Machine Learning

Lecture 1

Introduction to Machine Learning

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2023-2024

Content

Content

Organization

Information about the course in **Aula Global**

- Teachers contact
- Course description
- Homework
- Evaluation

Objective

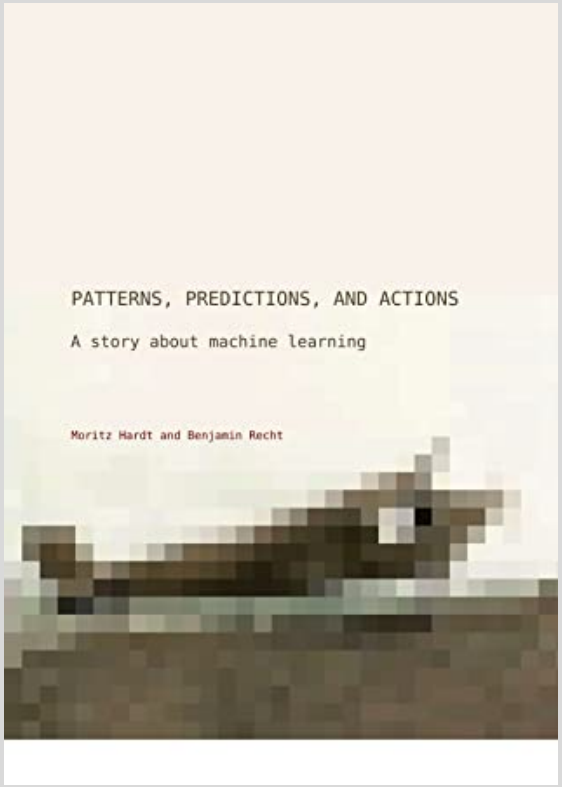
- Understand the mathematical principles of machine learning
- Solve mathematical exercises related to machine learning theory
- Recognize different types of machine learning problem
- Choose and implement appropriate machine learning algorithms
- Evaluate learning outcome and compare different algorithms
- Select appropriate values of hyperparameters through validation

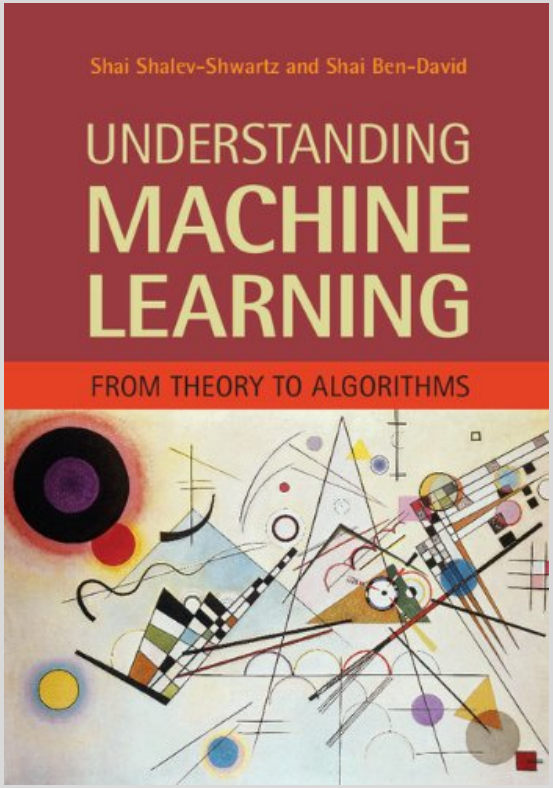
Prerequisites

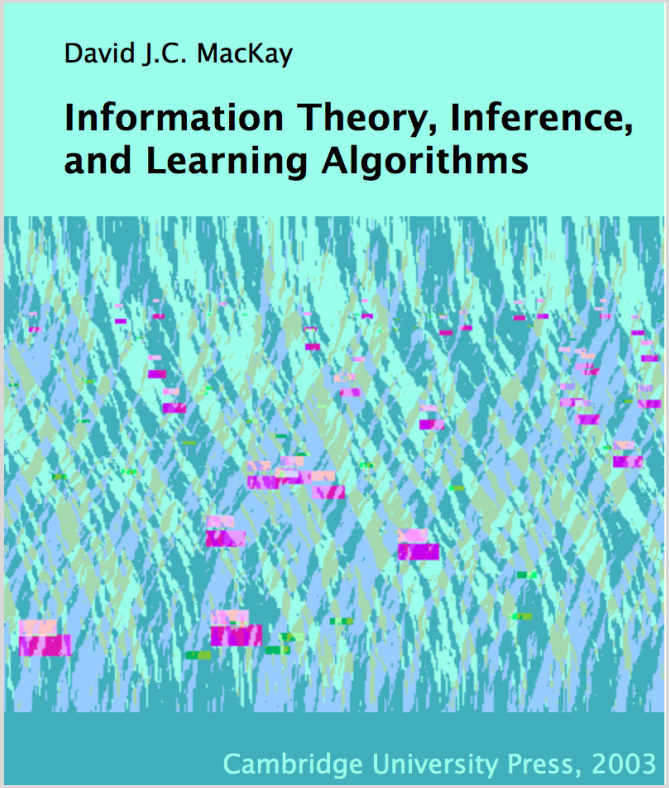
Students are expected to have basic knowledge in these topics:

- Linear algebra
- Calculus
- Probability theory/statistics

Books


PATTERNS, PREDICTIONS, AND ACTIONS
A story about machine learning
Moritz Hardt and Benjamin Recht


Shai Shalev-Shwartz and Shai Ben-David
UNDERSTANDING
MACHINE
LEARNING
FROM THEORY TO ALGORITHMS


David J.C. MacKay
Information Theory, Inference,
and Learning Algorithms
Cambridge University Press, 2003

Content

Definition of machine learning

From Wikipedia: “Machine learning algorithms build a model based on sample data [...] in order to make predictions or decisions without being explicitly programmed to do so.”

