

Introduction and Overview

Traditional Algorithms vs ML

Understanding Machine Learning

goals of this course

- understanding of foundational ML concepts and commonalities between different methods
- ability to properly use ML for scientific or business problems

schedule of lectures

1. introduction and overview
2. statistical learning
3. non-linear models
4. generalization
5. deep learning
6. transformers
7. generative models
8. causality
9. reinforcement learning

AI/ML Overview

Main Areas of Artificial Intelligence

- **computer vision**
(spatial structures, state-of-the-art: Convolutional Neural Networks)
- **natural language processing**
(sequential structures, state-of-the-art: transformers)
- **automated decision making, robotics**
(reinforcement learning)

All of these are enabled by one key ingredient:

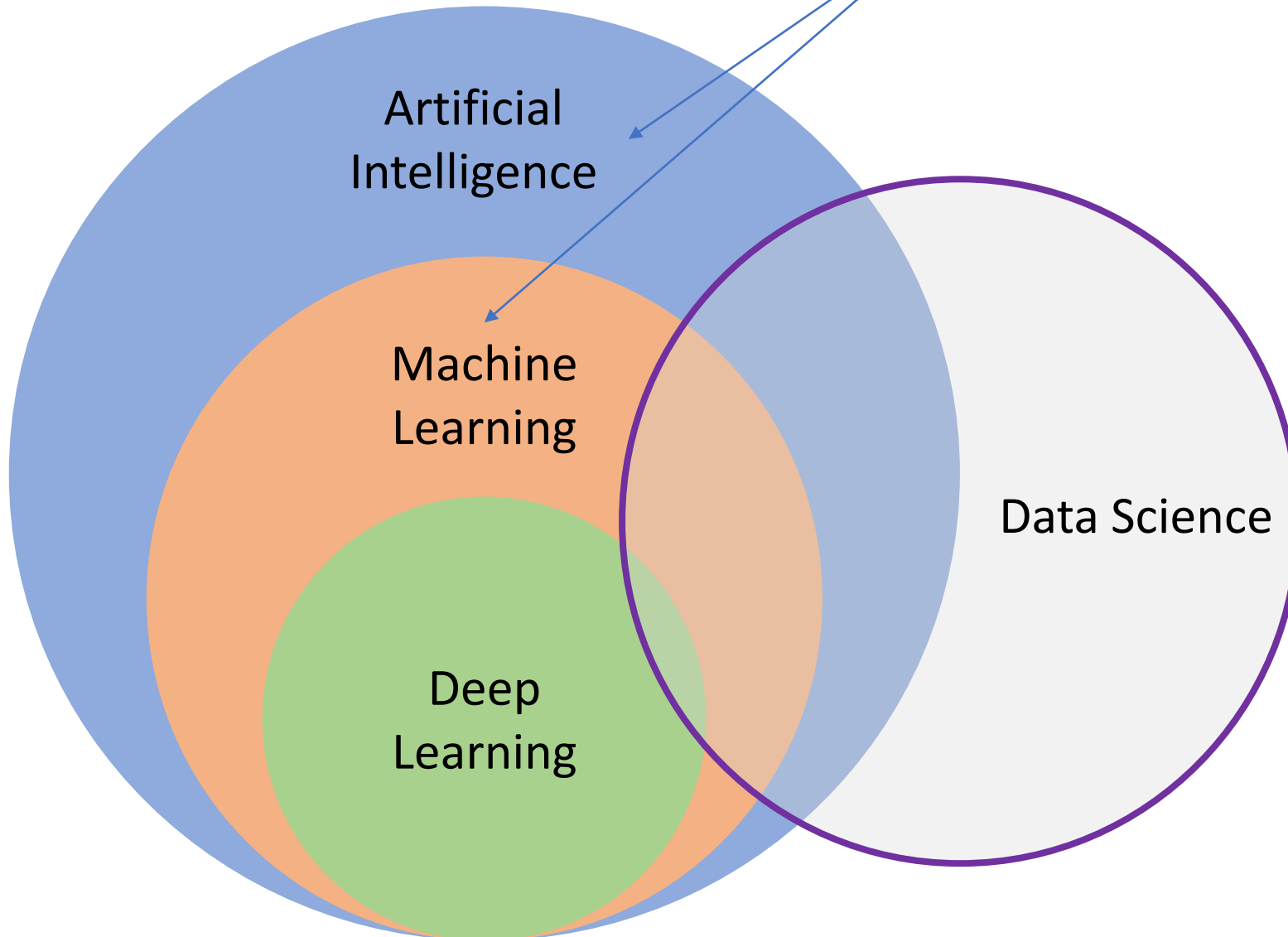
- *learning from experience* (**Machine Learning**)
- also: knowledge representation, automated reasoning (first indices in modern Large Language Models)



from wikipedia

agency:
perception – thought – action

Buzz Words ...



blend of diverse components from different domains
(statistics, optimization, computer science, ...)

Deep Learning:

special kind of ML
algorithms using (deep)
neural networks

Data Science:

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

Traditional Algorithms and GOFAI

traditional algorithms:

explicit (handcrafted) instructions for each situation

symbolic AI (aka GOFAI):

use knowledge by means of symbols (as representations), logic, search (e.g., expert systems like Deep Blue)

Public perception is changing over time: A modern chess program, nowadays disparaged as brute computing, would have been considered intelligent in the 50s.



from wikipedia

ML: Learning from Experience/Data

mainly exploiting statistical dependencies with the aim of **generalization** to new (e.g., future) data (compare with human reasoning by [analogies](#))

training (usually offline optimization):

ML algorithm + data = explicit algorithm (to be used at inference time)

→ reduction of complexity and much better generalizability compared to handcrafted algorithms

analogy: Humans do not hit the ground running (storage capacity of DNA limited) but have learning capabilities.

