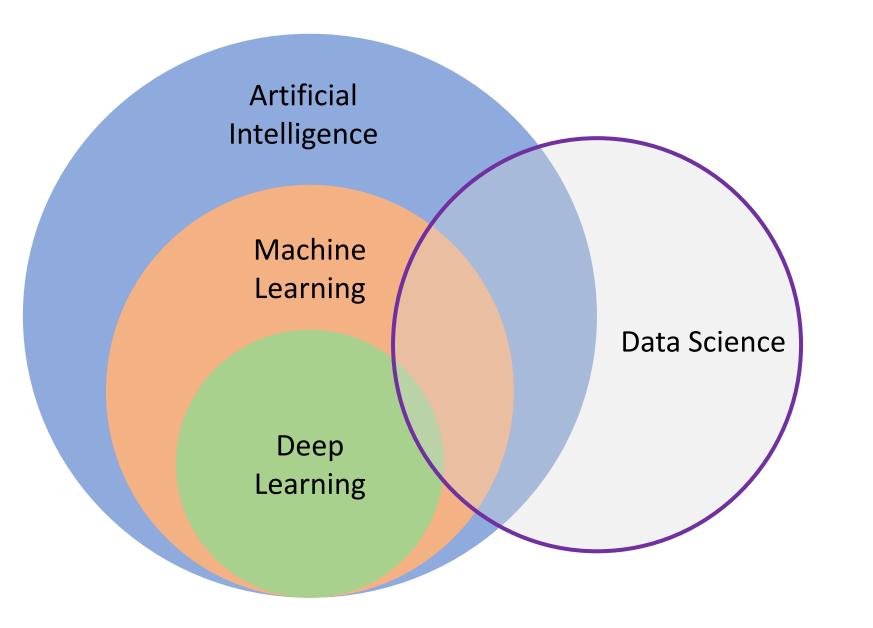
# Demand Forecasting



## Deep Learning:

special kind of ML algorithms using (deep) neural networks

Business Intelligence / Data Science:

extract knowledge from data (by means of ML, among other things)

# Automated Decision Making with AI in Retail

## replenishment

avoid waste or out-of-stock situations (lost sales)

## pricing

shape demand to maximize of revenue or profit

typically, thousands of products and stores: many individual decisions → automation crucial

decisions under uncertainty (random variables, many influencing factors) difficult for humans → statistical methods

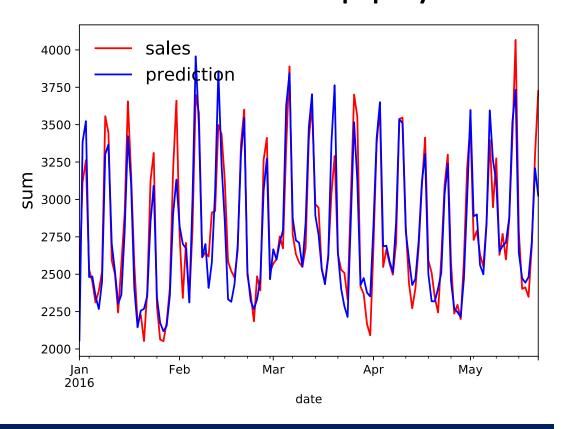
# Demand-Driven Decision Making

core component: demand forecasting used in subsequent (or entangled) decision making

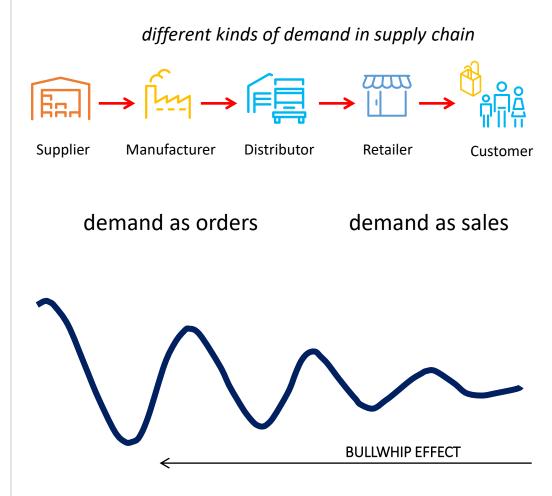
ordering / replenishment: minimization of costs for over- or underfulfilment of demand

dynamic pricing: shape demand by altering its causes (other possibility: individual customer targeting)

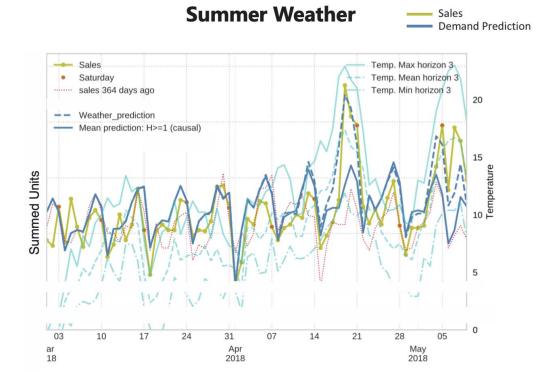
# Demand in Supply Chains

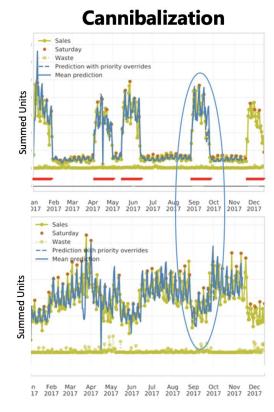


demand is a time-tagged random variable → time series regression

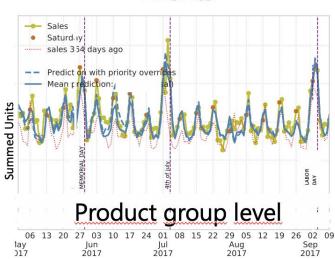


# Demand in Retail

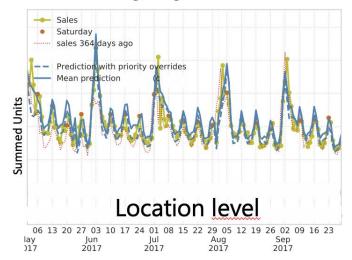




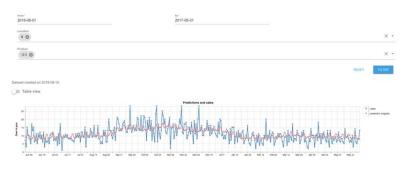
## **Events**



## **Payday Effect**



## **Seasonality**



# Time Series Modeling

# Types of Time Series Forecasting Information

## auto-correlation

- using past values of considered time series as function of lag
- identifying periodicity (seasonality) and trend

