Causal Inference and Deep Learning

Alexandro Guimarãe

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## Motivation

Causal Inference and Deep Learning

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Joshua Angrist, 2021 Nobel Prize Winner in Economics

 $"E conometrics is the {\it original data science."}$ 

- Suppose we have a treatment *T* , and an outcome *Y*
- We also have *covariates*, which cause both *Y* and *T* and can *confound* the treatment effect, and they are called X (high-dimensional)
- For instance, Y is the academic performance of the student, and T is the school providing tablets for studying
- Suppose that, for any given individual, there are two *potential outcomes* Y(t):
  - $Y(T=1) = Y(1) = Y_1$ , the outcome *with* the treatment;
  - $Y(T=0) = Y(0) = Y_0$ , the outcome *without* the treatment.

### The causal inference question

What is the *Average Treatment Effect* (ATE) of *T* on *Y*? Mathematically,

ATE = 
$$\mathbb{E}[Y_1 - Y_0] = \mathbb{E}[Y|T=1] - \mathbb{E}[Y|T=0]$$

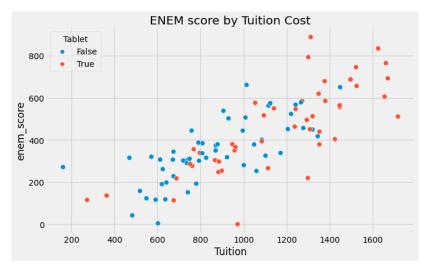
We can also ask what the effect of the treatment will be in each individual. This is known as Individual Treatment Effect (ITE) or Conditional Average Treatment Effect (CATE), and defined by

$$ITE = \mathbb{E}[Y_1 - Y_0 | X]$$

## Why Causal Inference is hard

The fundamental problem of Causal Inference

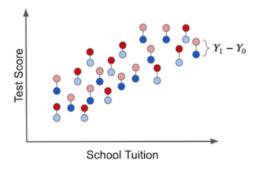
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We can only observe one potential outcome for each individual!

- We can achieve zero bias with randomization, i.e., creating control and treated groups coming from the same population.
- However, randomization is expensive, and sometimes just can't be done.

### Some thing we can do to learn from non-randomized observational data

- Covariate adjustment
- Propensity score re-weighting
- Doubly robust estimators
- Matching
- **...**

We could explicitly model the outcome based on treatment and covariates (*outcome modeling*).

Let's say there is a function h=h(x,T) and we would use an ML model, taking X and T as features, to fit it and predict Y, i.e.,

$$h(x,t) \approx \mathbb{E}[Y_t|T=t,x]$$

We could then estimate the ATE with

$$\widehat{ATE} = \frac{1}{n} \sum_{i=1}^{n} [h(x_i, 1) - h(x_i, 0)]$$

and the ITE with

$$\widehat{\text{ITE}}(x_i) = h(x_i, 1) - h(x_i, 0)$$

## Why neural networks?

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- They are almost **non-parametric models** (but so are trees);
- Neural networks naturally extract relevant information through representation learning;
- Causal inference in quantitative data, text, images, and graphs.

## First concepts

Causal Inference and Deep Learning

### Learning Representations for Counterfactual Inference

Fredrik D. Johansson CSE, Chalmers University of Technology, Göteborg, SE-412 96, Sweden

Uri Shalit

CIMS, New York University, 251 Mercer Street, New York, NY 10012 USA.

SHALIT@CS.NYU.EDG

\* Equal contribution

### Abstract

Observational studies are rising in importance due to the widespread accumulation of data in fields such as healthcare, education, employment. and evaluate. We consider the task of appropriate counterfactual questions such as, "Would this patient have lower blood sugar had she received a different medication?". We propose a new algorithmic framework for counterfactual inference which brings together ideas from domain adaptation and expresentation learning. In addition to a comparison with previous approaches to causal inference from observational data. Our deep learning algorithm significantly outperforms the provious state-of-the-art.