Hot Debate: Connectionism vs Symbolic AI

connectionists:

learn from (big) data without prior knowledge

symbolists:

use knowledge with only modest input data

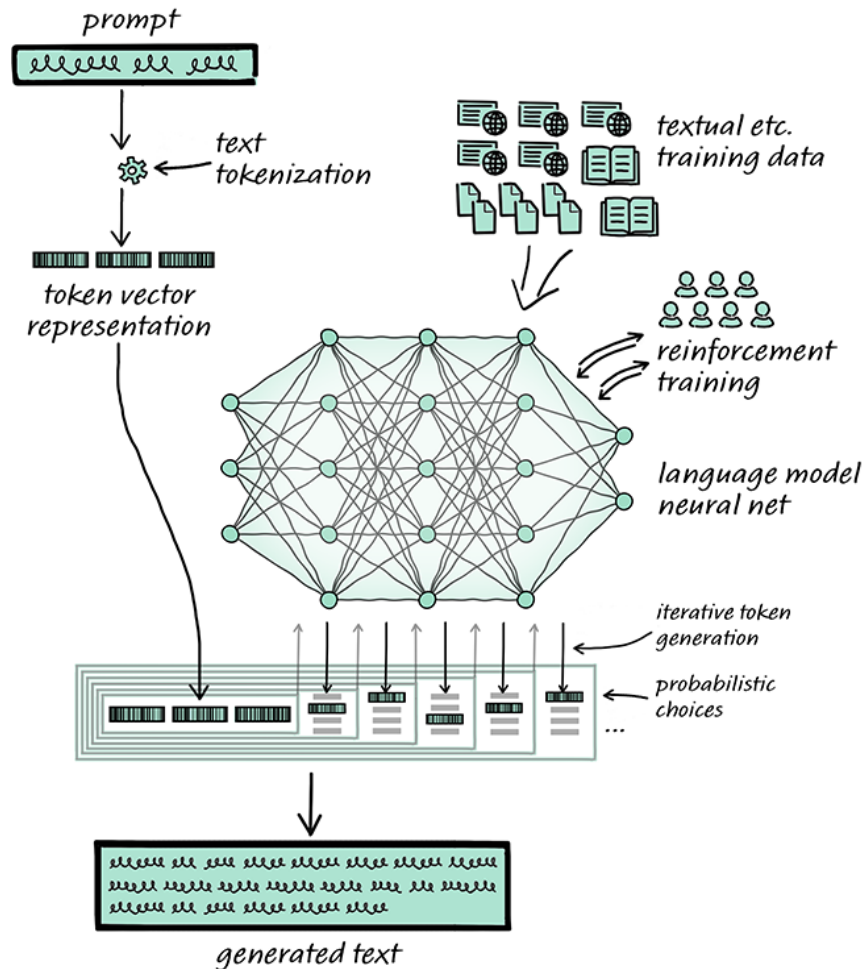
(crude) analogy: learning and evolution

philosophical: empiricist and rationalist schools of mind

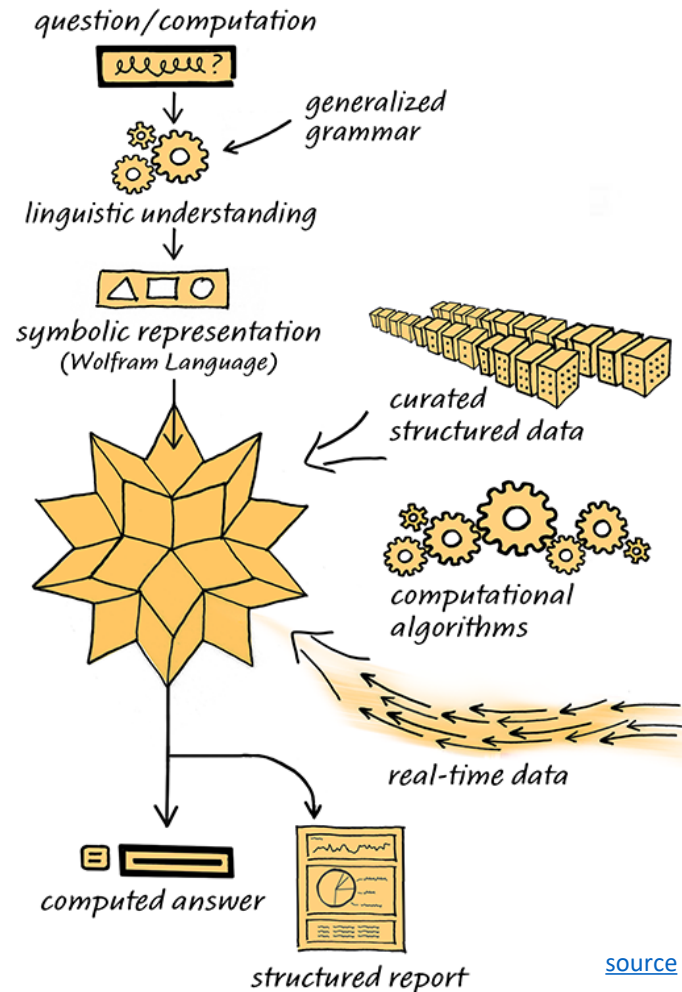
hybrid approaches often most successful (feature engineering for ML models also kind of symbolic knowledge representation)

Hybrid Approach for Language Models?

