Statistical Learning Theory

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[1] Slides based on Lecture 1b, 1c from David Rosenberg's course material.

Contents

Decision Theory

What types of problems are we solving?

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

Actions

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

Examples of Actions

- Produce a 0/1 classification (classical ML)
- Reject hypothesis that $\theta = 0$ (classical Statistics)
- Generate text (image captioning, speech recognition, machine translation)
- What's an action for predicting where a storm will be in 3 hours?

Inputs

In order to make the decision, we typically have additional context:

- Inputs [ML]
- Covariates [Statistics]

Examples of Inputs

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

Outcome

Inputs are often paired with **outputs** 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

Evaluation Criterion

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

Examples of Evaluation Criteria

- Is the classification correct?
- Does text transcription exactly match the spoken words?
  - Should we give partial credit? How?
- How far is the storm from the predicted location? (for point prediction)
- How likely is the storm's location under the predicted distribution? (for density prediction)

Typical Sequence of Events

Many problem domains can be formalized as follows:

1. Observe input x.
2. Take action a.
3. Observe outcome y.
4. Evaluate action in relation to the outcome

Three spaces:

- Input space: $\mathcal{X}$
- Action space: $\mathcal{A}$
- Outcome space: $\mathcal{Y}$

Formalization

Prediction Function

A **prediction function** (or **decision function**) gets input $x \in \mathcal{X}$ and produces an action $a \in \mathcal{A}$:

$$
\begin{aligned}
f: \quad \mathcal{X} &\to \mathcal{A} \\
x &\mapsto f(x)
\end{aligned}
$$

Loss Function

A **loss function** evaluates an action in the context of the outcome y.

$$
\begin{aligned}
\ell: \quad \mathcal{A} \times \mathcal{Y} &\to \mathrm{R} \\
(a, y) &\mapsto \ell(a, y)
\end{aligned}
$$

Evaluating a Prediction Function

Goal: find the optimal prediction function

Intuition: If we can evaluate how good a prediciton function is, we can turn this into an optimization problem.

- Loss function ℓ evaluates a *single* action
- How to evaluate the prediction function *as a whole*?
- We will use the standard **statistical learning theory** framework.

Statistical Learning Theory

Setup for Statistical Learning Theory

Define a space where the prediction function is applicable

- Assume there is a **data generating distribution** $P_{\mathcal{X}\times\mathcal{Y}}$.
- All input/output pairs (x, y) are generated i.i.d. from $P_{\mathcal{X}\times\mathcal{Y}}$.

Want prediction function $f(x)$ that "does well on average":

$$\ell(f(x), y) \text{ is usually small, in some sense}$$

How can we formalize this?

Risk

Definition

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

$$R(f) = \mathbb{E}_{(x,y) \sim P_{\mathcal{X} \times \mathcal{Y}}} \left[\ell(f(x), y) \right].$$

In words, it's the **expected loss** of f over $P_{\mathcal{X} \times \mathcal{Y}}$.

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 Prediction Function

Definition

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

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

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

- The risk of a Bayes prediction function is called the **Bayes risk**.
- A Bayes prediction function is often called the "**target function**", since it's the best prediction function we can possibly produce.

Example: Multiclass Classification

- Spaces: $\mathcal{A} = \mathcal{Y} = \{1, \ldots, k\}$
- 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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- Risk:

$$\begin{aligned} R(f) &= \mathbb{E}\left[1(f(x) \neq y)\right] \quad = 0 \cdot \mathbb{P}(f(x) = y) + 1 \cdot \mathbb{P}(f(x) \neq y) \\ &= \mathbb{P}(f(x) \neq y), \end{aligned}$$

which is just the misclassification error rate.

- Bayes prediction function is just the assignment to the most likely class:

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

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But we can't compute the risk!

- Can't compute $R(f) = \mathbb{E}\left[\ell(f(x), y)\right]$ because we **don't know** $P_{\mathcal{X}\times\mathcal{Y}}$.

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assume we have sample data.

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

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- Let's draw some inspiration from the Strong Law of Large Numbers:
  If $z_1, \ldots, z_n$ 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.

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The Empirical Risk

Let $\mathcal{D}_n = ((x_1, y_1), \dots, (x_n, y_n))$ 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

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

By the Strong Law of Large Numbers,

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

almost surely.

