

Vision-Language Pretraining: Current Trends and the Future

Part 3: Beyond statistical learning

Let's take a step back...

We use machine learning mostly to build **predictive models** that imitate real-world systems.

We build **statistical models**, which exploit the **correlations** yielding the best predictions, regardless of relevance to the task.

- › **Image recognition:** imitate a human labeller.

Predictive correlation: blue background / bird.



- › **Visual question answering (VQA):** imitate a human answering questions.

Predictions can be correct for the wrong reasons.

Training data is biased. Predictive correlations: question type / answer.

How many ...	• 2 (or 3)
Is/Are ...	• “Yes” (~80%) vs “no”
What sport ...	• Tennis
What animal ...	• Dog
What is the color of ...	Red, blue

What color is illuminated on the traffic light ?



Predicted answer: **Green.** ✓

We edit the input image and expect the answer to change:



Predicted answer: **Green.** ✗

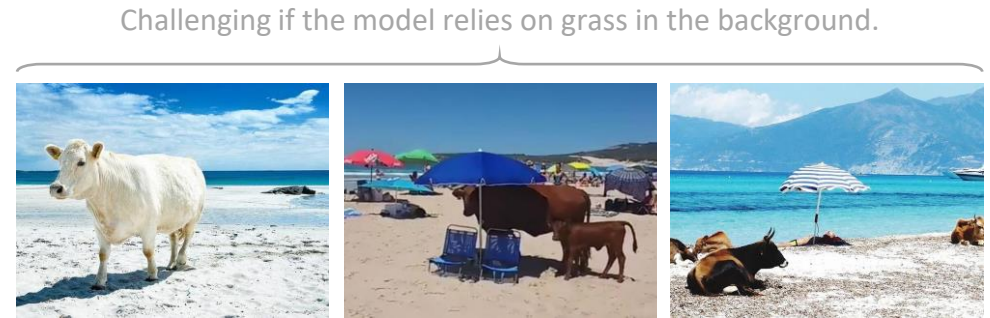
Statistical learning has limitations.

Predictions are reliable only **within the training distribution**.

Training data
(biased)



Test data
(out-of-distribution)



The features used by a model are **not necessarily the same** as for the real system we try to imitate. (e.g. human labeller)

*Formally, in causal language: the background is not a **cause** to the image label.*

⇔ *Intervening on the background (by **editing the image**) would **not** cause one to label it differently.*

A cow.



→
Intervention



Still a cow.

More limitations ! Statistical models only answer **predictive** questions.

- › Example: a model **predicting the imminent failure of a machine in a factory** from the noise it makes.
The model can't tell how to reduce the rate of failures. Soundproofing the factory will not work !
*The noise is not what causes the machine to fail (noise/failure is only a correlation). **Obvious by common sense.***
- › Example: an NLP model **predicting the popularity (future number of clicks)** of an online news article.
Interpretability methods may show that the model relies on headline length.
*But it doesn't mean we can alter popularity by changing headline lengths (only a correlation in tr. data). **Not as obvious !***

Even simple predictive questions should display:

- › Adversarial robustness = *Worst-case OOD generalization.*
- › Compositional and cross-task generalization = *Repurposing elements of learned knowledge.*
- › Robustness across distribution shifts = *Predictions in conditions not seen in training.*



All these settings violate the **assumption of i.i.d. training/test data** central to statistical learning.

Causal reasoning offers a framework of analysis to understand how to overcome these limitations.

- This talk:**
- Causal language/principles to help you navigate the literature.
 - Example applications: evaluating the robustness of V&L models.
 - Example applications: training better models.

- › Causality provides notations to describe **data-generating mechanisms** (more fundamental than the observed data itself).
The language of statistics, e.g. conditional probabilities, only describes observational properties such as correlations. Here, we aim to understand the “why” i.e. the reason for these observed correlations. Mechanisms are more fundamental than data: we can derive correlations from causal structure, but not the reverse.
- › “A causes B” $\equiv \textcircled{A} \rightarrow \textcircled{B} \equiv$ Setting A to a specific value can affect the distribution of B.
 $P(B|\textit{do}(A)) \neq P(B|A)$ A new ‘do’ operator represents **interventions**.
- › Causal learning = Learning the **data-generating mechanisms** of a **task** (and not just the correlations in a specific dataset).

Generalization ≠ generalization

In-domain (ID) generalization

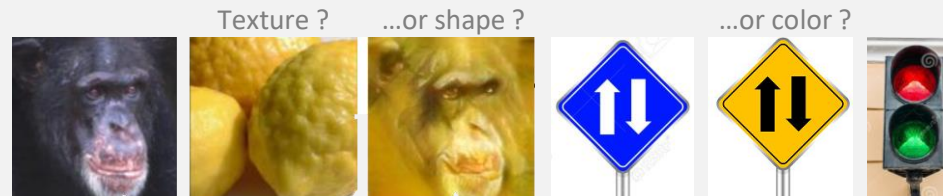
- › Classical use of the term.
- › Easier with more training data.
- › Inductive biases are indispensable, but some seem **universally** useful.

E.g. simple regularizers that favour simplicity/smoothness such as weight decay.

Out-of-distribution (OOD) generalization

- › Some correlations from the training data may be absent or misleading at test time.
- › More (of the same) data is not sufficient to improve OOD generalization.
- › Need **task-specific** information.

E.g. should we rely on texture/shape/color for object recognition ?



