Causal models are generative models What is special about them ?

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PEPR-IA-Causalite: M. Clausel (U. Nancy)

E. Gaussier, E. Devijver (U. Grenoble); E. Chzhen, M. Sebag (UPSaclay)





Summary

- A causal model is a generative model
- Why Positioning wrt Machine Learning
- What
- How
 Observational causal discovery
- An example: Causality and Human Resources analysis

Formal background

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Example

Pearl, 2009; Pearl & Mackenzie 2018

Variables

- Covariates X₁...X_d
- Outcome Y

genes G; smoke S

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cancer C



Intervention: do(X = v)

Setting the value of X to v

Definition: X is a cause of Y, noted $X \rightarrow Y$ iff

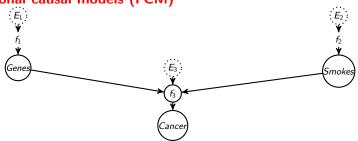
$$P(Y|do(X = v)) \neq P(Y|do(X = v'))$$

Beware: Intervening is *not* conditioning

- Conditioning: observing what happens for smokers
- Intervening: making everyone smoke; and observing what happens

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Functional causal models (FCM)



Variables

- Endogenous variables: X₁,...X_d
- Exogenous noise variables: independent, one for each variable

Noise variables E_1, E_2, E_3 model the known unknowns

Causal graph

Edge (X, Y) $(X \rightarrow Y)$ iff X is a direct cause of Y **Distribution**

Causal mechanism f_i

 $X_i \sim f_i(PA(X_i), E_i)$

with $PA(X_i)$ the immediate causes of X_i

$$P(X_1,\ldots,X_d)=\prod P(X_i|PA(X_i),\underbrace{E_i}_{a})$$

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Why Causal Modeling ? Position w.r.t. Machine Learning

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Ideally, Randomized Controlled Trials Alternative: Causal Discovery from Observational Data

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Dependency tests-based Score based Based on supervised learning

Structural Agnostic Modelling

An application to Human Resources

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The AI/ML/big data promise



Auguste Comte

$\textbf{Knowledge} \rightarrow \textbf{Prediction} \rightarrow \textbf{Control}$

Savoir pour prévoir afin de pouvoir

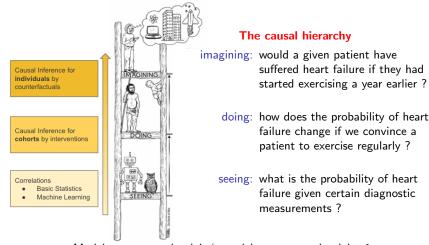
ML models will expectedly enable control:

= Interventions

- health and nutrition
- education
- economics/management
- climate

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Learning causal models



Pearl 2003, 2009, 2018; Schölkopf et al., 2021, Barenboim et al., 2022

Model accurate at level $i \not\rightarrow$ model accurate at level i+1

Mainstream Machine Learning: discriminative or generative modelling

Given a training set

iid samples $\sim P(X, Y)$

$$\mathcal{E} = \{(\mathbf{x}_i, y_i), \mathbf{x}_i \in \mathbb{R}^d, i \in [[1, n]]\}$$

Find

- Supervised learning: $\widehat{h}: X \mapsto Y$ or $\widehat{P(Y|X)}$
- Generative model P(X, Y)

Predictive modelling might be based on correlations If umbrellas in the street, Then it rains



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Using Machine Learning models out of their scope

If you can predict...



... can you make things happen ?

Causal models are generative models What is special about them ?

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Causal modeling for more trustworthy AI

Wanted: An AI with common decency

Fair no biases
 Accountable model can be explained
 Transparent decisions can be explained

The dark side of AI:

Robust

Zeynep Tufekci	We're building a dystopia just to make people click on ads	
C. O'Neill	Weapons of Math Destruction, 2016	
Timnit Gebru	www.technologyreview.com/2020/12/04/1013294/google-ai-ethics-	
	research-paper-forced-out-timnit-gebru	

Causal modeling for more trustworthy AI, 2

- Decreased sensitivity wrt data distribution
- Support interventions
- Hopes of explanations
- Hopes of bias detection

The robustness issue When it works



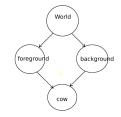
When it does not work



out-of-distribution generalization.

