Advanced Topics in Machine Learning

Winter Semester 2024/2025

Prof. Dr.-Ing. Christian Bergler | OTH Amberg-Weiden

Topics of Today: Advanced Deep Learning Strategies – Part III

- Self-Supervised Learning
- Active Learning

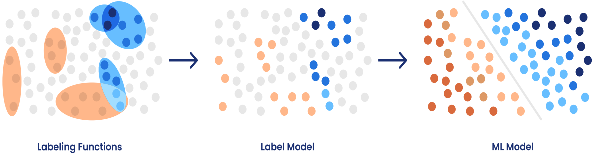
Topics of Today: Advanced Deep Learning Strategies – Part III

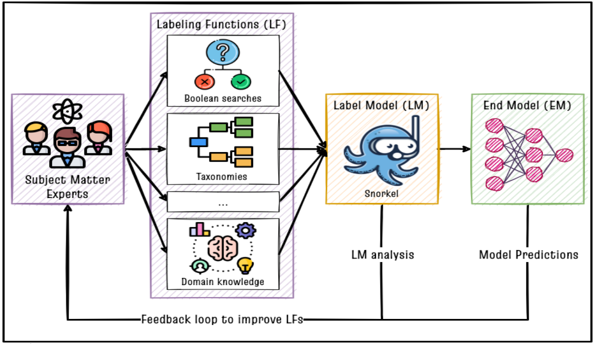
- Weak Supervision
- N-Shot Learning
- Causal Learning

Deep Learning Strategies – Part III

Weak Supervision

- Goal: How to transfer an unsupervised to a (weakly) supervised task!





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Deep Learning Strategies – Part III

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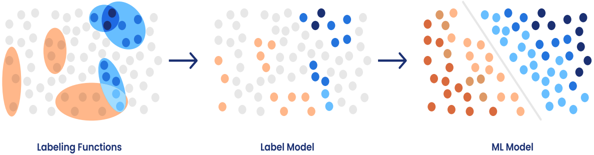
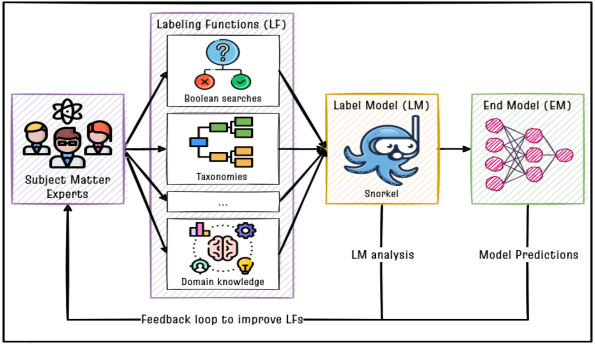
- Interpret & categorize high-level, scalable, and potentially noisy signal sources by applying multiple sources of supervision





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Deep Learning Strategies – Part III

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- Goal: How to transfer an unsupervised to a (weakly) supervised task!
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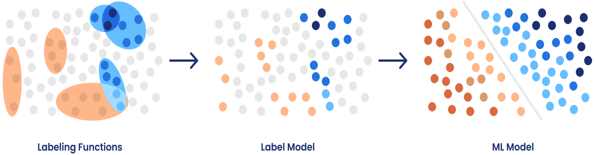

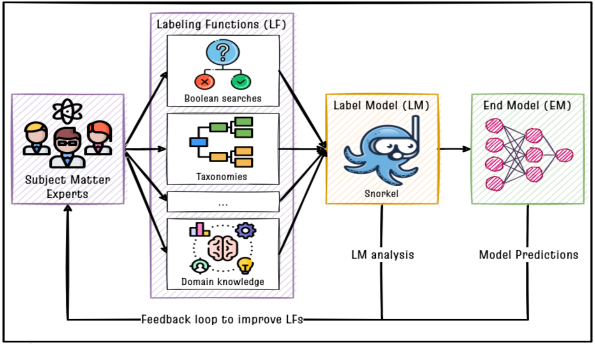

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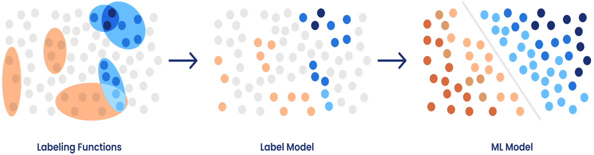

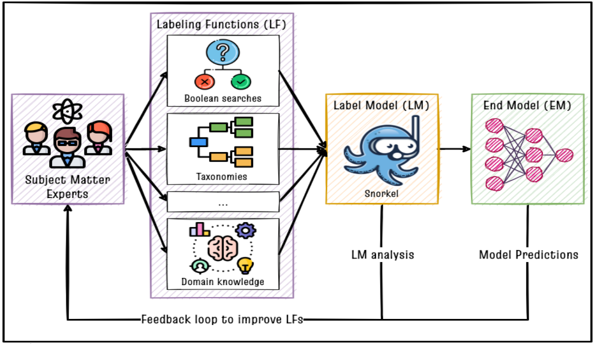

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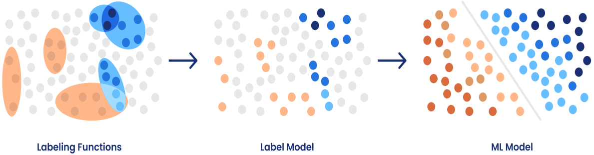
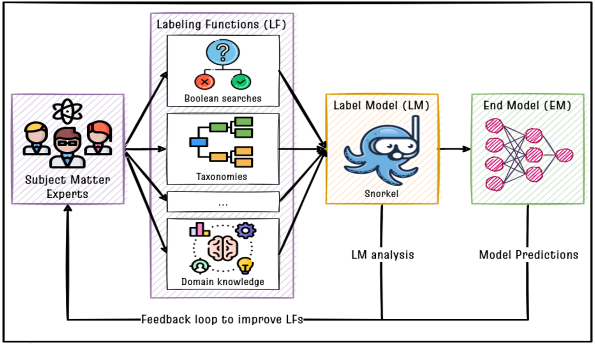
- Lack of precision: completely labeled, but often not precisely enough to recognize subtle differences





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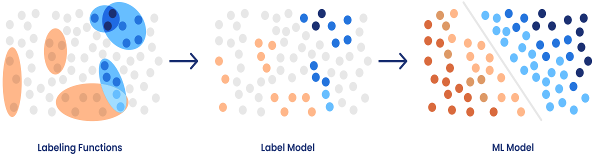

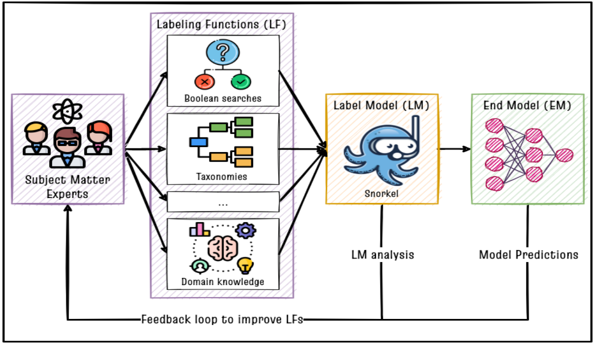

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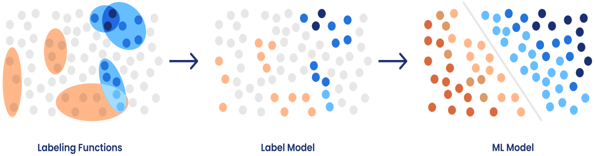

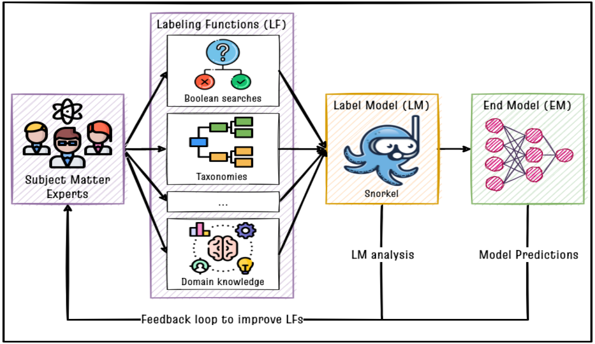

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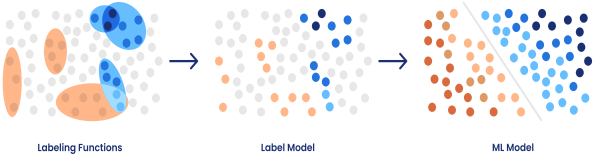

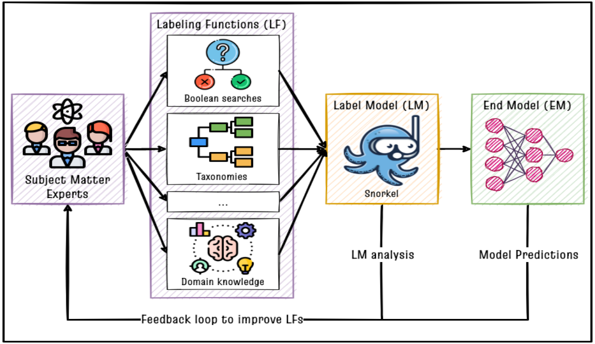

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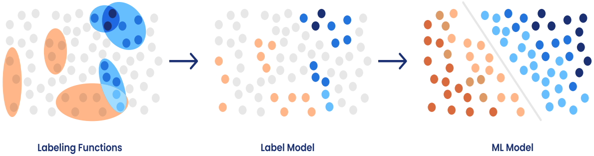
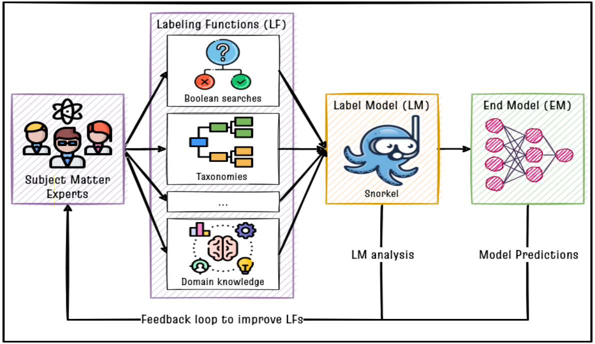
- Idea: trade-off 100,000 pretty good vs. 100 perfect data labels





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prob of diversity of 100 perfect is less than prob diversity of 100000 get rid of false classification: de noise

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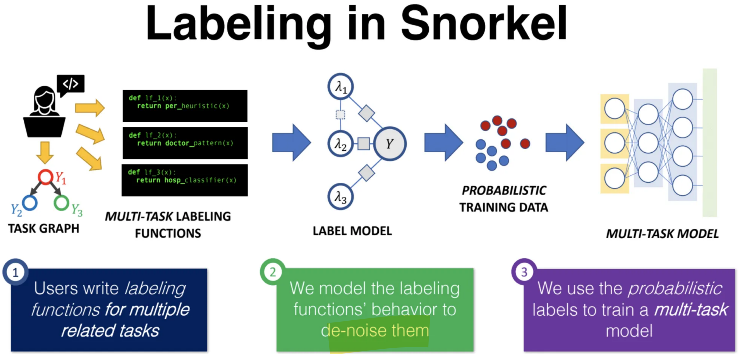
Snorkel Framework



- Labeling functions λ_N (simple functions/rules), providing multiple inconsistent or overlapping labels (commercialized version available here: Snorkel)
- Combine noisy weak labels in a labeling model to generate a consensusmore accurate final label
- Label model learns dependencies/reliabilities of the labeling functions, weighting each function according to its accuracy and overlap with others
- Probabilistic labels for each sample, allow to build a (weakly) supervised training set

Source: Link to Image

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Smart Labeling

- Labeling involves using automated or semi-automated techniques to label data intelligently (see pseudo-labeling, self-supervised approaches)

Source: Image from OTH-AW, Electrical Engineering, Media and Computer Science, Thomas Nierhoff – Vorlesung Advanced Topics in ML

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- Active Learning: label only the most uncertain or informative data points, making the labeling process more efficient

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Application: Cut-In Prediction Autonomous Vehicle

- Refers to predicting when another vehicle in adjacent lanes will “cut in” or merge into the lane occupied by the autonomous vehicle (critical for safe driving!)

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here patrren recognition is important

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- Unlabeled data: process large amounts of unlabeled driving data with weakly supervised trained models that learn to identify “cut-in” scenarios indirectly

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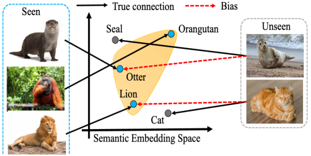
train model on weakly supervissed data sets. from sensor data, heuristics etc and unlabeled

N-Shot Learning – Zero-Shot, Single-Shot & Few-Shot Learning

Idea: Zero-shot, single/one-shot, and few-shot learning are learning paradigms where models identify/categorize or generate new categories with very few or even no labeled examples

- Zero-Shot Learning: identify new categories never seen in training by leveraging auxiliary semantic knowledge based on feature similarity via textual/visual embeddings!