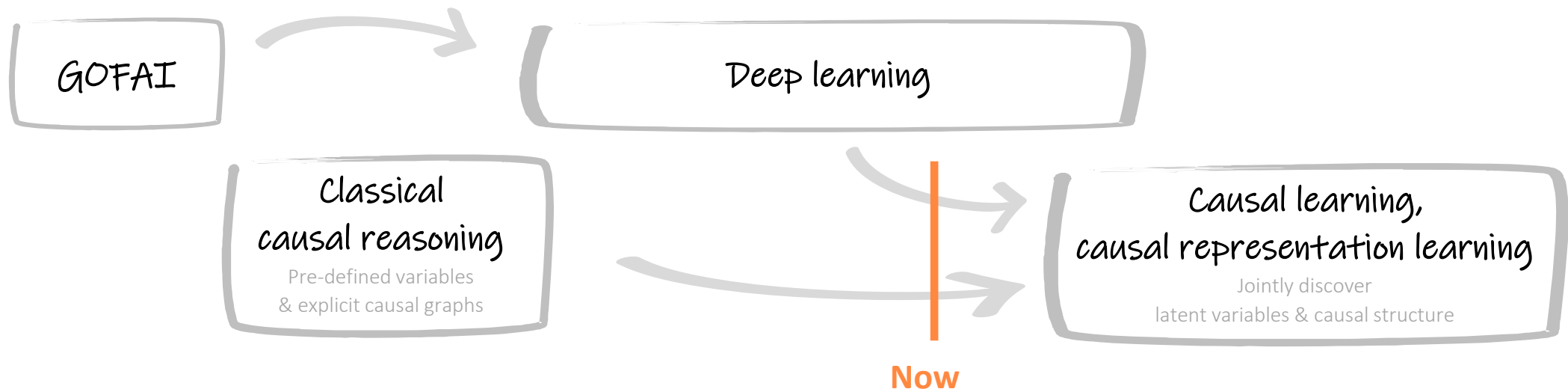
The disciplines of causality

Classical methods (economics, social science, biology, epidemiology, etc. rely on **predefined variables** & explicit causal graphs)

- › **Causal inference**: answering causal queries from observational data and a known causal graph (human-provided).
How much would people click on ads if we double the font size ? (provided a causal graph, and data from controlled and/or non-controlled experiments)
Would this specific person be in better health, had she been administered treatment X ?
- › **Causal discovery**: using data to refine a partially-known causal graph.
Is gene X responsible for health condition Y ?

Emerging area: extending ML with causal principles (high-dimensional data & causal relationships not modelled explicitly)

- › **Causal representation learning**: learning embeddings of raw data, disentangling its generative factors (causal parents).
Equivalent to: disentanglement, independent component analysis (ICA).
- › **Causal learning**: learning predictive models that rely on causal (not spurious) features.
Enable better transfer to unseen conditions, across datasets, across tasks.
Also aims at (implicitly) identifying generative factors.



And here's the key to enlightenment...

* in understanding current models' limitations 😊

Causal learning is difficult because we usually have only **observational data**. (passively collected)

- › Understanding causes/effects would be easy **if we could interact** with the real system: just act and observe the effects !

E.g. submitting every variation of an image to a labeller until she predicts a different label.

- › But a typical dataset only provides **i.i.d. samples of a joint distribution** e.g. over images/labels.

*A distribution is usually compatible with **multiple causal structures**.*

Even with 2 variables: a correlation between A and B can arise from $A \rightarrow B$ or $B \rightarrow A$ or $A \leftarrow C \rightarrow B$ (hidden common cause).

*This is why **spurious/robust** correlations are **indistinguishable**.*

- › **More observational data** does not help.

Biased/long-tailed distributions remain biased/long-tailed, even with lots of samples !

We need background knowledge, additional assumptions, or interventional/heterogeneous data.

↓ ↓
E.g. as custom architectures, losses, regularizers, ...

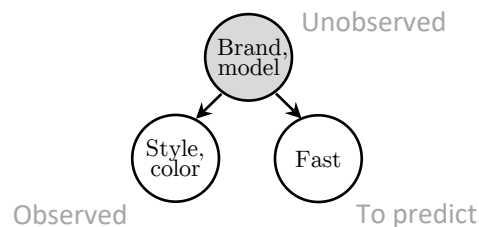
Making things concrete: statistical vs. causal learning

“Is this a fast car ?” (top speed >200 km/h)

Training images with labels ‘Fast’ ∈ {0,1}



Someone’s mental (causal) model:



- **Statistical learning is about correlations:** red = fast.
Reliable only if the training/test data are from similar distributions.

- **Causal learning is about mechanisms.**
It enables predictions in conditions unobserved during training (OOD).

Conditioned on **observing** the color
in the training distribution.

$$P(Fast \mid Color)$$

≠

$$P(Fast \mid \text{do}(Color))$$

Conditioned on an **intervention**.

What happens to
a re-painted car ?



Faster ? No !

More data (more images of red Ferraris) **can't help distinguishing** **spurious correlations** from **causal** ones.

Only 2 options to obtain knowledge of the data-generating process.

➤ **Existing task knowledge from humans.**

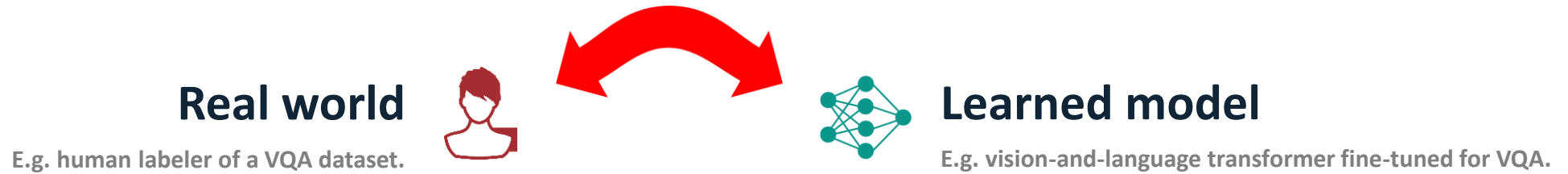
*Examples: custom architectures and losses,
hand-designed data augmentations,
interaction with human-designed simulator, etc.*

➤ **Heterogeneous/interventional data = non-i.i.d. samples.**

*Examples: data collected before/after interventions,
data from multiple environments (in time/location/subpopulation/...),
pairs of counterfactual examples,
non-stationary time series, etc.*

Back to vision and language:
How to evaluate a model's robustness ?