## exogenous variables

- using correlations of other variables to considered time series
- examples in demand forecasting: price, weather
- such effects lasting for some time create spurious auto-correlation

# Traditional Forecasting Methods

## direct use of auto-correlation:

- exponential smoothing
  - e.g., exponentially weighted moving average (EWMA):  $\hat{y}_t = \alpha \cdot y_{t-1} + (1 \alpha) \cdot \hat{y}_{t-1}$
  - potentially grouped by important lag like day of week or exogenous variables like promotion
- in general: (S)AR(I)MA(X)
- largely univariate time series models
- multivariate model by stacking: include univariate forecasts (e.g., EWMA) as feature in ML method

## decomposition-based approaches:

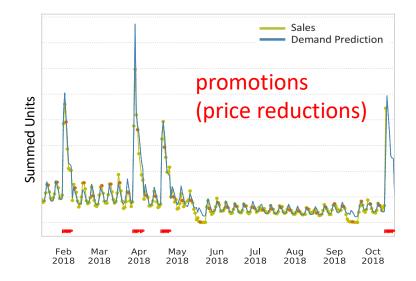
- additive components: trend, seasonality, holidays, others
- curve fitting (ML-like)
- Generalized Additive Models (e.g., multiplicative effects)
- example method: prophet
- natural way for multivariate model: training with several independent time series, distinguished by additional feature (e.g., product ID)

# Demand Forecasting with ML

#### many individual time series to consider

typical retail grocery chain:

- products (items): ~20k
- locations (stores): ~500
- daily/hourly aggregated sales



advantages of ML over traditional univariate time series forecasting:

**combined learning on all time series** of product-location combinations (rather than separately optimizing individual time series)

→ reduces variance by exploiting commonalities

**natural consideration of many exogenous variables** (prices, promotions, holidays, weather, ...)

→ reduces bias

#### to be noted:

- categorical features important (products and locations → high cardinality)
- mainly multiplicative effects
- demand (approximately) following Poisson (or rather negative binomial) distribution

# Beware of (Spurious) Auto-Correlation

difficult

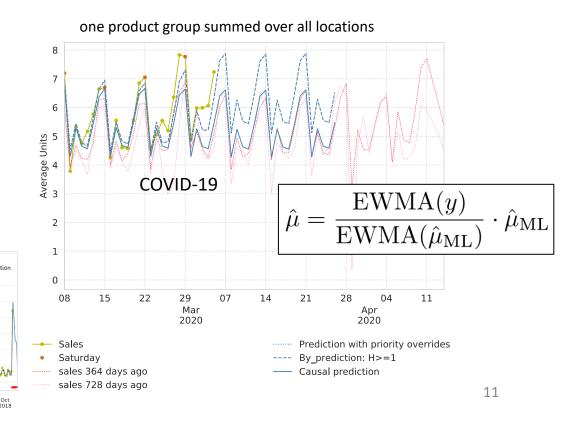
Most forecasting methods rely on lagged target information.

- univariate time series methods
- exponential smoothing features in ML model
- sequence modeling in deep learning (e.g., recurrent neural networks)

However, this makes learning of exogenous effects much harder.

- already blended in target autocorrelation
- delayed effects of short-lived structures/trends

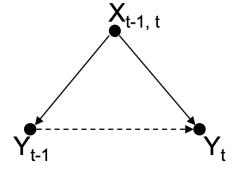
residual correction to capture missing trends)



# Temporal Confounding

auto-correlation often only spurious: common causes at consecutive times

→ no direct causal effects

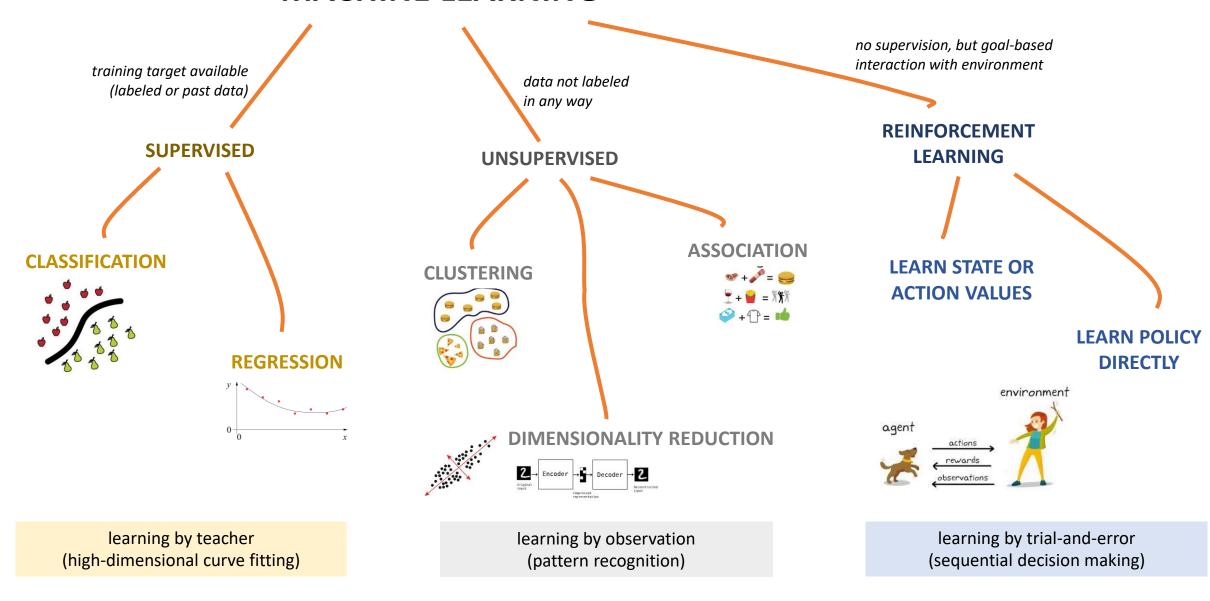


advantages of learning direct causal effects from exogenous information instead of confounded auto-correlation:

- explainability
- long-term forecasting
- predictability of rare events

# Quick Introduction to ML

## **MACHINE LEARNING**









# Supervised Learning Scenario

ML domain:

no deterministic dependencies between input and output

map inputs to output: y = f(x) (estimated:  $\hat{f}(x)$ ) random variables Y and  $\mathbf{X} = (X_1, X_2, \cdots, X_p)$  usually many dimensions

fit train data set of  $(y_i, x_i)$  pairs (i.i.d. assumption: random samples from underlying data-generating process) then apply learned statistical dependencies to test data set

## classification:

categorical target: y = 0 or y = 1 (e.g., image of cat or not), predict probabilities

regression:

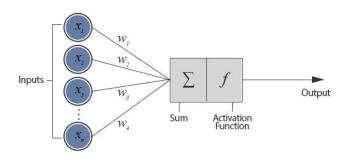
real-valued target:  $Y \in [0, \infty)$  (e.g., demand forecasting) or  $Y \in (-\infty, \infty)$ 

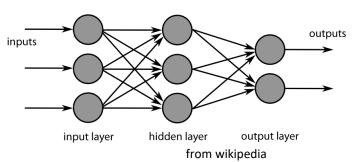
# Algorithmic Families

### linear (parametric) models

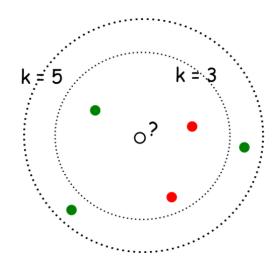
- linear regression
- Generalized Linear Models
- Generalized Additive Models

## **neural networks**: non-linear just by means of activation functions





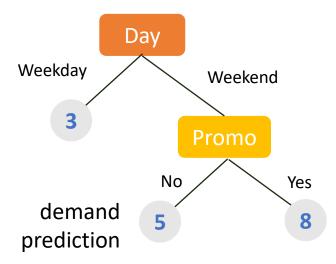
# nearest neighbors (local methods, instance-based learning) – non-parametric models



with k = 3, • with k = 5, •

**kernel/support-vector machines**: linear model (maximum-margin hyperplane) with kernel trick

#### decision trees

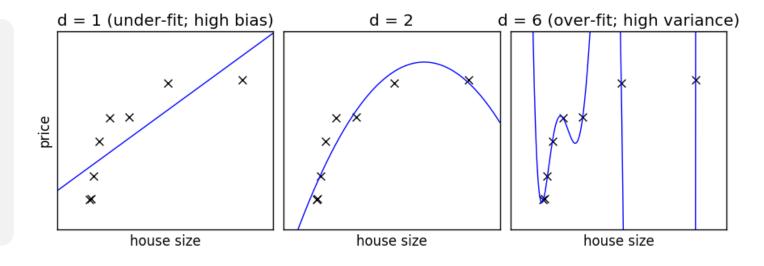


#### often used in ensemble methods

- bagging: random forests
- boosting: gradient boosting

## Common Core of Statistical Learning

curve fitting (e.g., least squares method or maximum likelihood estimation) through optimization methods (e.g., gradient descent) with the aim of generalization (by means of regularization techniques)



from scikit-learn documentation

At its heart, all the diverse statistical learning methods are reflections of the same underlying concept, and just differ in their applicability for different use cases.

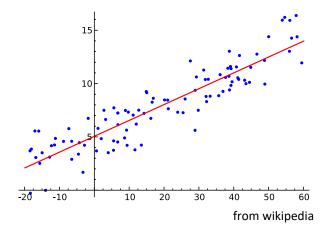
# Count Data & Multiplicative Effects: Generalized Linear Models

# Linear Regression

fit: 
$$\hat{f}(x_i)$$

$$y_i = \hat{\alpha} + \sum_{j=1}^p \hat{\beta}_j \ x_{ij} + \varepsilon_i$$
(model)

error term (noise): reflects assumed data distribution (here: Gaussian with same variance  $\sigma^2$  for all samples)



parameters to be estimated:

• 
$$\hat{\alpha}$$
,  $\hat{\beta}$ 

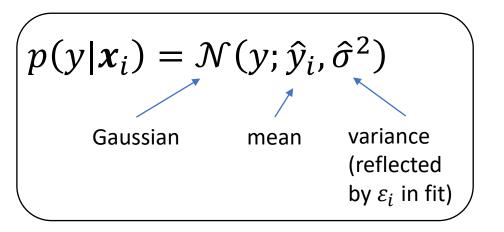
$$\Rightarrow \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \left( y_i - \hat{f}(x_i) \right)^2$$

(approximating assumed true  $\alpha$ ,  $\beta$ ,  $\sigma$ )

## predict:

$$\hat{y}_i = E[Y|X = x_i] = \hat{f}(x_i)$$

- conditional mean for squared loss of least squares method
- predict arbitrary quantile by means of quantile loss



# Multiplicative Model

- count data:  $Y \in [0, \infty)$
- Y follows Poisson (or negative binomial / Poisson-gamma) distribution

log-linear model (Gaussian errors in fit, Poisson with mean  $\hat{y}_i$  predicted):

$$\log(E[Y|X=x_i]) = \hat{\alpha} + \sum_{j=1}^p \hat{\beta}_j \; x_{ij}$$
 Single parameter 
$$\hat{y}_i$$

 further advantage: usually multiplicative effects for count data, i.e., variation proportional to level (small effects for small counts, large effects for large counts)

## Generalized Additive Models

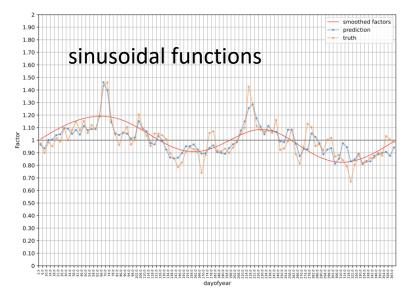
blending of Generalized Linear Models and additive models

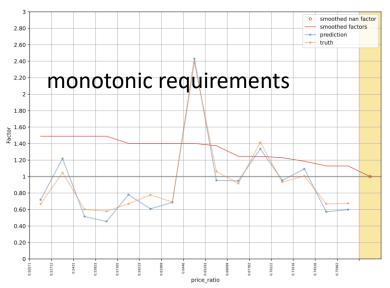
$$g(E[Y|X=x_i]) = \hat{\alpha} + \sum_{j=1}^{p} \hat{h}_j(x_{ij})$$

