

# Causality

Bernhard Schölkopf

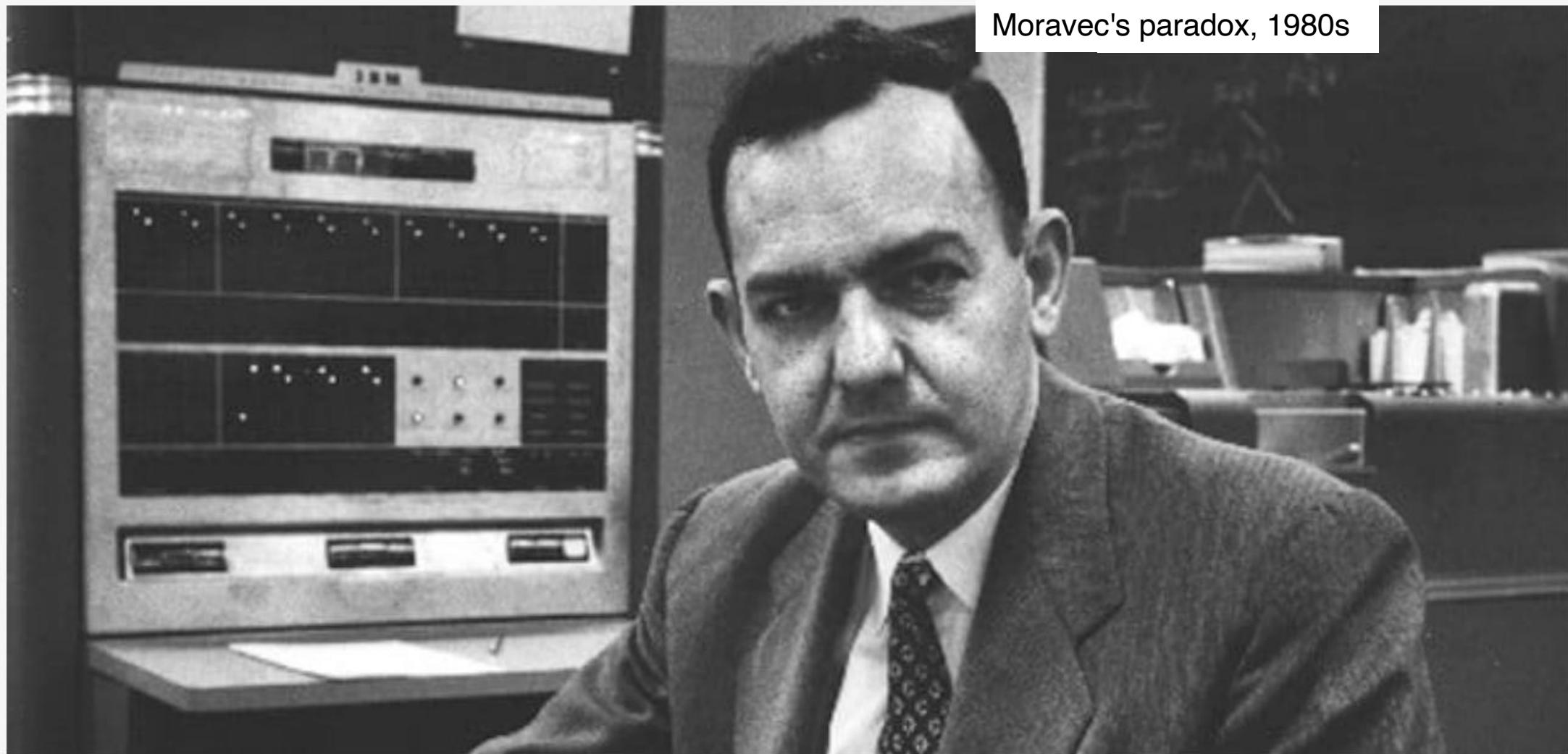
Max Planck Institute for Intelligent Systems & ETH Zürich

*Bernhard Schölkopf*



Max Planck ETH Center for Learning Systems

Moravec's paradox, 1980s



**"Machines will be capable, within twenty years, of doing any work a man can do"**



# THE NEURAL NET TANK URBAN LEGEND

*AI folklore tells a story about a neural network trained to detect tanks which instead learned to detect time of day; investigating, this probably never happened.*

NN, history, sociology, Google, bibliography

20 Sep 2011–14 Aug 2019 · finished · certainty: highly likely · importance: 4

SITE  
ME  
NEW:  
• MAIL  
• /R/GWERN

SUPPORT ON  
PATREON

## 1 Did It Happen?

- 1.1 Versions of the Story
  - 1.1.1 2010s
  - 1.1.2 2000s
  - 1.1.3 1990s
  - 1.1.4 1980s
  - 1.1.5 1960s

## 1.2 Evaluation

- 1.2.1 Sourcing
- 1.2.2 Variations
- 1.2.3 Urban Legends
- 1.2.4 Origin

## 2 Could it Happen?

- 2.1 Could Something Like it Happen?

## 3 Should We Tell Stories We Know Aren't True?

- 3.1 Alternative examples

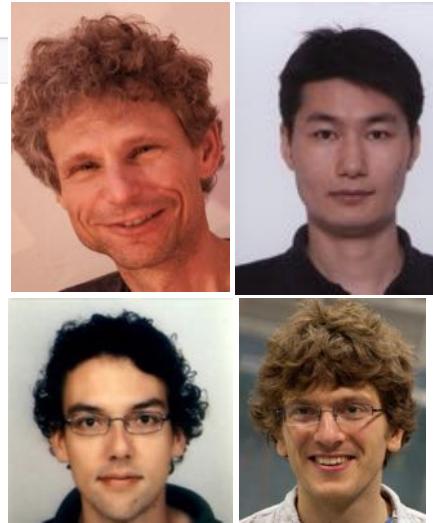
## 4 See Also

## 5 External Links

A cautionary tale in artificial intelligence tells about researchers training an neural network (NN) to detect tanks in photographs, succeeding, only to realize the photographs had been collected under specific conditions for tanks/non-tanks and the NN had learned something useless like time of day. This story is often told to warn about the limits of algorithms and importance of data collection to avoid “dataset bias”/“data leakage” where the collected data can be solved using algorithms that do not generalize to the true data distribution, but the tank story is usually never sourced.

I collate many extent versions dating back a quarter of a century to 1992 along with two NN-related anecdotes from the 1960s; their contradictions & details indicate a classic “urban legend”, with a probable origin in a speculative question in the 1960s by Edward Fredkin at an AI conference about some early NN research, which was subsequently classified & never followed up on.

I suggest that dataset bias is real but exaggerated by the tank story, giving a misleading indication of risks from deep learning and that it would be better to not repeat it but use real examples of dataset bias and focus on larger-scale risks like AI systems optimizing for wrong utility functions.



day (“environment”)

tank class

weather

image



MAX-PLANCK-GESELLSCHAFT

# Human-level object recognition?



cow	milk	agriculture	farm	cattle	livestock	dairy
beef	hayfield	field	grass	mammal	pasture	calf
farmland	rural	animal	pastoral	bull	grassland	



cow	beef	agriculture	cattle	milk	pasture	mammal
livestock	farmland	grass	farm	hayfield	rural	herd
dairy	pastoral	grassland	field	calf	bull	



cow	mammal	pasture	grass	animal	no person	nature
agriculture	livestock	hayfield	cattle	farm	rural	field
milk	grassland	beef	pastoral	country	sides	

*from Perona, 2017;  
cf. Lopez-Paz et al., 2016*

# Machine learning uses correlations rather than causality



beach sand travel no person water sea seashore  
summer sky outdoors ocean nature



no person water mammal cattle outdoors cow  
landscape travel sky livestock



water no person beach seashore sea sand mammal  
outdoors travel ocean surf sky

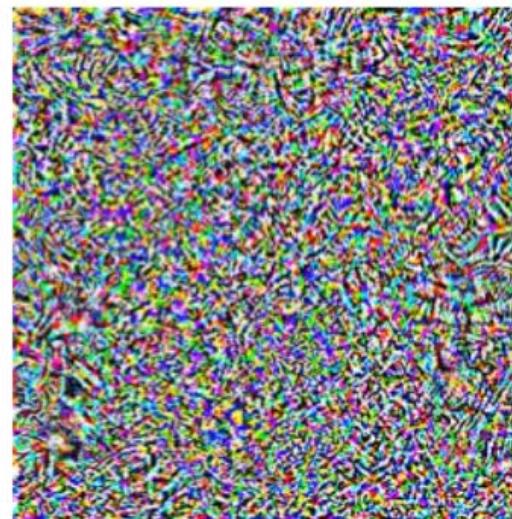
*from Perona, 2017;  
cf. Lopez-Paz et al., 2016*

# Adversarial Vulnerability

“pig”



+ 0.005 ×



=

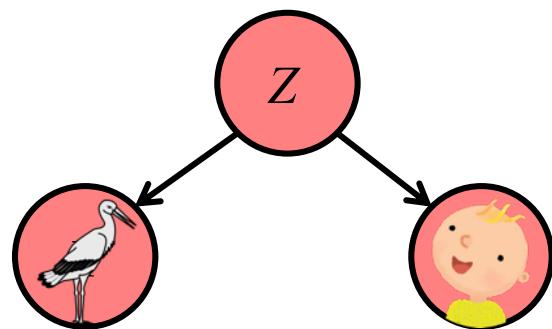


Image credit: [http://people.csail.mit.edu/madry/lab/blog/adversarial/2018/07/06/adversarial\\_intro/](http://people.csail.mit.edu/madry/lab/blog/adversarial/2018/07/06/adversarial_intro/)

C. Szegedy et al. Intriguing properties of neural networks. *arXiv:1312.6199*, 2013

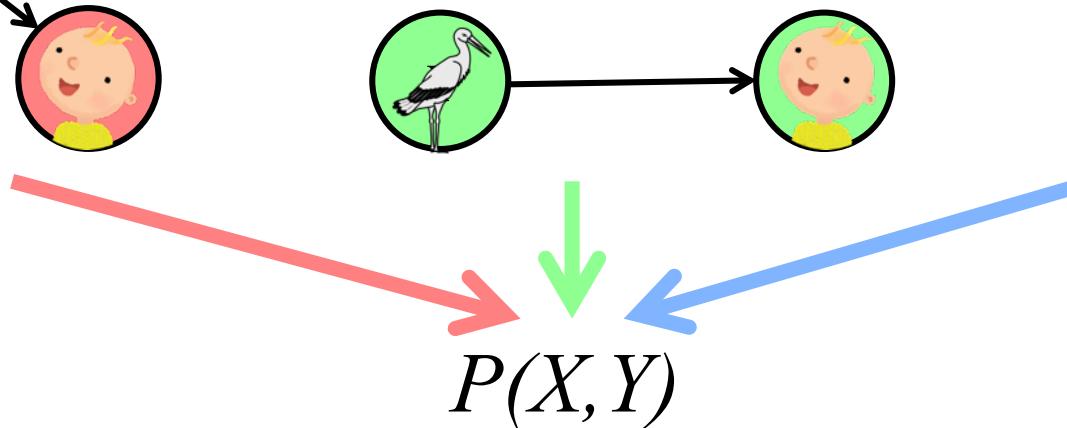
# Reichenbach's Common Cause Principle

(i) if  $X$  and  $Y$  are dependent, then there exists  $Z$  *causally* influencing both;



(ii)  $Z$  screens  $X$  and  $Y$  from each other (given  $Z$ ,  $X$  und  $Y$  become independent)

by permission of the  
University of Pittsburgh.  
All rights reserved.



$$\sum_z p(x|z)p(y|z)p(z)$$

$$p(x)p(y|x)$$

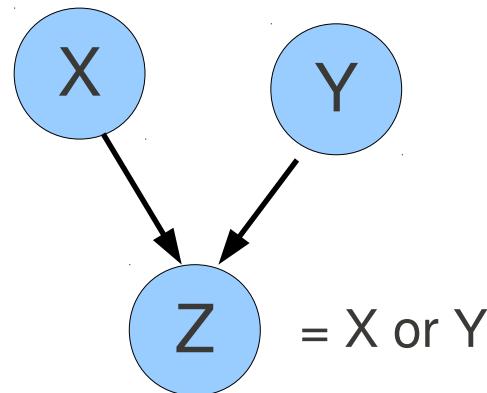
$$p(x|y)p(y)$$

Bernhard Schölkopf



# Correlation by conditioning on common effects

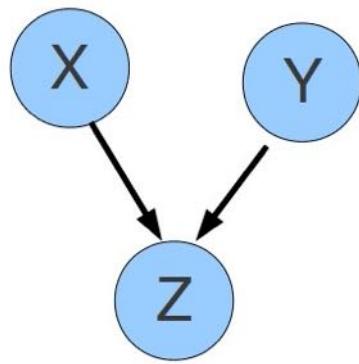
Berkson's paradox (1946)  
Example:  $X, Y, Z$  binary



$$X \perp\!\!\!\perp Y \quad \text{but} \quad X \not\perp\!\!\!\perp Y | Z$$

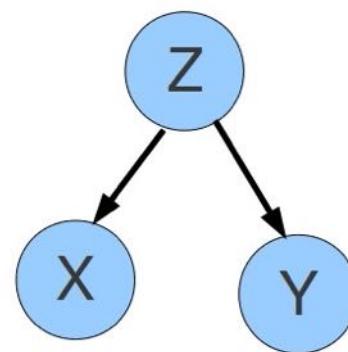
- assumption 1: there is no correlation between being a good speaker ( $X$ ) and being a good scientist ( $Y$ )
- assumption 2: to be successful, you need to be either a good speaker or a good scientist (or both)
- among the successful scientists, there is a *negative* correlation between being a good speaker and being a good scientist

# Asymmetry under inverting arrows



$$X \perp\!\!\!\perp Y$$

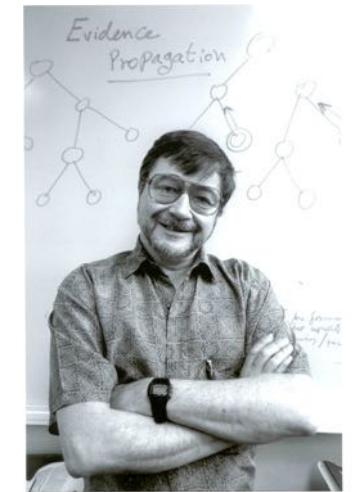
$$X \not\perp\!\!\!\perp Y | Z$$



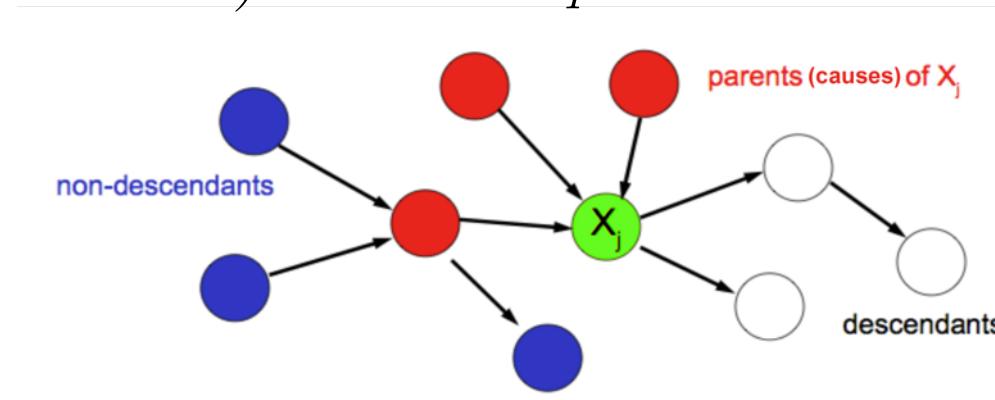
$$X \not\perp\!\!\!\perp Y$$

$$X \perp\!\!\!\perp Y | Z$$

# Definition of a Structural Causal Model (Pearl et al.)



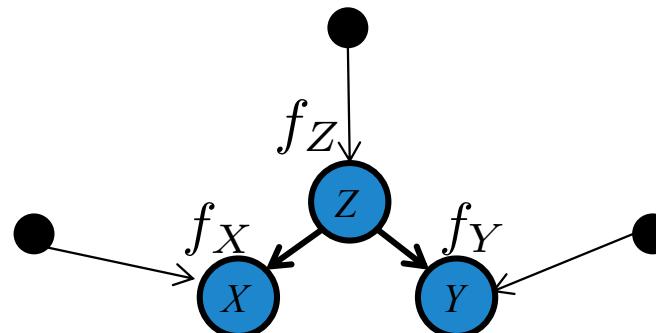
- directed acyclic graph  $G$  with vertices  $X_1, \dots, X_n$   
(following arrows does not lead to loops)
- Semantics: vertices = observables, arrows = direct causation
- $X_i := f_i(\text{PA}_i, U_i)$ , with independent RVs  $U_1, \dots, U_n$  that possess a joint density
- $U_i$  stands for “unexplained” (alternatively “noise” or “exogenous variable”)
- this is also called a *(nonlinear) structural equation model*



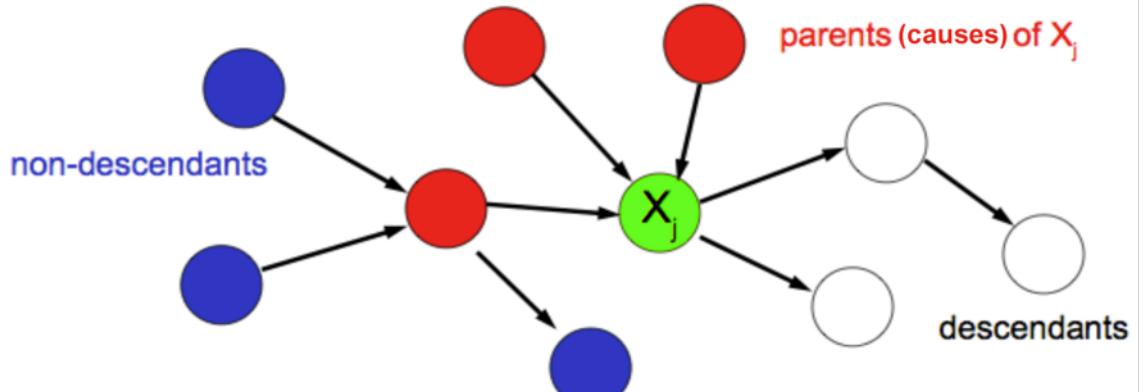
Bernhard Schölkopf

# Reichenbach's Principle and causal sufficiency

- Independence of noises is a form of "causal sufficiency:" if the noises were dependent, then Reichenbach's principle would tell us the causal graph is incomplete
- The SCM model satisfies Reichenbach's principle:
  1. functions of independent variables are independent, hence dependence can only arise in two vertices that depend (partly) on the same noise term(s).
  2. if we condition on these noise terms, the variables become independent

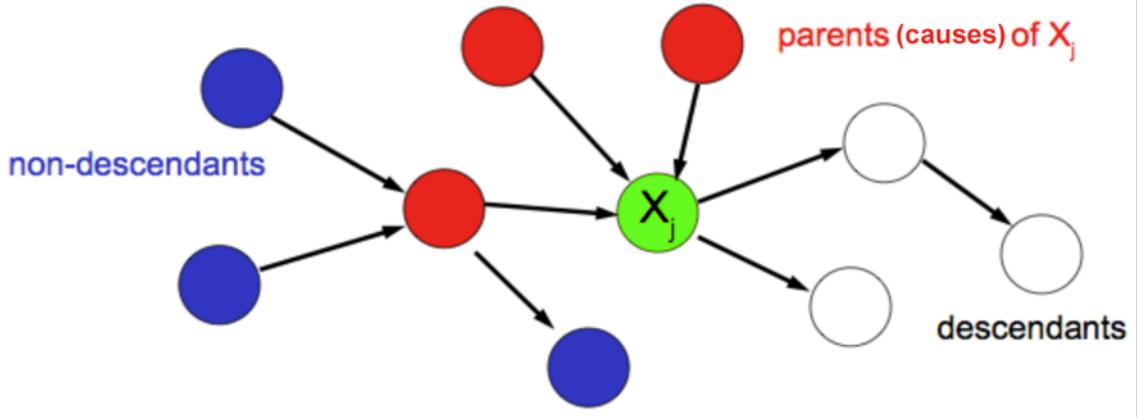


# Entailed distribution



- $X_i := f_i(\text{PA}_i, U_i)$ ,  
with independent  $U_1, \dots, U_n$ .
- Recursively substitute the parent equations to get  $X_i = g_i(U_1, \dots, U_n)$ ,  
with independent  $U_1, \dots, U_n$ .
- Each  $X_i$  is thus a RV and we get a joint distribution of  $X_1, \dots, X_n$ ,  
called the *observational distribution*.
- The distribution and the DAG form a *directed graphical model* and  
any directed graphical model can be written as a functional causal  
model.

# Entailed distribution



- A structural causal model entails a joint distribution  $p(X_1, \dots, X_n)$ .

## Questions:

- (1) What can we say about it?
- (2) Can we recover  $G$  from  $p$ ?

# Markov conditions (*Lauritzen 1996, Pearl 2000*)

**Theorem:** the following are equivalent:

- Existence of a structural causal model
- Local Causal Markov condition:  $X_i$  statistically independent of non-descendants, given parents (i.e.: every information exchange with its non-descendants involves its parents)
- Global Causal Markov condition: “d-separation” (characterizes the set of independences implied by local Markov condition — see below)
- Factorization  $p(X_1, \dots, X_n) = \prod_i p(X_i | \text{PA}_i)$

(subject to technical conditions)

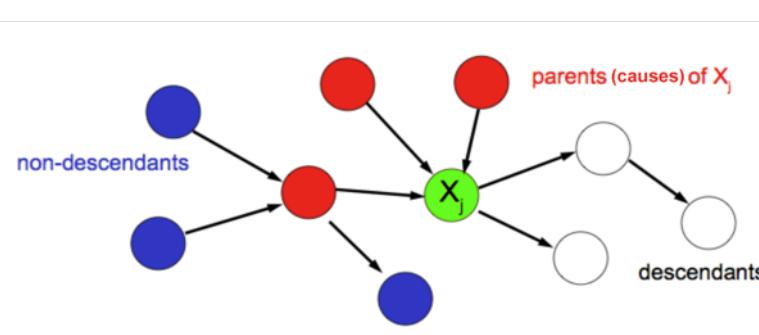
$p(X_i | \text{PA}_i)$  is called a *causal conditional* or *causal Markov kernel*.  
It corresponds to the structural “equation”  $X_i := f_i(\text{PA}_i, U_i)$ .

Not every conditional is causal — only those that condition on the parents in our DAG.

## Graphical Causal Inference (*Spirites, Glymour, Scheines, Pearl, ...*)

**Question:** How can we recover  $G$  from a single  $p$  (e.g., from the observational distribution)?

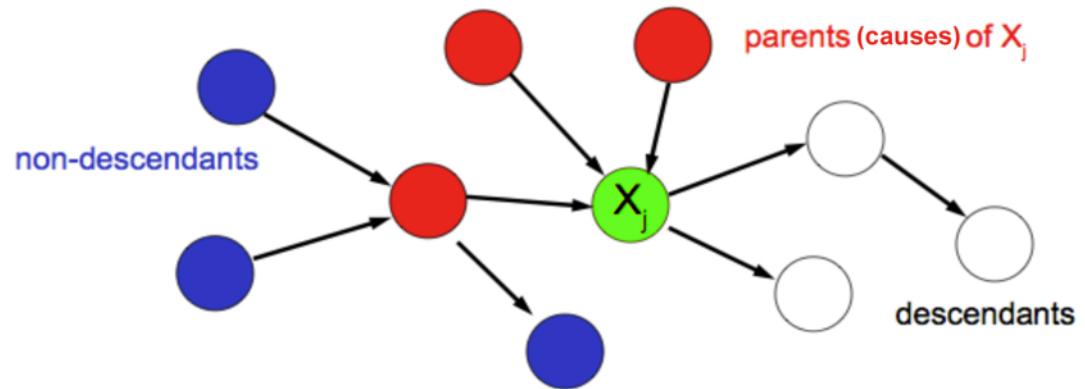
**Answer:** by conditional independence testing, infer a class containing the correct  $G$  (*i.e.*, track how the noise information spreads).



### Problems:

- Markov condition states  $(X \perp\!\!\!\perp Y | Z)_G \Rightarrow (X \perp\!\!\!\perp Y | Z)_p$ , but we need “faithfulness”  $(X \perp\!\!\!\perp Y | Z)_G \Leftarrow (X \perp\!\!\!\perp Y | Z)_p$  (*Spirites, Glymour, Scheines 2001*)  
Hard to justify for finite data (*Uhler, Raskutti, Bühlmann, Yu, 2013*).
- if the  $f_i$  are complex, then conditional independence testing based on finite samples becomes arbitrarily hard
- for **two variables** only, there are no conditional independences

# Interventions and shifts



- **Definition.** Replacing  $X_i := f_i(\text{PA}_i, U_i)$  with another assignment (e.g.,  $X_i := \text{const.}$ ) is called an *intervention* on  $X_i$ .
- The entailed distribution is called the *interventional distribution*.
- This contains as special cases: domain shift distribution and covariate shift distribution (see below).
- A general intervention corresponds to changing some *causal conditionals*  $p(X_i|\text{PA}_i)$

## Pearl's do-calculus

- Motivation: goal of causality is to infer the effect of interventions
- distribution of  $Y$  given that  $X$  is set to  $x$ :  $p(Y|do X = x)$  or  $p(Y|do x)$
- don't confuse it with  $p(Y|x)$
- can be computed from  $p$  and  $G$

# Difference between seeing and doing

$$p(y|x)$$

Probability a participant of this course can get a NeurIPS paper accepted

$$p(y \mid \text{do } x)$$

Probability that anyone can get a NeurIPS paper accepted after being made to participate in this course

# Computing $p(X_1, \dots, X_n | do x_i)$

from  $p(X_1, \dots, X_n)$  and  $G$

- Start with causal factorization

$$p(X_1, \dots, X_n) = \prod_{j=1}^n p(X_j | PA_j)$$

- Replace  $p(X_i | PA_i)$  with  $\delta_{X_i x_i}$

$$p(X_1, \dots, X_n | do x_i) := \prod_{j \neq i} p(X_j | PA_j) \delta_{X_i x_i}$$

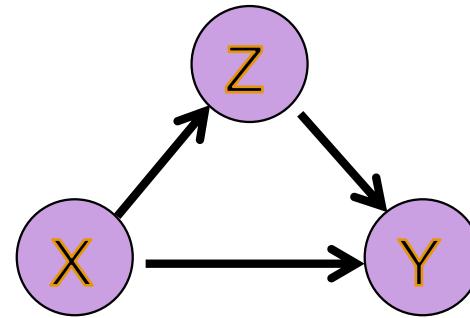
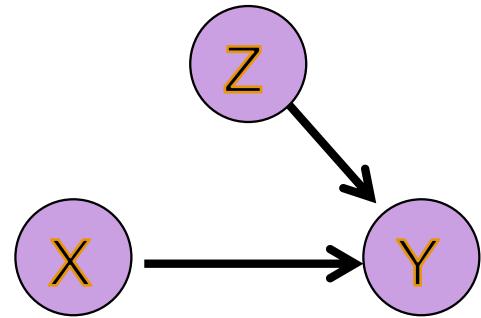
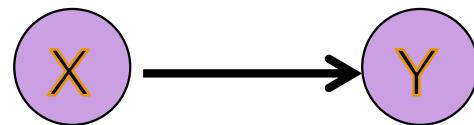
# Computing $p(X_k|do\ x_i)$

Sum over  $x_i$  to get

$$p(X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_n | do\ x_i) = \prod_{j \neq i} p(X_j | PA_j(x_i)).$$

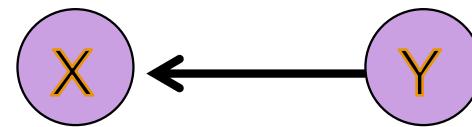
- i.e.: for  $j \neq i$ , drop  $p(X_j | PA_j)$  and substitute  $x_i$  for  $X_i$
- obtain  $p(X_k | do\ x_i)$  by marginalisation