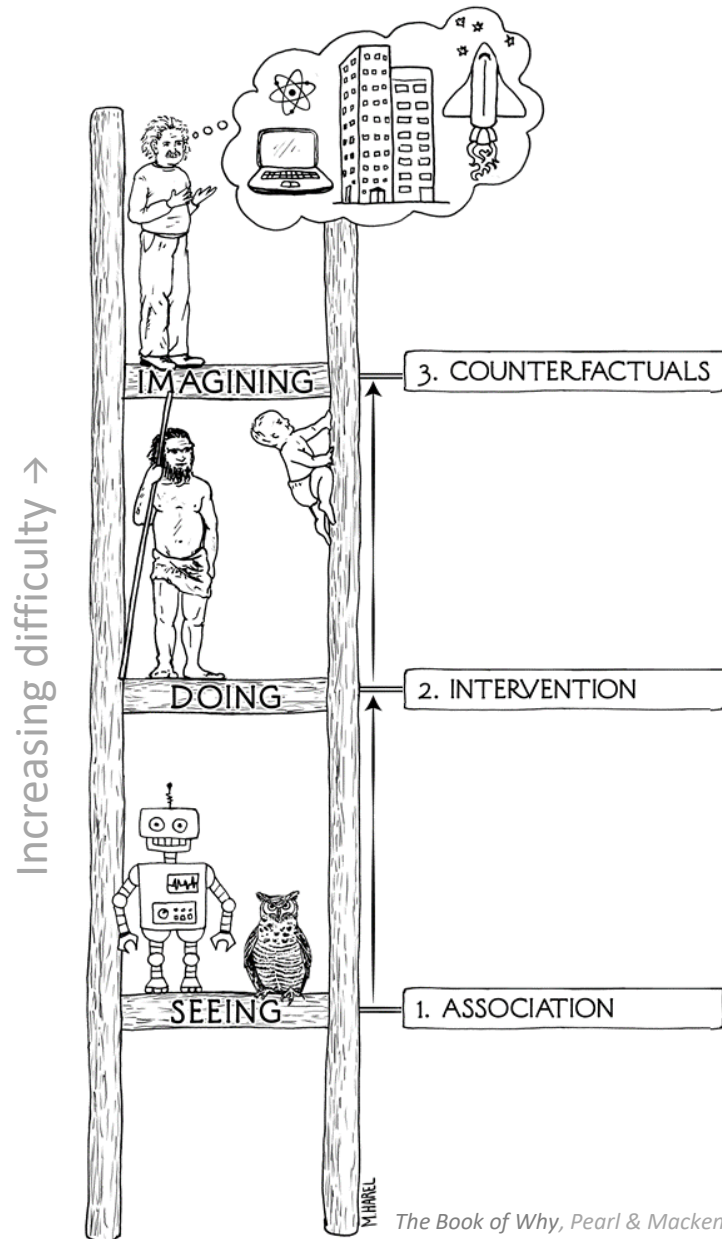
To imitate the real system faithfully,
we want to **mirror its causal mechanisms**.

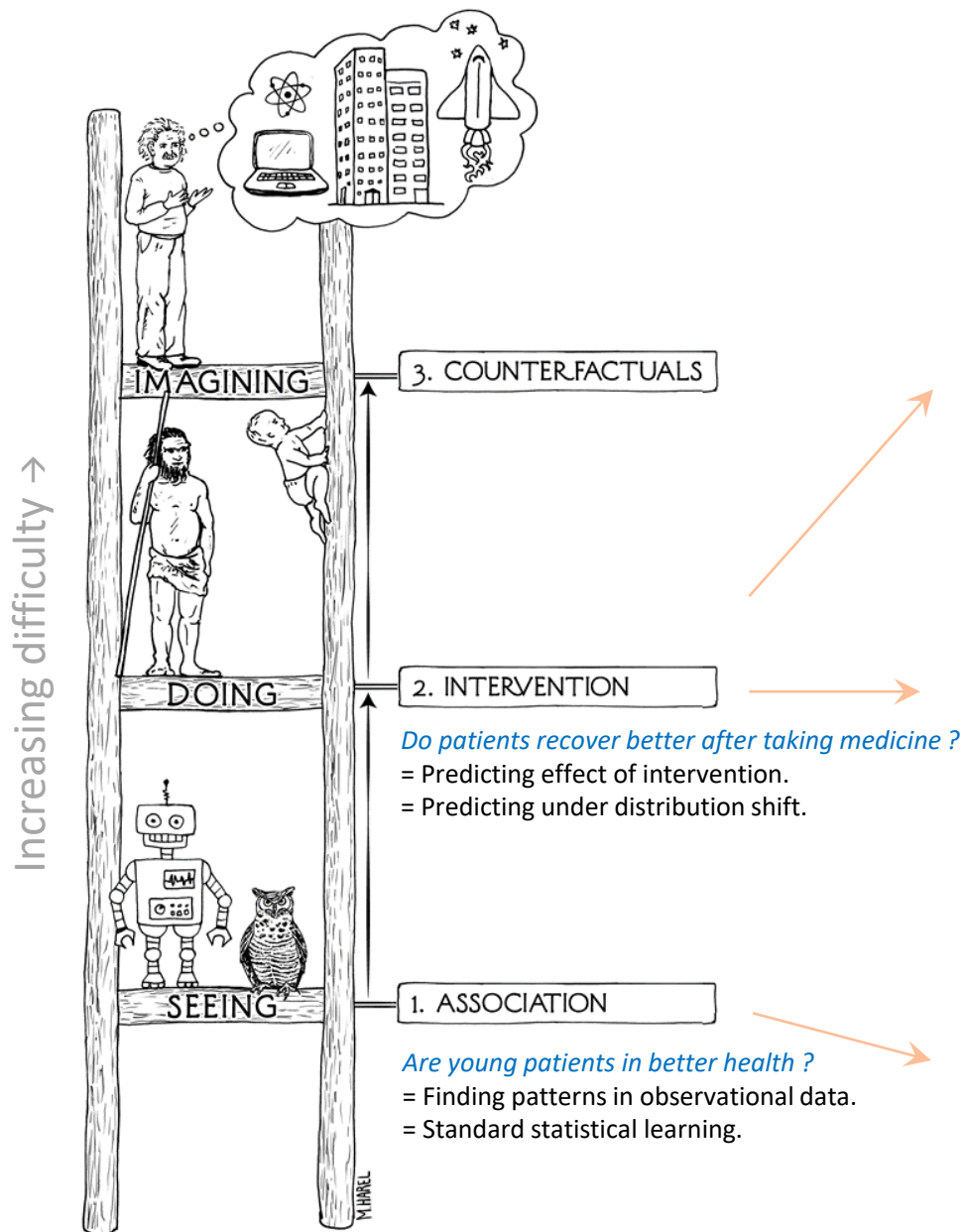


Does a VQA model { reliably answer questions about **novel/unusual (OOD)** scenes ?
rely on the **same features/reasoning** as a human ?
implement the same **causal structure** as the real system ?

