Causality

Correlation vs Causation

Understanding Machine Learning

Data-Generating Process

story behind the data as important as the data itself

Why are the statistical dependencies as observed?

→ data-generating process mostly governed by causal dependencies

but language of algebra symmetric

no way to tell that a storm causes barometer to go down and not the other way around → need for asymmetric mathematical language

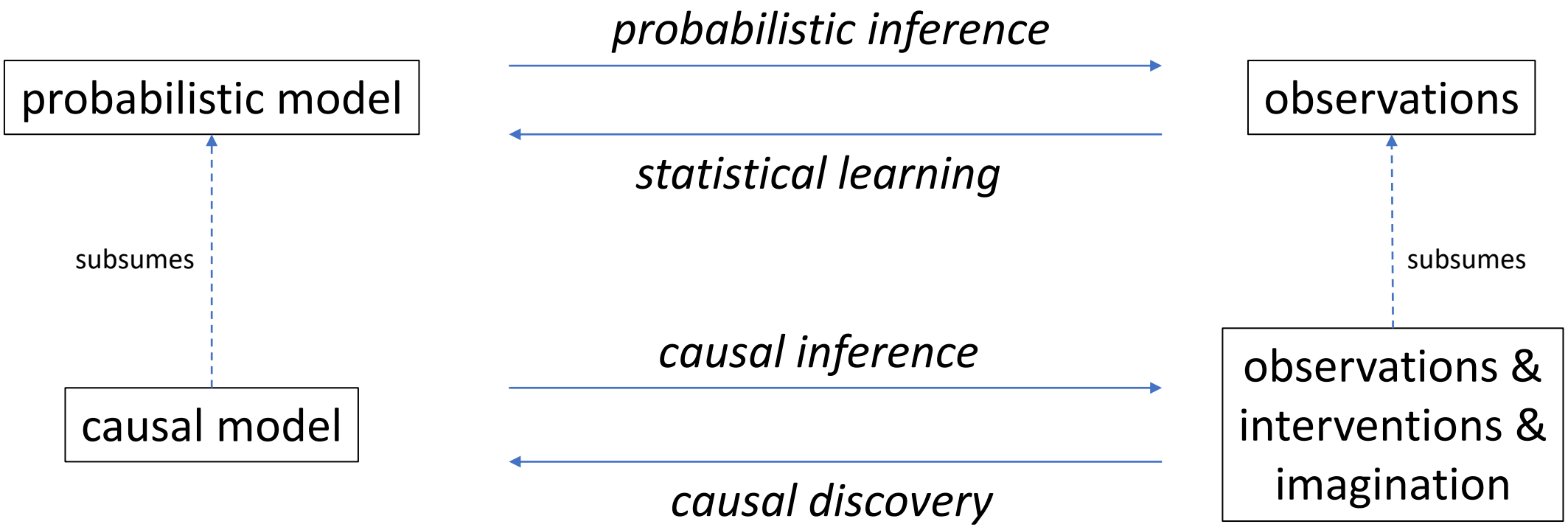
Levels of Causal Modeling

physical or deterministic models:
described by differential equations
needs somebody to come up with

causal models:
described by probabilities with causal structure
learned from data with causal assumptions

statistical models (including ML):
described by probabilities
can be learned from data

Probabilistic and Causal Models



from *Elements of Causal Inference* (Peters, Janzing, Schölkopf)

Causality and ML

causation as addition to ML: synonym for understanding

- no ML method can understand causes and effects from data (statistical dependencies) alone → need for causal assumptions (causal model)
- examples: transportability and robustness of models (generalization), handling of missing data, causal explainability

(see Pearl and Schölkopf 1 2 3)

but also: ML as help for causal discovery and inference

- counterfactuls (potential outcomes) need matching of individual cases
- adjusting for many confounders (e.g., propensity scores)

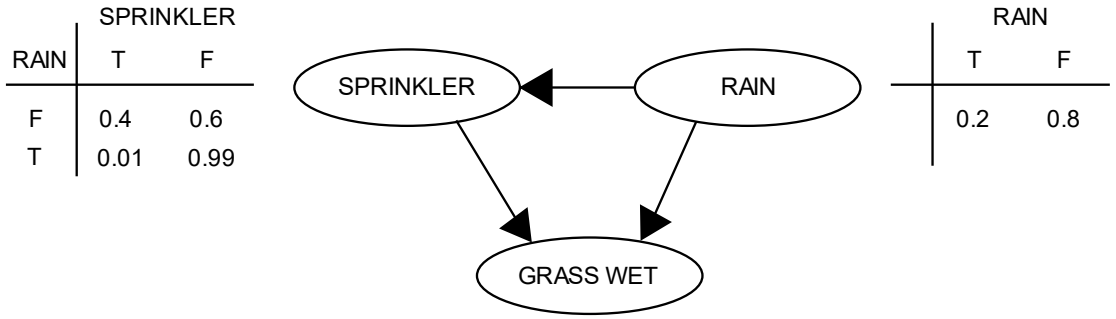
Graphical Models

Probabilistic Graphical Model

Directed Acyclic Graph (DAG): random variables (nodes) and their (conditional) dependencies (edges)

Bayesian network: DAG with updates on new evidence according to Bayes' rule (belief propagation)

- message from parent to child: update using conditional probabilities
- message from child to parent: update by multiplication with likelihood ratio



SPRINKLER	RAIN	GRASS WET T	GRASS WET F
F	F	0.0	1.0
F	T	0.8	0.2
T	F	0.9	0.1
T	T	0.99	0.01

from wikipedia

Markov Property

Each variable in a DAG is independent of its non-descendants conditional on its parents.

chain rule:

$A \rightarrow B \rightarrow C$: $P(A, B, C) = P(A)P(B|A)P(C|B)$

→ compact representation of conditional probability table

Conditional Independencies

DAG junctions:

- chains: $A \rightarrow B \rightarrow C$ (A and C conditionally independent given B)
- forks: $A \leftarrow B \rightarrow C$ (A and C conditionally independent given B)
- colliders: $A \rightarrow B \leftarrow C$ (A and C conditionally dependent given B)

d-separation (d means directional): conditional independencies in data corresponding to chains, forks, and colliders in a graph

→ allows for model testing

Toward Causal Diagrams

load graph with causal assumptions (model)

→ arrows give direction of cause-effect relationships

causal Markov property: Each variable in a causal graph is probabilistically independent of its non-effects conditional on its direct causes.

causal models (represented by graphs) allow to answer interventional and counterfactual (fictional) queries

often even without conducting experiments

Causal Inference

The Ladder of Causation

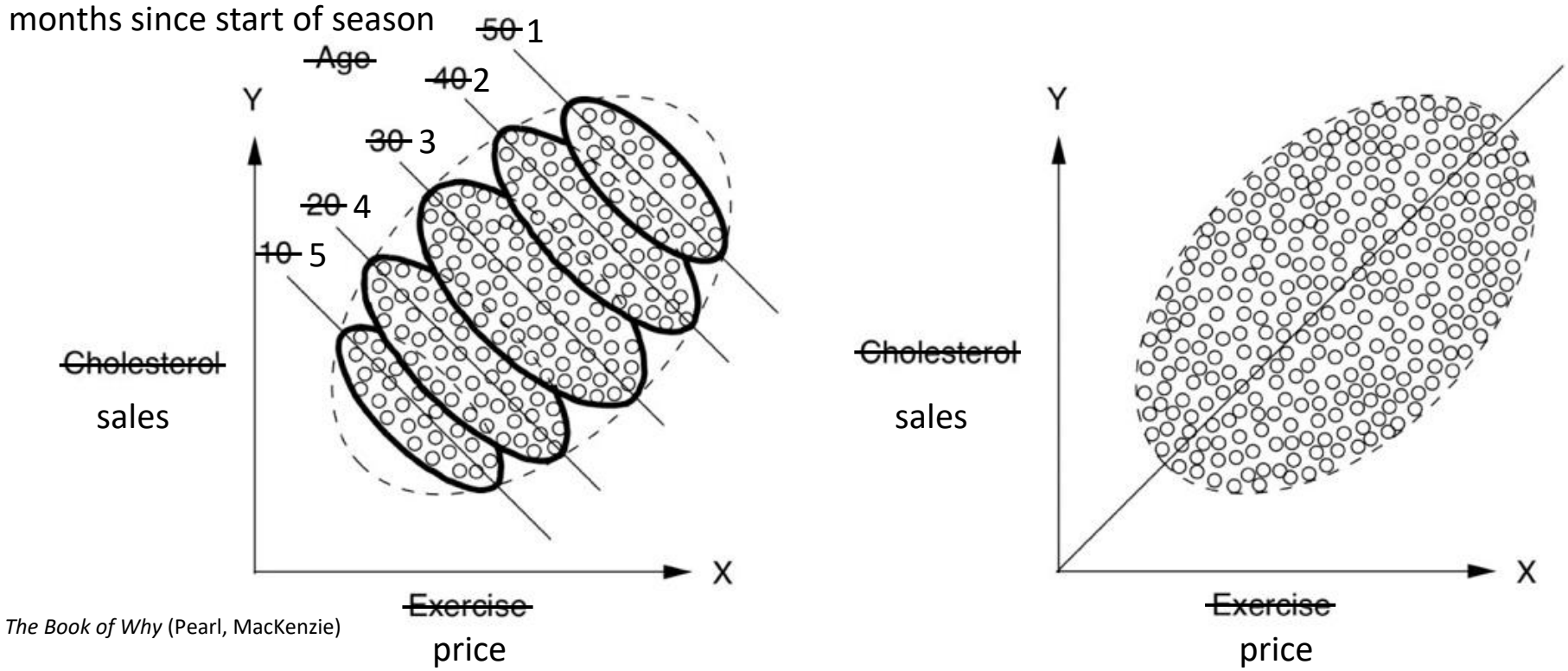
III	*imagining*	**counterfactuals**	What if I had done ...? Why?
II	*doing*	**intervention**	What if I do ...? How?
I	*seeing*	**association**	What if I see ...? → Realm of ML

from *The Book of Why* (Pearl, MacKenzie)

Simpson's Paradox

example: monthly sales of a fashion article in different shops during winter season

Lower price yields higher sales for each month individually, but lower sales overall?

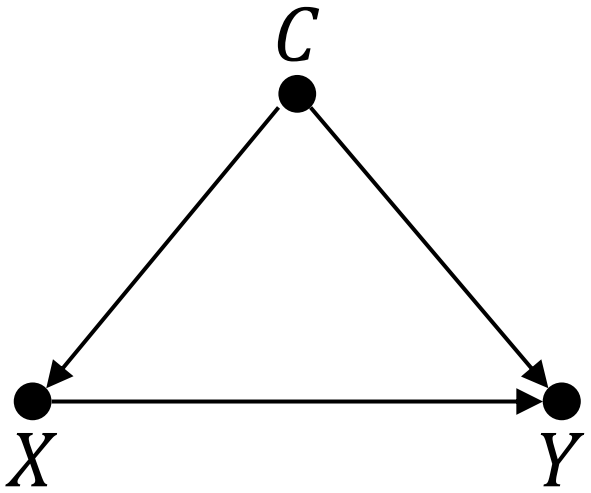


from *The Book of Why* (Pearl, MacKenzie)

