Learning Interpretable Concepts in Deep Learning: Desiderata from Causality and Neuro-Symbolic Reasoning Shortcuts

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SOTA Deep Learning models are Black-boxes

- High-dimensional, sub-symbolic inputs
- ✓ Learn from IID
- ✓ High performance in specific tasks

- X Not self-explainable
- X Cannot learn over time
- **X** Bad performances on OOD generalization



Concept Bottleneck Models

Pang Wei Koh^{*1} Thao Nguyen^{*12} Yew Siang Tang^{*1} Stephen Mussmann¹ Emma Pierson¹ Been Kim² Percy Liang¹

Abstract

We seek to learn models that we can interact with using high-level concepts: if the model did not think there was a bone spur in the x-ray, would it still predict severe arthritis? State-of-the-art models today do not typically support the manipulation of concepts like "the existence of bone spurs", as they are trained end-to-end to go directly from raw input (e.g., pixels) to output (e.g., arthritis severity). We revisit the classic idea of first predicting concepts that are provided at training time, and then using these concepts to predict the label. By construction, we can intervene on these concept bottleneck models by editing their predicted concept values and propagating these changes to the final prediction. On x-ray grading and bird identification, concept bottleneck models achieve competitive accuracy with standard end-to-end models, while enabling interpretation in terms of high-level clinical concepts ("bone spurs") or bird attributes ("wing color"). These



Figure 1. We study concept bottleneck models that first predict an intermediate set of human-specified concepts c, then use c to predict the final output y. We illustrate the two applications we consider: here x-ray grading and bird identification.

(Source: [1] Also: Concept Whitening [2])

- Concepts are "sparse"
- Concepts are "orthogonal"
- Concepts "activate highly" on concrete training examples
- Concepts "activate highly" on *parts of* training examples

Problems

Learn with label and concept supervision (concepts are specific for the application)

X The label/concept accuracy trade-off (supervision on concepts?)

X Spurious correlations in the learned concepts (aka Concept Leakage)

Promises and Pitfalls of Black-Box Concept Learning Models

Anita Mahinpei^{*1} Justin Clark^{*1} Isaac Lage¹ Finale Doshi-Velez¹ Weiwei Pan¹

Abstract

.G] 24 Jun 2021

Machine learning models that incorporate concept learning as in intermediate steps in their decision making process can match the performance of black-box predictive models while reating the ability to explain outcomes in human undextandable terms. However, we demonstrate that like concept representations learned by these models models information beyond the pre-defined conepts, and that matraff miligation strategies do be for the strategies of the strategies of the strategies and that matraff miligation strategies to be for the strategies of Leach et al. (2019). In each case, the neural network model learns to map raw input to concepts and them map those concepts to predictions. We call the mapping from input to concepts a Concept Learning Model (CHA), although this mapping may not always be trained independently from the downstream prediction task. Models that incorporate a CLM component have been shown to match the performance of complex black boxe predictions models with training the competition in the prediction models with training the docision in terms or informediate concepts.

Unfortunately, recent work noted that black-box CLMs do not learn as expected. Specifically, Margeloiu et al. (2021) demonstrate that outputs of CLMs used in Concept Bottle-

DO CONCEPT BOTTLENECK MODELS LEARN AS INTENDED?

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Yanzhi Chen University of Edinburgh Mateja Jamnik University of Cambridge Adrian Weller University of Cambridge The Alan Turing Institute

ABSTRACT

Concept butlencek models map from raw inputs to concepts, and then from conexpts to targets. Such models and to incorporate pre-specifich, high-level concepts into the learning procedure, and have been motivated to meet three desiderates interpretability predictability, and intervenability. However, we find that concept bottlencek, models struggle to meet these goals. Using post hos interpretability meaningth in input space, thus calling into question the usefulness of concept bottlencek in delets in their current from.

(Source: [3, 4])

Neuro-Symbolic models make also use of concepts

■ Neuro-Symbolic (NeSy) models/predictors are deemed to be trustworthy due to compliance to prior-knowledge.