Examples for  $p(.|do x) = p(.|x)$

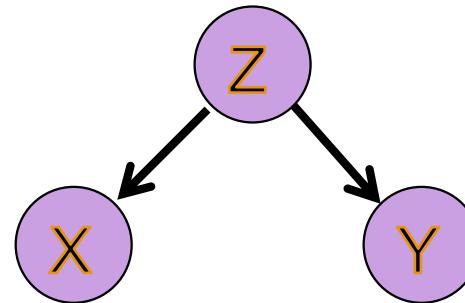


# Examples for $p(.|do x) \neq p(.|x)$

- $p(Y|do x) = P(Y) \neq P(Y|x)$



- $p(Y|do x) = P(Y) \neq P(Y|x)$

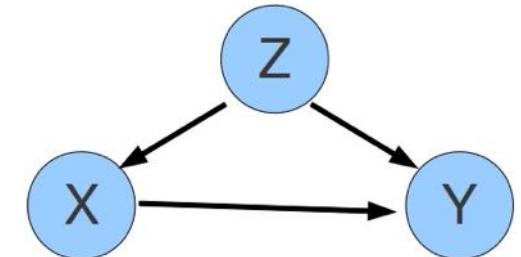


## Controlling for confounding / adjustment formula

$Y$  depends on  $X$  due to  $X \rightarrow Y$  and the confounder  $Z$

- Causal factorization

$$p(X, Y, Z) = p(Z) p(X|Z) p(Y|X, Z)$$



- Replace  $p(X|Z)$  with  $\delta_{Xx}$  and integrate out  $X$ :

$$\begin{aligned} p(X, Y, Z|do\ x) &= p(Z) \delta_{Xx} p(Y|X, Z) \\ p(Y, Z|do\ x) &= p(Z) p(Y|x, Z) \end{aligned}$$

- marginalize over  $Z$  to get the "adjustment formula"

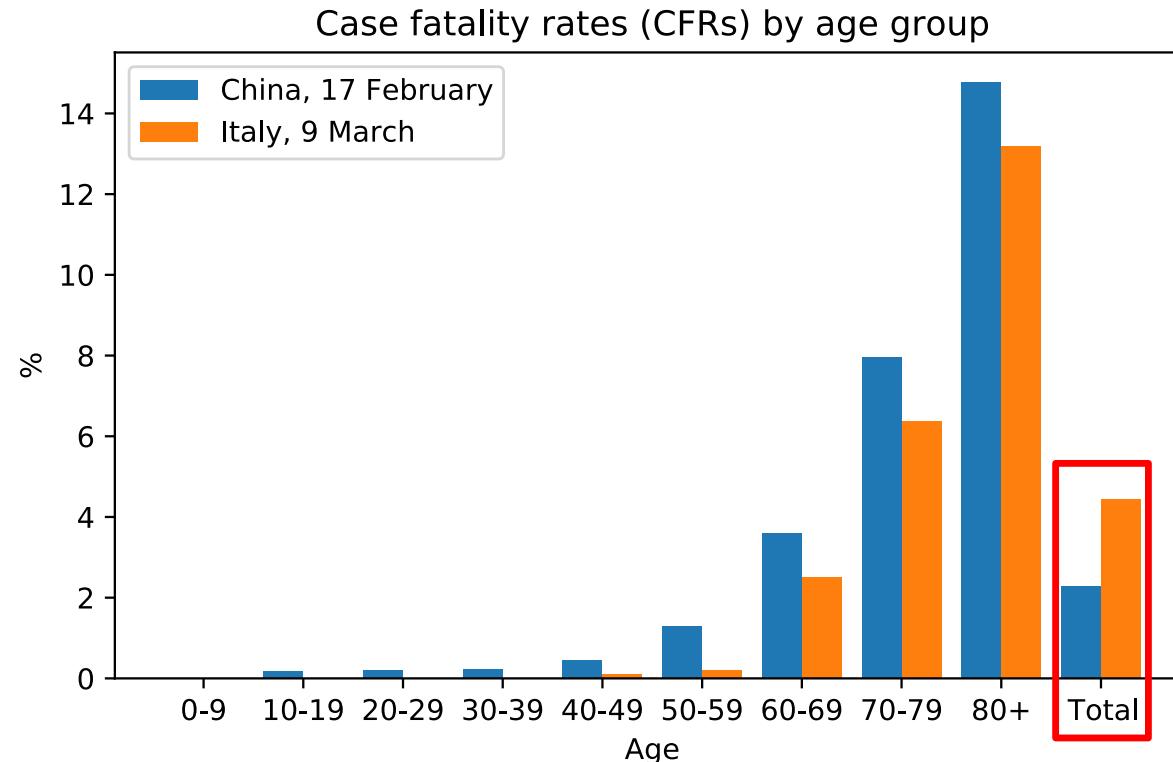
$$p(Y|do\ x) = \sum_z p(z) p(Y|x, z)$$



This is different from  $p(Y|x)$  (Simpson's paradox).

# Simpson's paradox in Covid-19 case fatality rates

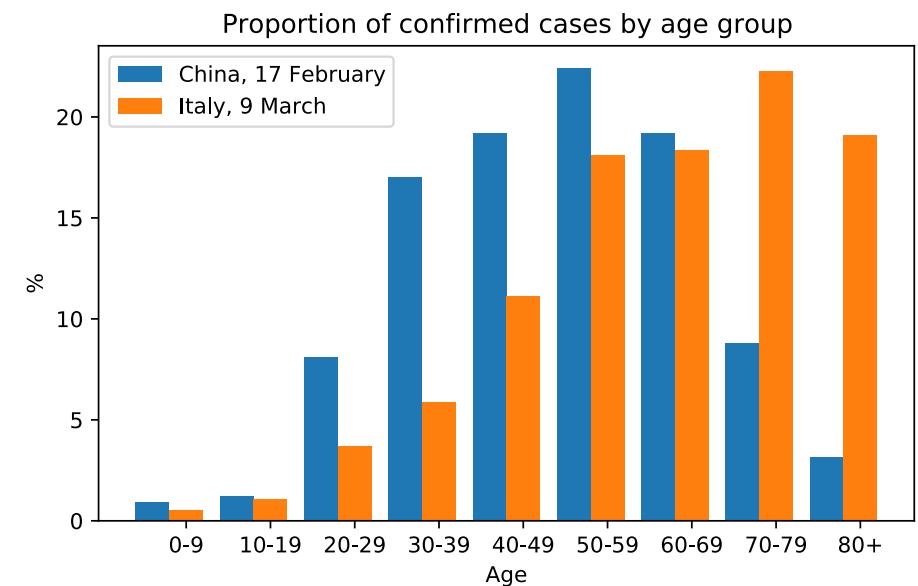
(v. Kügelgen, Gresele, <https://arxiv.org/abs/2005.07180> / IEEE Trans. AI)



Case fatality rates (CFRs) in Italy are *lower* for each age group, but *higher* overall.

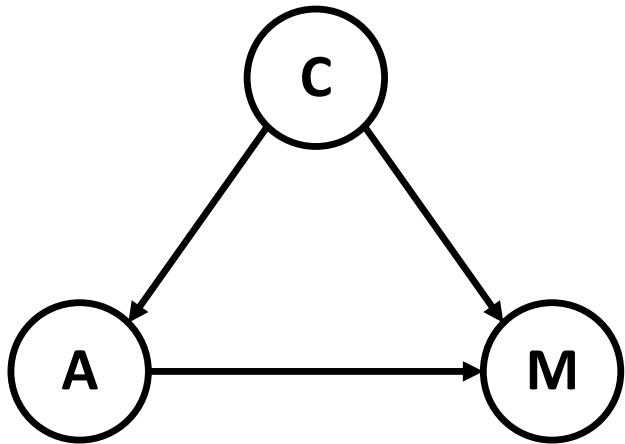
**Simpson's paradox:** opposite trends in grouped and aggregated data.

Here, it stems from a difference in case demographic:



Thanks to Elias Bareinboim

# Coarse-grained causal graph



## Data generating process:

- Randomly pick a **country C**
- Given **C**, sample a *positively-tested* patient with **age group A**
- Given **C** and **A**, sample **medical outcome, or mortality, M** (deceased at time of reporting?)

## Assumptions & meaning of directed arrows:

- **C → A**: general population demographic, inter-generational mixing, age-specific social-distancing, ...
- **A → M**: age-related health condition & other comorbidities.
- **C → M**: number of ventilators & ICU beds, ...

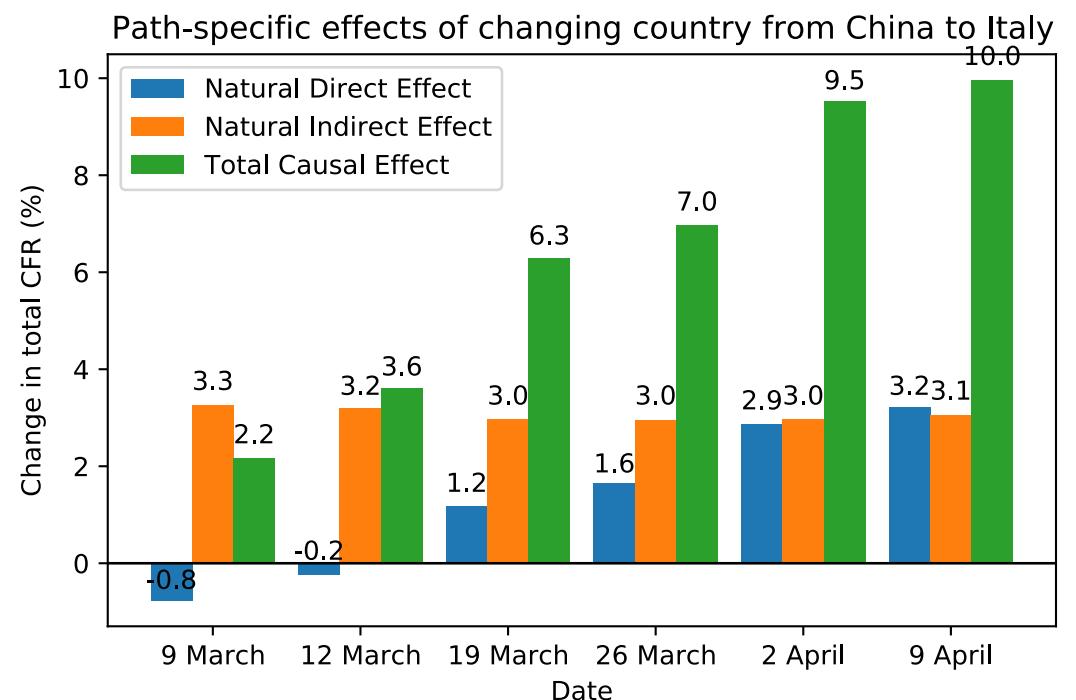
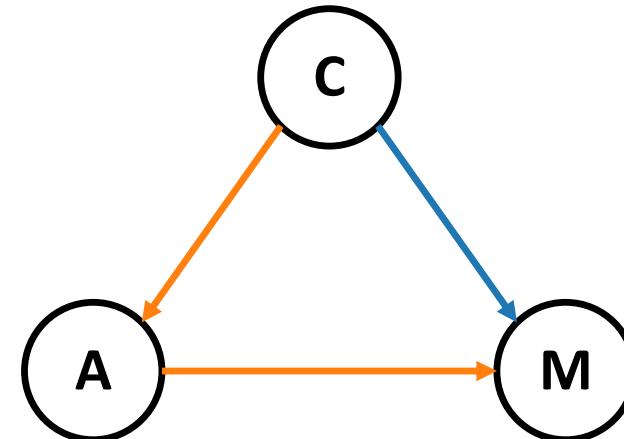
# Mediation analysis

*Only for linear models* can **total causal effect (TCE)** be decomposed into direct effect (DE) and indirect effect (IE),

$$TCE = DE + IE$$

Due to interactions, DE and IE are *not uniquely defined in general*, but depend on the state of the mediator.

- **Natural Direct Effect (NDE):** case demographic kept as in China while CFRs per age group changed to those in Italy.
- **Natural Indirect Effect (NIE):** CFRs per age group kept as in China, while case demographic changed to that in Italy.



Does it make sense to talk about  
causality without mentioning time?

Does it make sense to talk about  
statistics without mentioning time?

# Causality in differential equations

Consider the set of differential equations

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d,$$

with initial value  $\mathbf{x}(t_0) = \mathbf{x}_0$ .

**Picard–Lindelöf:** locally, if  $f$  is Lipschitz, there exists a unique solution  $\mathbf{x}(t)$

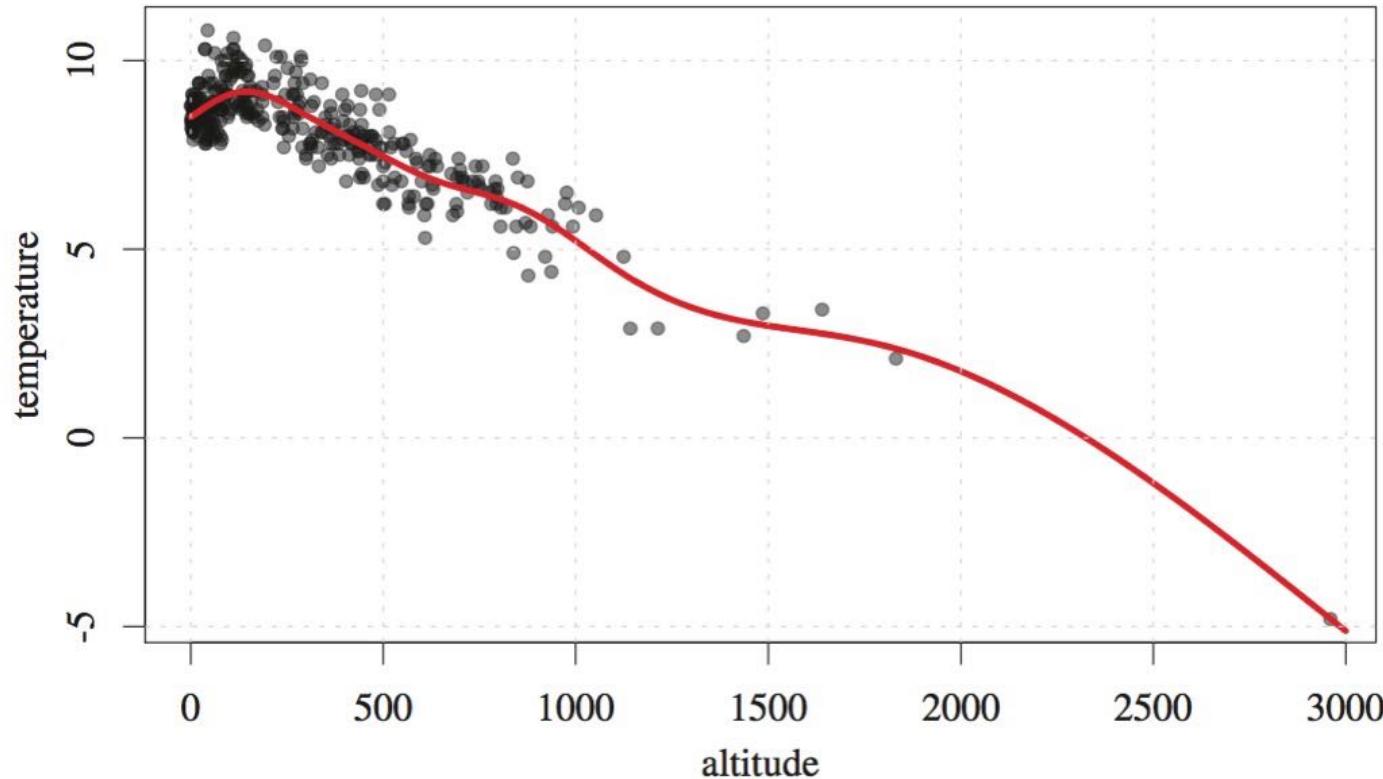
$\implies$  the immediate future of  $\mathbf{x}$  is implied by its past

Using  $dt$  and  $d\mathbf{x} = \mathbf{x}(t + dt) - \mathbf{x}(t)$ :

$$\mathbf{x}(t + dt) = \mathbf{x}(t) + dt \cdot f(\mathbf{x}(t)).$$

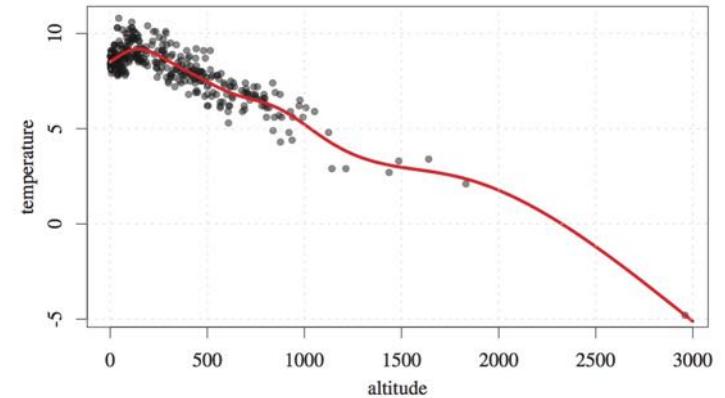
This tells us which entries of  $\mathbf{x}(t)$  cause the future of others  $\mathbf{x}(t + dt)$ , i.e., the causal structure.

# What is cause and what is effect?



$$\begin{aligned} p(a, t) &= p(a|t) \ p(t) & T \rightarrow A \\ &= p(t|a) \ p(a) & A \rightarrow T \end{aligned}$$

Bernhard Schölkopf



- **intervention** on  $a$ : raise the city, find that  $t$  changes
- hypothetical intervention on  $a$ : still expect that  $t$  changes, since we can think of a physical mechanism  $p(t|a)$  that is **independent** of  $p(a)$
- we expect that  $p(t|a)$  is **invariant** across, say, different countries in a similar climate zone

*Independent Causal Mechanisms*

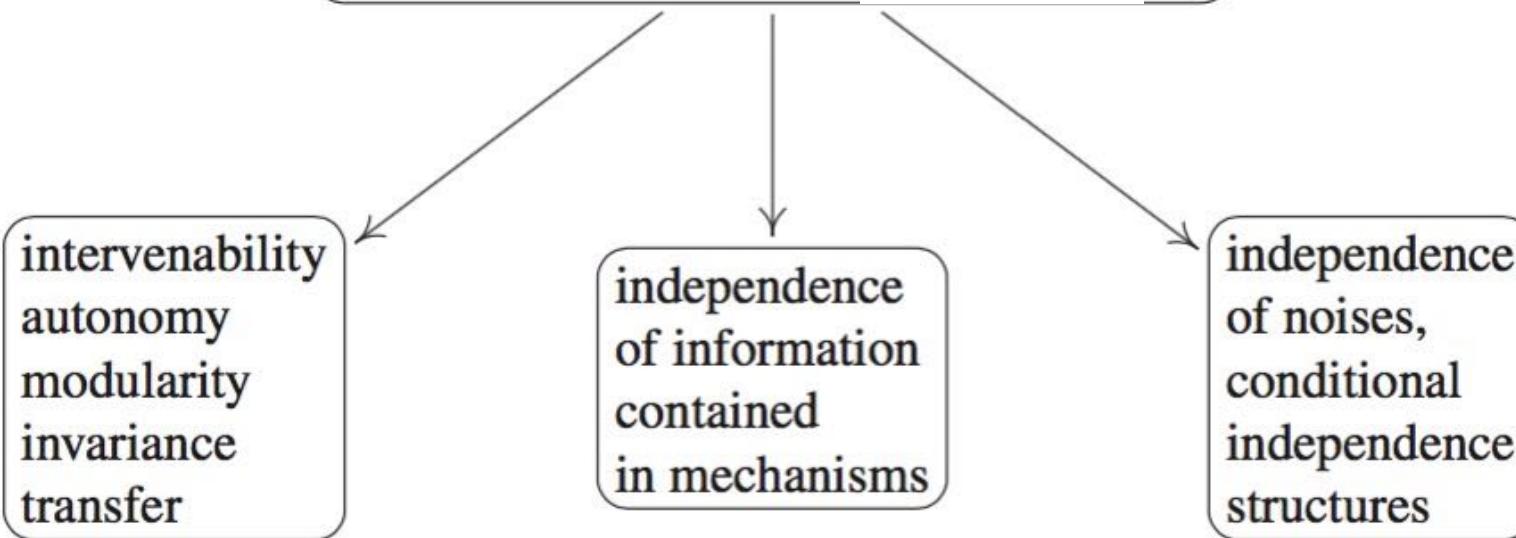
**Principle (ICM):**

*The causal generative process  
is composed of autonomous  
modules that do not inform  
or influence each other.*



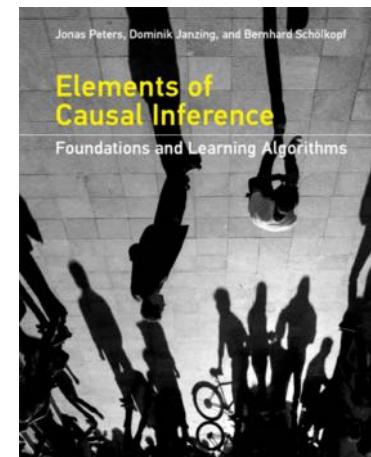
## (physical) independence of mechanisms

### Principle 2



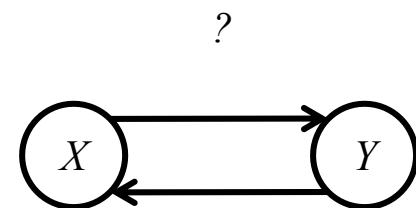
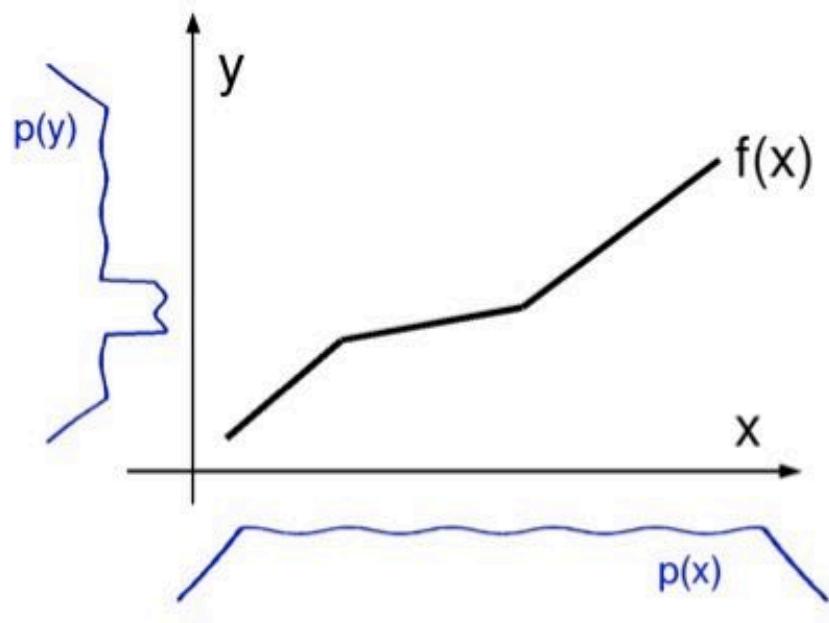
Peters, Janzing, Schölkopf. *Elements of Causal Inference: Foundations and Learning Algorithms*. MIT Press, 2017

[http://www.math.ku.dk/~peters/jonas\\_files/bookDRAFT11-online-2017-06-28.pdf](http://www.math.ku.dk/~peters/jonas_files/bookDRAFT11-online-2017-06-28.pdf)



# Independence of input and mechanism

- No noise on effect variable
- Assumption:  $y = f(x)$  with invertible  $f$



*Daniusis, Janzing, Mooij, Zscheischler, Steudel, Zhang, Schölkopf:*  
Inferring deterministic causal relations, *UAI*  
2010

# Causal independence implies anticausal dependence

Assume that  $f$  is a monotonically increasing bijection of  $[0, 1]$ .

View  $p_x$  and  $\log f'$  as RVs on the prob. space  $[0, 1]$  w. Lebesgue measure.

**Postulate (independence of mechanism and input):**

$$\text{Cov}(\log f', p_x) = 0$$

**Note:** this is equivalent to

$$\int_0^1 \log f'(x)p(x)dx = \int_0^1 \log f'(x)dx,$$

since  $\text{Cov}(\log f', p_x) = E[\log f' \cdot p_x] - E[\log f']E[p_x] = E[\log f' \cdot p_x] - E[\log f']$ .

**Proposition:** If  $f \neq Id$ ,

$$\text{Cov}(\log f^{-1}', p_y) > 0.$$

$u_x, u_y$  uniform densities for  $x, y$

$v_x, v_y$  densities for  $x, y$  induced by transforming  $u_y, u_x$  via  $f^{-1}$  and  $f$

Equivalent formulations of the postulate:

Additivity of Entropy:

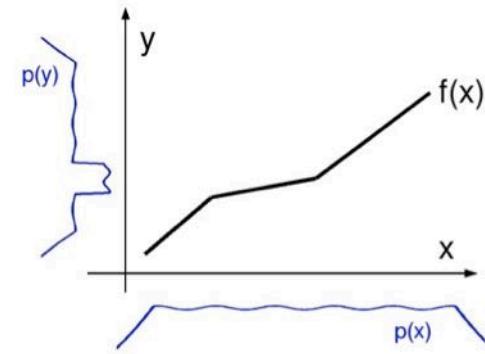
$$S(p_y) - S(p_x) = S(v_y) - S(u_x)$$

Orthogonality (information geometric):

$$D(p_x \| v_x) = D(p_x \| u_x) + D(u_x \| v_x)$$

which can be rewritten as

$$D(p_y \| u_y) = D(p_x \| u_x) + D(v_y \| u_y)$$



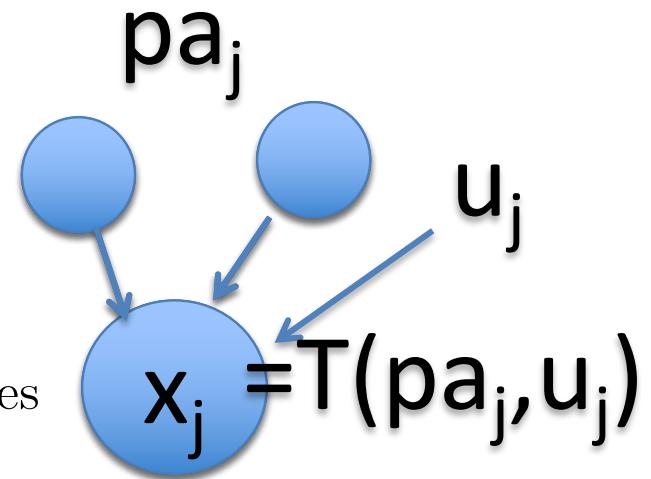
Interpretation:

irregularity of  $p_y$  = irregularity of  $p_x$  + irregularity introduced by  $f$

# Algorithmic structural causal model

- for every node  $x_j$  there exists a program  $u_j$  that computes  $x_j$  from its parents  $pa_j$

- all  $u_j$  are jointly independent
- the program  $u_j$  represents the causal mechanism that generates the effect from its causes
- $u_j$  are the analog of the unobserved noise terms in the statistical functional model



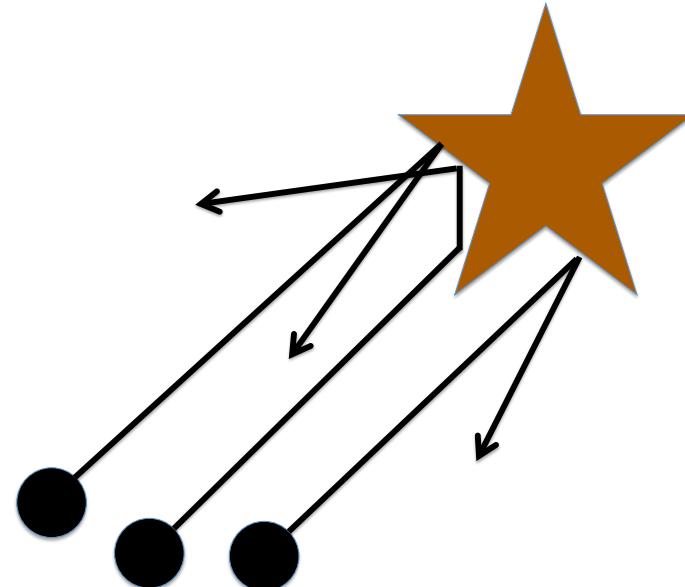
**Theorem:** this model implies the causal Markov condition (replacing Shannon entropy with Kolmogorov complexity).