ChatGPT



Wolfram|Alpha



[AlphaGeometry](#)

tool usage:
[LangChain](#)

Supercharging the Scientific Method

use ML and data to replace or enhance explicit methods relying on detailed domain knowledge ([Software 2.0](#))

- overcome our evolutionary limitations in math with clever learning algorithms and collecting data
- immediate impact on many aspects of industry, business, and science, formulated as narrow tasks with strictly defined inputs (aka weak AI)

more imminent than (still philosophical) long-term quest for human-level AI (aka strong AI, AGI), i.e., general-purpose intelligence

(although recent language models show multi-purpose capabilities)

Most Famous Applications

recommendations



chatbots



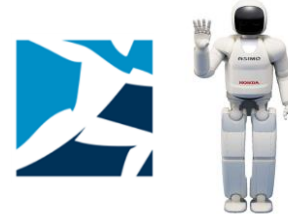
autonomous driving



translation



robotics



assistants (speech recognition)



OCR

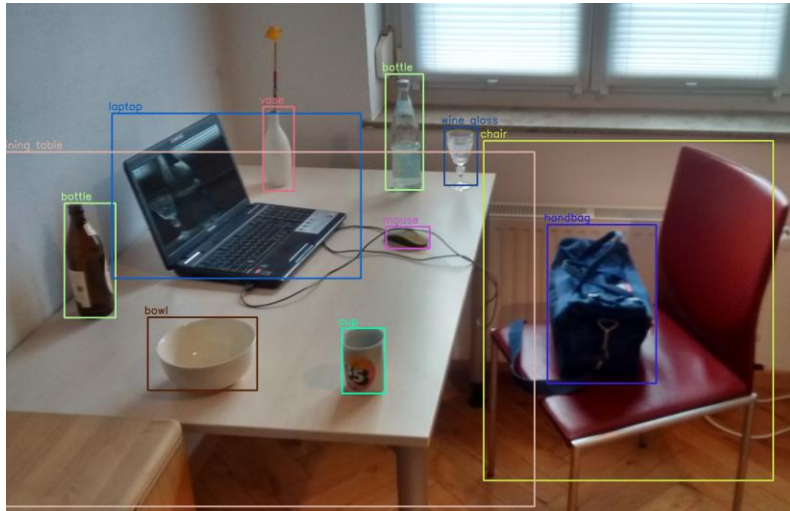


and many more ...

When to Use ML (= Learning from Data)

automation

too complex for rules



from wikipedia

examples: object recognition, all applications from previous slide

complexity / uncertainty

too complex for humans



examples: protein structure predictions (AlphaFold), demand forecasting

more scientific use cases: medicine (imaging, diagnosis, drug design), particle physics (analysis of collider experiments), material science (material properties and design of new materials), ...

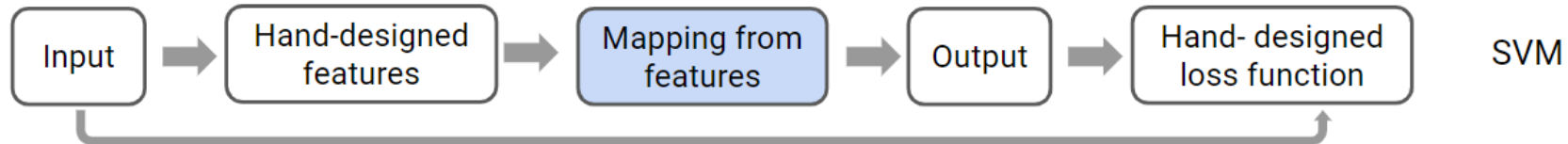
Ladder of Generalization

Rule-based systems

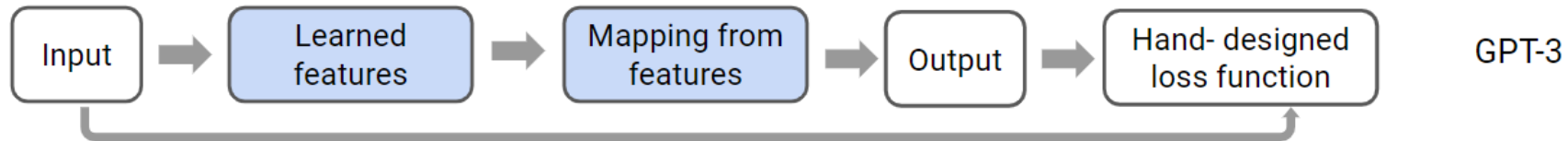


Learnable part of the system

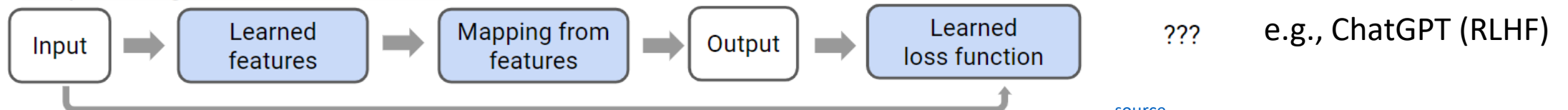
Classical machine learning



Deep learning: (self-)supervised learning



Deep learning: other RL formulations



[source](#)

