/the-future-of-deep-learning.html>



# SOFTWARE 2.0 (ANDREJ KARPATHY), NOV 2017

“Software 2.0 is written in neural network weights”

“a large portion of real-world problems [...] it is significantly easier to collect the data than to explicitly write the program.”

“Google is [...] re-writing large chunks of itself into Software 2.0 code.”

“neural networks as a software stack and not just a pretty good classifier”

“future of Software 2.0 is bright because [...] when we develop AGI, it will certainly be written in Software 2.0.”



# The Next AI Revolution (LeCun 2018)



**THE REVOLUTION  
WILL NOT BE SUPERVISED  
(nor purely reinforced)**

With thanks  
To  
Alyosha Efros

# UNSUPERVISED LEARNING

DARPA's program: Learning with less labels

Current trick: pre-training with word2vec, glove, BERT, filling the slots

In RL: intrinsic motivation

What are the principles?

- Energy-based, i.e., pull down energy of observed data, pull up every else
- Filling the missing slots (aka predictive learning, self-supervised learning)
- Multiple objectives, or no objective at all?
- Minimizing “actual” energy given a Markov blanket?
- Compress the history?
- Emergence from many simple interacting elements?

# SELF-SUPERVISED LEARNING (LECUN 2018)

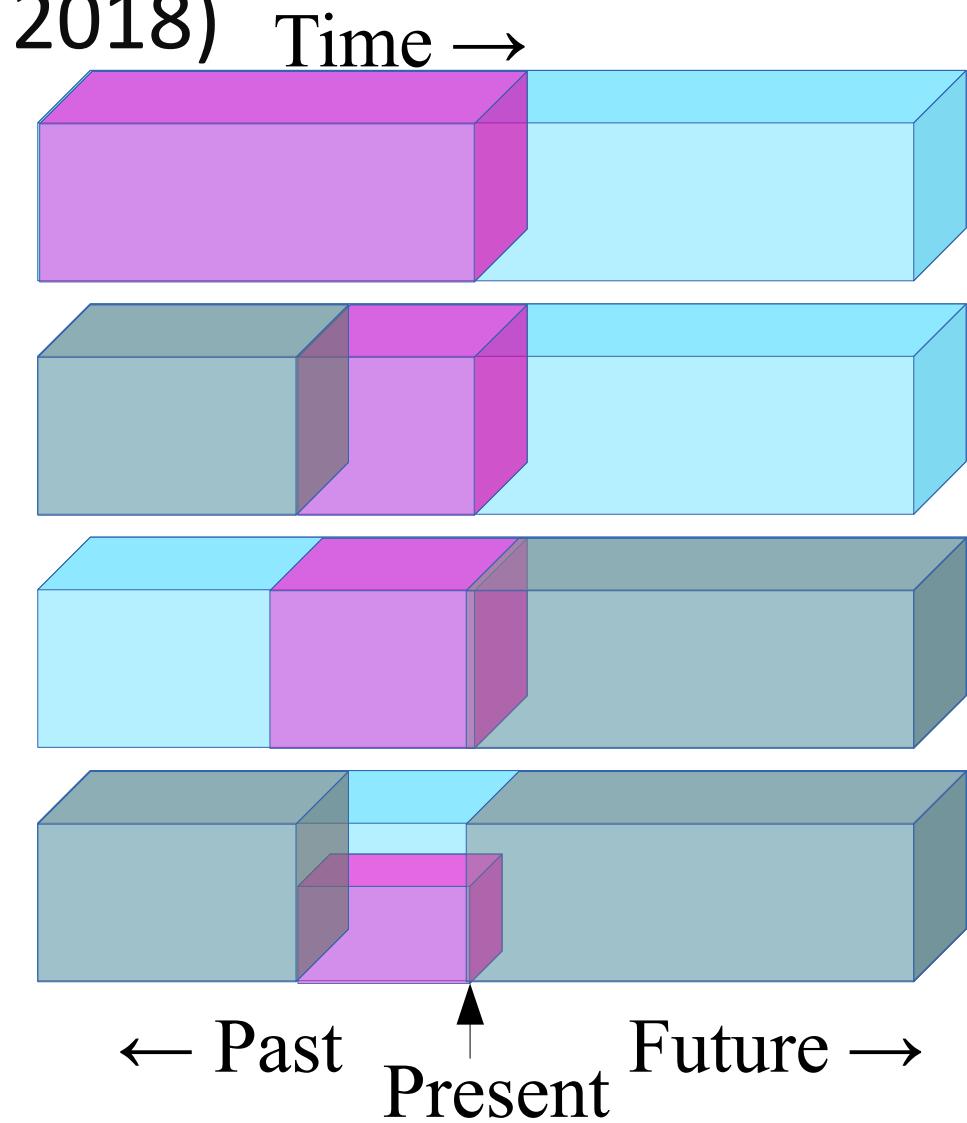
Predict any part of the input from any other part.

Predict the **future** from the **recent past**.

Predict the **past** from the **present**.

Predict the **top** from the **bottom**.

Predict the **occluded** from the **visible**  
Pretend there is a part of the input you  
don't know and predict that.



## COULD SELF-SUPERVISED LEARNING LEAD TO COMMON SENSE? (LECUN 2018)

**Successfully learning to predict everything from everything else would result in the accumulation of lots of background knowledge about how the world works.**

**Perhaps this ability to learn and use the regularities of the world is what we call common sense.**

**If I say “john picks up his briefcase and leaves the conference room”**

You can infer a lot of facts about the scene.

John is a man, probably at work, he is extending his arm, closing his hand around the handle of his briefcase, standing up, walking towards the door. He is not flying to the door, not going through the wall....



# DATA EFFICIENCY FROM DARPA

## Program on Learning with Less Labels

- “reducing the amount of labeled data required to build a model by **six or more orders of magnitude**, and by reducing the amount of data needed to adapt models to new environments to **tens to hundreds of labeled examples**.”

## Technical Area 1: Learn and Adapt Efficiently

- “given a dataset, algorithms must be able to automatically determine which exemplars they would like to have labeled, select from existing corpora or existing models for potential transfer, and create models of a given task without human intervention. Algorithms can create data as part of this process, but they cannot manually create labels. ”

## Technical Area 2: Limits of Machine Learning and Adaptation

- “seeks theories that prove tight bounds on learning in the presence of transfer and meta-transfer learning. The scope of this TA includes extensions to PAC (Probably Approximately Correct) learning theory (and variants) or alternative formalisms to prove tight class-specific problem bounds (e.g., extensions to VC theory), and statistical theory needed to characterize data complexity (e.g., extensions to Johnson-Lindenstrauss) and domain mismatch.”

Source: <https://www.darpa.mil/program/learning-with-less-labels>

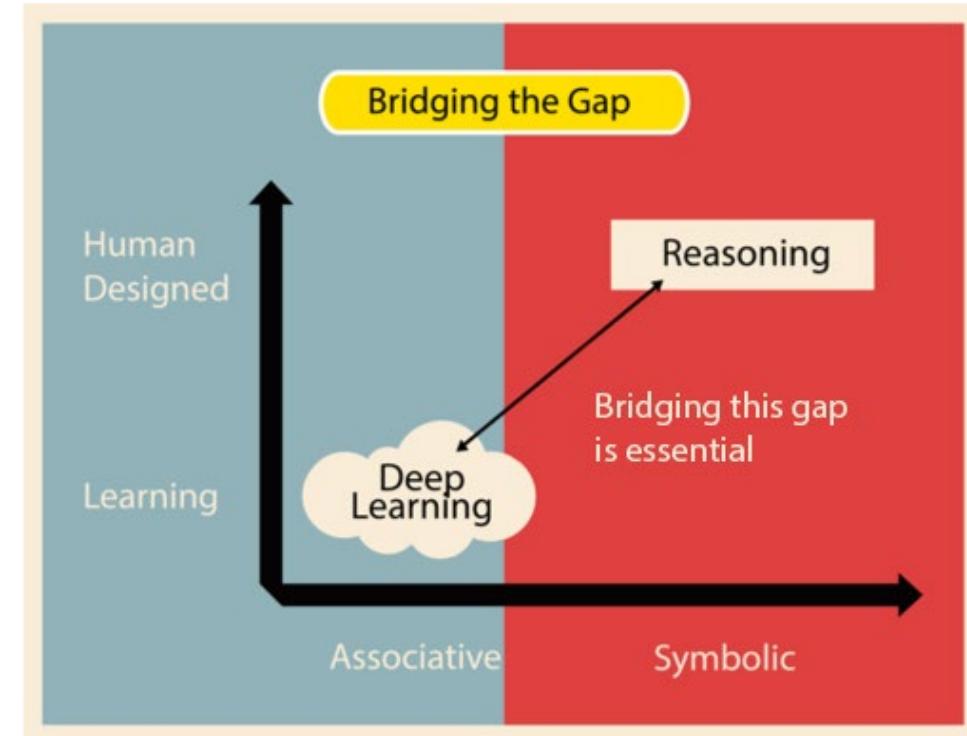
# “DEEP” REASONING

Fusion of perception (CV), communication (NLP), action (RL), and reasoning (classical AI)

Aka neural-symbolic integration

- Perception done by neural nets
- Symbolic integration needs reinforcement learning

<http://www.neural-symbolic.org/CoCoSym2018/index.html>



# (DEEP) REINFORCEMENT LEARNING

Rewards engineering → Rewards learning

Engineering more learning signals

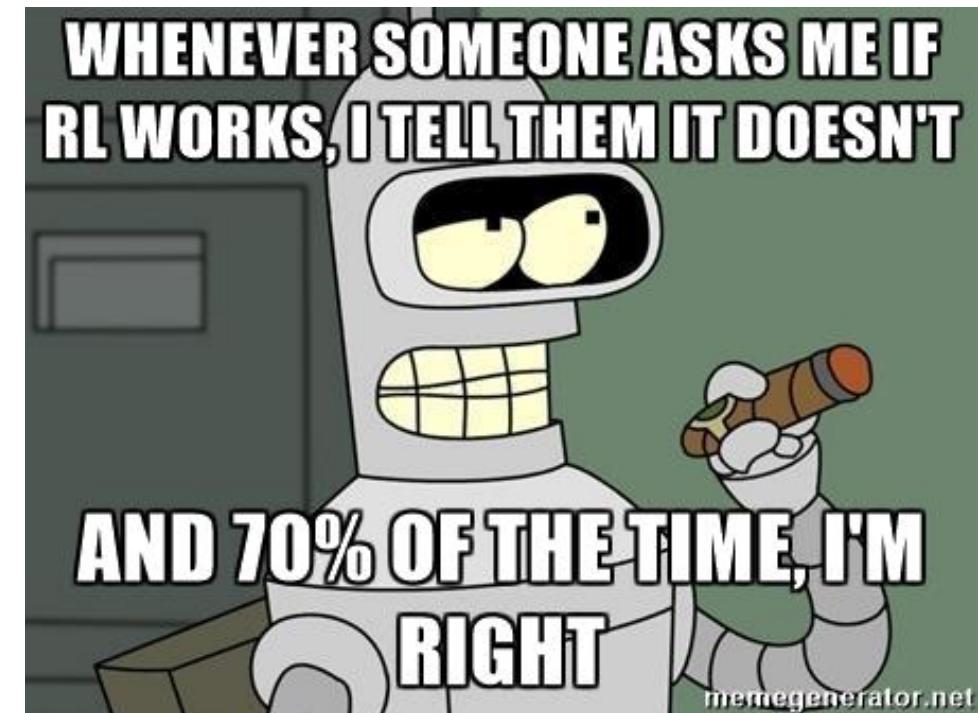
Model-based learning

Better priors

Model reuse

Uncertainty modelling

Hierarchical RL



<https://www.alexirpan.com/2018/02/14/rl-hard.html>

# THEORETICAL DL

Deep versus shallow, (over)-representation, generalization issues

- Role of compositionality on AI and learning.

Loss surface of deep nets, and whether SGD can find good local minima or global minima

Invariance and equivariance properties of CNNs

Limits of deep nets, especially RNNs, Graph NNs & neural Turing machines

Compressibility of RNNs & NTMs

The rise of Optimal Transport Theory (e.g., with GAN)

Complex-valued neural nets

[https://stats385.github.io/lecture\\_slides](https://stats385.github.io/lecture_slides)

<https://sites.google.com/site/deeplearningtheory/schedule>

<http://dalimeeting.org/dali2018/workshopTheoryDL.html>

<http://nips2018dltheory.rice.edu>

# PROBABILISTIC PROGRAMMING

Whether the brain is probabilistic/Bayesian is debatable, but probabilistic thinking is useful.

- This was the reason behind the conference of UAI and later AISTATS
- Related to Probabilistic Graphical Models (Bayesian nets, Markov random fields and Factor graphs), but more flexible.
- Naturally support probabilistic reasoning (aka inference, either marginalization or posterior estimation)

<http://probabilistic-programming.org/wiki/Home>

# ANY HOPE FOR LAWS OF INTELLIGENCE?

Be predictive (aka Popper's falsifiability)

Beauty (simple and revealing)

