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. X

Statistical learning has limitations.

Predictions are reliable only within the training distribution.









Test data (out-of-distribution)

Challenging if the model relies on grass in the background.







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.







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" $\equiv \triangle \rightarrow B \equiv$ Setting A to a specific value can affect the distribution of B. $P(B|do(A)) \neq P(B|A) = A \text{ new 'do' operator represents interventions}.$
- > 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

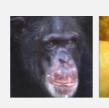
- > Classical use of the term.
- Easier with more training data.
- > Inductive biases are indispensable, but some seem universally useful.

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 <u>and a known causal graph</u> (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?

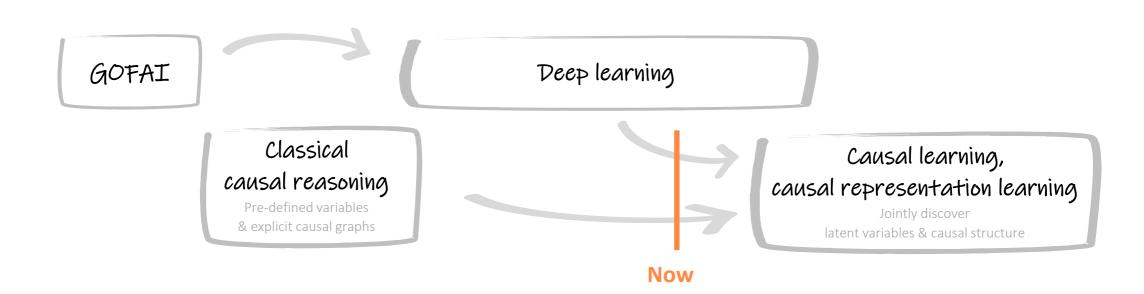
Emerging area: extending ML with causal principles (high-dimensional data & causal relationships not modelled explicitly)

- > 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...

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 $\triangle \rightarrow \mathbb{B}$ or $\triangle \leftarrow \bigcirc \rightarrow \mathbb{B}$ (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}



> 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.

 $P(Fast \mid Color)$

 \neq

 $P(Fast \mid do(Color))$

Conditioned on an intervention.

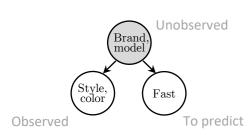
What happens to a re-painted car?





Faster? No!

Someone's mental (causal) model:



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.

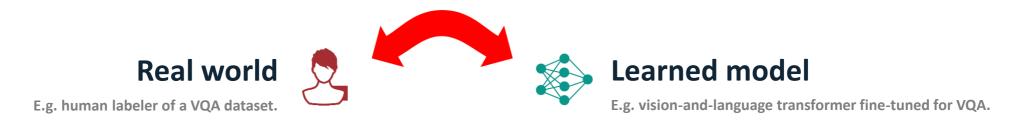
Examples: custom architectures and losses, hand-designed data augmentations, interaction with human-designed simulator, etc.

> 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?

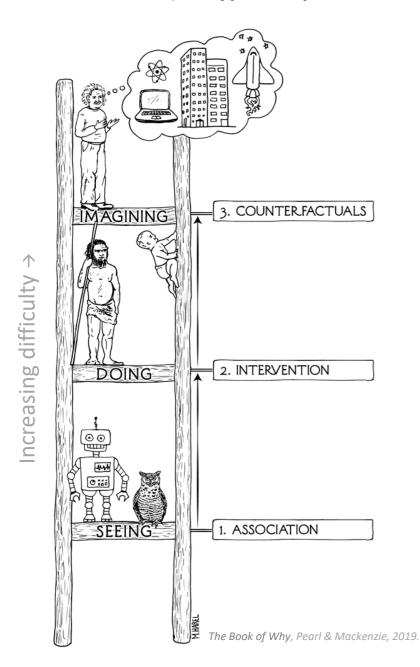
To imitate the real system faithfully, we want to mirror its causal mechanisms.