### 1. Introduction

Inferring causal relations is a fundamental problem in the sciences and commercial applications. The problem of questions (Lewis, 1973; Rubin, 1974; Pearl, 2009) such as "Would this nations have lower blood sugar had she received a different medication?", or "Would the user have clicked on this ad had it been in a different color?". In this for counterfactual inference, and show its efficacy in both simulated and real world tasks.

known as observational studies. Observational studies are studies where interventions and outcomes have been recorded, alone with appropriate context. For example, consider an electronic health record dataset collected over nceedings of the 33°4 International Conference on Machine Learning, New York, NY, USA, 2016. JMLR: W&CP volume

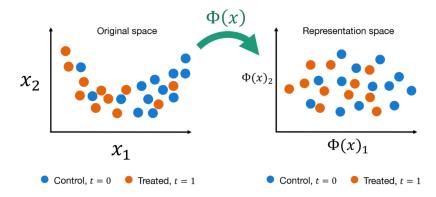
past diagnoses, as well as data relating to their diabetic status, and the causal question of interest is which of two existing anti-diabetic medications A or B is better for a given nations. Observational studies are rising in importance due to the widestread accumulation of data in fields such as healthcare, education, employment and ecology. We believe machine learning will be called on more and more to help make better decisions in these fields, and that researchers should be careful to pay attention to the ways in which these studies differ from classic supervised learning.

In this work we draw a connection between counterfactual inference and domain adaptation. We then introduce a form of negalarization by enforcing similarity between with different interventions. For example, the representations for patients who received medication A versus those who received medication B. This reduces the variance from such representations. In Section 4 we show our methods approximately minimizes an upper bound on a regret term in the counterfactual revime. The seneral method is outlined in Figure 1. Our work has commonalities with recent work on learning fair representations (Zernel et al., 2013; Louizos et al., 2015) and learning representations for transfer learning (Ben-David et al., 2007; Gará et al., 2015). In all these cases the learned representation has some invaricertain group such as racial minorities for fair representa-

In machine learning, counterfactual questions typically arise in problems where there is a learning arent which performs actions, and receives feedback or reward for that Learning Representations for Counterfactual Inference, 2016 (Fredrik D. Johansson, Uri Shalit, David Sontag.)

"We propose to perform counterfactual inference by amending the direct modeling approach, taking into account the fact that the learned estimator h must generalize from the factual distribution to the counterfactual distribution."

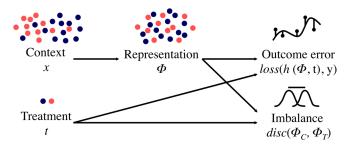
Instead of directly modeling h(X,T), we learn a representation  $\Phi(X)$  where the treated and control groups are similar or balanced, and only then apply  $h(\Phi(X),T)$ .

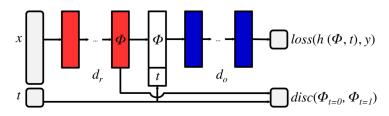


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Our networks should trade off between 3 main objectives:

- low-error prediction of the observed outcomes;
- low-error prediction of unobserved outcomes;
- balance between treatment populations in representation space.





Our objective is to minimize

$$B_{\alpha,\gamma}(\Phi,h) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} |h(\Phi(x_i),t_i) - y_i^{\mathrm{F}}|}_{\text{populations discrepancy}} + \underbrace{\frac{\gamma}{n} \sum_{i=1}^{n} |h(\Phi(x_i),1-t_i) - y_{\mathrm{nn}(i)}^{\mathrm{F}}|}_{\text{normalization}} + \underbrace{\frac{\gamma}{n} \sum_{i=1}^{n} |h(\Phi(x_i),1-t_i) - y_{\mathrm{nn}(i)}^{\mathrm{F}}|}_{\text{populations discrepancy}} + \underbrace{\frac{\gamma}{n} \sum_{i=1}^{n} |h(\Phi(x_i),1-t_i) - y_{\mathrm{nn}(i)}^{\mathrm{F}}|}_{\text{normalization}} + \underbrace{\frac{$$

where  $\alpha$  and  $\gamma$  are hyperparameters.

## The seminal paper

Causal Inference and Deep Learning

### Estimating individual treatment effect: generalization bounds and algorithms

#### Uri Shalit 11 Fredrik D. Johansson 12 David Sontag 23

### Abstract

There is intense interest in applying machine learning to problems of causal inference in fields such as healthcare, economics and education has important applications such as precision medicine. We rive a new theoretical analysis and family of algorithms for predicting indidata, under the assumption known as strong ignorability. The algorithms learn a 'balanced' representation such that the induced treated and control distributions look similar, and we give showing the expected ITE estimation error of a representation is bounded by a sum of the stanand the distance between the treated and control distributions induced by the representation. We use Interral Probability Metrics to measure distances between distributions, deriving explicit Discrepancy (MMD) distances. Experiments on real and simulated data show the new algorithms

#### 1 Introduction

Making predictions about causal effects of actions is a central problem in many domains. For example, a doctor decidize which medication will cause better outcomes for a rationt: a povernment deciding who would benefit most from subsidized job training; or a teacher deciding which study program would most benefit a specific student. In this paper we focus on the problem of making these predictions based on observational data. Observational data is Equal contribution CIMS, New York University, New York, NY 10003 IMIS, MIT, Cambridge, MA 02142 CSAIL, MIT, Cambridge, MA 02139. Correspondence ac Uri Shalit <shalit@cc.mva.elu>. Fredrik D. Johanson cfredrikj@mit.edu>, David Sontag <a href="mailto:choosafecuil.mit.edu">choonag@esuil.mit.edu></a>.

Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, PMLR 70, 2017. Copyright 2017

data which contains past actions, their outcomes, and possibly more context, but without direct access to the mechations (actions), and outcomes, but we do not have complete The hallmark of learning from observational data is that the actions observed in the data depend on variables which mister star effect the outcome, resulting in confounding: For example, richer patients might better afford certain medications, and job training might only be given to those motivated enough to seek it. The challenge is how to untargle these confounding factors and make valid predictions Specifically, we work under the common simplifying assumption of "no-hidden confounding", assuming that all the factors determining which actions were taken are ob measured a nationt's wealth or an employee's motivation.

As a learning problem, estimating causal effects from observational data is different from classic learning in that in our training data we never see the individual-level effect. For each unit, we only see their response to one of the posclose to what is known in the machine learning literature as "learning from logged bandit feedback" (Strehl et al., 2010; Swaminathan & Joschims, 2015), with the distinction that Our work differs from much work in casual inference in that we focus on the individual-level causal effect ("c. specific treatment effects" Shpitser & Pearl (2006); Pearl (2015)), rather than the average or population level. Our main contribution is to give what is, to the best of our knowledge, the first generalization-error1 bound for estimatine individual-level causal effect, where each individ ual is identified by its features x. The bound leads natu rally to a new family of representation-learning based algorithms (Bengio et al., 2013), which we show to match or

\*Our use of the term generalization is different from its use in

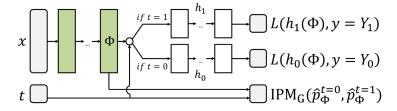
Estimating individual treatment effect: generalization bounds and algorithms, 2017 (Uri Shalit, Fredrik D. Iohansson, David Sontag.)

"The bound we derive points the way to a family of algorithms based on the idea of representation learning (Bengio et al., 2013): Jointly learn hypotheses for both treated and control on top of a representation which minimizes a weighted sum of the factual loss (the standard supervised machine learning objective), and the IPM distance between the control and treated distributions induced by the representation."

## Counterfactual Regression Net (CFRNet)

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- Now our network has 2 heads, and also 2 regression functions ( $h_0$  and  $h_1$ ), one for each potential outcome.
- The  $Y_1$  head is trained with samples from the treated group and the  $Y_0$  head is trained with samples from the control group.
- The IPM is an integral probability measure, which measures the distance between the 2 distributions in the representation space.

Our objective is now to find

$$\min_{h,\Phi} \frac{1}{n} \sum_{i=1}^{n} w_i \cdot L(h(\Phi(x_i), t_i), y_i) + \lambda \cdot \Re(h) + \alpha \cdot \text{IPM}_{G}(\{\Phi(x_i)\}_{i:t_i=0}, \{\Phi(x_i)\}_{i:t_i=1}),$$

where  $w_i = \frac{t_i}{2u} + \frac{1-t_i}{2(1-u)}$ ,  $u = \frac{1}{n}\sum_{i=1}^n t_i$ ,  $\Re(h)$  is a model complexity term and  $\alpha, \gamma$  are hyperparameters. Particularly, if  $\alpha = 0$ , the resulting architecture is called *Treatment Agnostic Representation Network* (TARNet).

Additionaly, this paper proves a bound on the expected error in estimating the ITE for a given representation. The expected *Precision in Estimation of Heterogeneous Effect* (PEHE), which is the MSE between predicted and true ITE, is bounded by

$$\epsilon_{\mathrm{PEHE}}(h,\Phi) \leq 2(\underbrace{\epsilon_{\mathrm{F}}^{t=0}(h,\Phi) + \epsilon_{\mathrm{F}}^{t=1}(h,\Phi)}_{\text{treatment and control losses}} + B_{\Phi} \underbrace{\mathrm{IPM}_{\mathrm{G}}(p_{\Phi}^{t=1},p_{\Phi}^{t=0})}_{\text{discrepancy}} - 2\sigma_{Y}^{2})$$