Elements of surprise

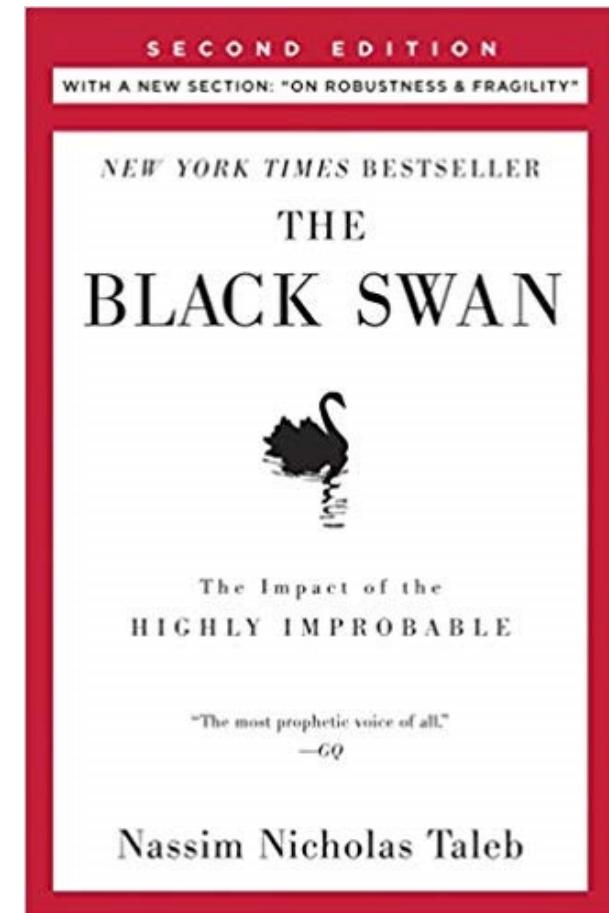
Universality

Invariance

Symmetry

Conservation of quantities

A discovery of an anti-thermal dynamics law



# THEORIES OF INTELLIGENCE

Penrose's consciousness theory

**Friston's free-energy principle**

Russell's bounded rationality

Domingos' Master algorithms

**Newell's unified theories of cognition**

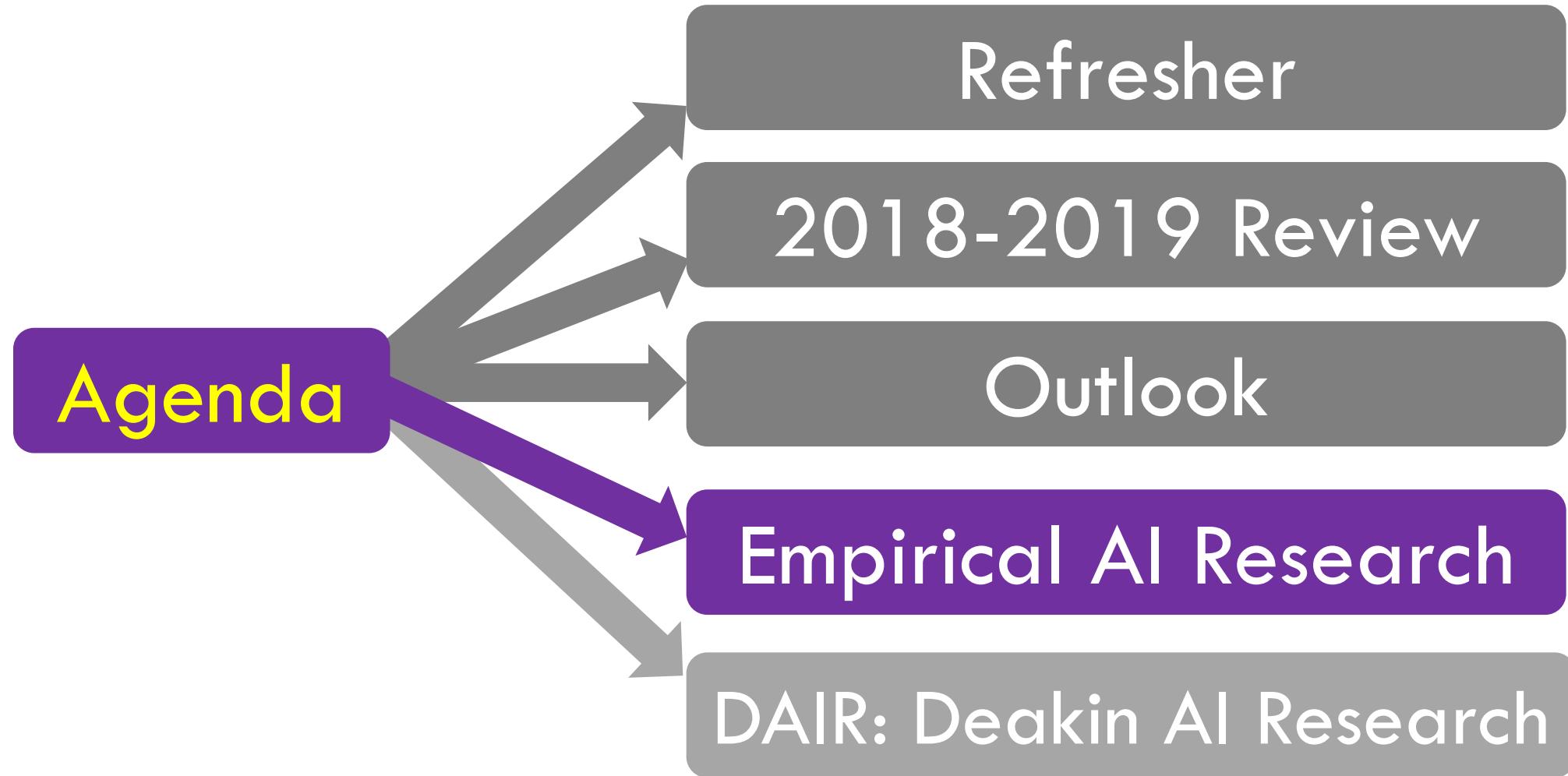
Cognitive architecture. The latest:  
Sigma (symbolic + factor graph)

**Priors of intelligence (innate)**

Intelligence as emerging phenomenon

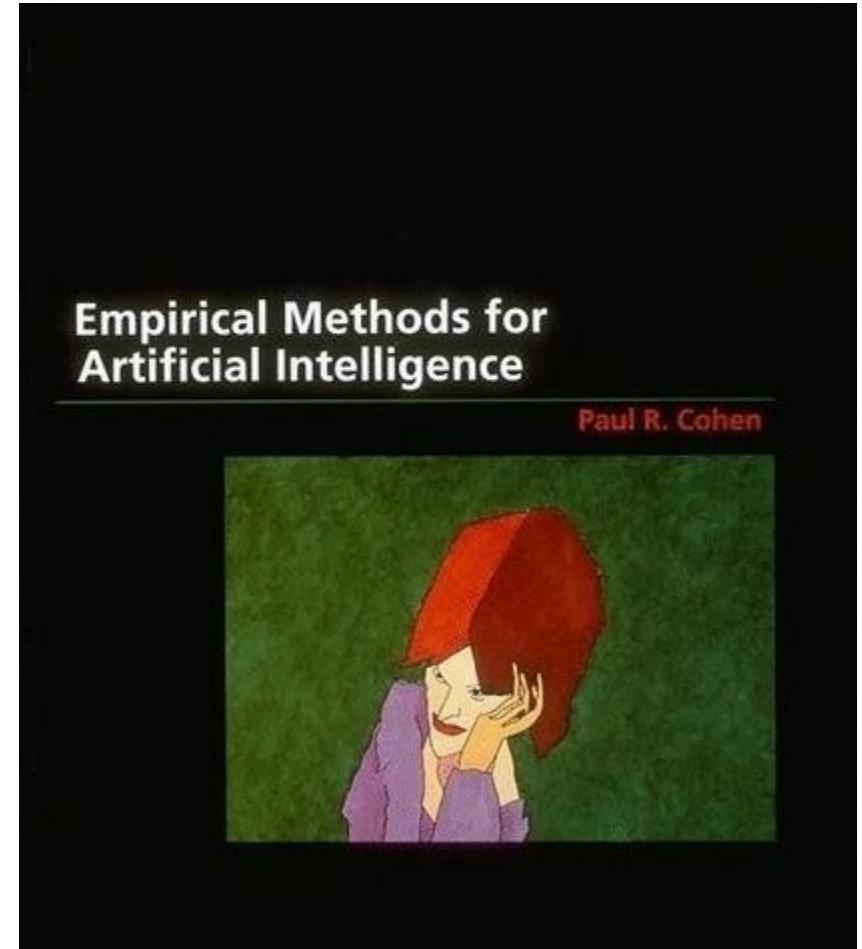
Minsky's society of minds

Quantum theories of cognition



# Empirical observations of empirical AI research

Concepts • Positioning • Planning •  
Empirical methods • Theorization





# em·pir·i·cal

/əm'pirik(ə)l/

adjective

based on, concerned with, or verifiable by observation or experience rather than theory or pure logic.  
"they provided considerable empirical evidence to support their argument"

Empirical != Ad-hoc

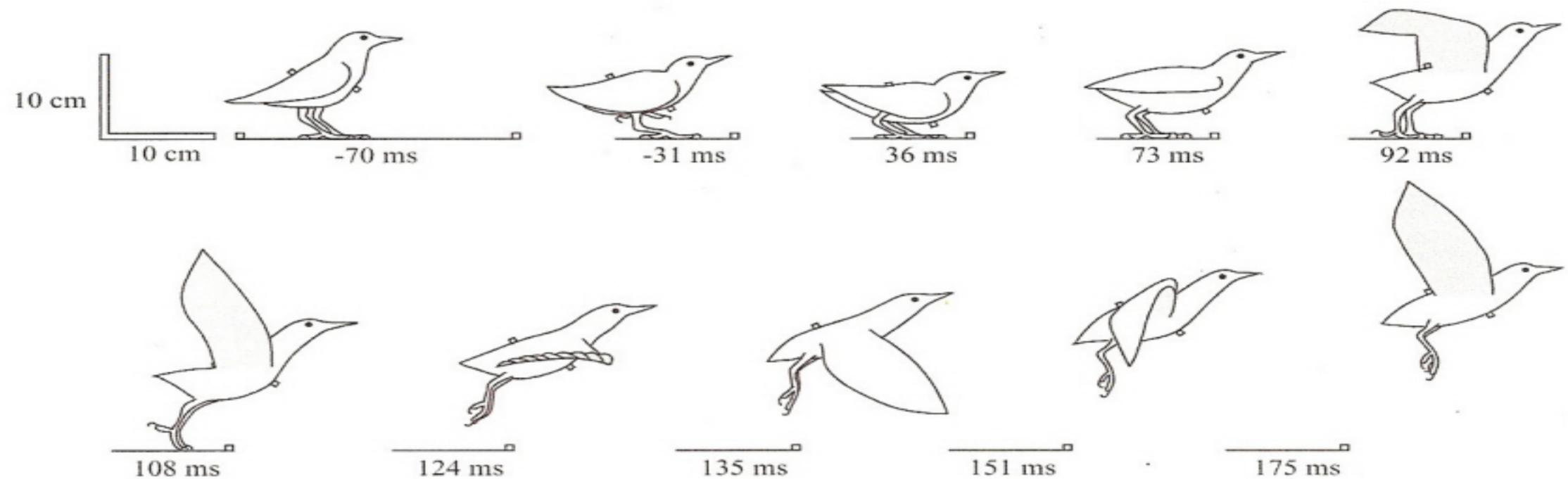
Empirical !=  
Applied research

Origin: Greek *empeirikos* ("experienced")

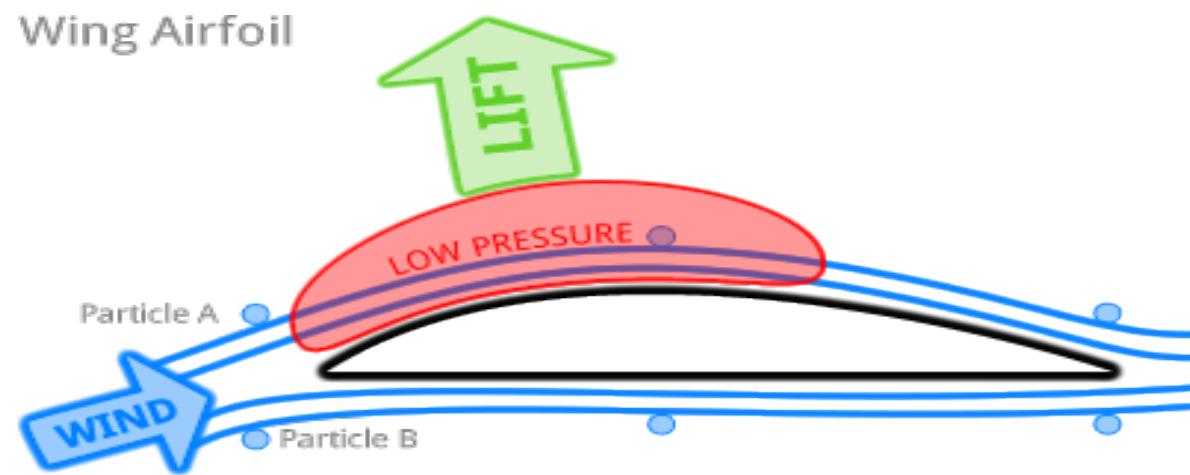


Source: QuestionPro

# HEAVIER-THAN-AIR FLIGHT: OBSERVATION



# HEAVIER-THAN-AIR FLIGHT: THEORY



## Enabling factors

- Aerodynamics
- Powerful engines
- Light materials
- Advances in control
- Established safety practices

Sources:

<http://aero.konelek.com/aerodynamics/aerodynamic-analysis-and-design>  
<http://www.foolishsailor.com/Sail-Trim-For-Cruisers-work-in-progress/Sail-Aerodynamics.html>

# WHY EMPIRICAL?

- Unless theoretically proven, we need realistic validation.
  - Physics theories are great, but they are based on assumptions → need experimental validation
- Toy theories don't scale → have zero impact → Winter AI.
  - Hence, the theories have gone down a bit, e.g., down the Chomsky hierarchy in NLP, and down to surface pattern recognition in CV.
- Real difficult problems lead to new theoretical set ups.
- Empirical observations offer insights, suggests problem formulation, induction and abduction
- Push the field forward. AI now strongly driven by industry.

# EMPIRICAL RESEARCH != IGNORANCE OF THEORY

Theory guides the search. It quantifies the goals. Making sure what we obtained is correct.

Current AI theories:

- Optimization. Mostly non-convex. Loss landscape of deep nets.
- Learnability and generalization. Learning dynamics, convergence and stability.
- Probabilistic inference. Quantification of uncertainty. Algorithmic assurance.
- First-order logic.
- Constraint satisfaction.

# IS EMPIRICAL ML/AI DIFFICULT?

**Yes!** This is the real world.  
It is messy and must be  
difficult.

- Robotics
- Healthcare
- Drug design

**No!** The “effective”  
solution space is small and  
constrained.

- Machine translation
- Self-driving cars
- Drug design

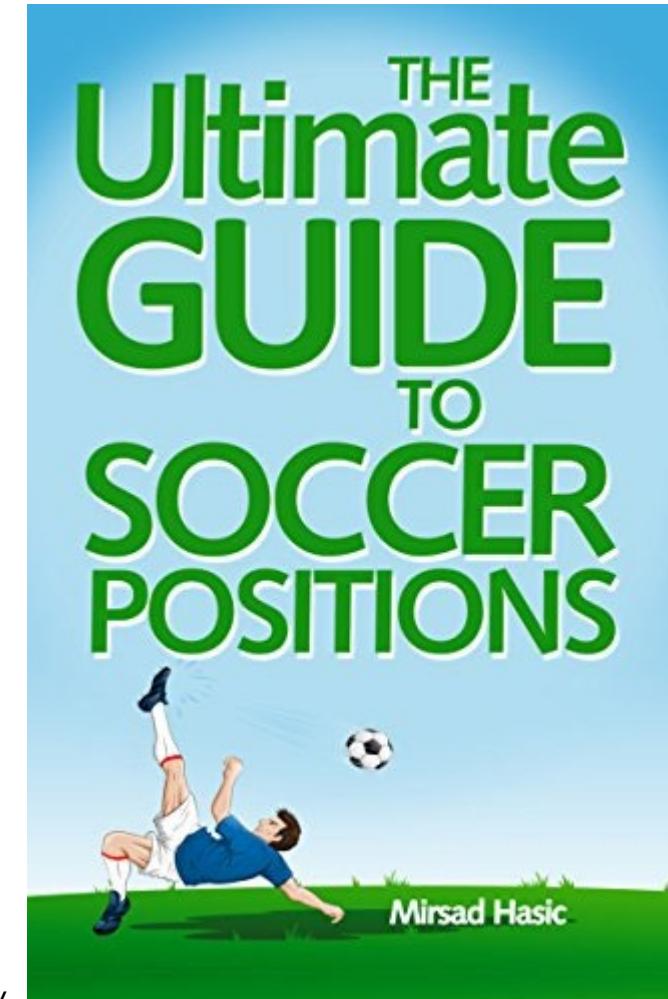
# TWO RESEARCH STYLES

**Methodological:** One method, many application scenarios. The method will fail at some point.

**Applied:** One app, many competing methods. Some methods are intrinsically better than others. E.g., CNN for image processing.

# HOW TO POSITION YOURSELF

“[...] the dynamics of the game will evolve. In the long run, the right way of playing football is **to position yourself intelligently and to wait for the ball to come to you**. You’ll need to run up and down a bit, either to respond to how the play is evolving or to get out of the way of the scrum when it looks like it might flatten you.” (*Neil Lawrence, 7/2015, now with Amazon*)





“Then ask yourself, what is your unique position? What are your strengths and advantages that people do not have? Can you move faster than others? It may be by having access to data, access to expertise in the neighborhood, or borrowing angles outside the field. Sometimes digging up old ideas is highly beneficial, too.

