

Foundations of Machine Learning

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- 1 Statistical Learning
- 2 Two Workhorses of Statistical Learning
- 3 The Learning Problem
- 4 Aproximation Error vs. Estimation Error
- 5 Prediction vs Causality

Statistical Learning

- Most Statistical Learning techniques fall into one of the following two categories:
 - 1 Supervised Learning: Data take the form $\{(x_1, y_1), \dots, (x_n, y_n)\}$ where y are the output variables.
 - The aim is to study the behavior of the output variable y (response variable) conditional on the independent variables x (predictor variables).
 - Mathematically: study and describe the distribution of y conditional on x .
 - 2 Unsupervised Learning: Data takes the form $\{x_1, \dots, x_n\}$, there are inputs but no output to supervise.
 - The aim is study the x variables (inputs), its patterns, clusters, etc.
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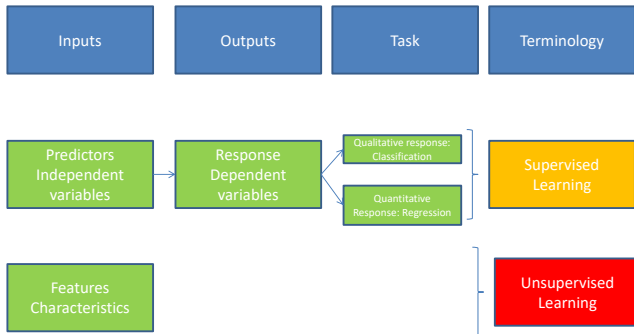
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- Terminology



- To illustrate the main ideas, let's focus on the classification task (applications: credit granting, fraud, customer profiling, etc).
- Suppose we have a sample $\tau_n = \{(x_1, y_1), \dots, (x_n, y_n)\}$ *independently* generated by a distribution $P(X, Y)$ where $y \in \{0, 1\}$.
- The distribution P is unknown.
- Assumption: sample is i.i.d.
- Denote Ξ the space of independent variables ($x \in \Xi$) and Υ the space of dependent variables ($y \in \Upsilon$).
- A **learning function** is a function $f : \Xi \rightarrow \Upsilon$. Intuitively, given an observation of x , the function selects a response $f(x)$.

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- The standard way to evaluate the performance of a learning function for the **classification** task is using a loss function.
- Let $L : \Xi \times \Upsilon \times \Upsilon \rightarrow \{0, 1\}$. Given an observation (x, y) , if $f(x) \neq y$ then $L(x, y, f(x)) = 1$ and $L(x, y, f(x)) = 0$ otherwise (standard Loss function for binary classification tasks).
- The most common way to measure the loss in a **regression** task is using the squared error: $L(x, y, f(x)) = (f(x) - y)^2$

Statistical Learning: Loss function

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- A Machine Learning algorithm M , is an algorithm that enable us to build a learning function form each sample τ_n .
- Let \mathbb{F} be the set of all learning functions (i.e., $f_n : \Xi \rightarrow \Upsilon$), then:

$$M : (\Xi \times \Upsilon)^n \rightarrow \mathbb{F} \quad (1)$$

is a machine learning algorithm.

- $M(\tau_n)$ is denoted by f_n . The learning function f_n depends on the size of the sample n . For different samples we get different Learning functions.

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- Approximation Error (bias) vs Estimation Error (Variance).
- Consistency.
- The problem of empirical risk minimization.
- Capacity.

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Two Workhorses of Statistical Learning

- Two workhorses (algorithms) of statistical learning are:
 - 1 K-Nearest Neighbors.
 - 2 Linear Regression Model.

Two Workhorses: K-Nearest Neighbors

- Suppose you have a concept of distance between predictors.
- Define k as the number of neighbors that the Learning function uses to classify.
- Given a sample τ_n and $x \in \Xi$, we identify the k points $\{x_{i_1}, \dots, x_{i_k}\}$ that are closest to x .
- The learning function in binary classification tasks is defined based on the number of $\{k : y_{i_k} = 1\}$: majority vote.
- For regression tasks we estimate the average.
- We denote these learning machines as $K - NN_n$.

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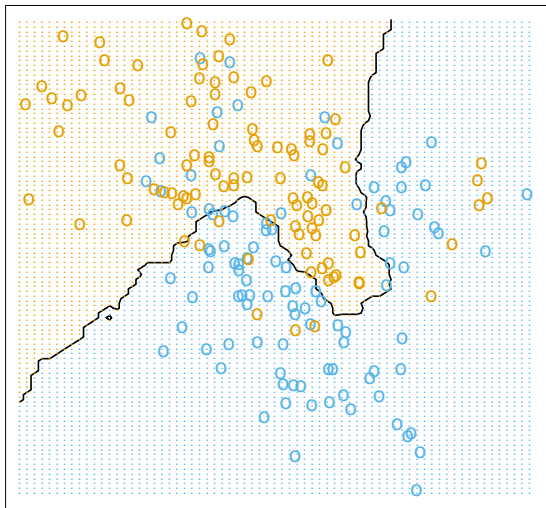
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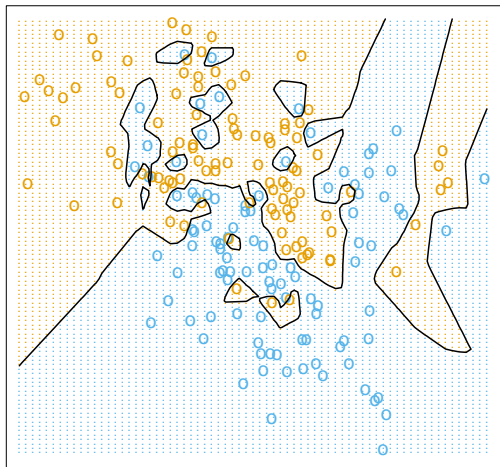
15-Nearest Neighbor Classifier