## smooth functions

- potentially non-parametric form
- describe non-linear effects
- estimated, e.g., via backfitting algorithm
- extension: add interaction terms between different features (e.g., different holiday effects for different products)

## **Cyclic Boosting**

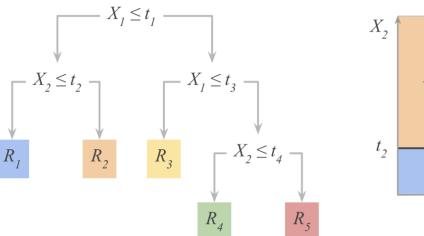


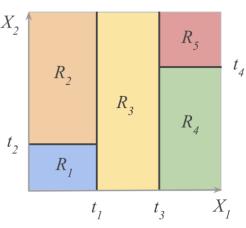


# Automatic Interaction Learning: Gradient Boosting

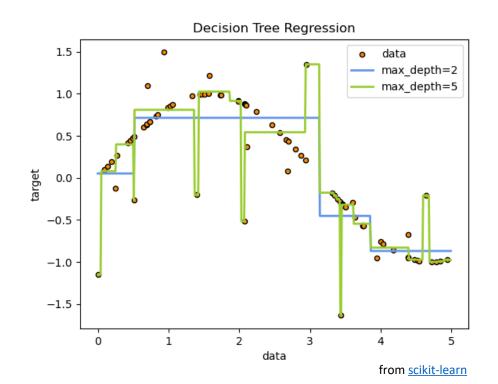
## **Decision Trees**

- non-parametric learning of simple decision rules
- usually, binary trees
- axis-parallel decision boundaries (box-shaped regions in feature space)
- fit constant  $\hat{c}$  in each box (note similarity to kNN)
  - classification: majority class of target
  - regression: average of target
- fully explainable models





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# Boosting

idea: sequentially learn and combine several "weak" learners (such as small decision trees, but in principle any ML algorithm) to construct a "strong" one  $\rightarrow$  gradually (in a greedy fashion) reducing bias of ensemble model

in simple terms: building a model from the training data, then creating a second model that attempts to correct the errors from the first model, ...

→ each subsequent weak learner is forced to concentrate on the examples that are missed by the previous ones in the sequence

not a committee of models typically, use simple, high-bias methods as individual models

# Gradient Boosting

## forward stagewise additive modeling:

- initialize  $\hat{f}_0(x) = 0$
- for m=1 to M
  - a) compute  $\operatorname*{argmin} \sum_{i=1}^N L\left(y_i, \hat{f}_{m-1}(\boldsymbol{x}_i) + \hat{h}_m(\boldsymbol{x})\right)$  b) set  $\hat{f}_m(\boldsymbol{x}) = \hat{f}_{m-1}(\boldsymbol{x}) + \hat{h}_m(\boldsymbol{x})$
- → functional gradient descent

## prominent implementations:

- XGBoost: uses second-order Taylor approximation in loss function (Newton-Raphson instead of gradient descent)
- <u>LGBM</u>: uses improved histogram-based algorithm
- CatBoost: uses kind of leave-one-out encoding for categorical features

 $L\left(y_{i},\hat{f}_{m-1}(\boldsymbol{x}_{i})\right) + \hat{h}_{m}(\boldsymbol{x}_{i}) \left[\frac{\partial L\left(y_{i},\hat{f}(\boldsymbol{x}_{i})\right)}{\partial \hat{f}(\boldsymbol{x}_{i})}\right]_{\hat{f}=\hat{f}_{m-1}}$ 

## Decision Tree Sizes for Boosting

consider degree to which features interact with each other in given data set (see ANOVA expansion)

- decision trees with single split (aka decision stumps): covering no interaction effects, just main effects of individual features
- decision trees with two splits: covering second-order interactions
- decision trees with three splits: covering third-order interactions (usually interaction order not much higher than  $\sim$ 5)

why boosting often works better than single large, low-bias model: uncorrelated learners, each focusing on a specific aspect of the data

# Embeddings & Feature Learning: Deep Learning

# Categorical Variables

tabular data usually heterogenous, often with sparse categorical variables (like color of an object)

→ need for an encoding for categorical variables

## different possibilities:

- ordinal encoding
- leave-one-out encoding (use mean of target for given category excluding current row)
- one-hot encoding (suffers from curse of dimensionality)
- embeddings

### stacking:

# Embeddings

representation of entities by vectors similarity between embeddings by, e.g.,

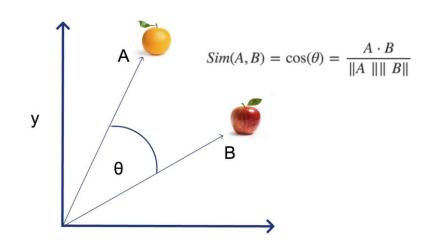
cosine similarity → semantic similarity

→ associations (natural language processing)

learned via co-occurrence (e.g., word2vec)

but general concept: embeddings of (categorical) features (e.g., products in recommendation engines)

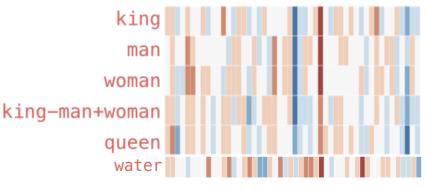
end-to-end learning: embeddings layer in deep neural network, e.g., multi-layer perceptron (MLP)

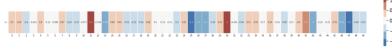






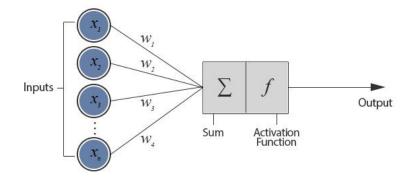
but also direction of difference vectors interesting (analogies):





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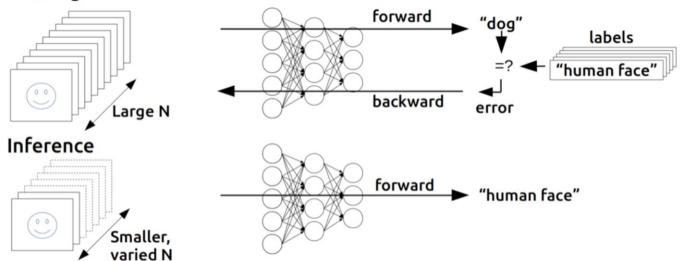
# (Deep) Neural Networks



back-propagation of errors (gradients of cost function according to weights) through layers via chain rule of calculus (avoiding redundant calculations of intermediate terms)

each node exchanges information only with directly connected nodes  $\rightarrow$  enables efficient, parallel computation

### Training



- forward pass: current weights fixed, predictions computed
- backward pass: errors computed from predictions and backpropagated → weights then updated according to loss gradients (via gradient descent)

<u>source</u>

# Examples for Feature Engineering

#### seasonality

day of week, payday, week of year

#### weather

event-like: first sunny weekend, snowstorm, ...