(Janzing & Schölkopf, IEEE Trans. Information Theory 2010)

Bernhard Schölkopf

# Gedankenexperiment

Particles scattered at an object



- incoming beam: ‘cause’
- scattering at object: ‘mechanism’
- outgoing beam: ‘effect’, contains information about the object

# Independence assumption

- $s$  initial state of a physical system
- $M$  the system dynamics applied for some fixed time

**Independence Principle:**  $s$  and  $M$  are algorithmically independent

$$I(s : M) \stackrel{+}{=} 0,$$

i.e., knowing  $s$  does not enable a shorter description of  $M$  and vice versa.

# Thermodynamic Arrow of Time

**Theorem [non-decrease of entropy].** Let  $M$  be a bijective map on the set of states of a system then  $I(s : M) \stackrel{+}{=} 0$  implies

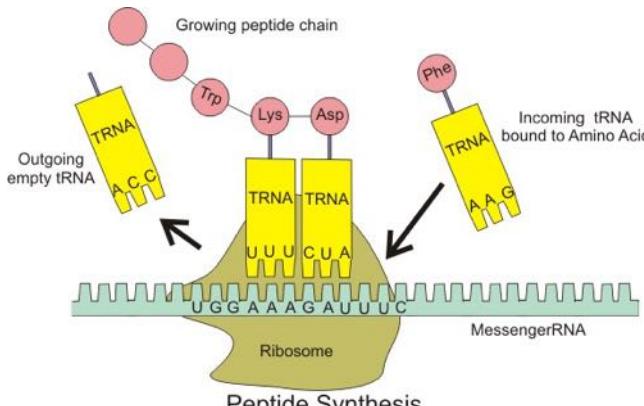
$$K(M(s)) \stackrel{+}{\geq} K(s)$$

Proof idea: If  $M(s)$  admits a shorter description than  $s$ , knowing  $M$  admits a shorter description of  $s$ : just describe  $M(s)$  and then apply  $M^{-1}$ .

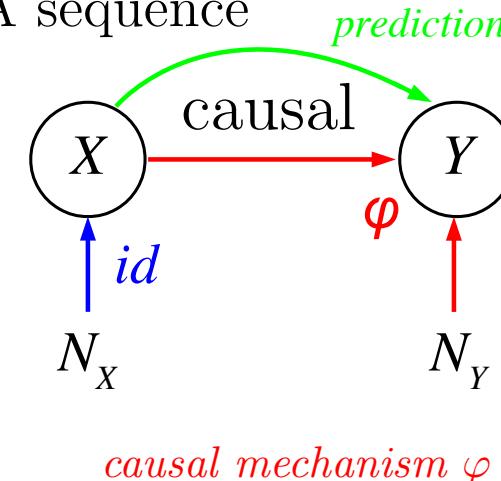
*Janzing, Chaves, Schölkopf.* Algorithmic independence of initial condition and dynamical law in thermodynamics and causal inference. New J. of Physics, 2016

# Using cause-effect knowledge

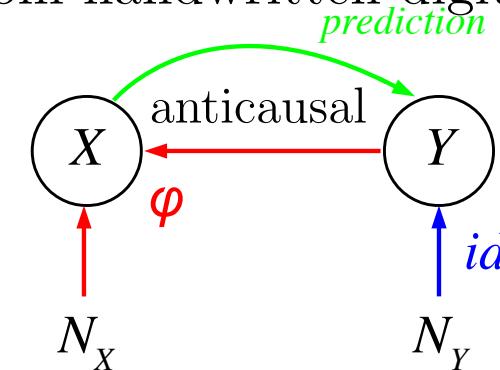
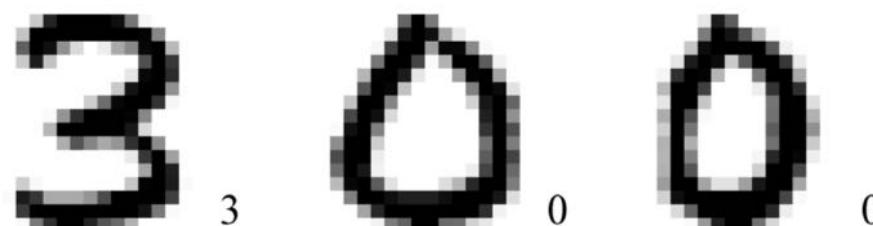
- example 1: predict protein from mRNA sequence



Source: [http://commons.wikimedia.org/wiki/File:Peptide\\_syn.png](http://commons.wikimedia.org/wiki/File:Peptide_syn.png)



- example 2: predict class membership from handwritten digit



# Covariate Shift and Semi-Supervised Learning

Assumption:  $p(C)$  and mechanism  $p(E|C)$  “independent”

Goal: learn  $X \mapsto Y$ , i.e., estimate (properties of)  $p(Y|X)$

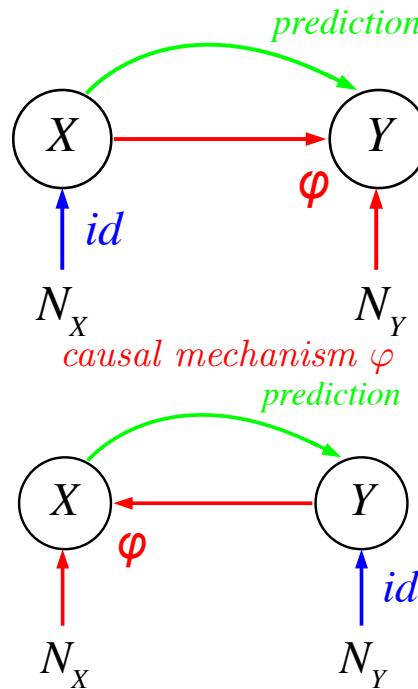
Semi-supervised learning: improve estimate by more data from  $p(X)$

Covariate shift:  $p(X)$  changes between training and test

## Causal learning

$p(X)$  and  $p(Y|X)$  independent

1. semi-supervised learning impossible
2.  $p(Y|X)$  invariant under change in  $p(X)$



## Anticausal learning

$p(Y)$  and  $p(X|Y)$  independent

hence  $p(X)$  and  $p(Y|X)$  dependent

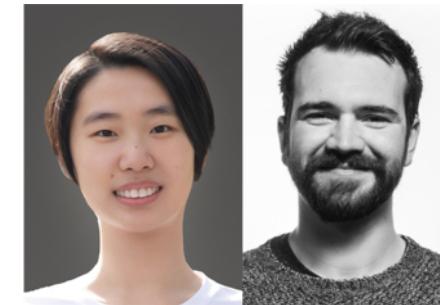
1. semi-supervised learning possible
2.  $p(Y|X)$  changes with  $p(X)$

Schölkopf, Janzing, Peters, Sgouritsa, Zhang, Mooij, 2012, cf. Storkey, 2009; Bareinboim & Pearl, 2012

- Experimental Meta-Analysis confirms prediction  
*Schölkopf et al., ICML 2012; von Kügelgen et al., UAI 2020, Jin et al., submitted*
- All known SSL assumptions link  $p(X)$  to  $p(Y|X)$ :
  - ***Cluster assumption***: points in same cluster of  $p(X)$  have the same  $Y$
  - ***Low density separation assumption***:  $p(Y|X)$  should cross 0.5 in an area where  $p(X)$  is small
  - ***Semi-supervised smoothness assumption***:  $E(Y|X)$  should be smooth where  $p(X)$  is large

# Independent Causal Mechanisms in NLP

(with Zhijing Jin & Julius von Kügelgen)



Prompt for annotators

? Given the English sentence above, can you write its Spanish translation?

Common NLP tasks:

Cause: [En] This is a beautiful world.

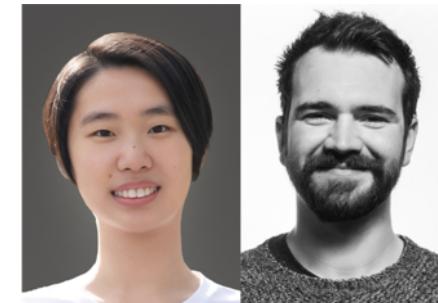
Effect: [Es] Este es un mundo hermoso.

Annotation process  
(Noise)

Category	Example NLP Tasks	Effect = CausalMechanism (Cause, Noise)
Causal learning	Summarization, question answering, parsing, tagging, data-to-text generation, information extraction	
Anticausal learning	Author attribute classification, question generation, review sentiment classification	
Other/mixed (depending on data collection)	Machine translation, language modeling, intent classification	

# ICM in NLP: Findings

(with Zhijing Jin & Julius von Kügelgen)

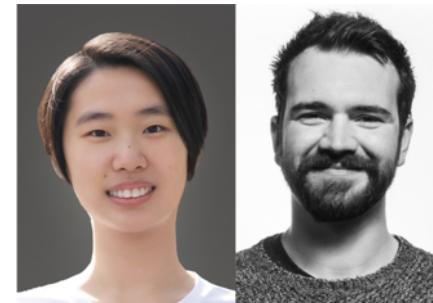


**Causal direction corresponds to shorter description of machine translation data in terms of minimum description length (MDL):**

Data ( $X \rightarrow Y$ )	MDL(X)	MDL(Y)	MDL(Y X)	MDL(X Y)	MDL(X)+MDL(Y X) vs. MDL(Y)+MDL(X Y)
En→Es	46.54	105.99	2033.95	2320.93	2080.49 < 2426.92
Es→En	113.42	55.79	3289.99	3534.09	3403.41 < 3589.88
En→Fr	20.54	53.83	503.78	535.88	524.32 < 589.71
Fr→En	53.83	21.6	705.28	681.12	759.11 > 702.72
Es→Fr	58.26	55.66	701.04	755.5	759.30 < 811.16
Fr→Es	56.14	54.34	665.26	706.53	721.40 < 760.87

# ICM in NLP: Findings

(with Zhijing Jin & Julius von Kügelgen)



**Implications of ICM for SSL and DA confirmed by NLP meta-study:**

Semi-supervised learning (SSL): *anticausal* > *causal*.

<b>Task Type</b>	<b>Mean <math>\Delta</math>SSL (<math>\pm</math>std)</b>	<b>According to ICM</b>
Causal	+0.04 ( $\pm$ 4.23)	Smaller or none
Anticausal	+1.70 ( $\pm$ 2.05)	Larger

Domain adaptation (DA): *causal* > *anticausal*.

<b>Task Type</b>	<b>Mean <math>\Delta</math>DA (<math>\pm</math>std)</b>	<b>According to ICM</b>
Causal	5.18 ( $\pm$ 6.57)	Larger
Anticausal	1.26 ( $\pm$ 1.79)	Smaller

# *Causal Modeling for Confounder Removal in Exoplanet Detection*



MAX-PLANCK-GESSELLSCHAFT

# *Milky Way Galaxy*

**Kepler Search Space**

← 3,000 light years →



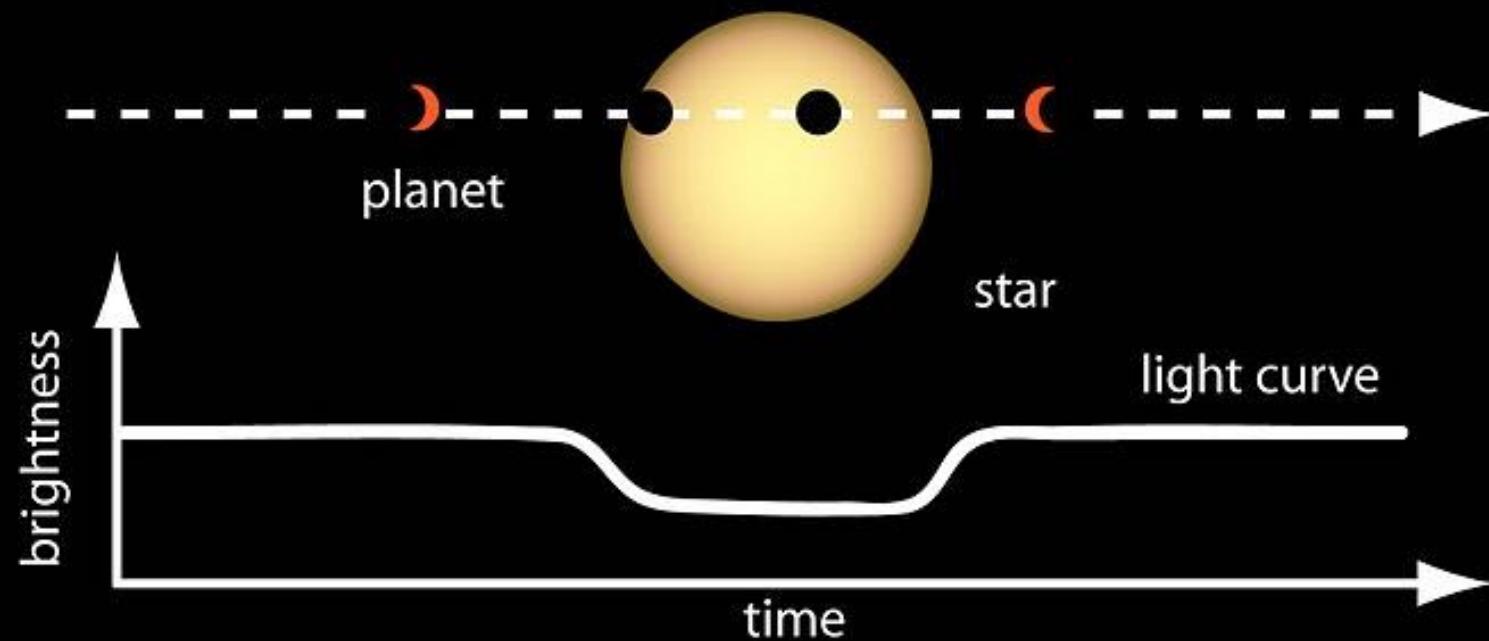
**Sun**

**Sagittarius Arm**

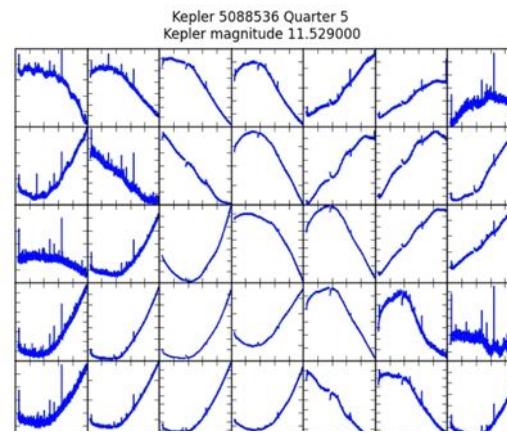
**Orion Spur**

**Perseus Arm**

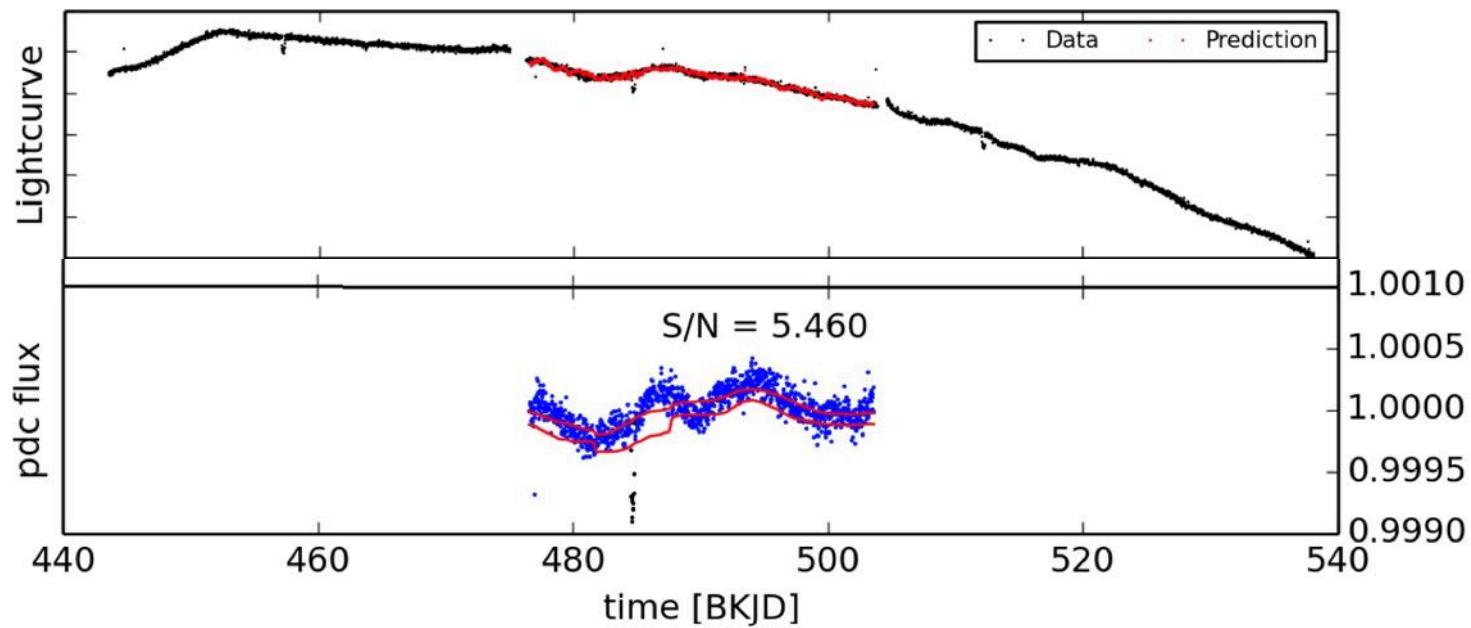
# Exoplanet Transits



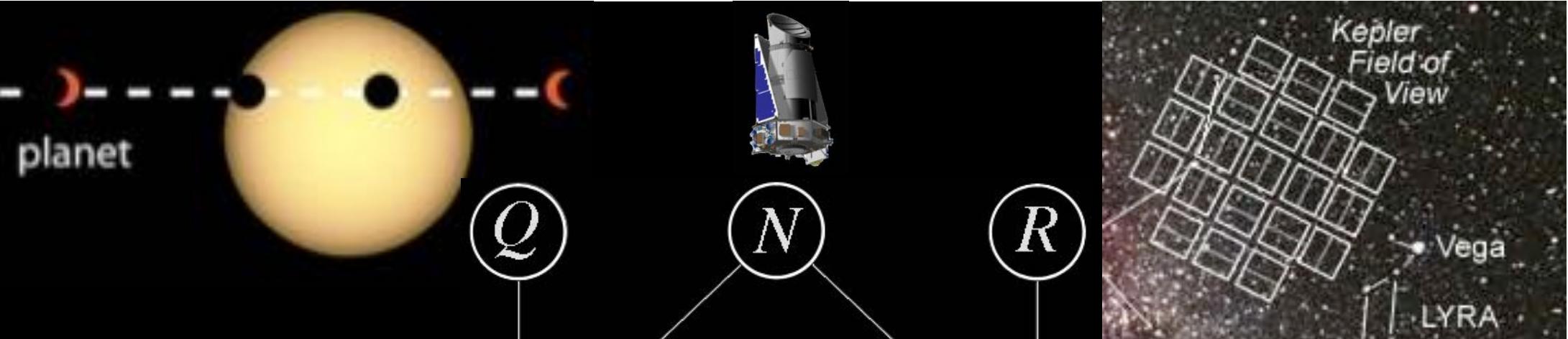
MAX-PLANCK-GESELLSCHAFT



KIC:5088536 Q5 Aperture flux Mag:11.529000 poly:0 Test Region:-12-12  
Star[Number:150 Pixels:3983 L2:1e+05] Auto[Window:3 Pixels:78 L2:1e+05]

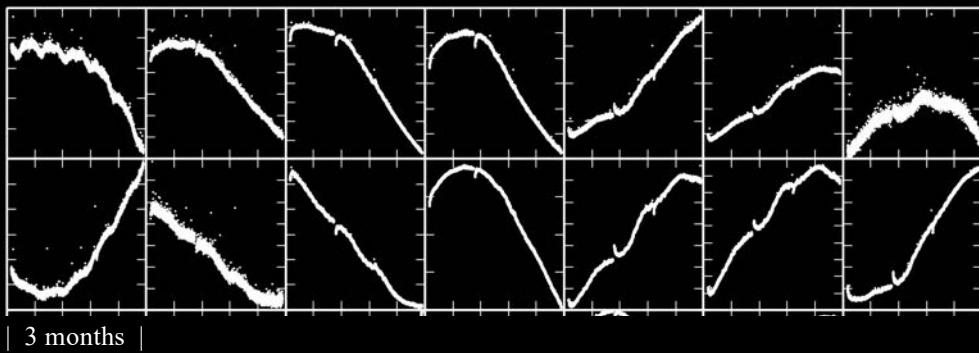


Bernhard Schölkopf

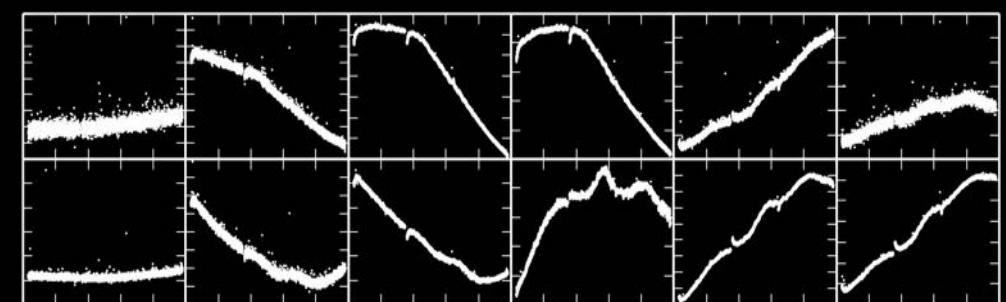


$$Q - E[Q] = Y - E[Y|X]$$

Kepler 5088536 Quarter 5  
CCD channel 25 Row 875 Column 322

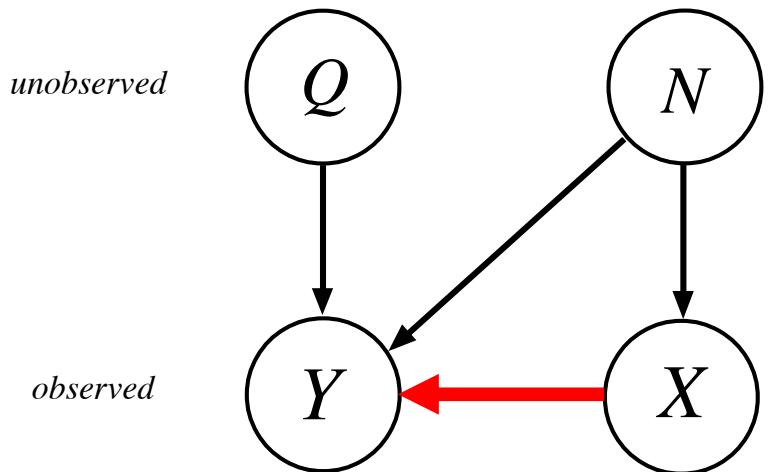


Kepler 5949551 Quarter 5  
CCD channel 25 Row 57 Column 756



MAX-PLANCK-GESELLSCHAFT

# Half-Sibling Regression



Idea: remove  $E[Y|X]$  from  $Y$  to reconstruct  $Q$ .

$$X \perp\!\!\!\perp Q$$

$X$  and  $Y$  share information  
(only) through  $N$

If we try to predict  $Y$  from  $X$ ,  
we only pick up the part due to  $N$

Bernhard Schölkopf

with David Hogg, Dan Foreman-Mackey, Dun Wang, Dominik Janzing,  
Jonas Peters, Carl-Johann Simon-Gabriel (ICML 2015)

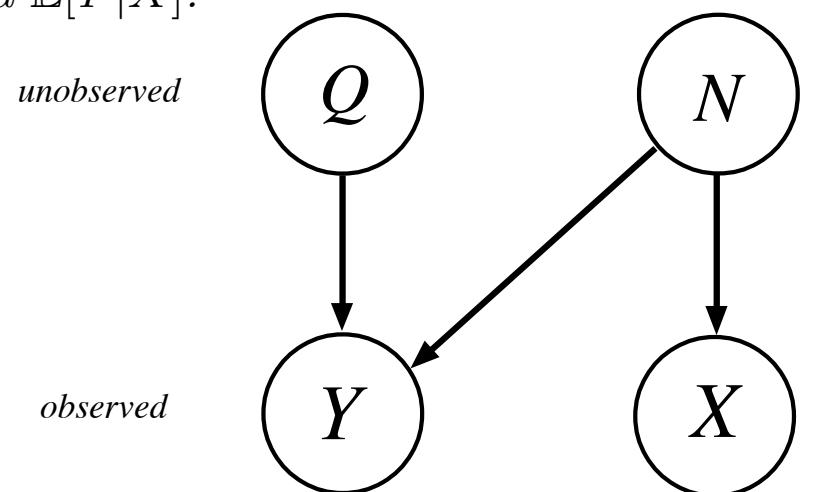
**Proposition.**  $Q, N, Y, X$  random variables,  $X \perp\!\!\!\perp Q$ , and  $f$  measurable.

Suppose

- $Y = Q + f(N)$  (*additive noise model*)
- $f(N) = \psi(X)$  for some  $\psi$  (*complete information*).

Then  $\hat{Q} := Y - \mathbb{E}[Y|X] = Q - \mathbb{E}[Q]$ .

$Q$  can be reconstructed, up to a constant offset, from  $Y$  and  $\mathbb{E}[Y|X]$ .



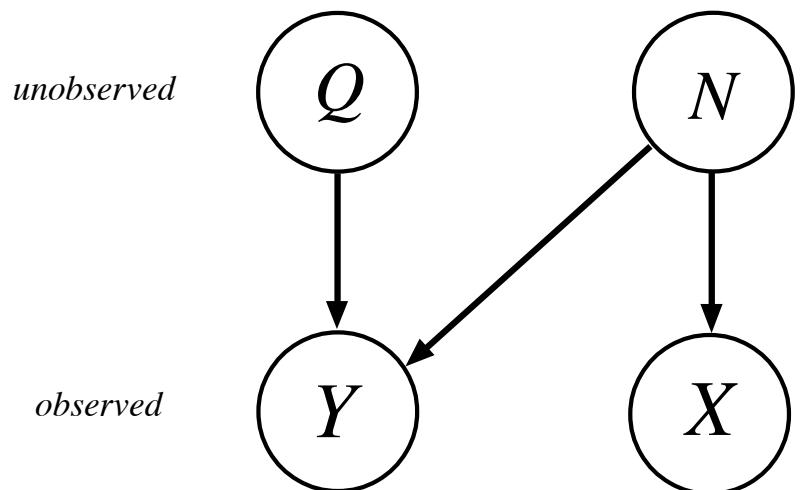
**Proposition.**  $Q, N, Y, X$  random variables,  $X \perp\!\!\!\perp Q$ , and  $f$  measurable.