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1) **Perception:** Extract (binary) **concepts** to be input for the reasoning

(2) **Reasoning:** Perform probabilistic reasoning from the concepts

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(1) **Perception:** Extract (binary) concepts to be input for the reasoning

(2) **Reasoning:** Perform probabilistic reasoning from the concepts

Changing the knowledge we can use the same concepts to solve different tasks.

Trustworthiness claim

NeSy predictors are learned with input-output samples (typically no concept supervision)

Claim: this is sufficient to solve the *symbol grounding problem*:

integrating the knowledge \implies recovering the intended concepts ? (False)



- A traffic light cannot move,
- · If an agent is crossing, it is either a pedestrian or a cyclist.



How to make sure the learned concepts/representations are interpretable?

- 1. Interpretability in Representation Learning. What is an interpretable representation?
- 2. Reasoning Shortcuts (in NeSy AI). Do NeSy AI models learn the intended concepts?

Our Work

Accepted at NeurIPS 2022

GlanceNets: Interpretable, Leak-proof Concept-based Models

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Published in MDPI Entropy



MDPI

Arrive Interpretability Is in the Mind of the Beholder: A Causal Framework for Human-Interpretable Representation Learning

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Accepted at ICML 2023

Neuro-Symbolic Continual Learning: Knowledge, Reasoning Shortcuts and Concept Rehearsal

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Accepted at NeurIPS 2023

Not All Neuro-Symbolic Concepts Are Created Equal: Analysis and Mitigation of Reasoning Shortcuts

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Andrea Passerini DISI University of Trento Trento, Italy andrea.passerini@unitn.it Interpretability of the concepts



What is **concept interpretability**? If any change a makes to their **mental representation** impacts the machine representation in a way that they can **understand**, they **the two concepts share the same name**.

- The formalization includes the human
- Alignment for **non-disentangled repr**

Leakage is lack of context-style separation
Link to causal abstractions







The Naming Game



 \Box Several generative factors $\mathbf{G} = (G_1, \ldots, G_n)$, encoding hair color, age, complexion, ...



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 \Box Model acquires latent factors Z_1, \ldots, Z_k



■ Communication is possible ⇔ same semantics

 \Box Assume subset of generative factors G_1 are understandable to a human agent. For instance, G_1 = age, G_2 = hair color, G_3 = complexion.



Interpretability as alignment.

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Example: if α is **the identity**, then **Z**_{1:3} are by construction interpretable!



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Example: if α is permutes elements, then $\mathbf{Z}_{1:3}$ are by construction interpretable!



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Example: If α is rescales individual elements, then $\mathbf{Z}_{1:3}$ are by construction interpretable!



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 \Box How much can we push?



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□ How much can we push? Let's be conservative



Interpretability as alignment.

Alignment

The map *alpha* from ground-truth concepts to machine concepts:

(1) mixes no two generative factors into the same learned concept (disentanglement)

2) is elementwise monotonic.



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Interpretability as alignment.

Effect of *intervening* on observed G_1 or unobserved G_{-1} factors:





1) Fit two concepts to recognize MNIST images of "4"s and "5"s using full concept annotations



2 Concept Leakage = Unintended Semantics

1) Fit two concepts to recognize MNIST images of "4"s and "5"s using full concept annotations

2 Use the learned concepts, predict parity of remaining digits (i.e., all except "4" and "5")









GlanceNets = VAE + concept supervision





GlanceNets = VAE + concept supervision + **open-set rejection**







GlanceNets = VAE + concept supervision + **open-set rejection**




Metrics:

- Accuracy
- Alignment (linear DCI)
- **CelebA** w/ supervision for 6 generative factors, realistic labels obtained via clustering.

Same # of concepts for both GlanceNets and Concept Bottleneck models [4].



Learning the concepts/symbols in Neuro-Symbolic AI











Learning on (input,output) samples (annotation on concepts is costly!) like DeepProbLog [6], Semantic Loss [7], and Logic Tensor Networks [8]

Probably, you'd expect that...

Knowledge + supervision on labels constrain the concepts to acquire the **right semantics**, i.e., to be grounded correctly.

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"if my NeSy model predicts correct actions in all examples of autonomous driving, then the concepts are good! For instance, red_light = \top iff there is a red traffic light in the dashcam image!"