## Treatment modeling and targeted regularization

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### Adapting Neural Networks for the Estimation of Treatment Effects

Claudia Shi<sup>1</sup>, David M. Blei<sup>1,2</sup>, and Victor Veitch<sup>2</sup>

<sup>1</sup>Department of Computer Science, Columbia Unitversity <sup>2</sup>Department of Statistics, Columbia University

### Abstract

This paper addresses the use of hemoral networks for the estimation of treatment desiret from observational and concernils, estimation proceeds in two sugges First, secret for each unit. Second, we plug these fitted models into adversariation of the effects. Nexual networks are autitated to the first models in the continuous of the effect. Nexual networks are until a those for the models in the first manner of the effects of the end of

#### 1 Introduction

We consider the estimation of causal effects from observational data. Observational data is often readly smallable in intensities where randomized content visials (ECT) are required or impossible. However, causal inference from observational data ment address (possible) conformating factors that affects but intensit and contense. Failure to adjust for conformative ratio in incerts consistions. To address this, a practitioner collects or oursities information in addition to intensit and outcome.

To address this, a practitioner collect can be destinted if the oversities contain all conformations and outcome states. The causal effect can be destinted if the oversities contain all conformations are destinated in the observation of the contract of the observation of

We consider how to use neural networks to estimate the reatment effect. The estimation of treatment for effects proceeds in two stages. First, we fit models for the conditional outcome  $(P_k, y = \mathbb{R}^V)^T | 1, 2, 3$  and the proposality score g(x) = P(T = 1|x). Then, we plug these fitted models into a downstream earlier constitution. The strong predictive performance of neural networks motivates their use for effects estimated in  $\{g_k, y_k\} \in \mathbb{R}^N : \{g_k\} \in \mathbb{R}^N : \{g_k\}$ 

In principle, using neural networks for the conditional outcome and propensity score models is straightforward. We can use a standard net to predict the outcome Y from the treatment and covariates, and another to predict the treatment from the covariates. With a suitable choice of training objective, the trained models will yield consistent estimates of the conditional outcomes and propensity scores. However, neural network research has focused on predictive performance. What is Adapting Neural Networks for the Estimation of Treatment Effects, 2019 (Claudia Shi, David M. Blei, Victor Veitch.)

"We propose two adaptations based on insights from the statistical literature on the estimation of treatment effects. The first is a new architecture, the Dragonnet, that exploits the sufficiency of the propensity score for estimation adjustment. The second is a regularization procedure, targeted regularization, that induces a bias towards models that have non-parametrically optimal asymptotic properties 'out-of-the-box'."

## Propensity Score

Measures the conditional distribution of T given X, and is given by g(X) = p(T = 1|X). A famous result states that the propensity score is sufficient for estimating the ATE controlling X.

If the ATE is identifiable form the observational data, then

$$\begin{split} \text{ATE} &= \mathbb{E}\left[\mathbb{E}[Y|X,T=1] - \mathbb{E}[Y|X,T=0]\right] \\ &= \mathbb{E}\left[\mathbb{E}[Y|g(X),T=1] - \mathbb{E}[Y|g(X),T=0]\right] \end{split}$$

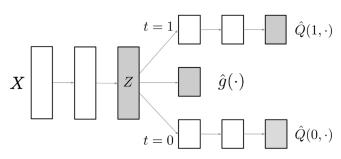
The intuition here is that, when controlling for X, the only part of X that is important is the one which confounds T. If it is not relevant for T, then it is not relevant for estimating treatment effect.

Using g in our estimation process means that we are not just modeling *outcomes*, but also the treatment itself.

## Dragonnet architecture

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Dragonnet is very similar to TARNet. The addition is the extra head g. This network tries to predict both outcome and treatment. The representation layer Z has a similar idea from the previous archtectures, but the reasoning here is leveraging the sufficiency of the propensity score and trading off predictive accuracy and propensity score propensity propensity

$$\hat{\theta} = \min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \underbrace{\left[ \left( Q(t_i, x_i; \theta) - y_i \right)^2 + \alpha \underbrace{\mathsf{CrossEntropy}}(g(x_i; \theta), t_i) \right]}_{\text{outcome loss}} + \alpha \underbrace{\mathsf{CrossEntropy}}(g(x_i; \theta), t_i) \underbrace{\mathsf{CrossEntropy}}_{\text{treatment loss}}$$

## Building a framework

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### Generalization Bounds and Representation Learning for Estimation of Potential Outcomes and Causal Effects