(a) a tapir made of accordion. a tapir with the texture of an accordion.

(b) an illustration of a baby hedgehog in a christmas sweater walking a dog

Source: https://medium.com/@vireshj/zero-shot-learning-understanding-machines-that-learn-like-humans-e670f83186b8
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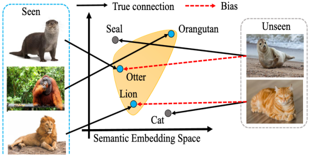

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zero shot for first time seeing few shot is for few times seeing

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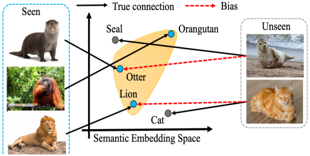
- Non-static set of classes, while unseen events will be stored in the high-dimensional feature space either near (related to “Knowns”) or far-apart (unrelated to “Knowns”)
- Class assignment for a first-time appearance of a new category requires pre-existing knowledge (embeddings, e.g. single-shot) describing the new class



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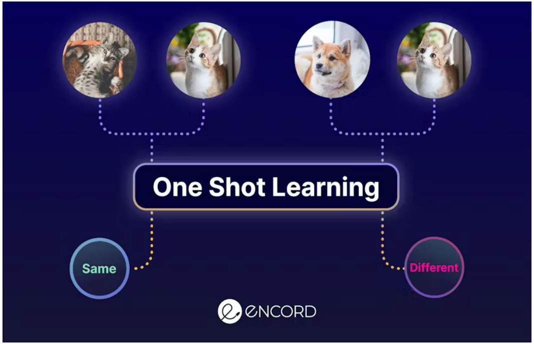

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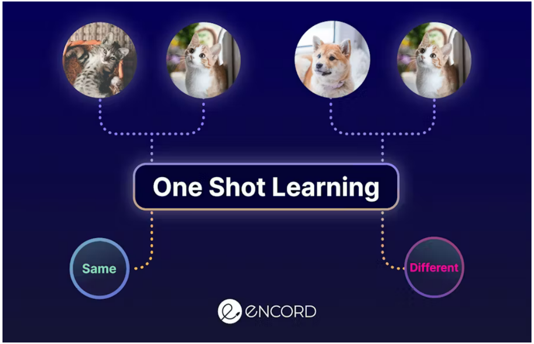

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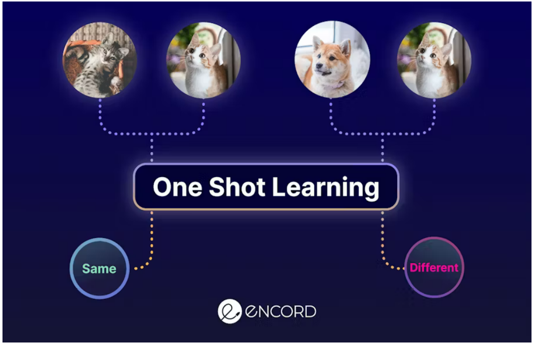

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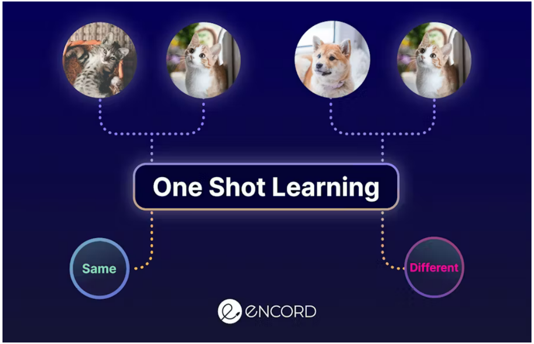
- Class assignment is based on distance-related outcome ("close enough") of an unseen sample w.r.t. the "single shot data point"



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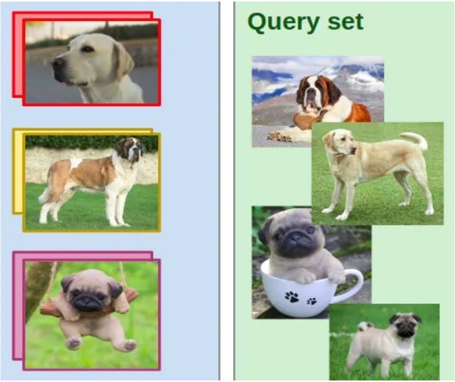

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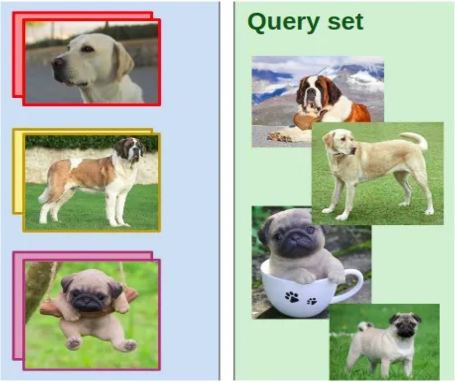

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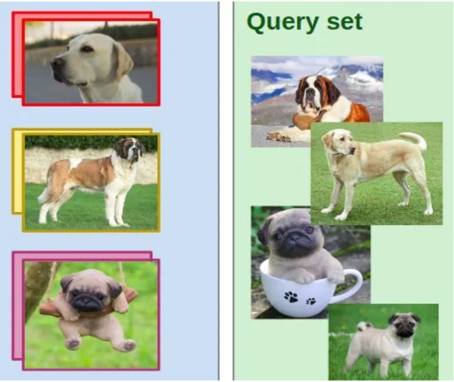
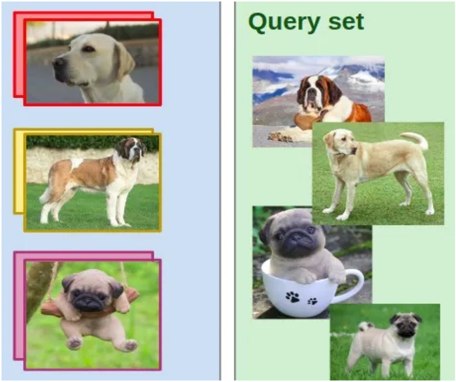
- Often a K-way N-Shot classification problem, with K as the number of classes and N as the class-specific small number of labels, together with Q many query images



Source: https://neptune.ai/blog/understanding-few-shot-learning-in-computer-vision

causal learning home work

- Few-Shot Learning: model learns from a small number of labeled examples, with more than zero/one images to compare against
- Number of labeled "shots" $N < 10$, usually between 2 to 5, while model generalization is based on this small set of instances
- Often a K-way N-Shot classification problem, with K as the number of classes and N as the class-specific small number of labels, together with Q many query images
- Classify Q query images among the K classes, with $K \times N$ samples in the training set are the only representatives



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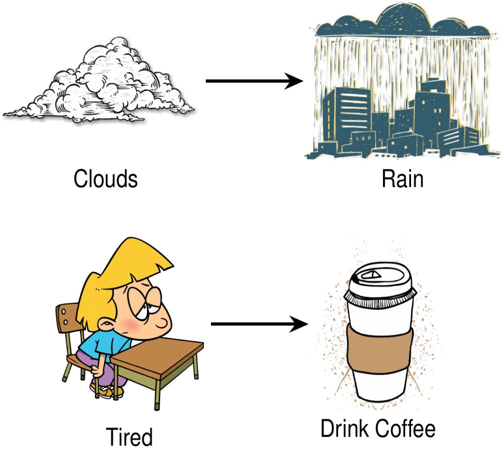
Deep Learning Strategies – Part III

Causal Learning

- Implies a direct cause-and-effect relationship ("explain the cause of an effect") between two variables (change one variable will directly impact the other in a predictable way)



Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Deep Learning Strategies – Part III

Causal Learning

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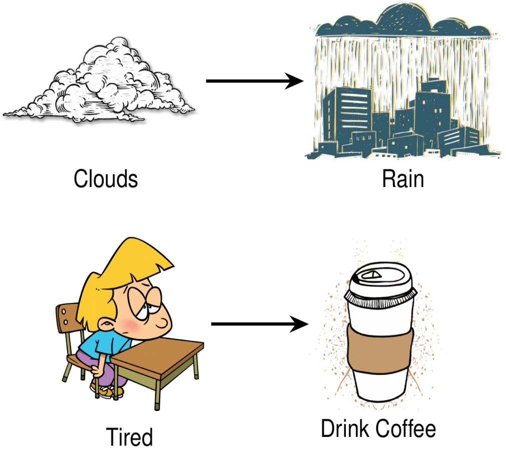
- Implies a direct cause-and-effect relationship (“explain the cause of an effect”) between two variables (change one variable will directly impact the other in a predictable way)
- Careful: correlation describes a statistical association between two variables and indicates a simultaneous change (trend!) $\rightarrow$ However, not necessarily causing the other!



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Deep Learning Strategies – Part III

Causal Learning

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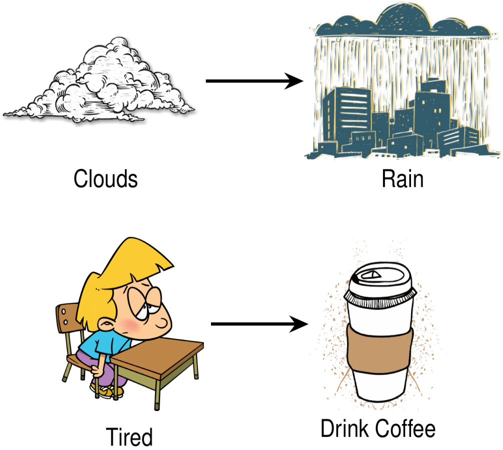
- Careful: correlation describes a statistical association between two variables and indicates a simultaneous change (trend!) $\rightarrow$ However, not necessarily causing the other!
- Causal inference often uses statistical methods to identify relationships that are not simply correlations but have a directional influence



Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Types of Causal Relationships

- Direct Causal Relationships: One variable directly affects another (e.g., smoking directly causes an increased risk of lung cancer)
- Indirect Causal Relationships: The effect of one variable on another is mediated through a third variable (e.g., education may lead to higher income, and higher income might then lead to better health outcomes)
- Bidirectional Causality: Some relationships may involve mutual causality, where two variables affect each other (e.g., diet and exercise can both affect each other over time)

Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Causal Learning

Source: Image from Nan Rosemary Ke, Stefan Bauer, "Causality and Deep Learning: Synergies, Challenges and the Future", Slide 29

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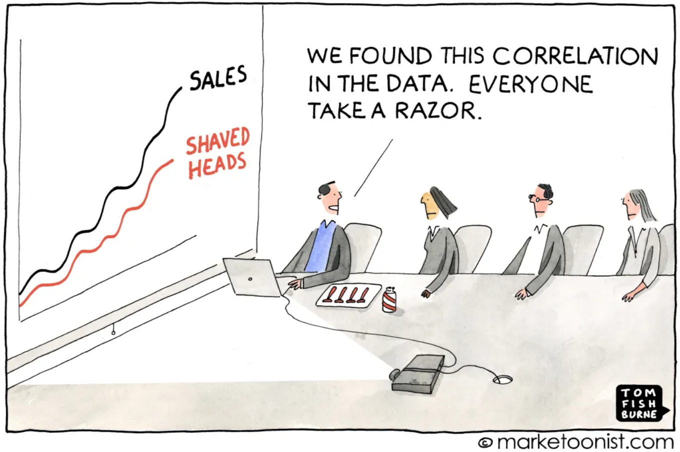
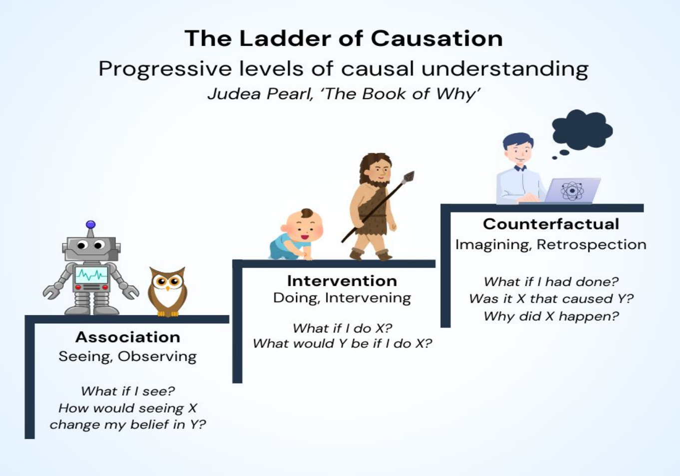
Correlation is NOT Causation!