Alternatively, just calm down, and do boring-but-important stuffs. Important problems are like the goal areas in ball games. The ball will surely come.”

<https://letdataspeak.blogspot.com/2016/12/making-dent-in-machine-learning-or-how.html>

# WISDOM OF THE ELDERS

## Max Planck

- Science advanced by one death at a time

## Geoff Hinton:

- When you have a cool idea but everyone says it is rubbish, then it is a really good idea.
- The next breakthrough will be made by some grad students

## Richard Hamming:

- After 7 years you will run out of ideas. Better change to a totally new field and restart.
- If you solve one problem, another will come. **Better to solve all problems for next year, even if we don't know what they are.**

<http://paulgraham.com/hamming.html>

# STRATEGIES TO SELECT RESEARCH AREAS

Ask what intelligence means, and what human brain would do

Set an intelligence level (bacteria, insect, fish, mouse, dog, monkey, human)

Check solvable unsolved problems. There are LOTS of them!!!

Look for impact

Look for being difference. Fill the gap. Be unique. Be recognizable.

Riding the early wave.

Ask what a physicist would do:

- Simplest laws/tricks that would do 99% of the job
- Minimizing some free-energy
- Looking for invariance, symmetry

# INSIGHTS FROM NEUROSCIENCE

Brain is the only known intelligence system

Can provide inspirations for AI

Can validate AI claims

Indeed, many AI concepts have had originated from neuroscience

- However, the influence is only at the initial step
- AI doesn't have the constraints that neuroscience does
- AI can do things that are impossible within neuroscience

Hassabis, Demis, et al. "Neuroscience-inspired artificial intelligence." *Neuron* 95.2 (2017): 245-258.

Schmidhuber, Jürgen. "Deep learning in neural networks: An overview." *Neural networks* 61 (2015): 85-117.

# NEUROSCIENCE CONCEPTS

Memory

Reinforcement learning

Control

Attention

Planning

Imagination

Symbolic manipulation

Emotion

Consciousness

Transfer learning

Continual learning

Spatial memory

Social interaction

Developmental

Catastrophic forgetting

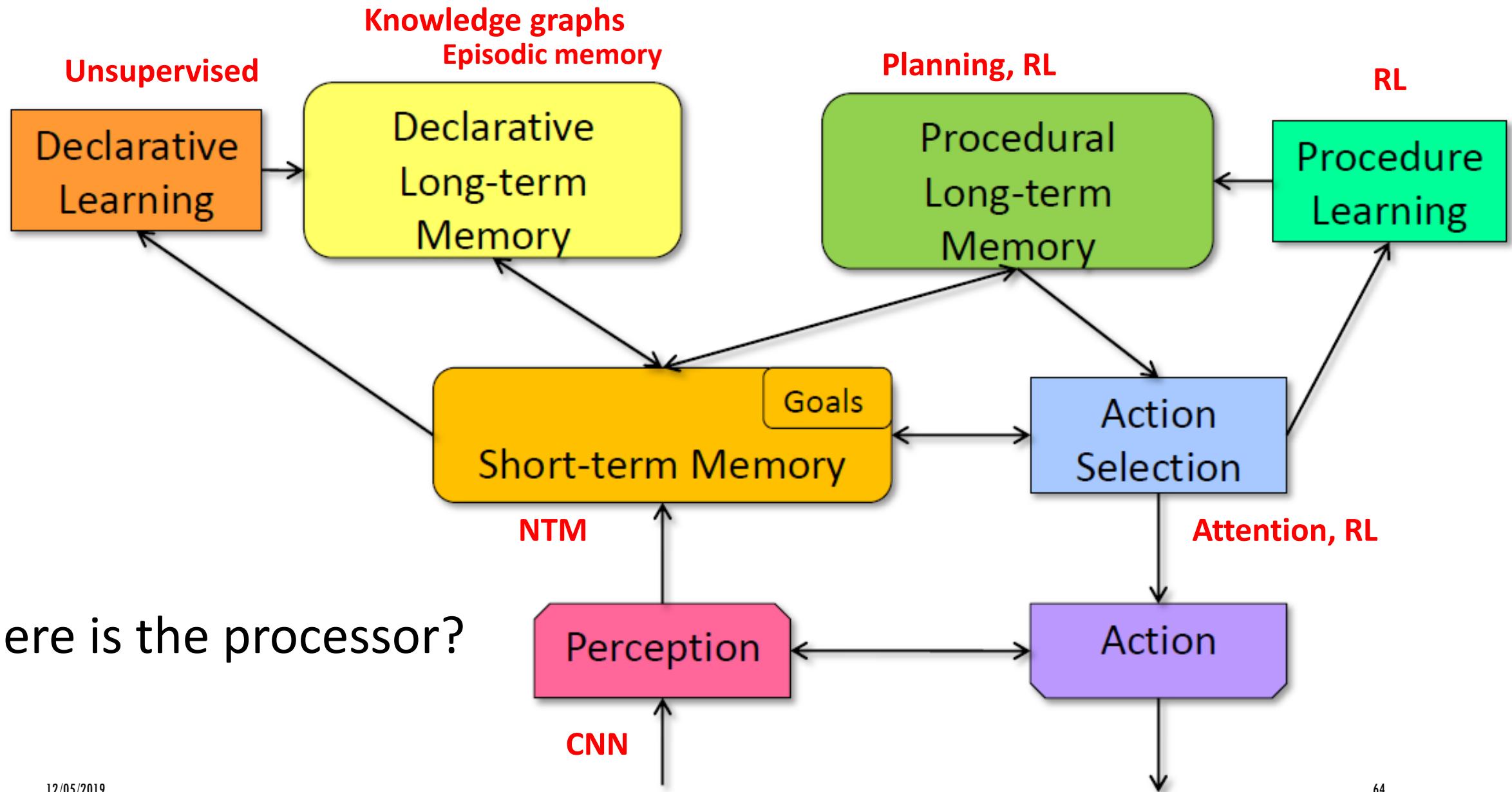
Nature versus nurture

# Newell's Time Scale of Human Action

<u>Scale (sec)</u>	<u>Time Units</u>	<u>System</u>	<u>Band</u>
$10^7$	months	Social	
$10^6$	weeks		
$10^5$	days		
$10^4$	hours	Task	Rational
$10^3$	10 min	Task	
$10^2$	minutes	Task	
$10^1$	10 sec	Unit task	Cognitive
$10^0$	1 sec	Operations	
$10^{-1}$	100 ms	Deliberate act	
$10^{-2}$	10 ms	Neural Circuit	Biological
$10^{-3}$	1 ms	Neuron	
$10^{-4}$	100 $\mu$ s	Organelle	

The diagram illustrates the mapping of various cognitive architectures onto Newell's Time Scale of Human Action. The architectures are represented by colored bars: LEABRA (green), SPAUN (green), EPIC (blue), Sigma (purple), ACT-R (blue), Soar (purple), and Companions (purple). The bars are positioned along the right edge of the table, corresponding to their approximate time scale:

- LEABRA:  $10^0$  to  $10^1$  sec
- SPAUN:  $10^{-1}$  to  $10^0$  sec
- EPIC:  $10^{-2}$  to  $10^{-1}$  sec
- Sigma:  $10^{-3}$  to  $10^0$  sec
- ACT-R:  $10^{-2}$  to  $10^0$  sec
- Soar:  $10^{-3}$  to  $10^0$  sec
- Companions:  $10^{-3}$  to  $10^0$  sec



# THINKING & LEARNING, FAST AND SLOW

## Thinking

- Fast: reactive, primitive, associative, animal like
- Slow: deliberative, reasoning, logical.

## Learning

- Fast: often memory-based, one-shot learning style, fast-weights, e.g., k-NN
- Slow: often model- based, iterative, slow-weights, e.g., backgrop

# UNSOLVED PROBLEMS (1)

Learn to organize and remember ultra-long sequences

Learn to generate arbitrary objects, with zero supports

Reasoning about object, relation, causality, self and other agents

Imagine scenarios, act on the world and learn from the feedbacks

Continual learning, never-ending, across tasks, domains, representations

Learn by socializing

Learn just by observing and self-prediction

Organizing and reasoning about (common-sense) knowledge

Grounding symbols to sensor signals

Automated discovery of physical laws

Solve genetics, neuroscience and healthcare

Automate physical sciences

Automate software engineering

# UNSOLVED PROBLEMS (2)

[Click here](#)

# LECUN'S LIST (2018)

**Deep Learning on new domains (beyond multi-dimensional arrays)**

Graphs, structured data...

**Marrying deep learning and (logical) reasoning**

Replacing symbols by vectors and logic by algebra **Self-supervised learning of world models**

Dealing with uncertainty in high-dimensional continuous spaces

**Learning hierarchical representations of control space**

Instantiating complex/abstract action plans into simpler ones

**Theory!**

**Compilers for differentiable programming.**

# A TYPICAL EMPIRICAL PROCESS

## Hypothesis generation

- Mostly by our brain
- But AI can help the process too!

## Hypothesis testing by experiments

### Two types:

- **Discovery:** it is there, awaiting to be found. Mostly theories of nature.
- **Invention:** not there, but can be made. Mostly engineering.

# HOW TO PLAN AN EMPIRICAL RESEARCH

Get the right people. Smart. Self-motivated. Can read maths. Can code. Can do dirty data cleaning.

Choose a right topic. Impactful ones at the right time. Looks for current failures. Set the targets.

Explore theoretical options.

Breaking into solvable parts

- Before: 3 years of PhD, one problem.
- Now: every 3-6 months to meet a conference deadline (Feb-March, May-June, Aug-Sept, Nov-Dec)

Collect data. LOTS of them. Clean up.

Code it up. In DL, it means using your favourite programming frameworks (e.g., PyTorch, TensorFlow)

Evaluate the options on some small data, then big data, then a variety of data

Repeat

**Question: When should we stop evaluating?**

# CHOOSING HIGH IMPACT PROBLEMS

Impact to the population (e.g., 100M people or more – Andrew Ng)

Start a new paradigm – a new trend

Ride the wave

No need to have a competitive mind – “Mine beats yours”

# CHOOSING IMPORTANT BUT LESS SHINY PROBLEMS

Computer vision & NLP are currently shiny areas. Dominated by industry. You can't compete well without good data, computing resources, incentives and high concentration of talent.

Some of the best lie in the intersection of areas. Esp. those with some domain knowledge (which you can learn fast).

- Biomedicine, e.g., drug design, genomics, clinical data.
- Sustainability, e.g., Earth health, ocean, crop management, land use, climate changes, energy, waste management.
- Social good, law, developing countries, access to healthcare and education, clean water, transportation.
- Value-alignment, ethics, safety, assurance.
- Accelerating sciences, e.g., molecule design/exploration, inverse materials design, quantum worlds.

# HOW TO BE PRODUCTIVE AND BE HAPPY

**Maximize your quantity and quality of enlightenment.**

Fail fast. Fail smart. Start small. Scale latter.

Use simplest possible method to confirm or reject a hypothesis

If the hypothesis is partially confirmed, refine the hypothesis, or improve the method, and repeat.

Time spent per experiment should be limited to an hour or similar range. Winning code seems to run for 2 weeks.

**Productivity = knowledge unit gained / time unit.**

# PATTERNS REPEATED EVERYWHERE

Lots of problems can be formulated in similar ways

We often need an intermediate representation, e.g., graphs that can be seen in many fields.

Solving the generic problems are often faster and generalizable.  
See Sutton's remarks.

Many domains can be solved at the same time. After all, we have just one brain that does everything.

Methods that survive need to be simple, generic and scalable.  
PCA, CNN, RNN, SGD are examples.

# METHODS VERSUS CONCEPTS

Methods come and go, but concepts stay

- Decision trees, kernels → Template matching, data geometry
- Random forests, gradient boosting → Smoothing, variance reduction
- Neural nets → Differentiable programming, function reuse, credit assignment

“Machine learning is the new algorithms”

- <https://nlpers.blogspot.com.au/2014/10/machine-learning-is-new-algorithms.html>

# RIDING THE EARLY WAVES

Neural network, cycle 1: 1985-1995

- Backprop

SVM:1995-2005

- Nice theory, strong results for moderate data

Ensemble methods: 1995-2005

- Nice theory, strong results for moderate data

Probabilistic graphical models: 1992-2002

- Nice theory, open up new thinking, difficult in practice

Topic models & Bayesian non-parametrics:  
2002-2012

- Nice theory, indirect applications

Feature learning: 2005-2015

- Little theory, toy results, great excitements

Neural network, cycle 2: 2012-present

- Differentiable programming, backprop + adaptive SGD
- Little theory, strong results for large data

**For PhD students: be an expert when the trend is at its peak!**

# MY OWN JOURNEY

**In 2004** I bet my PhD thesis on “Conditional random fields”. It died when I finished in 2008.

**In 2007** I bet my theoretical research area on Deep Learning, back then it was Restricted Boltzmann Machines. RBM died around 2012. But the field moves on and now reaches its peak.

**In 2012** I bet my applied research area on Biomedicine. This is super-hot now.

**In 2019** I am betting on “learning to reason” → cognitive architectures.

# THE 10 YEAR MINI-CYCLES IN ML

Neural network, cycle 1: 1985-1995

- Backprop

SVM: 1995-2005

- Nice theory, strong results for moderate data

Ensemble methods: 1995-2005

- Nice theory, strong results for moderate data

Probabilistic graphical models: 1992-2002

- Nice theory, open up new thinking, difficult in practice

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- Nice theory, indirect applications

Feature learning: 2005-2015

- Little theory, toy results, great excitements

Neural network, cycle 2: 2012-present

- Differentiable programming, backprop + adaptive SGD
- Little theory, strong results for large data

# THE CURSE OF TEXT BOOKS

**Truyen's law:** “whenever a universally accepted textbook is published, the field is saturated.”

- decision tree (1984),
- neural nets, cycle 1 (1995),
- information retrieval (1998),
- reinforcement learning (1998),
- multi-agent system (2001),
- ensemble methods (2001),
- kernels (2002),
- probabilistic graphical models (2006),
- structured output learning (2007),
- learning to rank (2009),
- Bayesian non-parametrics (2012), and
- deep learning (2016).

# HOW MUCH COMPUTING POWER?

The larger the better. It gives you freedom.

- Sutton (“the bitter lesson”): generic methods + lots of compute win!
- See the history of speech recognition, machine translation.

However, for faster discovery and learning, better maximize the number of reasonably good GPUs → more people, more parallel experiments.

On the other hand, little compute forces us to be smart. There are lots of important problems with lean data. See “You and your research” by Richard Hamming.

Our brain uses very little energy (somewhere like 10 Watts). There must be clever ways to arrange computation.