Note: **Interpretability methods** serve to compare (only qualitatively) a model's causal structure with our (mental) **causal model of the world** (i.e. what predictive features should be used). Here, we aim to do this **quantitatively** and **with data** (rather than expert knowledge).

Causal hierarchy: 3 types of queries to a model \Leftrightarrow Existing types of benchmarks used in machine learning.





- > Pairs of **counterfactual test examples** (aka. contrast sets) \approx interventions at instance level. Probing models near the desired decision boundary.



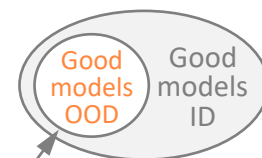
Towards Causal VQA,
 Agarwal et al., CVPR 2020.

- > Test sets from a **different distribution**. Increasingly popular to evaluate robustness. Formally: test data from intervention on variable(s) in the data-generating process. Examples: any cross-dataset (zero-shot) evaluation, VQA-CP (intervention on question type & answer), GQA-OOD.



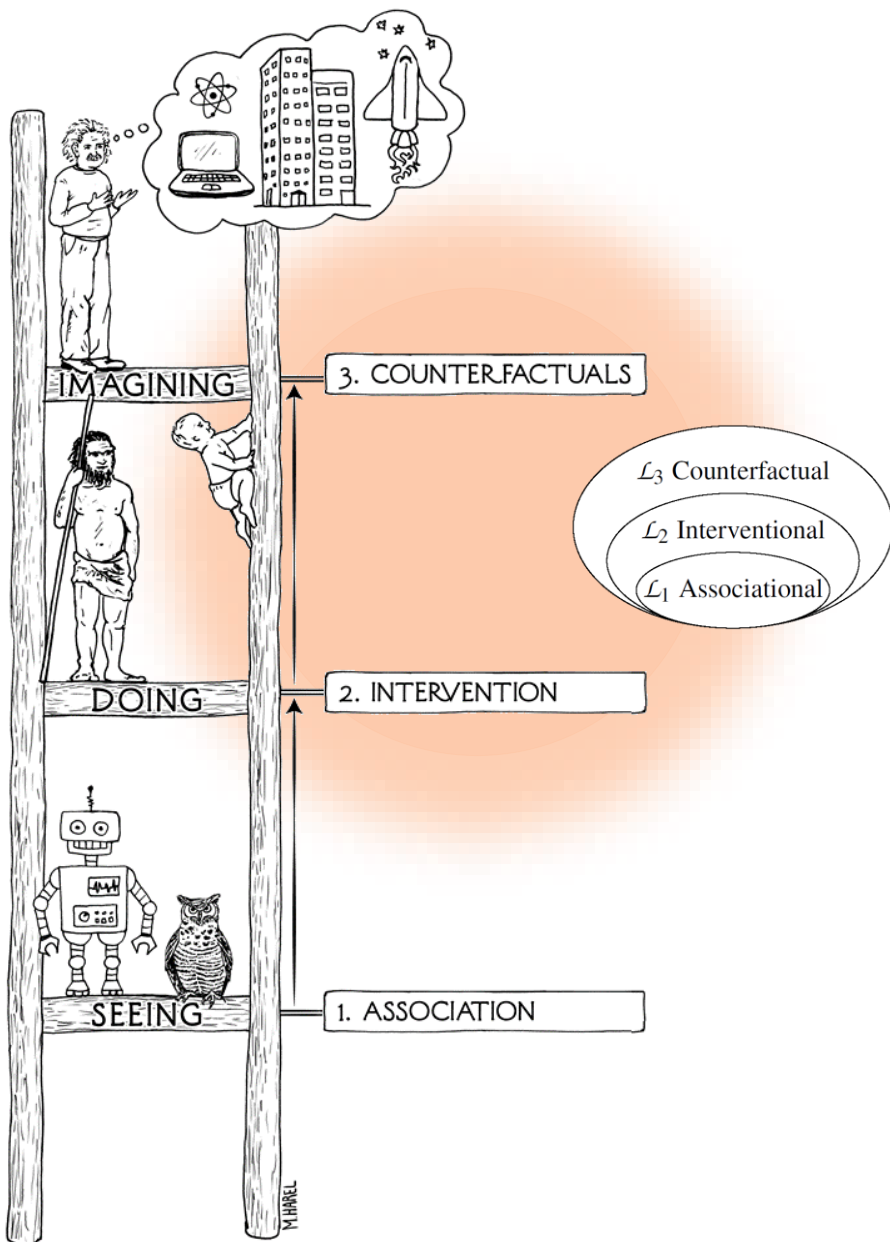
ImageNet-9 backgrounds challenge,
 Madry lab.

- > Standard evaluation: test set with **same distribution** as tr. data. Limitation: only measures in-domain (ID) generalization. Says nothing about generalization to **unusual** (OOD) data.



Small subset !