Perona, 2022

Tentative interpretation



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Causal models are generative models What is special about them ?

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Caveat

Causal models \neq efficient predictive models

Predicting Y

$$\widehat{Y} = 0.25X + 0.5Z$$

If interpreted as a causal model, suggests that Y depends on Z.

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An application to Human Resources

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Causal Discovery: The royal road

Gold standard: Randomized controlled trials, RCT

- Draw iid samples, form two subsets:
 - T=1: treatment group
 - T=0: control group
- Compute Average Treatment Effect (ATE); Conditional Average Treatment (CATE)

Notations

- Y: outcome (survival)
- X: covariates (age, gender,...)
- > $Y_i(0)$: outcome of the i-th sample if it does not get the treatment
- > $Y_i(1)$: outcome of the i-th sample if it does get the treatment

Challenges:

- For *i*-th individual, either $Y_i(0)$ or $Y_i(1)$ is known
- In many cases, no RCTs (infeasible; unethical; too expensive)

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Estimate the Average Treatment Effect

$$ATE = \mathbb{E}[Y(1) - Y(0)]$$

Under assumptions, it works

 $(X \perp T)$

 $ATE = \mathbb{E}[Y(1) - Y(0)]$ $= \mathbb{E}[Y(1)] - \mathbb{E}[Y(0)]$ linearity of expectation $= \mathbb{E}_{X}[\mathbb{E}[Y(1)|X]] - \mathbb{E}_{X}[\mathbb{E}[Y(0)|X]]$ expectation over covariates $= \mathbb{E}_{X}[\mathbb{E}[Y(1)|T = 1, X]] - \mathbb{E}_{X}[\mathbb{E}[Y(0)|T = 0, X]]$ no hidden confounder (no unbserved common causes) overlap assumption, T=1 and T=0 are observed in the data $= \mathbb{E}_X[\mathbb{E}[Y|T=1,X]] - \mathbb{E}_X[\mathbb{E}[Y|T=0,X]]$ consistency: $Y_i(1) \sim Y | T = 1, X = X_i$ (1)

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Estimating ATE: when it does not work $(X \not\perp T)$

The Simpson paradox: comparing treatments A and B of kidney stones

Reporting the survival rate:

Stone size	Treatment A	Treatment B
Small stones	93% (81/87)	87% (234/270)
Large stones	73% (192/263)	69% (55/80)
Total	78% (273/350)	83% (289/350)

Bottom line: treatment B dominates treatment A

Not really: treatment A applied more often on severe cases

(because it's more efficient)

because applied on more severe cases, A looks less efficient...

Observational Causal Discovery

WHAT

- Given data,
- Infer causal models
- Challenges: data quality; data quantity; learning criterion...

Some applications

For human resources Quality of life at work / economic profitability Coll. SECAFI, La fabrique de l'industrie; Kalainathan et al. 18

For health

Diet / Diabetes type 2.

Coll. INRAE Gasnikova et al. 21

Impact of pesticides on newborn diseases

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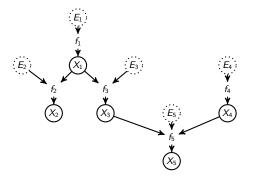
An application to Human Resources

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Observational causal discovery

Goal Given $\mathcal{D} \sim P(X_1, \dots, X_d)$ Find Functional





$$\begin{cases} X_1 = f_1(E_1) \\ X_2 = f_2(X_1, E_2) \\ X_3 = f_3(X_1, E_3) \\ X_4 = f_4(E_4) \\ X_5 = f_5(X_3, X_4, E_5) \end{cases}$$

Requirements on solutions

- Identifiability
- The causal graph is directed acyclic

unicity of the FCM solution

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Observational causal discovery, 2

Reichenbach principle

If $X \not\perp Y$, then exists Z s.t. $Z \to X$ and $Z \to Y$. 3 cases: $X \to Y$ or $Y \to X$ or $X \leftarrow Z \to Y$ (Z confounder)

Usual assumptions

Causal sufficiency: no unobserved common confounders

Causal Markov, Causal Faithfulness:

