Introduction to Statistical Learning Theory

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Decision Theory: High Level View

What types of problems are we solving?

- In data science problems, we generally need to:
  - Make a decision
  - Take an action
  - Produce some output

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- In data science problems, we generally need to:
    - Make a decision
    - Take an action
    - Produce some output
- Have some evaluation criterion

Actions

Definition

An *action* is the generic term for what is produced by our system.

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- What's an action for predicting where a storm will be in 3 hours?
- What's an action for a self-driving car?

Evaluation Criterion

Decision theory is about finding "optimal" actions, under various definitions of optimality.

Examples of Evaluation Criteria

- Is classification correct?
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  - Should we give partial credit? How?

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- Does text transcription exactly match the spoken words?
  - Should we give partial credit? How?
- How far is the storm from the prediction location? [for point prediction]
- How likely is the storm's location under the prediction? [for density prediction]

Real Life: Formalizing a Business Problem

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- Formalization may evolve gradually, as you understand the problem better

Inputs

Most problems have an extra piece, going by various names:

- Inputs [ML]
- Covariates [Statistics]

Examples of Inputs

- A picture
- A storm's historical location and other weather data
- A search query

“Outcomes” or “Output” or “Label”

Inputs often paired with *outputs* or *outcomes or labels*

Examples of outcomes/outputs/labels

- Whether or not the picture actually contains an animal
- The storm’s location one hour after query
- Which, if any, of suggested the URLs were selected

Typical Sequence of Events

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    - automated driving

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- What are the spaces for a support vector machine?

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- Typical sequence:
  1. Stakeholder presents problem to data scientist
  2. Data scientist produces decision function
  3. Engineer deploys "industrial strength" version of decision function

Evaluating a Decision Function

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- We will use the standard **statistical learning theory** framework.

Statistical Learning Theory

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  - what about stock market investing?
- What about fancier problems where this does not hold?
  - often can be reformulated or "reduced" to problems where it does hold
  - see literature on **reinforcement learning**

Setup for Statistical Learning Theory

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- How can we formalize this?

The Risk Functional

Definition

The **risk** of a decision function $f : \mathcal{X} \to \mathcal{A}$ is

$$R(f) = \mathbb{E}\ell(f(x), y).$$

In words, it's the **expected loss** of f on a new exampe (x, y) drawn randomly from $P_{\mathcal{X}\times\mathcal{Y}}$.

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Risk function cannot be computed

Since we don't know $P_{\mathcal{X}\times\mathcal{Y}}$, we cannot compute the expectation.
But we can estimate it...

The Bayes Decision Function

Definition

A **Bayes decision function** $f^*: \mathcal{X} \to \mathcal{A}$ is a function that achieves the *minimal risk* among all possible functions:

$$f^* = \arg\min_f R(f),$$

where the minimum is taken over all functions from $\mathcal{X}$ to $\mathcal{A}$.

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- A Bayes decision function is often called the "**target function**", since it's the best decision function we can possibly produce.

Example 1: Least Squares Regression

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- target function:

$$f^*(x) = \mathbb{E}[y|x]$$

Example 2: Multiclass Classification

- spaces: $\mathcal{A} = \mathcal{Y} = \{0, 1, \ldots, K-1\}$
- 0-1 loss:

$$\ell(a, y) = 1(a \neq y) := \begin{cases} 1 & \text{if } a \neq y \\ 0 & \text{otherwise.} \end{cases}$$

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- target function is the assignment to the most likely class

$$f^*(x) = \underset{1 \leqslant k \leqslant K}{\arg\max}\, \mathbb{P}(y = k \mid x)$$

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assume we have sample data.

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- Let's draw some inspiration from the Strong Law of Large Numbers:
  If $z, z_1, \ldots, z_n$ are i.i.d. with expected value $\mathbb{E}z$, then

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} z_i = \mathbb{E}z,$$

  with probability 1.

The Empirical Risk Functional

Let $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$ be drawn i.i.d. from $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$.

Definition

The **empirical risk** of $f : \mathcal{X} \to \mathcal{A}$ with respect to $\mathcal{D}_n$ is

$$\hat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(x_i), y_i).$$

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By the Strong Law of Large Numbers,

$$\lim_{n\to\infty} \hat{R}_n(f) = R(f),$$

almost surely.

That's a start...

Empirical Risk Minimization

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Definition

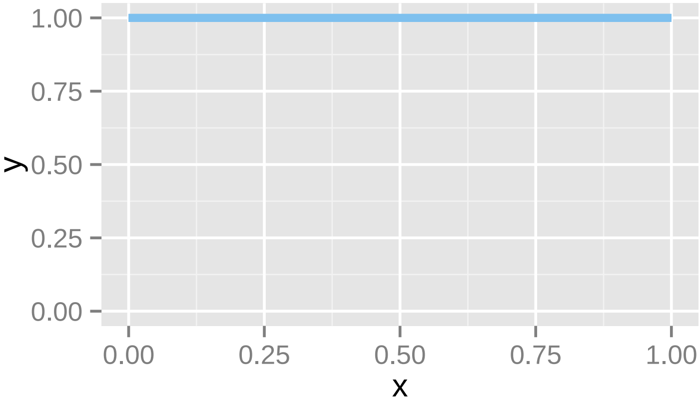
A function $\hat{f}$ is an **empirical risk minimizer** if

$$\hat{f} = \arg\min_{f} \hat{R}_n(f),$$

where the minimum is taken over all functions.