Source: Image from https://censemaking.com/2022/08/03/the-fear-and-folly-of-data/

Ladder of Causation



- Organizes causal reasons into three hierarchical levels: association, intervention, counterfactuals
- From simply observing data to fully understanding & reasoning about causal mechanisms

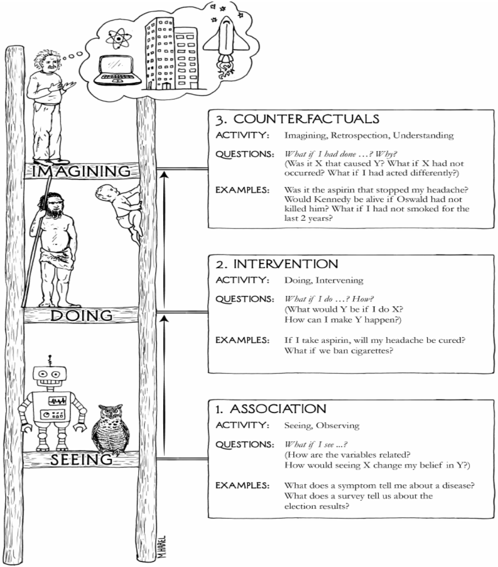
Source: Image from https://www.linkedin.com/posts/causai-bv_ladderofcausation-causalai-decisionmaking-activity-7177992092458057729-hiP9

Deep Learning Strategies – Part III

Causal Learning

Association

- Observing correlations/dependencies of variables: "What happens if we change this variable?"



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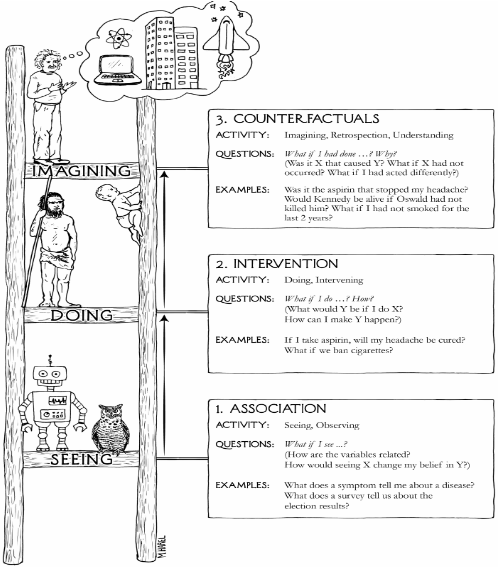
Deep Learning Strategies – Part III

Causal Learning

Association

- Observing correlations/dependencies of variables: “What happens if we change this variable?”
- However, no explanation why one thing happens because of another (purely observational!)



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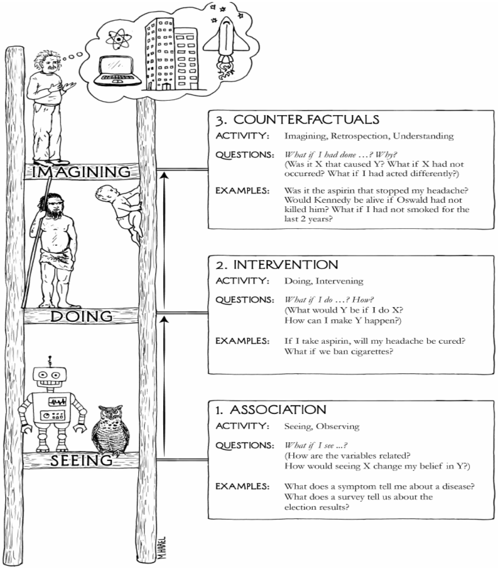

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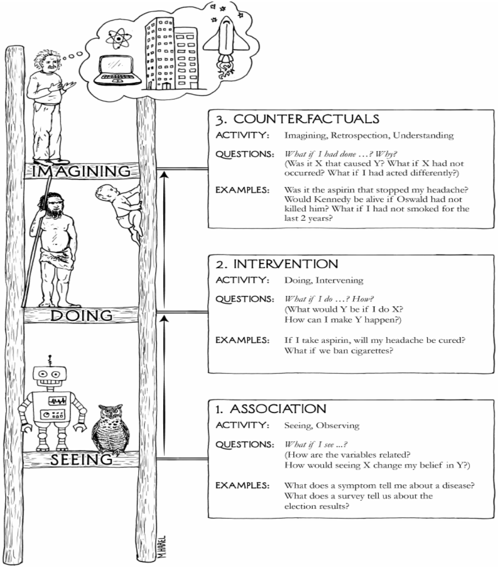

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- However, no explanation why one thing happens because of another (purely observational!)
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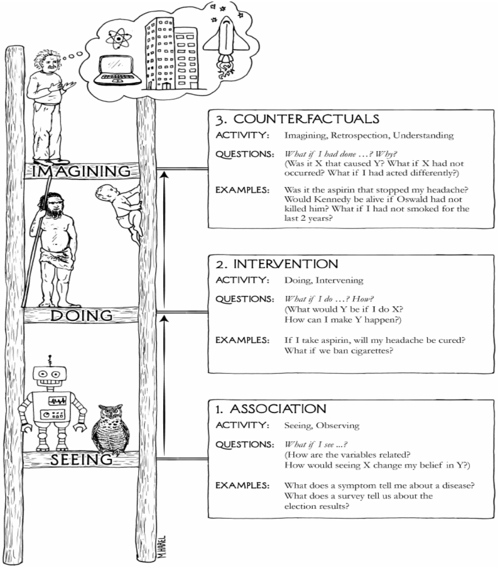
- Methods: traditional statistical methods, ML (linar regression, classification, clustering)
- Association alone do not determine if a relationship is causal (correlation between ice cream sales and drowning incidents does not imply that buying ice cream causes drowning)



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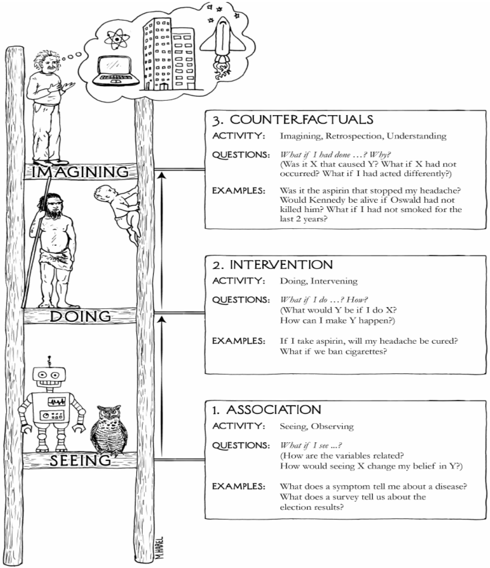
Deep Learning Strategies – Part III

Causal Learning

Intervention

- Moving beyond observation by introducing actions to change the system and observing the results: "What if I do this?"



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Deep Learning Strategies – Part III

Causal Learning

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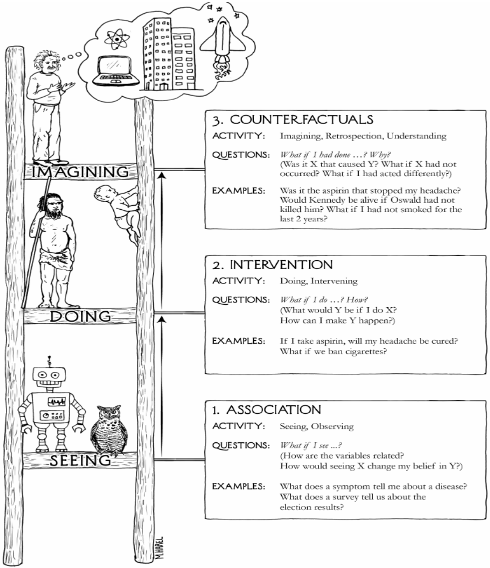
- Moving beyond observation by introducing actions to change the system and observing the results: "What if I do this?"
- Represent causal relationship by showing how changes in one variable affect another



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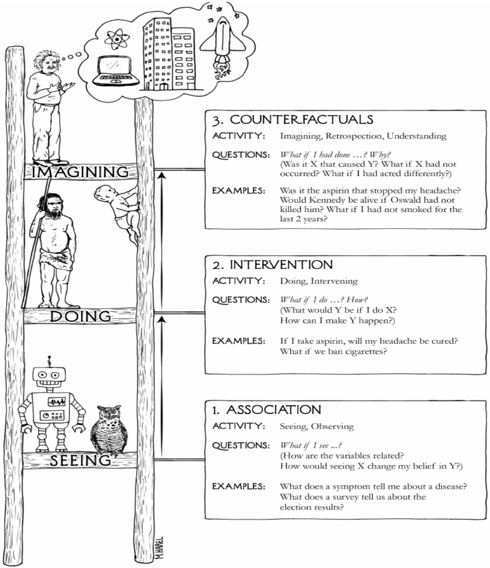

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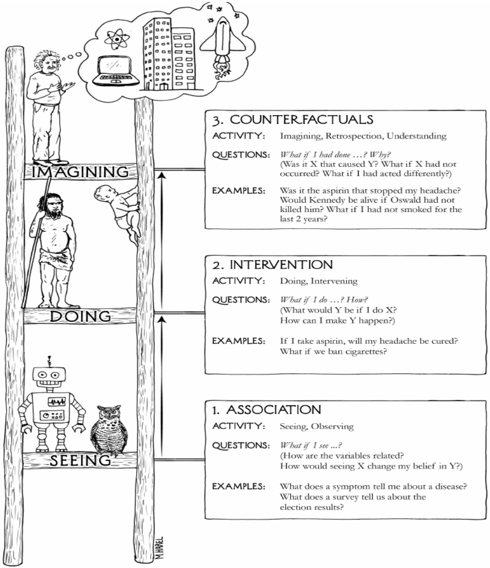
- Represent causal relationship by showing how changes in one variable affect another
- Question: "What will happen to Y if I change X?"
- Methods: randomized controlled trials, where the experimenter manipulates the independent variable $P(Y|do(X))$ (e.g. giving patients a treatment placebo) to observe the effect on a dependent variable (like recovery rates)



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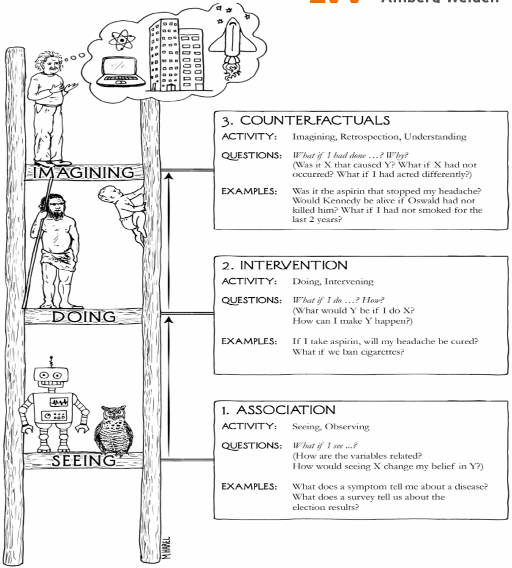
Deep Learning Strategies – Part III

Causal Learning

Counterfactuals

- Asking about hypothetical alternatives to what actually happened, what would have happened "if"



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Deep Learning Strategies – Part III

Causal Learning

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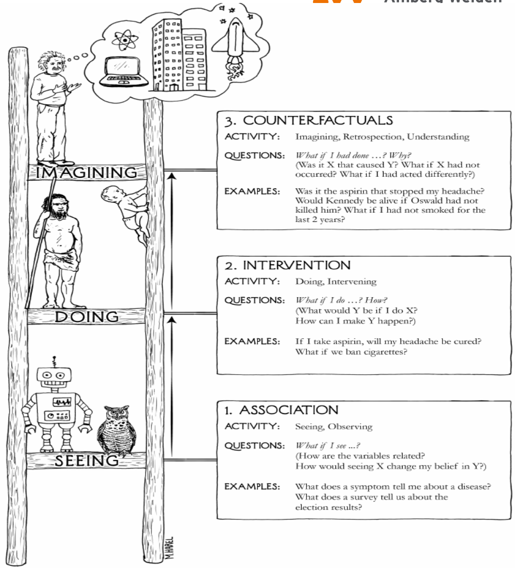
- Asking about hypothetical alternatives to what actually happened, what would have happened "if"
- Alternative realities by imagining what the outcome would have been if a different action or condition had been in place



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Deep Learning Strategies – Part III