# BUT ... BY ALL MEANS, ADVANCE SCIENCE

**J. Pearl:** Uncertainty in AI (1980s-1990s) & causality (2000s-present)

**G. Hinton** (Turing Award): parallel distributed processing (1980s-present)

**J. Schmidhuber:** Agent that learns to do, and to learn (1980s-present)

**C. Sutton:** Agent that learns by reinforcement (1980s-present)

**M. Jordan:** Probabilistic inference (1990s-present)

## WARNING! PREDICTION V.S. UNDERSTANDING

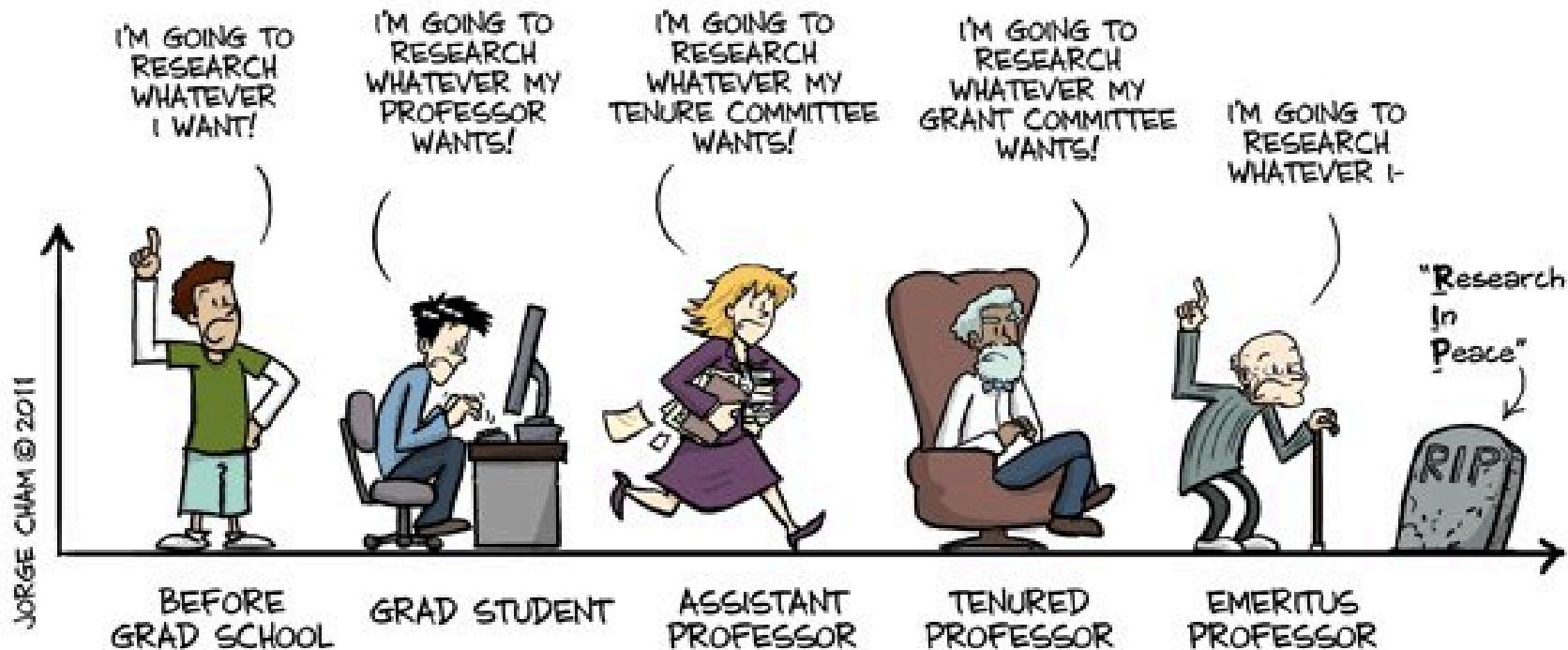
We can predict well without understanding (e.g., planet/star motion Newton).

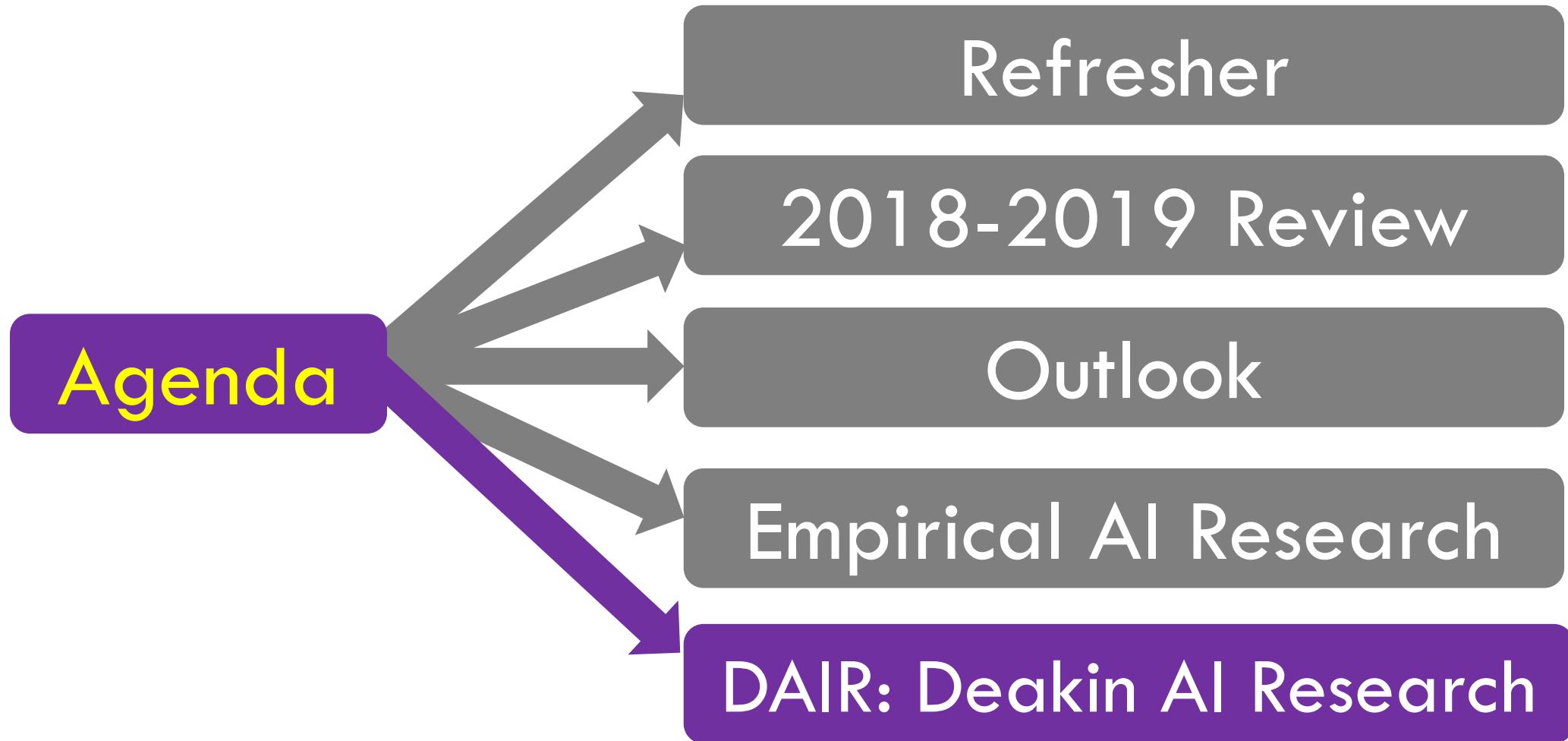
**Guessing** the God's many complex behaviours versus **knowing** his few universal laws.

- Without theorization, we can have intelligent behaviours, but not true intelligence.
- Might **abduction** (selecting the simplest explaining theory) be the goal.

# A NECESSARY CAUTION

## THE EVOLUTION OF INTELLECTUAL FREEDOM





# DAIR: Deakin AI Research

Part of the newly found Applied AI Institute



# THE TEAM @DAIR



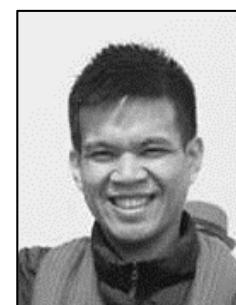
A/Prof. Truyen Tran



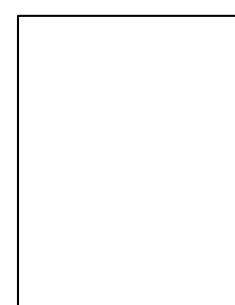
Dr Vuong Le



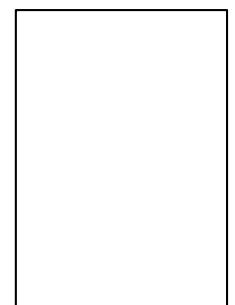
Dr Phuoc Nguyen



Dr Khanh Tran



Dat Tran @UTS



Romero Barata



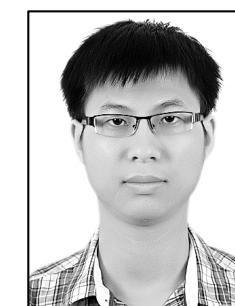
Dung Nguyen



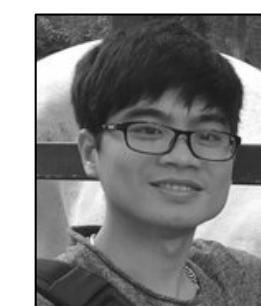
Tung Hoang



Tin Pham



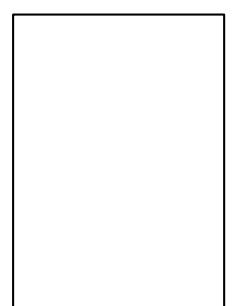
Kien Do



Thao Le



Hung Le



Duc Nguyen

## Fundamentals

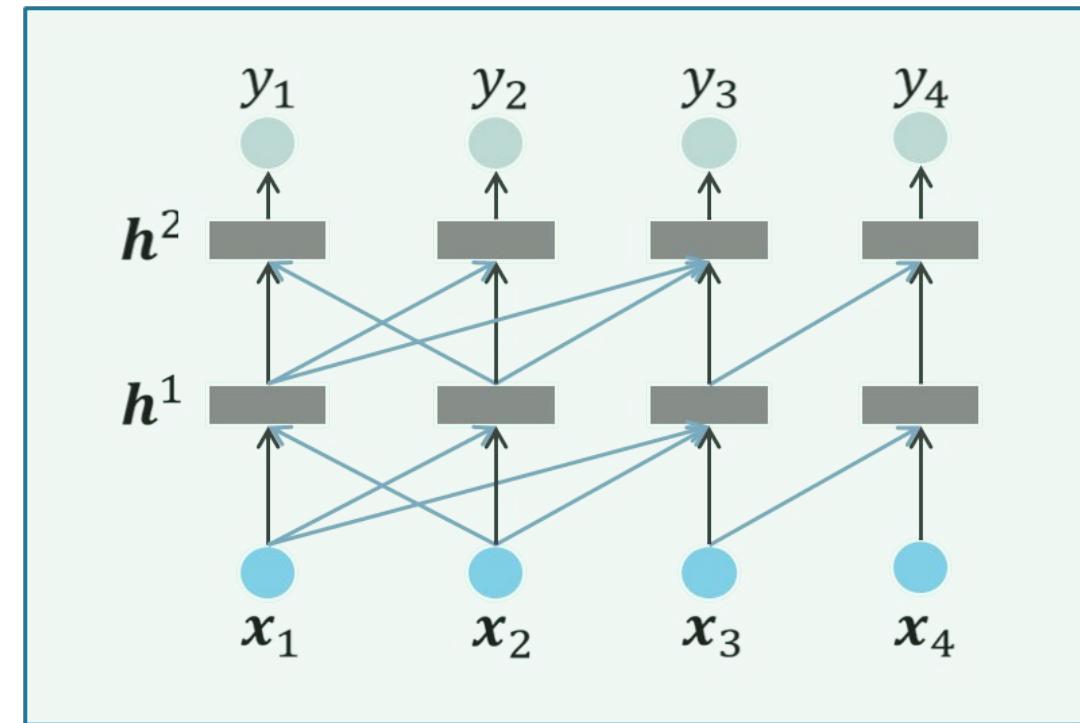
- New inductive biases
- Memory and Turing machines
- Learning to reason
- Learning with less labels
- Deep reinforcement learning

## Applied projects

- Vision: Visual reasoning
- NLP: QA and dialog systems
- Accelerating physical & bio sciences
- Transforming healthcare
- Automating software developments
- Building smarter smart homes
- Value-aligned ML

# NEW INDUCTIVE BIASES

- Search for new priors
- In DL, we have a small set of primitive operators (signal filtering, convolution, recurrence, gating, memory and attention)
- Sets, tensors, sequences, trees, graphs.
- Inspirations from neocortex
  - Columns, thalamus routing, memory structures.



# GRAPH: WHAT WE HAVE DONE

Column Network (CLN): Generic message passing architecture (AAAI'17)

Relation basis for knowledge graph completion (ICPR'18)

Graph with virtual nodes (IJCAI'17 workshop)

Graph Memory Network (ICLR'18) → Relational Dynamic Memory Network (In submission to MLJ)

- Support **graph-graph interaction** (e.g., chemical-chemical interaction)

# GRAPH: WHAT WE HAVE DONE (2)

Graph transformation policy network (Submitted to ICLR'19)

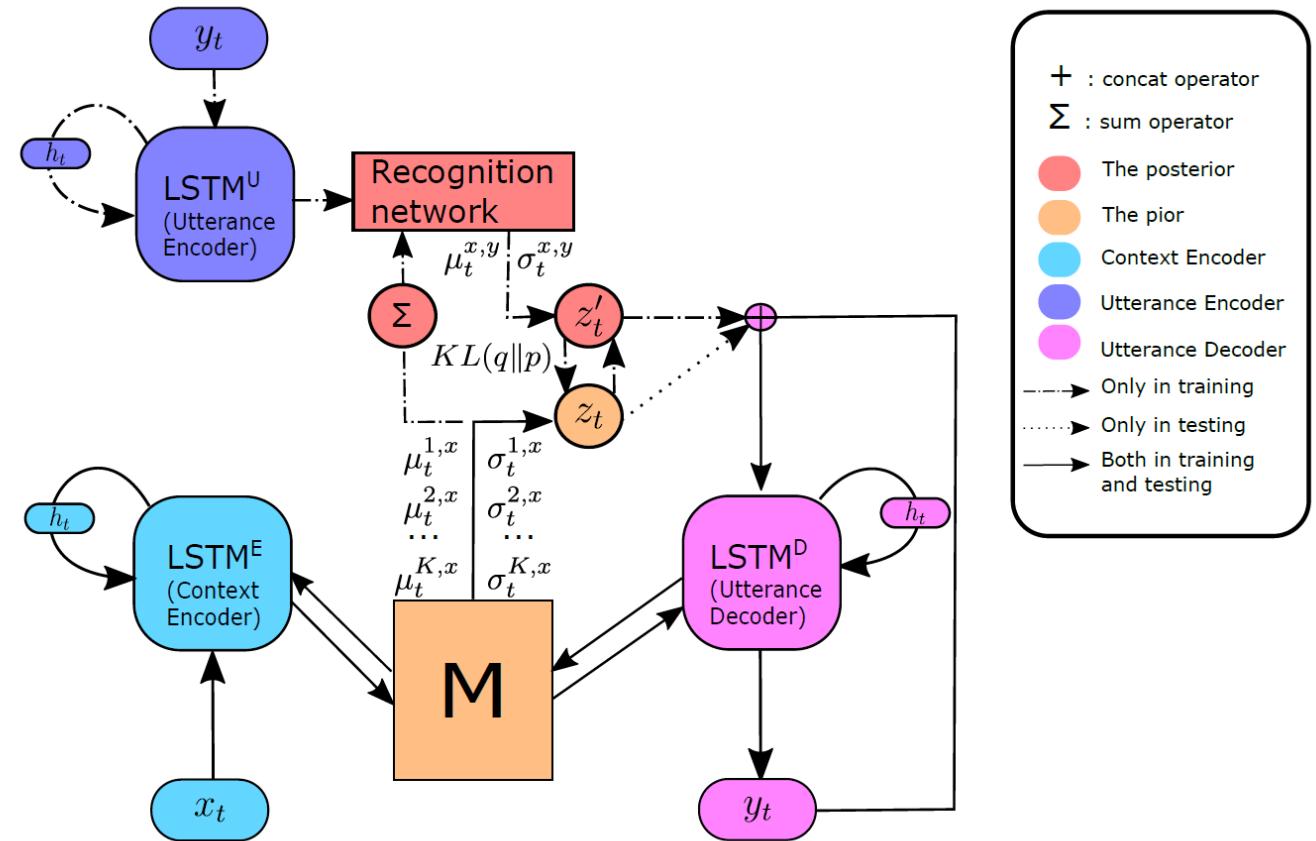
Graph Attentional Multi-label Learning (GAML): Graph2X,  
where X = set (MLJ, Minor revision)