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"if my NeSy model predicts correct actions in all examples of autonomous driving, then the concepts are good! For instance, red_light = \top iff there is a red traffic light in the dashcam image!"

This would be ideal: concepts with the right semantics generalize to new tasks (as required by, e.g., NeSy verification [9]) and support interpretability.

 $K_1 = (pedestrian \lor red \Rightarrow stop)$



Task: predict stop vs. go using concepts "pedestrian", "red", and "green".

 $K_1 = (pedestrian \lor red \Rightarrow stop)$



Task: predict stop vs. go using concepts "pedestrian", "red", and "green".

Perfect accuracy by predicting pedestrians as red lights!!!

 $K_2 = (emergency \land \neg pedestrian \Rightarrow go) \land K_1$



■ Task: ... but now if there is an emergency, we can ignore "red" lights

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- 2. What are the root causes?
- 3. What are *natural* mitigation strategies?
- 4. Do RSs appear in real-world tasks?

Formalization (but not covered today :))

Data generation: $\mathbf{g} \in \mathcal{G} \subset \mathbb{N}^k$ and $\mathbf{s} \in \mathbb{R}^q$. The joint distribution is factorized $p(\mathbf{G})p(\mathbf{S})$ and there exist:

 $p^{*}(\mathbf{X} \mid \mathbf{G}, \mathbf{S}) \text{ and } p^{*}(\mathbf{Y} \mid \mathbf{G}; \mathsf{K})$ where $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^{n}$ and $\mathbf{y} \in \mathcal{Y} \subset \mathbb{N}^{\ell}$. Typically, $\ell < k$. Learning in DPL, with $\mathcal{C} = \mathcal{G}$: $p_{\theta}(\mathbf{Y} \mid \mathbf{X}; \mathsf{K}) = \sum_{\mathbf{c} \in \mathcal{C}} p^{*}(\mathbf{Y} \mid \mathbf{c}; \mathsf{K}) p_{\theta}(\mathbf{c} \mid \mathbf{X})$

trained with
$$\max_{ heta} \prod_{(\mathbf{x}, \mathbf{y}) \in \mathcal{D}} p_{ heta}(\mathbf{y} \mid \mathbf{x}; \mathsf{K})$$

Technical Assumptions:

A1 There exists invertible (and differentiable over s) $f : (\mathbf{g}, \mathbf{s}) \mapsto \mathbf{x}$ underlying $p^*(\mathbf{X} \mid \mathbf{G}, \mathbf{S}): p^*(\mathbf{x} \mid \mathbf{g}, \mathbf{s}) = \delta(\mathbf{x} - f(\mathbf{g}, \mathbf{s}))$

A2 The knowledge K is deterministic: there exists $\beta_{\mathsf{K}} : \mathbf{g} \mapsto \mathbf{y}$ such that $p^*(\mathbf{y} \mid \mathbf{g}; \mathsf{K}) = \mathbb{1}\{\mathbf{y} = \beta_{\mathsf{K}}(\mathbf{g})\}$



The data generation process.





- G are (binary or discrete) ground-truth concepts
- S are (real-valued) stylistic factors



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- We consider two key properties:
 - 1. Optimality when \mathbf{Y} is correct $\wedge \mathsf{K}$ is satisfied
 - 2. Intended Semantics when $(\forall x, c = g)$
- Def A Reasoning Shortcut (RS) occurs whenever the model achieves optimality but learns unintended concepts.



The NeSy model extracts C and computes Y.





 $\begin{array}{l} \mbox{Generative process} + \\ \mbox{the NeSy predictor.} \end{array}$



Every NeSy predictor entails a map α : $\mathbf{g} \mapsto \mathbf{c}$ from ground-truth to learned concepts. Ideally, it'd be the **identity**!



Map α entailed by a NeSy predictor.



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We consider those α 's that are optimal for the reasoning $\beta_{\kappa} : \mathbf{g} \mapsto \mathbf{y}$, underlying the prior knowledge.



Map α and knowledge $\beta_{\mathbf{K}}$.

$\widehat{1}$ How many Reasoning Shortcuts?