Causal Learning

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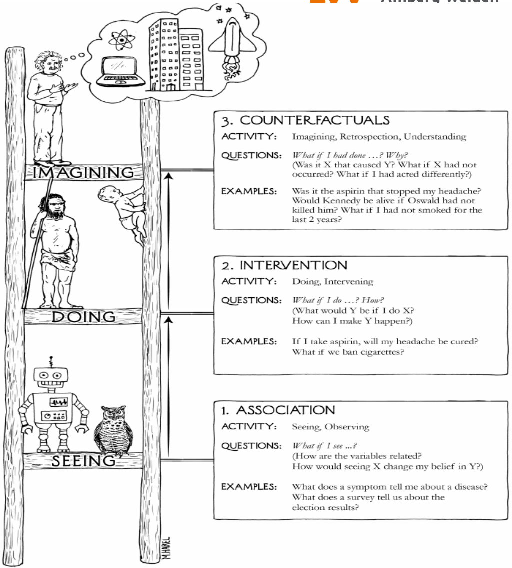

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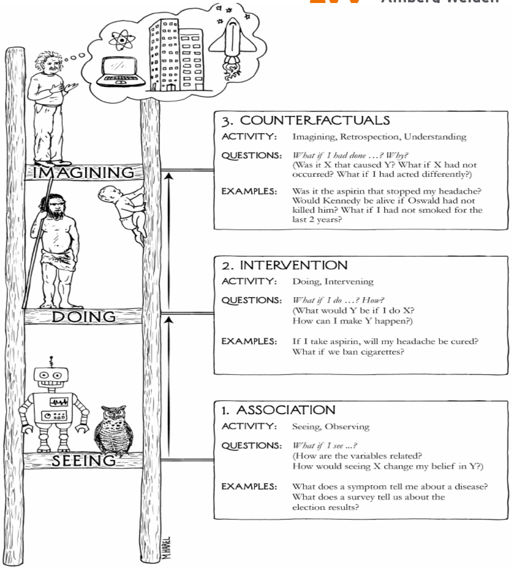
- Question: "What would have happened to Y if X had been different?"
- Methods: structural causal models (SCMs), provide a framework for understanding causal relationships at a deeper level by specifying equations reflecting mechanisms of causation



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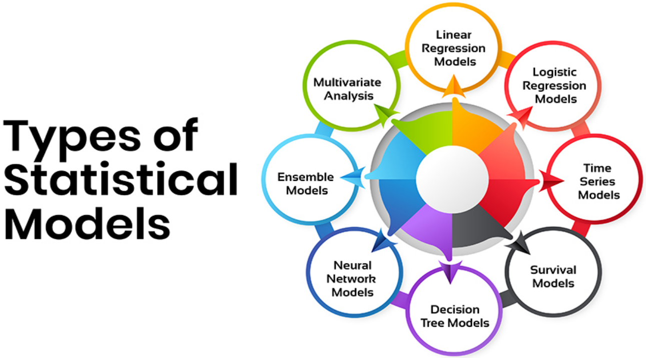

- Current ML-Models or statistical models can only do "Association"

Source: https://www.dasca.org/world-of-data-science/article/what-is-statistical-modeling-in-data-science
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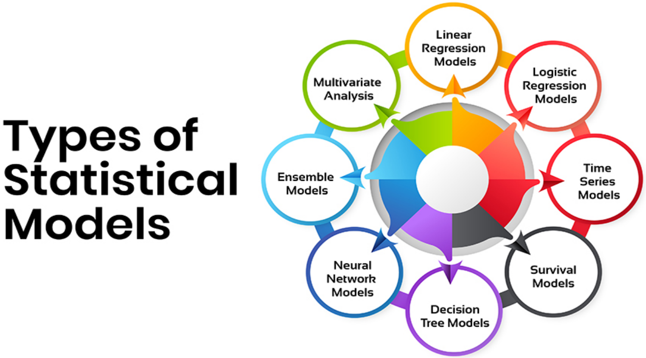
Deep Learning Strategies – Part III

Causal Learning



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- Statistical inference $\rightarrow P(Fire|Smoke), P(Smoke|Fire)$

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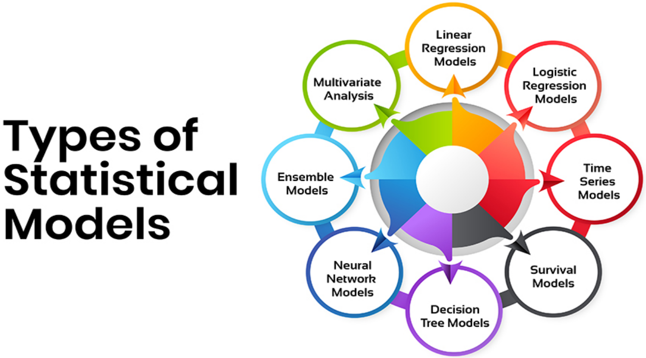
Causal Learning



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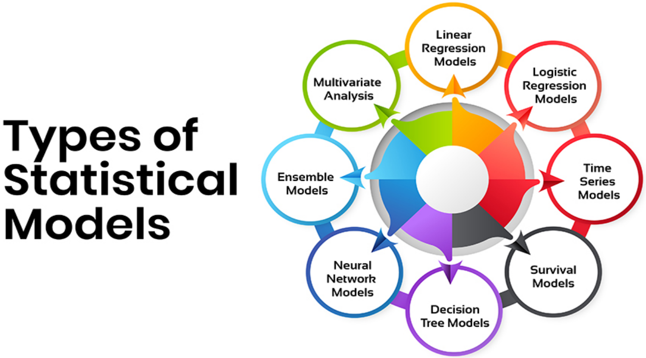

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- Statistical inference → $P(Fire|Smoke)$, $P(Smoke|Fire)$
- No Causal Inference → Yes: Fire causes Smoke, No: Smoke causes Fire
- Successful because: massive amount of data, high number of parameters, strong computational power, independent and identically distributed (i.i.d.) assumption

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Deep Learning Strategies – Part III

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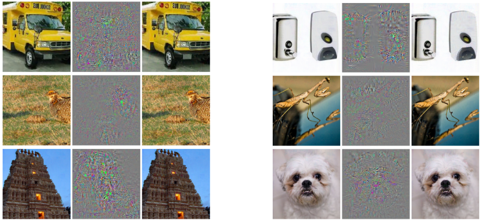

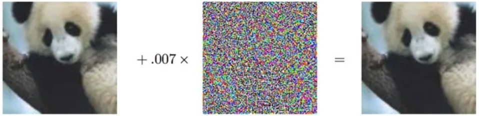

Source: Szegedy et al., Intriguing properties of neural networks, Figure 5

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Deep Learning Strategies – Part III

Causal Learning

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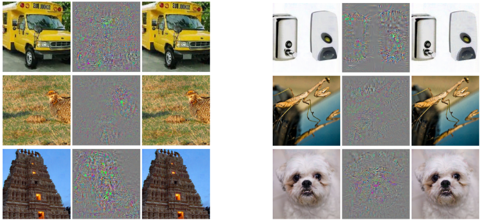

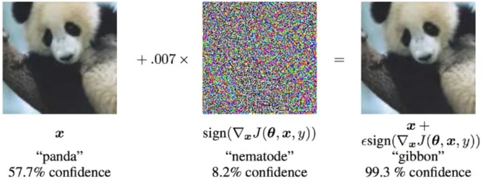

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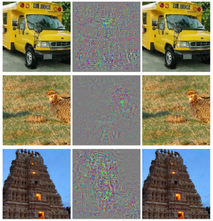
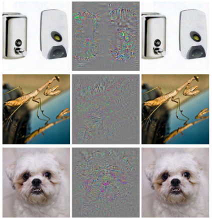
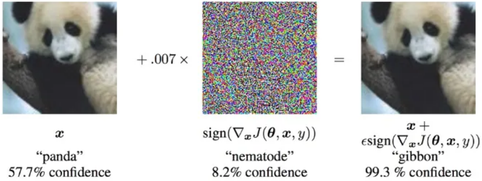
  - Temporal: properties evolve over time
  - Contextual: data in one environment/setup not representative in another, different devices, methods, sources







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Deep Learning Strategies – Part III

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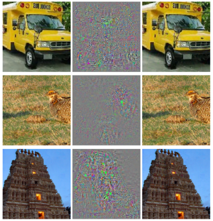
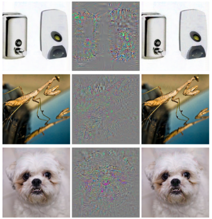
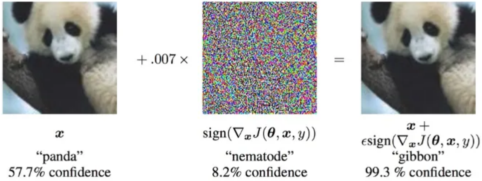
- Introducing an unexpected distribution change?







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Common Causal Principles

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- If Z is not observed (hidden), it is a confounding variable, affecting both the cause and the effect, making it difficult to establish a true causal relationship

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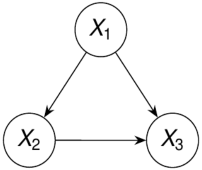
- Explains the connection between causality and statistical dependence
- Postulated by Hans Reichenbach in 1956: given two observations X and Y are statistically dependent $\rightarrow P(X, Y) \neq P(X)P(Y)$, then an event Z which causally influences both results in $P(X, Y|Z) = P(X|Z)P(Y|Z)$
- If Z is not observed (hidden), it is a confounding variable, affecting both the cause and the effect, making it difficult to establish a true causal relationship
- Example: exercise frequency (Z), body weight (X), cholesterol levels (Y) $\rightarrow$ without considering Z, it might appear that body weight directly affects cholesterol, however, exercise impacts both independently

Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Causal Graphical Models (CGMs)

- Directed Acyclic Graphs (DAGs) or Bayesian Networks ("acyclic" part $\rightarrow$ no loops, flow in one direction without cycling back)

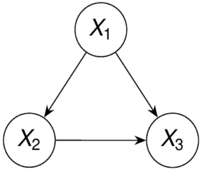


$$p(X_1, X_2, X_3) = p(X_1)\, p(X_2 \mid X_1)\, p(X_3 \mid X_1, X_2)$$

Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Causal Graphical Models (CGMs)

- Directed Acyclic Graphs (DAGs) or Bayesian Networks ("acyclic" part $\rightarrow$ no loops, flow in one direction without cycling back)
- Causal relationships of variables using graph structures



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Causal Graphical Models (CGMs)

- Directed Acyclic Graphs (DAGs) or Bayesian Networks (“acyclic” part $\rightarrow$ no loops, flow in one direction without cycling back)
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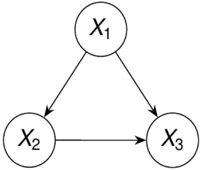
- How different variables in a system influence each other, clarifying potential cause-and-effect paths



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Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

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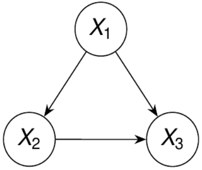
Causal Graphical Models (CGMs)

- Directed Acyclic Graphs (DAGs) or Bayesian Networks ("acyclic" part $\rightarrow$ no loops, flow in one direction without cycling back)
- Causal relationships of variables using graph structure:
- How different variables in a system influence each other, clarifying potential cause-and-effect paths
- Variables X (observations) as nodes and causal relationships between them as directed edges



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Causal Graphical Models (CGMs)

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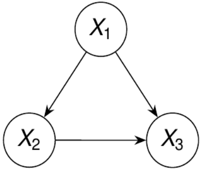
- Causal relationships of variables using graph structures
- How different variables in a system influence each other, clarifying potential cause-and-effect paths
- Variables X (observations) as nodes and causal relationships between them as directed edges
- Causal Markov condition (Causal Independence!): $P(X_1, ..., X_n) = \prod_{i=1}^{n} P(X_i | PA_i)$, with PA_i as the parents of X_i, having a direct causal link (e.g. $X_1 \rightarrow X_2$)



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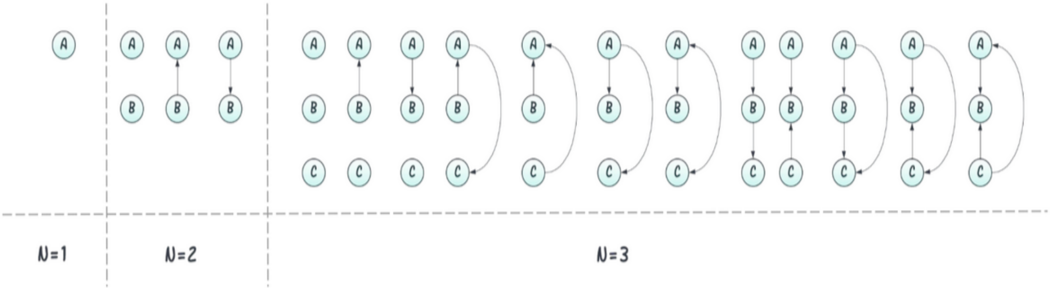
Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

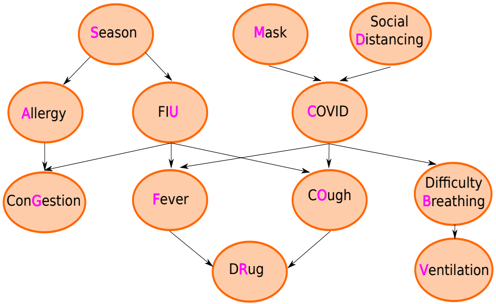
Space of causal graphs (i.e. DAGs) grows **super-exponentially**.