#### events (e.g., holidays)

time window around event (e.g., monotonic)

#### promotion

days since start of promotion period

#### price

ratio of reduced and normal price, price-demand elasticity

### product information

text (name/description) or image embeddings

# Feature Engineering vs Feature Learning

shallow learning:

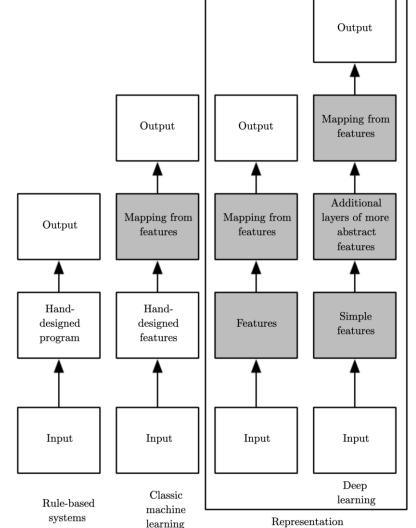
representation encoded in features

→ feature engineering

deep learning:

representation encoded in network

→ feature/representation learning (hierarchy of concepts learned from raw data in deep graph with many layers)



source

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learning

## Tabular vs Unstructured Data

deep learning methods dominate applications on unstructured data (like text or images), but not necessarily on tabular data

typical characteristics of tabular data difficult to handle for deep learning:

- irregular patterns in target function (neural networks require piecewise continuous targets)
- uninformative features
- non-rotationally invariant data (linear combinations of features misrepresent the information)

tree-based models (e.g., gradient boosting) can naturally deal with these situations

## Black-Box Models

To build trust in AI systems, individual predictions/actions need to be fully transparent, i.e., explainable.

(do not confuse explainability with causality though)

Unfortunately, complex models like deep learning methods are difficult to interpret.

→ need for model-agnostic methods to explain black-box models examples: local surrogates (<u>LIME</u>), Shapley values (<u>SHAP</u>)

<u>overview</u>

# Deep Learning Methods for Sequential Data

→ direct inclusion of auto-correlation in ML model (but remember: mainly spurious)

## convolutional neural networks (CNN)

- main application computer vision: images correspond to regular 2D grids of data (pixels)
- time series data as 1D grid at regular time intervals
- parameter sharing via convolutions (and pooling) → highly regularized feed-forward networks
- fixed time window (kernel)
- multivariate time series model via different input channels

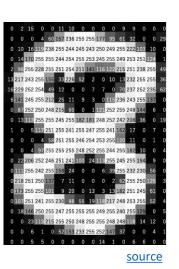
### recurrent neural networks (RNN)

- main application natural language processing (NLP): sequence of words (tokens)
- time series data as time-tagged stream
- parameter sharing via recurrent nodes → context-awareness (input from past activations)
- variable-length time series
- multivariate time series model via more input nodes

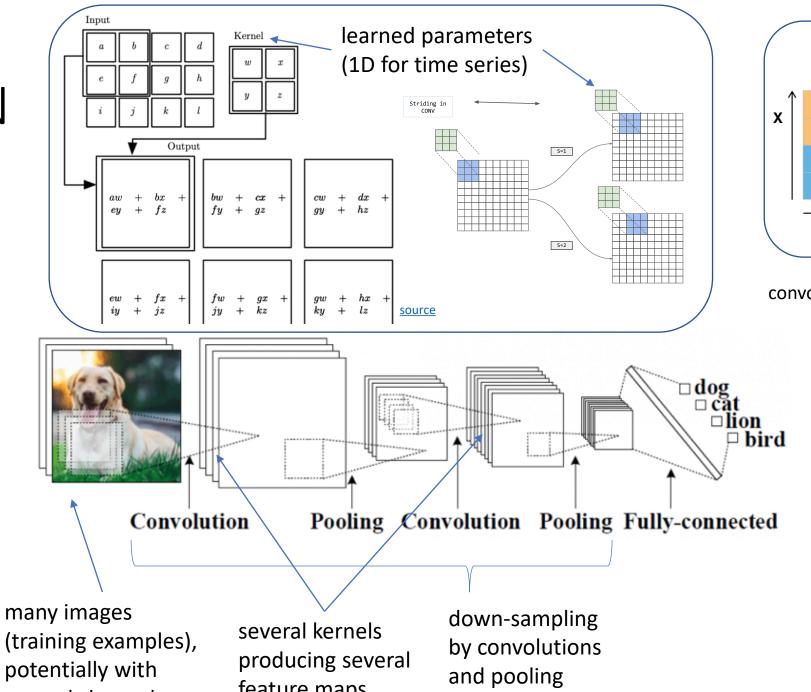
#### transformers

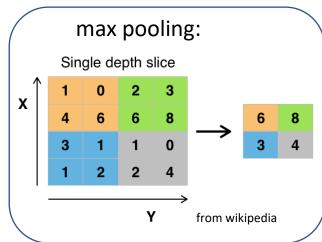
- main application NLP (largely replaced RNNs), but also computer vision
- time series data as directed graph (attention in edges)
- masked self-attention to focus on relevant past time steps and positional encoding to include order of sequence
- multivariate time series model via input concatenation

## **CNN**

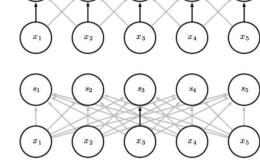


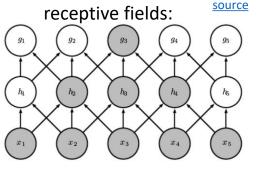
1D for time series





convolutional vs fully-connected layer:





(training examples), potentially with several channels

feature maps

# RNN: Back-Propagation through Time

interaction with delay of single time step computational graph with repeated pieces: hidden layer: several  $h^{(...)}$   $h^{(t-1)}$   $h^{(t-1)}$ 

recurrent neurons

#### input layer:

- NLP: one-hot encoded words or embeddings
- time series: lagged target (e.g., sales) or exogenous time series (e.g., price)

parameter/weight sharing over time

Unfold

single model operating on all time steps

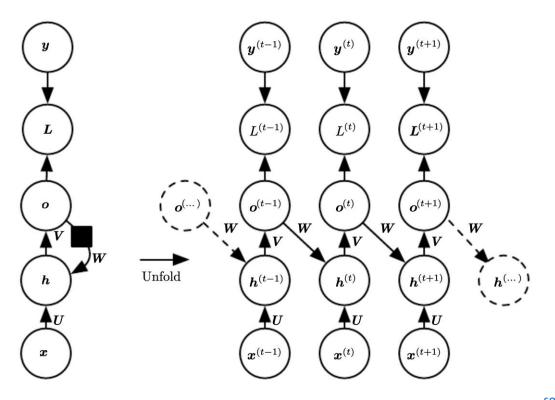
 $oldsymbol{x}^{(t+1)}$ 

activation of recurrent

nodes at that point in time

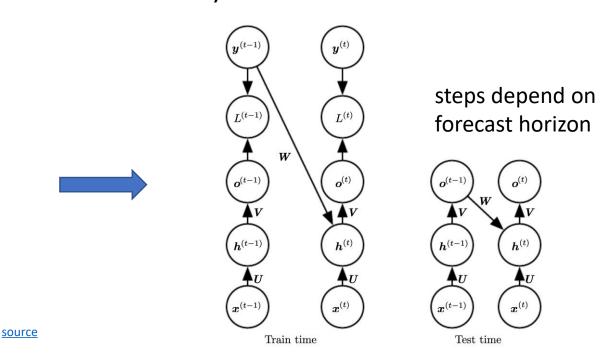
## Teacher Forcing

e.g., RNN:

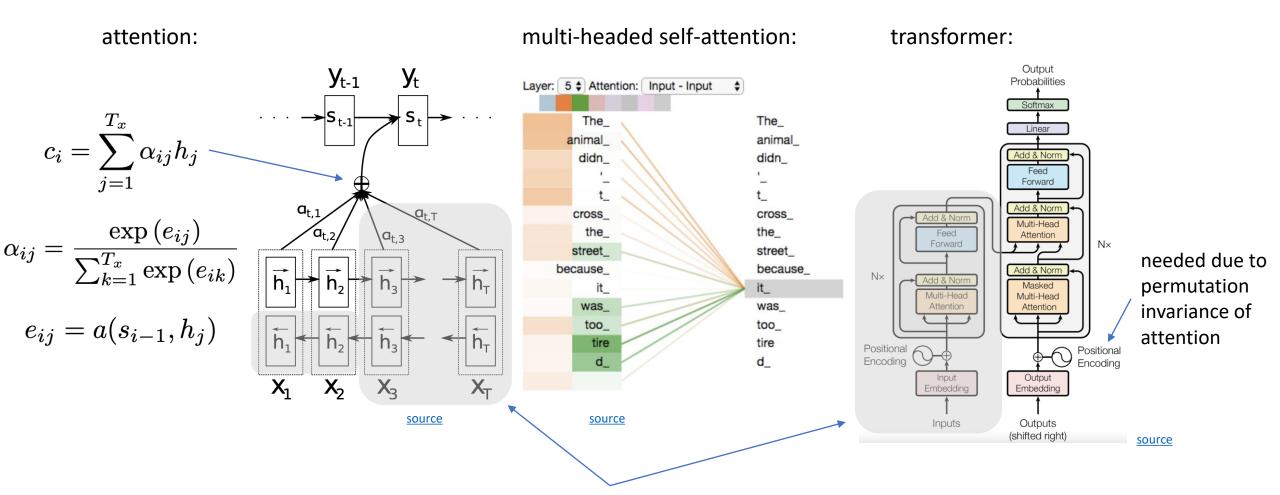


instead of feeding model output back into itself, use target values directly for feedback from output to hidden layer

example demand forecasting: sales from day before (different to usage as input from last slide)



## Transformer



time series: masked self-attention (only attending to past) → decoder-only (auto-regressive)

# Demand Forecasting Subtleties

## Censored Target

using sales data from past as target quantity to reflect unobservable demand

BUT: sales data correspond to censored demand due to

- out-of-stock situations
- markdown sales: reduced prices for items, e.g., nearing its best before date → increased sales compared to demand at usual, unreduced price

need for (probabilistic) target correction in these situations to enable unbiased demand forecasts

## Cannibalization and Halo Effects

sample interactions: demand decreases (cannibalization) or increases (halo) due to other products in promotion at the same time

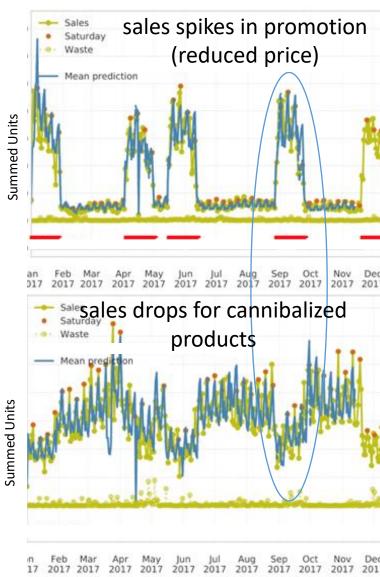
- ➤ additional ML model(s) after demand forecasting
- prediction residuals as target (all other effects
- aptured)

  learn individual effect for each product pair
  (product matrix with separate models for each row)

  reduction (or promotion flag) of different other

  - feature selection to avoid overfitting (e.g., lasso)





# Order Optimization: Need for PDF Predictions

# Prediction of Full Probability Distributions

### quantile regression:

estimate quantile  $\tau$  of distribution instead of conditional mean by minimizing

$$(1 - \tau) \sum_{y_i < \hat{q}} (y_i - \hat{q}) + \tau \sum_{y_i \ge \hat{q}} (y_i - \hat{q})$$