Increasing difficulty →

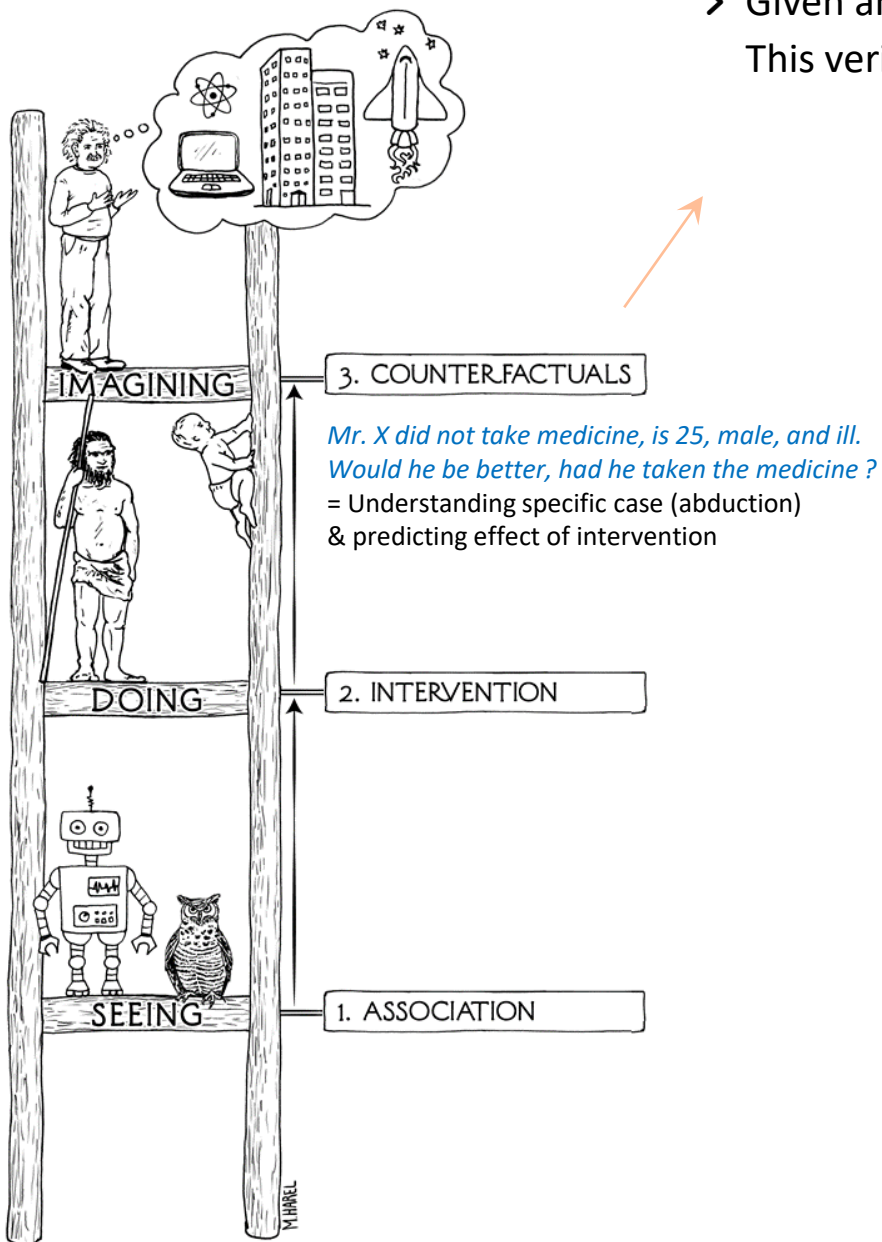


Each level requires strictly more causal information.

Some benchmarks are clearly better (more demanding) than others.

To evaluate robustness, we should design benchmarks matching levels 2/3.

Increasing difficulty →



- Given an image/Q/A triplet, ask the model to **generate plausible images** for alternative answers.
This verifies that the model understands **which visual clues matter**.

Input to the model:

What color is illuminated ?

Green.

Alternative answer: red.



Correct output:



- Given an image/Q/A triplet, ask the model to **generate plausible images** for alternative answers. This verifies that the model understands **which visual clues matter**.

*Mr. X did not take medicine, is 25, male, and ill.
Would he be better, had he taken the medicine ?*
= Understanding specific case (abduction)
& predicting effect of intervention

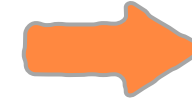


Input to the model:

What color is illuminated ?

Green.

Alternative answer: red.



Correct output:



The more **demanding** the evaluation, the more **difficult** the data collection/benchmark design.
Fundamentally, the evaluator has to “know more” than the evaluatee !

Implications for evaluation

The more **demanding** the evaluation, the more **difficult** the data collection/benchmark design.

...because the evaluator fundamentally needs to “know more” than the evaluatee !

Ultimate evaluation: direct comparison of a model with the real system. (e.g. human in the loop)

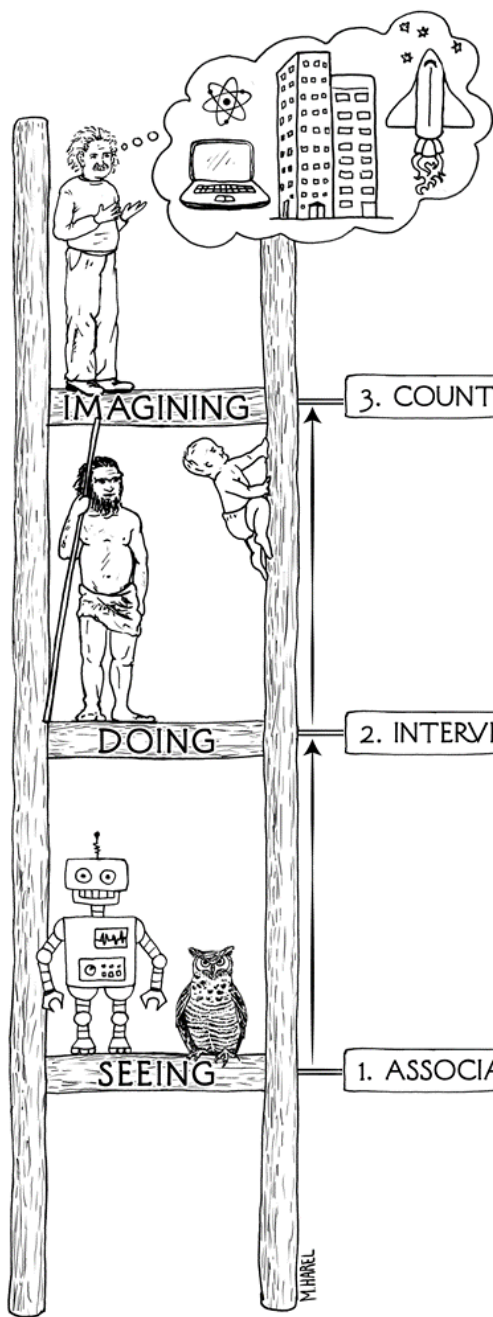
The more **simple/automated** the evaluation, the more likely it can be **gamed**.