 $P(X_1,\ldots,X_d) == \prod P(X_i | PA(X_i), E_i)$

Observational Causal Discovery

Main approaches

- Dependence/independence tests based
- Score-based
- Learning-based

Main drawbacks

- Find a graphical model: doubly exponential
- ▶ Data hungry: Tests in $O(d^3)$ + multiple hypothesis testing
- Representativity and biases in data

Observational Causal Discovery based on tests, 1

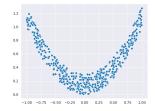
Independent variables X and Y (X \perp Y)

 $X \perp Y$ iff P(X, Y) = P(X).P(Y)

Dependency tests

Correlation

limited to linear dependencies



$$Y = X^2 + \varepsilon$$

Correlation(X, Y) ≈ 0

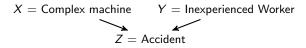
HSIC, Hilbert-Schmitt Independence Criterion

Gretton et al. 05

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Observational Causal Discovery based on tests, 2

Conditional dependence a.k.a. V-structure

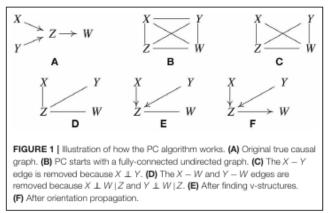


X and Y are independent; but given Z = true they are not independent (either the machine is complex or the worker is inexperienced...)

Observational Causal Discovery based on tests, 3

Algorithms

- Find dependencies and conditional independencies
- Constraint propagation



PC Algorithm (PC) Spirtes et al. 00; Glymour et al., 20 Non-linear extensions (CI tests): PC-HSIC (KCI-test), PC-RCIT

Zhang 12, Strobl 17

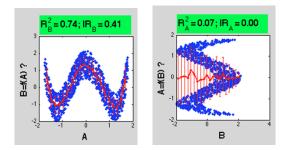
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Observational Causal Discovery based on scores, 1

Leveraging Occam's razor principle

Janzig 19

 \rightarrow the causal model as the one being the simplest model that fits the data.



Intuition

If
$$X \to Y$$
, then $p(X, Y) = p(Y|X).p(X)$

Observational Causal Discovery based on scores, 2

Bayesian Information Criterion

$$BIC(\mathcal{G}) = -2\ln L + k * \ln n$$

with L: Likelihood of the model, k: number of parameters, n: Number of samples

The graph is optimized with the operators:

- add edge
- remove edge
- revert edge

Alg: Greedy Equivalence Search (GES)

Chickering 02, 20

Observational Causal Discovery based on scores, 2

Leveraging the data inverse covariance matrix Θ

Loh Buhlman 2014; Shimizu et al. 06, Dong et al. 23

 $\mathbf{X} = B^t \mathbf{X} + \mathbf{E}$

Then

lf

$$(I - B) D^{-1} (I - B)^{t} = \Theta$$
 (2)

with $D = Diag(var(E_1), \dots var(E_d))$

Issues

- Estimating Θ
- Enforcing DAG-ness
- Solution of Eq. 2 not unique

Zheng et al. 18

Observational Causal Discovery based on Machine Learning

Guyon et al, 2014-2015; 2019

Pair Cause-Effect Challenges

Gather data: a sample is a pair of variables (A_i, B_i)

lts label ℓ_i is the "true" causal relation (e.g., age "causes" salary)

Input

$$\mathcal{E} = \{ (A_i, B_i, \ell_i), \ell_i \text{ in } \{ \rightarrow, \leftarrow, \bot \!\!\!\bot \} \}$$

Example A_i, B_i	Label ℓ_i
A_i causes B_i	\rightarrow
B_i causes A_i	\leftarrow
A_i and B_i are independent	

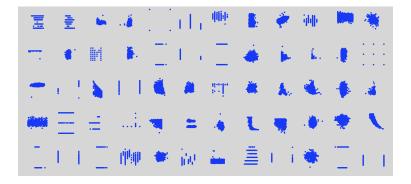
Output

using supervised Machine Learning

Hypothesis : $(A, B) \mapsto$ Label

Guyon et al, 2014-2015

Pair (A_i, B_i) can be represented by a distribution = an image:



The Cause-Effect Pair Challenge

Learn a causality classifier (causation estimation)

Like for any supervised ML problem from images

ImageNet 2012



More

Guyon et al., eds, Cause Effect Pairs in Machine Learning, 2019.