Two Workhorses: K-Nearest Neighbors

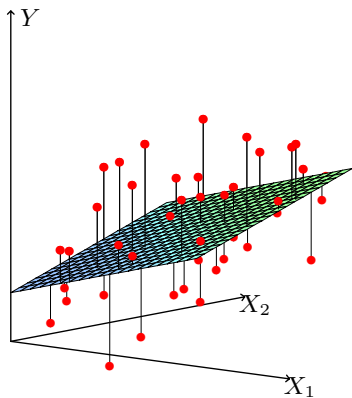
- Note that this learning function fits better *in-sample* and is more *complex* than the previous one.

1-Nearest Neighbor Classifier



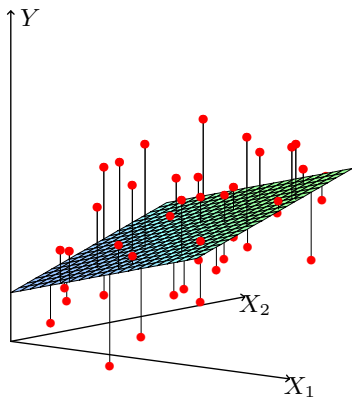
Two Workhorses: Linear Regression

- Suppose that $y_i = \beta_n^T x_i$ where we include a 1 as the first coordinate in every vector x_i (the constant in the linear regression model).
- Defining $\hat{\beta}_n$ as the estimator of ordinary least squares.
- Note that $\hat{\beta}_n$ defines a learning function $f_n^{OLS}(x) = 1$ if $\beta_n^T x > 0,5$ and zero otherwise.



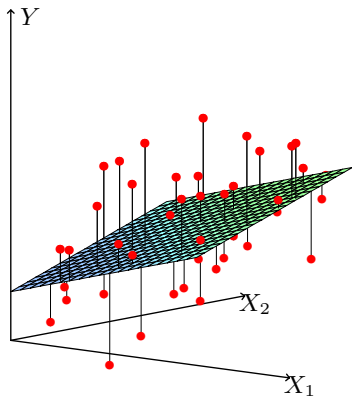
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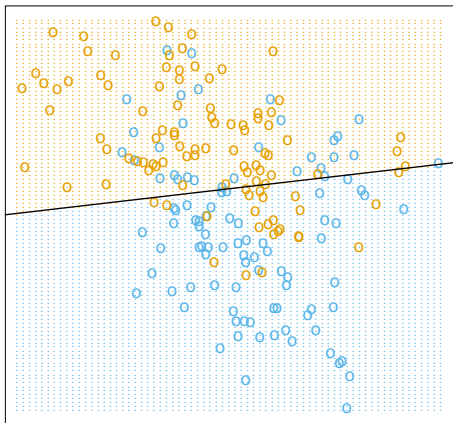
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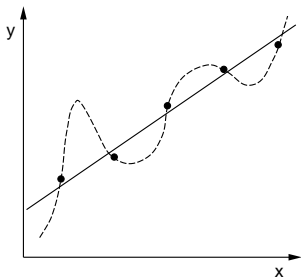
Two Workhorses: Linear Regression Model

- Black line corresponds to $\beta_n^T x_i = 0,5$.



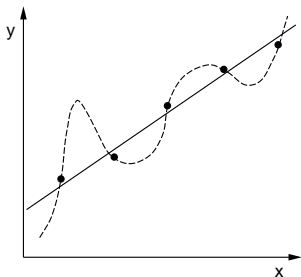
Statistical Learning: The Classification Task

- The Overfitting problem.
- Note that if the true model is the straight line, the empirical error of the curve is zero but the curve generalizes badly. The line's empirical error is larger than zero but the line generalizes better. And viceversa.
- In the first case, the curve is more complex, the variance is high and the bias is low. In the second case, the line is less complex, the variance is low but the bias is high.



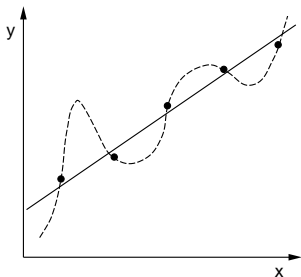
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Risk

- Given a learning function f , the risk of f is defined as:

$$R(f) = E_P[L(X, Y, f(X))]$$

where P is the joint distribution of X, Y , the true data generatig process.