Generative AI

more recently: generative applications

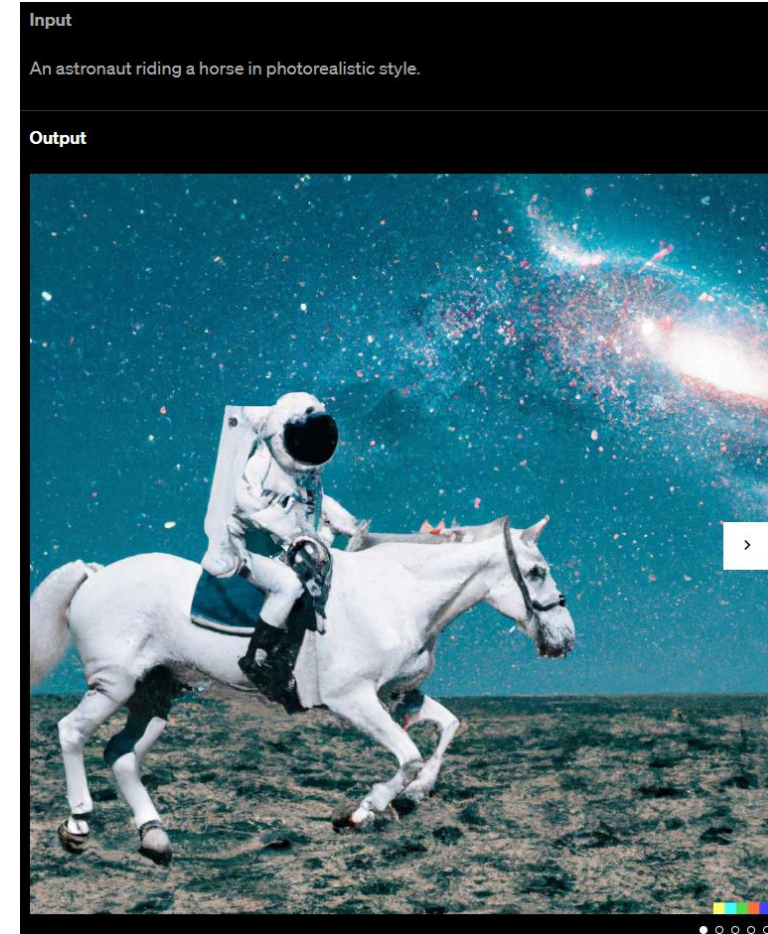
- rather than predictive (or discriminative) ones
- e.g., image generation, conversational AI, new proteins or materials

Depending on the application, there are currently two dominant approaches:

- text generation: large language models (transformer)
- image synthesis: diffusion models

up next: video synthesis → dynamics/physics understanding/simulation

example: DALL-E 2



Learning Paradigms

Supervised Learning

learning by teacher → usually rather narrow tasks (passive approach)

Target Quantity

- **known in training:** labeled samples or observations from past
- to be **predicted** for unknown cases (e.g., future values)

Features

input information that is

- correlated to target quantity
- known at prediction time



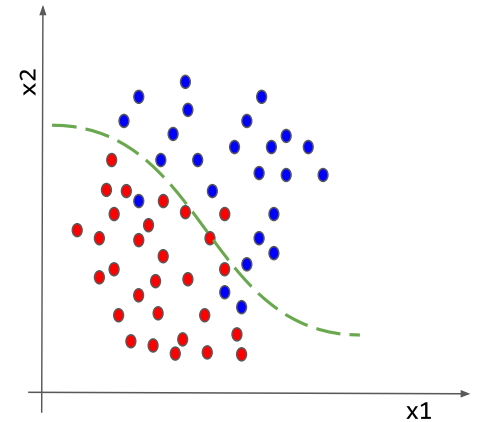
Example: Spam Filtering

Classify emails as spam or no spam

use accordingly **labeled**
emails as training set

use information like
occurrence of specific
words or email length
as **features**

features x_1 and x_2
spam, no spam



Reinforcement Learning

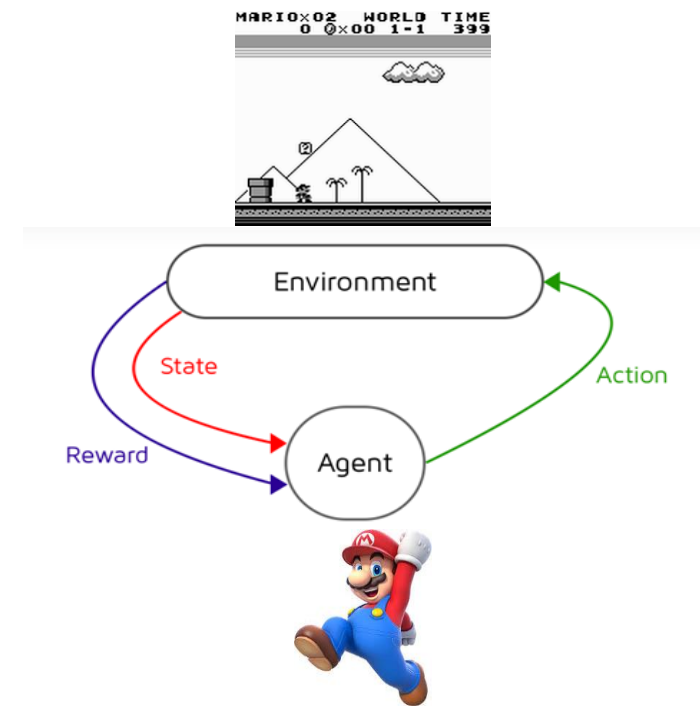
learning by trial-and-error (exploration and exploitation)

- goal-based approach → active and more generic than supervised learning (but sparse reward signals)
- receiving feedback from the environment, no supervision
- formalization of sequential decision making (delayed rewards)

corresponds to search for best action policy to reach a given goal (e.g., win a game)

using learning from examples (data) to guide the search

RL setup usually more difficult (e.g., non-differentiable as a whole) than supervised learning one but RL can be cast as supervised-learning setup: express rewards by more intricate loss function



Unsupervised Learning

learning by observation

no target information → kind of “vague” pattern recognition (but plenty of data)

can be cast as **self-supervised learning**:

- input-output mapping like supervised learning
- but generating labels itself from input information
- learning of semantic feature representations
- e.g., word2vec, BERT, GPT

generative AI as unsupervised learning: generate variations of training data

How Much Information is the Machine Given during Learning?

