Machine Learning: Generalization 1

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Machine learning is about programming with data

- Minimizing a loss function on a data set produces a program.
- How do we know if the program is correct?

Correctness of classical programs

- A program is correct if it has the desired behavior on **all** input.
- Correctness is achieved through mathematical proofs and careful engineering.

Correctness of learned programs

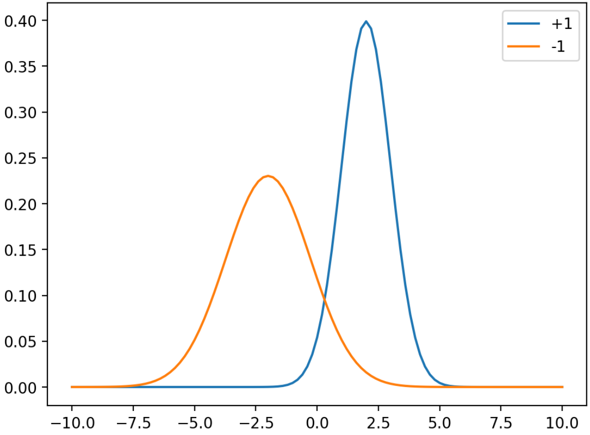
$$\boxed{\text{training set}} \xrightarrow{\text{training}} \text{classifier}$$

- Imagine we have trained a binary classifier.
- We know the loss on the training set.
- Even on the training set, the loss might not be 0.
- Can we say anything about the loss outside of the training set?
- Is it even possible? What assumptions do we need?

The big picture

- What is generalization? PAC learning and ERM
- When is generalization possible? Uniform convergence and VC dimension
- How to achieve generalization? Overfitting, underfitting, and regularization
- Generalization of neural networks. Universal approximation, overparameterization, and interpolation

What happens if the data is Gaussian?



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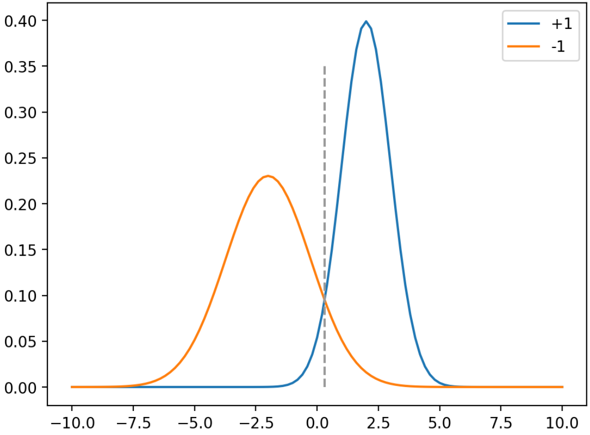

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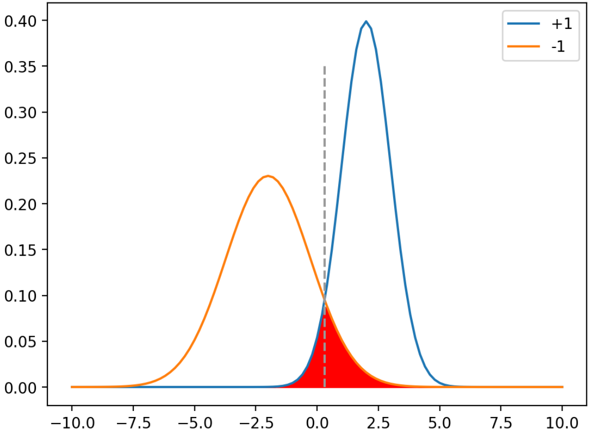

Gaussian data

- We need to know
  - the two distributions are Gaussian
  - their means
  - their variances.
- The decision boundary
  - can be found without training
  - is optimal (in the sense that no other boundary achieves a lower error).
- Next questions
  - What if we don't know the means?
  - What if we don't know the variances?
  - What if the two distributions are not Gaussian?
  - What if we don't know what the distributions are?