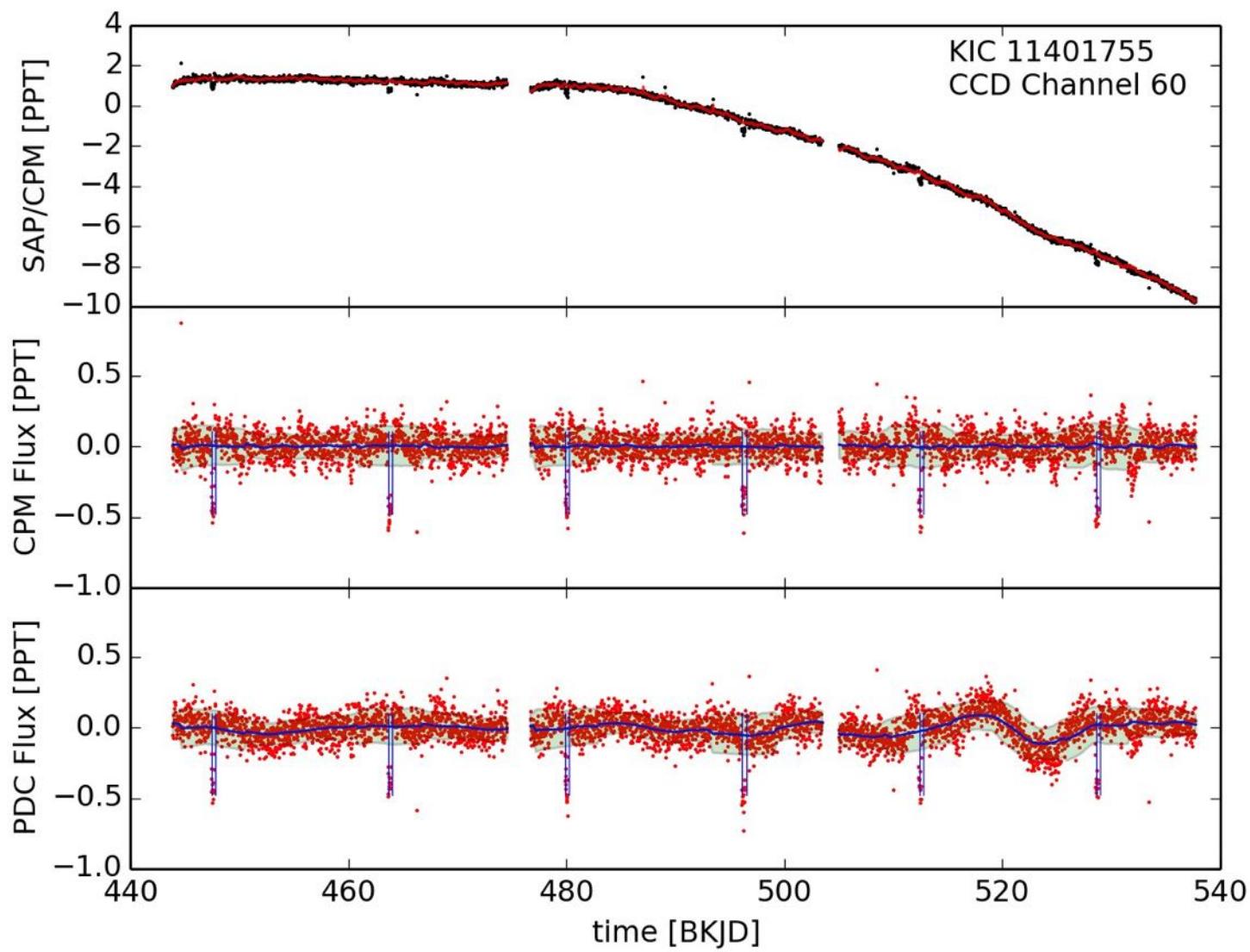
Suppose

- $Y = Q + f(N)$  (additive noise model)

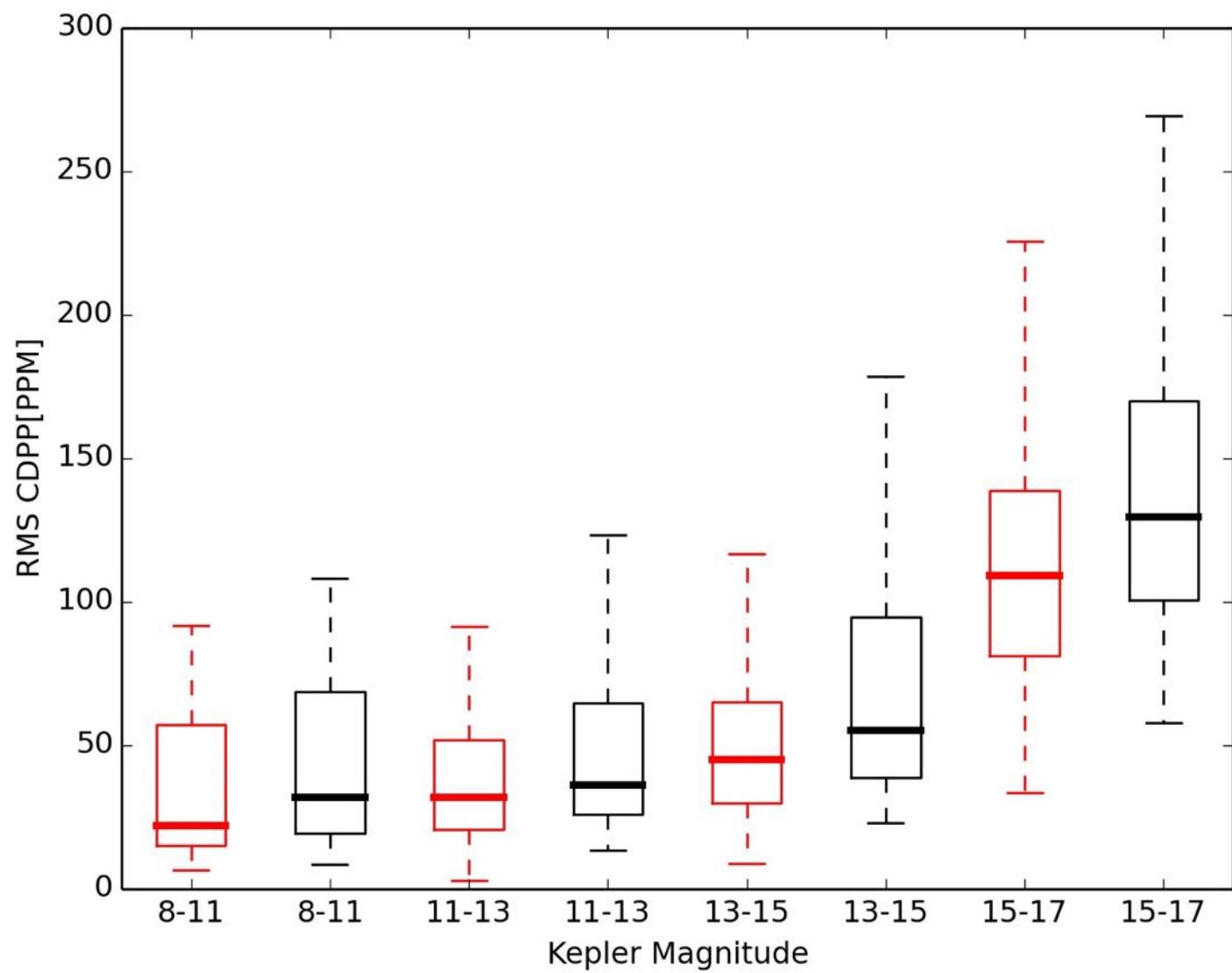
Then  $E[(\hat{Q} - (Q - E[Q]))^2] = E[\text{Var}[f(N)|X]]$ .

If  $f(N)$  can (in principle) be predicted well from  $X$ ,  
then  $Q$  can be reconstructed well.





Bernhard Schölkopf



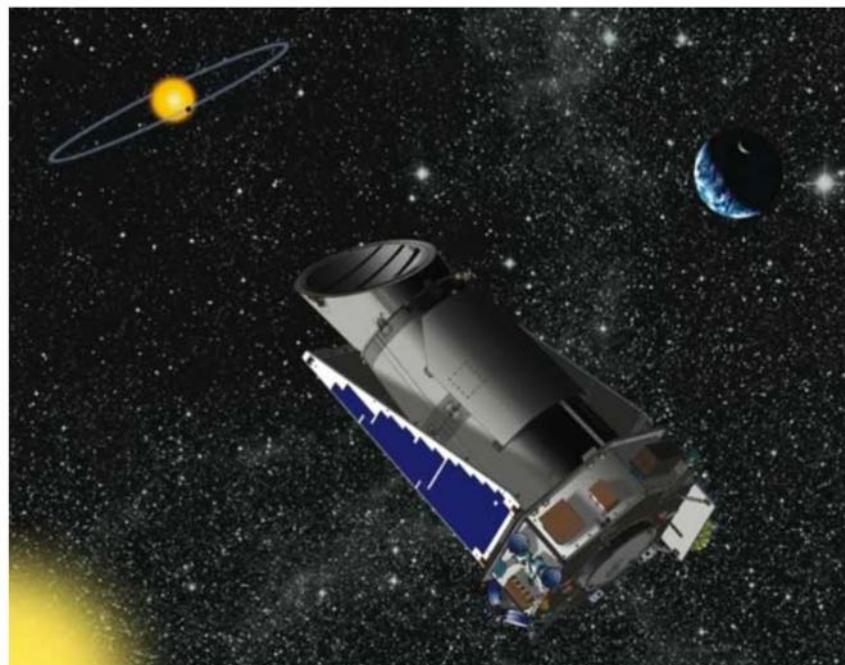
Bernhard Schölkopf



MAX-PLANCK-GESELLSCHAFT

# Planet-Hunting Kepler Spacecraft Suffers Major Failure, NASA Says

By [Mike Wall](#) May 15, 2013 Science & Astronomy



An artist's interpretation of the Kepler observatory in space. (Image: © NASA.)

*This story was updated at 5:20 p.m. EDT.*

The planet-hunting days of NASA's prolific Kepler space telescope, which has discovered more than 2,700 potential alien worlds to date, may be over.

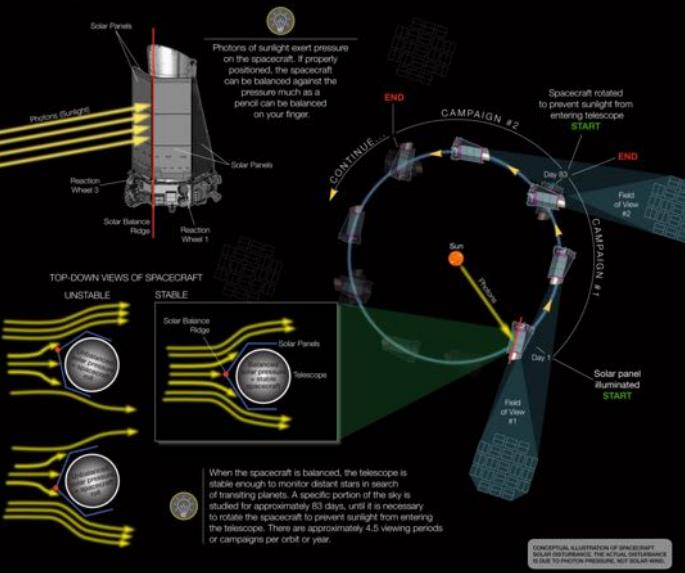
The second of Kepler's four [reaction wheels](#) — devices that allow the observatory to maintain its position in space — has failed, NASA officials announced Wednesday (May 15).

Bernhard Schölkopf



MAX-PLANCK-GESELLSCHAFT

## Kepler's Second Light: How K2 Will Work



Credits: NASA Ames/W Stenzel

## NASA'S K2 MISSION: WHERE K2 WILL OBSERVE

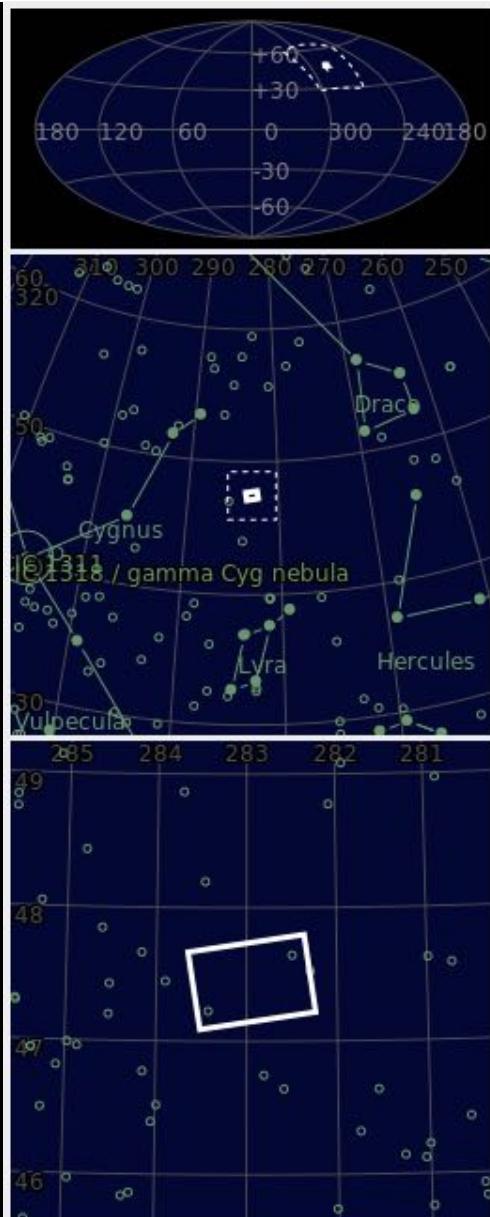
FIELD 1

The search for planets continues today!  
May 30, 2014

MILKY WAY GALAXY

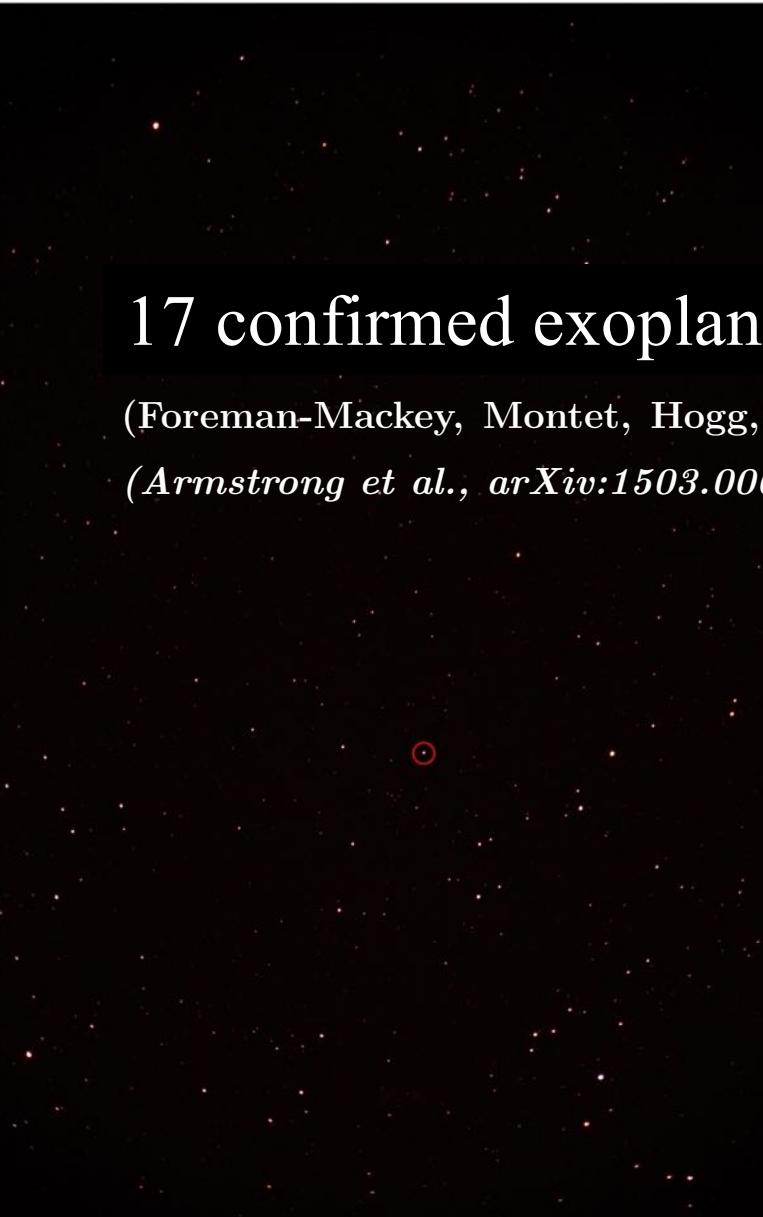
ECLIPTIC PLANE





## 17 confirmed exoplanets

(Foreman-Mackey, Montet, Hogg, Morton, Wang, Schölkopf, arXiv:1502.04715):  
(Armstrong et al., arXiv:1503.00692; Montet et al., arXiv:1503.07866 ).



## A SYSTEMATIC SEARCH FOR TRANSITING PLANETS IN THE *K2* DATA

DANIEL FOREMAN-MACKEY<sup>1</sup>, BENJAMIN T. MONTET<sup>2,3</sup>, DAVID W. HOGG<sup>1,4,5</sup>,  
 TIMOTHY D. MORTON<sup>6</sup>, DUN WANG<sup>1</sup>, AND BERNHARD SCHÖLKOPF<sup>7</sup>

<sup>1</sup> Center for Cosmology and Particle Physics, Department of Physics, New York University,

4 Washington Place, New York, NY 10003, USA; [danfm@nyu.edu](mailto:danfm@nyu.edu)

<sup>2</sup> Cahill Center for Astronomy and Astrophysics, California Institute of Technology, Pasadena, CA 91125, USA

<sup>3</sup> Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA

<sup>4</sup> Max-Planck-Institut für Astronomie, Königstuhl 17, D-69117, Heidelberg, Germany

<sup>5</sup> Center for Data Science, New York University, 726 Broadway, 7th Floor, New York, NY 10003, USA

<sup>6</sup> Department of Astrophysics, Princeton University, Princeton, NJ 08544, USA

<sup>7</sup> Max Planck Institute for Intelligent Systems, Spemannstrasse 38, D-72076, Tübingen, Germany

Received 2015 February 16; accepted 2015 May 12; published 2015 June 18

### ABSTRACT

Photometry of stars from the *K2* extension of NASA’s *Kepler* mission is afflicted by systematic effects caused by small (few-pixel) drifts in the telescope pointing and other spacecraft issues. We present a method for searching *K2* light curves for evidence of exoplanets by simultaneously fitting for these systematics and the transit signals of interest. This method is more computationally expensive than standard search algorithms but we demonstrate that it can be efficiently implemented and used to discover transit signals. We apply this method to the full Campaign 1 data set and report a list of 36 planet candidates transiting 31 stars, along with an analysis of the pipeline performance and detection efficiency based on artificial signal injections and recoveries. For all planet candidates, we present posterior distributions on the properties of each system based strictly on the transit observables.

*Key words:* catalogs – methods: data analysis – methods: statistical – planetary systems – stars: statistics

### 1. INTRODUCTION

The *Kepler* Mission was incredibly successful at finding transiting exoplanets in the light curves of stars. The Mission

a few percent of the data are actually stored and downloaded to Earth, there is not enough information in the data to derive or infer a complete or accurate flat-field map. Therefore, work on

**Table 2**  
The Catalog of Planet Candidates and their Observable Properties

EPIC	Kepler mag	R.A. (J2000)	Decl. (J2000)	P (days)	$t_0$ [BJD-2456808]	$R_p/R_\star$
201208431	14.41	174.745640	-3.905585	$10.0040^{+0.0018}_{-0.0016}$	$7.5216^{+0.0098}_{-0.0090}$	$0.0349^{+0.0034}_{-0.0026}$
201257461	11.51	178.161109	-3.094936	$50.2677^{+0.0083}_{-0.0074}$	$20.3735^{+0.0147}_{-0.0098}$	$0.0334^{+0.0054}_{-0.0017}$
201295312	12.13	174.011630	-2.520881	$5.6562^{+0.0007}_{-0.0007}$	$3.7228^{+0.0086}_{-0.0091}$	$0.0175^{+0.0020}_{-0.0009}$
201338508	14.36	169.303502	-1.877976	$10.9328^{+0.0022}_{-0.0021}$	$6.5967^{+0.0088}_{-0.0081}$	$0.0339^{+0.0025}_{-0.0030}$
201338508	14.36	169.303502	-1.877976	$5.7350^{+0.0006}_{-0.0006}$	$0.8626^{+0.0054}_{-0.0055}$	$0.0331^{+0.0025}_{-0.0023}$
201367065	11.57	172.334949	-1.454787	$10.0542^{+0.0004}_{-0.0004}$	$5.4186^{+0.0018}_{-0.0018}$	$0.0354^{+0.0022}_{-0.0011}$
201367065	11.57	172.334949	-1.454787	$24.6470^{+0.0014}_{-0.0016}$	$4.2769^{+0.0030}_{-0.0029}$	$0.0272^{+0.0016}_{-0.0013}$
201384232	12.51	178.192260	-1.198477	$30.9375^{+0.0029}_{-0.0052}$	$19.5035^{+0.0053}_{-0.0039}$	$0.0260^{+0.0011}_{-0.0011}$
201393098	13.05	167.093771	-1.065755	$28.6793^{+0.0105}_{-0.0116}$	$16.6212^{+0.0305}_{-0.0177}$	$0.0231^{+0.0028}_{-0.0020}$
201403446	11.99	174.266344	-0.907261	$19.1535^{+0.0050}_{-0.0050}$	$7.3437^{+0.0116}_{-0.0143}$	$0.0154^{+0.0014}_{-0.0013}$
201445392	14.38	169.793665	-0.284375	$10.3527^{+0.0011}_{-0.0011}$	$5.6110^{+0.0047}_{-0.0051}$	$0.0349^{+0.0045}_{-0.0025}$
201445392	14.38	169.793665	-0.284375	$5.0644^{+0.0006}_{-0.0006}$	$5.0690^{+0.0059}_{-0.0064}$	$0.0274^{+0.0025}_{-0.0020}$
201465501	14.96	176.264468	0.005301	$18.4488^{+0.0015}_{-0.0015}$	$14.6719^{+0.0035}_{-0.0032}$	$0.0531^{+0.0061}_{-0.0039}$
201505350	12.81	174.960319	0.603575	$11.9069^{+0.0005}_{-0.0004}$	$9.2764^{+0.0013}_{-0.0013}$	$0.0446^{+0.0009}_{-0.0006}$
201505350	12.81	174.960319	0.603575	$7.9193^{+0.0001}_{-0.0001}$	$5.3840^{+0.0006}_{-0.0006}$	$0.0747^{+0.0016}_{-0.0013}$
201546283	12.43	171.515165	1.230738	$6.7713^{+0.0001}_{-0.0001}$	$4.8453^{+0.0012}_{-0.0011}$	$0.0481^{+0.0020}_{-0.0012}$
201549860	13.92	170.103081	1.285956	$5.6083^{+0.0005}_{-0.0006}$	$4.1195^{+0.0045}_{-0.0047}$	$0.0283^{+0.0041}_{-0.0023}$
201555883	15.06	176.075940	1.375947	$5.7966^{+0.0002}_{-0.0002}$	$5.3173^{+0.0027}_{-0.0050}$	$0.0604^{+0.0068}_{-0.0032}$
201565013	16.91	176.992193	1.510249	$8.6381^{+0.0003}_{-0.0002}$	$3.4283^{+0.0016}_{-0.0015}$	$0.1538^{+0.0355}_{-0.0243}$
201569483	11.77	167.171299	1.577513	$5.7969^{+0.0000}_{-0.0000}$	$5.3130^{+0.0002}_{-0.0003}$	$0.3587^{+0.0379}_{-0.0334}$
201577035	12.30	172.121957	1.690636	$19.3062^{+0.0013}_{-0.0013}$	$11.5790^{+0.0025}_{-0.0027}$	$0.0380^{+0.0023}_{-0.0012}$
201596316	13.15	169.042002	1.986840	$39.8415^{+0.0136}_{-0.0155}$	$21.8572^{+0.0120}_{-0.0101}$	$0.0267^{+0.0034}_{-0.0022}$
201613023	12.14	173.192036	2.244884	$8.2818^{+0.0006}_{-0.0007}$	$7.3752^{+0.0055}_{-0.0052}$	$0.0205^{+0.0012}_{-0.0008}$
201617985	14.11	179.491659	2.321476	$7.2823^{+0.0007}_{-0.0008}$	$4.6337^{+0.0050}_{-0.0050}$	$0.0333^{+0.0072}_{-0.0032}$
201629650	12.73	170.155528	2.502696	$40.0492^{+0.0186}_{-0.0259}$	$4.5363^{+0.0202}_{-0.0172}$	$0.0241^{+0.0025}_{-0.0020}$
201635569	15.55	178.057026	2.594245	$8.3681^{+0.0002}_{-0.0002}$	$3.4514^{+0.0015}_{-0.0014}$	$0.0991^{+0.0120}_{-0.0078}$
201649426	13.22	177.234262	2.807619	$27.7704^{+0.0001}_{-0.0001}$	$13.3476^{+0.0001}_{-0.0001}$	$0.4365^{+0.0777}_{-0.0583}$
201702477	14.43	175.240794	3.681584	$40.7365^{+0.0026}_{-0.0025}$	$3.5451^{+0.0026}_{-0.0025}$	$0.0808^{+0.0043}_{-0.0114}$
201736247	14.40	178.110797	4.254747	$11.8106^{+0.0016}_{-0.0019}$	$3.8483^{+0.0093}_{-0.0071}$	$0.0347^{+0.0030}_{-0.0024}$
201754305	14.30	175.097258	4.557340	$19.0726^{+0.0048}_{-0.0049}$	$1.4893^{+0.0128}_{-0.0133}$	$0.0297^{+0.0042}_{-0.0030}$
201754305	14.30	175.097258	4.557340	$7.6202^{+0.0012}_{-0.0011}$	$3.6813^{+0.0061}_{-0.0057}$	$0.0281^{+0.0034}_{-0.0026}$
201779067	11.12	168.542699	4.988131	$27.2429^{+0.0001}_{-0.0001}$	$12.2599^{+0.0002}_{-0.0003}$	$0.2535^{+0.0369}_{-0.0259}$
201828749	11.56	175.654342	5.894323	$33.5093^{+0.0023}_{-0.0018}$	$5.1554^{+0.0037}_{-0.0032}$	$0.0267^{+0.0021}_{-0.0020}$
201855371	13.00	178.329775	6.412261	$17.9715^{+0.0015}_{-0.0017}$	$9.9412^{+0.0033}_{-0.0038}$	$0.0311^{+0.0030}_{-0.0017}$
<b>201912552</b>	12.47	172.560460	7.588391	$32.9410^{+0.0039}_{-0.0032}$	$28.1834^{+0.0057}_{-0.0105}$	$0.0513^{+0.0035}_{-0.0056}$
201929294	12.97	174.656969	7.959611	$5.0084^{+0.0001}_{-0.0001}$	$4.5703^{+0.0022}_{-0.0012}$	$0.1163^{+0.0011}_{-0.0014}$

## STELLAR AND PLANETARY PROPERTIES OF *K2* CAMPAIGN 1 CANDIDATES AND VALIDATION OF 17 PLANETS, INCLUDING A PLANET RECEIVING EARTH-LIKE INSOLATION

BENJAMIN T. MONTEL<sup>1,2</sup>, TIMOTHY D. MORTON<sup>3</sup>, DANIEL FOREMAN-MACKEY<sup>4,5</sup>, JOHN ASHER JOHNSON<sup>2</sup>, DAVID W. HOGG<sup>4,5,6</sup>, BRENDAN P. BOWLER<sup>1,8</sup>, DAVID W. LATHAM<sup>2</sup>, ALLYSON BIERYLA<sup>2</sup>, AND ANDREW W. MANN<sup>7,9</sup>

<sup>1</sup> Cahill Center for Astronomy and Astrophysics, California Institute of Technology, Pasadena, CA 91125, USA; [btm@astro.caltech.edu](mailto:btm@astro.caltech.edu)

<sup>2</sup> Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA

<sup>3</sup> Department of Astrophysics, Princeton University, Princeton, NJ 08544, USA

<sup>4</sup> Center for Cosmology and Particle Physics, Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA

<sup>5</sup> Center for Data Science, New York University, 726 Broadway, 7th Floor, New York, NY 10003, USA

<sup>6</sup> Max-Planck-Institut für Astronomie, Königstuhl 17, D-69117 Heidelberg, Germany

<sup>7</sup> Department of Astronomy, The University of Texas at Austin, Austin, TX 78712, USA

*Received 2015 March 27; accepted 2015 July 2; published 2015 August 5*

### ABSTRACT

The extended *Kepler* mission, *K2*, is now providing photometry of new fields every three months in a search for transiting planets. In a recent study, Foreman-Mackey and collaborators presented a list of 36 planet candidates orbiting 31 stars in *K2* Campaign 1. In this contribution, we present stellar and planetary properties for all systems. We combine ground-based seeing-limited survey data and adaptive optics imaging with an automated transit analysis scheme to validate 21 candidates as planets, 17 for the first time, and identify 6 candidates as likely false positives. Of particular interest is K2-18 (EPIC 201912552), a bright ( $K = 8.9$ ) M2.8 dwarf hosting a  $2.23 \pm 0.25 R_{\oplus}$  planet with  $T_{\text{eq}} = 272 \pm 15$  K and an orbital period of 33 days. We also present two new open-source software packages which enable this analysis. The first, *isochrones*, is a flexible tool for fitting theoretical stellar models to observational data to determine stellar properties using a nested sampling scheme to capture the multimodal nature of the posterior distributions of the physical parameters of stars that may plausibly be evolved. The second is *vespa*, a new general-purpose procedure to calculate false positive probabilities and statistically validate transiting exoplanets.