Y. LeCun

- ▶ “Pure” Reinforcement Learning (**cherry**)
 - ▶ The machine predicts a scalar reward given once in a while.
 - ▶ **A few bits for some samples**
- ▶ Supervised Learning (**icing**)
 - ▶ The machine predicts a category or a few numbers for each input
 - ▶ Predicting human-supplied data
 - ▶ **10→10,000 bits per sample**
- ▶ Self-Supervised Learning (**cake génoise**)
 - ▶ The machine predicts any part of its input for any observed part.
 - ▶ Predicts future frames in videos
 - ▶ **Millions of bits per sample**



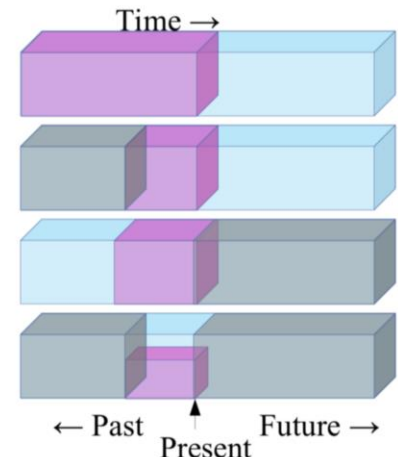
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Self-Supervised Learning

Y. LeCun

- ▶ Predict any part of the input from any other part.
- ▶ Predict the **future** from the **past**.
- ▶ Predict the **future** from the **recent past**.
- ▶ Predict the **past** from the **present**.
- ▶ Predict the **top** from the **bottom**.
- ▶ Predict the **occluded** from the **visible**
- ▶ **Pretend there is a part of the input you don't know and predict that.**



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Example for Unsupervised Learning

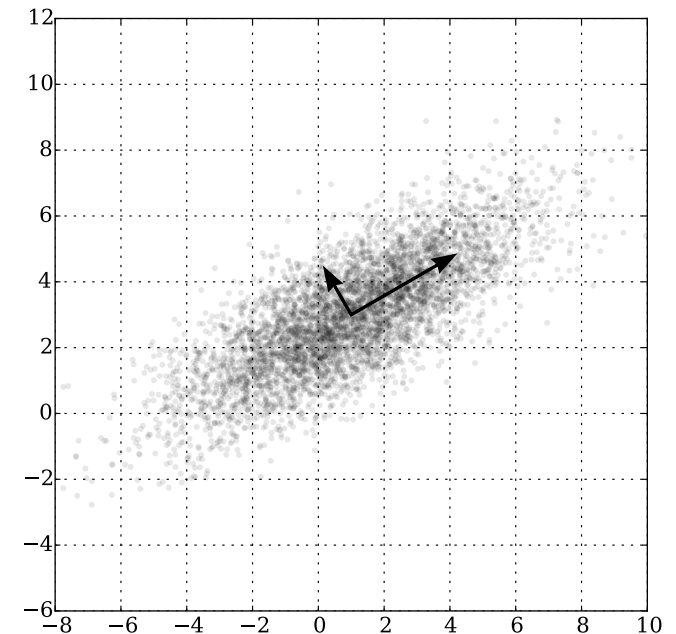
dimensionality reduction by principal component analysis (PCA)

using only first few principal components (eigenvectors of data's covariance matrix)

intuition: fitting p -dimensional ellipsoid to data

- axes representing principal components
 - large axis \rightarrow high variance, small axis \rightarrow low variance
 - successively choose directions of maximum variance
- \rightarrow account for as much variability (uniqueness) of data set as possible


often used as lower-dimensional features in other (supervised) methods



from wikipedia

Fitting / Statistical Learning

Notation

- random variable: X
 - vector of p random variables X_j (features): \mathbf{X}
 - observation of random variable X : x
 - matrix of n observations of p features x_{ij} : \mathbf{X}
 - vector of observations: \mathbf{x}
 - vector of n observations x_i : \mathbf{x}
 - vector of observation of p features x_j : \mathbf{x}
 - column vector: \mathbf{x}
 - row vector: \mathbf{x}^T
 - parameter: β
 - vector of parameters β_k : $\boldsymbol{\beta}$
 - probability that X takes on value x_0 : $P(X = x_0)$
 - probability distribution: $p(x) = P(X = x)$
- 
- design matrix

Supervised Learning Scenario

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

classification

- categorical target (e.g., image of cat or not $\rightarrow y = 0$ or $y = 1$)
- predict probability to belong to specific class

regression

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



... ML ...



ML domain:
no deterministic dependencies
between input and output

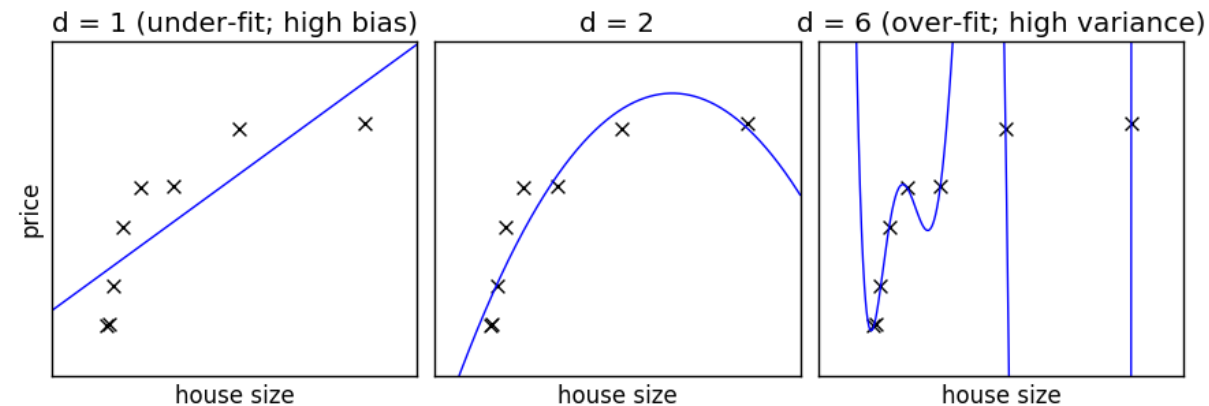
Curve Fitting / Parameter Estimation

fit train data set of (y_i, x_i) pairs

→ minimization of cost function

- e.g., least squares method, maximum likelihood estimation
- usually many dimensions (features X_j)