Column Bundle: Generic architecture for multi-X learning,  
where X = view, instance, label, task

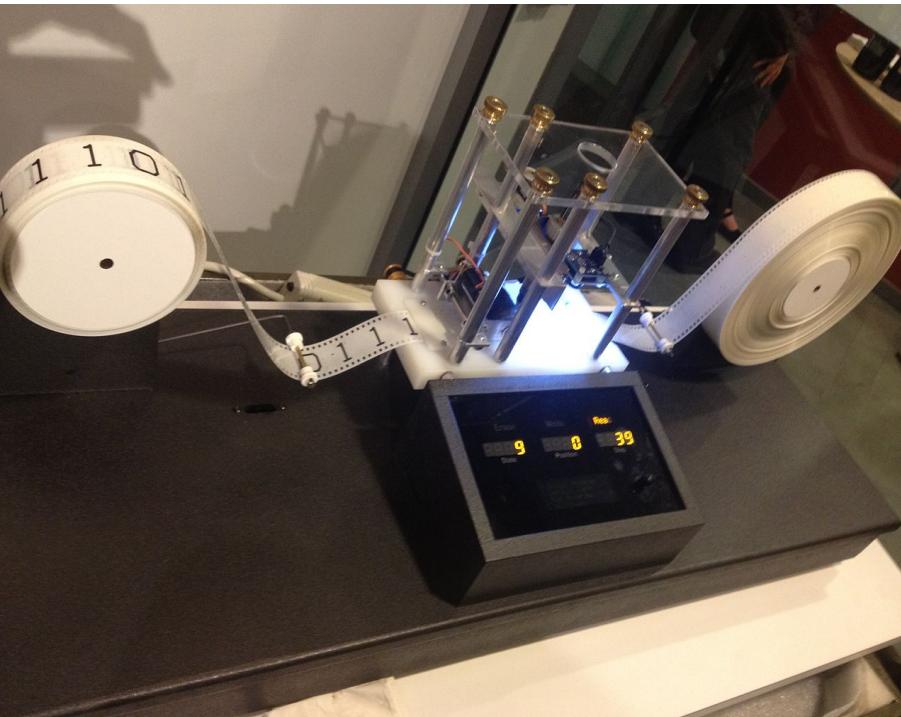
Matrix representation of graphs & relation

# MEMORY-AUGMENTED NEURAL NETWORKS

- Complex, long-range dependencies demand external memory
- Resemble how modern computer works (CPU & RAM)



# MEMORY AND TURING MACHINES



Can we learn from data a model that is as powerful as a Turing machine?

It is possible to invent a *single machine* which can be used to compute *any* computable sequence. If this machine **U** is supplied with the tape on the beginning of which is written the string of quintuples separated by semicolons of some computing machine **M**, then **U** will compute the same sequence as **M**.

Wikipedia

# MANN: WHAT WE HAVE DONE

Dual-view in sequences (KDD'18)

Bringing variability in output sequences (NIPS'18)

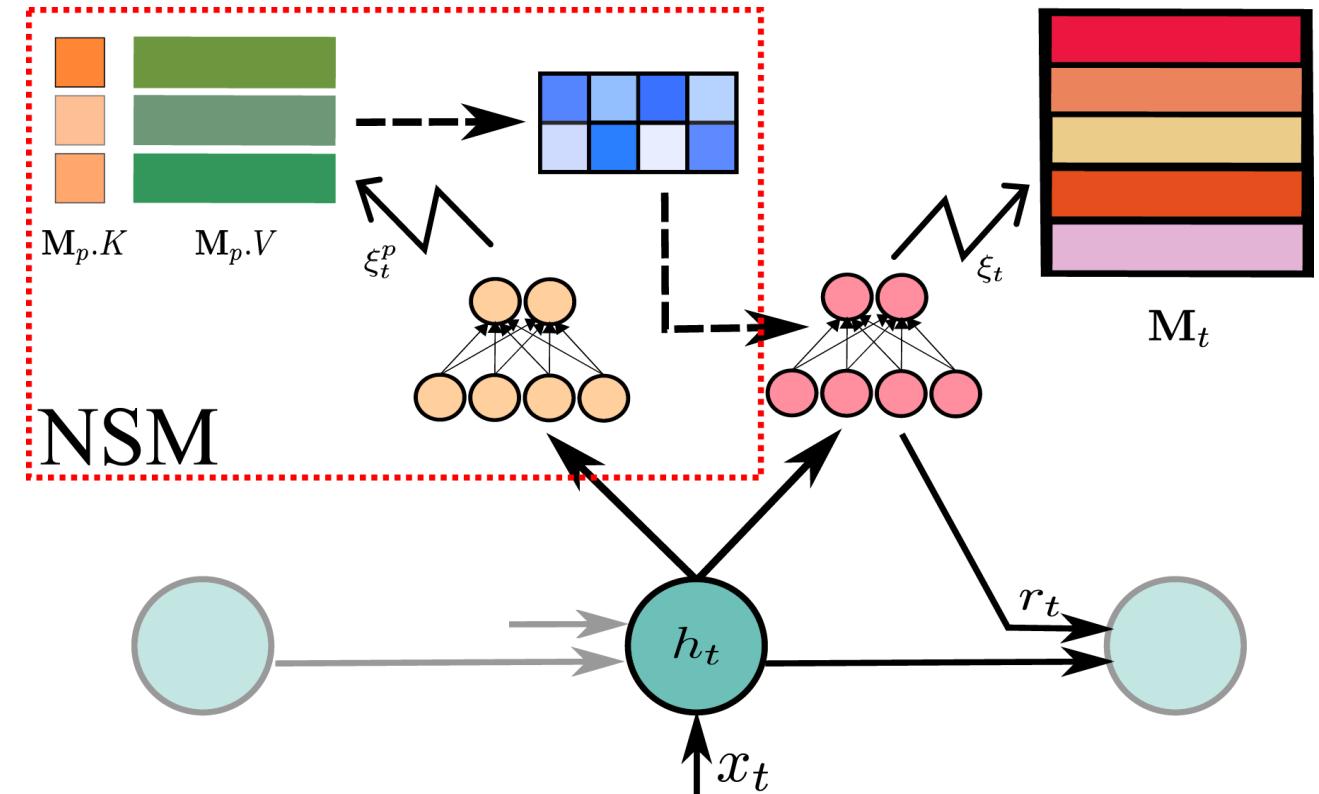
Bringing relational structures into memory (ICPR'18)

Learning to skim read (ICLR'19)

Learning to program (on going)

# ON GOING: NEURAL STORED-PROGRAM MEMORY

- Truly Turing machine:  
programs can be stored and  
called when needed.
- Can solve BIG problem with  
many sub-modules.
- Can do continual learning.
- Can help mitigate  
catastrophic forgetting.



# LEARNING TO REASON (L2R)

- L2R is learning to decide if a knowledge base entails a predicate.
- Can be cast as QA.
- Where neural meets symbolic
- Deep learning solves symbol grounding problem
- Integrating if fast and slow thinking
- Role of episodic memory to piece things together
- Role of working memory to support deliberative multi-step reasoning
- Knowledge-base L2R

# CURRENT WORKS

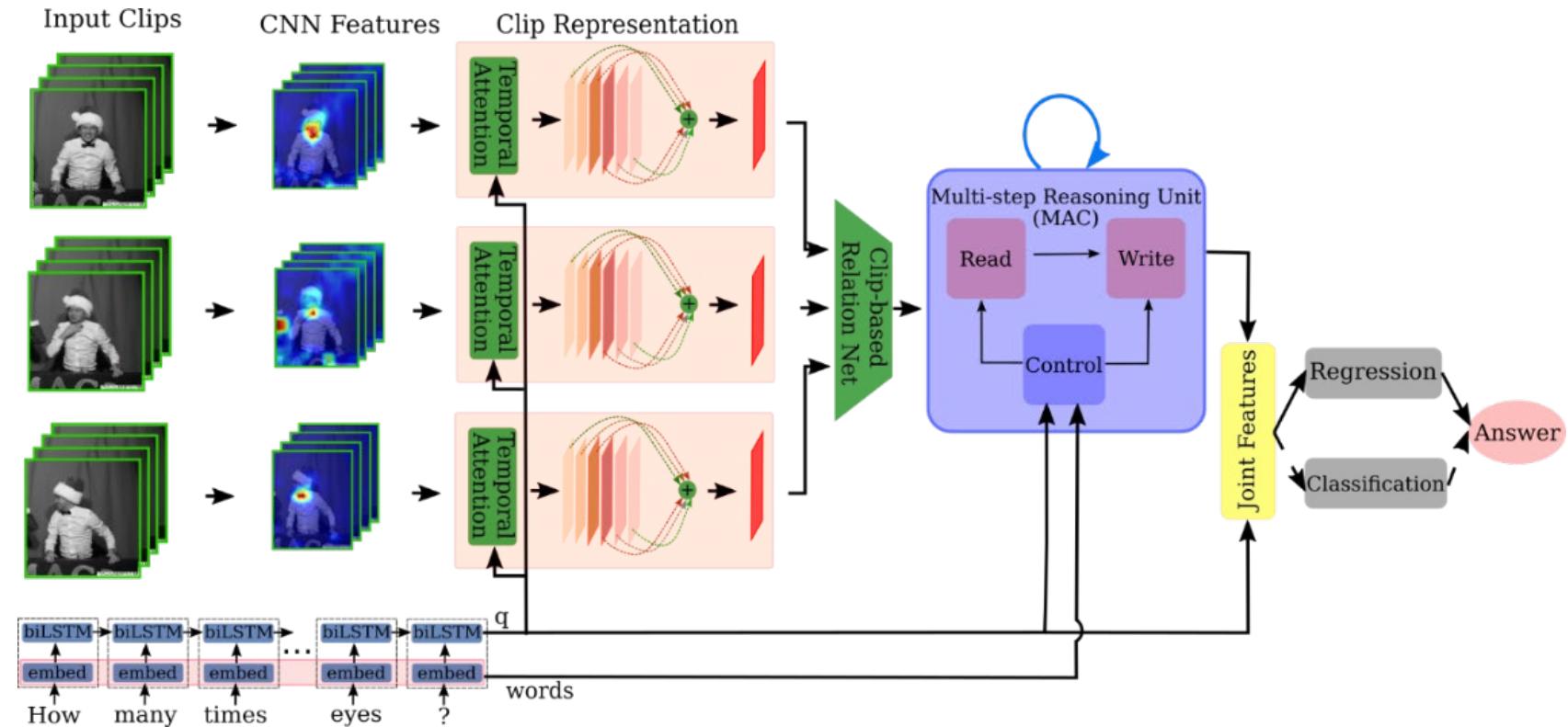
Graph reasoning

Video question answering

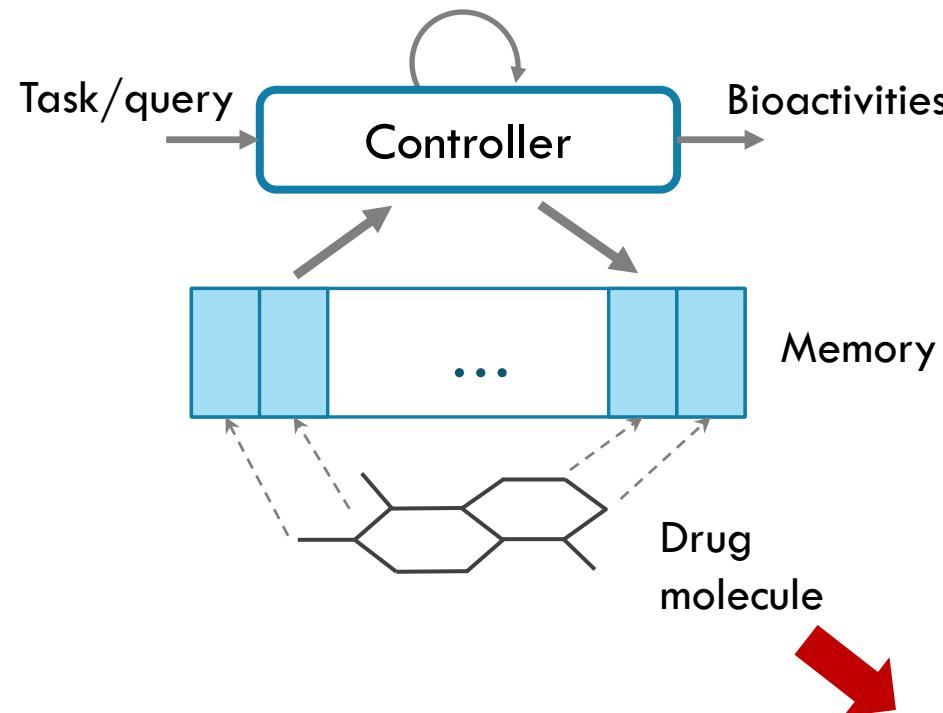
Protein-drug design: affinity prediction (drug as query) & drug generation  
(bioactivities as answers, what is the question?)

