

Towards compositional understanding of the world by deep learning Yoshua Bengio

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Current AI is far from Human-Level AI

- Sample complexity is high for supervised learning, even more for RL
 - Real-world actions can be lethal, experience is limited & costly
 - We don't have a good simulator of the real world (esp. involving humans)
- High-level concepts provided by human designers or labelers
- Errors made by trained systems reveal that their 'understanding' is very shallow and superficial
- The dream of deep learning discovering and disentangling high-level explanatory variables is far from achieved



Learning Multiple Levels of Abstraction

(Bengio & LeCun 2007)

- The big payoff of deep learning is to allow learning higher levels of abstraction
- Higher-level abstractions would disentangle the factors of variation, which allows much easier generalization, transfer, reasoning, and language understanding
- These factors are composed to form observed data



How to Discover Good Disentangled Representations

- How to discover abstractions?
- What is a good representation? (Bengio et al 2013)
- Need clues (= priors) to help disentangle the underlying factors (not necessarily statistically independent), such as
 - Spatial & temporal scales
 - Marginal independence
 - Simple dependencies between factors
 - Consciousness prior
 - Causal / mechanism independence
 - Controllable factors





System 1 vs System 2 Cognition

Two systems (and categories of cognitive tasks):

- System 1
 - Cortex-like (state controller and representations)
 - intuitive, fast heuristic, UNCONSCIOUS, non-linguistic
 - what current DL does quite well
- System 2
 - Hippocampus (memory) + prefrontal cortex
 - slow, logical, sequential, CONSCIOUS, linguistic, algorithmic
- what classical symbolic AI was trying to do
- Grounded language learning: combine both systems

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



Compositionality to bypass 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 can give an **exponential** gain in representational power

Distributed representations / embeddings: feature learning

Deep architecture: multiple levels of feature learning

Prior assumption: compositionality is useful to describe the world around us efficiently

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: humans are good at systematic generalization (e.g., combining known words in new ways unlikely under the training distribution)





The Need for Meta-Learning



Meta-Learning / Learning to Learn

- Generalize the idea of hyper-parameter optimization
 - Inner loop optimization (normal training), a fn of meta-params

$$\theta_t(\omega) = \operatorname{approxmin}_{\theta} C(\theta, \omega, \mathcal{D}_{train}^t)$$

• Outer loop optimization (meta-training), optimize meta-params

$$\omega = \operatorname{approxmin}_{\omega} \sum_{t} L(\theta_t(\omega), \omega, \mathcal{D}_{test}^t))$$

 Meta-parameters can be the learning rule itself (Bengio et al 1991; Schmidhuber 1992), learn 2 optimize

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- Meta-learn an objective or reward function, or a shared encoder
- Meta-learning can be used to learn to generalize or transfer
- Can backprop through $\,\, heta_t$, use RL, evolution, or other tricks

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Learning to Generalize and Adapt End-to-End

- We can optimize through the sequence
 - see regular training data (and learn from it)
 - see (a few) out-of-distribution examples (and optionally fine-tune / adapt to them)
- if these steps involve some meta-parameters which can be tuned so that we optimize the generalization performance in the second step
 - 0-shot generalization = out-of-distribution generalization
 - k-shot generalization: the learner is allowed to use a few examples of the modified distribution, we are doing transfer learning
 transfer learning





Beyond iid: Hypotheses about how the environment changes, Independent Mechanisms and the Small Change Hypothesis

- Independent mechanisms:
 - changing one mechanism does not change the others (Peters, Janzig & Scholkopf 2017)
- Small change:
 - Non-stationarities, changes in distribution, involve few mechanisms at a time (e.g. the result of a single-variable intervention)
- How can we discover these independent mechanisms, i.e., factor knowledge?



The Need for Sparsely Interacting Modules



On the Relation between Abstraction, Thought and Attention

- A thought is a low-dimensional object, few aspects of the state
- Attention allows us to focus on a few elements out of a large set
- Soft-attention allows this process to be trainable with gradient-based optimization and backprop

Attention focuses on a few appropriate abstract or concrete elements of mental representation





The Attention Revolution in Deep Learning

• Attention mechanisms exploit GATING units, have unlocked a breakthrough in machine translation:

Neural Machine Translation (ICLR'2015)



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The Consciousness Prior Bengio 2017, arXiv:1709.08568

- 2 levels of representation:
 - High-dimensional abstract representation space (all known concepts and factors) *h*
 - Low-dimensional conscious thought *c*, extracted from *h*



Why do I call it a Prior?