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Theorem (informal): # of Reasoning Shortcuts

Under assumptions ${}^{\rm TM}\!$, the # of these $\alpha{}'{\rm s}$ for NeSy predictors ${}^{\rm s}$ is:

$$\sum_{oldsymbol{lpha}\in\mathcal{A}}\mathbb{1}ig\{ig \wedge_{\mathbf{g}\in\mathsf{supp}(\mathbf{G})}(oldsymbol{eta}_{\mathsf{K}}\circoldsymbol{lpha})(\mathbf{g})=oldsymbol{eta}_{\mathsf{K}}(\mathbf{g})ig\}\geq 1$$





Map α and knowledge $\beta_{\mathbf{K}}$.

$$\begin{array}{c|c} \hline C1 + C2 = Y \\ \uparrow & \uparrow \\ \hline C_1 & C_2 \\ \uparrow & \uparrow \\ \hline nn & nn \\ \uparrow & 1 \\ \hline Z & 3 \\ \end{array} \rightarrow Y=5$$

Inference in DeepProbLog with the same neural network

$$\begin{cases} \mathbf{0} + \mathbf{1} = 1 \\ \mathbf{0} + \mathbf{2} = 2 \end{cases}$$

Problem. How many optimal solutions?

G	С
0•	•0
1•	•1
2•	•2

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Example: MNIST-Addition with few sums.





$$\sum_{oldsymbol{lpha}\in\mathcal{A}}\mathbb{1}ig\{igwedge_{\mathbf{g}\in\mathsf{supp}(\mathbf{G})}(oldsymbol{eta}_{\mathsf{K}}\circoldsymbol{lpha})(\mathbf{g})=oldsymbol{eta}_{\mathsf{K}}(\mathbf{g})ig\}\geq 1$$



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Causes of RSs can be read off of it:

 (\mathcal{K}) Structure of **knowledge** K, via β_{K}





$$\sum_{\boldsymbol{\alpha} \in \mathcal{A}} \mathbb{1} \Big\{ \bigwedge_{\mathbf{g} \in \mathsf{supp}(\mathbf{G})} \underbrace{(\boldsymbol{\beta}_{\mathsf{K}} \circ \boldsymbol{\alpha})(\mathbf{g}) = \boldsymbol{\beta}_{\mathsf{K}}(\mathbf{g})}_{objective} \Big\} \geq 1$$

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Multi-task learning consists on solving more tasks in parallel





Concept supervision involves regressing on the ground-truth concepts



Reconstruction penalty for recovering the original input from the learned concepts



Disentanglement = independent variations of the concepts

Table 1: **Impact of different mitigation strategies on the number of deterministic optima**: R is reconstruction, C supervision on C, MTL multi-task learning, and DIS disentanglement. All strategies reduce the number of α 's in Eq. (6), sometimes substantially, but require different amounts of effort to be put in place. Actual counts for our data sets are reported in Appendix C.2.

MITIGATION	REQUIRES	Constraint on α	ASSUMPTIONS	RESULT
None	-	$\bigwedge_{\mathbf{g}\insupp(\mathbf{G})}\left((\beta_{K}\circ\alpha)(\mathbf{g})=\beta_{K}(\mathbf{g})\right)$	A1, A2	Theorem 2
MTL	Tasks	$\bigwedge_{\mathbf{g}\insupp(\mathbf{G})}\bigwedge_{t\in[T]}\left((\beta_{K^{(t)}}\circ\alpha)(\mathbf{g})=\beta_{K^{(t)}}(\mathbf{g})\right)$	A1, A2	Proposition 4
С	Sup. on \mathbf{C}	$\bigwedge_{\mathbf{g}\in\mathcal{S}\subset\mathrm{supp}(\mathbf{G})}\bigwedge_{i\in I}\left(\alpha_i(\mathbf{g})=g_i\right)$	A1	Proposition 5
R	-	$\bigwedge_{\mathbf{g},\mathbf{g}'\insupp(\mathbf{G}):\mathbf{g}\neq\mathbf{g}'}\left(\alpha(\mathbf{g})\neq\alpha(\mathbf{g}')\right)$	A1, A3	Proposition 6

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Plenty of experiments: no existing mitigation strategy is sufficient in all cases!