Source: Image from Nan Rosemary Ke, Stefan Bauer, "Causality and Deep Learning: Synergies, Challenges and the Future", Slide 26

Bayesian Network

#	COVID	Mask	Soc. Distance	FIU	Cough	Fever	Ventilate	Season	ConGestion	Difficulty Breath	Drug	Allergy
1	1	0	1	0	1	0	1	Spring	0	0	1	0
2	0	1	0	1	0	1	0	Summer	1	1	0	0
3	1	1	1	0	0	0	1	Fall	1	0	1	1
4	0	0	1	1	1	0	0	Winter	0	1	0	0
...	...	...	...	...	...	...	...	...	...	...	...	...
500	0	1	1	1	0	0	0	Summer	0	0	1	1

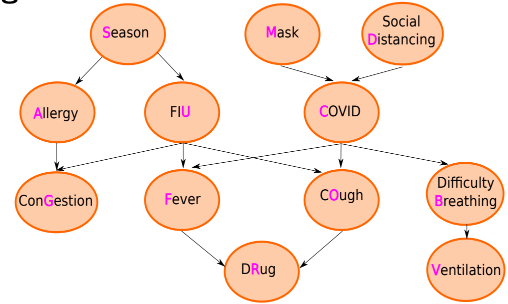


Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

Deep Learning Strategies – Part III

Causal Learning

Bayesian Network



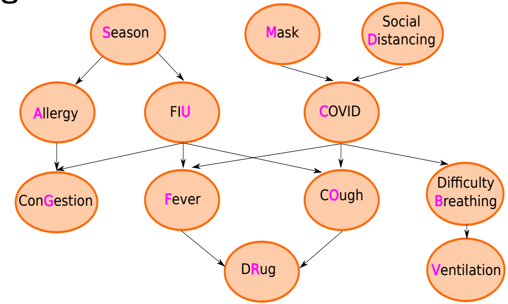
- Random (dependent/independent) variables, e.g. Fever/COVID and Allergy/Cough

Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

Deep Learning Strategies – Part III

Causal Learning

Bayesian Network



- Random (dependent/independent) variables, e.g. Fever/COVID and Allergy/Cough
- Joint (dependent) probability: from COVID $\rightarrow$ Fever – $P(F, C) = P(F|C)P(C)$ – or from Fever $\rightarrow$ COVID – $P(F, C) = P(C|F)P(F)$

Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

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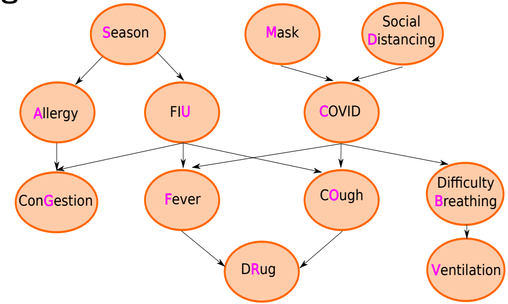
Bayesian Network



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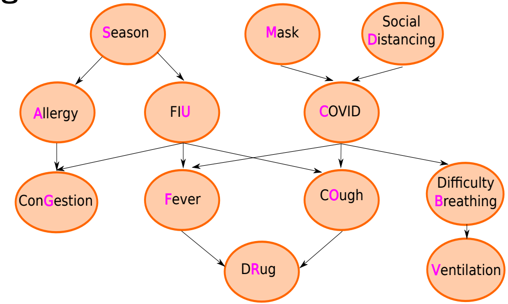
Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

Deep Learning Strategies – Part III

Causal Learning

Bayesian Network



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- Causality (single direction!) would mean either F is causing C or C is causing F

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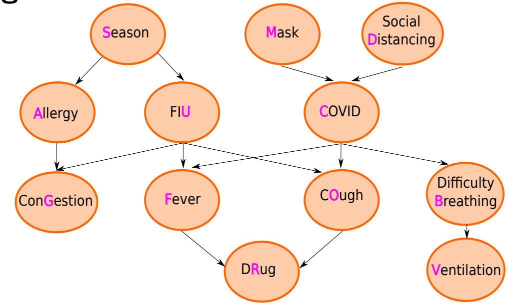
Bayesian Network



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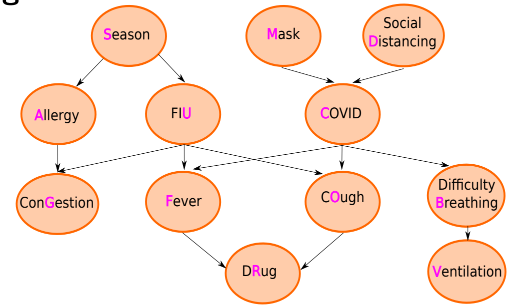
- Causality (single direction!) would mean either F is causing C or C is causing F
- How to read statistical dependence as causal dependence?

Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

Deep Learning Strategies – Part III

Causal Learning

Bayesian Network



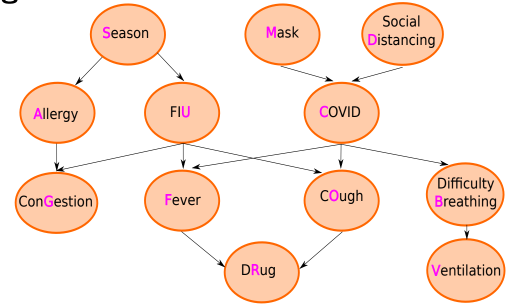
- In general: read a conditional probability $P(X|Y_1, ..., Y_n) \neq P(X)$, as X is "caused" by $Y_1, ..., Y_n$

Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

Deep Learning Strategies – Part III

Causal Learning

Bayesian Network



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- However: above relation just indicates association, meaning how X is associated with $Y_1, \ldots, Y_n$, also possible: $P(Y_1, \ldots, Y_n|X) \neq P(Y_1, \ldots, Y_n)$

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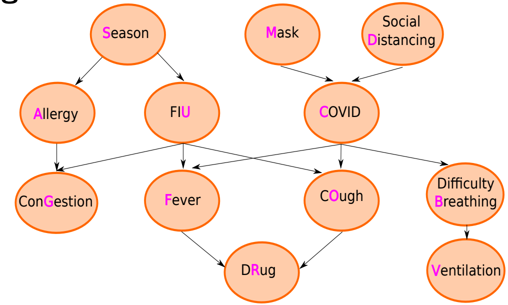
Bayesian Network



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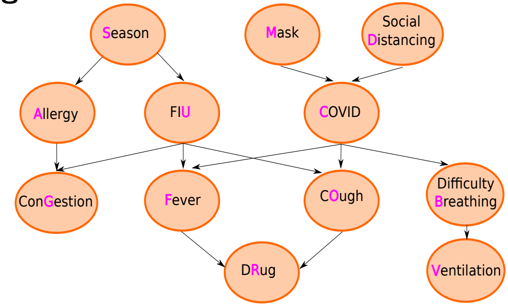

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- However: above relation just indicates association, meaning how X is associated with $Y_1, ..., Y_n$, also possible: $P(Y_1, ..., Y_n|X) \neq P(Y_1, ..., Y_n)$
- Still: No Causality!
- Goal: Given data D, what is causing what (the other)?

Source: YouTube – easy learning – Causality 1: Bayesian networks are not causal, Link

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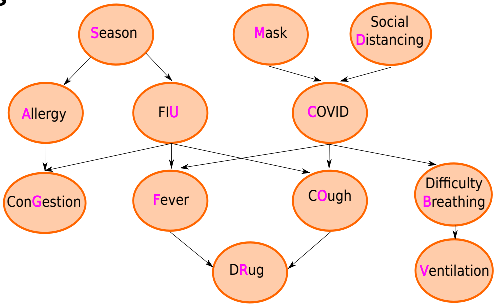
Bayesian Network



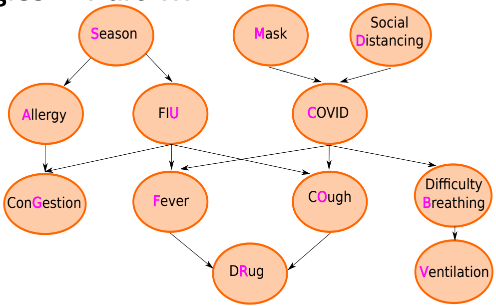
- Consider binary variables COVID $\in$ {COVID, –COVID} and Fever $\in$ {Fever, –Fever}

Source: YouTube – easy learning – Causality 2: Intervention, Link

Deep Learning Strategies – Part III

Causal Learning

Bayesian Network



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- COVID is detected by a test, Fever by temperature, while observations result in:

$$P(\text{Fever}|\text{COVID}) > P(\text{Fever}|\text{–COVID})$$

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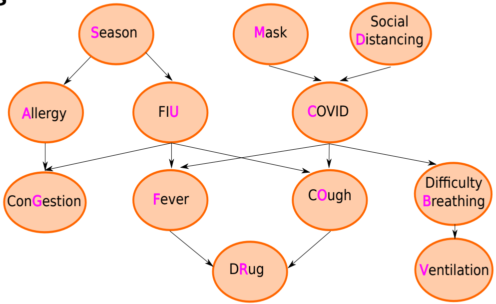
Source: YouTube – easy learning – Causality 2: Intervention, Link

Causal Learning

Bayesian Network



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- Observing one of them, increases probability of the other! $\rightarrow$ Statistical dependence (correlation!) – Which one causes the other, how to figure it out – more data?

Source: YouTube – easy learning – Causality 2: Intervention, Link

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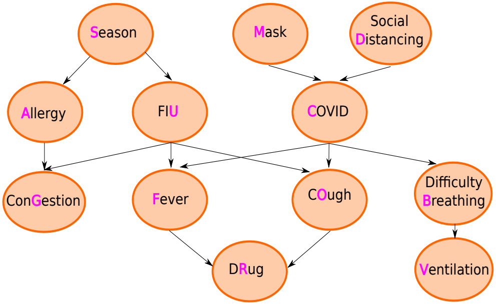
Observation vs. Intervention



- Just by observing, it is not possible to determine what is causality!

Source: YouTube – easy learning – Causality 2: Intervention, Link

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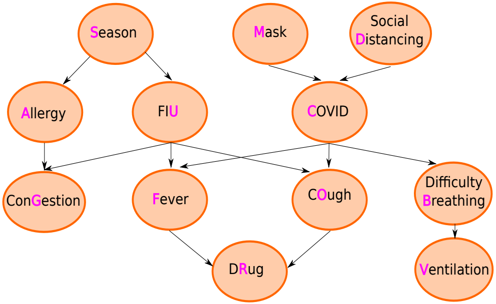

- Just by observing, it is not possible to determine what is causality!
- Why??? – How do we know that COVID is causing ($\rightarrow$) Fever and not vice versa?