How to learn robust models ?

Maybe overkill: we may expect only small shifts



Let's aim for the best: a predictor that generalizes to **any** distribution shift.
= which relies on the **causal parents** of the target variable.



A model capable of level i requires knowledge/data relevant to level $j \geq i$.

⇒ Levels strictly increase in difficulty.

What we really care about.

Standard dataset

⇒ We cannot learn to **reason about interventions** (levels 2/3) from **observational data** (level 1).

3. COUNTERFACTUALS

$$P(Y_x | x', y')$$

$$\mathcal{L}_3$$

Counterfactual data

E.g. pairs of counterfactual examples.

2. INTERVENTION

$$P(Y | do(X))$$

$$\mathcal{L}_2$$

Interventional data

E.g. data collected before/after a controlled intervention; multiple tr. environments.

1. ASSOCIATION

$$P(X, Y)$$

$$\mathcal{L}_1$$

Observational data

E.g. standard dataset, i.i.d. samples from the joint distribution.

Learning from multiple environments

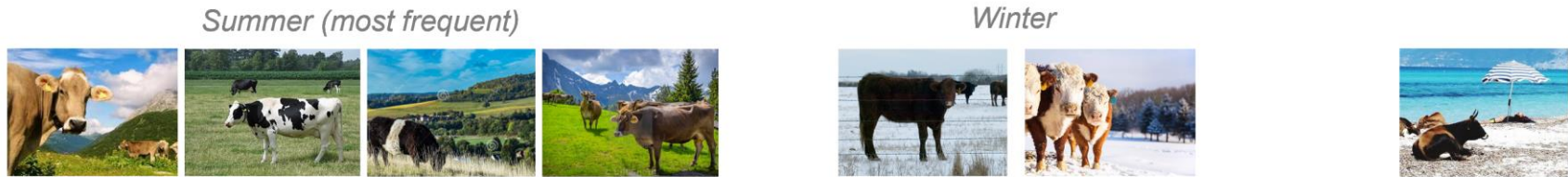
- › Training data divided in multiple subsets. One **environment** = one **intervention** e.g. on a selection bias.

*Examples: **pictures** from geographical locations, **text** from periods of time, **dialogue** from subgroups of people, **reviews** for sentiment analysis from different domains, ...*

Cell phones



Cows



Fire hydrants



Training examples over time →

OOD Test cases

Learning from multiple environments with invariant risk minimization (IRM)

- › We want a mapping from words/pixels to a representation encoding high-level concepts that causally affect the target.

Invariant risk minimization (IRM): “To learn invariances across environments, find a data representation such that the optimal classifier on top of that representation matches for all environments.”

[1] Invariant risk minimization, Arjovsky et al., 2019.

- › The resulting model will make predictions based on features that are invariant across training environments, and therefore also in new test environments (under certain conditions).
- › **Some remaining challenges:** optimization difficult, getting data from many diverse environments, trade-off between generalization and lower in-domain performance.
- › There are applications of IRM in NLP, e.g. to sentiment classification: OOD generalization is improved by removing spurious reliance on single words that typically correlate highly with the target in the training data.

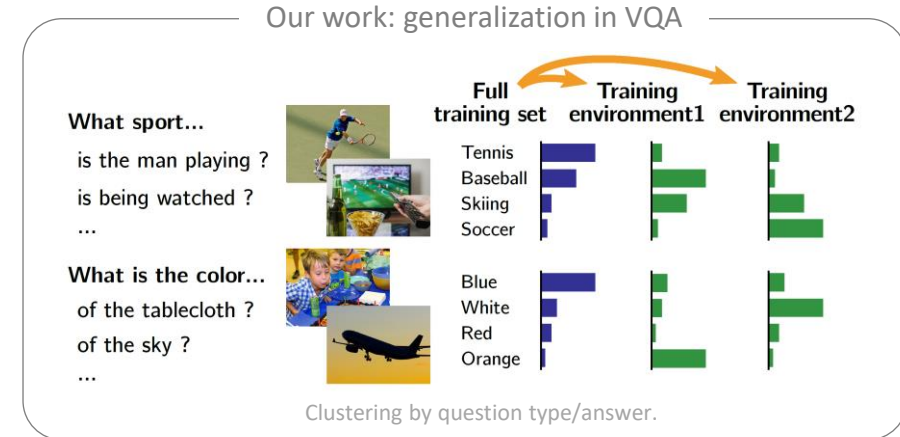
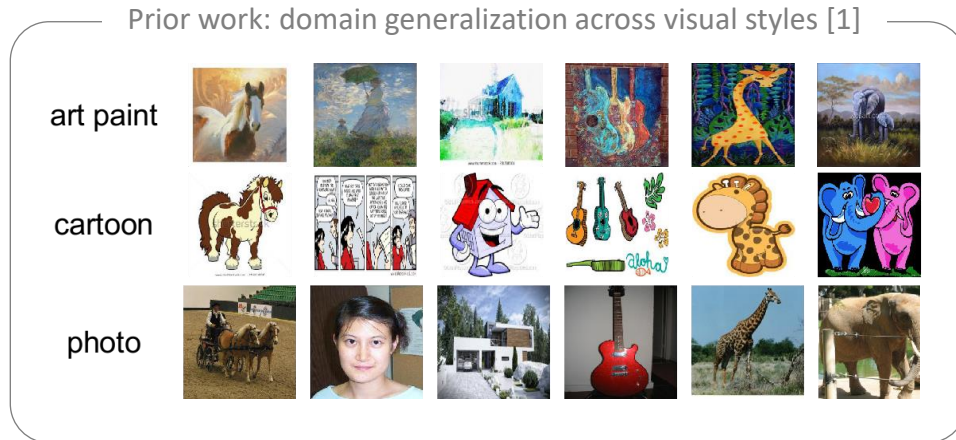
[2] An Empirical Study of Invariant Risk Minimization, Choe et al. 2020.