Machine learning problems

In which of the following problems can machine learning help?

- Predict on which weekday the next market crash will occur
- Classify an email as spam or not spam
- Find the shortest path between two nodes in a graph
- Recognize cancerous cells in the X-ray image of a patient
- Guess when the next world-wide pandemia will occur

Characteristics of machine learning problems

- There exists an underlying pattern that we can exploit
- Describing (or programming) the pattern is difficult
- However, one can obtain many observations (data) of the pattern
- Machine learning algorithms can learn the pattern (or an approximation) from data

Machine learning problems

In which of the following problems can machine learning help?

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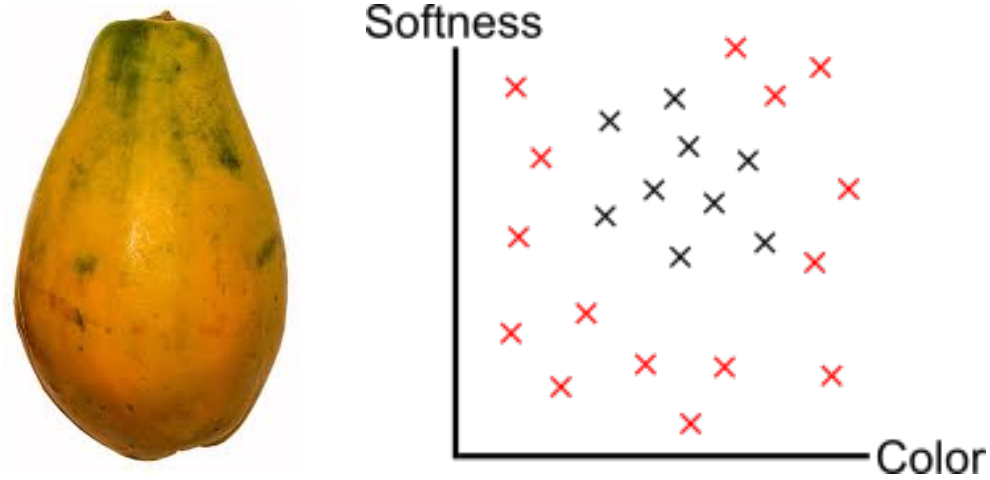
Intuition

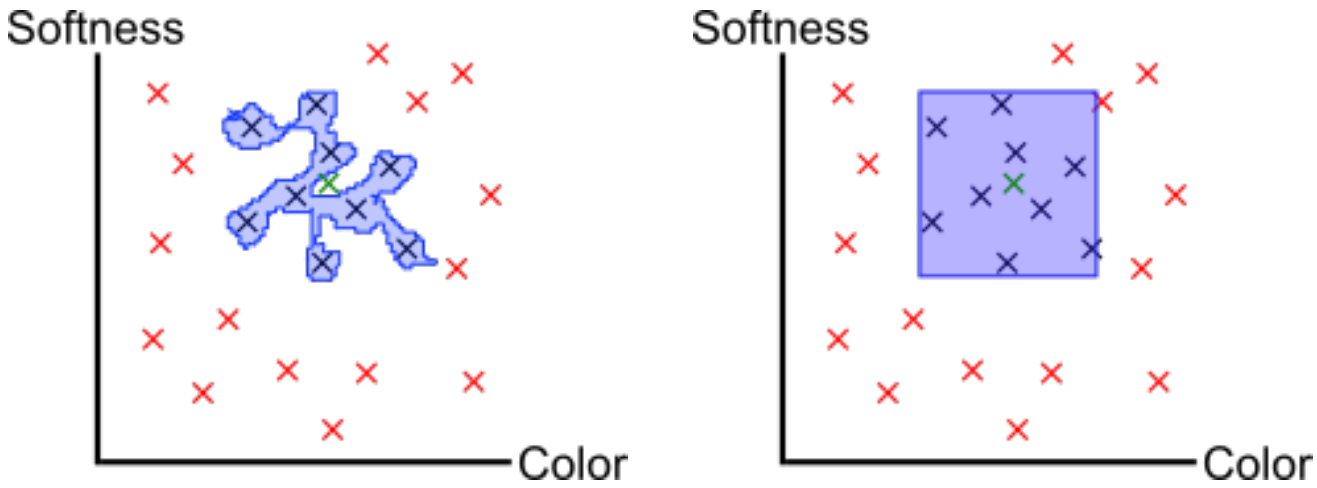
- There exists a set of objects or concepts that we want to analyze
- Key assumption: objects of the same type have similar features
- If this assumption does not hold, learning is hopeless

Example [Understanding Machine Learning]