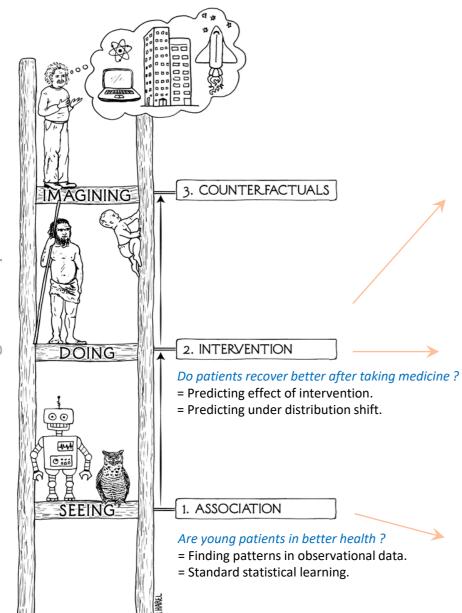


Does a VQA model

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).





Pairs of counterfactual test examples (aka. contrast sets) ≈ 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.

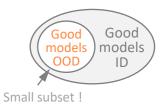
Examples: any cross-dataset (zero-shot) evaluation, VQA-CP (intervention on question type & answer), GQA-OOD.

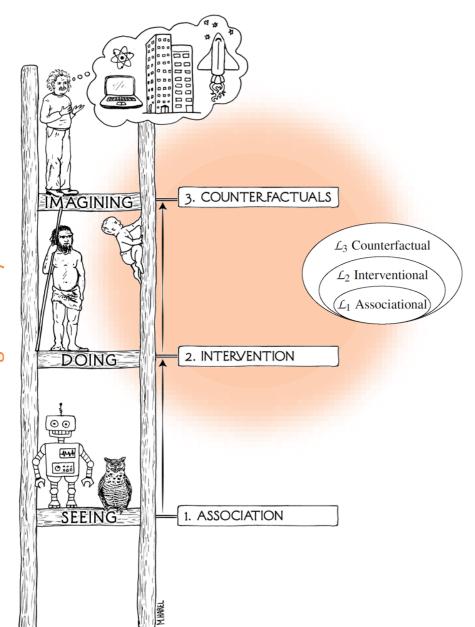




ImageNet-9 backgrounds challenge, Madry lab.

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.

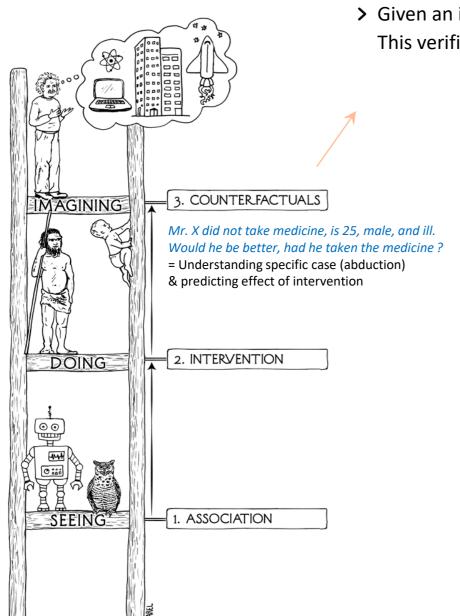




Each level requires strictly more causal information.

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

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



> 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:



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 evaluee!

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.