d: degree of fitted polynomial → number of parameters



from scikit-learn documentation

apply learned statistical dependencies from training to new test data set

different (y_i, x_i) pairs considered as random samples (whereby x values are taken for granted in discriminative models) of underlying data-generating process (i.i.d. assumption), for both train and test data sets

Generalization

generalization as core of ML:

empirical risk minimization (training error) as proxy for minimizing unknown population risk (test error, aka generalization error or out-of-sample error)

generalization gap: difference between test and training error

- **interpolation** to unencountered samples from training environment
- **extrapolation** to testing conditions differing from training environment (aka out-of-distribution)

curse of dimensionality: many features (dimensions) → lots of data needed to densely sample volume

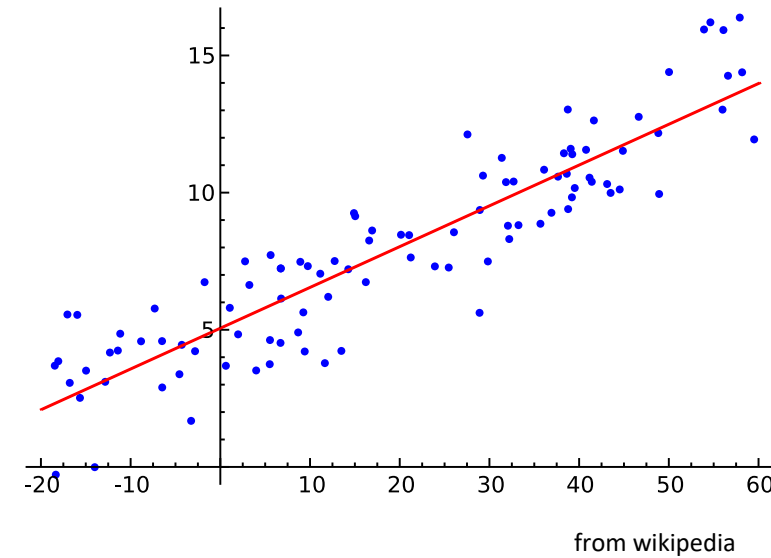
but reality is friendly: most high-dimensional data sets reside on lower-dimensional manifolds (manifold hypothesis) → enabling effectiveness of ML

→ need for appropriate **inductive bias** (different forms: model design, regularization, ...)

Generalized Linear Models (GLM)

Linear Regression

$$y_i = \alpha + \sum_{j=1}^p \beta_j x_{ij} + \varepsilon_i \quad (\text{model})$$



y : dependent variable / target

\mathbf{x} : p independent variables / features

$\alpha, \boldsymbol{\beta}$: $p + 1$ parameters

ε : error term / statistical noise

} vector (\mathbf{y}) or matrix (\mathbf{X}) of given data

→ to be fitted

reflects assumed data distribution (here: Gaussian with same variance σ^2 for all samples)

- \mathbf{X} and Y jointly distributed random variables

- $\hat{f}(\mathbf{x})$: predict, e.g., conditional mean of conditional density function $p(y|\mathbf{x})$

consider given \mathbf{x} values for this

↑
depending on used loss function

(conditional mean for squared loss of least squares method)

Linear Regression

fit: $\hat{f}(\mathbf{x}_i)$

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

predict:

Gaussian

$$\hat{y}_i = E[Y|\mathbf{X} = \mathbf{x}_i] = \hat{f}(\mathbf{x}_i) = \hat{\alpha} + \sum_{j=1}^p \hat{\beta}_j x_{ij}$$

$$p(y|\mathbf{x}_i) = \mathcal{N}(y; \hat{y}_i, \hat{\sigma}^2)$$

Gaussian

mean

variance

to be estimated:

- $\hat{\alpha}, \hat{\beta}$

$$\rightarrow \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{f}(\mathbf{x}_i))^2$$

(approximating assumed true α, β, σ)

Multiplicative Model

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

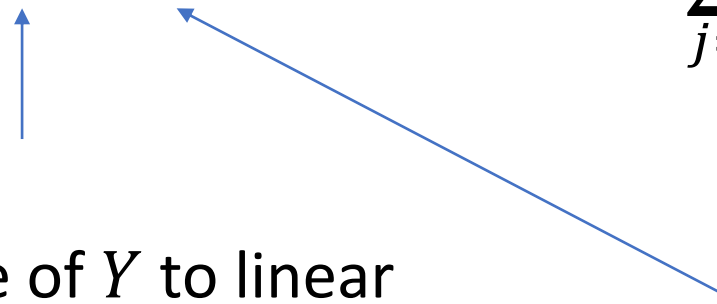
log-linear model (Gaussian errors in fit, Poisson with mean \hat{y}_i predicted):

$$\log(\underbrace{E[Y|\mathbf{X} = \mathbf{x}_i]}_{\hat{y}_i}) = \hat{\alpha} + \sum_{j=1}^p \hat{\beta}_j x_{ij}$$

↑
single parameter

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

Scheme of GLMs

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


link function g :