Source: YouTube – easy learning – Causality 2: Intervention, Link

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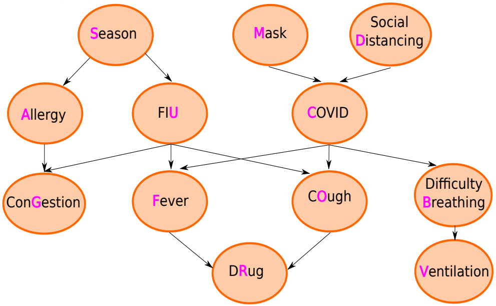

- Just by observing, it is not possible to determine what is causality!
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- Intervene via experimental verification!!! (by observing people with COVID, it is likely to observe Fever; observing Fever, is very often not COVID-related, e.g. fire/smoke)

Source: YouTube – easy learning – Causality 2: Intervention, Link

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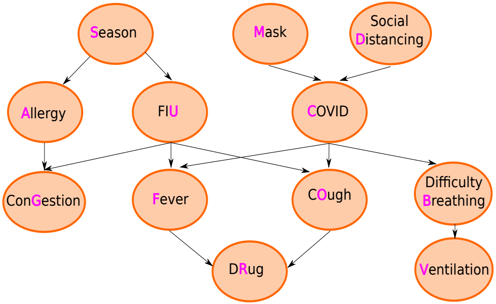

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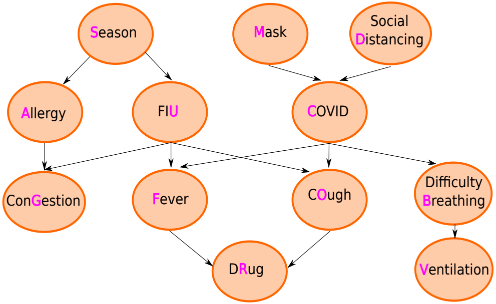
- Force variables to certain values and check changes in the other variable

Source: YouTube – easy learning – Causality 2: Intervention, Link

Deep Learning Strategies – Part III

Causal Learning

Observation vs. Intervention



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- Intervene via experimental verification!!! (by observing people with COVID, it is likely to observe Fever; observing Fever, is very often not COVID-related, e.g. fire/smoke)
- Force variables to certain values and check changes in the other variable
- Intervention $\rightarrow$ Causality!!! (...Find causal relationships)

Source: YouTube – easy learning – Causality 2: Intervention, Link

Intervention – Do-Operator

- Definition "Intervention": an ideal intervention on a given random variable Z is described by forcing its value to z, denoted $\mathrm{do}(Z := z)$ or $\mathrm{do}(z)$

Source: YouTube – easy learning – Causality 2: Intervention, Link

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- Constraint: when intervening on one variable, no other variable should be intervened

Source: YouTube – easy learning – Causality 2: Intervention, Link

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- Constraint: when intervening on one variable, no other variable should be intervened
- $\text{do}(\text{COVID} := 1)$ or $\text{do}(\text{COVID} := 0) \rightarrow$ Expectation: affect the likelihood of Fever, because COVID is a cause of fever (being the effect/sympotme of COVID)

Source: YouTube – easy learning – Causality 2: Intervention, Link

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- Constraint: when intervening on one variable, no other variable should be intervened
- $\mathrm{do}(\mathrm{COVID} := 1)$ or $\mathrm{do}(\mathrm{COVID} := 0) \rightarrow$ Expectation: affect the likelihood of Fever, because COVID is a cause of fever (being the effect/sympotme of COVID)
- $\mathrm{do}(\mathrm{Fever} := 1)$ or $\mathrm{do}(\mathrm{Fever} := 0) \rightarrow$ Expectation: does not affect the likelihood of COVID, because Fever is NOT a cause of COVID (not a sympotme of Fever)

Source: YouTube – easy learning – Causality 2: Intervention, Link

- Intervene on Fever (induce/remove fever) and observe COVID (person has/has not COVID), should not result in any probability difference of seeing/causing COVID:

$$P(\text{COVID}|\text{do}(\text{Fever})) = P(\text{COVID}|\text{do}(\text{–Fever}))$$

indicating that Fever does not cause COVID!

$$P(\text{COVID}|\text{see}(\text{Fever})) > P(\text{COVID}|\text{see}(\text{–Fever}))$$

Different from the observational relation!

Source: YouTube – easy learning – Causality 2: Intervention, Link

- Intervene on Fever (induce/remove fever) and observe COVID (person has/has not COVID), should not result in any probability difference of seeing/causing COVID:

$$P(\text{COVID}|\text{do}(\text{Fever})) = P(\text{COVID}|\text{do}(-\text{Fever}))$$

  indicating that Fever does not cause COVID!

$$P(\text{COVID}|\text{see}(\text{Fever})) > P(\text{COVID}|\text{see}(-\text{Fever}))$$

  Different from the observational relation!

- However: intervene on COVID and observe Fever, lead to:

$$P(\text{Fever}|\text{do}(\text{COVID})) > P(\text{Fever}|\text{do}(-\text{COVID}))$$

  COVID causes Fever!

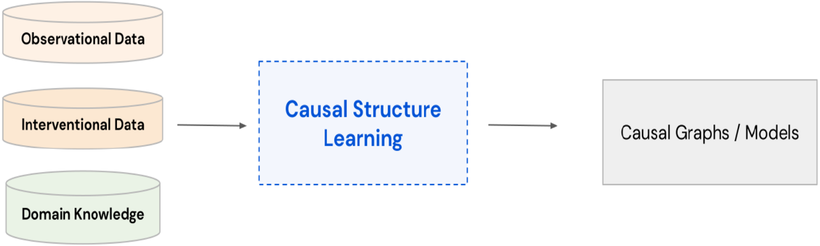
$$P(\text{Fever}|\text{COVID}) > P(\text{Fever}|-\text{COVID})$$

  Interventional and observational relation is in line!

Source: YouTube – easy learning – Causality 2: Intervention, Link

Deep Learning Strategies – Part III

Causal Learning

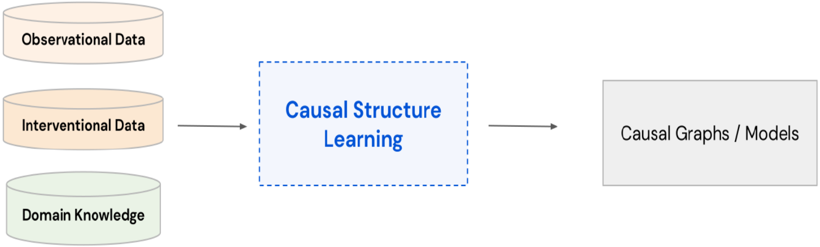


- Observational Data: collected without actively manipulating variables, just observing the natural state of the system (correlations/associations)

Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Deep Learning Strategies – Part III

Causal Learning



- Observational Data: collected without actively manipulating variables, just observing the natural state of the system (correlations/associations)
- Interventional Data: collected by actively changing or intervening on specific variables, to reveal causal relationships

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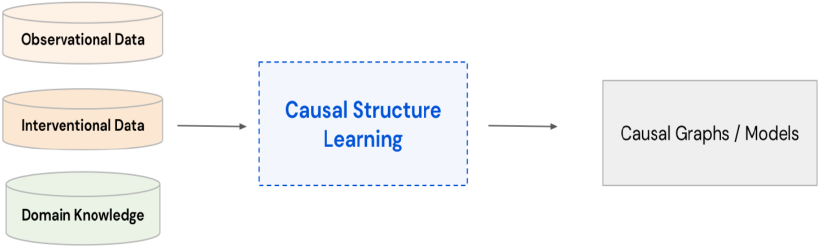
Deep Learning Strategies – Part III

Causal Learning



- Observational Data: collected without actively manipulating variables, just observing the natural state of the system (correlations/associations)
- Interventional Data: collected by actively changing or intervening on specific variables, to reveal causal relationships
- Domain Knowledge: includes expert understanding, assumptions, or prior information about the system being studied, to help guiding the interpretation of observational data and the design of meaningful interventions

Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

- Average Causal Effect (ACE): Binary variable $Z \in \{0, 1\}$, causes variable Y, if the average causal effect (ACE) of Z on $Y = y$ is defined as:

$$ACE(Z \to Y_y) = P(Y = y|\text{do}(Z := 1)) - P(Y = y|\text{do}(Z := 0))$$

is non-zero!

Source: YouTube – easy learning – Causality 3: Defining causality: Structural causal models (SCM), Link

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$$P(Y|\text{do}(z_0)) \neq P(Y|\text{do}(z_1))$$

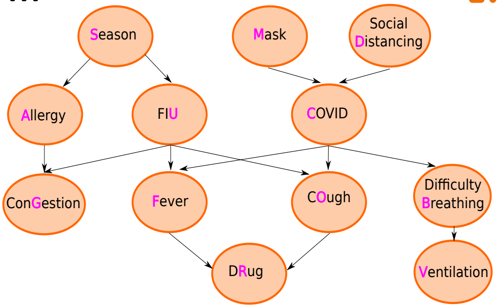
- However: Let $Y = X \oplus Z$ be the XOR-Function of X and Z, then:

$$P(Y|\text{do}(X = 0)) = P(Y|\text{do}(X = 1)) = P(Y)$$

  $\rightarrow$ Better Definition as Deterministic Function!

Source: YouTube – easy learning – Causality 3: Defining causality: Structural causal models (SCM), Link

Causality as Deterministic Function!



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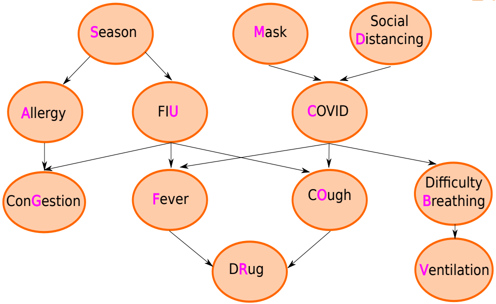

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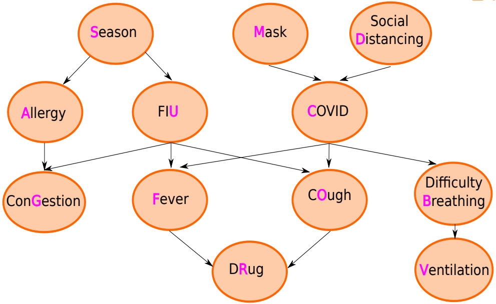

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- Each Variable X (here: C, O, R – referred to as endogenous) have such exogenous (here: U_C, U_O, U_R) variables, used together with a deterministic function of is endogenous and exogenous parents
- $C := f_C(U_C) = U_C$, $O := f_O(C, U_O)$, $R := f_R(O, U_R)$
  $\rightarrow$ Structural Causal Model (SCM)

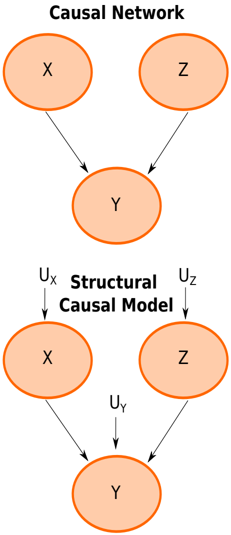
Source: YouTube – easy learning – Causality 3: Defining causality: Structural causal models (SCM), Link

Structural Causal Models (SCMs)

- SCM defined as a touple $< V, U, P_U, F >$ with:

1. V as the set of endogenous random variables
2. $U = \{U_X | X \in V\}$ as set of exogenous/latent/noise random variables
3. P_U is the joint distribution over U satisfying $P_U(U) = \prod_X P_U(U_X)$
4. F set of functions f_X, how values are assigned to each variable $X \in V$, based on a subset of endogenous variables $Pa_X \subset V \setminus \{X\}$ (parents), with a parent exogenous variable $U_X \subset U$, leading to:

$$X := f_X(Pa_X, U_X)$$



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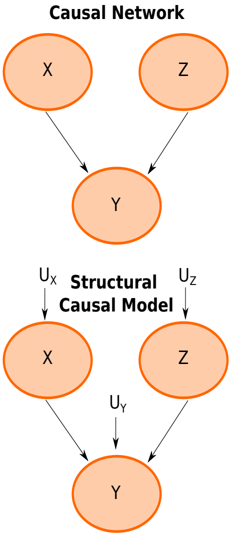
- Causal graph (network) over nodes V, where the parents of each node are linked to it (assume the graph as DAG)



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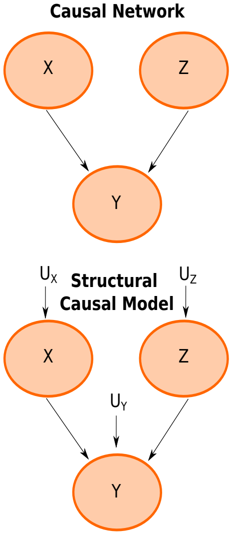
- Parents of a variable V are also called direct causes (one hierarchy level above), while the ancestors are known as indirect causes (multiple previous hierarchy levels)



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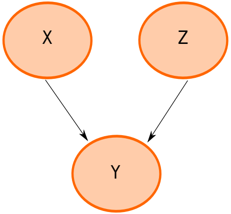
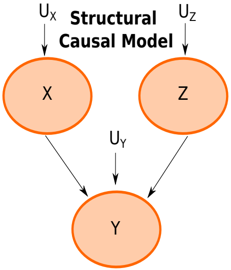
Causal Network



Structural Causal Model



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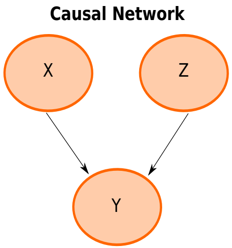

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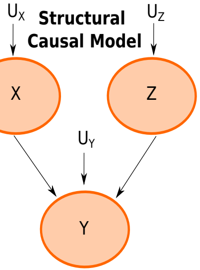

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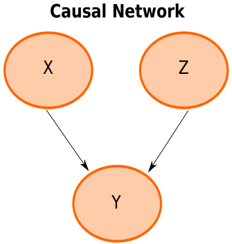
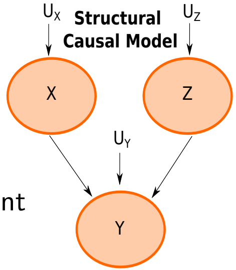
- Observational distribution of all endogenous variables V refers to the joint probability distribution $P(V) = \prod_X P(X|Pa_X)$