Conditional software execution

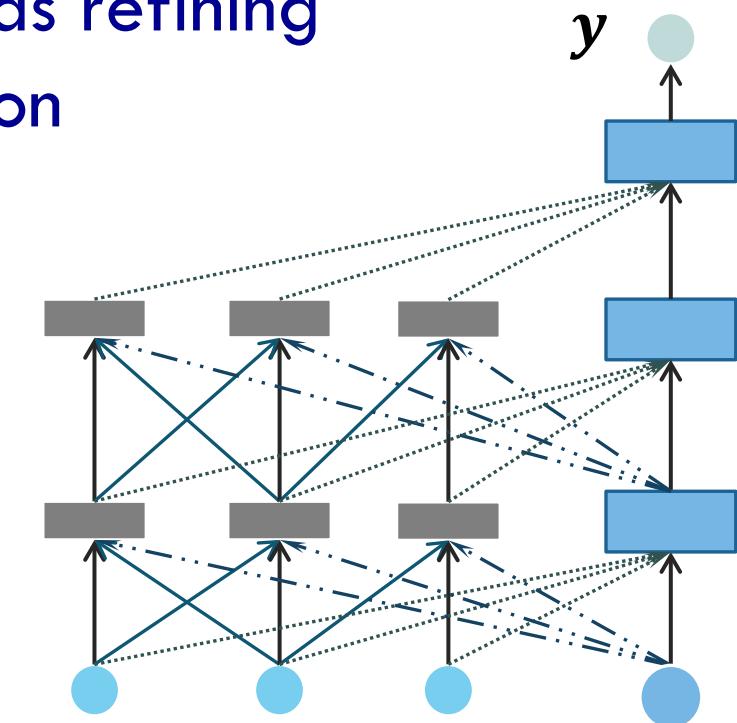
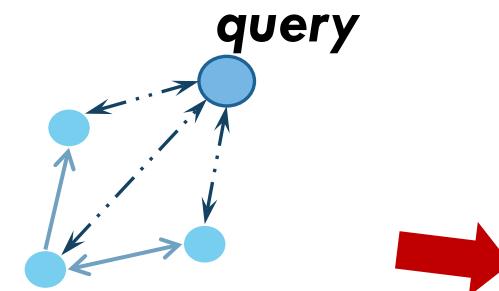
Knowledge graph querying and completion



# QUERYING A GRAPH



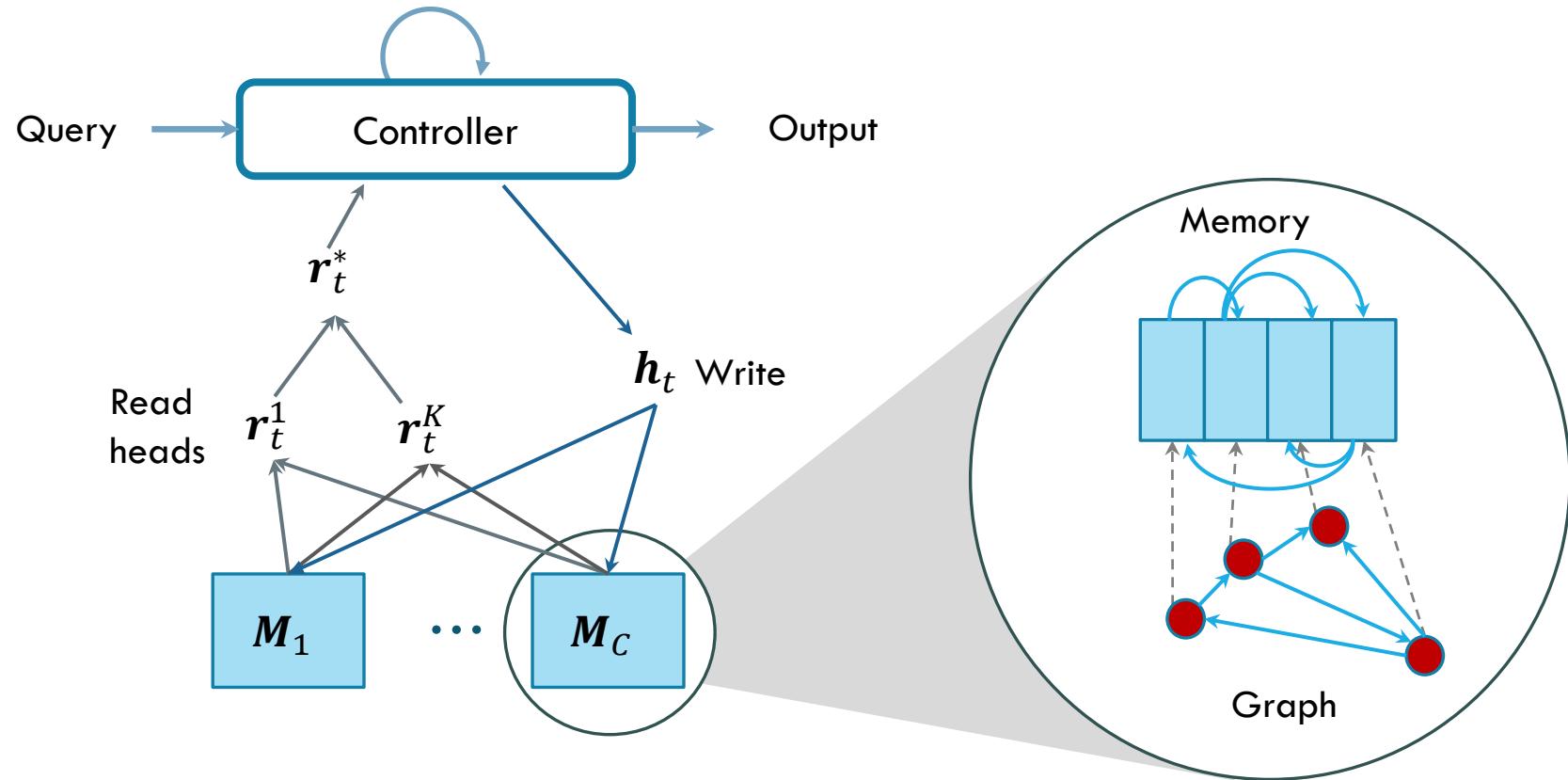
Message passing as refining  
atom representation



#Ref: Pham, Trang, Truyen Tran, and Svetha Venkatesh. "Graph Memory Networks for Molecular Activity Prediction." ICPR'18.

# QUERYING MULTIPLE GRAPHS

A working  
memory view



Pham, Trang, Truyen Tran, and Svetha Venkatesh. "Relational dynamic memory networks." *arXiv preprint arXiv:1808.04247*(2018).

# VIDEO QA: OUR NEW STOTA RESULTS

Repetition Count



Question: How many times does the man kick his legs?

Preds: (GT) 6    **(ST-TP) 4**    (Ours) 6

Repeating Action



Question: What does the man do 5 times?

Preds: (GT) shake finger    **(ST-TP) turn**    (Ours) shake finger

State Transition



Question: What does the man do after squat?

Preds: (GT) stretch hand out    **(ST-TP) inhale**    (Ours) stretch hand out

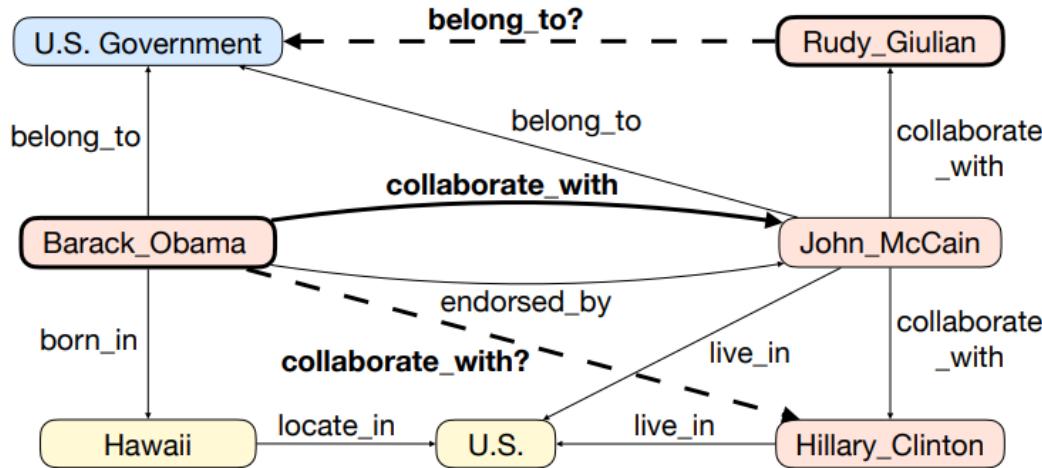
Frame QA



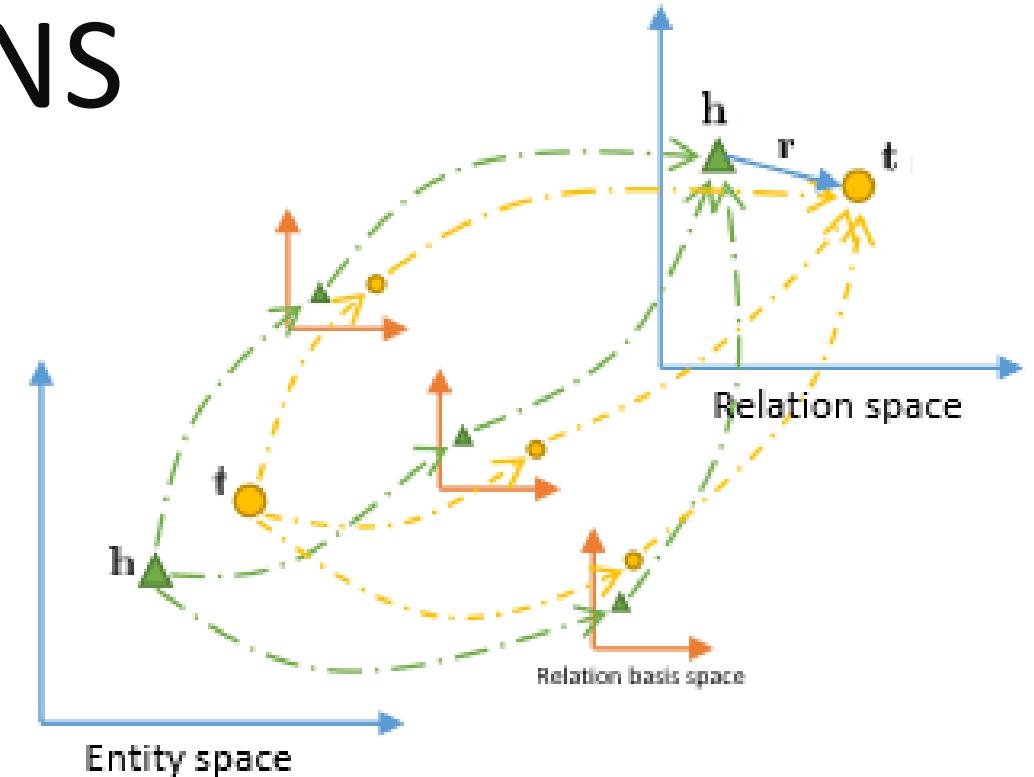
Question: what is having its head rubbed ?

Preds: (GT) bird    **(ST-TP) dog**    (Ours) bird

# INFERRING RELATIONS



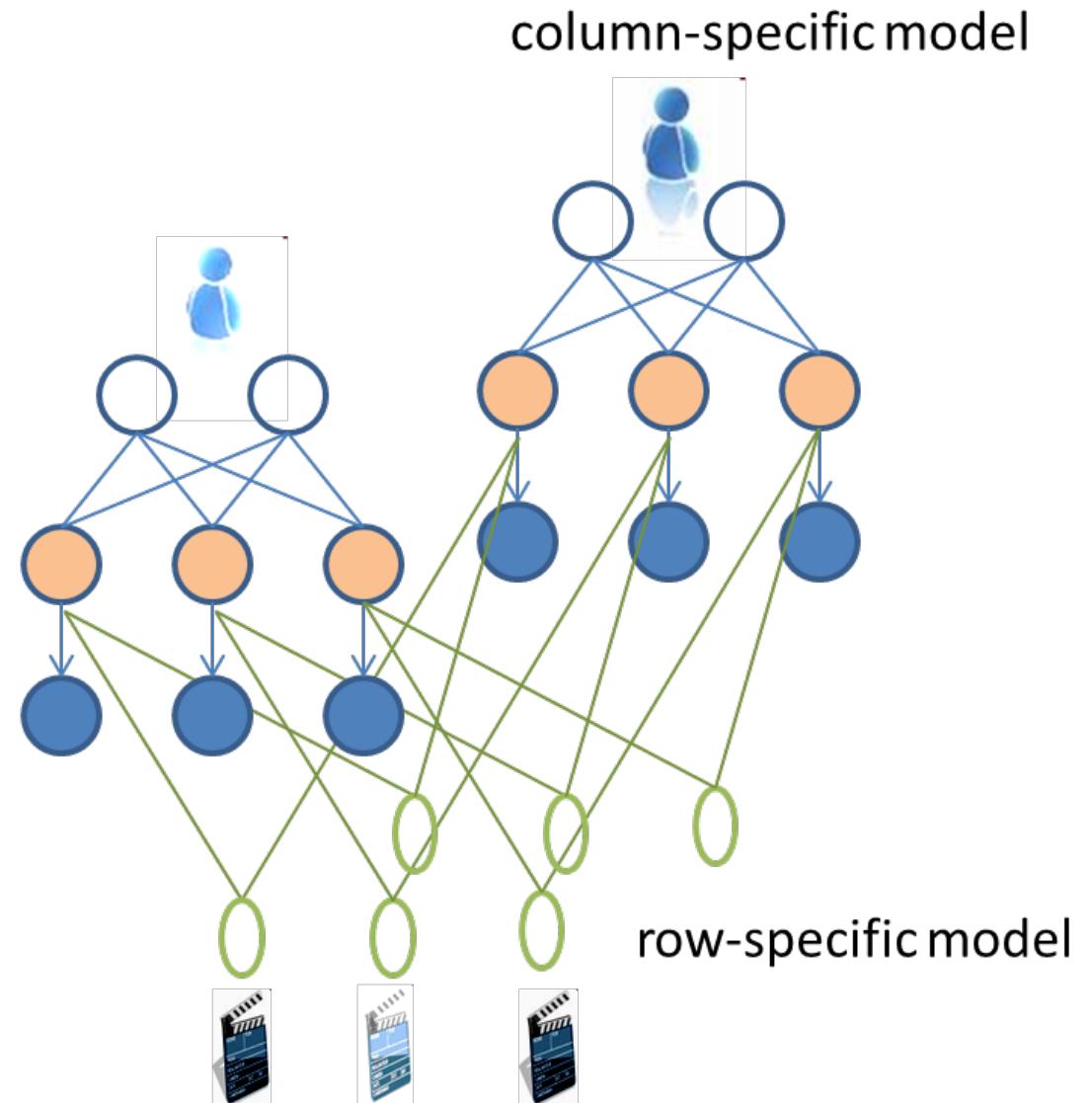
<https://www.zdnet.com/article/salesforce-research-knowledge-graphs-and-machine-learning-to-power-einstein/>



Do, Kien, Truyen Tran, and Svetna Venkatesh. "Knowledge graph embedding with multiple relation projections." 2018 24th International Conference on Pattern Recognition (ICPR). IEEE, 2018.