- linking range of Y to linear predictor
- canonical forms for different Y distributions (e.g., log for Poisson, identity for Gaussian → linear regression)

Y following probability distribution from exponential family (e.g., Poisson or Gaussian)

Classification: Logistic Regression

- predict probability p_i for $y = 1$ respectively $y = 0$ for each sample
- link function: logit (log-odds)
- Y following Bernoulli distribution

$$\begin{aligned}\text{logit}(E[Y|\mathbf{X} = \mathbf{x}_i]) &= \ln\left(\frac{p_i}{1 - p_i}\right) \\ &= \hat{\alpha} + \sum_{j=1}^p \hat{\beta}_j x_{ij}\end{aligned}$$

Toward Non-Linear Models

Generalized Additive Models (GAM)

blending of GLMs and additive models

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

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., \mathbf{X}_3 and \mathbf{X}_4

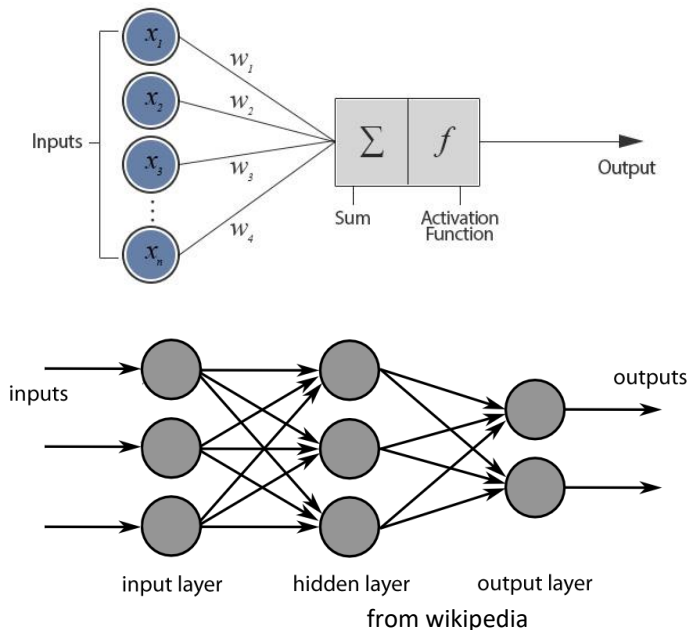
[Cyclic Boosting](#)

Algorithmic Families and Linear Building Blocks

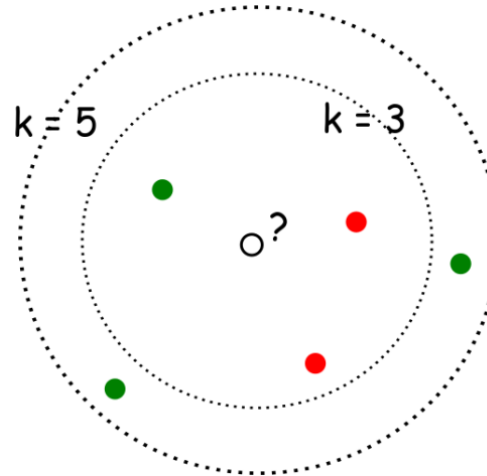
linear (parametric) models

- linear regression
- GLM
- GAM

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



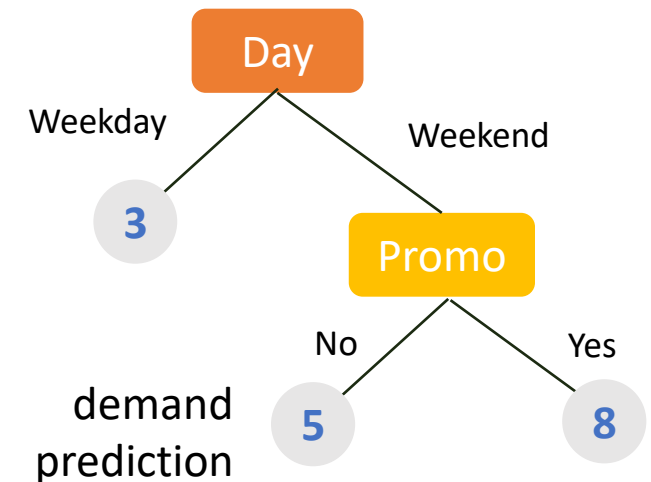
nearest neighbors (local methods, instance-based learning) – non-parametric models



with $k=3$, ●
with $k=5$, ●

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

decision trees: rule learning



often used in ensemble methods

- bagging: random forests
- boosting: gradient boosting

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.

(need to find method with best inductive bias for the task at hand → generalization capability)

ML Workflow

Modeling

extract features

- help the ML algorithm to better understand the data
- impose assumptions hard to discover in the raw data

choose ML algorithm

- from open-source libraries like scikit-learn or pytorch, rarely write an own one
- many different algorithms available, differently suited for given task

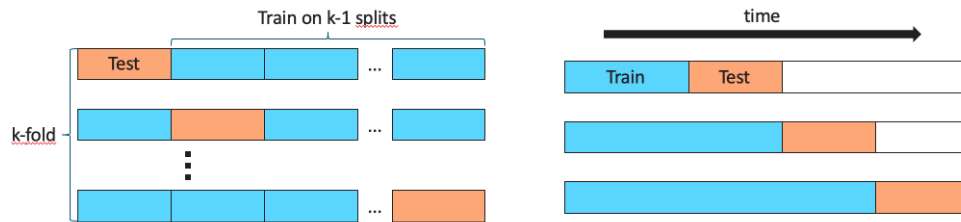
execute hyperparameter tuning

- variety of different forms
- model settings not all automatically adjusted by the machine