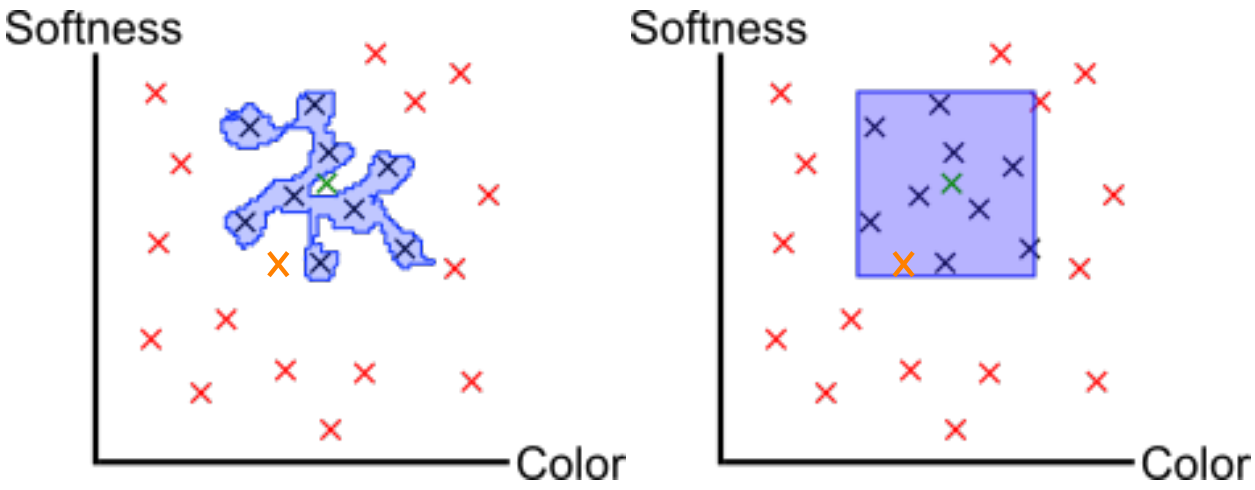
- Papayas can be described by two features: softness and color
- Papayas are either tasty (x) or not tasty (x)
- We can obtain many observations of papayas: softness, color, and tastiness

Example (cont.)



- Machine learning algorithms attempt to find a pattern that explains the relationship between features (softness, color) and label (tastiness)
- Many possible patterns exist for explaining this relationship!

Prediction



- Given an unseen papaya (x), predict whether or not it is tasty
- Record features (softness, color) and use pattern model to predict tastiness
- Prediction depends on model! Need a way to measure performance of models

Areas of machine learning

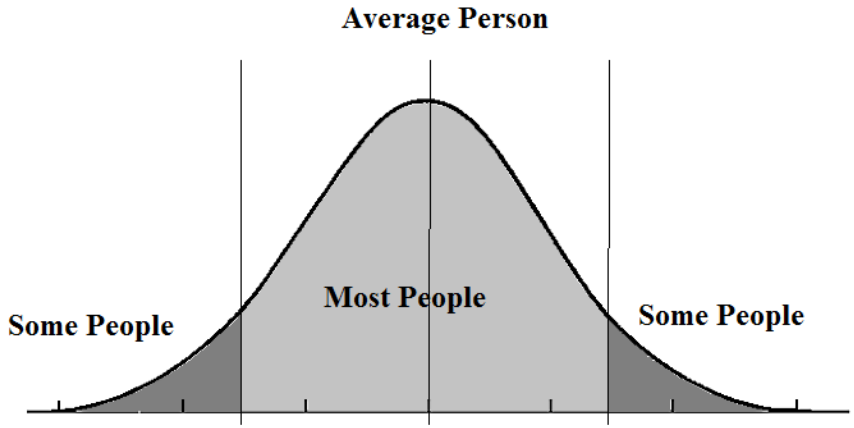
- Supervised learning: data contains (feature,label) pairs, objective is to predict target for unseen examples
- Unsupervised learning: data only contains feature examples, objective is to find patterns in features
- Reinforcement learning: algorithms can perform actions that modify features, objective is to perform actions that maximize long-term reward

Content

Domain set

- Assume that there exists a set of features $\mathcal{X}^1, \ldots, \mathcal{X}^d$
- Objects or concepts are described by feature vectors $(x^1, \ldots, x^d)$
- An input is given by $x = (x^1, \ldots, x^d) \in \mathcal{X}^1 \times \cdots \times \mathcal{X}^d \equiv \mathcal{X}$
- $\mathcal{X}$ is called the domain set, input set, or sample space
- d is the number of dimensions, e.g. $d = 2$ in the papaya example

Input distribution



- Not all inputs are equally likely
- Assume that inputs follow a probability distribution $\mathcal{D}$
- We can sample an input $x \sim \mathcal{D}$ from the probability distribution

Target set

- Target set (label space) $\mathcal{Y}$ represents what we want to predict
- The machine learning problem depends on the form of $\mathcal{Y}$:

$\mathcal{Y} = \{c_1, \ldots, c_k\}$:	classification (target is a class)
$\mathcal{Y} = \mathbb{R}$:	regression (target is a real number)
$\mathcal{Y} = [0, 1]$:	logistic regression (target is a probability)

- For example, $\mathcal{Y} = \{\text{tasty}, \text{not tasty}\}$ in the papaya example