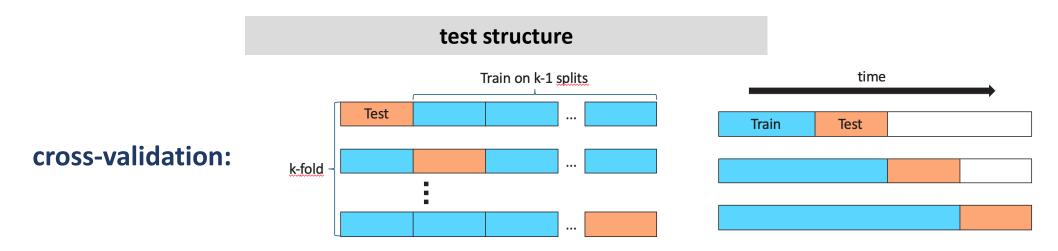
instead of squared error loss (choice of loss function defines point estimate)

possible with various ML methods, including neural networks and tree-based methods (like random forests or gradient boosting)

## PDF assumption for model and estimation of its parameters:

assume, e.g., Gaussian or negative binomial  $\rightarrow$  estimate mean and variance (with different ML models or corresponding likelihood)

## Model Evaluation



decide on acceptance of model changes by accuracy measure: improved model vs baseline (current best)

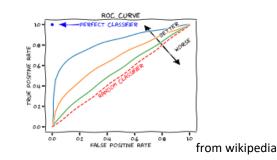
## measure (out-of-sample) accuracy of predictions

(loss function in training as proxy of this)

#### regression

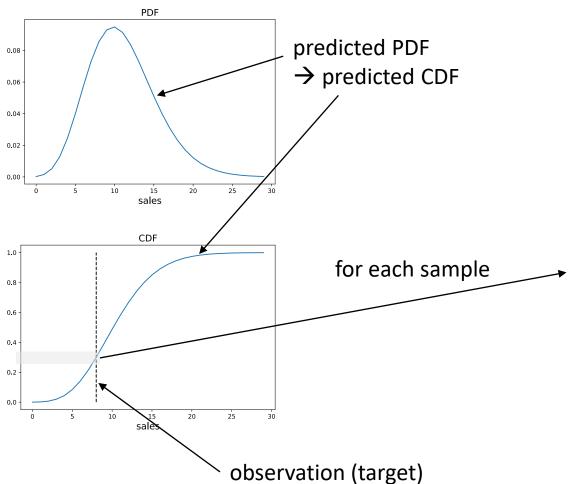
- point estimate: absolute (MAD, MSE, ...) or relative (MAPE, ...) metrics
- full probability distribution: a bit tricky

#### classification

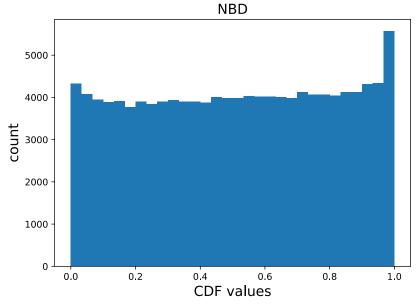


## Evaluation of PDF Predictions: Histogram of CDF Observations

individual prediction/observation:



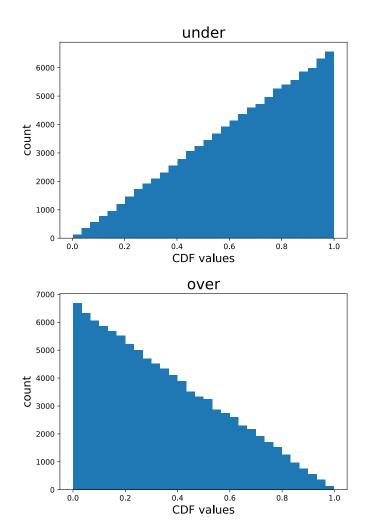
many (or all) predictions/observations:



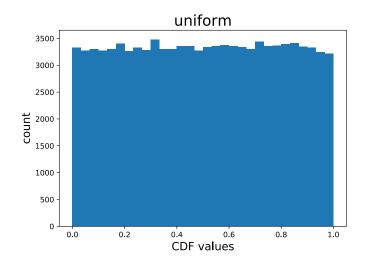
subtlety for discrete PDFs:

histogram filled using random numbers according to the CDF intervals (e.g., for 3 actual sales: random pick between discrete CDF values for 2 and 3)

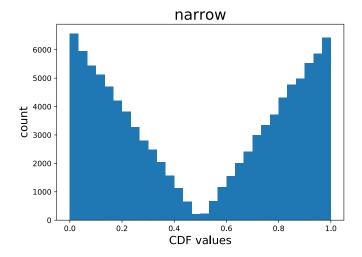
## Interpretation of CDF Histogram

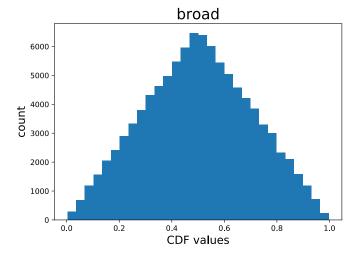






quantitative evaluation: measure deviation from uniform distribution (e.g., earth mover's distance)





## Replenishment

loss: deviation between predicted value and truth

- 1. demand forecasts in form of full, individual probability distributions
- 2. order proposals by individually choosing the quantile minimizing expected costs (scaled losses)

simplistic: **order quantity = upcoming demand - current inventory** (ignoring delivery lead times and shrinkage beyond demand, e.g., waste)

potential add-on: (probabilistic) inventory estimation

assumption for two-step approach: demand (not sales) not affected by subsequent action of ordering

In fact, stock level can have small effects on demand. For example, full shelves might increase demand.