Confounding

causal effect of X on Y confounded by common cause C:

$$X \leftarrow C \rightarrow Y$$



→ spurious correlation between X and Y

(overlaying potential true causal effect of X on Y)

common cause principle:

every correlation either due to a direct causal effect linking the correlated entities or brought about by a third factor (confounder)

Example: Pricing in Retail

price setting for a product can be considered a demand shaping method

the idea is a causal effect: lower price leads to higher demand

→ by estimating this causal effect one can find an optimal price according to a given policy (like maximizing profit)

problem: confounders influencing both pricing in past (obverved) data and demand, e.g., lowering prices on weekends only for grocery or lowering prices toward end of a season for fashion (most sales at beginning of season)

Example: Temporal Confounding

forecasting of times series can rely on endogenous (past values of the time series to forecast in the future) or exogenous (other variables) information

- endogenous information means auto-correlation
- auto-correlation often spurious (temporal confounding, e.g., common causes at consecutive times), i.e., no direct causal effects

most state-of-the-art forecasting methods rely mainly on endogenous information, i.e., temporal confounding

but learning of direct causal effects from exogenous information offers several advantages, like explainability, long-term forecasting, predictability of rare events

one simple possible solution: no use of target auto-correlation in (quasi-causal) ML model, but subsequent residual correction

Interventions

aim:

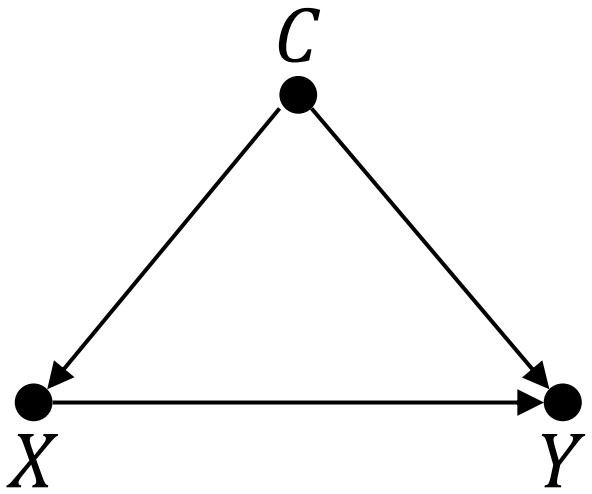
prediction of (average) causal effect of (yet untried) actions (interventions)

two ways:

- intervene via randomized controlled trials (RCT): set action randomly and check effect → physically disassociate cause from confounders
- causal model: emulating interventions by smart calculations → predict effects of potential interventions from observational studies only, i.e., without experiment

Solution for Average Causal Effects

causal effect of X on Y confounded by common cause C



solution for computation of average causal effect:

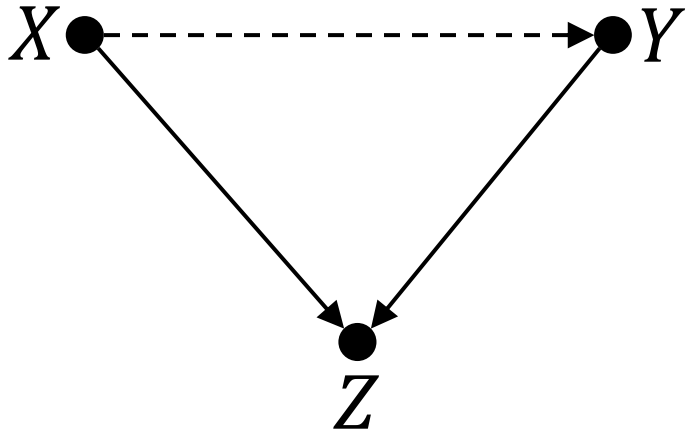
adjust for C (if there are measurements of C), i.e., stratification of data in terms of C

$$\sum_c P(Y|X, C = c)\, P(C = c)$$

fashion example: adjust for months-in-season groups

Colliders and Mediators

unwanted effects of adjusting for third variable on causal effect between X and Y:

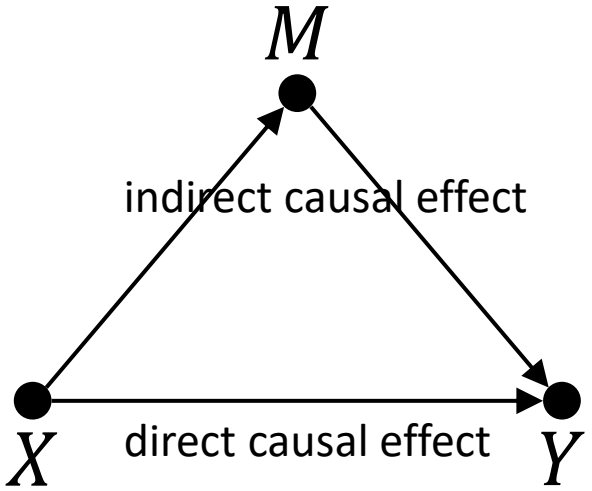


collider Z

- correlation without causation (exception to common cause principle)
- selection bias

mediator M (mechanism of effects)

→need for counterfactual description



Back-Door Criterion

to stop information flow from X to Y (d-separation):

