

COL866: Foundations of Data Science

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Machine Learning

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Generalization bounds

- One of the main tasks in Machine Learning is **classification**.
 - The goal is to **learn** a rule for labeling data (given a few labeled examples).
- The data comes from an **instance space** \mathcal{X} and typically $\mathcal{X} = \mathbb{R}^d$ or $\mathcal{X} = \{0, 1\}^d$.
- So, a data item is typically described by a d -dimensional **feature vector**.
 - For example in spam classification, the features could be the presence (or absence) of certain words.
- For performing the learning task, the learning algorithm is given a set S of *training examples* that are items from \mathcal{X} along with their correct classification.
- The main idea is **generalization**. That is, use one set of data to perform well on new data that the learning algorithm has not seen.

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- For performing the learning task, the learning algorithm is given a set S of *training examples* that are items from \mathcal{X} along with their correct classification.
- The main idea is **generalization**. That is, use one set of data to perform well on new data that the learning algorithm has not seen.
- The hope is that if the training data is **representative** of what the future data will look like, then we can try learning some **simple** rules that work for the training data and perhaps that will work well for the future data.

- Let us now try to formalize the ideas in the previous slide with respect to binary classification.
- Future data being **representative** of the training set:
 - There is a distribution D over the instance space \mathcal{X} .
 - Training set S consists of points drawn independently at random from D .
 - The new points are also drawn from D .
- A **target concept** w.r.t binary classification is simply a subset of $c^* \subseteq \mathcal{X}$ denoting the positive data items of the classification task.
- The learning algorithm's goal is to produce a set $h \subseteq \mathcal{X}$ called **hypothesis** that is close to c^* w.r.t. distribution D .
- The **true error** of hypothesis h is defined as $err_D(h) = \Pr[h \Delta c^*]$, where Δ denotes symmetric difference and the probability is over the distribution D .
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- In many learning scenarios, a hypothesis is not an arbitrary subset of \mathcal{X} but constrained to be a member of a **hypothesis class** (also called **concept class**) denoted by \mathcal{H} .
 - Consider example $\mathcal{X} = \{(-1, -1), (-1, 1), (1, -1), (1, 1)\}$ and \mathcal{H} consists of all subsets that can be formed using a *linear separator*. What is $|\mathcal{H}|$?

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- In many learning scenarios, a hypothesis is not an arbitrary subset of \mathcal{X} but constrained to be a member of a **hypothesis class** (also called **concept class**) denoted by \mathcal{H} .
- We would like to argue that for all $h \in \mathcal{H}$ the probability that there is a large gap between true error and training error is small.
 - Question: How large should S be the above to be true?

Theorem

Let \mathcal{H} be a hypothesis class and let $\varepsilon, \delta > 0$. If a training set S of size

$$n \geq \frac{1}{\varepsilon} (\ln |\mathcal{H}| + \ln 1/\delta),$$

is drawn from distribution D , then with probability at least $(1 - \delta)$ every $h \in \mathcal{H}$ with true error $\text{err}_D(h) \geq \varepsilon$ has training error $\text{err}_S(h) > 0$. Equivalently, with probability at least $(1 - \delta)$, every $h \in \mathcal{H}$ with training error 0 has true error at most ε .

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- The above result is called the **PAC-learning guarantee** since it states that if we can find an $h \in \mathcal{H}$ consistent with the sample, then this h is *Probably Approximately Correct*.
- What if we manage to find a hypothesis with small disagreement on the sample? Can we say that the hypothesis will have small true error?

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Theorem (Uniform convergence)

Let \mathcal{H} be a hypothesis class and let $\varepsilon, \delta > 0$. If a training set S of size

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- The above theorem essentially means that conditioned on S being sufficiently large, good performance on S will translate to good performance on D .

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- The above theorem follows from the following tail inequality.

Theorem (Chernoff-Hoeffding bound)

Let x_1, \dots, x_n be independent $\{0, 1\}$ random variables such that $\forall i, \Pr[x_i = 1] = p$. Let $s = \sum_{i=1}^n x_i$. For any $0 \leq \alpha \leq 1$,

$$\Pr[s/n > p + \alpha] \leq e^{-2n\alpha^2} \quad \text{and} \quad \Pr[s/n < p - \alpha] \leq e^{-2n\alpha^2}.$$

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- Let us do a case study of *Learning Disjunctions*.
- Consider a binary classification context where the instance space $\mathcal{X} = \{0, 1\}^d$.
- Suppose we believe that the target concept is a disjunction over a subset of features. For example, $c^* = \{x : x_1 \vee x_{10} \vee x_{50}\}$.
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- What is the size of the concept class \mathcal{H} ? $|\mathcal{H}| = 2^d$
- So, if the sample size $|S| = \frac{1}{\epsilon}(d \ln 2 + \ln(1/\delta))$ then good performance on the training set generalizes to the instance space.
- Question: Suppose the target concept is indeed a disjunction, then given any training set S is there an algorithm that can at least output a disjunction consistent with S .

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- What do we mean by a rule being simple?
- Different people may have different description languages for describing rules.
- How many rules can be described using fewer than b bits?

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- What do we mean by a rule being simple?
- Different people may have different description languages for describing rules.
- How many rules can be described using fewer than b bits? $< 2^b$

Theorem (Occam's razor)

Fix any description language, and consider a training sample S drawn from distribution D . With probability at least $(1 - \delta)$ any rule h consistent with S that can be described in this language using fewer than b bits will have $\text{err}_D(h) \leq \epsilon$ for $|S| = \frac{1}{\epsilon}(b \ln 2 + \ln(1/\delta))$. Equivalently, with probability at least $(1 - \delta)$ all rules that can be described in fewer than b bits will have $\text{err}_D(h) \leq \frac{b \ln(2) + \ln(1/\delta)}{|S|}$.

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- The theorem is valid irrespective of the description language.
- It does not say that complicated rules are bad.
- It suggests that Occam's rule is a good policy since simple rules are unlikely to fool us since there are not too many of them.

End