# LEARNING WITH LESS LABELS

- A hallmark of intelligence.
- Representation learning
- Deep generative models
- Continual learning



# WORKS DONE

Restricted Boltzmann machines  
(2009-2016)

- Bimodal RBM (UAI'09)
- Mixed-variate RBM (ACML'11)
- Ordinal matrix RBM (ACML'12)
- Tensor-variate RBM (AAAI'15)

Continual learning, solve  
catastrophic forgetting (on going)

Deep generative models

- GAN as continual learning (ICML'18 workshop)
- Generalization and stability analysis of GAN (ICLR'19)
- Inverse design (SDM'19)
- **Learn within supported domain, and explore unsupported domain at the same time (on going)**

# DEEP REINFORCEMENT LEARNING

New priors

RL equipped with memory

Multi-agent RL

Relational reasoning

Theory of AI/machine mind

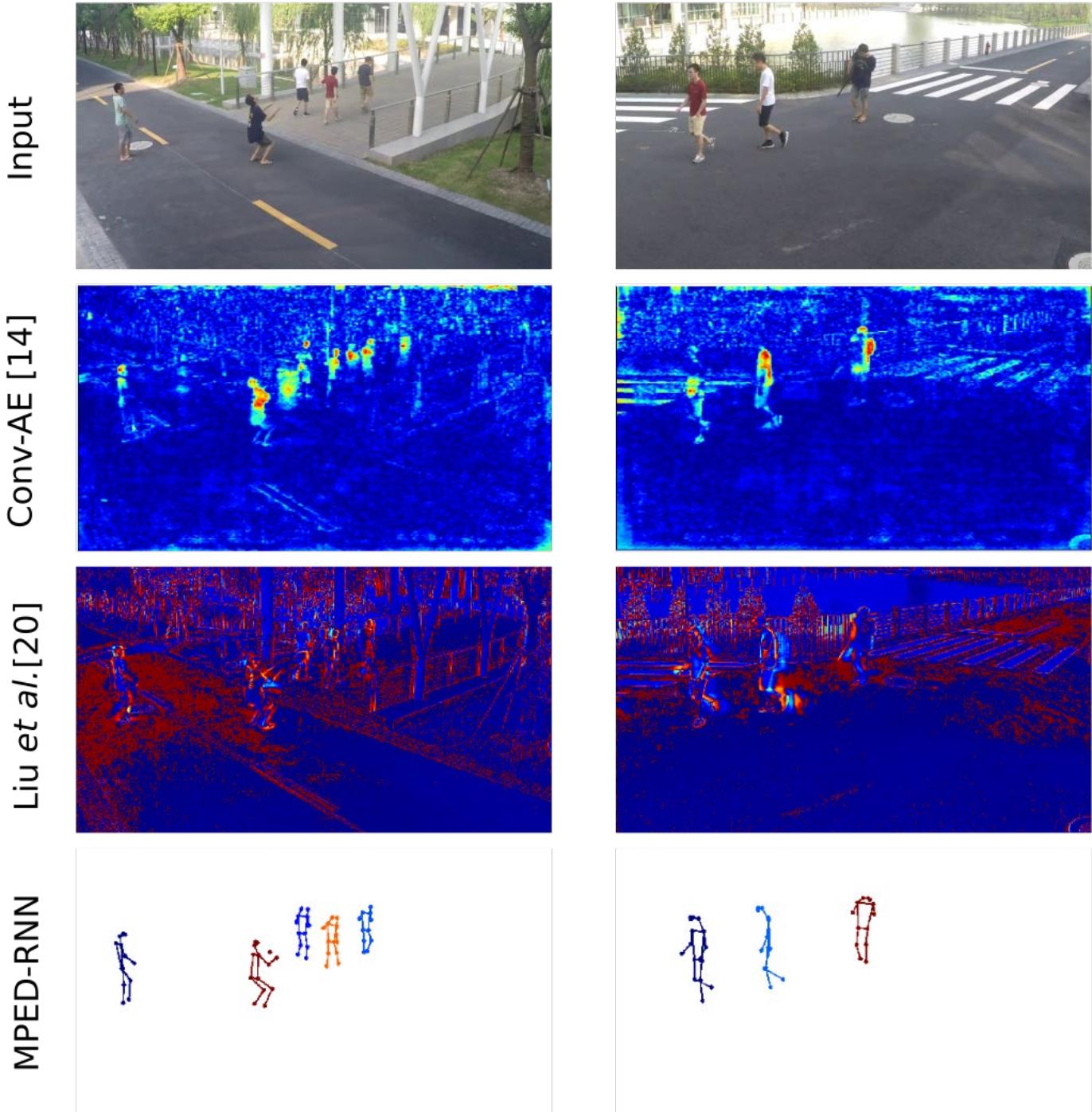
Psychological games

RL for structured prediction

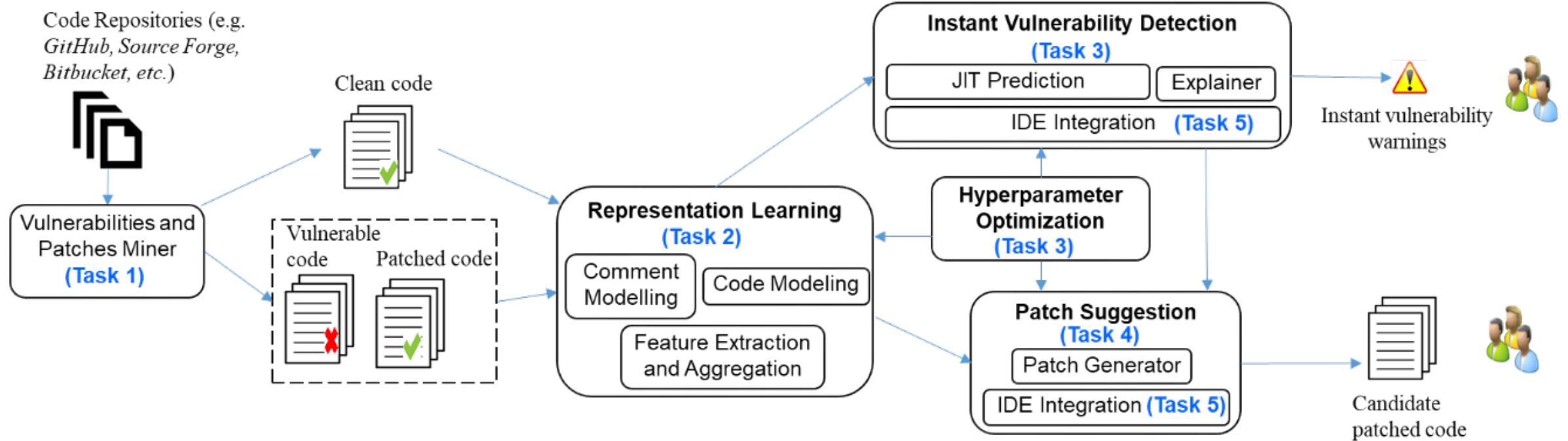
# HUMAN BEHAVIOUR UNDERSTANDING

CVPR'19

12/05/2019



# AI FOR AUTOMATED SOFTWARE ENGINEERING



# WORKS DONE

Project delay prediction with deep networked classification (ASE'15)

Code language model with LSTM (FSE'16 WS)

Defect prediction with Tree-LSTM (MSR'19)

Unsupervised feature learning for vulnerability detection (TSE, 2019)

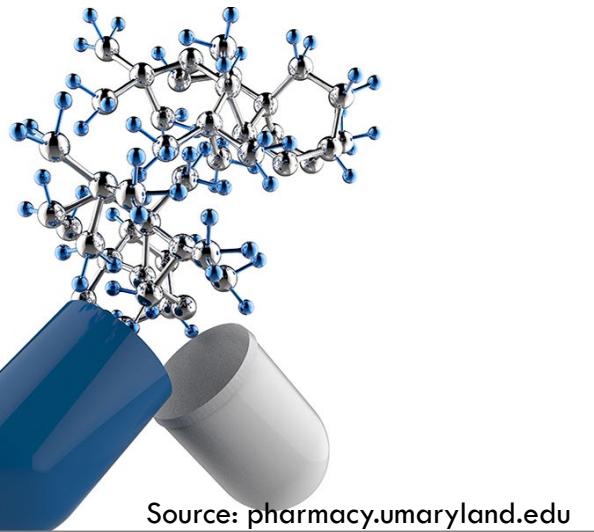
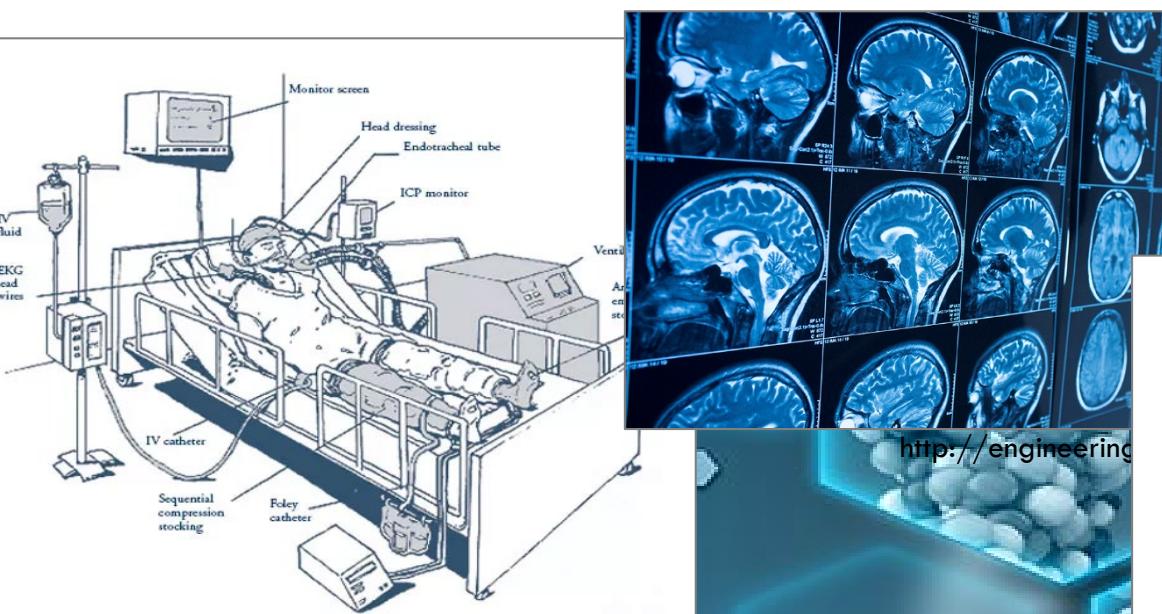
Deep learning for story point estimation (TSE, 2018)

Graph with virtual nodes for software code modelling (IJCAI'17 WS)

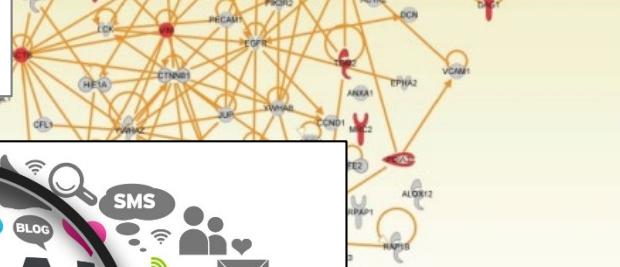
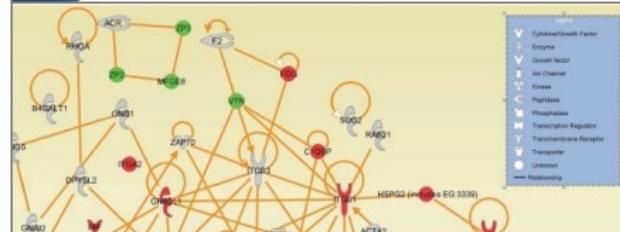
Code repair (on going)

Code translation (on going)

Program synthesis (on going)



Source: [pharmacy.umaryland.edu](http://pharmacy.umaryland.edu)



[openi.nlm.nih.gov](http://openi.nlm.nih.gov)



# AI FOR BIOMEDICINE



[marketingland.com](http://marketingland.com)

# CONTEXT

## 2012-2016: Health focused

- Electronic Medical Records, ICU, EEG/ECG
- Social media health, wearable devices
- Intervention tools (Toby PlayPad)



## 2017-present: Genomics focused

- Cell functions modelling
- Drug bioactivity prediction
- Drug response against gene expressions
- BioNLP: Natural Language Processing for biology



## 2017-present: PAGI - Program in Advanced Genomic Investigation

- Deakin + Garvan Partnership
- “Big Data” machine learning approach to genomics
- Leveraging computing power to crunch data
- Whole-genome sequencing



# CONVERSATIONAL AI

Memory-augmented chatbot

Lifelong conversational agent

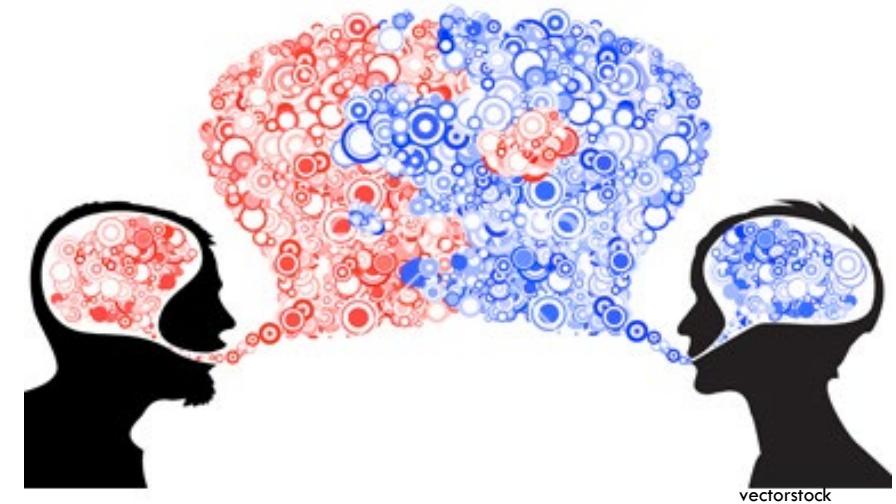
Chatbot with persona and ethics

Chatbot with theory of human mind

Multi-agent communication

Learning from instructions

Clinical dialog systems



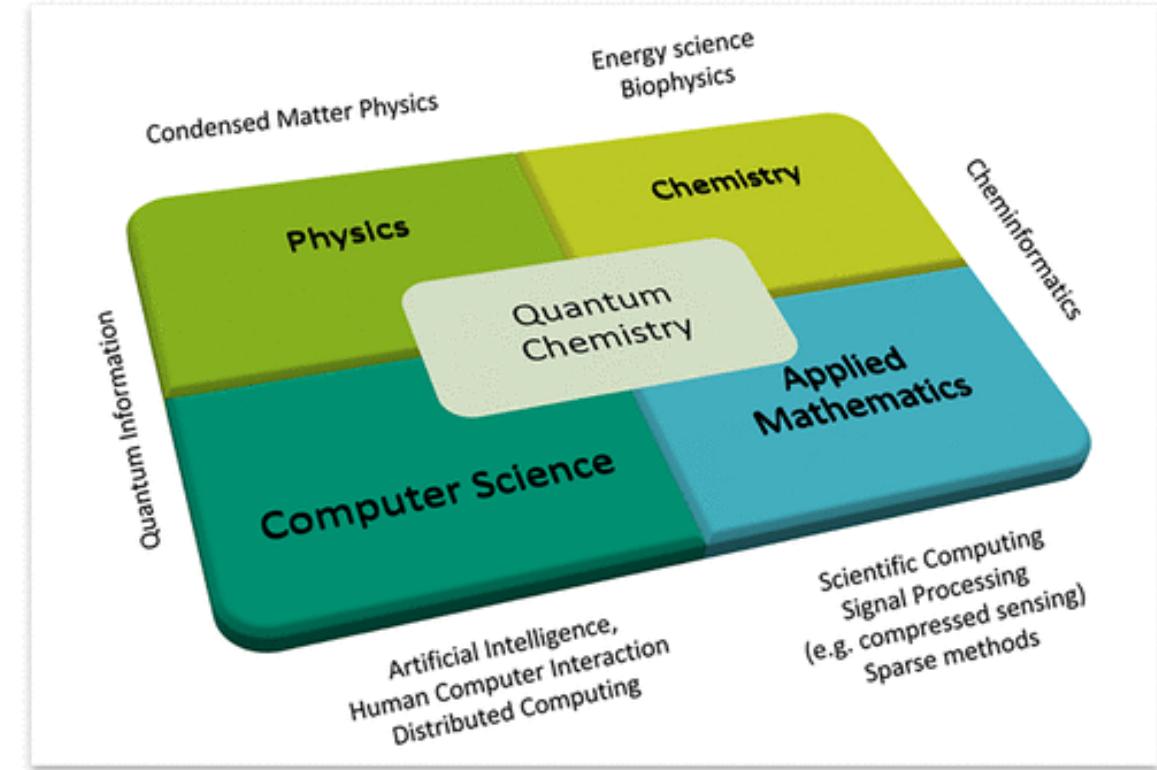
vectorstock

# VARIATIONAL MEMORY ENCODER DECODER, NIPS'18

Input context	Response
<b>Reddit comment:</b> What is your favorite scene in film history ? Mine is the restaurant scene in the Godfather.	<b>Seq2Seq:</b> The scene in <b>Seq2Seq-att:</b> The final <b>DNC:</b> The scene in <b>CVAE:</b> Inception god! Not by a shark /* Amour great /* Pro thing you know 3 dead <b>VMED (K=3):</b> The opening scene from history movie /* The scene in a shot nights! Robin movie /* The psycho scene in fight from
<b>Reddit comment:</b> What actor will win an Oscar in the next 10 years ?	<b>Seq2Seq:</b> Colin <b>Seq2Seq-att:</b> Liam Neeson <b>DNC:</b> Tom Gyllenhaal <b>CVAE:</b> Daryl and Aaron /* Carefully count Alfred Deniro /* Ponyo Joker possible <b>VMED (K=3):</b> Edward or Leo Dicaprio goes on /* Dicaprio will /* Dicaprio Tom has actually in jack on road