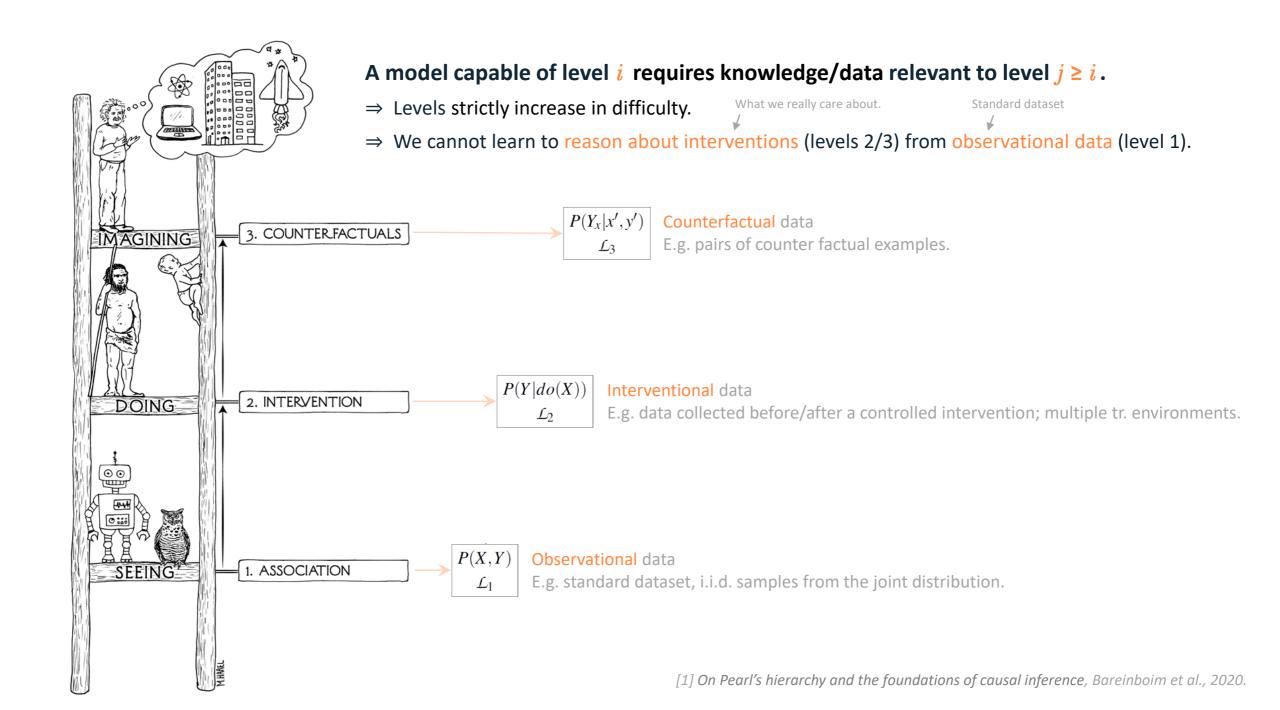
How to learn robust models?

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.



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, ...



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."

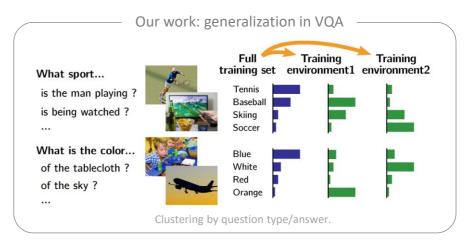
 [1] Invariant risk minimization, Arjovsky et al., 2019.
- > The resulting model will make predictions based on features that are invariant across training environments, and therefore also in new test environments (under certain conditions).
- > **Some remaining challenges**: optimization difficult, getting 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: $(x,y) \sim P_1(X,Y) = P(Y|X) P(X|do(Z = z_1))$

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

Each environment shows an intervention on a variable Z 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?

From annotators...

and use of the soundtrack. Negative

Great movie, I loved it. Great editing and use of the soundtrack. Positive Bad movie, I hated it. Weak editing

Minimal edits of movie reviews. [1]



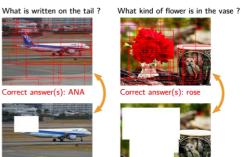






...or generated using heuristics and side annotations.





Inpainting/masking of relevant regions using human attention. [2]

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.

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



- [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.

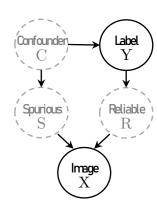
Causal principles help explain the effectiveness of data augmentation and contrastive learning.

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:

 $\label{eq:augmenting} \textit{Augmenting images with } \textit{geometric transformations} = \textit{intervening on camera parameters}.$

 $\mbox{\it Augmenting VQA questions with } \mbox{\it rephrasings} \qquad = \mbox{\it intervening on annotators' writing style.}$

Samples from $P(X,Y \mid do(S))$, 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?

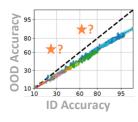
- > Assumptions/heuristics in existing methods are often hidden, and almost surely task/dataset-specific.
 - Example: line of works claiming debiasing by removing easy-to-learn features (~ half a dozen paper in the past year).
 - The hidden assumption: the second-easiest features are the good ones. Not 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.



- [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 at 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.