Generalization

Generalization

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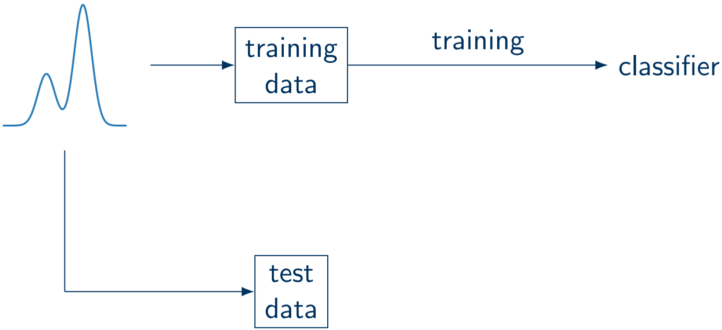
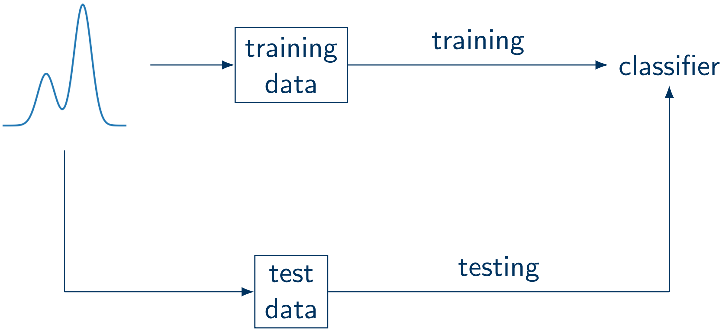


Generalization



Generalization

- A data set is said to be **i.i.d. (independent and identically distributed)** if the data points come from the same distribution and are statistially independent from each other.
- A function (or program) is said to **generalize** to data within a distribution if the function achieves a low error on data drawn from that distribution *in expectation*.
- In particular, if a function generalizes then the function has to achieve a low error on both the training set and the test set.
- We do not know the distribution, and only have data drawn from the distribution.
- The only assumption is i.i.d. data.

Generalization

- There exists a distribution $\mathcal{D}$ where both the training data and the test data are drawn from.
- The training set $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ includes i.i.d. samples drawn from $\mathcal{D}$.
- The **training error** for a loss ℓ and a program h is defined as

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

- If we have a test set S', then $L_{S'}(h)$ is the error on the test set (or test error for short) for a program h.

Generalization

- The **generalization error** for a program h is defined as

$$L_{\mathcal{D}}(h) = \mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(y, h(x))]. \tag{2}$$

- The test error $L_{S'}(h)$ of a program h is an estimate of the generalization error $L_{\mathcal{D}}(h)$.

$$\mathbb{E}_{S\sim\mathcal{D}^n}[L_S(h)] = \mathbb{E}_{S'\sim\mathcal{D}^{n'}}[L_{S'}(h)] = L_{\mathcal{D}}(h) \tag{3}$$

- The goal of learning is to find a program h with low generalization error $L_{\mathcal{D}}(h)$.

Learning algorithms and hypothesis classes

- A learning algorithm A is a function that takes a data set of size m and returns a function from the hypothesis class $\mathcal{H}$.

- A hypothesis class $\mathcal{H}$ is the set of possible programs of a particular form.

- For example, a linear classifier is $\mathcal{H} = \{x \mapsto w^\top x : w \in \mathbb{R}^d\}$.

Probably approximately correct

A hypothesis class $\mathcal{H}$ is PAC-learnable with a learning algorithm A if for any distribution $\mathcal{D}$, and any $\epsilon > 0$ and $0 \leq \delta \leq 1$, there exists $N > 0$ such that

$$\mathbb{P}_{S \sim \mathcal{D}^n}\left[L_{\mathcal{D}}(A(S)) - \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') > \epsilon\right] < \delta \tag{4}$$

for any $n \geq N$.

Probably approximately correct

- The data set S is is a random variable.
- $A(S)$ is a program returned by A after training on S.
- $L_{\mathcal{D}}(A(S))$ is also a random variable.
- $\min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h')$ is the best error we can achieve among all programs in $\mathcal{H}$.
- ϵ is the error tolerance, the approximately correct part.
- δ is the confidence probability, the probably part.

