MLCC 2019
Statistical Learning: Basic Concepts

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Outline

Learning from Examples

Data Space and Distribution

Loss Function and Expected Risk

Stability, Overfitting and Regularization

Learning from Examples

- Machine Learning deals with systems that are trained from data rather than being explicitly programmed

- Here we describe the framework considered in statistical learning theory.

Supervised Learning

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The data, called *training set*, is a set of n input-output pairs (examples)

$$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}.$$

We Need a Model to Learn

- We consider the approach to machine learning based on the *learning from examples* paradigm
- **Goal:** Given the training set, *learn* a corresponding I/O relation
- We have to postulate the existence of a model for the data
- The model should take into account the possible *uncertainty* in the task *and* in the data

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Data Space

- The inputs belong to an input space X, we assume that $X \subseteq \mathbb{R}^D$
- The outputs belong to an output space Y, typycally a subset of $\mathbb{R}$
- The space $X \times Y$ is called the *data space*

Examples of Data Space

We consider several possible situations:

- Regression: $Y \subseteq \mathbb{R}$
- Binary classification $Y = \{-1, 1\}$
- Multi-category (multiclass) classification $Y = \{1, 2, \ldots, T\}$.
- ...

Modeling Uncertainty in the Data Space

- **Assumption:** $\exists$ a fixed unknown distribution $p(x, y)$ according to which the data are **identically and independently sampled**
- The distribution p models different sources of **uncertainty**
- **Assumption:** p factorizes as $p(x, y) = p_X(x)p(y|x)$

Marginal and Conditional

$p(y|x)$ can be seen as a form of *noise* in the output

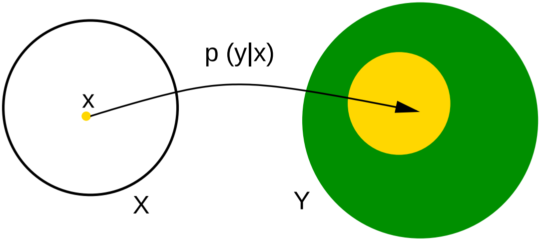

Figure: For each input x there is a distribution of possible outputs $p(y|x)$.

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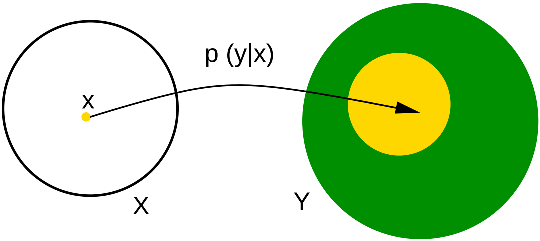

Figure: For each input x there is a distribution of possible outputs $p(y|x)$.

The marginal distribution $p_X(x)$ models uncertainty in the sampling of the input points.

Data Models

- In **regression**, the following model is often considered:

$$y = f^*(x) + \epsilon$$

where:

  - f^*: fixed unknown (*regression*) function
  - ϵ: random noise, e.g. standard Gaussian $\mathcal{N}(0, \sigma I)$, $\sigma \in [0, \infty)$

- In **classification**,

$$p(1|x) = 1 - p(-1|x), \forall x$$

Noiseless classification, $p(1|x) = \{1, 0\}, \forall x \in X$

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Loss Function

Goal of learning: Estimate "best" I/O relation (not the whole $p(x, y)$)

- We need to fix a *loss function*

$$\ell : Y \times Y \to [0, \infty)$$

  $\ell(y, f(x))$ is a point-wise error measure. It is the cost of when predicting $f(x)$ in place of y

Expected Risk and Target Function

The *expected loss (or expected risk)*

$$\mathcal{E}(f) = \mathbb{E}[\ell(y, f(x))] = \int p(x,y)\ell(y, f(x))dxdy$$

can be seen as a measure of the error on past as well as future data.

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Given ℓ and a distribution, the "best" I/O relation is the *target function*

$$f^* : X \to Y$$

that minimizes the expected risk

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- The goal of learning is to find an *estimator* of the target function from data

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The latter requirement needs some care since f_S depends on the training set and hence is **random**

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- **Learning rates** provide finite sample information, for all $\epsilon >$ if $n \geq n(\epsilon)$, then

$$\mathbb{E}_S[\mathcal{E}(f_S) - \mathcal{E}(f^*)] \leq \epsilon,$$

- $n(\epsilon)$is called **sample complexity**

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- **Fitting**: an estimator should *fit* data well
- **Stability**: an estimator should be stable, it should not change much if data change slightly

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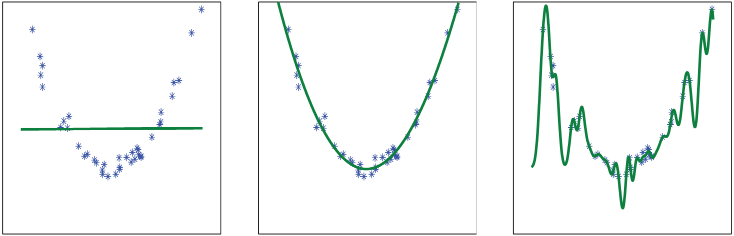

We say that an algorithms **overfits**, if it fits the data while being unstable

We say that an algorithms **oversmooth**, if it is stable while disregarding the data

Regularization as a Fitting-Stability Trade-off

- Most learning algorithms depend on one (or more) **regularization parameter**, that controls the trade-off between *data-fitting* and *stability*
- We broadly refer to this class of approaches as **regularization algorithms**, our main topic of discussion

Wrapping up

In this class, we introduced the basic definitions in statistical learning theory, including the key concepts of overfitting, stability and generalization.

Next Class

We will introduce the a first basic class of learning methods, namely local methods, and study more formally the fundamental trade-off between overfitting and stability.