- There is something very special about the kind of high-level variables which we manipulate with language:
 - we can predict some given very few others
 - E.g. "if I drop the ball, it will fall on the ground"
 - corresponds to a sparse factor graph
 - Each factor captures an independent piece of knowledge
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- Strong interactions between few variables

 $P(V) \propto \prod \phi(V_{s_k})$ where V_{s_k} is the subset of Vwith indices s_k

Learn Generative Models in Latent Space, not Pixel Space

- For human-like brains, generative models are useful for planning (**model-based RL**), imagination, counterfactuals, inference over causes and explanations, high-level credit assignment
 - NONE OF THIS REQUIRES WORKING IN PIXEL SPACE
- Current generative models are trained wrt pixel-space objectives, how to train purely in the space of abstract representations? We want the encoder mapping pixel space to abstract space to be trained wrt the high-level goals too.
- There is an issue of possible collapse of representations if we maximize predictability (e.g. max likelihood) in latent space





Deep InfoMax or DIM (Hjelm et al & Bengio ICLR 2019)

Integrating System 1 and System 2

- System 2 model is very coarse and imperfect, unlike system 1
- System 2 abstract concepts need to be grounded via system 1
- System 2 thinking allows counterfactual reasoning, i.e., imagining scenarios which did not and will not happen, as an exercise (e.g. for credit assignment, if I had done that...), allows generalization far from the training data, imagine dangerous scenarios without having to take the actual risks
- System 2 is too slow and inefficient, compile to system 1 into habits and intuitive behavior



Separating Knowledge in Small Re-Usable Pieces

- Pieces which can be re-used combinatorially
- Pieces which are stable vs nonstationary, subject to interventions



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Wrong Knowledge Factorization Leads to Poor Transfer

- With the wrong factorization P(B) P(A|B), a change in ground truth P(A) influences both modules, all the parameters
 - poor transfer: all the parameters must be adapted
- This is the normal situation with standard neural nets: every parameter participates to every relationship between all the variables
 - this causes catastrophic forgetting, poor transfer, difficulties with continual learning or domain adaptation, etc



Recurrent Independent Mechanisms

Goyal et al, arXiv:1909.10893

Multiple recurrent sparsely interacting modules, each with their own dynamics, with object (key/value pairs) input/outputs selected by multihead attention



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Recurrent Independent Mechanisms

Goyal et al, arXiv:1909.10893

Copyin k _T	ng	k_{A}	$h_{ m size}$	Train(50) CE	Test(200) CE	Sequenti k _T	ial I	$\frac{\mathbf{MNIS}}{k_{\mathrm{A}}}$	\mathbf{ST} h_{size}	16 x 16 Accuracy	19 x 19 Accuracy	24 x 24 Accuracy
RIMs	6 6 6	5 4 3 2	600 600 600 600	0.01 0.00 0.00 0.00	3.5 0.00 0.00 0.00	RIMs	6 6 6	6 5 4	600 600 600	85.5 88.3 90.0	56.2 43.1 73.4	30.9 22.1 38.1
	5	3	500 300	0.00	0.00	LSTM	-	-	300 600	86.8 84.5	42.3 52.2	25.2 21.9
LSTM	-	-	600	0.00	3.56	EntNet	-	-	-	89.2	52.4	23.5
NTM DMC	-	-	-	0.00	2.54	RMC	-	-	-	89.58	54.23	27.75
KMC Transf	- orm	- ers -	-	0.00	0.13	DNC Transfor	- rme	- rs -	-	87.2 91.2	44.1 51.6	19.8 22.9

RIMs generalize better than SOTA methods for sequential learning to out-of-distribution data (longer sequences, larger images).



The Need for Causal Understanding



Learning « How the world ticks »

- So long as our machine learning models « cheat » by relying only on superficial statistical regularities, they remain vulnerable to out-of-distribution examples
- Humans generalize better than other animals thanks to a more accurate internal model of the **underlying causal relationships**
- To predict future situations (e.g., the effect of planned actions) far from anything seen before while involving known concepts, an essential component of reasoning, intelligence and science

Deep Learning Objective: discover high-level representation capturing cause and effect variables

- What are the right representations?
 - Causal variables explaining the data
 - Pixels are not causal variables
- How to discover them? (learn the mythical encoder)
- How to discover their causal relationship, the causal graph?



Turning a Hindrance into a Useful Signal

ArXiv paper, Bengio et al 2019: A Meta-Transfer Objective for Learning to Disentangle Causal Mechanisms

- Changes in distribution (nonstationarities in agent learning, transfer scenarios, etc) are seen as a bug in ML, a challenge
- Turn them into a feature, an asset, to help discover causal structure, or more generally to help **factorize knowledge**:
- Tune knowledge factorization (e.g. causal structure) to maximize fast transfer
- "Nature does not shuffle environments, we shouldn't" L. Bottou



Small Change → Small Sample Complexity

Few parameters need to change \rightarrow small L2 change \rightarrow few examples needed to recover from the change



Under the right parametrization *→* fast adaptation to interventions



Empirical Confirmation: Correct Causal Structure Leads to Faster Adaptation



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 $A \rightarrow B$ is the structure: faster online adaptation to modified distribution = lower NLL

A Novel Approach to Causality: Disentangling the Causes

Bengio et al 2019: A Meta-Transfer Objective for Learning to Disentangle Causal Mechanisms

- Realistic settings: causal variables are not directly observed
- Need to learn an encoder which maps raw data to causal space
- Consider both the encoder parameters and the causal graph structural parameters as meta-parameters trained together wrt proposed meta-transfer objective





Experiments successful in 2-D with simple linear mappings, Bengio et al 2019.