## Need for Probability Distributions instead of mere Point Estimators

#### one best (usually different) quantile for each (out-of-sample) error measure

examples for error measures and their optimal point estimators:

- mean squared error (MSE) optimized by mean
- mean absolute error/deviation (MAD) optimized by median

but usually **individual cost function** for each product (possibly even for different dates of one product),

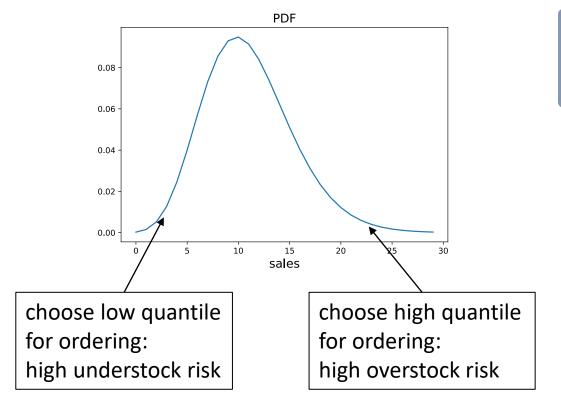
individual, optimal quantile as point estimator

#### possible approaches:

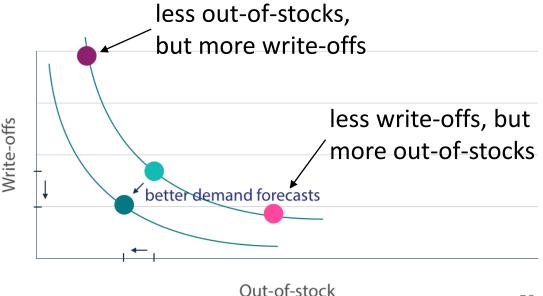
- many quantile regressions: for each individual, optimal point estimator use corresponding loss function
- full, individual probability distributions, i.e., probability density functions (PDF) for the continuous case

# Order Optimization

costs refer to scaled demand losses: assign costs to out-of-stocks (lost sales), write-offs (waste), ... → full **multi-dimensional cost function** as sum of different costs



complete cost functions often not available in practice → simulate impact of quantile choice on different KPIs (by means of full PDF predictions)



# Demand Shaping: ML and Causality

## 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  $\rightarrow$  need for asymmetric mathematical language

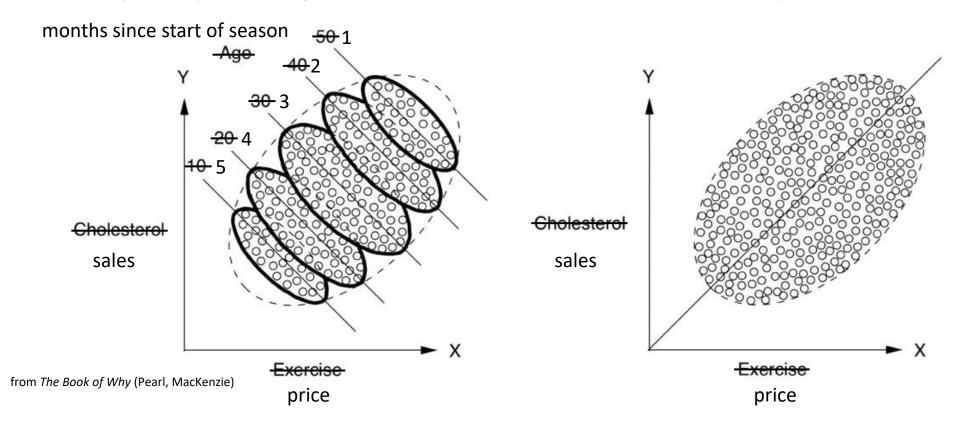
## The Ladder of Causation

	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?

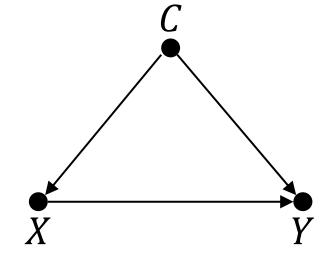


# Confounding

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

$$X \leftarrow C \rightarrow Y$$

 $\rightarrow$  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)

# Confounders for Pricing

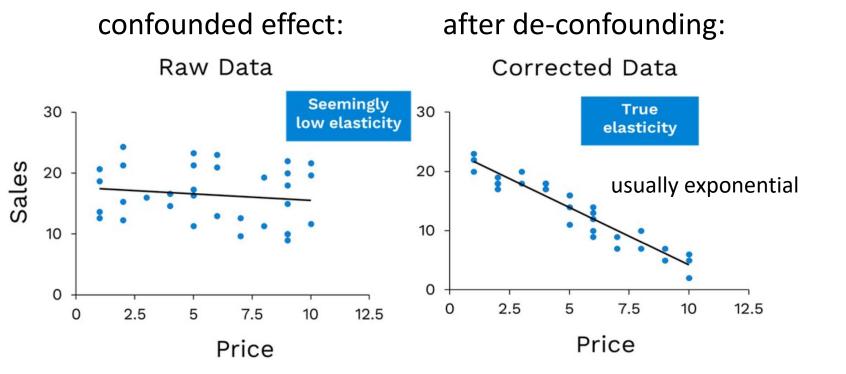
price setting for a product can be considered a demand shaping method the idea is a causal effect: lower price leads to higher demand

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

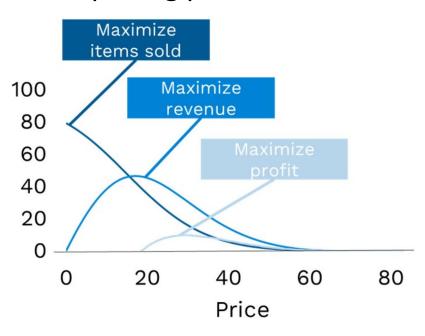
problem: confounders influencing both pricing in past (obverved) data and demand, e.g., lowering prices on weekends only for grocery or lowering prices toward end of a season for fashion (most sales at beginning of season)

# Demand Shaping with Causal Inference

dynamic pricing: influencing demand of different products by price setting



use for pricing policies:



customer targeting: influence individual customer demand by sending coupons

## Counterfactuals

#### fundamental problem of causal inference:

only one realization: What happened? And what could have happened instead?

→ cannot observe different **potential outcomes (individual causal effect)** 

example for application of **causal what-if scenario**:

individual (e.g., per product-location-date combination) demand shaping via price setting

ML and data not enough to describe causal structure

→ need for causal assumptions as add-on to ML (going beyond curve fitting)

## Potential Outcomes with ML

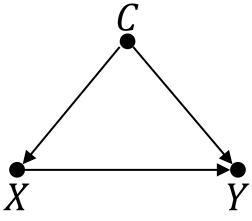
deconfounding

by RCTs or

independence weights (inverse propensity scores)

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

## 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):

$$P(Y|do(X)) \propto \sum_{c} \frac{P(Y|X,C=c)}{P(X|C=c)}$$

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)

alternative: A/B test