- $X \rightarrow Z \rightarrow Y$ → adjust for Z
- $X \leftarrow Z \rightarrow Y$ → adjust for Z
- $X \rightarrow Z \leftarrow Y$ → do **not** adjust for Z

back-door path: any path from X to Y starting with an arrow pointing into X

de-confounding X and Y means blocking all back-door paths

(which need to be identified before)

do-Calculus

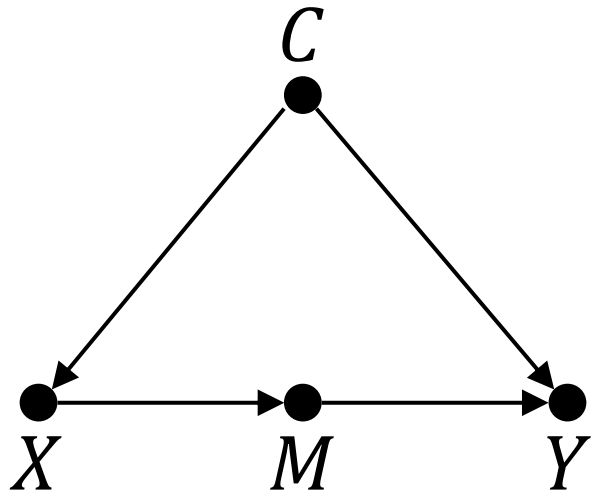
effect of intervention represented by $P(Y|do(X))$

aim: calculate $P(Y|do(X))$ in terms of data such as $P(Y|X, A, B, \dots)$
no do-operator remaining → can be calculated from observational data

$do(X)$ means removing all arrows of a causal diagram going into X

definition of confounding: $P(Y|X) \neq P(Y|do(X))$
back-door adjustment: $P(Y|do(X)) = \sum_c P(Y|X, C = c)\ P(C = c)$

Front-Door Criterion



unobservable confounder → no back-door adjustment

front-door adjustment by means of observable mediator M:

$$P(Y|do(X)) = \sum_m P(M = m|X) \sum_x P(Y|X = x, M = m)\, P(X = x)$$

adjust for two variables: M and X

derived from simple axioms of do-calculus:

- observation of W irrelevant to Y: $P(Y|do(X), Z, W) = P(Y|do(X), Z)$
- Z blocking all back-door paths: $P(Y|do(X), Z) = P(Y|X, Z)$
- no causal paths from X to Y: $P(Y|do(X)) = P(Y)$

Individual Causal Effects

Counterfactuals

so far: average causal effects over (sub-)populations by means of interventions (RCTs, do-calculus)

individual causal effects, acting on individual units u, as counterfactuals:

What happened? and *What could have happened?*

only one realization per individual: cannot simply measure difference between respective potential outcomes (all but one purely hypothetical)

counterfactual notation (had X been x): $Y_{X=x}(u)$

Estimation of Individual Causal Effects

impossible to correctly estimate individual causal effects by means of statistical interpolation techniques (impute missing data of potential outcomes)

→ need for additional causal assumptions (a causal model)

two different approaches:

1. structural causal models (Pearl): guided by causal graph and response functions
2. Rubin causal model (potential outcomes): guided by structural assumptions (e.g., the need for adjusting for all confounders)

Structural Causal Models (SCM)

also known as structural equation models (SEM)

modeler needs to specify which (causal graph) and how (deterministically, e.g., linearly) variables interact

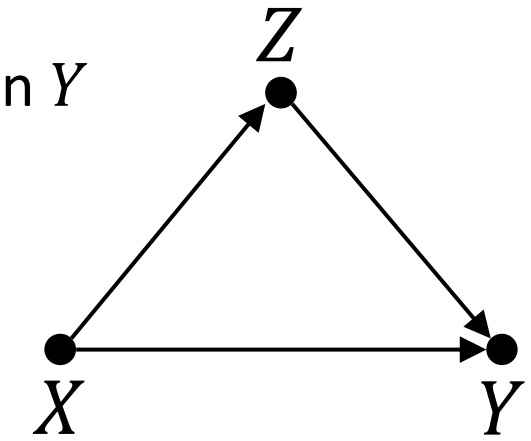
→ average and individual causal effects can be inferred from the model

example: direct and indirect (via mediator Z) causal effects of X on Y

$$Y(u) = f_Y(X(u), Z(u), U_Y(u))$$

$$Z(u) = f_Z(X(u), U_Z(u))$$

U: effects from unobserved (exogenous) variables



Counterfactual Queries in SCM

receipt for counterfactual queries on individual u:

1. abduction: use data to estimate individual $U(u)$ (potentially ML)
2. action: do-operation to change model according to counterfactual query (erasing arrows)
3. prediction: use modified model and updated information on $U(u)$ to estimate individual causal effect

connection to generative models:

unobserved variables U in SCMs correspond to latent noise variables in generative models

→ both use reparametrization trick: randomness as exogenous model input (rather than intrinsic component)

Potential Outcomes with ML

deconfounding

by RCTs or

independence weights (inverse propensity scores)

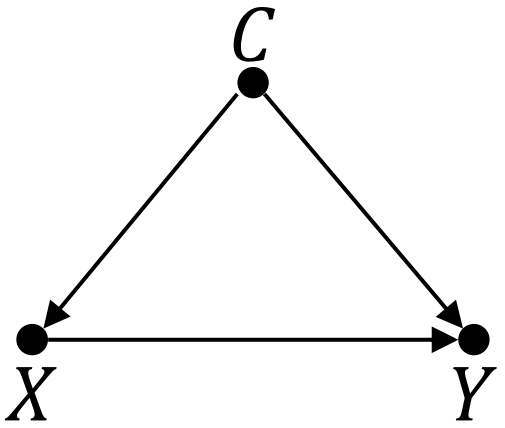
prediction of individual causal effect with ML model (generalization by function approximation)

mimicking RCT: propensity score (probability of u being subject to action) matching (importance weighting)

(see also doubly-robust methods)

can be seen as reverse engineering of artificial control group: find (averaged) similar individuals in data as potential outcome partners