Fredrik D. Johansson<sup>\*1</sup>, Uri Shalit<sup>2</sup>, Nathan Kallus<sup>3</sup>, David Sontag<sup>4</sup>

<sup>1</sup>Chalmers University of Technology <sup>2</sup>Technion, Israel Institute of Technology <sup>3</sup>Cornell Tech <sup>4</sup>Massachusetts Institute of Technology

### Abstract

Practitioners in diverse fields such as healthcare, economics and education are eager to apply machine learning to improve decision making. The cost and impracticality of performing experiments and a recent monumental increase in electronic record keeping has brought attention to the problem of evaluating decisions based on non-experimental observational data. This is the setting of this work. In particular, we study estimation of individual-level causal effects, such as a single patient's response to alternative medication, from recorded contexts, decisions and outcomes. We give generalization bounds on the error in estimated effects based on distance measures between groups receiving different treatments, allowing for sample re-weighting. We provide conditions under which our bound is tight and show how it relates to results for unsupervised domain adaptation. Led by our theoretical results, we devise representation learning algorithms that minimize our bound, by regularizing the representation's induced treatment group distance, and encourage sharing of information between treatment groups. We extend these algorithms to simultaneously learn a weighted representation to further reduce treatment group distances. Finally, an experimental evaluation on real and synthetic data shows the value of our proposed representation architecture and regularization

#### 1 Introduction

Evaluating intervention decisions is a key question in many diverse fields including medicine, concouncies, and echanicals, in medicine, an equilar advise of treatment for a patient in the intensive one unit may mean the difference between life and death. In public policy, job refreshem have impact to the mempleyment run and the economy of a nation. To evaluate such interventions, we must study their consist effect—the difference in an outcome of intervent under alternative decises of intervention. Since early one option may be carried out at a time, any data to support such evaluations only reveals the outcome of the action takes and never the outcome of the action take many whether the action takes mad never the outcome of the action take man, which remains a unixone constricted.

Generalization Bounds and Representation Learning for Estimation of Potential Outcomes and Causal Effects, 2021 (Fredrik D. Johansson, Uri Shalit, Nathan Kallus, David Sontag.)

"We give generalization bounds on the error in estimated effects based on distance measures between groups receiving different treatments, allowing for sample reweighting. We provide conditions under which our bound is tight and show how it relates to results for unsupervised domain adaptation."

<sup>\*</sup>Correspondence to: fredrik.iohansson@chalmers.se

- Selecting hyperparameters in supervised learning is fairly straightforward. We just have to experiment with different values and pick the combination that is best offers the best prediction on the validation set.
- In causal inference we have no access to our counterfactuals, which is what we are trying to predict, so how could we select the best hyperparameters for our observatoinal data?
- This paper proposes an experimental setup with baseline estimators as well as a hyperparameter selection method, based on nearest neighbors.

To substitute the ground-truth potential outcomes, we use pseudo-labels for the CATE. Suppose j(i) is the nearest "counterfacutal" neighbor of the sample i in Euclidean distance, such that  $t_{j(i)} \neq t_i$ . The metric

$$\widehat{\text{MSE}}_{\text{nn}}(f) := \frac{1}{n} \sum_{i=1}^{n} \left[ (1 - 2t)(y_{j(i)} - y_i) - (f(x_i, 1) - f(x_i, 0)) \right]^2$$

is computed in the validation set for each hyperparameter combination, and the best combination is selected.

- Models depend too much on training data and are not good at generalization;
- Machine Learning models assume that real-world data will have the same distribution as the one used in training;
- humans learn with no such assumption, by learning the underlying structure of reality, in other words, a causal model.

## How can Machine Learning evolve?

Causal Inference and Deep Learning

### Towards Causal Representation Learning

Bernhard Schölkopf †, Francesco Locatello †, Stefan Bauer \*, Nan Rosemary Ke \*, Nal Kalchbrenner Anirudh Goyal, Yoshua Bengio

Abstract—The two fields of machine learning and graphical - natural language processing [58], and speech recognition [85]. Astron — The Ires leibts of machine marring and graphical causality arose and developed separately. However, there is now cross-polination and increasing interest in both fields to benefit from the advances of the other. In the present paper, we review crucial open problems of machine learning, including transfer and generalization, thereby assaying how causality can contribute to modern machine learning research. This also applies in the opposite direction; we note that most work in casuality starts from the premise that the causal variables are given. A central problem for AI and causality is, thus, causal proposentation learning, the discovery of high-level causal variables from low level observations. Finally, we delineate some implications of were proposed to uncellically test centralization of classification causality for machine learning and propose key research areas and detection methods with respect to simple algorithmically at the intersection of both communities.