Labelling function

- The unknown pattern that we are trying to learn
- Mathematically, the pattern is a labelling function $f : \mathcal{X} \to \mathcal{Y}$
- For a given input $x \in \mathcal{X}$, the label is $y = f(x) \in \mathcal{Y}$
- In practice, labelling is noisy, and two identical inputs may have different labels

Training set

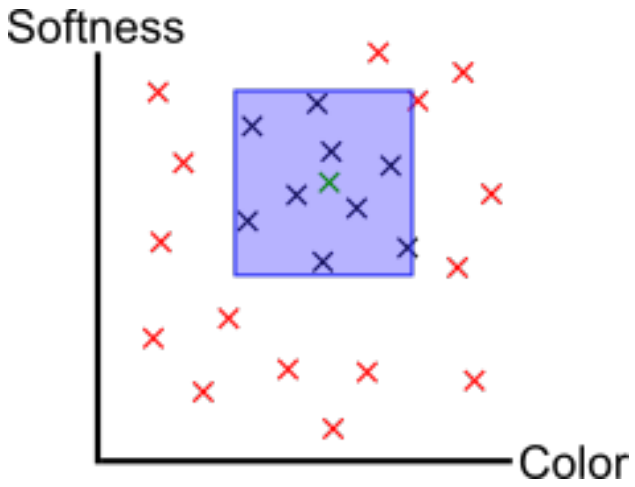
- Data is obtained by observing multiple labelled examples
- The result is a training set $S = ((x_1, y_1), \ldots, (x_m, y_m))$
- Each data point (x_i, y_i), $1 \leq i \leq m$, consists of an input $x_i \sim \mathcal{D}$ and a label $y_i = f(x_i)$
- Technically, S is a sequence and not a set, since two distinct data points (x_i, y_i) and (x_j, y_j), $1 \leq i < j \leq N$, may be identical
- Some algorithms process the data points in S sequentially

Supervised learning problem

To summarize, a supervised learning problem consists of:

- A domain set $\mathcal{X} = \mathcal{X}^1 \times \cdots \times \mathcal{X}^d$
- An unknown probability distribution $\mathcal{D}$ on $\mathcal{X}$
- A target set $\mathcal{Y}$
- An unknown labelling function $f : \mathcal{X} \to \mathcal{Y}$
- A training set $S = ((x_1, y_1), \ldots, (x_m, y_m))$ sampled from $\mathcal{D}$ and f

Hypothesis class



- Since the space of functions is enormous, the learner usually restricts the space of candidate functions
- Hypothesis class $\mathcal{H}$: set of functions considered by the learner
- Each hypothesis $h \in \mathcal{H}$ is a function from $\mathcal{X}$ to $\mathcal{Y}$, i.e. $h : \mathcal{X} \to \mathcal{Y}$
- Papaya example: set of rectangles in two dimensions

Loss function

- Need a way to measure the performance of a hypothesis $h \in \mathcal{H}$
- Loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$: measures the error between a prediction $\hat{y}$ and the true label y
- Loss is a (non-negative) cost: lower is better
- Many different loss functions exist
  - Classification or 0-1 loss: $\ell(\hat{y}, y) = [\![\hat{y} \neq y]\!]$
  - Squared loss: $\ell(\hat{y}, y) = (\hat{y} - y)^2$

True loss vs. training loss

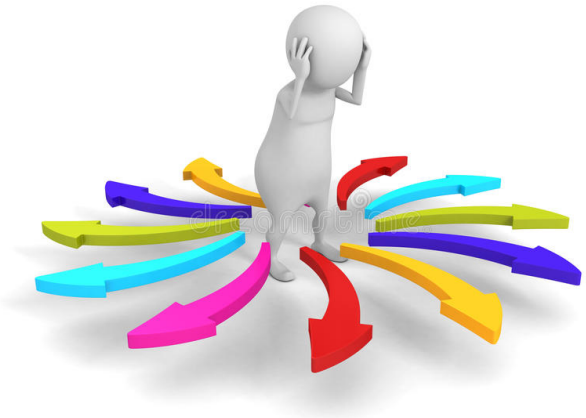
- Loss can measure the performance of a hypothesis $h \in \mathcal{H}$
- True loss $L_{\mathcal{D},f}(h)$, also known as generalization error or risk, measures the mistakes of h on the entire domain set $\mathcal{X}$

$$L_{\mathcal{D},f}(h) = \mathbb{E}_{x \sim \mathcal{D}} \left\{ \ell(h(x), f(x)) \right\}$$

- Training loss $L_S(h)$, also known as empirical risk, measures the mistakes of h on the training set $S = ((x_1, y_1), \ldots, (x_m, y_m))$

$$L_S(h) = \frac{1}{m} \sum_{i=1}^{m} \ell(h(x_i), y_i)$$

Learning algorithm



- A learning algorithm should output a hypothesis $h \in \mathcal{H}$ that approximates f well
- We would like h to minimize the true loss $L_{\mathcal{D},f}(h)$
- However, $L_{\mathcal{D},f}(h)$ is unobservable since $\mathcal{D}$ and f are unknown

Empirical risk minimization

- Basic principle of supervised learning
- Given a hypothesis class $\mathcal{H}$ and a training set S, return the hypothesis that minimizes the empirical risk (i.e. training loss)
- Formally,

$$h_S = \mathrm{ERM}_{\mathcal{H}}(S) \in \arg\min_{h \in \mathcal{H}} L_S(h),$$

- Note that if $f \in \mathcal{H}$, $L_S(h_S) = 0$

Supervised learning

To summarize, given a supervised learning problem, the learner chooses the following:

- A hypothesis class $\mathcal{H}$ of candidate labelling functions
- A loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
- An algorithm $\mathcal{A}$ that minimizes the empirical risk

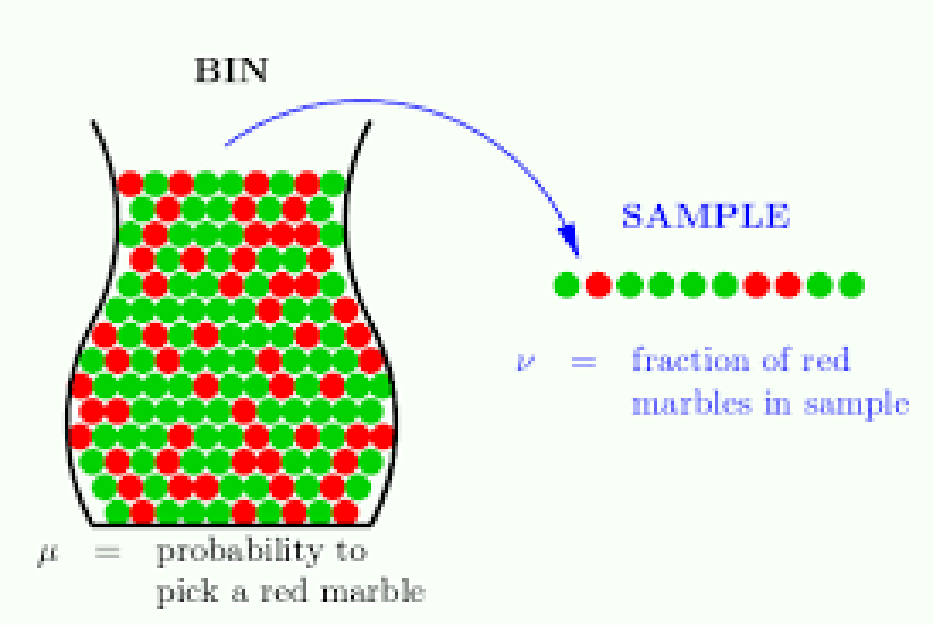
Generalization properties

- Trivially, we have

$$L_{\mathcal{D},f}(h) = L_S(h) + (L_{\mathcal{D},f}(h) - L_S(h))$$

- For a fixed $h \in \mathcal{H}$, how well does $L_S(h)$ approximate $L_{\mathcal{D},f}(h)$?
- Depends on quality of the training set $S = ((x_1, y_1), \ldots, (x_m, y_m))$
- If we are unlucky, $L_S(h)$ is not representative of $L_{\mathcal{D},f}(h)$
- With high probability, $L_S(h)$ approximates $L_{\mathcal{D},f}(h)$ well

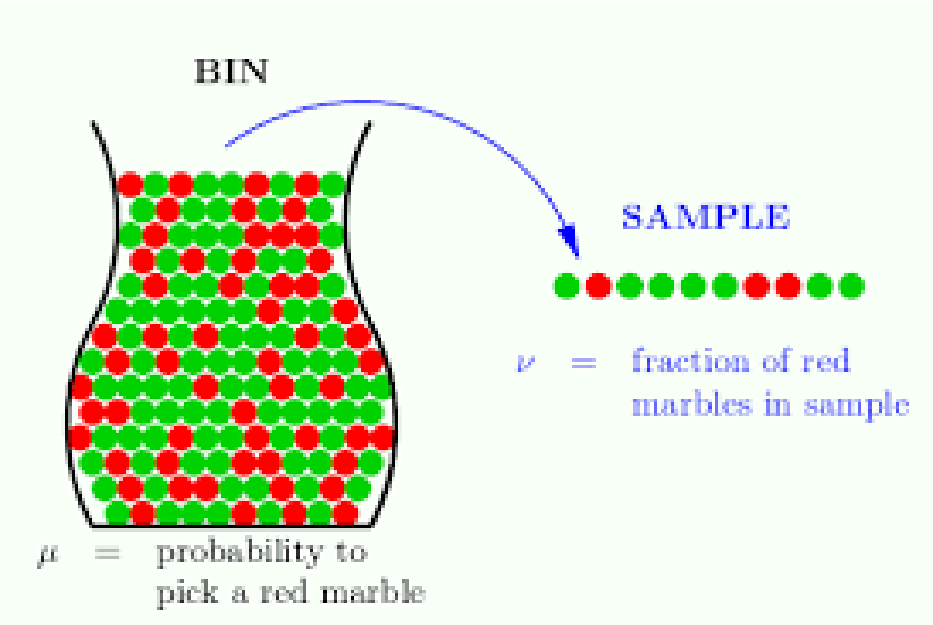
Bin analogy



- Large bin with red and green marbles, proportion red/green = μ
- Randomly pick m marbles, record proportion ν of red marbles
- Hoeffding's inequality (holds for any ϵ):