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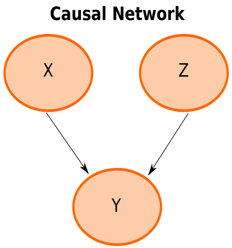
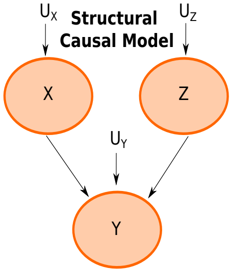
Structural Causal Models (SCMs)

- The causal network $\mathcal{G}$ is an I-Map for $P(V) = \prod_X P(X|Pa_X)$ (Bayesian Network Factorization) with $P(X|Pa_X)$ obtained from $X = f_X(Pa_X, U_X)$





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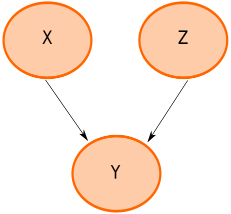
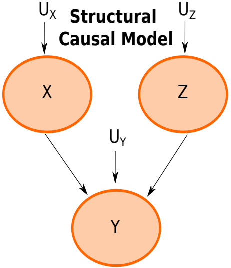
Causal Network



Structural Causal Model



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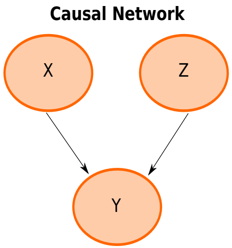

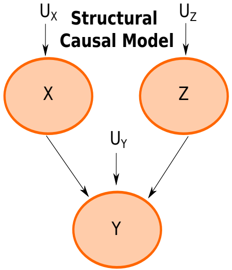

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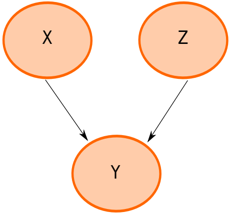
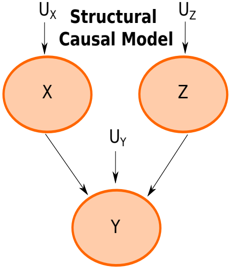


Structural Causal Model



Deep Learning Strategies – Part III
Causal Learning

Structural Causal Models (SCMs)

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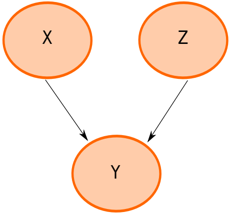
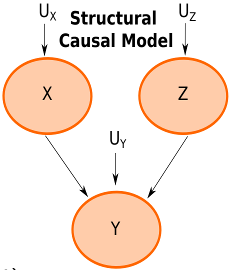
- Example I-MAP Graph: $X \rightarrow Y \rightarrow Z$ – with $X =$ Having Disease, $Y =$ Taking Medication, $Z =$ Observing Side Effects
- Captures direct dependencies ($X \rightarrow Y$, $Y \rightarrow Z$) and conditional independencies (X and Z are independent given Y, disease X alone not directly lead to side effects Z, only through the medication Y – parents!!!)

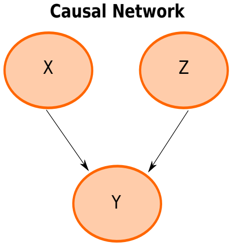
Causal Network

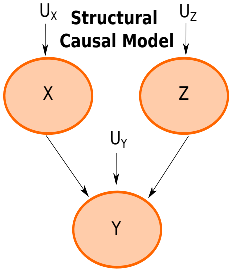




Structural Causal Models (SCMs) – Example XOR

- $P(V) = P(X = x, Z = z, Y = y)$





Source: YouTube – easy learning – Causality 3: Defining causality: Structural causal models (SCM), Link

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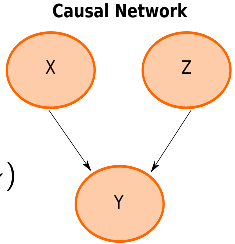

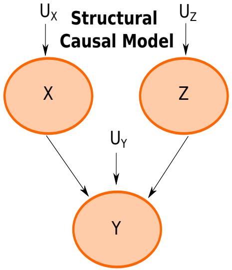

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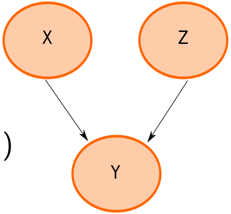
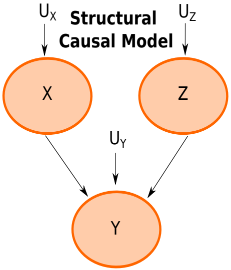
Causal Network





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Deep Learning Strategies – Part III

Causal Learning

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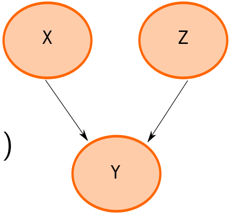
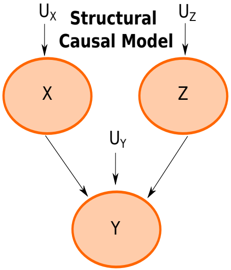
Causal Network





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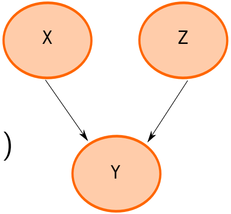
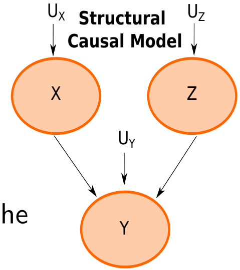
- Note: From an SCM it is possible to compute the joint distribution of the given variables!

Causal Network





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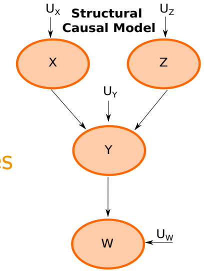
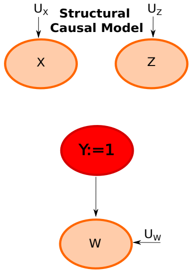
Structural Causal Models (SCMs) – Example XOR – Intervention

- Causal network turns into a Bayesian network if augmented with CPDs (prior probabilities, conditional probabilities) answering probability queries $P(Y|Z=z)$ for all $z \in Val(Z)$, $Z, Y \subseteq V$





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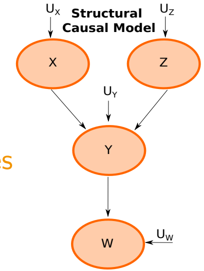

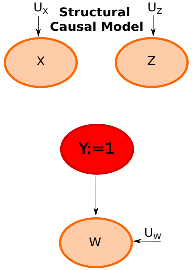

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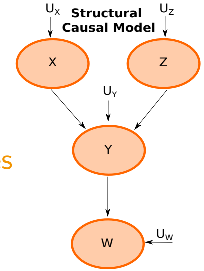
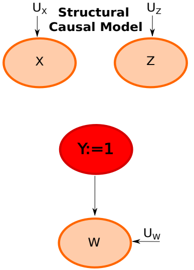
- Intervention in SCMs (do-operation): setting $Y := 1$

  Before: $X := U_X,\ Z := U_Z,\ Y := X \oplus Z + U_Y,\ W := 2Y + U_W$

  After: $X := U_X,\ Z := U_Z,\ Y := 1,\ W := 2Y + U_W \rightarrow U_W = W - 2$





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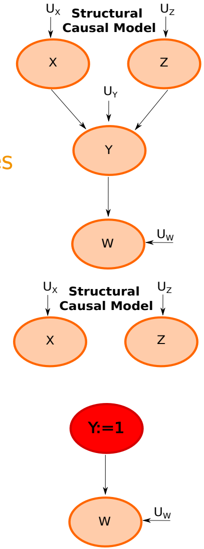
Structural Causal Models (SCMs) – Example XOR – Intervention

- Causal network turns into a Bayesian network if augmented with CPDs (prior probabilities, conditional probabilities) answering probability queries $P(Y|Z = z)$ for all $z \in Val(Z)$, $Z, Y \subseteq V$
- Conditional Probability Distribution (CPD): function that defines the probability of a random variable, given the values of its parent variables in a graph $P(X|Pa_X)$
- Intervention in SCMs (do-operation): setting $Y := 1$

  Before: $X := U_X, \; Z := U_Z, \; Y := X \oplus Z + U_Y, \; W := 2Y + U_W$

  After: $X := U_X, \; Z := U_Z, \; Y := 1, \; W := 2Y + U_W \rightarrow U_W = W - 2$
- Y does not depend on its endogenous/exogenous parents Pa_Y (all incoming links in the graph are removed!) $\rightarrow$ Perfect intervention!



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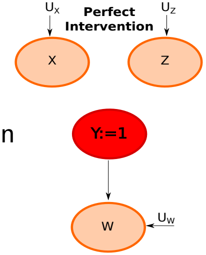
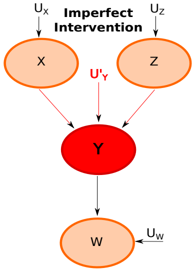
Deep Learning Strategies – Part III

Causal Learning

Structural Causal Models (SCMs) – Example XOR – Intervention

- In a perfect intervention the variable Y has a fixed/static value, based on its intervened value





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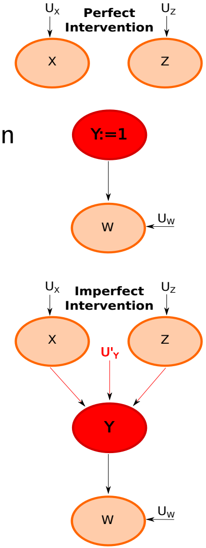
Structural Causal Models (SCMs) – Example XOR – Intervention

- In a perfect intervention the variable Y has a fixed/static value, based on its intervened value
- However: there exist also an imperfect/parametric intervention, known as mechanism change (f' assignment) (still some remaining parents) $\rightarrow$ $Y := f(Pa_Y, U_Y) \rightarrow Y := f'(Pa_Y, U'_Y)$ (e.g. $Y := X - Z + U'_Y$)



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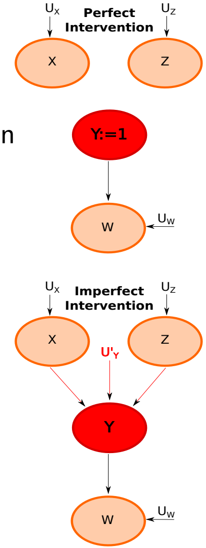
- Every intervention leads to a CPD change w.r.t. Y from:

  $Y : P(Y|Pa_Y)$ to $P^{\star}(Y|Pa_Y)$



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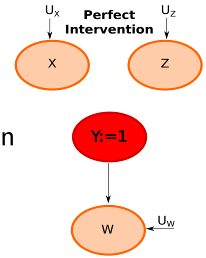

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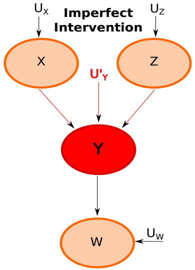
- Every intervention leads to a CPD change w.r.t. Y from:

  $Y : P(Y|Pa_Y)$ to $P^\star(Y|Pa_Y)$
- After every intervention there exist still a (new) SCM (causal network), with different dependencies and a intervention distribution $P(V\backslash Z, \mathrm{do}(Z))$ a intervention distribution over all the variables V



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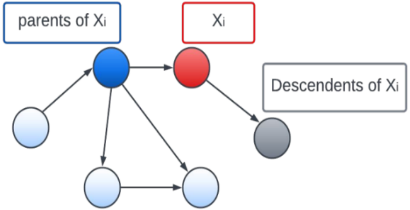
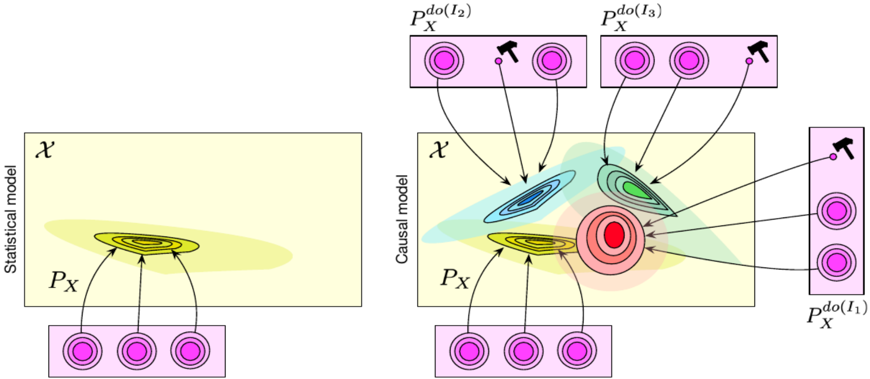
Describing the causal mechanisms of a system.