Probably approximately correct

- Imagine we do the following experiment many many times.
  1. Draw a training set S and obtain a trained program $A(S)$.
  2. Evaluate $L_{\mathcal{D}}(A(S)) - \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h')$.
  3. Repeat

- On average, the chance of seeing $L_{\mathcal{D}}(A(S)) - \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') > \epsilon$ is δ.

- Think of ϵ and δ as something small, close to 0.

- With high probability $1 - \delta$, the two terms $L_{\mathcal{D}}(A(S))$ and $\min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h')$ only differ by a small amount ϵ.

- With high probability, the program learned by A achieves a similar error to the best program in $\mathcal{H}$.

PAC learning

- PAC learnability is merely a definition.
- The minimum number of samples required, N, also known as **sample complexity**, is a function of $\mathcal{H}$, ϵ, and δ.
- We can now ask, "is the set of linear classifiers PAC learnable if we minimize the zero-one loss on a training set?"

Empirical risk minimization

- Minimizing the loss on a training set is also known as **empirical risk minimization (ERM)**.

$$A_{\mathrm{ERM},\mathcal{H}}(S) = h_{\mathrm{ERM}} = \operatorname*{argmin}_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i)) \tag{5}$$

- The set of linear classifiers is $\mathcal{H}_{\mathrm{lin}} = \{w \mapsto w^\top x : w \in \mathbb{R}^d\}$.
- We can now formally ask, "is the set of linear classifiers $\mathcal{H}_{\mathrm{lin}}$ PAC learnable with ERM?"
- And if so, how does the sample complexity N depends on $\mathcal{H}_{\mathrm{lin}}$, ϵ, and δ?

The universe of all programs

- Instead of choosing the set linear classifiers $\mathcal{H}_{\text{lin}} = \{x \mapsto w^\top x : w \in \mathbb{R}^d\}$, can we choose $\mathcal{H}_{\text{universe}} = \{\text{any function in the universe}\}$?

- We can now ask, "is $\mathcal{H}_{\text{universe}}$ PAC learnable with ERM or with any other learning algorithms?"

Probably approximately correct

A hypothesis class $\mathcal{H}$ is PAC-learnable with a learning algorithm A if for any distribution $\mathcal{D}$, and any $\epsilon > 0$ and $0 \leq \delta \leq 1$, there exists $N > 0$ such that

$$\mathbb{P}_{S\sim\mathcal{D}^n}\left[L_{\mathcal{D}}(A(S)) - \min_{h'\in\mathcal{H}} L_{\mathcal{D}}(h') > \epsilon\right] < \delta \tag{6}$$

for any $n \geq N$.

No free lunch theorem

Suppose $|\mathcal{X}| = 2m$. For any learning algorithm A, there is a distribution $\mathcal{D}$ and $f : \mathcal{X} \to \{0, 1\}$ such that $L_{\mathcal{D}}(f) = 0$, but

$$\mathbb{P}_{S \sim \mathcal{D}^m} \left[L_{\mathcal{D}}(A(S)) \geq \frac{1}{10} \right] \geq \frac{1}{10}. \tag{7}$$

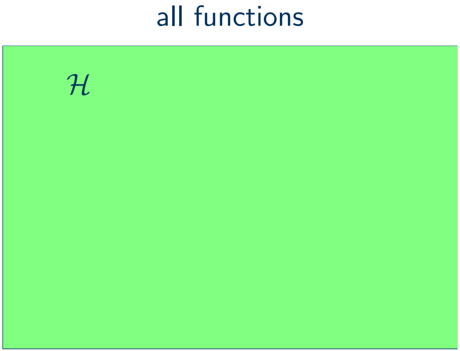
No free lunch theorem

- The 2 and 10 are arbitrary constants.
- In words, for any learning algorithm, there exists a distribution and a perfect function, but the learning algorithm has a sufficiently large error with sufficiently high probability.
- What is the problem?
- A cheater is an algorithm that knows $\mathcal{D}$.
- The universe always includes whatever the cheater can find.
- Don't compare to the cheater that knows $\mathcal{D}$. Instead, compare to the best in the hypothesis space.

No free lunch theorem

all functions

No free lunch theorem



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