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The Cause-Effect Pair Challenge, Limitation

Using predictive ML to estimate the causation sense: where is the problem ?

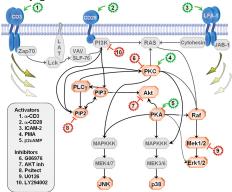
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The Cause-Effect Pair Challenge, Limitation

Using predictive ML to estimate the causation sense: where is the problem ? Predictive learning requires **examples**: many, representative,...

Where do the CEP examples come from ?

- Common sense (age causes salary...)
- Variations on regulatory genes



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Structure Agnostic Modeling

Kalainathan et al. 22

Principle

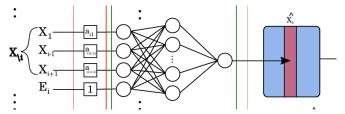
For each X_i, learn a Markov kernel

 $X_i \sim f_i$ (Subset of **X**, E_i)

Rk: Sufficient subset of X: Markov blanket (X_i) (causes, effects, spouses) Yu et al., 2018

- Learn simultaneously all kernels
 Rk: Avoids combinatorial search for structure
- Add regularization
 To enforce parsimony (MB(X_i))
 To enforce DAGness (PA(X_i))

Structure Agnostic Modeling, 2



The *i*-th neural net

• Learns conditional distribution $P(X_i|X_{\setminus i})$ as $\hat{f}_i(X_{\setminus i}, E_i)$

$$f_i(X_{i}, E_i) = \sum_k \beta_{i,k} \phi_{i,k}(\mathsf{a}_{i,1}X_1, \dots, \mathsf{a}_{i,d}X_d, E_i)$$

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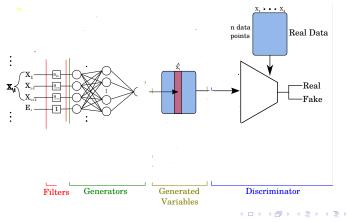
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Structure Agnostic Modeling, 2

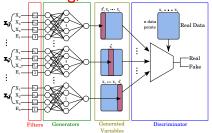
Adversarial training Goodfellow 14; 17; Arjovsky Bottou 2017

- Generate $\{\tilde{x}_i^{(j)}\}$ with *j*-th component of $\tilde{x}_i^{(j)}$ set to $\hat{f}_i(x_i, \epsilon)$, $\epsilon \sim \mathcal{N}(0, 1)$
- Discriminate true from generated data

 $\min_{G} \max_{D} \mathbb{E}_{x}[log(D(x))] + \mathbb{E}_{\hat{x}}[log(1 - D(x))]$



Structure Agnostic Modeling, 3



Given observational data
$$\{x_1, \ldots, x_n\} \sim P(X_1, \ldots, X_d)$$
 x_i in \mathbb{R}^d

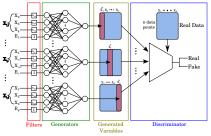
Adversarial learning

- Generate $\{\tilde{x}_i^{(j)}\}$ with *j*-th component of $\tilde{x}_i^{(j)}$ set to $\hat{f}_i(x_i, \epsilon)$, $\epsilon \sim \mathcal{N}(0, 1)$
- ▶ Discriminator *D* among observational data $\{x_i\}$ and generated data $\{\tilde{x}_i^{(j)}, i = [[1, n]], j = [[1, d]]\}$
- Learning criterion (adversarial + sparsity)

$$\min_{G} \max_{D} \left(\mathbb{E}_{x}[log(D(x))] + \mathbb{E}_{\hat{x}}[log(1 - D(x)] + \lambda \sum_{i,j} |a_{i,j}| \right)$$

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Structure Agnostic Modeling, 4



Structure of causal graph: $A = (a_{i,j})$

Competition between discriminator and sparsity term $||A||_1$

- Avoids combinatorial search for structure
- Cycles are possible
- DAGness achieved by enforcing constraints on trace of exp(A)