*Key words:* catalogs – planetary systems – planets and satellites: detection – stars: fundamental parameters

**Table 3**  
Planet Properties for All Objects of Interest

# Habitable Zone Gallery

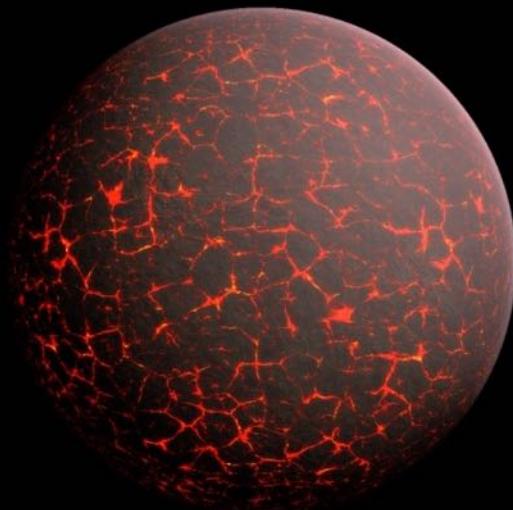
[Home](#) [Plots](#) [Table](#) [Gallery](#) [Movies](#) [About](#) [Links](#)

This site is dedicated to tracking the orbits of exoplanets in relation to their Habitable Zones.

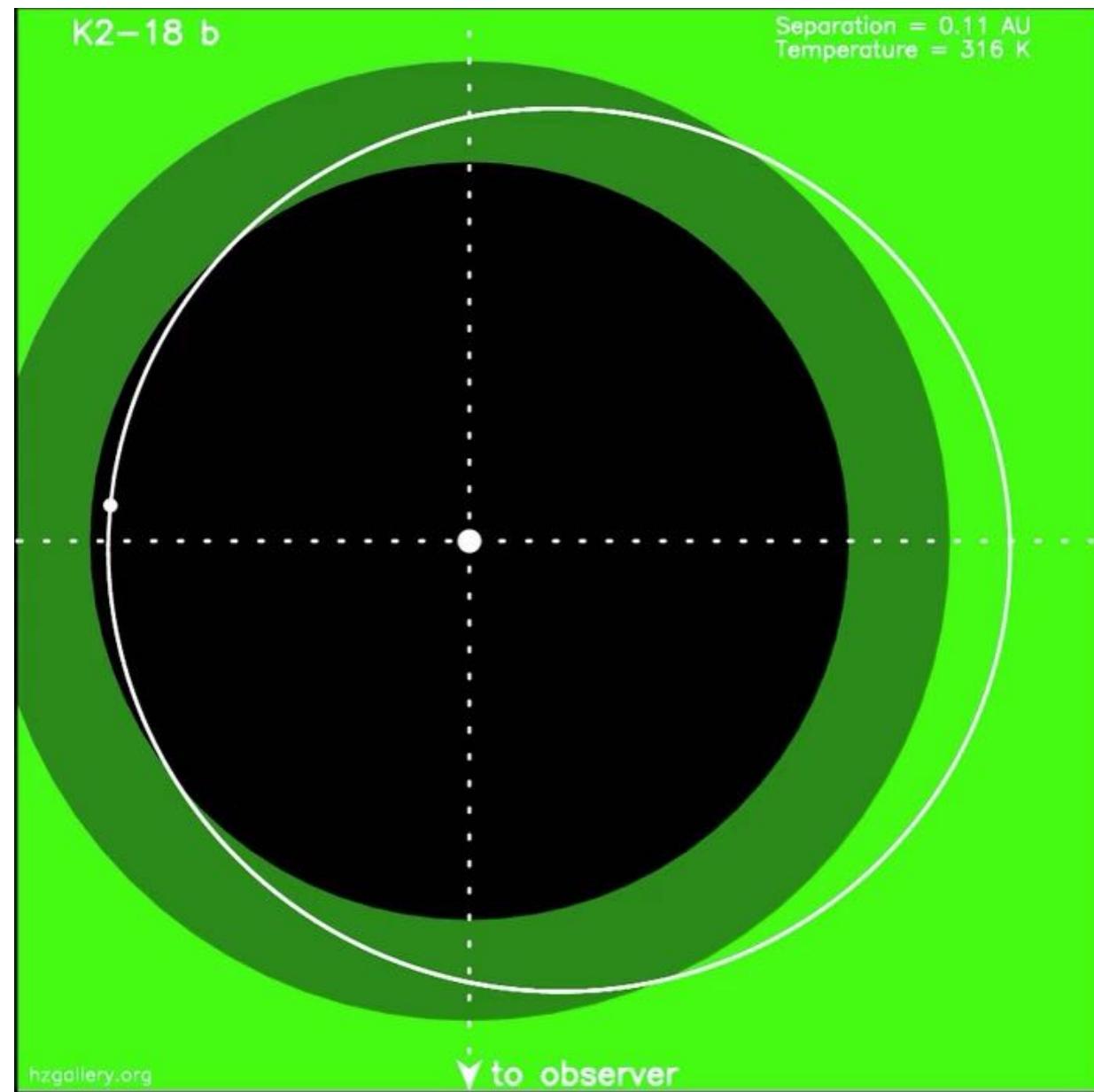
Planets: 3706 Systems: 2806

Planets with orbits entirely within the Habitable Zone: 129 [?]

Updated: 2019 08 29 14:39:34 PDT



*"The Earth is the only world known so far to harbor life. There is nowhere else, at least in the near future, to which our species could migrate. Visit, yes. Settle, not yet. Like it or not, for the moment the Earth is where we make our stand." - Carl Sagan*



## Water found on a potentially life-friendly alien planet

A super-Earth about 111 light-years away is “the best candidate for habitability that we know right now,” astronomers say.



## Water found on most habitable known world beyond solar system

**But humans would not fare well on planet K2-18b despite wispy clouds and huge red sun**



Astronomische Sensation

### Wasser dampf auf Planet K2-18b

News outlets that said otherwise are just crying wolf—but they’re not the only ones at fault

By Laura Kreidberg on September 23, 2019



#### Observations

#### No, the Exoplanet K2-18b Is Not Habitable

News outlets that said otherwise are just crying wolf—but they’re not the only ones at fault

By Laura Kreidberg on September 23, 2019

3 MINUTE READ



NASA

Missions | Galleries | NASA TV | Follow

Humans in Space | Moon to Mars | Earth | Space Tech | Flight | So

Credits: ESA/Hubble,  
M. Kornmesser

Hubble

NASA's Hubble Finds Water Vapor on Habitable-Zone Exoplanet for 1st Time

## Water Vapor on the Habitable-Zone Exoplanet K2-18b

BJÖRN BENNEKE,<sup>1</sup> IAN WONG,<sup>2,3</sup> CAROLINE PIAULET,<sup>1</sup> HEATHER A. KNUTSON,<sup>4</sup> IAN J.M. CROSSFIELD,<sup>5</sup> JOSHUA LOTHIRINGER,<sup>6</sup> CAROLINE V. MORLEY,<sup>7</sup> PETER GAO,<sup>8,3</sup> THOMAS P. GREENE,<sup>9</sup> COURTNEY DRESSING,<sup>8</sup> DIANA DRAGOMIR,<sup>5,10</sup> ANDREW W. HOWARD,<sup>11</sup> PETER R. McCULLOUGH,<sup>6</sup> ELIZA M.-R. KEMPTON,<sup>12,13</sup> JONATHAN J. FORTNEY,<sup>14</sup> AND JONATHAN FRAINÉ<sup>15</sup>

<sup>1</sup>Institute for Research on Exoplanets and Department of Physics, Université de Montréal, Montreal, QC, Canada

<sup>2</sup>Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA, 02139, USA

<sup>3</sup>51 Pegasi b Fellow

<sup>4</sup>Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125, USA

<sup>5</sup>Department of Physics and Kavli Institute of Astronomy, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA, 02139, USA

<sup>6</sup>Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

<sup>7</sup>Department of Astronomy, University of Texas, Austin, TX 78712, USA

<sup>8</sup>Department of Astronomy, University of California - Berkeley , Berkeley, CA, 94720, USA

<sup>9</sup>NASA Ames Research Center, Moffett Field, CA, 94035, USA

<sup>10</sup>NASA Hubble Fellow

<sup>11</sup>Department of Astronomy, California Institute of Technology, Pasadena, CA 91125, USA

<sup>12</sup>Department of Astronomy, University of Maryland, College Park, MD 20742, USA

<sup>13</sup>Department of Physics, Grinnell College, 1116 8th Avenue, Grinnell, IA 50112, USA

<sup>14</sup>Department of Astronomy, University of California, Santa Cruz, CA 95064, USA

<sup>15</sup>Center for Extrasolar Planetary Systems, Space Science Institute, Boulder, CO 80301, USA

## ABSTRACT

Ever since the discovery of the first exoplanet, astronomers have made steady progress towards finding and probing planets in the habitable zone of their host stars, where the conditions could be right for liquid water to form and life to sprawl. Results from the Kepler mission indicate that the occurrence rate of habitable-zone Earths and super-Earths may be as high as 5–20%. Despite this abundance, probing the conditions and atmospheric properties on any of these habitable-zone planets is extremely difficult and has remained elusive to date. Here, we report the detection of water vapor and the likely presence of liquid water clouds in the atmosphere of the 8.6 M<sub>⊕</sub> habitable-zone planet K2-18b. With a 33 day orbit around a cool M3 dwarf, K2-18b receives virtually the same amount of total radiation from its host star (1441 ± 80 W/m<sup>2</sup>) as the Earth receives from the Sun (1370 W/m<sup>2</sup>), making it a good candidate to host liquid water clouds. In this study we observed eight transits using HST/WFC3 in order to achieve the necessary sensitivity to detect water vapor. While the thick gaseous envelope of K2-18b means that it is not a true Earth analogue, our observations demonstrate that low-mass habitable-zone planets with the right conditions for liquid water are accessible with state-of-the-art telescopes.

**Keywords:** planets and satellites: individual (K2-18b) – planets and satellites: atmospheres

## 1. INTRODUCTION

The recent discovery of the transiting 8.63 ± 1.35 M<sub>⊕</sub> exoplanet K2-18b in the habitable zone of a bright,

nearby M3-dwarf provides us with an opportunity to carry out the spectroscopic study of the atmosphere of a habitable-zone planet outside our solar system (Montet et al. 2015, Benneke et al. 2017, Cloutier et al. 2019). K2-18b is an intriguing planet because its equilibrium temperature (265 ± 5 K at an albedo of  $A = 0.3$ ) is potentially very close to that of the Earth (257 K). The planet’s predicted temperature provides the right con-

Corresponding author: Björn Benneke  
 benneke@astro.umontreal.ca

## Water vapour in the atmosphere of the habitable-zone eight-Earth-mass planet K2-18 b

Angelos Tsiaras<sup>①\*</sup>, Ingo P. Waldmann<sup>②\*</sup>, Giovanna Tinetti<sup>③</sup>, Jonathan Tennyson and Sergey N. Yurchenko

In the past decade, observations from space and the ground have found water to be the most abundant molecular species, after hydrogen, in the atmospheres of hot, gaseous extrasolar planets<sup>1–3</sup>. Being the main molecular carrier of oxygen, water is a tracer of the origin and the evolution mechanisms of planets. For temperate, terrestrial planets, the presence of water is of great importance as an indicator of habitable conditions. Being small and relatively cold, these planets and their atmospheres are the most challenging to observe, and therefore no atmospheric spectral signatures have so far been detected<sup>4</sup>. Super-Earths—planets lighter than ten Earth masses—around later-type stars may provide our first opportunity to study spectroscopically the characteristics of such planets, as they are best suited for transit observations. Here, we report the detection of a spectroscopic signature of water in the atmosphere of K2-18 b—a planet of eight Earth masses in the habitable zone of an M dwarf—with high statistical confidence (Atmospheric Detectability Index = 5.0, ~3.6σ (refs. <sup>5,6</sup>)). In addition, the derived mean molecular weight suggests an atmosphere still containing some hydrogen. The observations were recorded with the Hubble Space Telescope/Wide Field Camera 3 and analysed with our dedicated, publicly available, algorithms<sup>7,8</sup>. Although the suitability of M dwarfs to host habitable worlds is still under discussion<sup>9–13</sup>, K2-18 b offers an unprecedented opportunity to gain insight into the composition and climate of habitable-zone planets.

Atmospheric characterization of super-Earths is currently within reach of the Wide Field Camera 3 (WFC3) on board the Hubble Space Telescope (HST), combined with the recently implemented spatial scanning observational strategy<sup>14</sup>. The spectra of three hot transiting planets with radii less than 3.0 Earth radii ( $R_{\oplus}$ ) have been published so far: Gliese 1214 b<sup>15</sup>, HD 97658 b<sup>16</sup> and 55 Cancri e<sup>17</sup>. The first two do not show any evident transit depth modulation with wavelength, suggesting an atmosphere covered by thick clouds or made of molecular species heavier than hydrogen, while only the spectrum of 55 Cancri e has revealed a light-weight atmosphere, suggesting hydrogen–helium (H<sub>2</sub>–He) still being present. In addition, transit observations of six temperate Earth-size planets around the ultra-cool dwarf TRAPPIST-1—planets b, c, d, e, f and g<sup>18</sup>—have not shown any molecular signatures and have excluded the presence of cloud-free H<sub>2</sub>–He atmospheres around them.

K2-18 b was discovered in 2015 by the Kepler spacecraft<sup>19</sup> and is orbiting around an M2.5 (metallicity [Fe/H] = 0.123 ± 0.157 dex (units of decimal exponent), effective temperature  $T_{\text{eff}} = 3,457 \pm 39$  K, stellar mass  $M_{\star} = 0.359 \pm 0.047$  solar masses ( $M_{\odot}$ )), stellar radius  $R_{\star} = 0.411 \pm 0.038$  solar radii ( $R_{\odot}$ )<sup>20</sup> dwarf star, 34 pc away from the Earth. The star–planet distance of 0.1429 AU (ref. <sup>21</sup>) suggests a

planet within the star’s habitable zone (~0.12–0.25 AU) (ref. <sup>20</sup>), with effective temperature between 200 K and 320 K, depending on the albedo and the emissivity of its surface and/or its atmosphere. This crude estimate accounts for neither possible tidal energy sources<sup>22</sup> nor atmospheric heat redistribution<sup>23,24</sup>, which might be relevant for this planet. Measurements of the mass and the radius of K2-18 b (planetary mass  $M_{\star} = 7.96 \pm 1.9$  Earth masses ( $M_{\oplus}$ ) (ref. <sup>22</sup>), planetary radius  $R_{\star} = 2.279 \pm 0.0026 R_{\oplus}$  (ref. <sup>20</sup>)) yield a bulk density of  $3.3 \pm 1.2$  g cm<sup>-3</sup> (ref. <sup>24</sup>), suggesting either a silicate planet with an extended atmosphere or an interior composition with a water (H<sub>2</sub>O) mass fraction lower than 50% (refs. <sup>25,26</sup>).

We analyse here eight transits of K2-18 b, obtained with the WFC3 camera on board the HST. We used our publicly available tools, specialized for HST/WFC3 data<sup>27</sup>, to perform the end-to-end analysis from the raw data to the atmospheric parameters. The techniques used here have been validated by the analysis of the largest catalogue of exoplanetary spectra from WFC3. Details can be found in Methods, and links to the data and the codes used can be found in ‘Data availability’ and ‘Code availability’, respectively. Along with the data, we provide descriptions of the data structures and instructions on how to reproduce the results presented here. Our analysis resulted in the detection of an atmosphere around K2-18 b with an Atmospheric Detectability Index<sup>28</sup> (ADI; a positively defined logarithmic Bayes factor) of 5.0, or approximately 3.6σ confidence<sup>29,30</sup>, making K2-18 b the first habitable-zone planet in the super-Earth mass regime (1–10  $M_{\oplus}$ ) with an observed atmosphere around it.

More specifically, nine transits of K2-18 b were observed as part of the HST proposals 13665 and 14682 (principal investigator: Björn Benneke), and the data are available through the Mikulski Archive for Space Telescopes (MAST; see ‘Data availability’). Each transit was observed during five HST orbits, with the G141 infrared grism (1.1–1.7 μm), and each exposure was the result of 16 up-the-ramp samples in the spatial scanning mode. The ninth transit observation suffered from pointing instabilities, and we therefore decided not to include it in this analysis. We extracted the white and the spectral light curves from the reduced images, following our dedicated methodology<sup>27,28</sup>, which has been integrated into an automated, self-consistent and user-friendly Python package named Iraclis (see ‘Code Availability’). No systematic variations of the white light curve,  $R_{\star}/R_{\oplus}$ , appeared between the eight different observations. This level of stability among the extracted broadband transit depths is not always guaranteed, as consistency problems among different observations emerged in previous analyses<sup>28,31</sup>.

In our analysis, we found that the measured mid-transit times were not consistent with the expected ephemeris<sup>20</sup>. We used these results to refine the ephemeris of K2-18 b to  $P = 32.94007 \pm 0.00003$  days and  $T_0 = 2457363.2109 \pm 0.0004$  BJD<sub>TDB</sub> (ref. <sup>20</sup>), where  $P$

Department of Physics & Astronomy, University College London, London, UK. \*e-mail: [atsiaras@star.ucl.ac.uk](mailto:atsiaras@star.ucl.ac.uk); [ingo@star.ucl.ac.uk](mailto:ingo@star.ucl.ac.uk)

NATURE ASTRONOMY | [www.nature.com/natureastronomy](http://www.nature.com/natureastronomy)

<http://people.tue.mpg.de/bs/K2-18b.html>

**Recent Discoveries From Planet K2 18b! (Super Earth)**  
234K views • 1 year ago

**Could K2-18b Sustain Life?**  
10K views • 3 months ago

**Der erste Exoplanet mit Wasser! Leben auf K2-18b...**  
51K views • 2 years ago

**Hubblecast 124 Light: Exoplanet K2-18b**  
131K views • 2 years ago

**Animation of Exoplanet K2-18b (Artist's Impression)**  
66K views • 2 years ago

**Animation of Exoplanet K2-18b (Artist's Impression)**  
6.4K views • 2 years ago

**Episode 2: Rain on K2-18b**  
796 views • 1 year ago

**Cele mai recente descoperiri despre Planeta K2 18B (SUPE...**  
210K views • 1 year ago

**K2-188 EXOPLANET**  
44K views • 2 years ago

**Water Discovered on Exoplanet K2-18b in 'Goldilocks Zone'**  
44K views • 2 years ago

**Wie finden wir eine zweite Erde?**  
3.8K views • 1 year ago

**K2-18b / රුජුවාට් අමාන ප්‍රාග්‍රැමයක නිවේදී ඇත / NASA's...**  
30 views • 1 year ago

**K2-18b экзопланетасы атмосферасынан су буы...**  
250 views • 2 years ago

**K2-18**  
No views • 1 month ago

**CIENTISTAS ENCONTRAM ÁGUA PELA PRIMEIRA VEZ E...**  
29 views • 2 years ago

**NASA's Hubble Finds exoplanet with Water Vapor**  
68 views • 1 year ago

**What is the most Earth-like Exoplanet?**  
1.7K views • 7 months ago

**We have discovered over 4000 exoplanets, out of this, what is the most Earth-Like exoplanet discovered...  
4K**

**मिस गाई एक नई पृथी || जानिए क्या है #Super-Earth (K2-18b) ||**  
133 views • 2 years ago

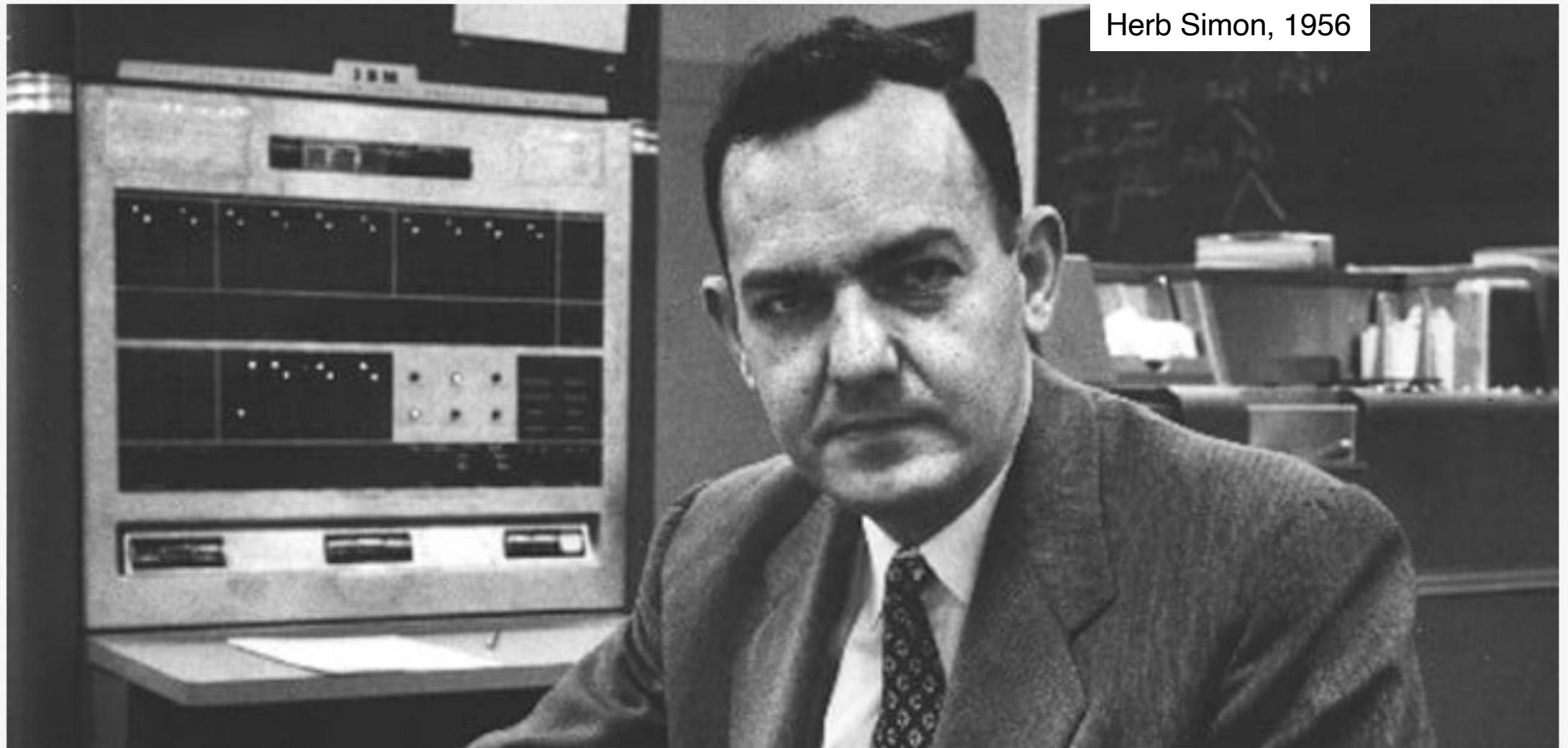
**Top Science Discoveries of 2019**  
2.2K views • 1 year ago

**Fique Sabendo - Vizinhos interplanetários?**  
55 views • 2 years ago

*Bernhard Schölkopf*



MAX-PLANCK-GESELLSCHAFT



Herb Simon, 1956

**"Machines will be capable, within twenty years, of doing any work a man can do"**

# Toward causal representation learning

**Core Problem of Statistical Representations:** Representation learning only includes *statistical* information — it does not capture interventions, reasoning, planning.

**Core Problem of Causal Representations:** SCMs are usually at the *symbolic* level — they assume the causal variables are given.

<https://arxiv.org/abs/2102.11107>

# Independent mechanisms and the disentangled factorization

## Factorization

- independent noises in the causal graph:

$$p(X_1, \dots, X_n) = \prod_{I=1}^n p(X_i \mid \text{PA}_i)$$



# Independent mechanisms and the disentangled factorization

Disentangled (causal) factorization

<https://arxiv.org/abs/1911.10500>

<https://arxiv.org/abs/2102.11107>

- independent noises in the causal graph:

$$p(X_1, \dots, X_n) = \prod_{I=1}^n p(X_i | \text{PA}_i)$$

- independent mechanisms: changing one  $p(X_i | \text{PA}_i)$  does not change the other  $p(X_j | \text{PA}_j)$  ( $j \neq i$ ); they remain **invariant**

(Janzing & Schölkopf, IEEE Trans. Inf. Th. 2010; Schölkopf et al., ICML 2012),

cf. *autonomy, (structural) invariance, separability, exogeneity, stability, modularity*: (Aldrich, 1989; Pearl, 2009)

Special case: If the graph has no edges, disentanglement reduces to statistical independence:

$$p(X_1, \dots, X_n) = \prod_{I=1}^n p(X_i)$$

In general, the causal factors will not be statistically independent, and independence-based methods struggle to find them (Träuble et al., ICML 2021)



# Entangled factorizations

Disentangled (causal) factorization

$$p(X_1, \dots, X_n) = \prod_{I=1}^n p(X_i \mid \text{PA}_i)$$

Entangled (non-causal) factorizations

e.g.,

$$p(X_1, \dots, X_n) = \prod_{I=1}^n p(X_i \mid X_{i+1}, \dots, X_n).$$

- cannot intervene on  $p(X_i \mid X_{i+1}, \dots, X_n)$
- changing one  $p(X_i \mid \text{PA}_i)$  will usually change **many** of the  $p(X_i \mid X_{i+1}, \dots, X_n)$

# Causal viewpoint on distribution shift

Disentangled causal factorization

$$p(X_1, \dots, X_n) = \prod_{I=1}^n p(X_i | \text{PA}_i)$$

with independent mechanisms  $p(X_i | \text{PA}_i)$ .

**Sparse Mechanism Shift Hypothesis:** small distribution changes manifest themselves sparsely in the disentangled factorization, i.e., they should usually not affect all factors simultaneously.

Here, a shift can be passive (e.g., distribution drift) or active (intervention, action).

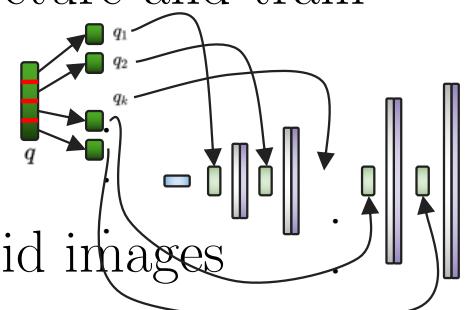
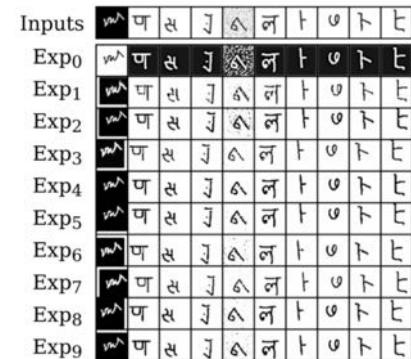
Stated in (*Parascandolo et al., arXiv:1712.00961 (2017); Bengio et al., arXiv:1901.10912 (2019), Schölkopf, arXiv:1911:10500 (2019)*); see also (*Schölkopf et al., ICML 2012, Schölkopf, Janzing, Lopez-Paz 2016, Zhang et al., ICML 2013, Huang, Zhang et al., JMLR 2020*)

# Causal training

**ICM training:** encourage independence of mechanisms

**Structural training:** embed SCM structure into decoder architecture and train by reconstruction error

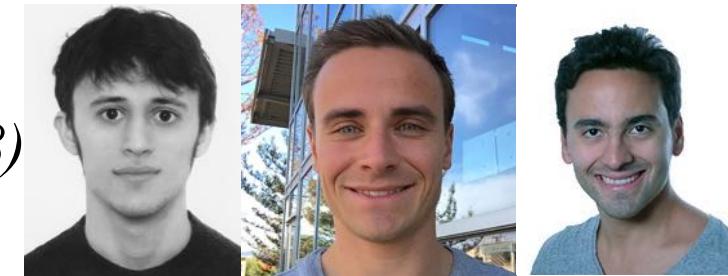
**Counterfactual training:** require that interventions (e.g., after reconstruction in an autoencoder).