Bonus: We prove that optimal maps α 's are the extremes of the simplex of optimal solutions in Probabilistic Logic. This can be leveraged to be agnostic about which RS to pick!









































In this setting, the number of Reasoning Shortcuts scales like:



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$$\sim 10^{78}$$



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If we **disentangle** the concepts, Reasoning Shortcuts completely vanish!

0+0	_	0
0 + 1	_	1
÷		
9 + 9	=	18



In this setting, the number of Reasoning Shortcuts scales like:



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Frequency in % of RSs over 30 optimal runs.

		XOR			MNIST-Addition		
	DPL	SL	LTN	DPL	SL	LTN	
-	100%	100%	100%	96.7%	82.9%	100%	
DIS	0%	0%	0%	0%	0%	0%	

In this setting, the number of Reasoning Shortcuts scales like:



(4) BDD-01A: Real-world Autonomous Vehicle Data Set [10]



4) BDD-OIA: Real-world Autonomous Vehicle Data Set [10]

Predict one or more actions:

- move_forward / stop
- turn_left

• . . .

• turn_right

20-ish concepts including:
red_light / green_light
obstacle / road_clear

(b) HT-PURCE (c) HT-COMPARENT (c) HT-COM

Predicted (C)

Top: No supervision on concepts **Bottom**: Full supervision on concepts + entropy

Learn to solve a sequence of NeSy predictions over *different episodes/tasks*

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- We show that here Reasoning Shortcuts are also likely to happen and standard CL strategies fail to preserve the intended concepts

- Learn to solve a sequence of NeSy predictions over *different episodes/tasks*
- We show that here Reasoning Shortcuts are also likely to happen and standard CL strategies fail to preserve the intended concepts



E. Marconato, G. Bontempo, E. Ficarra, S. Calderara, A. Passerini, and S. Teso; Neuro-Symbolic Continual Learning: Knowledge, Reasoning Shortcuts, and Concept Rehearsal, ICML (2023).
Take-home message:

- Interpretability of concepts can be framed within a Causal framework and allows to define properly some notions, like *interpretability*, concept leakage, and completeness.
- Reasoning shortcuts constitute a severe problem for perception (the maps a) + reasoning (the knowledge K), undermining trustworthiness and interpretability.
 - Existing mitigation strategies are not effective and more research is needed!
- Fruitful intersection between Concept Learning, NeSy AI with Causal Representation Learning.



DeepProbLog (left), Semantic Loss (center), and Logic Tensor Networks (right) pick similar Reasoning Shortcuts.

Future extension to learning end-to-end

New works are appearing to learn both the **concepts** and the **knowledge**:

- DSL (Deep Symbolic Learning) [12]
- ROAP (Regularize, Overparametrize, and Amoritize for Programs) [13]



Figure 1: Architecture of Deep Symbolic Learning for the Sum task. Red arrows represent the backward signal during learning.

- This problem is even less constrained than before:
 - RSs affecting models with prior knowledge transfer to models learning the knowledge
 - More RSs can appear by mistaking the knowledge



Do LLMs synthesize Reasoning Shortcuts?

(123234345 + 987876765 = 1111111110									
Rad	Deg	x!	()	%	AC			
Inv	sin	In	7	8	9	÷			
π	cos	log	4	5	6	×			
е	tan	4	1	2	3	-			
Ans	EXP	xy	0		=	+			

Do LLMs synthesize Reasoning Shortcuts?

ChatGPT 3.5 ~						
	Continue until you reach the leftmost column. In this case, you'll end up with:					
I	123234345 + 967878785 					
	So, 123234345 + 987876765 = 1110113110.					

© 123234345 + 9878767655 = 11111111110							
Rad	Deg	×I	()	%	AC	
Inv	sin	In				+	
π	cos	log				×	
e	tan	4				-	
Ans	EXP	×۳			=	+	

- LLMs (without plugins) fail in reasoning:
 - Shortcut behavior in NLI [14]
 - Failures in reasoning benchmarks [15]
 - Non-unique solutions in modular arithmetic [16]
 - Pitfalls of out-of-distribution generalization on Dyck grammars with 2-layer transformers [17]

Because of an interplay of wrong concepts and/or wrong knowledge?

Thank you for your attention!



paper

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code

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