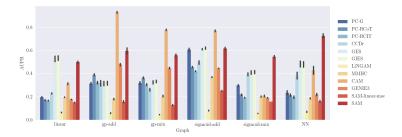
Zheng et al., 18

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Validation on synthetic graphs

Experimental setting on synthetic graphs **causal mechanisms:** linear; sigmoid additive or mixed; Gaussian Process additive or mixed; NN

Comparative performance, Area Under Precision Recall Curve (d = 100)

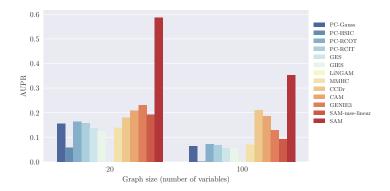


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On simulated biological datasets

On SynTREN graphs

Comparative performance, Area Under Precision Recall Curve



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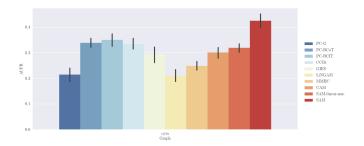
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On Sachs, 2005

On protein network problem

Sachs et al., 05

Comparative performance, Area Under Precision Recall Curve



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Quantitative results

Computational time (sec., per graph) CPU: 48-core Intel(R) Xeon(R) CPU E5-2650 CPU. GPU: Nvidia RTX 2080Ti GPU

AUPR	Linear	GP AM	GP Mix	Sigmoid AM	Sigmoid Mix	NN	CPU Time	GPU Time
PC-GAUSS	0.19 (0.01)	0.31 (0.02)	0.32 (0.02)	0.61 (0.02)	0.30 (0.01)	0.23 (0.03)	13	
PC-HSIC	-	-	-	-	-	-	-	
PC-RCOT	0.18 (0.01)	0.39 (0.02)	0.36 (0.01)	0.45 (0.01)	0.22 (0.01)	0.21 (0.02)	31,320	
PC-RCIT	0.17 (0.01)	0.32 (0.02)	0.31 (0.01)	0.52 (0.01)	0.19 (0.01)	0.19 (0.02)	46,440	
GES	0.53 (0.04)	0.32 (0.03)	0.32 (0.02)	0.61 (0.01)	0.41 (0.03)	0.48 (0.04)	1	
GIES	0.53 (0.03)	0.31 (0.03)	0.33 (0.02)	0.62 (0.02)	0.41 (0.02)	0.48 (0.04)	5	
MMHC	0.20 (0.01)	0.18 (0.01)	0.21 (0.01)	0.37 (0.01)	0.20 (0.01)	0.19 (0.01)	5	
LINGAM	0.06 (0.01)	0.06 (0.01)	0.04 (0.01)	0.08 (0.01)	0.05 (0.01)	0.07 (0.01)	5	
CAM	0.31 (0.01)	0.93 (0.01)	0.78 (0.01)	0.77 (0.01)	0.20 (0.01)	0.43 (0.05)	45,899	
CCDR	0.23 (0.01)	0.31 (0.04)	0.26 (0.02)	0.49 (0.02)	0.39 (0.02)	0.38 (0.05)	3	
GENIE3	0.18 (0.01)	0.48 (0.02)	0.45 (0.01)	0.45 (0.01)	0.19 (0.01)	0.22 (0.02)	511	
SAM-lin-mse	0.15 (0.003)	0.16 (0.02)	0.13 (0.01)	0.25 (0.004)	0.16 (0.002)	0.16 (0.01)	3,076	74
SAM-mse	0.21 (0.01)	0.30 (0.03)	0.20 (0.01)	0.33 (0.005)	0.20 (0.01)	0.26 (0.03)	12,896	118
SAM-lin	0.41 (0.01)	0.29 (0.02)	0.22 (0.01)	0.51 (0.01)	0.46 (0.02)	0.47 (0.04)	8,746	516
SAM	0.50 (0.02)	0.60 (0.04)	0.56 (0.02)	0.62 (0.02)	<u>0.55</u> (0.02)	<u>0.72</u> (0.03)	15,361	519

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Causal Modeling and Human Resources

Position of the problem

A Quality of life at work

- B Economic performance
- ... are correlated

Question: Are there causal relationships ?