Independence Weights with ML



scenario: X binary (for simplicity), several confounders C

aim: prediction of individual causal effect using observational data only

i. ML model to predict past action policy $P(X|C)$ (beware: need to include all C)

ii. inverse propensity score weighting of each unit (to adjust for multiple confounders):

$$P(Y|do(X)) = \sum_z P(Y|X, Z = z)\, P(Z = z) = \sum_z \frac{P(Y, X, Z = z)}{P(X|Z = z)}$$

alternative: A/B test

iii. train ML model on deconfounded data to predict Y with X and C as features

iv. individual causal effect as difference between predictions for setting feature $x = 1$ and $x = 0$, respectively (what-if scenario)

Causal Discovery

Causal Discovery from Observations

conditional independence testing can reveal aspects of causal graphs by means of observed statistical dependencies

subject to causal Markov property and causal faithfulness assumption: conditional independence only between d-separated variables in a DAG

hard for finite data sets without additional assumptions

→ need for approximative methods

Causal Discovery Methods

causal Bayesian networks: estimating relationships between all variables without the need to specify interactions before (like in SEMs)

restriction of function classes (e.g., smoothness): breaking cause-effect symmetry (e.g., by means of additive noise model)

meta-learning of causal structure based on speed of adaption to modified distributions (Bengio)

Graph Neural Networks (GNN)

Example: Application in Particle Physics

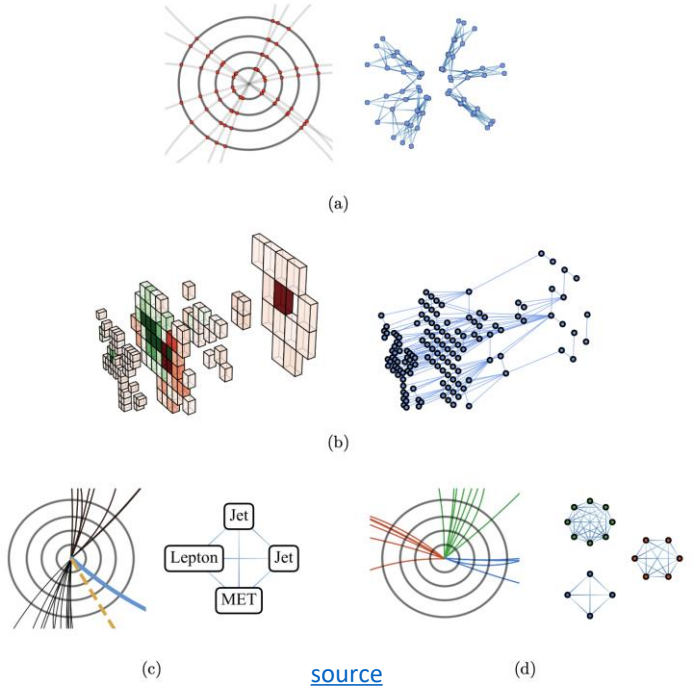
ML used in particle physics experiments for quite some time, e.g., for signal classification in detector measurements

but usual ML methods often require unnatural data representations

many problems graph-like → GNN

many applications (review), e.g.,

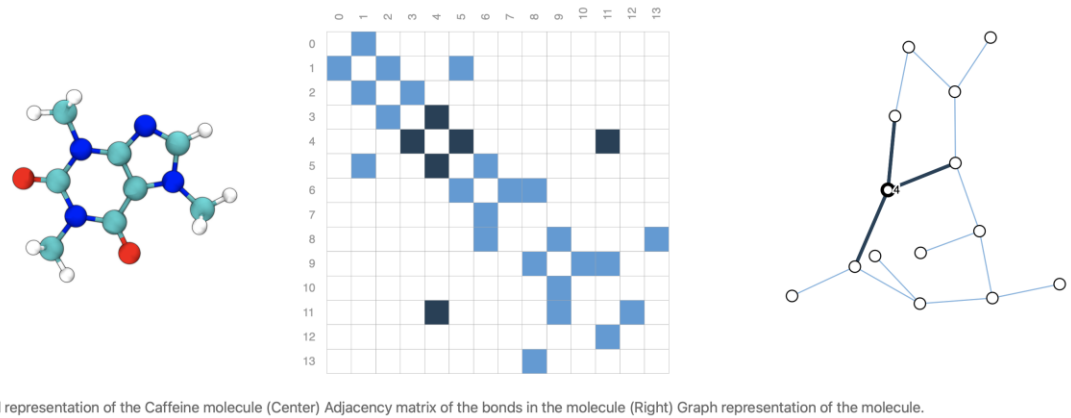
- jet reconstruction and classification
- classification of astrophysical neutrinos