Learning Neural Causal Models from Unknown Interventions: Avoiding Super-exponential Search

Ke et al & Bengio arXiv:1910.01075

- Most causal induction methods search over super-exponential number of possible graphs
 Difficult to scale to larger graphs
- How to bypass the super-exponential search?
 Learn ensemble of structured causal models (SCM)
 - More efficient, does not have to search through superexponential set of possible DAGs.



Multivariate Categorical MLP Conditionals



Comparative Results

Asia graph, CE on ground truth edges, comparison against other causal induction methods

Our method	(Eaton & Murphy, 2007a)	(Peters et al., 2016)	(Zheng et al., 2018)
0.0	0.0	10.7	3.1

Evaluating the consequences of a previously unseen intervention

	fork3	chain3	confounder3	collider3
Our Model	-0.4502	-0.3801	-0.2819	-0.4677
Baseline	-0.5036	-0.4562	-0.3628	-0.5082

Ke et al & Bengio arXiv:1910.01075 Learning Neural Causal Models from Unknown Interventions



Observing Other Agents

- Can infants figure out causal structure in spite of being almost passive observers?
- Yes, if they exploit and infer the interventions made by other agents
- Our approach does not require the learner to know what the action/intervention was (but it could do inference over interventions)
- But more efficient learning if you can experiment and thus test hypotheses about cause & effect



The Need for the Agent Perspective in Deep Learning



The Agent Perspective for Deep Learning

- Classical deep learning and ML only considered a fixed data distribution
- Agents can modify their environment through their actions
- There may be multiple agents, also leading to non-stationarities, changing distribution
- Difficult to generalize out-of-distribution
- Need for the agents to "really understand" their environment
- Acting purposely can help to gather knowledge, discover good representations



Jointly Learning Natural Language and a World Model

- Should we first learn a world model and then a natural language description of it?
- Or should agents jointly learn about language and about the world?
- I lean towards the latter.
- Consider top-level representations from supervised ImageNet classifiers. They tend to be much better and easier to learn than those learned by unsupervised learning. Why?
- Because language (here object categories) provides to the learner clues about relevant semantic high-level factors from which it is easier to generalize.
- See my earlier paper on cultural evolution, which posits that culture can help a learner escape from poor optimization, guide (through curricula) the learner to better explanations about the world.

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Grounded Language Learning

BabyAl Platform Chevalier-Boisvert et al & Bengio ICLR 2019

Purpose: simulate language learning from a human and study data efficiency

Comprises:

- a gridworld with partial observability (Minigrid)
- a compositional natural-looking Baby language with over 10^19 instructions
- 19 levels of increasing difficulty
- a heuristic stack-based expert that can solve all levels



(b) PutNextLocal: "put the blue key next to the green ball"

github.com/mila-udem/babyai



Early Steps in Baby AI Project



(a) GoToObj: "go to the blue ball"



(b) PutNextLocal: "put the blue key next to the green ball"





(c) BossLevel: "pick up the grey box behind you, then go to the grey key and open a door". Note that the green door near the bottom left needs to be unlocked with a green key, but this is not explicitly stated in the instruction.

- Designing and training experts for each level, which can serve as teachers and evaluators for the Baby AI learners
- Partially observable, 2-D grid, instructions about objects, locations, actions

go to the red ball

open the door on your left

put a ball next to the blue door

open the yellow door and go to the key behind you

put a ball next to a purple door after you put a blue box next to a grey box and pick up the purple box

Acting to Guide Representation Learning & Disentangling



(E. Bengio et al, 2017; V. Thomas et al, 2017; more recently see Warde-Farley et al ICLR 2019, Kim et al ICML 2019)

- Some factors (e.g. objects) correspond to 'independently controllable' aspects of the world
 - Corresponds to maximizing mutual information between intentions (goalconditioned policies) and changes in the state (trajectories), conditioned on the current state.
- Can only be discovered by acting in the world
 - Control linked to notion of objects & agents

Causal but agent-specific & subjective: affordances
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Four Tools for More Compositional Deep Learning

- 1. Meta-Learning (to adapt quickly to changes in distribution)
- 2. Sparsely interacting mechanisms at the top level (consciousness prior)
- 3. High-level variables are causal and their dependencies are represented in a modular way
- 4. System 1 and system 2 together actively acquire a world model and corresponding semantic concepts (grounded language learning), can be composed for reasoning and planning, and representations of actions and state are linked (affordances)



Looking Forward

- Build a world model which meta-learns causal effects in abstract space of causal variables, able to quickly adapt to changes in the world and generalize out-of-distribution
- Acting to acquire that knowledge (exploratory behavior)
- Bridging the gap between system 1 and system 2, old neural nets and conscious reasoning, all neural