$$\mathbb{P}\left[|\nu - \mu| > \epsilon\right] \leq 2e^{-2m\epsilon^2}$$

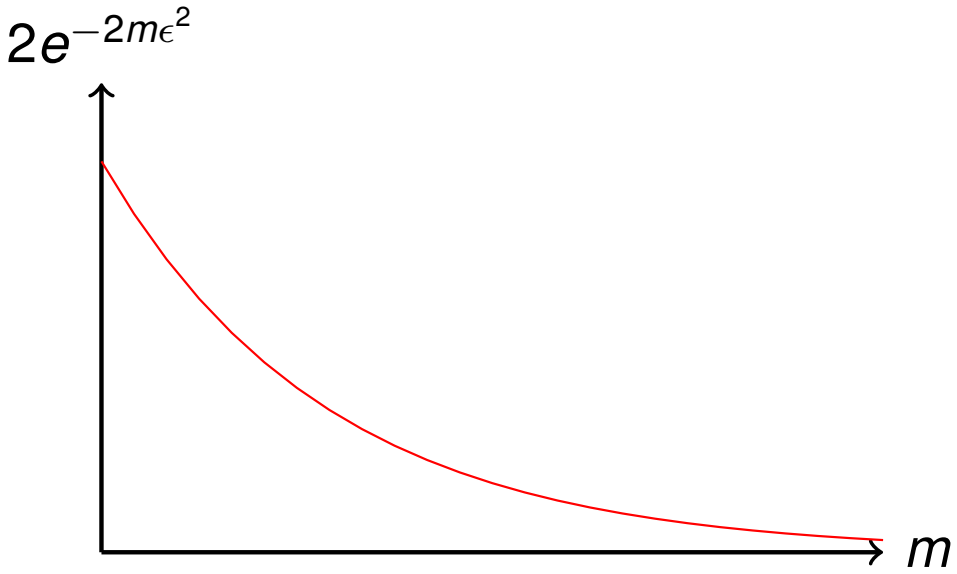
Bin analogy



- Marbles: inputs in $\mathcal{X}$, red: $h(x) \neq f(x)$, green: $h(x) = f(x)$
- Then $L_{\mathcal{D},f}(h) = \mu$, $L_S(h) = \nu$
- Hoeffding's inequality:

$$\mathbb{P}\left[|L_S(h) - L_{\mathcal{D},f}(h)| > \epsilon\right] \leq 2e^{-2m\epsilon^2}$$

Growth of upper bound



- Probability of S being bad decreases as a function of m

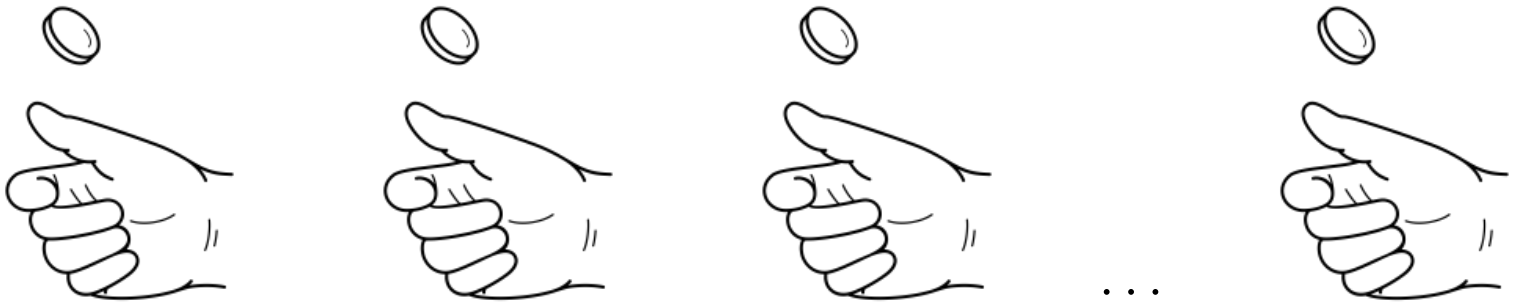
Generalization

- Empirical risk minimization returns a hypothesis

$$h_S = \mathrm{ERM}_{\mathcal{H}}(S) \in \arg\min_{h \in \mathcal{H}} L_S(h)$$

- How well does $L_S(h_S)$ approximate $L_{\mathcal{D},f}(h_S)$?
- Bias due to the fact that we select h with smallest $L_S(h)$

Coin flipping



- Assume that K people each flip a coin 10 times
- In expectation, each person will get 5 heads and 5 tails
- However, probability of getting 10 heads (or 10 tails) $\approx 0.1\%$
- Analogously, the h with smallest $L_S(h)$ may have been lucky

Generalization

- For each hypothesis $h \in \mathcal{H}$, bound the probability of S being bad

$$2e^{-2m\epsilon^2} + 2e^{-2m\epsilon^2} + \ldots + 2e^{-2m\epsilon^2}$$

- Union bound on Hoeffding's inequality yields

$$\mathbb{P}\left[|L_S(h_S) - L_{\mathcal{D},f}(h_S)| > \epsilon\right] \leq 2|\mathcal{H}|e^{-2m\epsilon^2}$$

Noisy labels

- In practice, two identical inputs may have different labels
- As an alternative to the labelling function f, we can model this as a conditional probability distribution $\mathbb{P}(y|x)$
- On input x, the label is y with probability $\mathbb{P}(y|x)$
- Even more compactly, we can define a joint probability distribution $\mathcal{D}$ on $\mathcal{X} \times \mathcal{Y}$ and sample data points $(x, y) \sim \mathcal{D}$

Content

Naïve empirical risk minimization

Empirical risk minimization

- For each hypothesis $h \in \mathcal{H}$, compute the loss $L_S(h)$
- Return hypothesis with smallest $L_S(h)$

Iterates over all hypotheses in $\mathcal{H}$ and all data points in S!