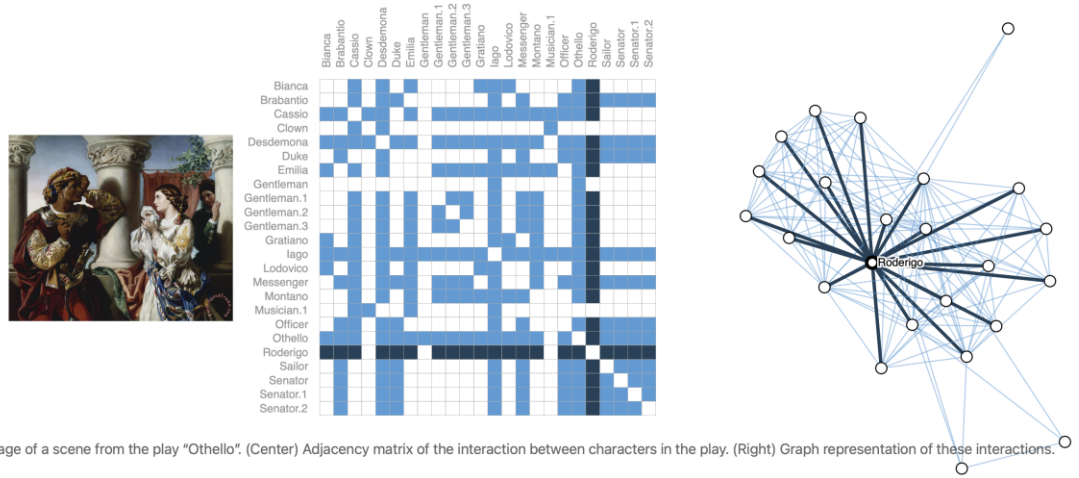
source

Graph Data

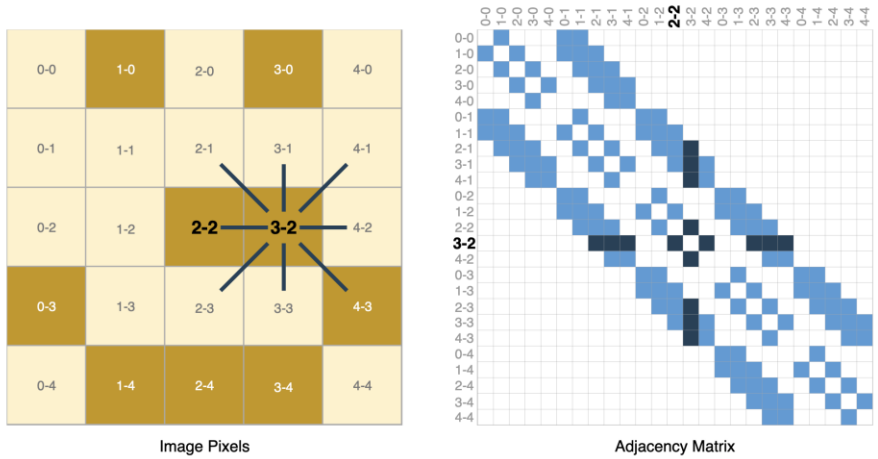
graphs: molecules, delivery routes, or social networks, but also images or text



(Left) 3d representation of the Caffeine molecule (Center) Adjacency matrix of the bonds in the molecule (Right) Graph representation of the molecule.



(Left) Image of a scene from the play "Othello". (Center) Adjacency matrix of the interaction between characters in the play. (Right) Graph representation of these interactions.



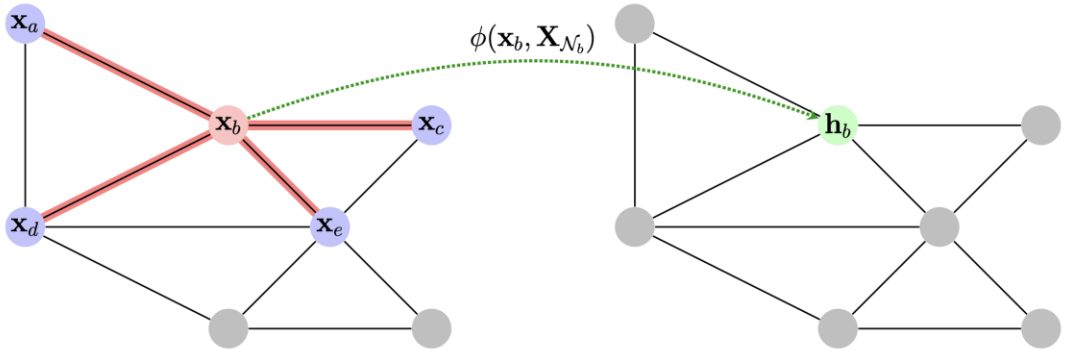
nodes × nodes adjacency matrix

all taken from [this](#) nice introduction to GNNs

Neural Networks on Graph Data

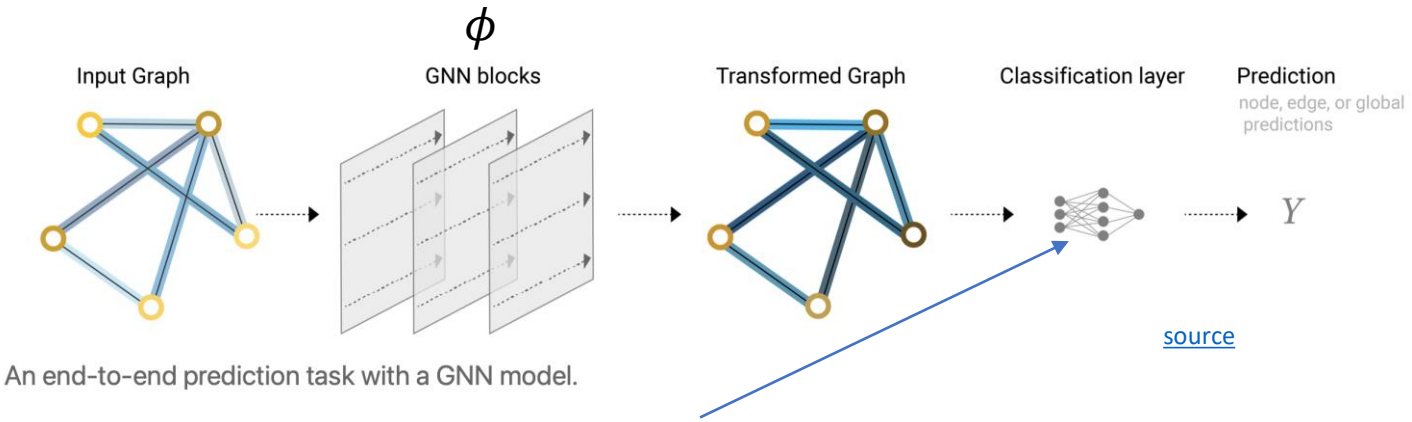
often, transductive setting: just one partially labelled graph rather than training and test graphs/samples (as in usual inductive ML setting)

graph can be specified with adjacency matrix as well as node (vertex), edge (link), and global attributes/features → learned as representation (graph encoder, embeddings)



source

GNNs: neural networks operating on graph data



source

different tasks:

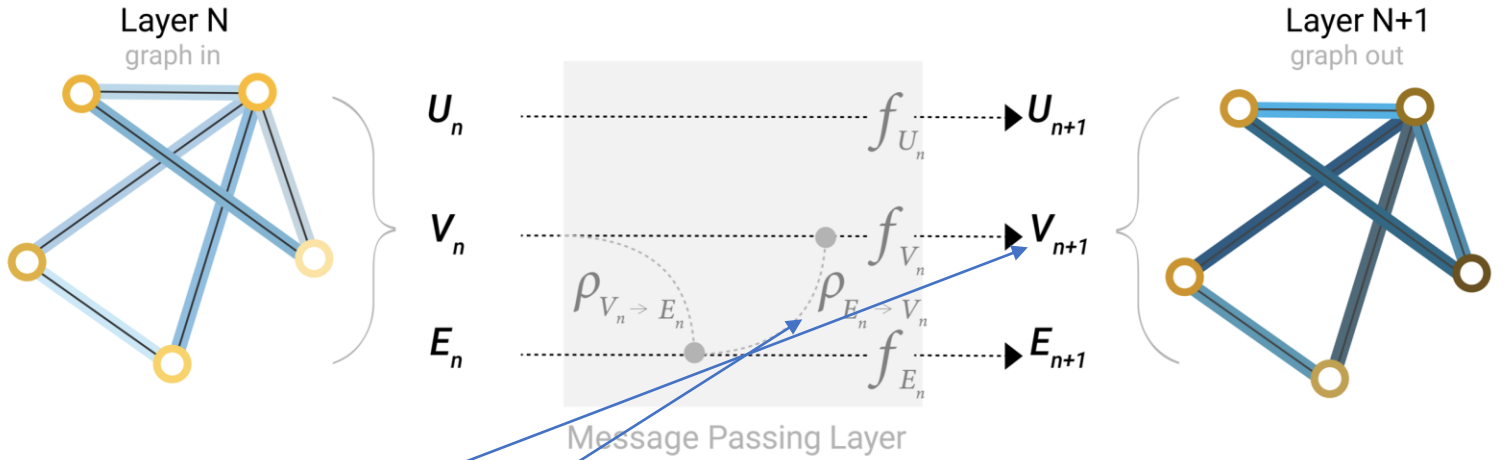
- graph-level: predict property of entire graph (e.g., molecule binding to receptor or labeling of image)
- node-level: predict the identity of nodes (e.g., image segmentation)
- edge-level: e.g., image scene understanding

global pooling layer: aggregation of node/edge representations (can also be node/edge predictions via adjacency instead of global one)

potentially also generative (decoder): e.g., generating routes for traveling salesman problem