Evaluation

test structure

cross-validation



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

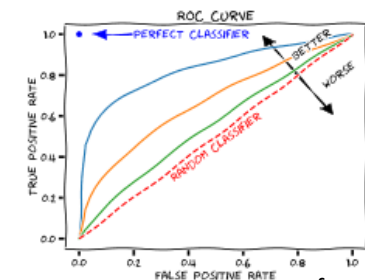
measure (out-of-sample) accuracy of predictions
(loss function in training as proxy of this)

regression

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

classification

ROC curve (true and false positive rates)



MACHINE LEARNING

training target available
(labeled or past data)

SUPERVISED

CLASSIFICATION



REGRESSION

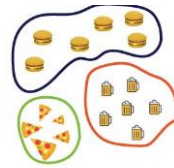


learning by teacher
(high-dimensional curve fitting)

data not labeled
in any way

UNSUPERVISED

CLUSTERING

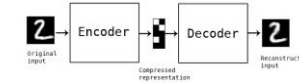
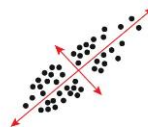


GENERATIVE MODELS

ASSOCIATION



DIMENSIONALITY REDUCTION



learning by observation
(pattern recognition)

no supervision, but goal-based
interaction with environment

REINFORCEMENT LEARNING

LEARN STATE OR ACTION VALUES

LEARN POLICY DIRECTLY

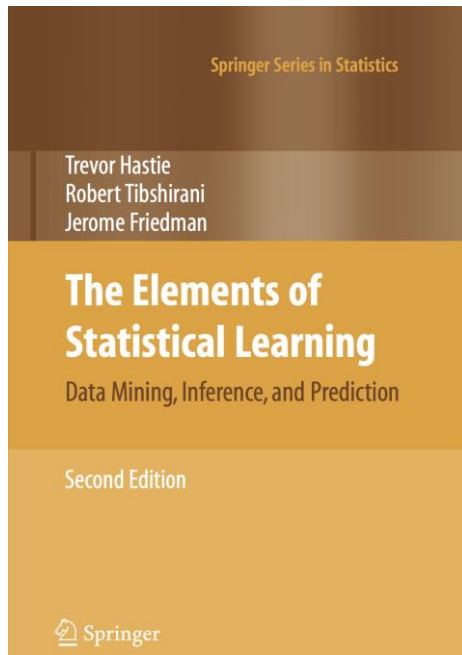


learning by trial-and-error
(sequential decision making)

unsupervised and reinforcement learning can
both be cast as supervised-learning setup

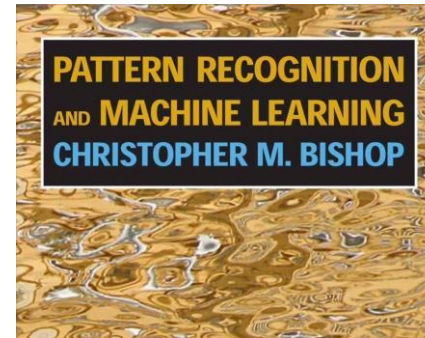
Literature

nice book on the foundations of ML
(relevant for the whole course):

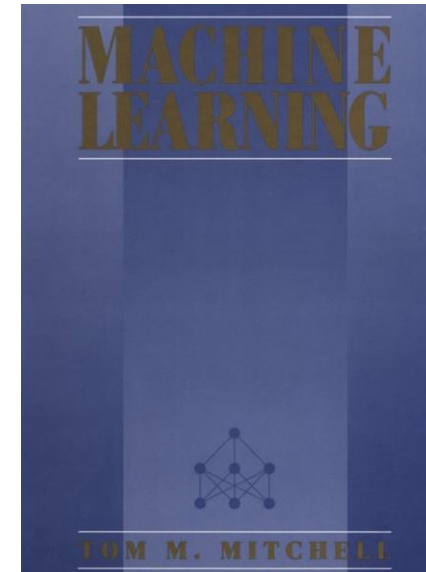


[Hastie](#)

other general overviews:



[Bishop](#)



[Mitchell](#)

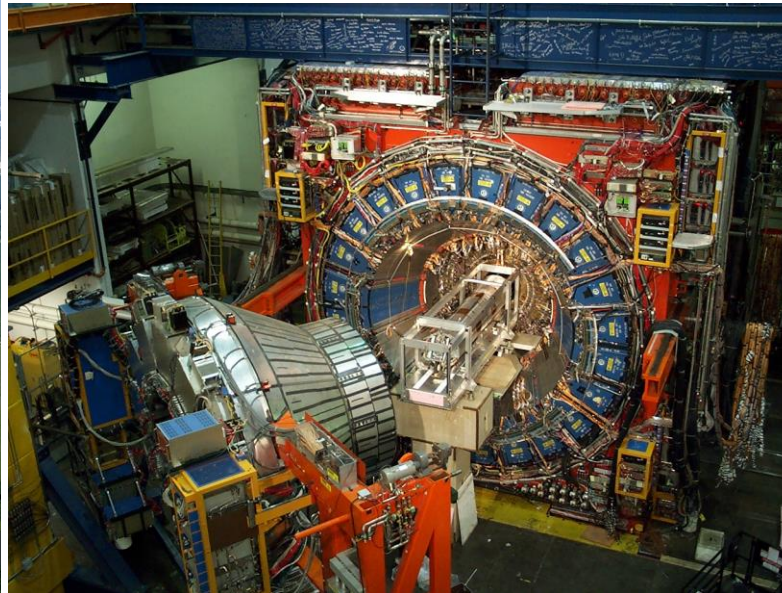
Scientific Application: ML in Particle Physics

example: classification of decay signatures in particle colliders

Tevatron accelerator at Fermilab



CDF detector at Tevatron



charmed baryon signals filtered out of background