**Sparse mechanism shift training:** require that interventions/interventions, only a sparse set of causal represent

# Learning independent mechanisms

(with Parascandolo, Kilbertus, Rojas-Carulla, ICML 2018)



- Data drawn from  $p(x)$ , transformed by  $M$  mechanisms  $f_1, \dots, f_M$
- Goal: learn the independent mechanisms / factors of variation
- Method: generative model with competing mechanisms

9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

Original data

9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

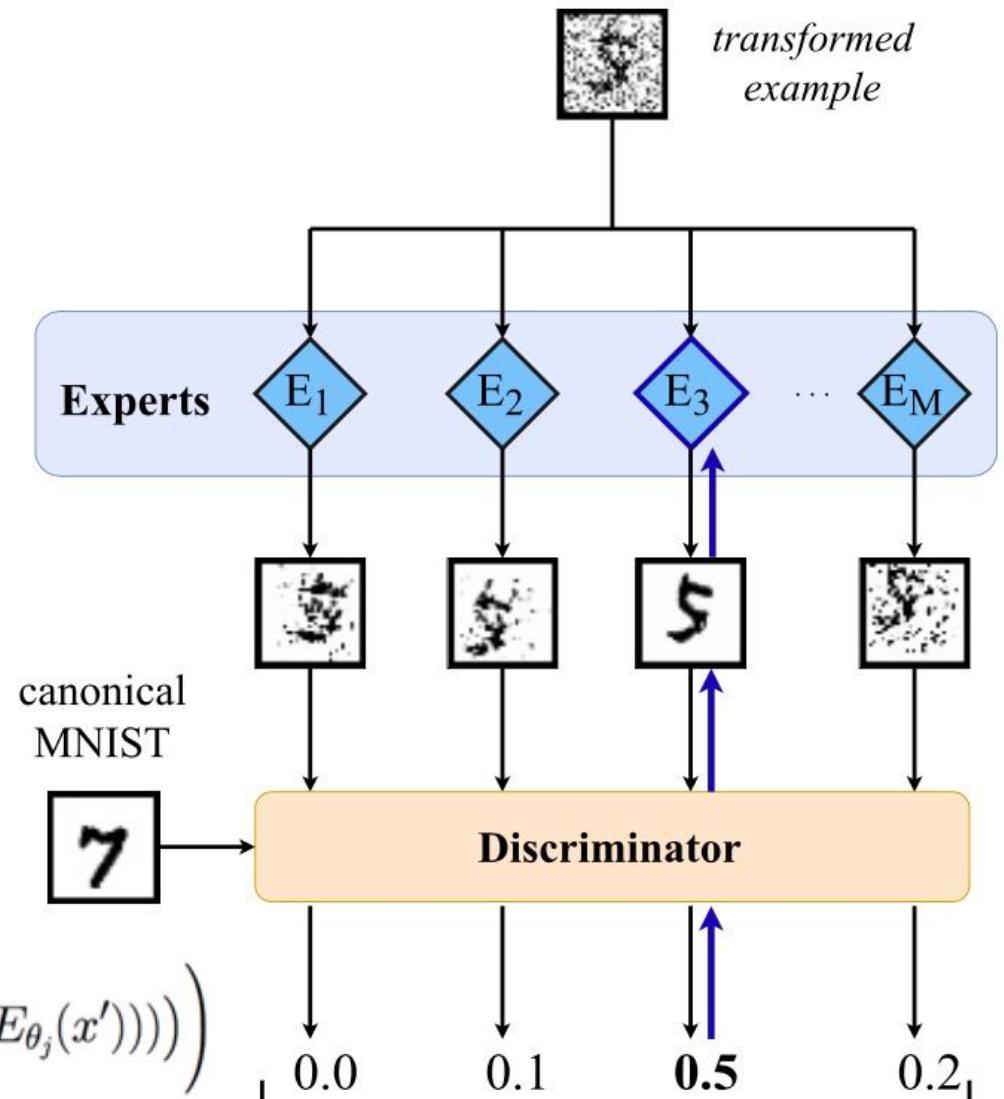
9	2	4	2	2	2	9	6
---	---	---	---	---	---	---	---

Transformed data

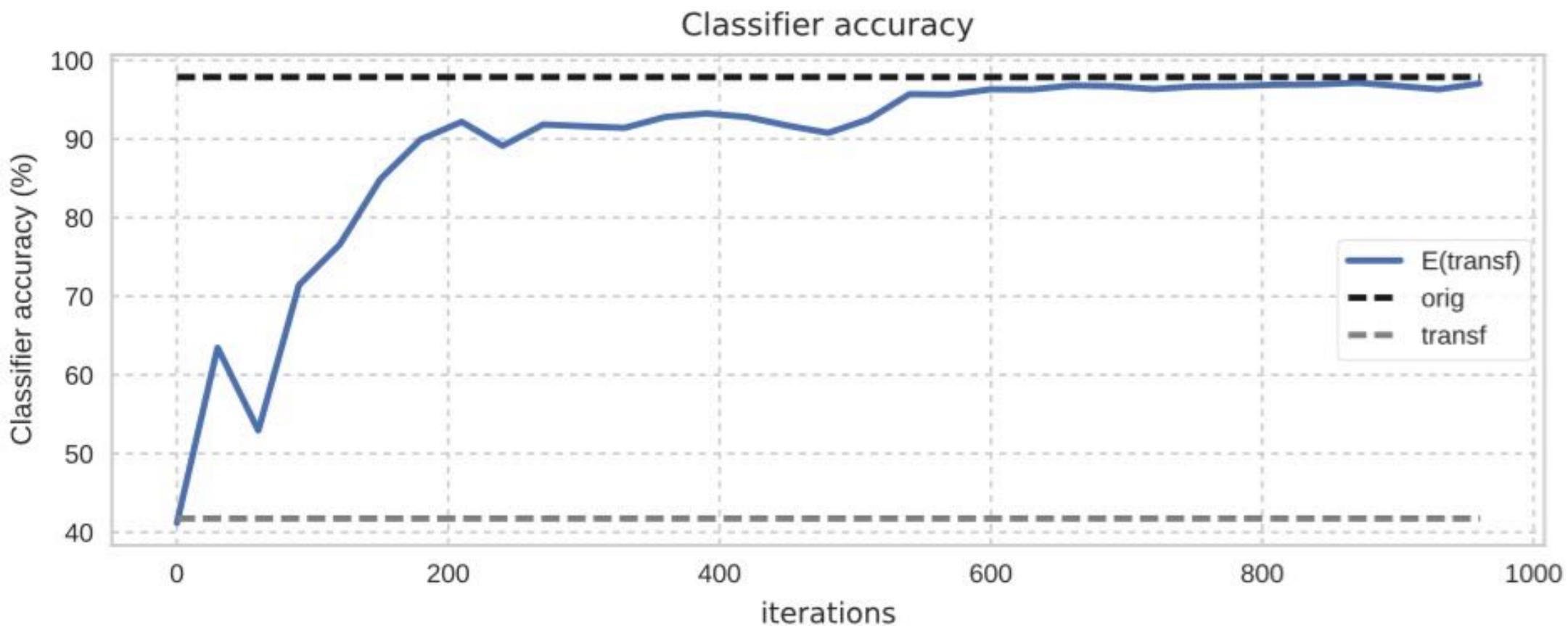
## Method

- Mechanisms initialized  $\approx$  identity
- The highest scoring mechanism against the discriminator  $D$  wins the example and is updated to increase the score
- $D$  is trained on the original data and against the winning outputs

$$\max_{\theta_D} \left( \mathbb{E}_{x \sim P} \log(D_{\theta_D}(x)) + \frac{1}{N'} \sum_{j=1}^{N'} \mathbb{E}_{x' \sim Q} (\log(1 - D_{\theta_D}(E_{\theta_j}(x')))) \right)$$



# Accuracy of a CNN trained on MNIST for different test sets



# Generalizing to Omniglot characters

## Inputs

Expo

Exp1

Exp<sub>2</sub>

Exp<sub>3</sub>

Exp4

Exp5

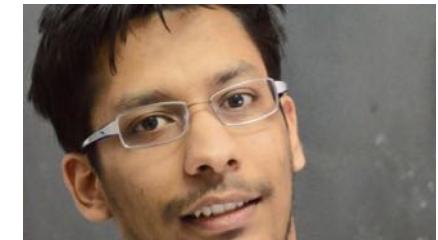
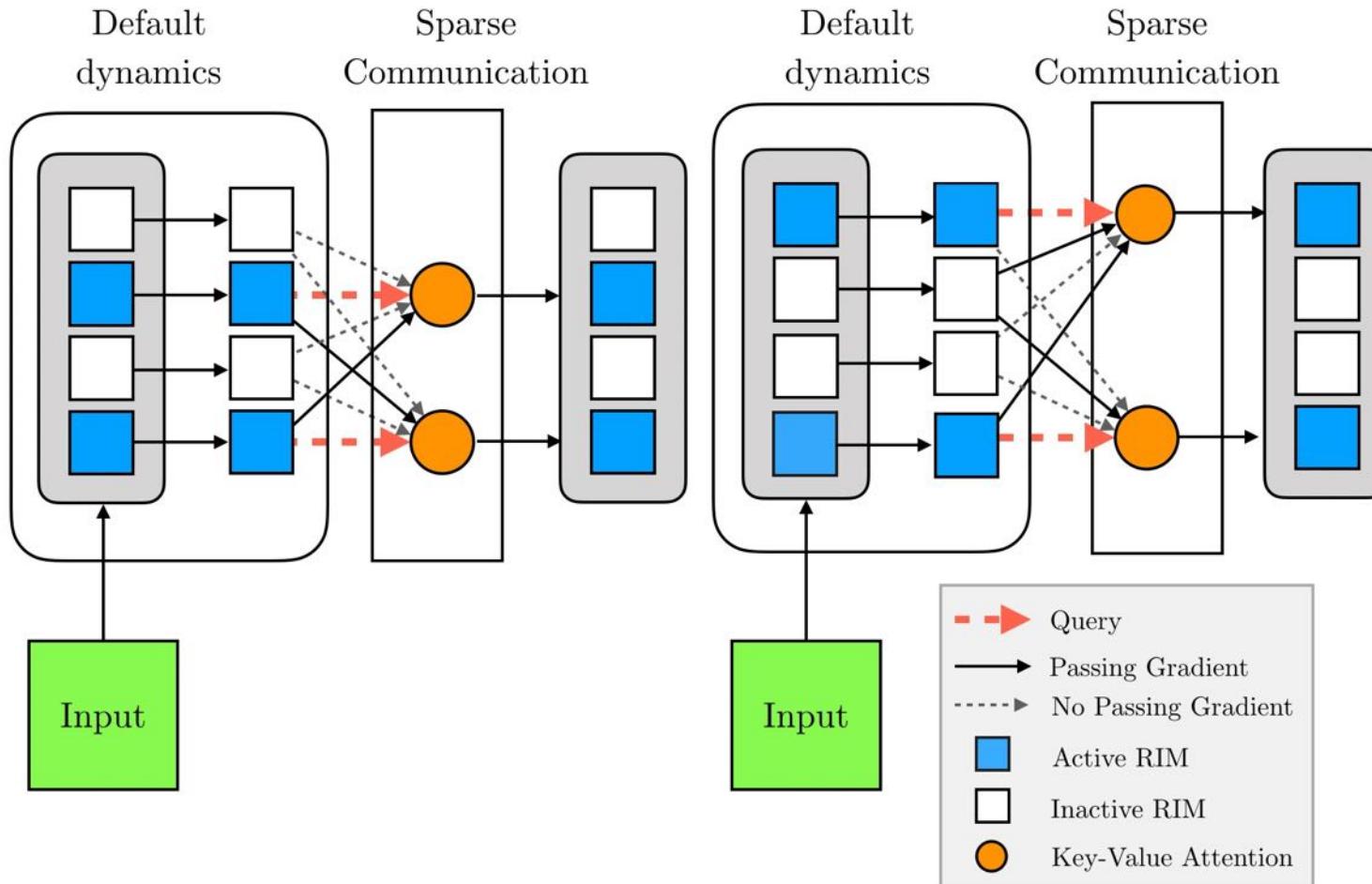
Exp6

Exp7

Expo

Expo

# Recurrent Independent Mechanisms



with **Anirudh Goyal**,  
Alex Lamb,  
Jordan Hoffmann,  
Shagun Sodhani,  
Sergey Levine,  
Yoshua Bengio

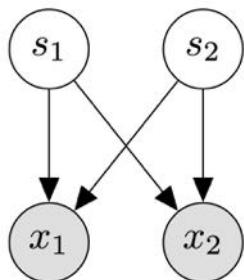
*ICLR 2021*

A. Goyal, A. Lamb, J. Hoffmann, S. Sodhani, S. Levine, Y. Bengio, and B. Schölkopf, 2019. Recurrent independent mechanisms.  
[arXiv:1909.10893](https://arxiv.org/abs/1909.10893).

# Causality for nonlinear ICA

(<https://arxiv.org/abs/2106.05200>)

with Luigi Gresele\*, Julius von Kügelgen\*, Vincent Stimper, Michel Besserve



Observe:

Goal:

Problem:

Recently:

New:

nonlinear mixtures,  $x = f(s)$ , of independent sources  $s$   
recover the unobserved sources (blind source separation)

impossible in general [Hyvärinen & Pajunen, '99]

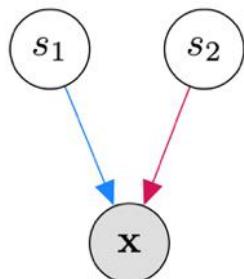
use auxiliary variables [Hyvärinen et al., '16, '17, '19]

interpret mixing as *causal* process & constrain  $f$  using the ICM principle



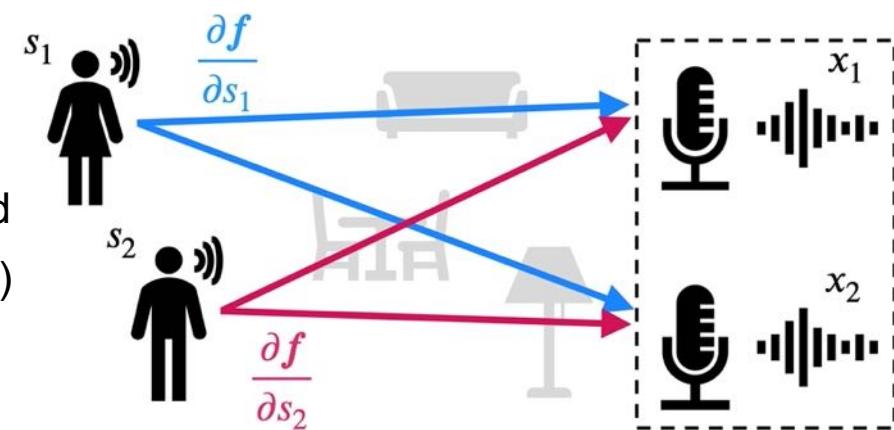
ICM usually applied to **cause distribution**  $p_c$  and **mechanism**  $p_{e|c}$  (or  $f$ ),  
e.g., cause-effect discovery

But: in nonlinear ICA, cause (source distribution) is unobserved



**Independent mechanism analysis (IMA):**

- ICM at level of mixing function
- contributions  $\frac{\partial f}{\partial s_i}$  of each source to observed distribution be "independent" (not statistical)
- speakers' positions not fine-tuned to room acoustics and microphone placement



# Independent mechanism analysis

IMA Principle: the influences of each source on the observed distribution are independent in the sense that:

$$\log |\mathbf{J}_f(\mathbf{s})| = \sum_{i=1}^n \log \left\| \frac{\partial \mathbf{f}}{\partial s_i}(\mathbf{s}) \right\|$$

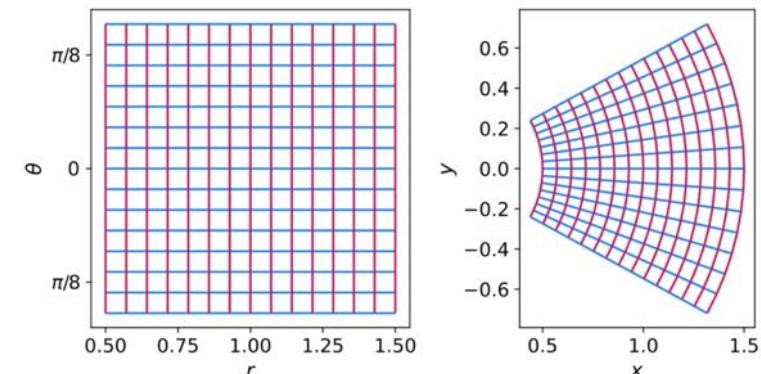
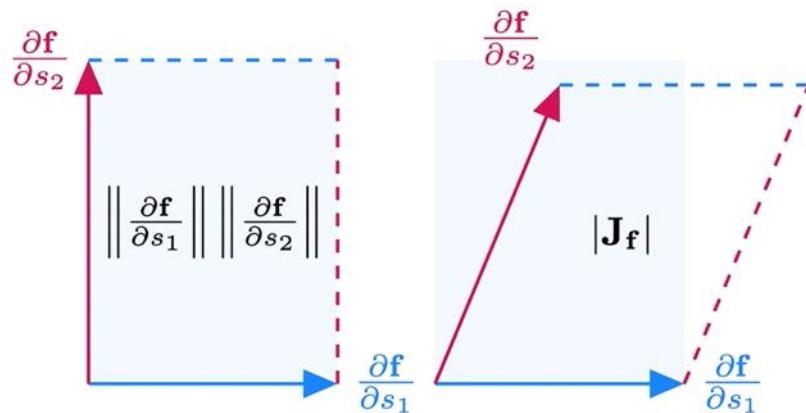
Geometric interpretation: corresponds to an *orthogonality condition* on the columns of the Jacobian.

Contrast function:

$$C_{IMA}(f, p_s) = \int \left( \sum_{i=1}^n \log \left\| \frac{\partial f}{\partial s_i}(\mathbf{s}) \right\| - \log |\mathbf{J}_f(\mathbf{s})| \right) p_s(\mathbf{s}) d\mathbf{s}$$

- $\geq 0$ , with equality iff.  $f$  is an *orthogonal coordinate transformation*
- *invariant to reparametrisation* of the sources by permutation and *element-wise invertible nonlinearities*

with Luigi Gresele\*, Julius von Kügelgen\*, Vincent Stimper, Michel Besserve



# Independent mechanism analysis

with Luigi Gresele\*, Julius von Kügelgen\*, Vincent Stimper, Michel Besserve



## Theory

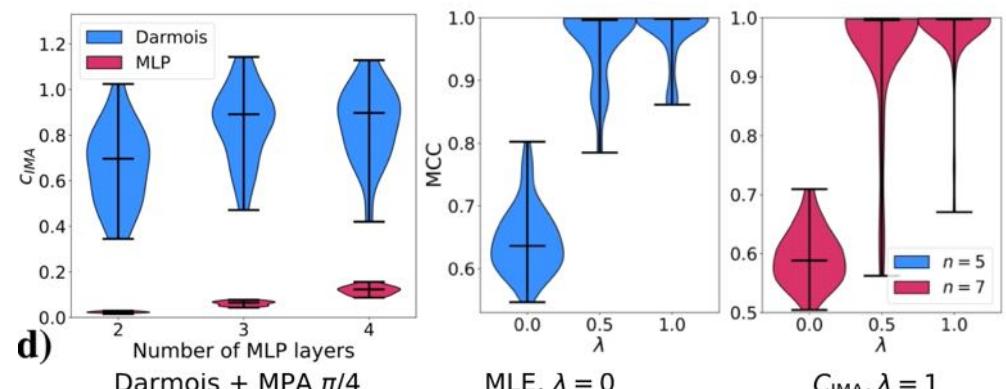
Can rule out (in the sense that  $C_{IMA}$  is larger for) well-known spurious ICA solutions:

- Darmois (inverse CDF) construction
- Measure-preserving automorphisms (MPA)

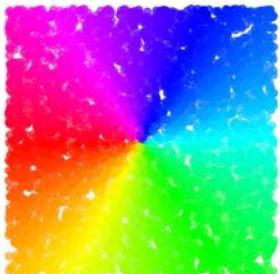
Consistent with existing identifiability results for linear ICA, and conformal maps.

## Experimental results

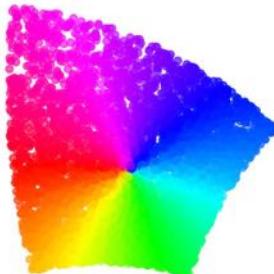
Even when assumptions are not perfectly satisfied, IMA seems useful to distinguish spurious solutions and recover the true sources



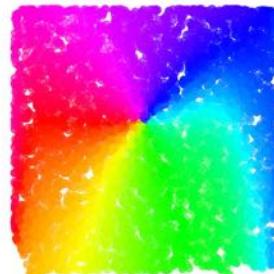
Ground truth



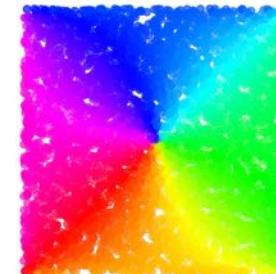
Observations



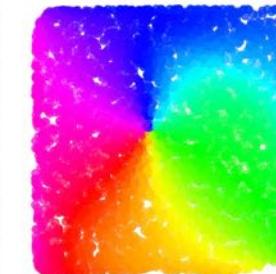
Darmois



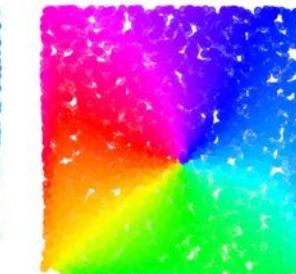
MPA  $\pi/4$



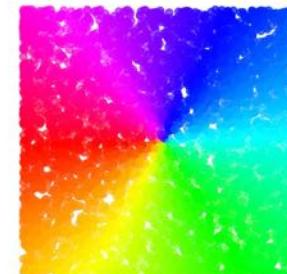
Darmois + MPA  $\pi/4$



MLE,  $\lambda = 0$



$C_{IMA}, \lambda = 1$



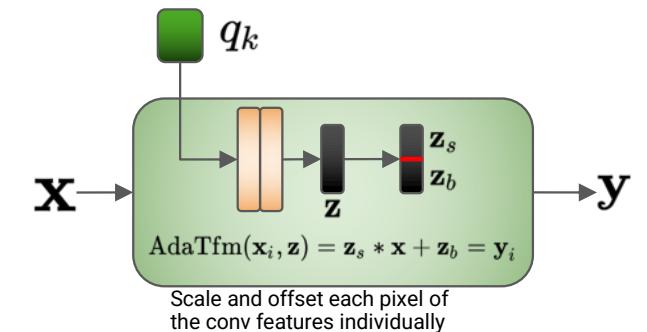
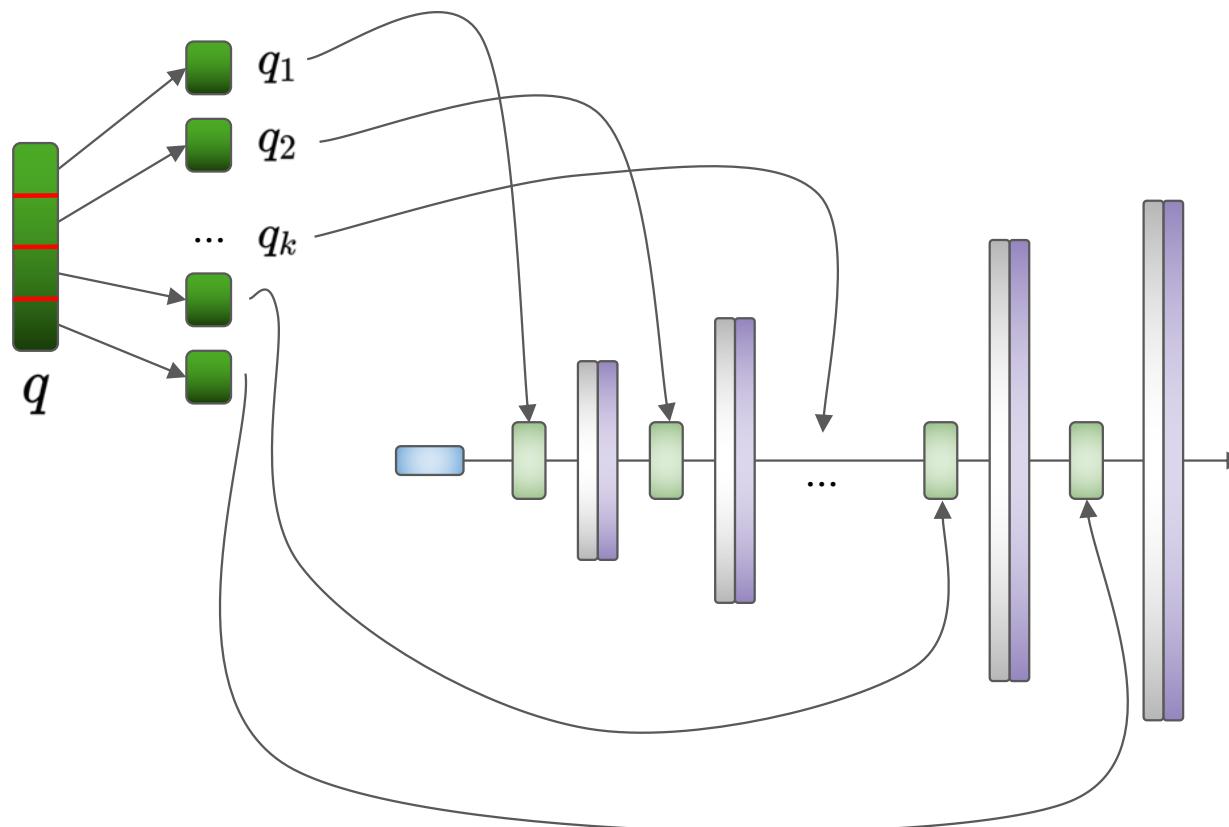
# Structural Decoders

Leeb et al.

arXiv 2006.07796



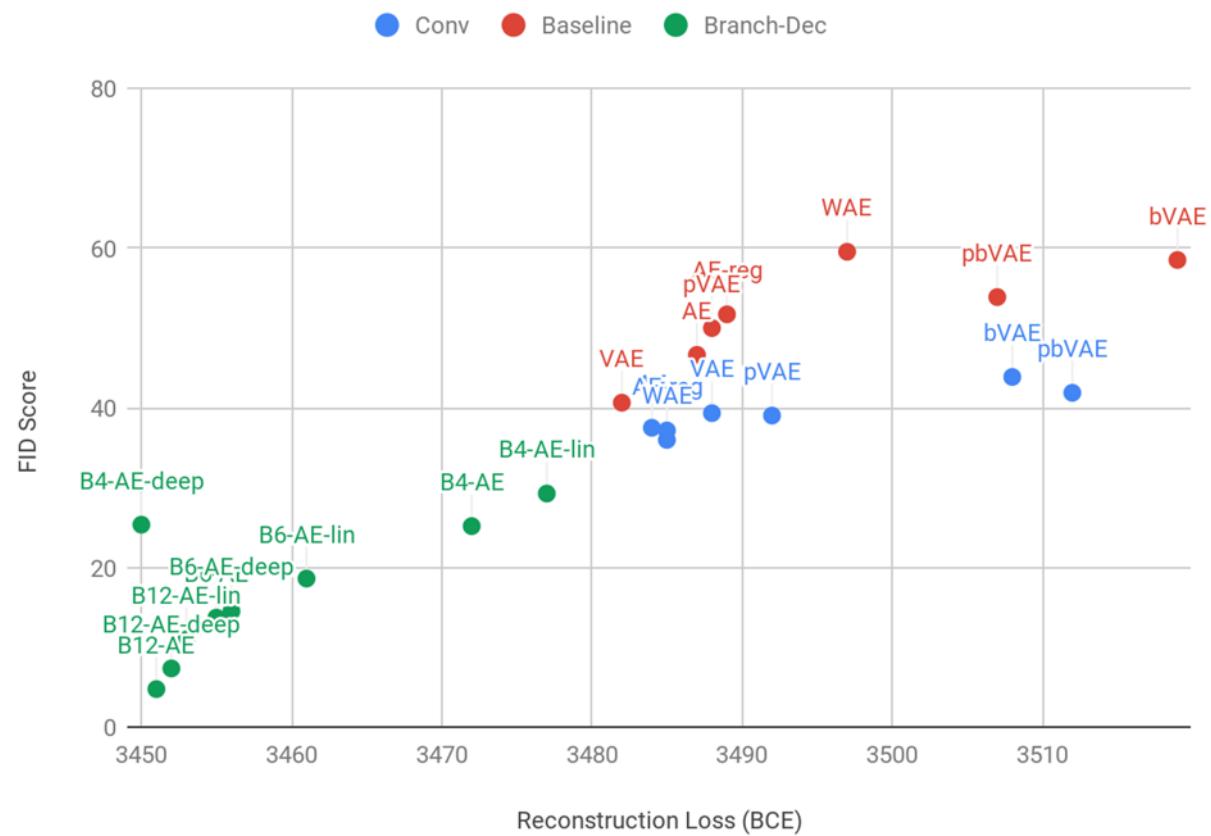
→ ~200-700k parameters



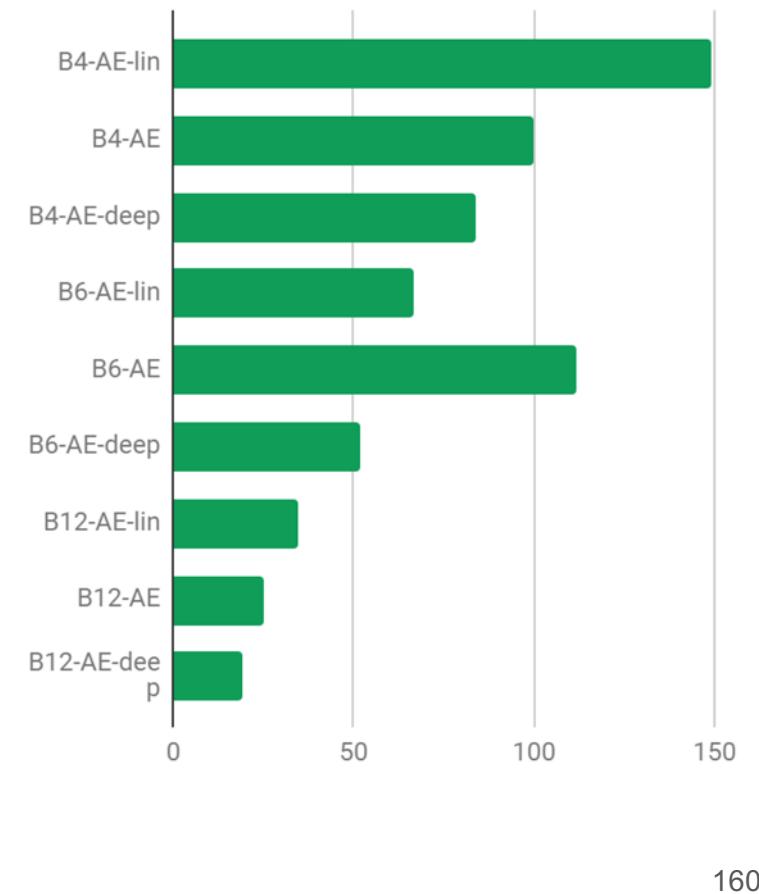
- Static features
- Adaptive Transform
- Vector Split
- Convolution
- Fully-connected
- Bilinear Upsampling