GNN Layers and Message Passing

updating node, edge, and global-context representations by message passing



$$h_b = \phi\left(x_b, \oplus_{z \in \mathcal{N}_b} \psi(x_b, x_z)\right)$$

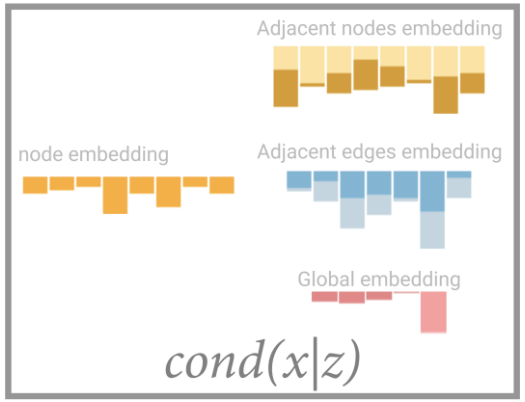
with learnable parameters

update function $f = $, …

pooling function ρ

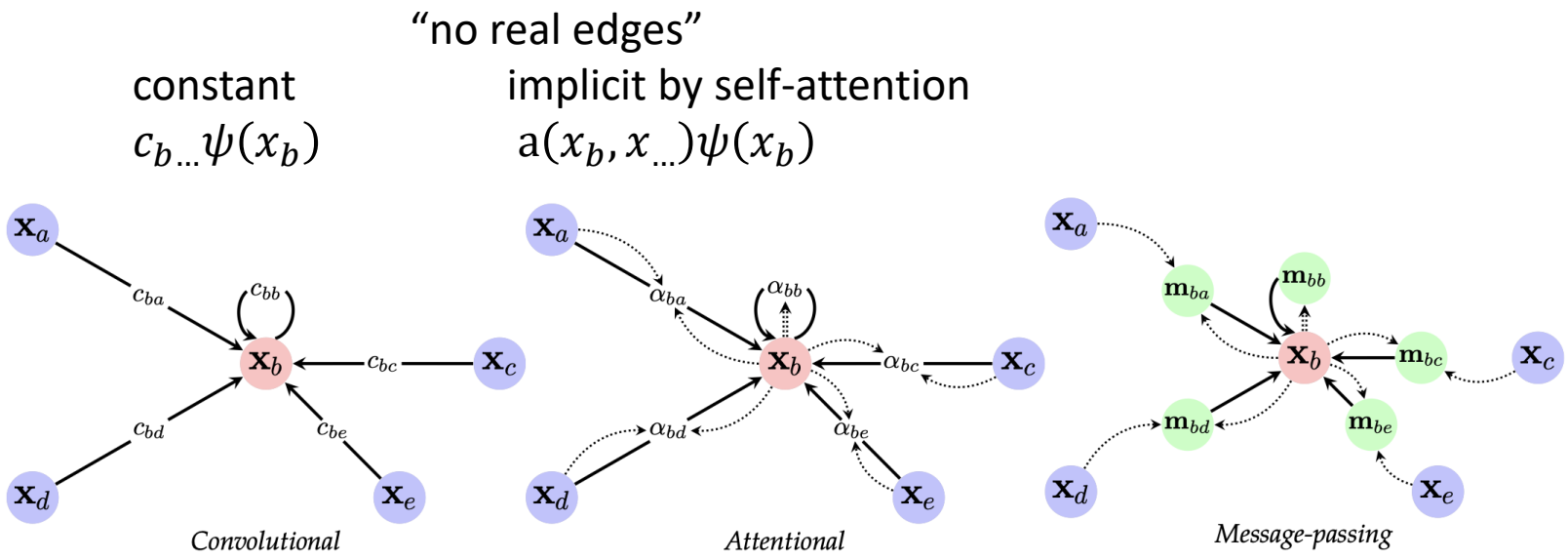
attributes

each message passing layer corresponds to one hop in graph
→ need for lots of stacking to reach full graph
→ add global representation U (context vector) connected to all nodes and edges



source

Different Types of GNN Layers



source

convolutional special case of attentional GNN layers (GAT)

both convolutional and attentional special cases of message passing GNN layers

GNNs very general deep learning architecture: most other architectures special cases of GNNs with additional geometric structure (i.e., different inductive biases)

e.g., transformers in NLP operating over complete graph of words

The Bigger Picture: Symmetries

idea of Geometric Deep Learning (borrowed from geometry):

derive different inductive biases and network architectures from symmetries and invariances

CNN from translation invariance of convolutions

GNNs from permutation invariance of graph nodes:

need for permutation-equivariant GNN layers with permutation-invariant aggregations (e.g., element-wise sum)

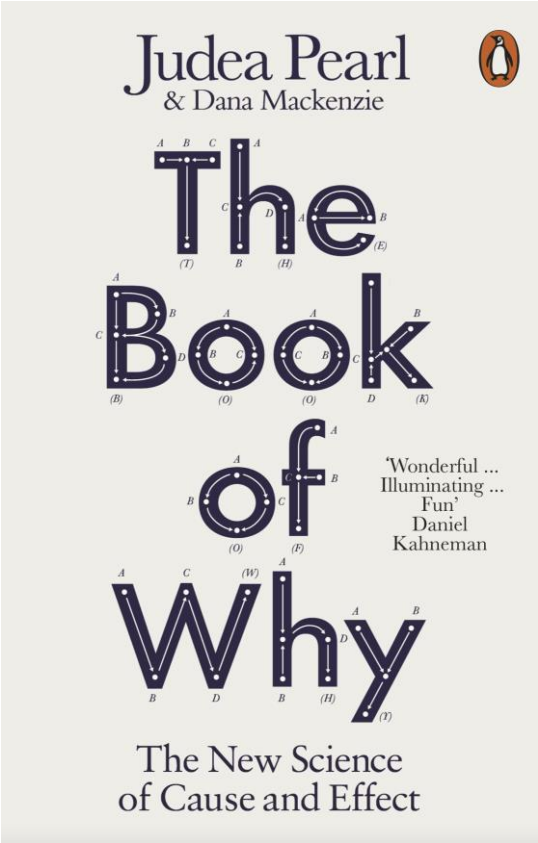
Link to Causality

neural causal models: connect SCMs and neural networks (gradient descent)

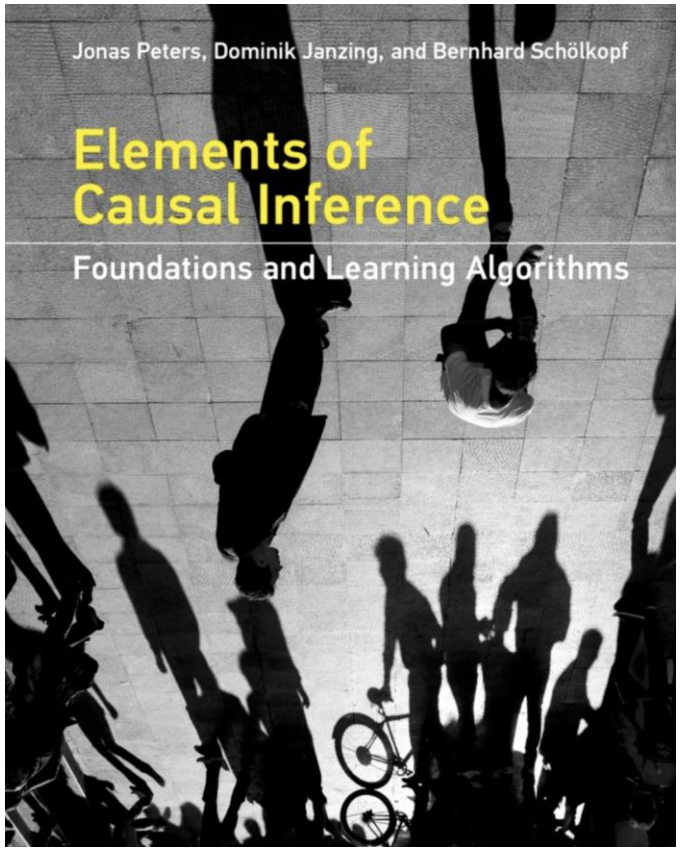
one step further: connection between SCMs and GNNs

Literature

gentle but geniune introduction, including most ideas:



… and with a little bit more maths ☺:



Fictional Thinking

fictional thinking (imagination of non-existent things) drastically improved human's communication and collaboration abilities (see *Sapiens: A Brief History of Humankind* from Harari)

counterfactual causal reasoning as base of human's fictional capabilities

enrich ML with causality:

- not only important for long-term goal of human-level AI
- also enabling better human-AI interaction (common causal language)