Online learning

- Process data points one at a time
- Update the candidate hypothesis after seeing each data point
- Sequential: order of the data points matter!
- For the moment, assume $|\mathcal{Y}| = 2$, $f \in \mathcal{H}$ and finite $|\mathcal{H}|$

Consistent learner

Consistent learner

- Initialize $\mathcal{H}_1 \leftarrow \mathcal{H}$
- For $t = 1, 2, \ldots$
  1. Get x_t
  2. Pick some $h \in \mathcal{H}_t$ and predict $h(x_t)$
  3. Get $y_t = f(x_t)$ and update $\mathcal{H}_{t+1} = \{h \in \mathcal{H}_t : h(x_t) = y_t\}$

Consistent learner

Theorem

The consistent learner will make at most $|\mathcal{H}| - 1$ *mistakes.*

Halving learner

Halving learner

- Initialize $\mathcal{H}_1 \leftarrow \mathcal{H}$
- For $t = 1, 2, \ldots$
  1. Get x_t
  2. Pick MAJORITY$(h(x_t) : h \in \mathcal{H}_t)$
  3. Get $y_t = f(x_t)$ and update $\mathcal{H}_{t+1} = \{h \in \mathcal{H}_t : h(x_t) = y_t\}$

Halving learner

Theorem

The halving learner will make at most $\log_2(|\mathcal{H}|)$ *mistakes.*

Halving learner

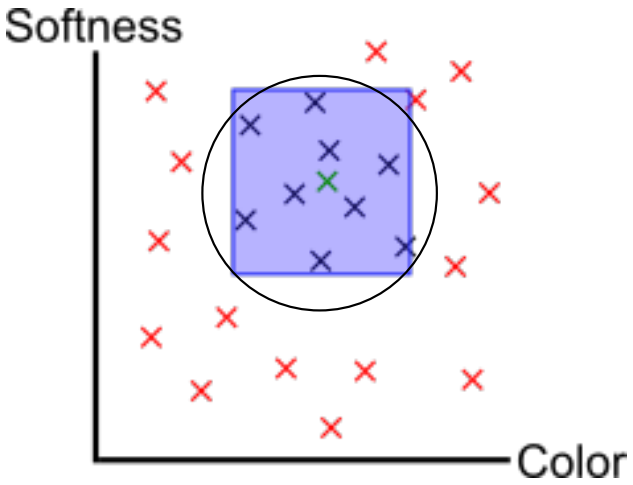
Advantages:

- Makes very few mistakes!
- No need to store a training set or compute a loss function

Disadvantages:

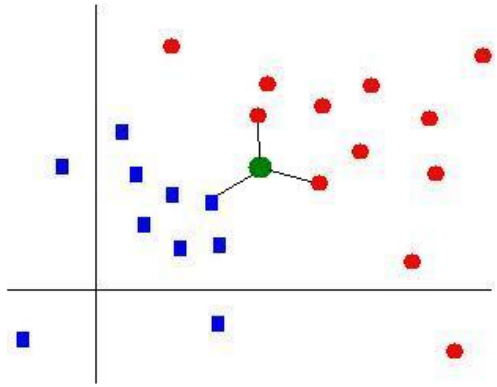
- Assumes $f \in \mathcal{H}$ (else we may exclude best hypothesis)
- In each time step, iterates over all hypotheses in $\mathcal{H}$!

Algorithmic properties



- We cannot always assume $f \in \mathcal{H}$ and $|\mathcal{H}|$ small (or even finite)
- Important that algorithms are computationally efficient
- Even minimizing the empirical risk is often expensive (NP-hard)
- Usually algorithms are specialized to the hypothesis class $\mathcal{H}$ and loss function ℓ

k nearest neighbors



- Assume that there exists a distance function $\rho : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
- Given $S = ((x_1, y_1), \ldots, (x_m, y_m))$ and $x \in \mathcal{X}$, let $\pi_1(x), \ldots, \pi_m(x)$ be a permutation of $1, \ldots, m$ according to their distance from x
- k nearest neighbors: make prediction based on the k nearest neighbors in S

k nearest neighbors

k nearest neighbors

- Get input x
- Return MAJORITY$(y_{\pi_i(x)} : i \leq k)$

No need for a hypothesis class or a loss function!

k nearest neighbors

Theorem

$$\mathbb{E}_{S\sim\mathcal{D},f}[L_{\mathcal{D},f}(h_S)] \leq 2L_{\mathcal{D},f}(h^*) + 4c\sqrt{d}m^{-\frac{1}{d+1}}$$

h^* is the optimal hypothesis

Constant c bounds how much f can change as a function of distance

Content

Consistent learner

Prove that the consistent learner makes at most $|\mathcal{H}| - 1$ mistakes

Consistent learner

- Initialize $\mathcal{H}_1 \leftarrow \mathcal{H}$
- For $t = 1, 2, \ldots$
  1. Get x_t
  2. Pick some $h \in \mathcal{H}_t$ and predict $h(x_t)$
  3. Get $y_t = f(x_t)$ and update $\mathcal{H}_{t+1} = \{h \in \mathcal{H}_t : h(x_t) = y_t\}$