[3] Invariant Rationalization, Chang et al., JMLR 2020.

Unshuffling data to improve generalization in VQA

- Learning from multiple **training sets** / **training environments**.

For VQA, we create environments by clustering the training data. [3]



- Intuition: **spurious correlations** vary across environments, while **causal mechanisms** remain constant.

Data from environment 1: $(x,y) \sim P_1(X,Y) = P(Y|X) P(X|\text{do}(Z = z_1))$

from environment 2: $(x,y) \sim P_2(X,Y) = P(Y|X) P(X|\text{do}(Z = z_2))$

Each environment shows
an **intervention** on a variable Z
sp spuriously correlated with labels Y .



- With a **well-chosen clustering** and modified objective [2] the model is **less reliant on answer prior** & generalizes better.

Task-specific, human-provided. No free lunch !

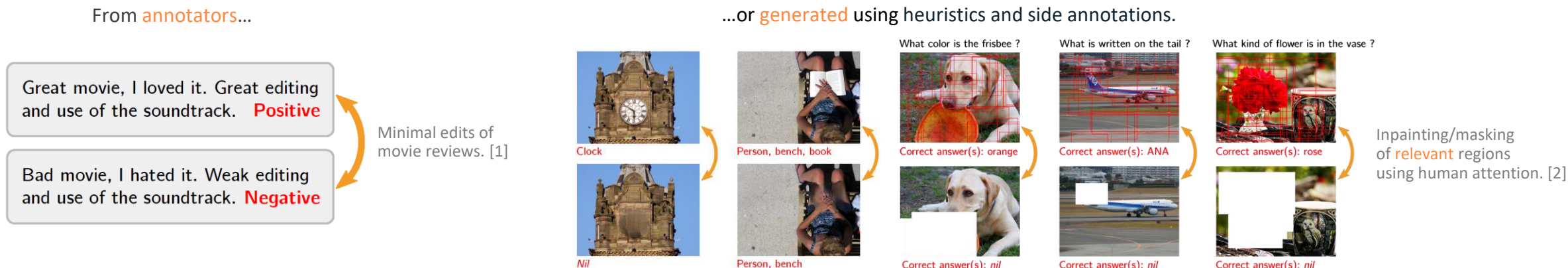
[1] Domain generalization – PACS Benchmark, <https://domaingeneralization.github.io>.

[2] Invariant risk minimization, Arjovsky et al., 2019.

[3] Unshuffling data for improved generalization in visual question answering, Teney et al., CVPR 2021.

Learning from pairs of counterfactual training examples.

> Pairs of similar examples with a different label. How to obtain them ?



Each pair shows **which features** (= causal parents) **are relevant for flipping the label**.

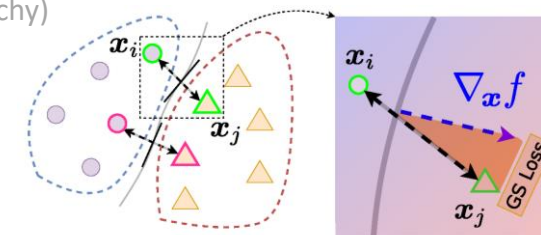
Used as data augmentation: they **improve generalization** more than the same amount of standard (i.i.d.) data.

> One step further: the causal information is in the **relation across each pair**. [3] (Level 3 in the causal hierarchy)

We can do better than treating them as individual examples !

New **auxiliary loss** to exploit these relations.

- ① Compute **vector differences** (in feature space) across a pair,
- ② Align the **classifier's gradient** (and decision boundary) with it.



> This gives additional improvements in **generalization across datasets** in VQA, image tagging, textual entailment, sentiment analysis.

[1] Learning the Difference that Makes a Difference with Counterfactually-Augmented Data, Kaushik et al., ICLR 2019.

[2] Towards Causal VQA: Revealing and Reducing Spurious Correlations by Invariant and Covariant Semantic Editing, Agarwal et al., CVPR 2020.

[3] Learning What Makes a Difference from Counterfactual Examples and Gradient Supervision, Teney et al., ECCV 2020.

Causal principles help explain the effectiveness of data augmentation and contrastive learning.

Data augmentation simulates interventions.

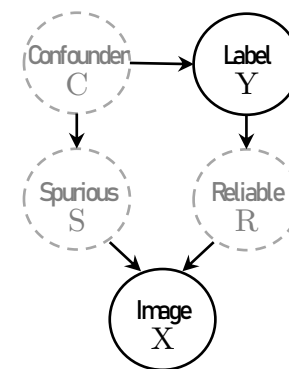
- › We design (by hand) transformations $(x, y) \rightarrow (x', y)$ that produce additional training examples.



- › Causal explanation: images contain **spurious** and **reliable** features.

Both are correlated with labels Y because of a selection bias (confounder C).

We want a model robust OOD = robust against changes of C .



- › This cannot be learned with samples from $P(X, Y)$. However, it can be learned by **observing interventions**.

*Data augmentation **simulates interventions** on S . For example:*

Augmenting images with geometric transformations = intervening on camera parameters.

Augmenting VQA questions with rephrasings = intervening on annotators' writing style.

} *Samples from $P(X, Y \mid \text{do}(S))$, which carry info about causal structure.*

- › Root source of improvements = specification (in the transformations) of **invariances** over (X, Y) that are valid for **this task's** data-generating process.

Causal explanations help select effective augmentations [1].