- Notice that P is unknown so you cannot actually estimate the risk of a learning function. We will develop techniques to estimate this risk.
- Notice also that $R(f)$ is just the out of sample error of the learning function f (also called test error).
- The analogous in-sample error (also called training error) is the called the empirical risk.

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Learning Problem

- Define \mathbb{F}_0 as a set of functions (i.e., a subset of \mathbb{F} the set of all functions).
- The learning problem is to solve:

$$f^* = \operatorname{argmin}_{f \in \mathbb{F}_0} R[f] \quad (2)$$

Note that \mathbb{F}_0 can be the set of all functions. When we want to make the space \mathbb{F}_0 explicit, we define f^* as $f_{\mathbb{F}_0}$.

- If $\mathbb{F}_0 = \mathbb{F}$ then f^* is called the Bayes Classifier (f_{Bayes}).
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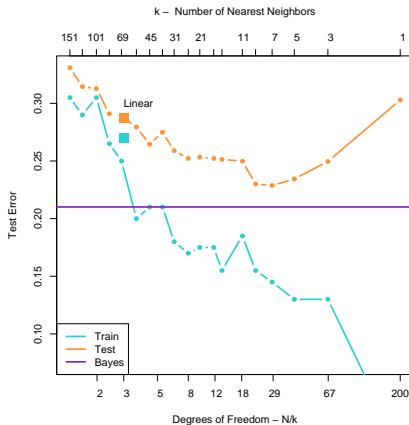
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Bias vs. Variance Tradeoff



- Simulation exercise: 200 examples (training set), 10,000

Bias vs. Variance Tradeoff

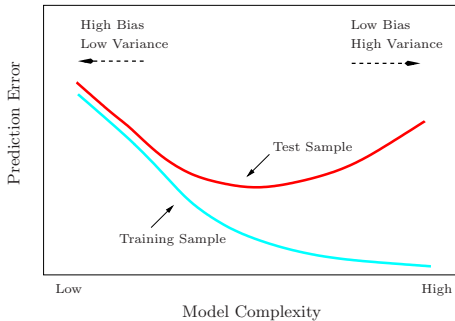
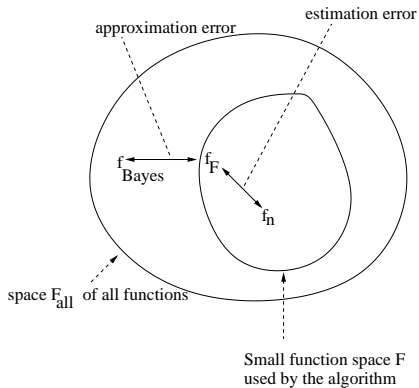
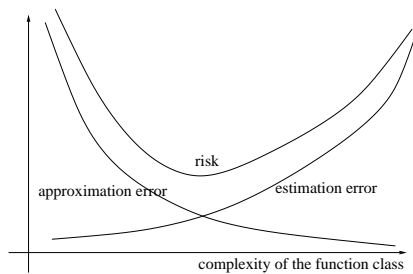


FIGURE 2.11. Test and training error as a function of model complexity.

Approximation Error vs. Estimation Error



Aproximation Error vs. Estimation Error



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Introduction

- Defining y as the interest variable, we don't know how y relates to x_0 (exogenous variable: economic policy) and x (covariates).
- The aim is to maximize a known function $\Pi(x_0, y)$.
- The decision depends on:

$$\frac{\partial \Pi}{\partial x_0} = \frac{\partial \Pi}{\partial x_0}(x_0, y) + \frac{\partial \Pi}{\partial y}(x_0, y) \frac{\partial y}{\partial x_0}(x_0)$$

- 1 Even though Π is known, the effect of x_0 depends on y (prediction problem).
 - 2 The second term depends on how x_0 affects y (causality problem).
- Note that both effects depend on the prediction y .
 - Therefore, a policymaker must solve both problems.

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- The aim is to maximize a known function $\Pi(x_0, y)$.
- The decision depends on:

$$\frac{\partial \Pi}{\partial x_0} = \frac{\partial \Pi}{\partial x_0}(x_0, y) + \frac{\partial \Pi}{\partial y}(x_0, y) \frac{\partial y}{\partial x_0}(x_0)$$

- 1 Even though Π is known, the effect of x_0 depends on y (prediction problem).
 - 2 The second term depends on how x_0 affects y (causality problem).
- Note that both effects depend on the prediction y .
 - Therefore, a policymaker must solve both problems.

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Example

- Suppose that the interest variable y is defined based on whether it rains or not. The decision in a problem could be a ritual so that it does not rain. In another problem the decision could be to carry or not umbrella.
- The objective function can be the utility generated by going to the park a Sunday.
- The task of doing a ritual is a causality problem:

$$\frac{\partial \Pi}{\partial x_0}(x_0, y) = 0$$

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- It may be the case that $\frac{\partial y}{\partial x_0}(x_0) \neq 0$.

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