accomplish, we observe that the former is rather limited at some the potential to lead to insights into the inductive biases of crucial feats where natural intelligence excels. These include state-of-the-art architectures. So far, there has been no definitive transfer to new problems and any form of generalization that - consensus on how to solve these problems, although progress is not from one data point to the next (xampled from the has been made using data augmentation, pre-training, selfsame distribution), but rather from one problem to the next - supervision, and architectures with suitable inductive biases both have been termed generalization, but the latter is a much w.r.t. a perturbation of interest (233, 59, 63, 137, 137, 139, 63, harder form thereof, sometimes referred to as hovicontal, strong. has been argued [158] that such fixes may not be sufficient. or our-of-distribution generalization. This shortcoming is not und generalizing well outside the i.i.d. setting requires learning too surprising, given that machine learning often disregards not more statistical associations between variables, but an information that animals use heavily: interventions in the world, underlying coasel model. The latter contains the mechanisms domain shifts, temporal structure - by and large, we consider these factors a misance and try to engineer them away. In accordance with this, the majority of current successes of machine [IES 237 218 D4 IES IES]. collected independent and identically distributed (i.i.d.) data. To illustrate the implications of this choice and its relation to causal models, we start by highlighting key research challenges.

 considerion.
 Schillepf is at the Max Planck Institute for Intelligent Systems, Max-Planck-Ring 4, 7205 Tablegen, Germany, Institute Languages, app. do.
 F. Locatello is at ETH Zurich, Computer Science Department and the Max N. R. Ke is at Mila and the University of Montreal, rese-

years Lettymation.

Kalchbrener is at Google Rocarch Ametedam, calkingcogle.com.

Gogal is at Mila and the University of Menteral,

a substantial body of literature explored the pobustness of the prediction of state-of-the-art deep neural network architectures. which the data comes from. In computer vision [73, 228]. from aberrations like camera blar, noise or compression quality (108, 1124, 170, 206), or from shifts, rotations, or generated interventions like spatial shifts, blar, changes in control over background and rotation [11], as well as images collected in multiple environments (FQ). Studying the failure If we compare what machine learning can do to what animals — modes of does neural networks from simule interventions has giving rise to the observed statistical dependences, and allows b) Issue 2 - Learning Reunable Mechanisms: Infants'

understanding of physics relies upon objects that can be tracked over time and behave consistently [52, 229]. Such a representation allows children to quickly learn new tasks as a) June 1 - Rebustness: With the widownest adoption their knowledge and intuitive understanding of physics can of deep learning approaches in computer vision [IOI, 140]. he re-used [IS, 52, 134, 1250]. Similarly, intelligent agents that robustly solve real-world tasks need to re-use and re-purpose their knowledge and skills in novel securios. Machine learning models that incorporate or learn structural knowledge of an environment have been shown to be more efficient and peneralize better fF4 IIR IIR R4 II97 212 R 274 28 76 R3 physical causal mechanisms, many modules can be expected to to adapt a few modules in its internal representation of the and rudbpoyal \$11 Prignal 1, con
Y. Buggo is at Mila, the University of Montrud, CIFAR Souter Fellow world [228] [848]. When learning a causal model, one should Towards Causal Representation Learning, 2021 (Bernhard Schölkopf, Francesco Locatello, Stefan Bauer, Nan Rosemary Ke, Nal Kalchbrenner, Anirudh Goyal, Yoshua Bengio.)

"...causality, with its focus on representing structural knowledge about the data generating process that allows interventions and changes, can contribute towards understanding and resolving some limitations of current machine learning methods."

### **Papers**

- Learning Representations for Counterfactual Inference
- Estimating individual treatment effect: generalization bounds and algorithms, 2017
- Adapting Neural Networks for the Estimation of Treatment Effects, 2019
- Generalization Bounds and Representation Learning for Estimation of Potential Outcomes and Causal Effects, 2021
- Towards Causal Representation Learning, 2021

### **External Material**

- Joshua Angrist interview
- Causal Inference for The Brave and True
- Yoshua Bengio Talk on Causal Representation Learning
- Deep Learning of Potential Outcomes
- Deep Learning for Causal Inference Tutorial GitHub
- Causal Inference class in MIT's Machine Learning for Healthcare (Spring 2019) course