Consistent learner

- Assume the algorithm makes a mistake in round t

Consistent learner

- Assume the algorithm makes a mistake in round t
- Then the hypothesis h used for prediction will not be part of $\mathcal{H}_{t+1}$

Consistent learner

- Assume the algorithm makes a mistake in round t
- Then the hypothesis h used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t| - 1$

Consistent learner

- Assume the algorithm makes a mistake in round t
- Then the hypothesis h used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t| - 1$
- After k mistakes, $|\mathcal{H}_t| \leq |\mathcal{H}| - k$

Consistent learner

- Assume the algorithm makes a mistake in round t
- Then the hypothesis h used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t| - 1$
- After k mistakes, $|\mathcal{H}_t| \leq |\mathcal{H}| - k$
- Since $f \in \mathcal{H}$ and f never makes mistakes, $|\mathcal{H}_t| \geq 1$ for each t

Consistent learner

- Assume the algorithm makes a mistake in round t
- Then the hypothesis h used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t| - 1$
- After k mistakes, $|\mathcal{H}_t| \leq |\mathcal{H}| - k$
- Since $f \in \mathcal{H}$ and f never makes mistakes, $|\mathcal{H}_t| \geq 1$ for each t
- Hence $|\mathcal{H}| - k \geq |\mathcal{H}_t| \geq 1$, which is equivalent to $k \leq |\mathcal{H}| - 1$

Halving learner

Prove that the halving learner makes at most $\log_2(|\mathcal{H}|)$ mistakes

Halving learner

- Initialize $\mathcal{H}_1 \leftarrow \mathcal{H}$
- For $t = 1, 2, \ldots$
  1. Get x_t
  2. Pick $\textsc{Majority}(h(x_t) : h \in \mathcal{H}_t)$
  3. Get $y_t = f(x_t)$ and update $\mathcal{H}_{t+1} = \{h \in \mathcal{H}_t : h(x_t) = y_t\}$

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Halving learner

- Assume the algorithm makes a mistake in round t
- Then the hypotheses used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t|/2$

Halving learner

- Assume the algorithm makes a mistake in round t
- Then the hypotheses used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t|/2$
- After k mistakes, $|\mathcal{H}_t| \leq |\mathcal{H}|/2^k$

Halving learner

- Assume the algorithm makes a mistake in round t
- Then the hypotheses used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t|/2$
- After k mistakes, $|\mathcal{H}_t| \leq |\mathcal{H}|/2^k$
- Since $|\mathcal{H}_t| \geq 1$ for all t, we have $|\mathcal{H}|/2^k \geq |\mathcal{H}_t| \geq 1$

Halving learner

- Assume the algorithm makes a mistake in round t
- Then the hypotheses used for prediction will not be part of $\mathcal{H}_{t+1}$
- It follows that $|\mathcal{H}_{t+1}| \leq |\mathcal{H}_t|/2$
- After k mistakes, $|\mathcal{H}_t| \leq |\mathcal{H}|/2^k$
- Since $|\mathcal{H}_t| \geq 1$ for all t, we have $|\mathcal{H}|/2^k \geq |\mathcal{H}_t| \geq 1$
- Solving for k yields $k \leq \log_2(|\mathcal{H}|)$

Memorizing predictor

Consider the following predictor (assuming $\mathcal{Y} = \{0, 1\}$)

Note that this predictor fails on any input x not in S such that $f(x) = 1$

Memorizing predictor

- Get x
- Return y_i if there exists (x_i, y_i) in S such that $x = x_i$, else 0

Show that there exists a polynomial p_S that determines the memorizing predictor by defining $h(x) = 1$ whenever $p_S(x) \geq 0$

Memorizing predictor

Make p_S equal to 0 in each data point (x_i, y_i) s.t. $y_i = 1$, else < 0

Memorizing predictor

Make p_S equal to 0 in each data point (x_i, y_i) s.t. $y_i = 1$, else < 0

For a single data point (x_1, y_1) such that $y_1 = 1$,

$$p_S(x) = -\|x - x_1\|^2$$

Memorizing predictor

Make p_S equal to 0 in each data point (x_i, y_i) s.t. $y_i = 1$, else < 0

For a single data point (x_1, y_1) such that $y_1 = 1$,

$$p_S(x) = -\|x - x_1\|^2$$

For multiple data points,

$$p_S(x) = -\prod_{i \in [m]: y_i = 1} \|x - x_i\|^2$$

Expected training loss

Fix some hypothesis $h \in \mathcal{H}$. Show that the expected value of $L_S(h)$ equals $L_{\mathcal{D},f}(h)$, i.e. that

$$\mathbb{E}_{S \sim \mathcal{D}}[L_S(h)] = L_{\mathcal{D},f}(h)$$

Expected training loss

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$$\begin{cases} \mathbb{E}_{S\sim\mathcal{D}}[L_S(h)] = \mathbb{E}_{S\sim\mathcal{D}}\left\{\dfrac{1}{m}\displaystyle\sum_{i=1}^{m}\ell(h(x_i), f(x_i))\right\} \\ \qquad\qquad = \dfrac{1}{m}\displaystyle\sum_{i=1}^{m}\mathbb{E}_{x_i\sim\mathcal{D}}\left\{\ell(h(x_i), f(x_i))\right\} \end{cases}$$

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\begin{cases}
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\end{cases}
$$