# AI for molecules

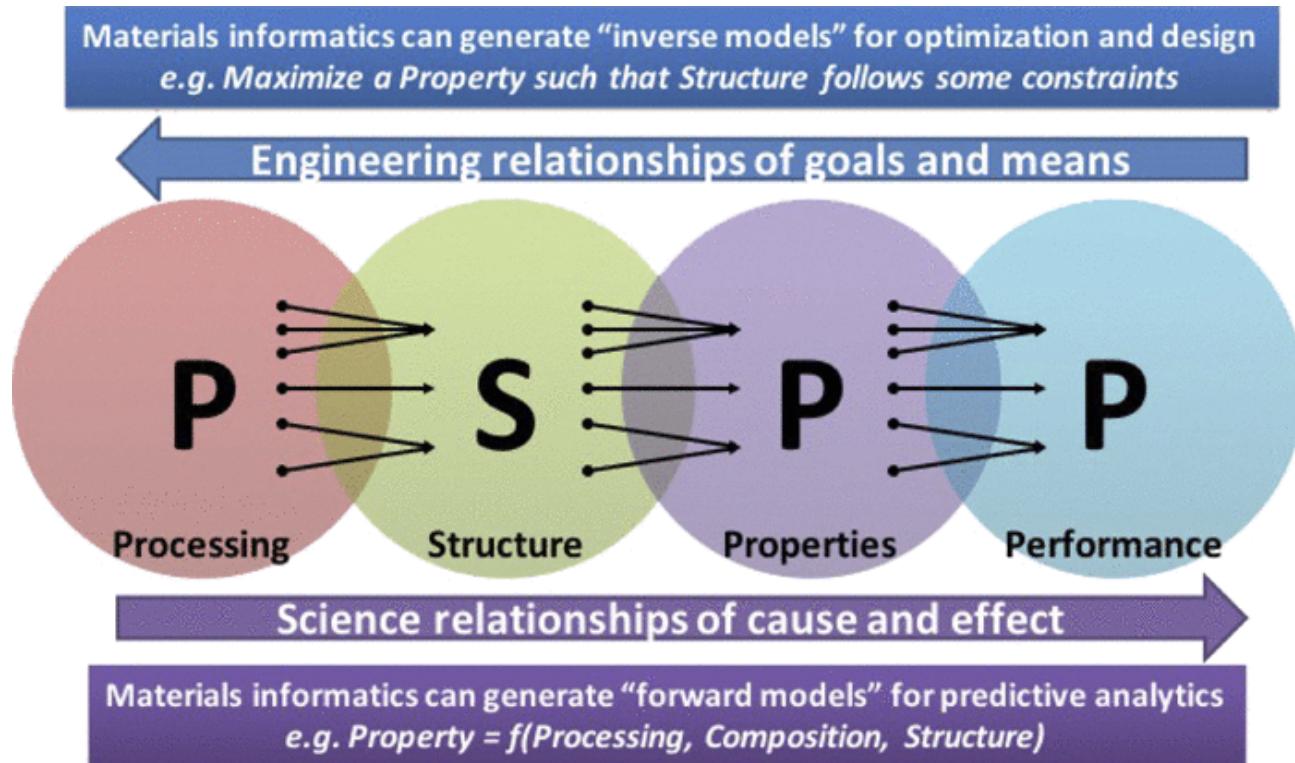
- Represent atom/molecular space
- Predict molecular properties
- Estimate chem-chem interaction
- Predict chemical reaction
- Fast search for new molecules
- Plan chemical synthesis



<https://pubs.acs.org/doi/full/10.1021/acscentsci.7b00550>

# AI for materials

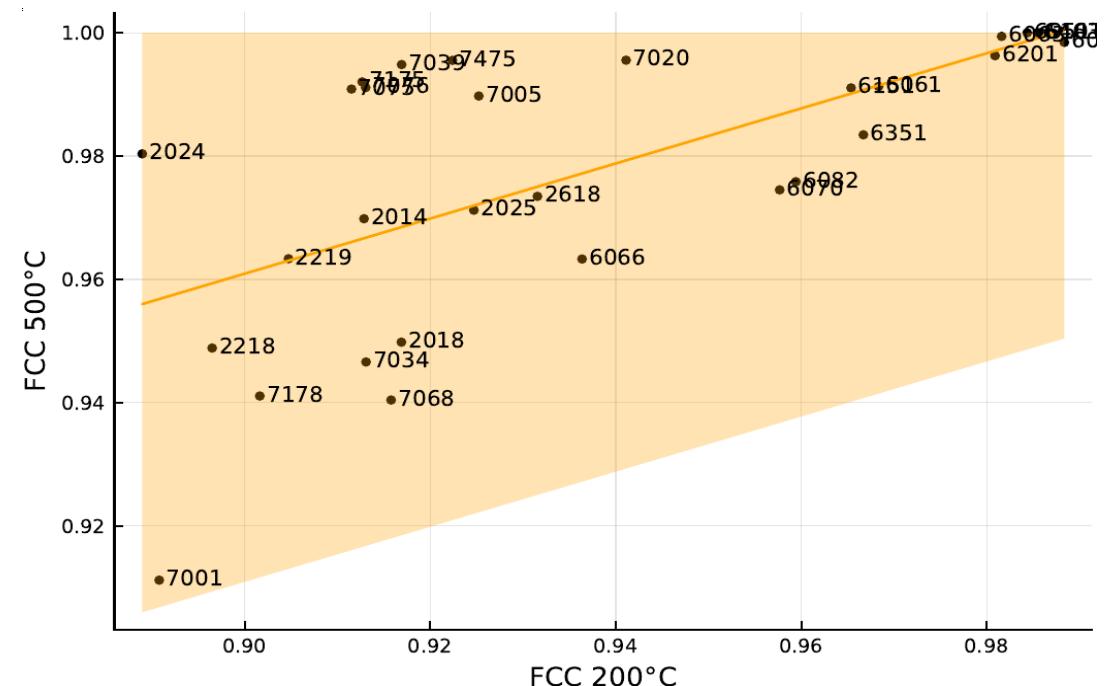
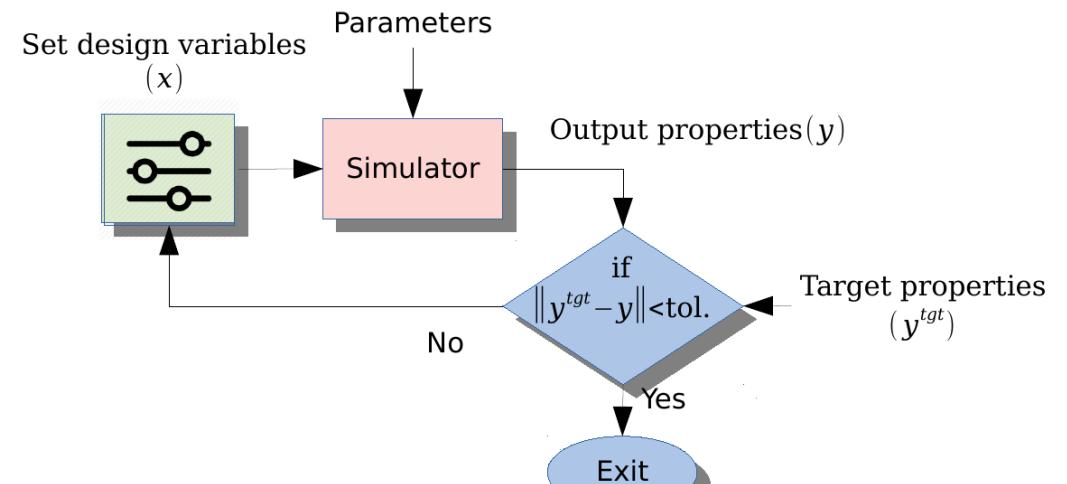
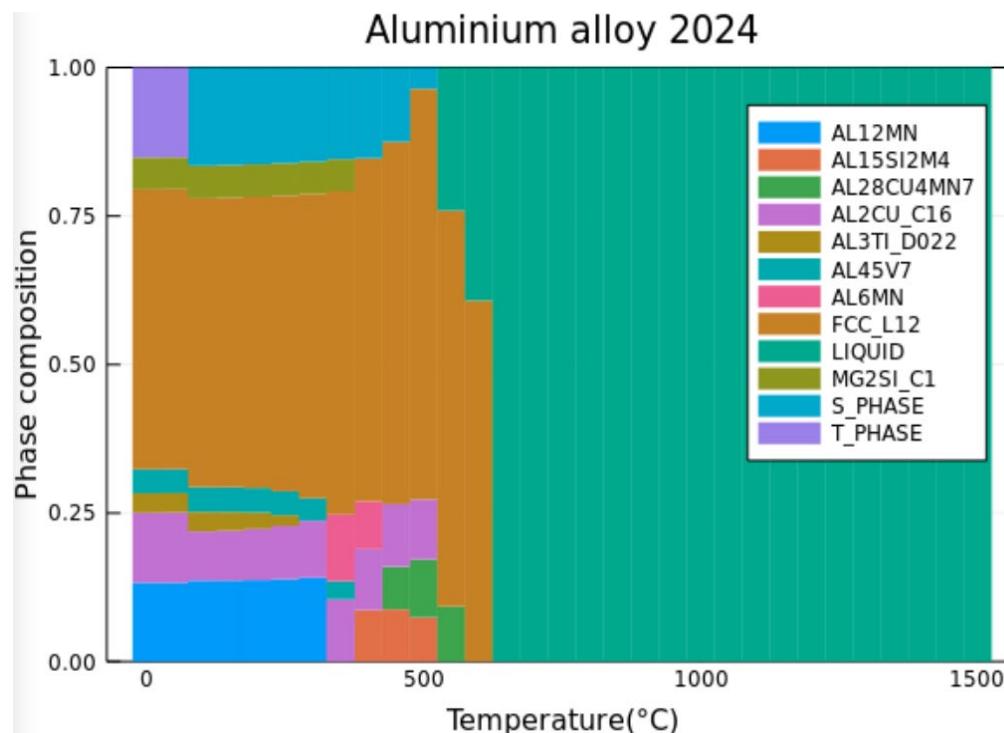
- Characterise the space of materials
- Represent crystals
- Map alloy composition → phase diagram
- Inverse design: Map phase diagram → alloy composition
- Generate alloys
- Optimize processing parameters



Agrawal, A., & Choudhary, A. (2016). Perspective: Materials informatics and big data: Realization of the “fourth paradigm” of science in materials science. *Appl Materials*, 4(5), 053208.

# Alloy space exploration

- Scientific innovations are expensive
- One search per specific target
- Availability of growing data



# BUILDING A SMARTER HOME

## **Short-term:** Anomaly detection

- Trajectories modelling with spatio-temporal models under irregular timing
- Fast adapting to changing condition
- Robust against noise

## **Mid-term:** A conversational agent that understands context and history

- Agents with episodic memory
- Contextual reasoning
- Knowledge and commonsense

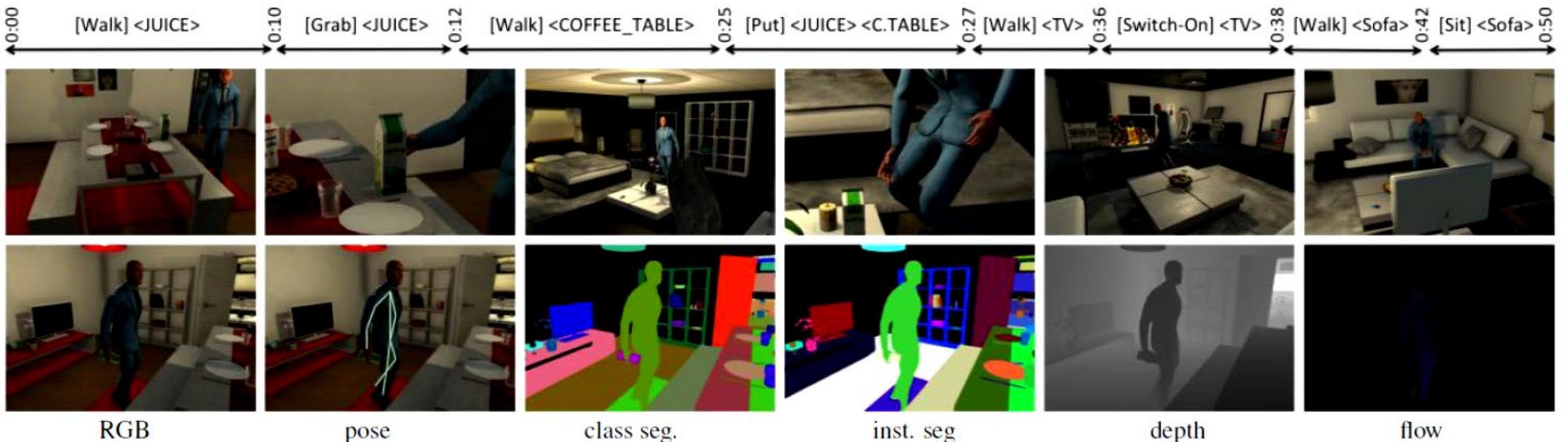
## **Long-term:** Developing a lifelong digital companion

- Lifelong learning
- Theory of human mind



# A NOVEL, CONTEXT-AWARE, UNSUPERVISED LEARNING PLATFORM TO LEVERAGE SENSING AND ANOMALY DATA

**Description:** Bring some juice to the coffee table, and relax by watching television from the sofa in the living room.



#REF: Puig, Xavier, Kevin Ra, Marko Boben, Jiaman Li, Tingwu Wang, Sanja Fidler, and Antonio Torralba. "VirtualHome: Simulating Household Activities via Programs." In CVPR. 2018.

# NEW DEEP GENERATIVE MODELS FOR SMART-HOME SENSORY DATA

**Represent, learn and infer about human activities:**

- Infer person's locations
- Count and disambiguate multiple persons (residents and visitors)
- Recognise interwoven and concurrent activities
- Detect anomalies

**Model multi-resolution activities from multi-modal, noisy sensory data.**

- Integrate temporal resolutions (minutes to months) & spatial resolutions (person bounding box to entire home).

**Handle (dynamic) contexts in a residential care.**

- Adapt automatically without human intervention.

# KEY TECHNICAL CHALLENGES

- Learning from minimal, unobtrusive sensing;
- Incremental, lifelong unsupervised learning with sparse, delayed feedbacks;
- Robustly handling spurious anomalies that arise from routine environmental signals (e.g. pets, outside light changes, wind, etc.);
- Transfer from simulated home to real home.

# VALUE-ALIGNED MACHINE LEARNING

Value regularisation in the context of conversational AI

Personalised values

Value-centric multi-agent communication

Theory of others' values

Learning to reason legally with values



Thank you!

We're hiring

PhD & Postdocs

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