# Quantitative Results

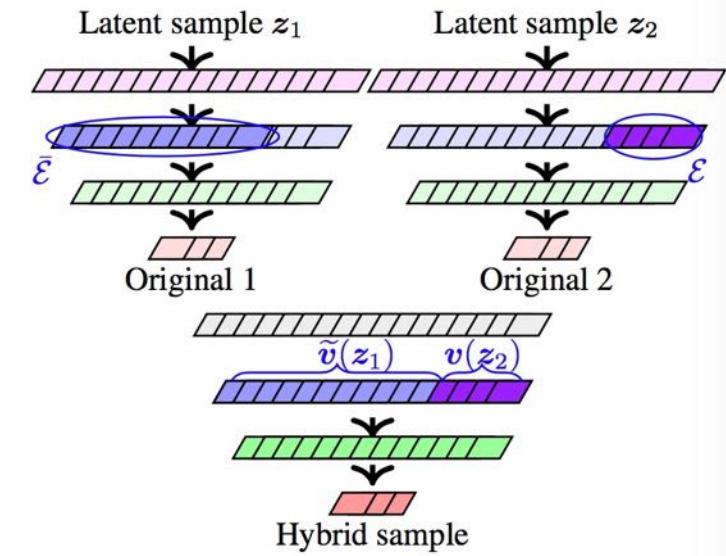
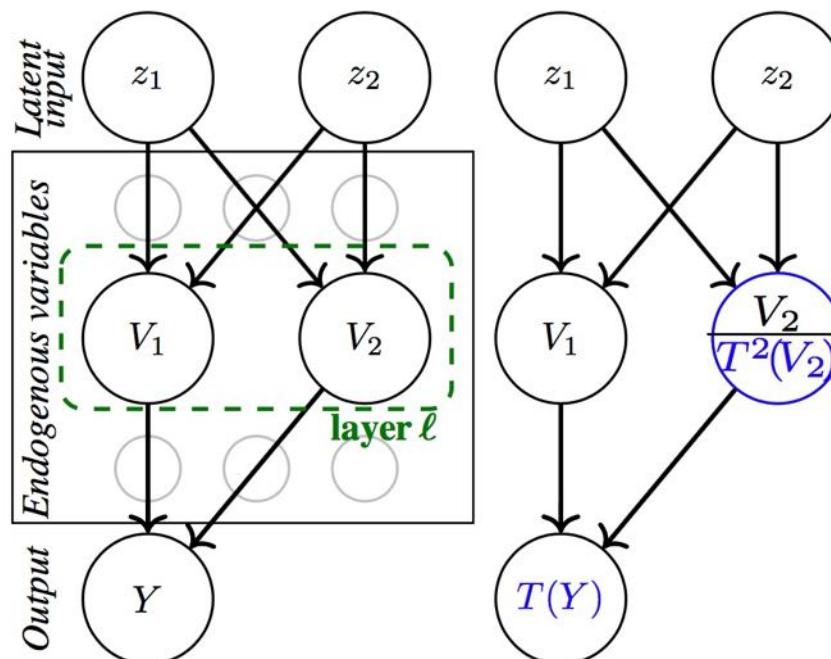
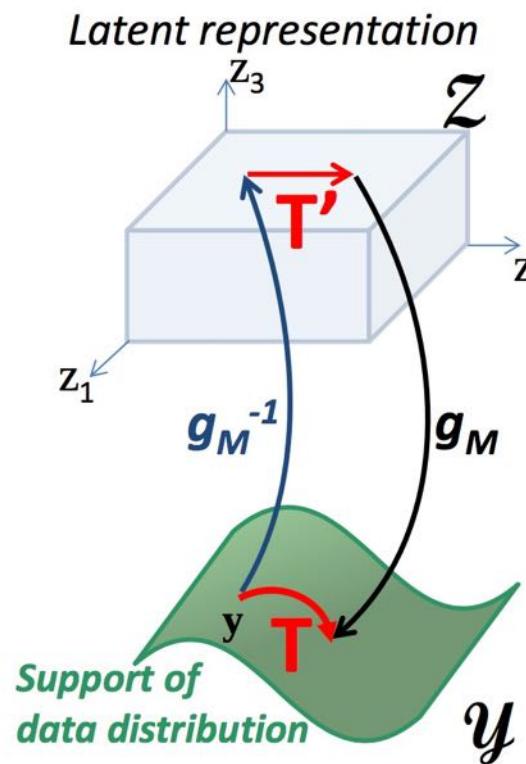
Reconstruction Quality



FID Score for Gen (Hyb)



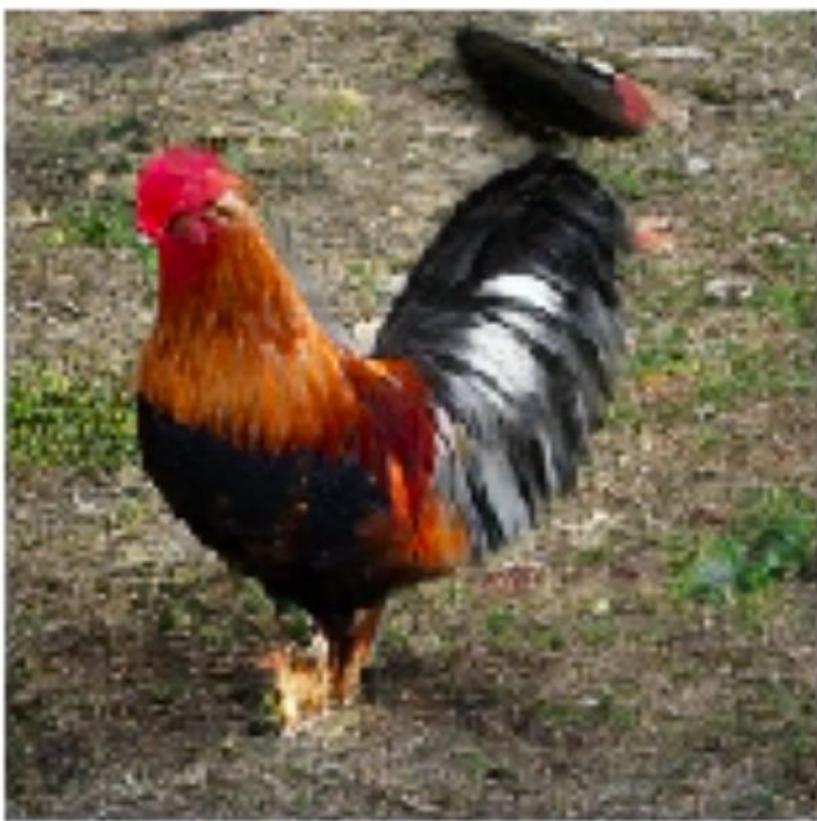
# Interventional Representations (Besserve et al., ICLR 2020)



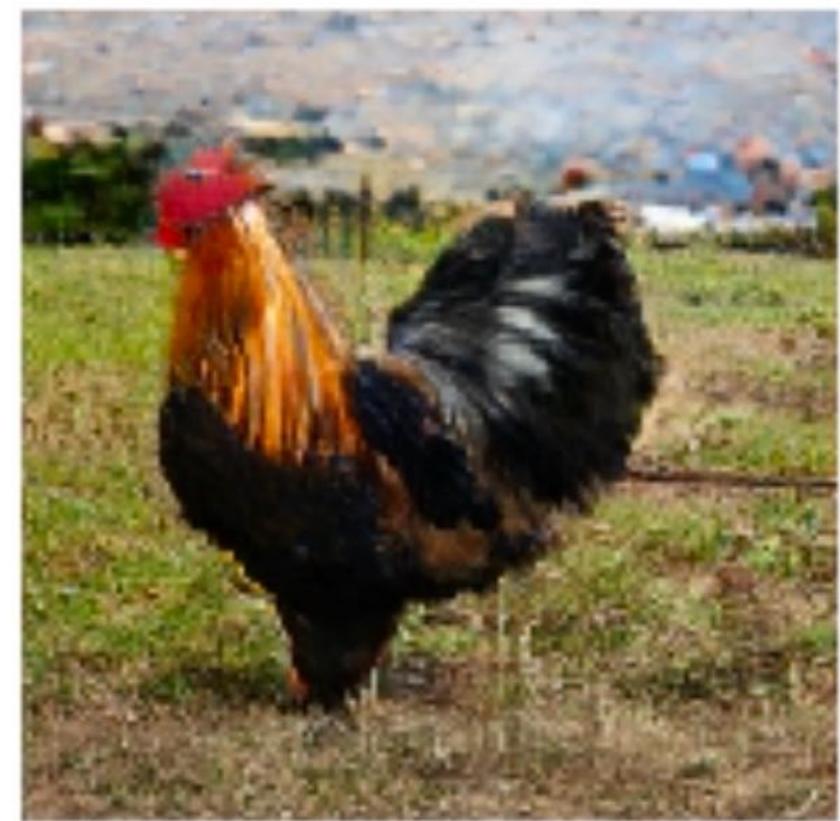
Bernhard Schölkopf

# Interventional Representations (Besserve et al., ICLR 2020)

Original



Counterfactual



# Interventional Representations (*Besserve et al., ICLR 2020*)

Original 1



Hybrid



Original 2



Bernhard Schölkopf



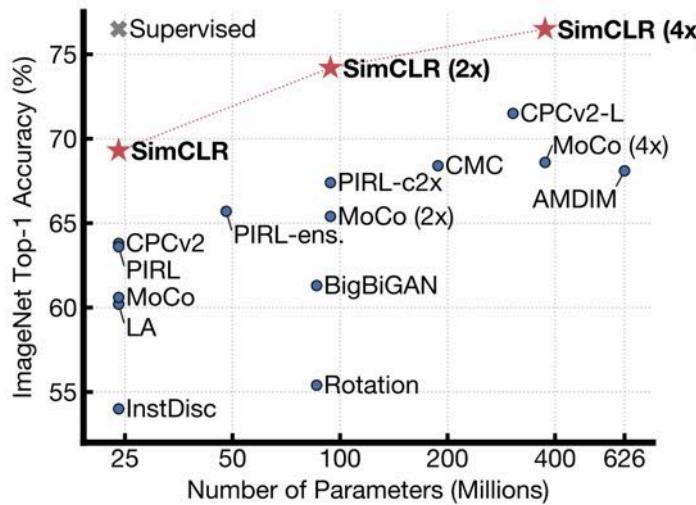
MAX-PLANCK-GESELLSCHAFT

# Self-supervised learning provably isolates content from style

(<https://arxiv.org/abs/2106.04619>)

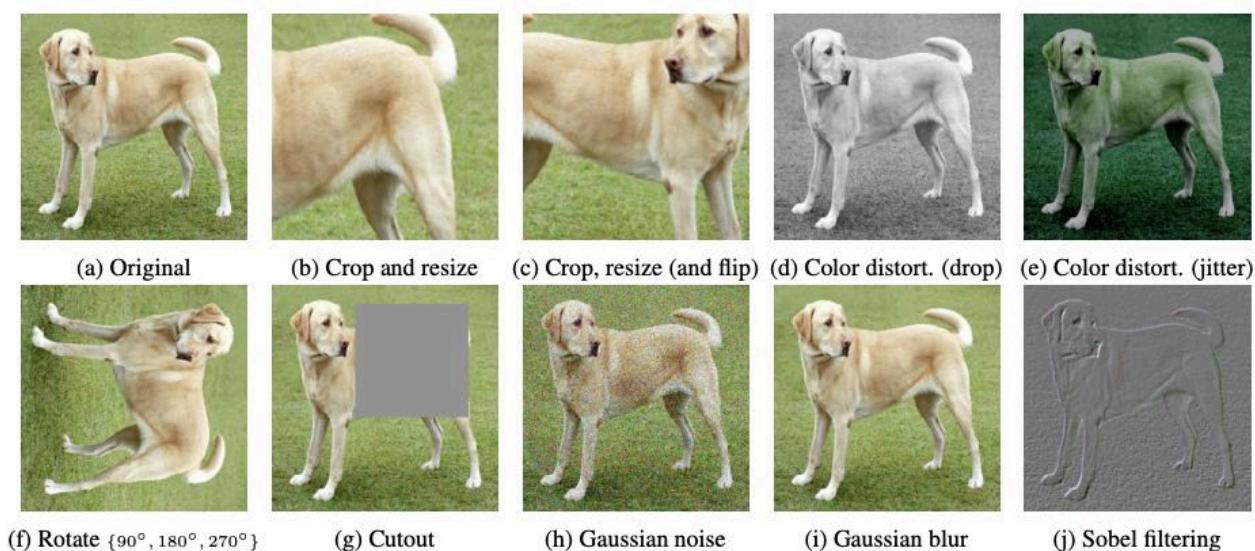


with **Julius von Kügelgen\***,  
**Yash Sharma\***, **Luigi Gresele\***,  
Wieland Brendel, Michel  
Besserve, Francesco Locatello



Self-supervised learning using contrastive training learn a representation which is insensitive to augmentation but sensitive to changing the example (NCE).

Can think of both as interventions.



Figures from:

*SimCLR: A Simple Framework for Contrastive Learning of Visual Representations.*  
Chen, Kornblith, Norouzi, Hinton (ICML 2020); <https://arxiv.org/abs/2002.05709>

# Self-supervised learning provably isolates content from style



with **Julius von Kügelgen\***,  
**Yash Sharma\***, **Luigi Gresele\***,  
Wieland Brendel, Michel  
Besserve, Francesco Locatello

Formalise generation  $\mathbf{x} = f(\mathbf{z})$  and augmentation  $\tilde{\mathbf{x}} = f(\tilde{\mathbf{z}})$  processes as latent variable model with unknown content-style partition  $\mathbf{z} = (\mathbf{c}, \mathbf{s})$ , interpreting style change as an intervention.

- *invariant content c*: shared between pairs  $(\mathbf{x}, \tilde{\mathbf{x}})$  of views;
- *varying style s*: may change across pairs  $(\mathbf{x}, \tilde{\mathbf{x}})$  of views.

Allow causal dependence of style on content (*Causal3DIdent* dataset).

Given data  $(\mathbf{x}, \tilde{\mathbf{x}})$  (nonlinear mixtures of content and style):

**Theory:** Can identify\* invariant content partition in generative and discriminative learning with entropy maximisation (e.g., SimCLR).

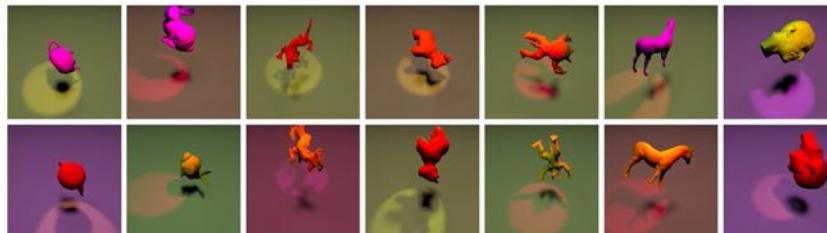
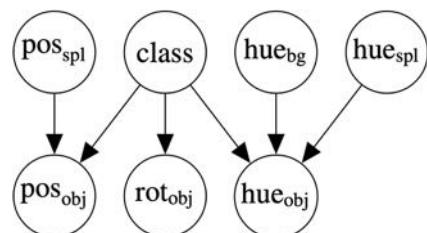
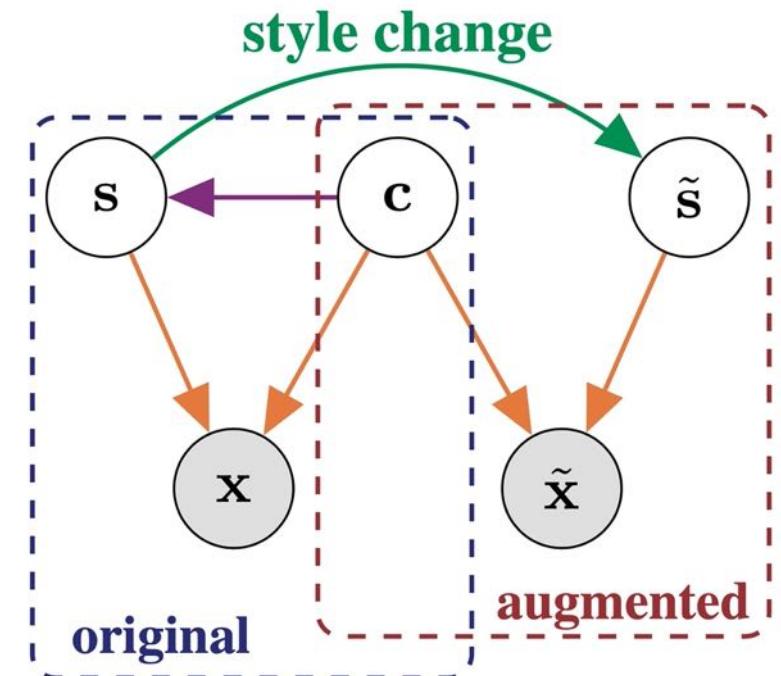


Figure 2: (Left) Causal graph for the *Causal3DIdent* dataset. (Right) Two samples from each object class.



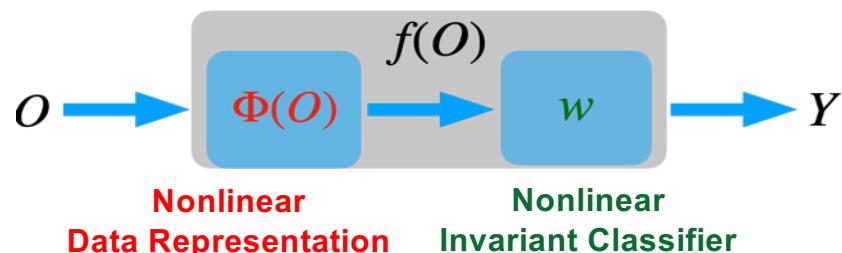
\*up to invertible transformation

# Nonlinear Invariant Risk Minimization

(with Chaochao Lu, Yuhuai Wu, José Miguel Hernández-Lobato, [arXiv:2102.12353](https://arxiv.org/abs/2102.12353))

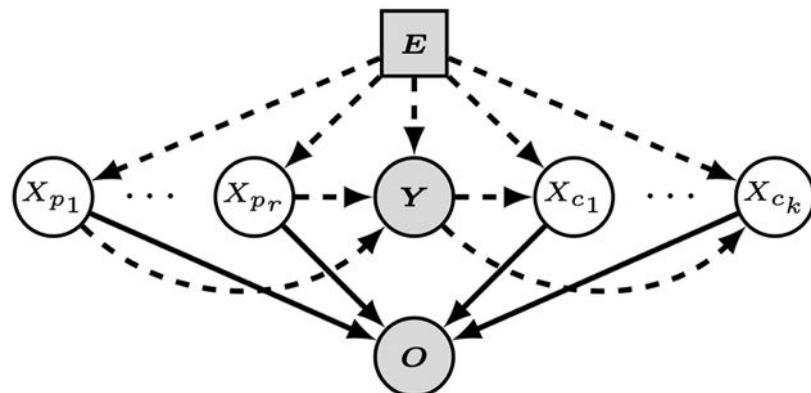


## Problem



**Key Idea:**  
**Data representation  $\Phi(O)$  should be the direct cause of  $Y$ .**

## Assumption on Causal Graphs



This assumption is more general than the common Independence assumption in latent variable models.

## Assumption on the Prior

$$P(X | Y, E) = P(X_{p_1}, \dots, X_{p_r} | Y, E) \prod_{i \in I_C} P(X_i | Y, E)$$

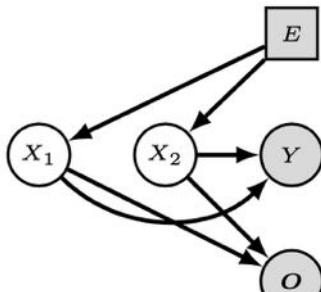
$\downarrow$

$$p_{T,\lambda}(X | Y, E) = \frac{\mathcal{Q}(X)}{\mathcal{Z}(Y, E)} \cdot \exp(\langle T(X), \lambda(Y, E) \rangle)$$

The prior is assumed to be a general exponential family distribution leading to IDENTIFIABILITY.

# Experimental Results

(with Chaochao Lu, Yuhuai Wu, José Miguel Hernández-Lobato, [arXiv:2102.12353](https://arxiv.org/abs/2102.12353))



Data Generating Process

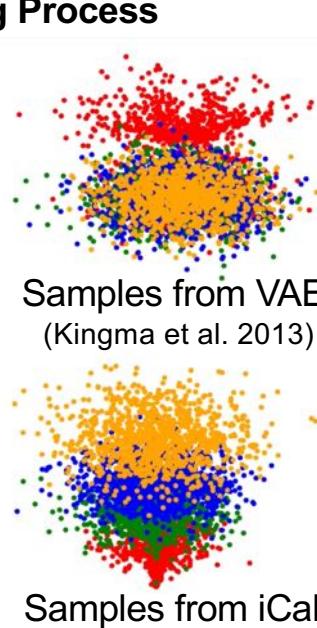


Original Data



Samples from VAE  
(Kingma et al. 2013)

$$\begin{aligned} E &\sim \mathcal{U}\{0.2, 2, 3, 5\} \\ X_1 &\sim \mathcal{N}(X_1|E, 1) \\ X_2 &\sim \mathcal{N}(X_2|2E, 2) \\ Y &\sim \mathcal{N}(Y|X_1 + X_2, 1) \\ O &= g(X_1, X_2) \end{aligned}$$



Samples from iVAE  
(Khemakhem et al. 2020)



Color	Red	Green
Y=0	$p_e$	$1 - p_e$
Y=1	$1 - p_e$	$p_e$

- **2 Training Envs:**  $\{p_e = 0.1, p_e = 0.2\}$
- **1 Testing Env:**  $\{p_e = 0.9\}$

Table 2: Colored Fashion MNIST. Comparisons in terms of accuracy (%) (mean  $\pm$  std deviation).

METHOD	TRAIN	TEST
ERM	$83.17 \pm 1.01$	$22.46 \pm 0.68$
ERM 1	$81.33 \pm 1.35$	$33.34 \pm 8.85$
ERM 2	$84.39 \pm 1.89$	$13.16 \pm 0.82$
ROBUST MIN MAX	$82.81 \pm 0.11$	$29.22 \pm 8.56$
F-IRM GAME	$62.31 \pm 2.35$	$69.25 \pm 5.82$
V-IRM GAME	$68.96 \pm 0.95$	$70.19 \pm 1.47$
IRM	$75.01 \pm 0.25$	$55.25 \pm 12.42$
<b>iCaRL (ours)</b>	<b><math>74.87 \pm 0.36</math></b>	<b><math>73.56 \pm 0.75</math></b>
ERM GRayscale	$74.79 \pm 0.37$	$74.67 \pm 0.48$
OPTIMAL	75	75

# Source-Free Adaptation to Measurement Shift via Bottom-Up Feature Restoration

(Cian Eastwood et al., <https://arxiv.org/abs/2107.05446>)

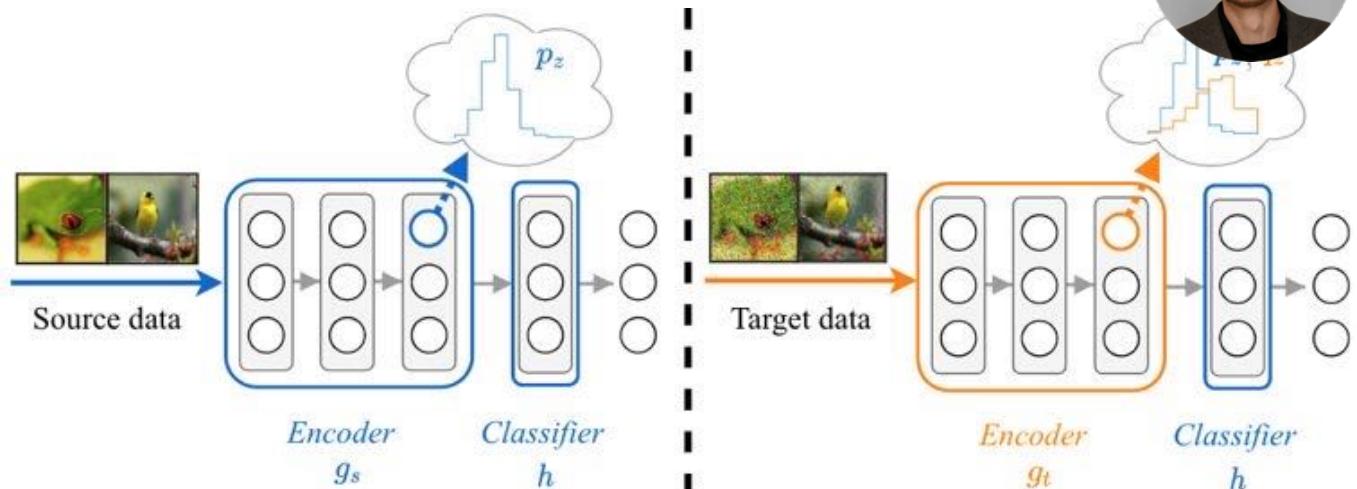


Source-free domain adaptation

- Development: train + equip model
- Deployment: adapt, no source data

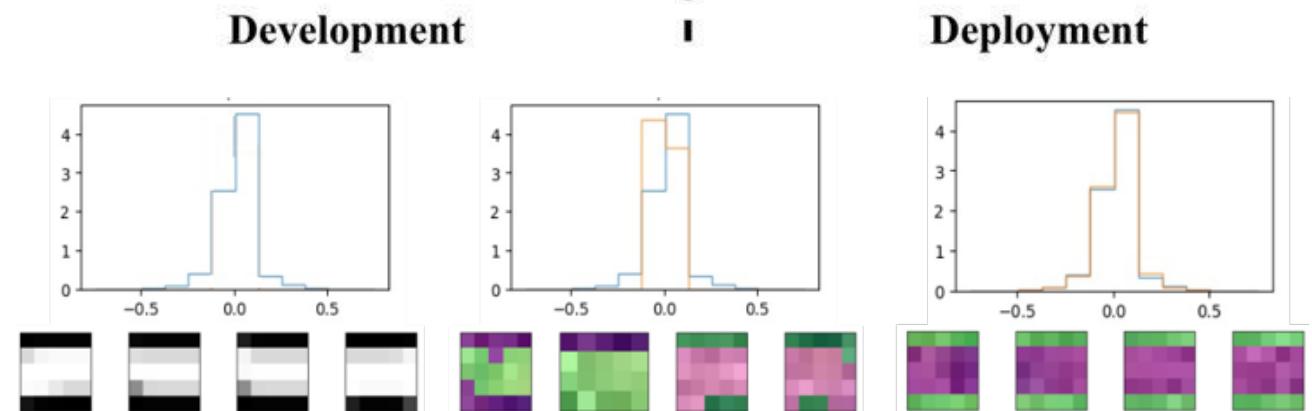
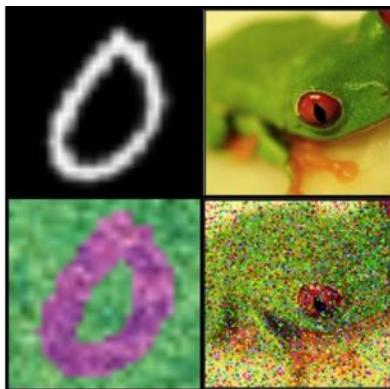
Measurement shift (cf. Storkey, 2009)

- New sensor, same underlying features



Feature restoration

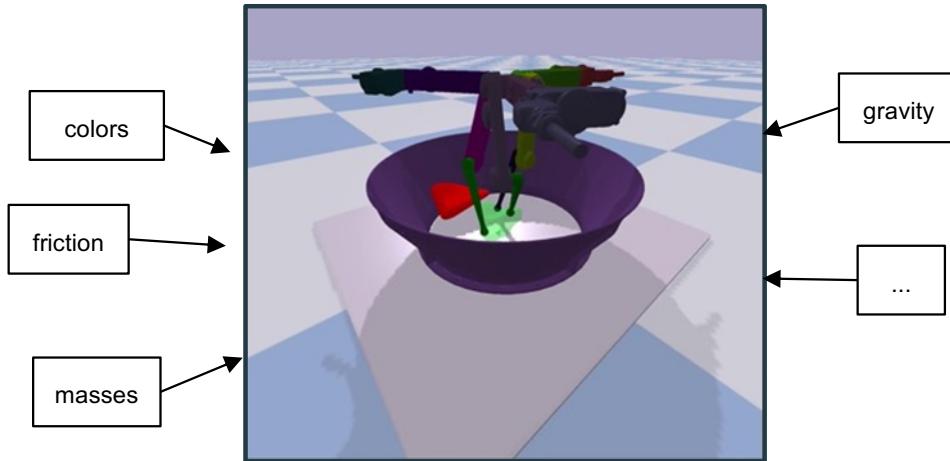
- Goal: extract same features, new env.
- Method: align (marginal) feature dists.