➔ No universal augmentation !

Similar case in self-supervised/contrastive learning [2]: augmentations = counterfactuals (intervention on style, leaving content unchanged).

[1] Selecting Data Augmentation for Simulating Interventions, Ilse et al. ICML 2021.

[2] Self-supervised learning with data augmentations provably isolates content from style, von Kugelgen et al., NeurIPS 2021.

- ✓ Causal language and principles.
- ✓ Evaluating V&L models.
- ✓ Training better models.

Take-aways

Causality is useful for ML.

- › The **capabilities & evaluation of ML models** have outgrown the framework of statistical learning (and its i.i.d. assumption).
- › **Causal language** helps formalizing existing concepts.
E.g. distribution shifts, OOD testing, challenge sets, data augmentation, disentanglement, adversarial examples, ...
Conditional probabilities cannot describe interventions, causal relationships, or invariances.
- › **Causal principles indicate hard limits** on what can be learned from a given type of data and assumptions.
Comparable to information theory for designing communication systems: not indispensable but darn useful !

When reading papers claiming improved OOD generalization, remember the only 2 possible explanations:

- › **Better inductive biases** that make the model **closer to the true causal structure** of the task.
Architecture, augmentations, losses, optimizer, ...
Good accidentally ? Opportunity to discover useful properties of real-world data.
Good by design ? What are the limits of applicability of the domain knowledge/heuristics used ?
- › **Additional training signals** that reveal some of the causal structure of the task.
I.i.d. samples are not sufficient.
Alternatives: assumptions (= partial knowledge) about the data-generating process, interventional data (not only w/ RL), multiple training environments, pairs of counterfactual examples, time series, meta data about data collection, ...
Possibly where the most promising future work lies !

Open question: how weak (universal) can the assumptions be for causal learning/OOD generalization ?

- › Assumptions/heuristics in existing methods are **often hidden**, and almost surely **task/dataset-specific**.

*Example: line of works claiming debiasing by removing **easy-to-learn features** (~ half a dozen paper in the past year).*

The hidden assumption: the **second-easiest features** are the good ones. Not true in general !

*Still, maybe a useful heuristic **in NLP**: simple to learn = always spurious ??*

[1] A Too-Good-to-be-True Prior to Reduce Shortcut Reliance, Dagaev et al. 2021.

[2] Rich Feature Construction for the Optimization-Generalization Dilemma (discussion in Section 5.2), Zhang et al. 2022.

- › We cannot do **model selection** with in-domain validation data (without further assumptions).

[3] Evading the simplicity bias: Training a diverse set of models discovers solutions with superior OOD generalization, Teney et al. CVPR 2022.

- › OOD **Benchmarks** can be misused. Example: VQA-CP, many useless papers (still being) published that overfit the OOD test set.

[4] On the Value of OOD Testing: An Example of Goodhart's Law, Teney et al., NeurIPS 2020.

Open question: how to explain OOD capabilities of large V&L models ?

- › Some OOD improvements naturally follow from ID improvements. **Effective robustness** is rare. →

[5] Accuracy on the Line: On the Strong Correlation Between OOD and ID Generalization, Miller et al. ICML 2021.

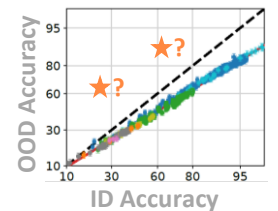
[6] Why do classifier accuracies show linear trends under distribution shift, Mania et al. 2020.

- › Effective robustness is lost during fine-tuning.

[7] The Evolution of OOD Robustness Throughout Fine-Tuning, Andreassen et al., 2021.

- › CLIP is exceptionally robust OOD: its data is large and diverse, but also filtered/selected/weighted.

[8] Data Determines Distributional Robustness in CLIP, Fang et al., 2022.



Further reading

Improving ML with causality (introductions and reviews):

- › *Causality for Machine Learning*, Cloudera report, 2020.
- › *Causal Inference in Natural Language Processing: Estimation, Prediction, Interpretation and Beyond*, Feder et al., 2021.
- › *Towards Causal Representation Learning*, Scholkopf et al. 2021.
- › *From Statistical to Causal Learning*, Scholkopf and Kuegelgen, 2022.
- › *Causality matters in medical imaging*, Castro et al., Nature Communications, 2020.

Not covered here: relevance of causality to fairness:

- › *Causal Reasoning for Algorithmic Fairness*, Loftus et al., 2018.
- › *Avoiding Discrimination through Causal Reasoning*, Kilbertus et al., NeurIPS 2017.
- › *On the Fairness of Disentangled Representations*, Locatello et al., NeurIPS 2019.

Also not covered here: improving causal inference (answering causal questions) with ML:

- › *Causal Effects of Linguistic Properties*, Pryzant et al., 2021.

Personal paper collection: damienteney.info/papers See folders “Causality” and “Biases”. PDFs are highlighted, some also commented. Very personal selection !

Extra slides

Advantages of a causal model

- › The causal structure of the data-generating process is **more informative** than statistical information.

$P(B|A)$ Conditional distribution = Filtering an observed distribution.
≠

$P(B|do(A))$ Interventional distribution = Forcing a variable to a specific value.

- › Learning causal structure = learning **invariants**.

Causal relationships hold true across environments, by definition.

*They allow predicting the effect of interventions **in conditions not seen** during training.*

- › **Always preferable** to a statistical model ? No.

If training/test distributions are similar, predictions can be better/easier using all correlations (incl. spurious ones).

Because causal correlations being more noisy/difficult to learn (than spurious ones).

E.g. if red cars are always fast and cows are always on green grass (and vice versa!), predictions are easy using just color!



Do we always want to rely **only** on causal features ?

- › No, we can safely use contextual cues **when training/test distributions are guaranteed to stay similar**.

E.g. use background for recognition.



- › Trade-off: greater **predictive accuracy** vs. **better generalization** to distribution shifts.
- › It's important to make these assumptions & choices explicit.
E.g. for medical imaging , in high-stakes ML, for understanding/eliminating unfair biases.