A
ightarrow B ; or B
ightarrow A; or $\exists C \ / \ C
ightarrow A$ and C
ightarrow B

Answering the question is key to evolve management strategies.

Data

- Gathered by Group Alpha Secafi (trade union advisor)
- Tax files + social audits for 408 firms

employee's perspective firm's perspective

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Data

Firms

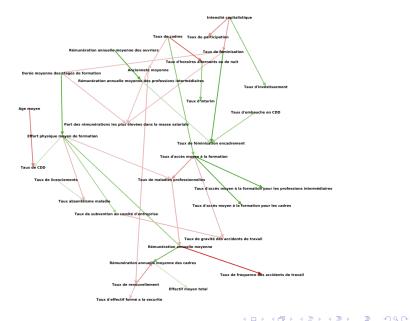
Category 1	255	Chocolatier, Lesieur, Dassault, Compagnie des fromages,
Category 2	312	ArcelorMittal, St Gobain, Lafarge, Vallourec, Michelin,
Category 3	197	Air Liquide, Thales, Mersen, Filtrauto, Fenwick,
Category 4	105	Hispano-Suiza, TurboMéca, Sanofi, Snecma,

Variables

- Total number of employees, av. salary, productivity, profits, ...
- age, Average seniority, Physical effort, Permanent contract rate, Manager rate, Fixed-term contract rate, Temporary job rate, Shift and night work, Turn-over
- Frequency & Gravity of work injuries, Safety expenses, Safety training expenses, Absenteism (diseases), Occupational-related diseases
- Percentage of women (employees, managers); wage gap

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Phase 1: General Causal Relations



Causal models are generative models What is special about them ?

General Causal Relations

Access to training \nearrow

- Gravity of work injuries
- \blacktriangleright \searrow Occupational-related diseases

Termination rate 🗡

Absenteism (diseases)

Percentage of managers *∧*

- Access to training
- \blacktriangleright Shift or night working hours

Age 🗡

- Fixed-term contract rate
- Productivity (weak impact)

?

▶ Productivity $\nearrow \rightarrow$ Participation rate \nearrow

Global relations between QLW and performance ?

Failure

Nothing conclusive

Interpretation

- ▶ Exist confounders (controlling QLW and performance) $C \rightarrow A$ and $C \rightarrow B$
- One such confounder is the activity sector
- In different activity sectors, causal relations are different (hampering their identification)
- ➤ ⇒ Condition on confounders (independently handle the activity sectors)

Conditioning on confounder ! Focus on Low-tech industry

Taux d'accès moyen à la formation
Durée moyenne des stages de formation
Taux de CDD
Taux d'interim
Taux d'embauches en CDI
Taux de gravité des accidents de travail
Taux de fréquence des accidents de travail
Turn-over CDI
Taux de démissions
Taux de licenciements Age moyen
Rémunération annuelle moyenne
Taux d'investissement
Intensité capitalistique
Taux de maladies professionnelles
raux de maladies professionnelles
Productivité
Taux de participation
Pentabilité d'exploitation

Rentabilité d'exploitation Causal models are generative models What is special about them ? 문 🛌 🖻

Category 1 (low-tech industry)

► Average salary ↗, Productivity ↗

very significant

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- Occupational-related diseases , Productivity
- ► Temporary job rate ↗, Gravity of work injuries ↗

Conclusion

SAM: Feasibility of causal generative modelling

- + Avoid combinatorial optimization + parallelization
- + Covers large families of causal mechanisms
- Better than competitors; still limited

Applications

- Always: Confirmatory studies needed
- Always: Confounders.

Open source: SAM + Causal Toolbox

- Causal Discovery Tolbox
- SAM

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Perspectives

Relaxing the requirements

From identifiability to stability

Change of representation

- Dimensionality reduction
- Handling confounders
- Causal structures in latent space

Divide and Conquer

- Subsets of variables (e.g., MB(X_i))
- Partial solutions G_i
- Reconcile G_i

We are hiring ! https://sites.google.com/view/causali-t-ai/home

Wang Blei 2021 Karlsson Krijthe 2023 Roy et al, 2023

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