- **Variables:** $\mathbf{X} = \{X_1, \ldots, X_N\}$
- **Noise:** $U = \{U_1, \ldots, U_N\}$
- **Causal parents of Xi** $X_{pa(i,G)}$
- **Structural Equations:** (Causal Mechanisms) $X_i = f_i\big(X_{pa(i,\mathbf{G})}, U_i\big) \quad \forall i \in \{1, \ldots N\}$

Source: Image from Nan Rosemary Ke, Stefan Bauer, "Causality and Deep Learning: Synergies, Challenges and the Future", Slide 22



- Statistical (Bayesian) Model: can only capture one probability distribution
- Causal Model: every intervention defines new joint distribution intervention

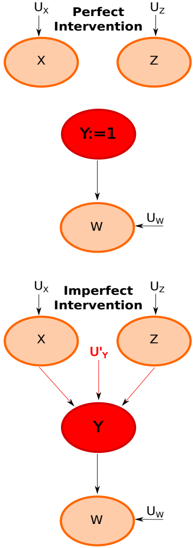
Source: FAU Erlangen-Nuremberg, Pattern Recognition Lab, K.Breininger, V. Christlein, Advanced Deep Learning – Interpretable/Causal Deep Learning

Source: Image from Nan Rosemary Ke, Stefan Bauer, "Causality and Deep Learning: Synergies, Challenges and the Future", Slide 22

Source: Schölkopf et al., "Toward Causal Representation Learning"

Structural Causal Models (SCMs) – Example XOR – Mutilated Network

- Converting an intervention to an observation query (remove all do's)



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Structural Causal Models (SCMs) – Example XOR – Mutilated Network

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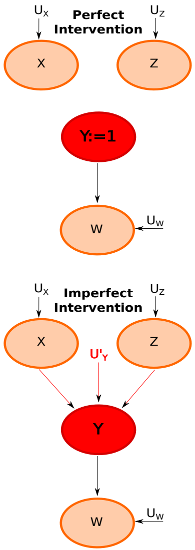
- In case of the previous Bayesian Network, and for a perfect intervention query, $P(Y|\mathrm{do}(z), x)$ is transformed to $P(Y|z, x)$, by removing all incoming edges to the intervened nodes Z, and set a fixed intervention value $Z = z$



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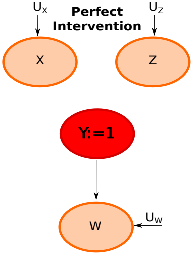
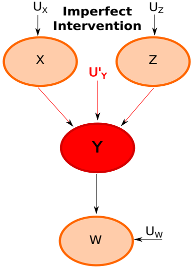
- Mutilated Network: $\mathcal{B}_{Z:=z}$, given a Bayesian Network $\mathcal{B}$, while removing all incoming links to the set of nodes Z and setting $Z = z$ (static value), $P(Z = z') = 1$ if $z' = z$, otherwise 0





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Deep Learning Strategies – Part III

Causal Learning

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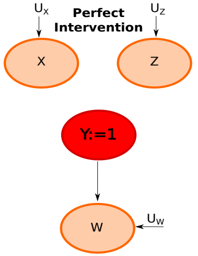

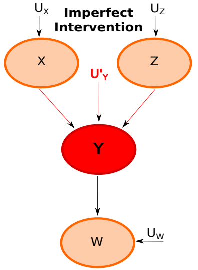

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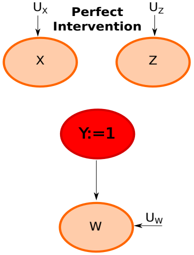
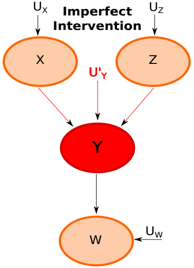
- Answering intervention queries: $P(Y|\text{do}(z), x) = P_{\mathcal{B}_{Z:=z}}(Y|z, x)$
- Modularity: conditional probability of a node is only affected if intervention is on its parents $P(Y|Pa_Y, \text{do}(z)) = P(Y|Pa_Y), \;\forall Y \notin Z$





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Causal Learning

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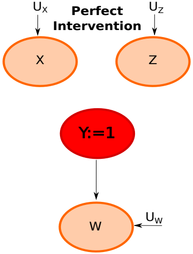
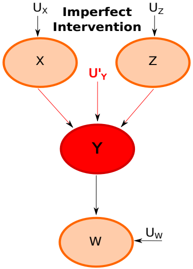
Structural Causal Models (SCMs) – Example XOR – Causal (Bayesian) Model

- **Causal (Bayesian) Network $\mathcal{C}$ (CBN):** over a set of random variables V (joint distribution P), $\mathcal{C}$ is a Bayesian network $\mathcal{B}(\mathcal{G}, P_{\mathcal{C}})$, with $\mathcal{G}$ is an I-Map for P, over V, answering both probability queries:
  1. $P(Y|x) = P_{\mathcal{C}}(Y|x)$ and intervention queries:
  2. $P(Y|Pa_Y, \mathrm{do}(z)) = P_{\mathcal{C}_{Z:=z}}(Y|Pa_Y), \;\; \forall Y \notin Z, \;\; z \in \mathrm{Val}(Z)$



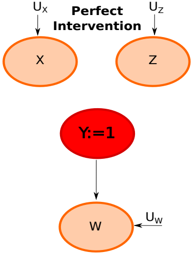


Source: YouTube – easy learning – Causality 4: Causal Bayesian Networks, Link

Deep Learning Strategies – Part III

Causal Learning

Structural Causal Models (SCMs) – Example XOR – Causal (Bayesian) Model



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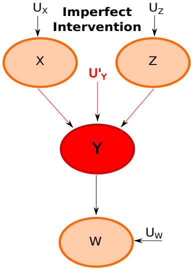
- Recap: Causal Hierarchy

1. Association (Seeing!) – Probabilistic query $P(Y|X)$ (e.g. probability of developing cancer given that the individual smokes?) – BN, CBN, SCM
2. Intervention (Doing!) – Invervention query $P(Y|\text{do}(X))$ (e.g. What is the prob. of developing cancer if individuals stop smoking?) – CBN, SCM
3. Counterfactual (Imagining!) – Counterfactual query $P(Y_{X=1}|X = 0)$ (e.g. What would have happpened if individuals had quitted smoking?) – SCM



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Structural Causal Models (SCMs) – Counterfactual Queries

- Bayesian Network (BN) is able to answer probabilistic queries (associations), while Causal Bayesian Networks (CBN) & SCM can also handle intervention queries

Source: YouTube – easy learning – Causality 6: Counterfactual Queries, Link

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Structural Causal Models (SCMs) – Counterfactual Queries

- Bayesian Network (BN) is able to answer probabilistic queries (associations), while Causal Bayesian Networks (CBN) & SCM can also handle intervention queries
- What about the last topic, addressing counterfactual queries?

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Structural Causal Models (SCMs) – Counterfactual Queries

- Bayesian Network (BN) is able to answer probabilistic queries (associations), while Causal Bayesian Networks (CBN) & SCM can also handle intervention queries
- What about the last topic, addressing counterfactual queries?
- Example: There was a fork in the road, where a decision must be made – take the freeway ($X = 1$) or go on a surface street ($X = 0$). The person took the surface street with a lot of traffic and arrived one hour later ($Y = 1$). He asked hisself – If he had taken the freeway, he would have gotton home earlier!!!

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- Such an unrealized situation from the past, wrapped in an "if-statement" is known as counterfactual $\rightarrow$ How to model a counterfactual query/situation?

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Structural Causal Models (SCMs) – Counterfactual Queries

- Let Y be the arriving time ($Y = 1$ for being late, $Y = 1$ for being in time)

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Structural Causal Models (SCMs) – Counterfactual Queries

- Let Y be the arriving time ($Y = 1$ for being late, $Y = 1$ for being in time)
- Causal inference: prediction of Y from the past, by intervening on the road (change from surface road $X = 0$ to freeway $X = 1$): $P(Y|\text{do}(X = 1))$

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- Counterfactual inference: reformulate as: $P(Y_{X=1}|X = 0, Y = 1)$

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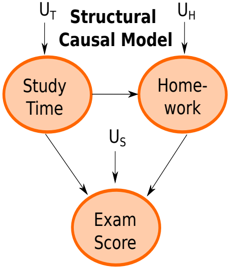
Structural Causal Models (SCMs) – Counterfactual Queries

- Example Counterfactual Event:
  - $T := U_T, \quad H := 0.5T + U_H, \quad S := 0.7T + 0.4H + U_S$

    with: T as the students studying time, H as the number of completed homeworks, S student's exam score, U_T student's free time at home, U_H student's intelligence, U_S student's anxiety



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  - Let $T = 0.5$, $H = 1$, and $S = 1.5$ for a particular student, resulting in:
    $U_T := T = 0.5$, $U_H = H - 0.5T = 1 - 0.5 \cdot 0.5 = 0.75$,
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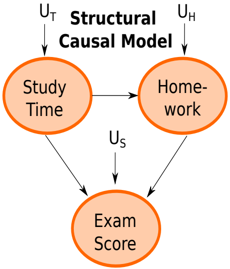

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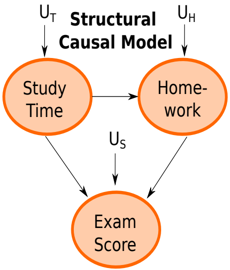

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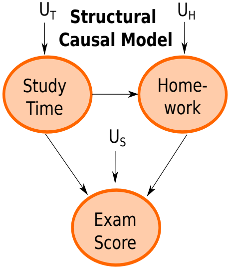

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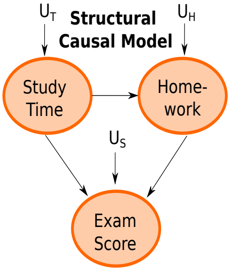
  - Counterfaction: $P(S_{H=2}|T = 0.5, H = 1, S = 1.5)$



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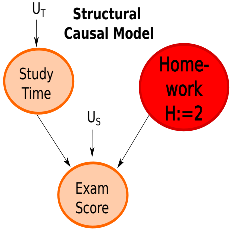
Structural Causal Models (SCMs) – Counterfactual Queries

- Example Counterfactual Event
  - Create mutilated graph, by removing all incoming links to the invervened node $Z = H$, with $P(H = 2) = 1$



Source: YouTube – easy learning – Causality 6: Counterfactual Queries, Link

Structural Causal Models (SCMs) – Counterfactual Queries

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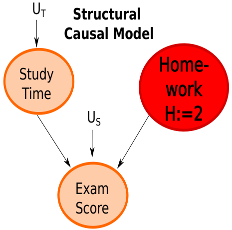

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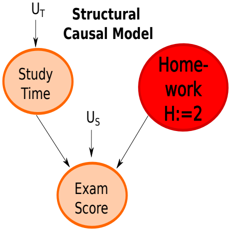

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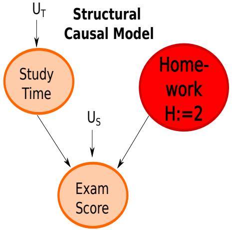

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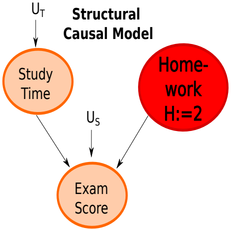

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  3. Prediction – Use the mutilated model and the value of U to compute the value of Y, the consequence of the counterfactual

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Summary – Difference BN, CBN and SCM

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1. BN is a directed acyclic graph (DAG) that represents probabilistic relationships among variables, while each random variable (node) connection represents a conditional dependence $\rightarrow$ No causation, only correlations, and conditional independencies

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2. Example: Bayesian Network, with nodes: Flu → Fever, Flu → Cough, while the model/graph shows the association between Flu and Fever, as well as Flu and Cough, however, no information that Flue causes both

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5. Example: same graph w.r.t. causation, show that Flu causes Fever and Cough, while intervening Flu causes an impact with resepct to Fever and Cough

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1. SCM is a causal model providing a more formal framework than a CBN, using a set of structural equations that specify how each variable is generated as a function of its causal parents and some random "noise" term, along with a causal DAG structure

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2. SCMs allow for both causal inference and formal intervention analysis, while being used for counterfactual reasoning, interventions, and predicting causal effects
3. SCM would not only represent Flu causing Fever & Cough, but also provide equations – Fever$=f(\text{Flu}, U_F)$, Cough$=g(\text{Flu}, U_C)$ – specifying how Flu influences Fever & Cough under different conditions

Further Questions?

https://www.oth-aw.de/hochschule/ueber-uns/personen/bergler-christian/

Source: https://emekaboris.medium.com/the-intuition-behind-100-days-of-data-science-code-c98402cdc92c