Empirical Risk Minimization

$P_{\mathcal{X}} = \text{Uniform}[0,1]$, $Y \equiv 1$ (i.e. Y is always 1).



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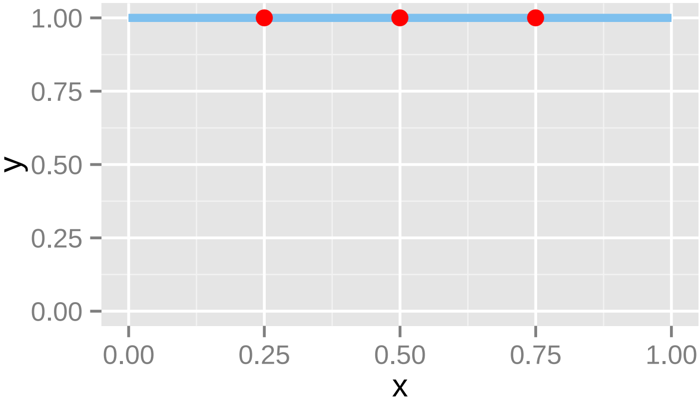

A sample of size 3 from $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$.

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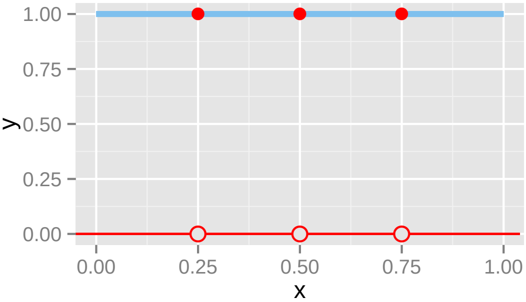

A proposed decision function:

$$\hat{f}(x) = 1(x \in \{0.25, 0.5, 0.75\}) = \begin{cases} 1 & \text{if } x \in \{0.25, .5, .75\} \\ 0 & \text{otherwise} \end{cases}$$

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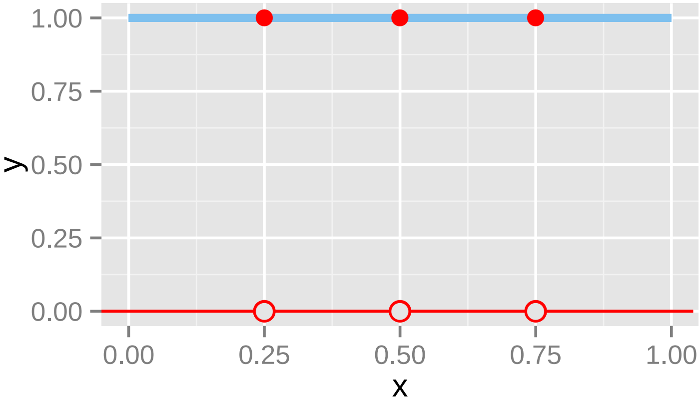

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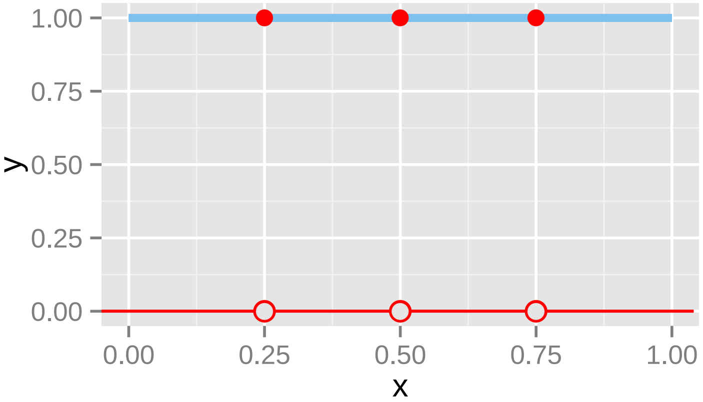

Under square loss or 0/1 loss: $\hat{f}$ has Empirical Risk = 0 and Risk = 1.

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- One approach: "Constrained ERM"
  - Instead of minimizing empirical risk over all decision functions,
  - constrain to a particular subset, called a **hypothesis space**.

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Example hypothesis spaces?

Constrained Empirical Risk Minimization

- Hypothesis space $\mathcal{F}$, a set of [decision] functions mapping $\mathcal{X} \to \mathcal{A}$
- **Empirical risk minimizer** (ERM) in $\mathcal{F}$ is

$$\hat{f}_n = \underset{f \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

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$$\hat{f}_n = \underset{f \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- **Risk minimizer** in $\mathcal{F}$ is $f^*_{\mathcal{F}} \in \mathcal{F}$, where

$$f^*_{\mathcal{F}} = \underset{f \in \mathcal{F}}{\arg\min} \mathbb{E}\ell(f(x), y).$$