# CausalWorld: A Robotic Manipulation Benchmark for Causal Structure and Transfer Learning



Ahmed and Träuble et al.,  
arXiv: 2010.04296,  
ICLR 2021



**Evaluate different generalization aspects** by intervening on a large range of different defining variables of the hierarchical causal generative world model of the robotic environment.

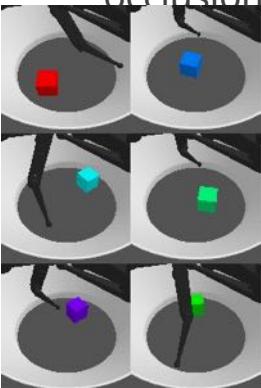
Benchmark with many challenging environments and fully documented code: <https://github.com/rr-learning/CausalWorld>



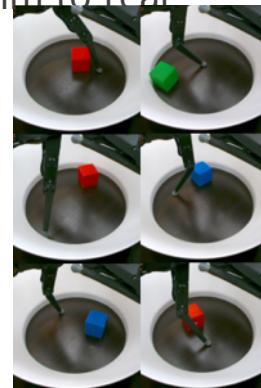
# On the Transfer of Disentangled Representations in Realistic Settings

## New Disentanglement Dataset

More complex and realistic, correlations between factors, occlusions, sim-to-real



1 million  
simulated



1800 real  
(labeled)

## Out-of-Distribution Generalization of Downstream Tasks



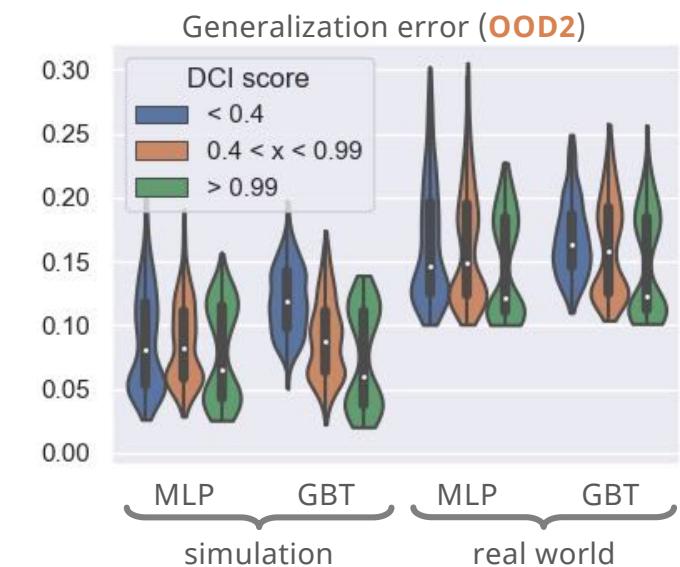
Task: predict value of non-OOD factors

- Train downstream task on pre-trained representations
- Test it OOD but still in the VAE's training distribution (OOD1)
- Test it OOD w.r.t. the VAE itself (OOD2)



Dittadi and Träuble et al.,  
arXiv: 2010.14407,  
ICLR 2021

Disentanglement has **minor role** when represent. function is OOD



# Causal Curiosity: RL Agents Discovering Self-supervised Experiments for Causal Representation Learning

- Curiosity to discover causation in an environment.
- **Reward-free**
- Set of environments with interventions on causal factors
- Use Kolmogorov Complexity as reward to RL agent
- Agents producing self-supervised experiments to test out mass, size etc.

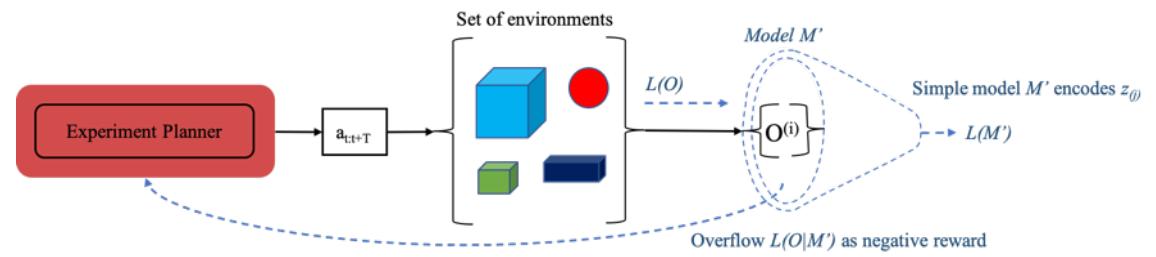


Fig 1: Experiment Discovery

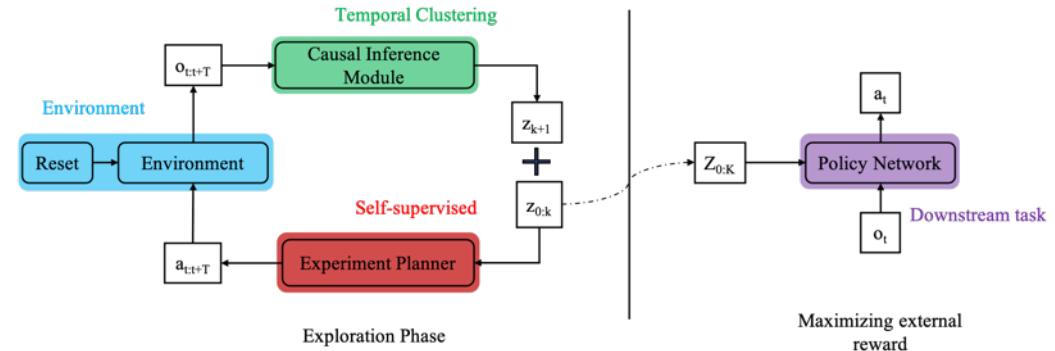


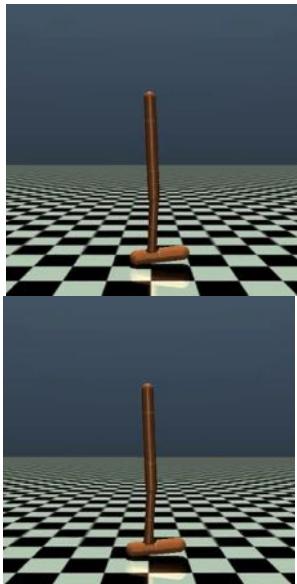
Fig 2: Performing experiments sequentially to learn causal representations.  
Representations used for downstream transfer.

Sontakke, Sumedh A., Arash Mehrjou, Laurent Itti, and Bernhard Schölkopf. "Causal Curiosity: RL Agents Discovering Self-supervised Experiments for Causal Representation Learning." *arXiv preprint arXiv:2010.03110* (2020). To appear at ICML 2021

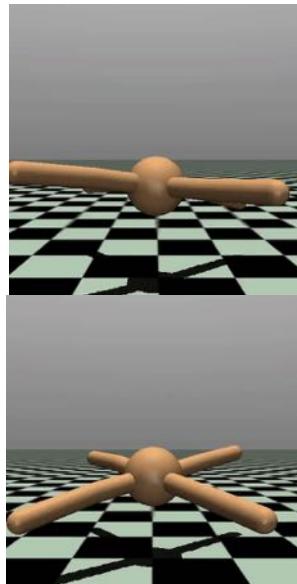


## Discovered Behaviors - Mujoco

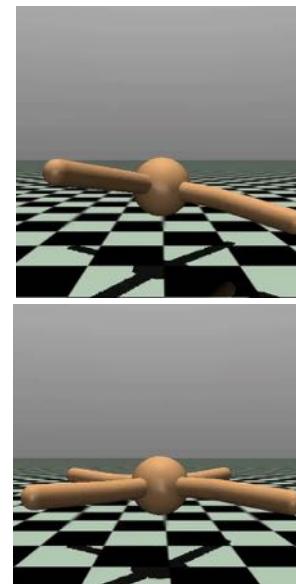
Heavy



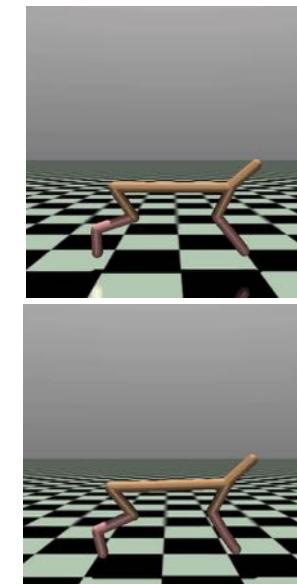
Light



Hop



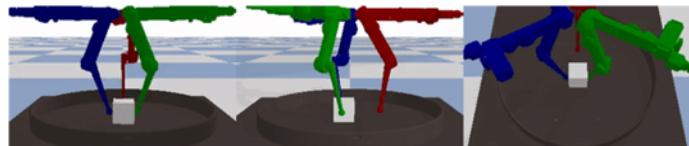
Pirouette



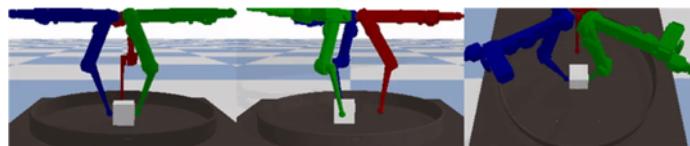
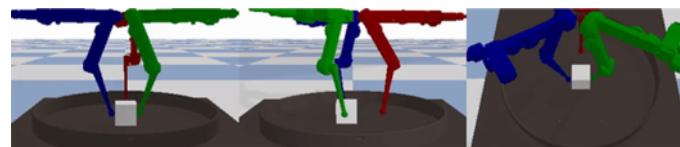
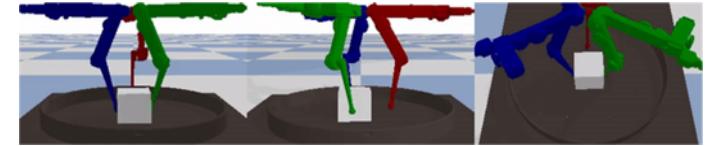
Leap

Pushup

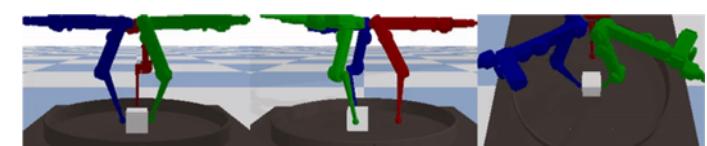
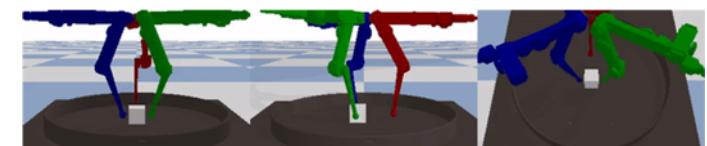
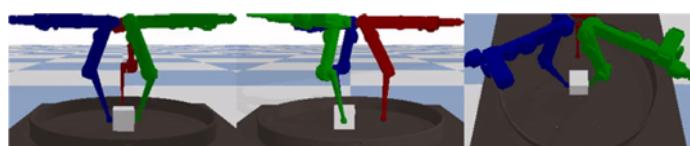
# Discovered Behaviors - CausalWorld



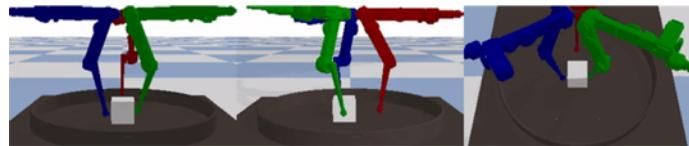
Lifting Behaviors



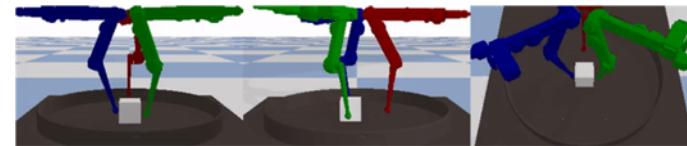
Rotate Behaviors



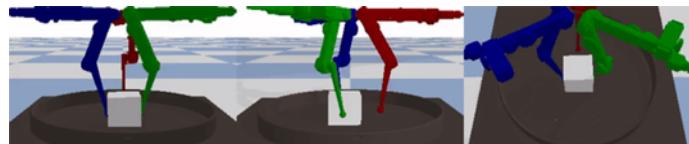
## Discovered Behaviors - CausalWorld



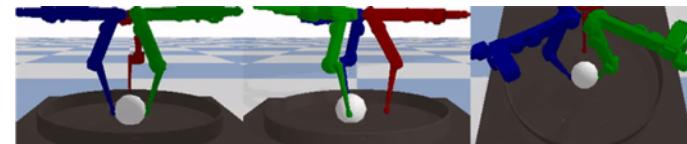
Dribble



Pushing along y



Pushing along x



Roll

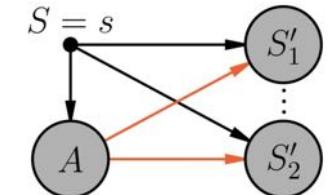
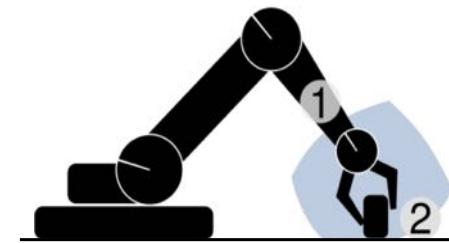
# Causal Influence Detection for Reinforcement Learning

(with Maximilian Seitzer and Georg Martius, arXiv:2106.03443)



## Observations

- Real-world agents have limited interventional range
- Causal influence of agent on environment occurs only sparsely



Robot can control object

## Idea

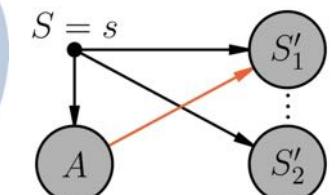
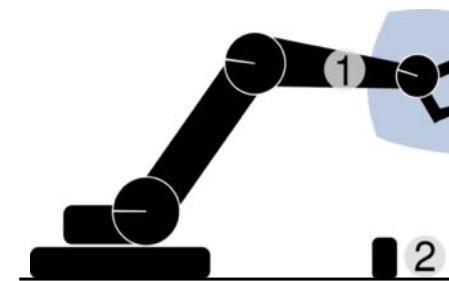
- Use causal influence to speed-up reinforcement learning

## Method

- Define measure of *causal action influence* as a conditional mutual information

$$C(s) := I(S', A \mid S = s)$$

- Estimate it from data using neural networks



Causal influence on object impossible

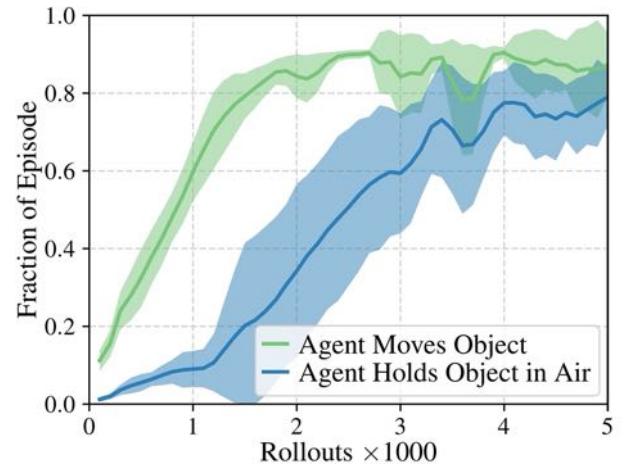
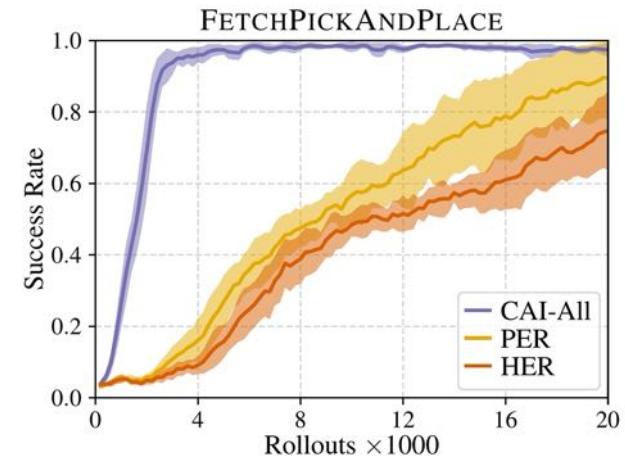
# Causal Influence Detection for Reinforcement Learning

(with Maximilian Seitzer and Georg Martius, arXiv:2106.03443)



## Results

- Focusing on states with causal influence (exploration and prioritization)
  - Highly increased sample-efficiency on robotic manipulation tasks
- Maximizing causal influence as intrinsic motivation
  - Agent quickly discovers interesting behaviors (grasping, lifting)



Brockmann et al. OpenAI Gym, arXiv:1606.01540

# Generative scene models as causal models

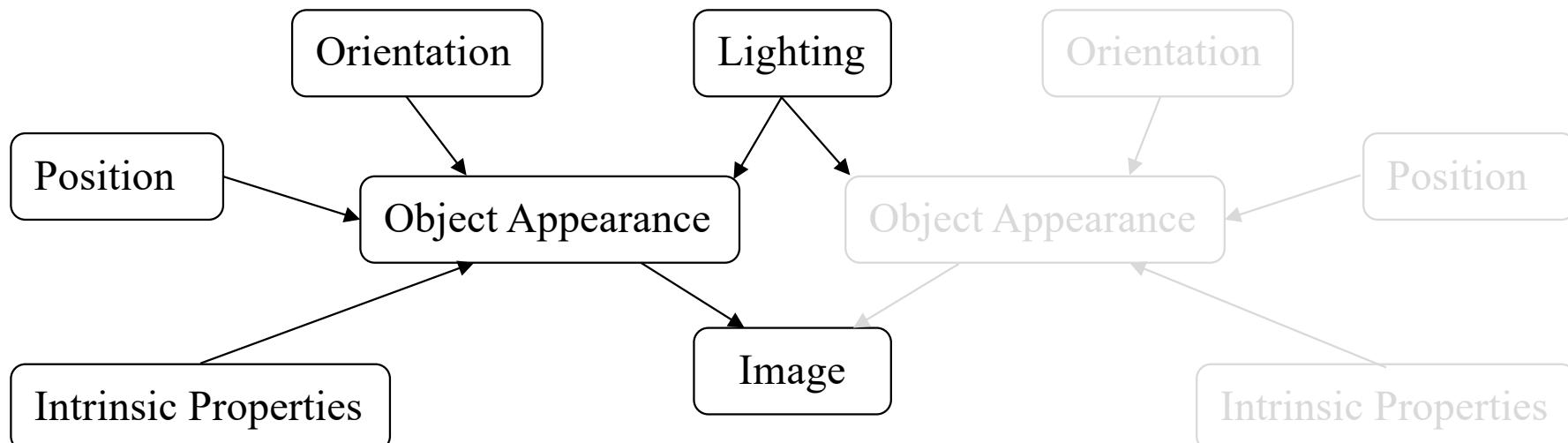
Disentangled (causal) factorization

<https://arxiv.org/abs/1911.10500>

- independent noises in the causal graph:

$$p(X_1, \dots, X_n) = \prod_{i=1}^n p(X_i | \text{PA}_i)$$

- independent mechanisms: changing one  $p(X_i | \text{PA}_i)$  does not change the other  $p(X_j | \text{PA}_j)$  ( $j \neq i$ ); they remain **invariant** (implies intervenability)





Presented at the ICLR 2020 workshop “Causal learning for decision making”

## TOWARDS CAUSAL GENERATIVE SCENE MODELS VIA COMPETITION OF EXPERTS

**Julius von Kügelgen<sup>\*†1,2</sup>, Ivan Ustyuzhaninov<sup>\*†3</sup>,**  
**Peter Gehler<sup>†4</sup>, Matthias Bethge<sup>†3,4</sup>, Bernhard Schölkopf<sup>†1,4</sup>**  
<sup>1</sup>Max Planck Institute for Intelligent Systems Tübingen, Germany  
<sup>2</sup>Department of Engineering, University of Cambridge, United Kingdom  
<sup>3</sup>University of Tübingen, Germany  
<sup>4</sup>Amazon Tübingen, Germany  
`{jvk,bs}@tuebingen.mpg.de,`  
`{ivan.ustyuzhaninov,matthias.bethge}@bethgelab.org,`  
`pgehler@amazon.com`

### ABSTRACT

Learning how to model complex scenes in a modular way with recombinable components is a pre-requisite for higher-order reasoning and acting in the physical world. However, current generative models lack the ability to capture the inherently compositional and layered nature of visual scenes. While recent work has made progress towards unsupervised learning of object-based scene representations, most models still maintain a global representation space (i.e., objects are not explicitly separated), and cannot generate scenes with novel object arrangement and depth ordering. Here, we present an alternative approach which uses an inductive bias encouraging modularity by training an ensemble of generative models (*experts*). During training, experts compete for explaining parts of a scene, and thus specialise on different object classes, with objects being identified as parts that re-occur across multiple scenes. Our model allows for controllable sampling of individual objects and recombination of experts in physically plausible ways. In contrast to other methods, depth layering and occlusion are handled correctly, moving this approach closer to a causal generative scene model. Experiments on simple toy data qualitatively demonstrate the conceptual advantages of the proposed approach.

### 1 INTRODUCTION

Proposed in the early days of computer vision Grenander (1976); Horn (1977), *analysis-by-synthesis* is an approach to the problem of visual scene understanding. The idea is conceptually elegant and appealing: build a system that is able to synthesize complex scenes (e.g., by rendering), and then understand analysis (inference) as the inverse of this process that decomposes new scenes into their constituent components. The main challenges in this approach are the need for generative models of objects (and their composition into scenes) and the need to perform tractable inference given new

*Tangemann, Schneider et al., 2021*



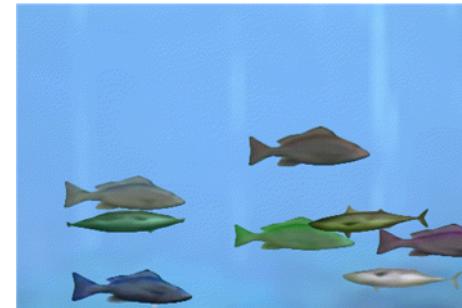
Training set



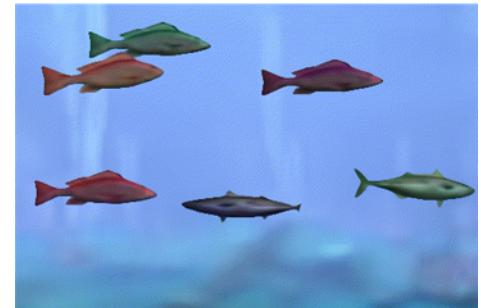
# of objects



fish identities



position



# Towards causal machine learning

learn *world models* (aka *digital twins*) that are

## (1) data-efficient

- use data from multiple tasks in multiple environments
- use re-usable components that are robust across tasks, i.e., causal (independent) mechanisms
  - disentanglement as a causal problem
  - bias RL to search for invariance / find models where shifts are sparse

## (2) interventional

- move representation learning towards interventional representations:  
*"thinking is acting is an imagined space"* (Konrad Lorenz) ---  
planning, reasoning, ...





# Toward Causal Representation Learning

*This article reviews fundamental concepts of causal inference and relates them to crucial open problems of machine learning, including transfer learning and generalization, thereby assaying how causality can contribute to modern machine learning research.*

By BERNHARD SCHÖLKOPF<sup>✉</sup>, FRANCESCO LOCATELLO<sup>✉</sup>, STEFAN BAUER<sup>✉</sup>, NAN ROSEMARY KE,  
NAL KALCHBRENNER, ANIRUDH GOYAL, AND YOSHUA BENGIO<sup>✉</sup>

**ABSTRACT** | The two fields of machine learning and graphical causality arose and are developed separately. However, there is, now, cross-pollination and increasing interest in both fields to benefit from the advances of the other. In this article, we review fundamental concepts of causal inference and relate them to 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 causality starts from the premise that the causal variables are given. A central problem for AI and causality is, thus, causal representation learning, that is, the discovery of high-level causal variables from low-level observations. Finally, we delineate some implications of causality for machine learning and propose key research areas at the intersection of both communities.

**KEYWORDS** | Artificial intelligence; causality; deep learning; representation learning.

---

Manuscript received August 14, 2020; revised December 29, 2020; accepted February 8, 2021. Date of publication February 26, 2021; date of current version April 30, 2021. (Bernhard Schölkopf and Francesco Locatello contributed equally to this work. Stefan Bauer and Nan Rosemary Ke contributed equally to this work.) (Corresponding author: Francesco Locatello.)

Bernhard Schölkopf and Stefan Bauer are with the Max Planck Institute for Intelligent Systems, 72076 Tübingen, Germany (e-mail: bs@tuebingen.mpg.de).

## I. INTRODUCTION

If we compare what machine learning can do to what animals accomplish, we observe that the former is rather limited at some crucial feats where natural intelligence excels. These include transfer to new problems and any form of generalization that is not from one data point to the next (sampled from the same distribution), but rather from one problem to the next—both have been termed *generalization*, but the latter is a much harder form thereof, sometimes referred to as *horizontal, strong, or out-of-distribution generalization*. This shortcoming is not too surprising, given that machine learning often disregards information that animals use heavily: interventions in the world, domain shifts, and temporal structure—by and large, we consider these factors a nuisance and try to engineer them away. In accordance with this, the majority of current successes of machine learning boil down to large-scale pattern recognition on suitably 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.

### A. Issue 1—Robustness



MAX-PLANCK-GESELLSCHAFT

# A Modeling Taxonomy

Task	statistical model	causal model	differential equation model	animal
Predict in i.i.d. setting, pattern recognition, “generalization”	y	y	y	y
Predict under shift & intervention, “horizontal generalization”	n	y	y	y
Think/Reason, “act in an imagined space”	n	?	?	y
Learn from data	y	?	n	y
Provide physical insight, understand predictions	n	?	y/?	n

Thank You