Empirical Risk Minimization

Definition

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

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

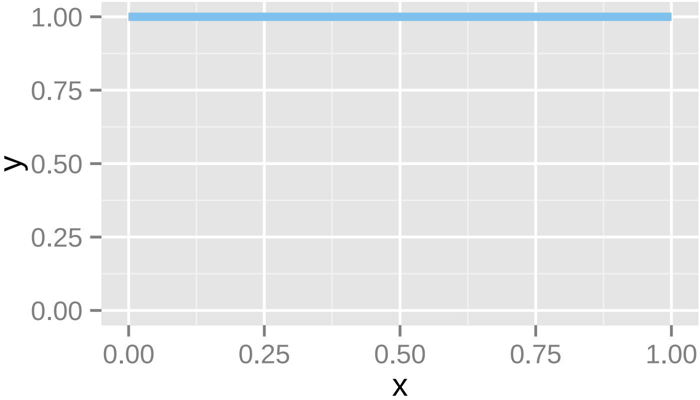
where the minimum is taken over all functions.

We want risk minimizer, is empirical risk minimizer close enough?

In practice, we only have a finite sample.

Empirical Risk Minimization

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



$\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$.

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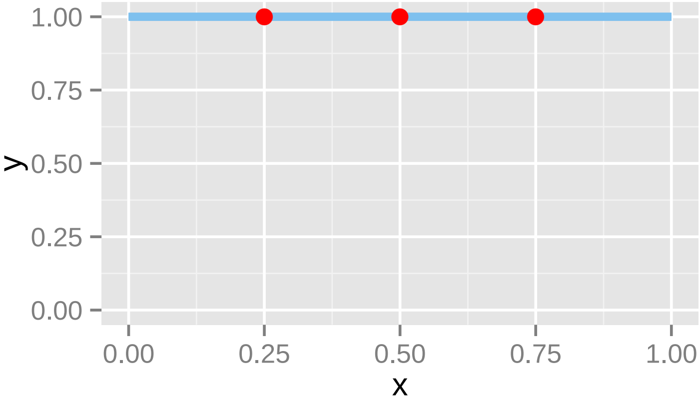

A sample of size 3 from $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$.

Empirical Risk Minimization

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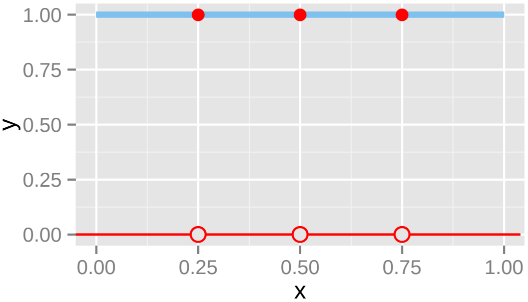

A proposed prediction function:

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

Empirical Risk Minimization

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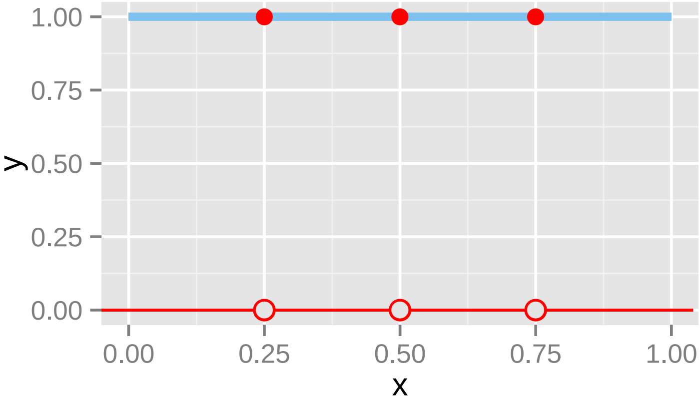


Under square loss or 0/1 loss: $\hat{f}$ has Empirical Risk = 0 and Risk = 1.

- ERM led to a function f that just memorized the data.
- How to spread information or **generalize** from training inputs to new inputs?
- Need to smooth things out somehow...
  - A lot of modeling is about spreading and extrapolating information from one part of the input space $\mathcal{X}$ into unobserved parts of the space.
- One approach: "Constrained ERM"
  - Instead of minimizing empirical risk over *all* prediction functions,
  - constrain to a particular subset, called a **hypothesis space**.

Hypothesis Spaces

Definition

A **hypothesis space** $\mathcal{F}$ is a set of functions mapping $\mathcal{X} \to \mathcal{A}$. It is the collection of prediction functions we are choosing from.

Want Hypothesis Space that

- Includes only those functions that have desired "regularity", e.g. smoothness, simplicity
- Easy to work with

Most applied work is about designing good hypothesis spaces for specific tasks.

Constrained Empirical Risk Minimization

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

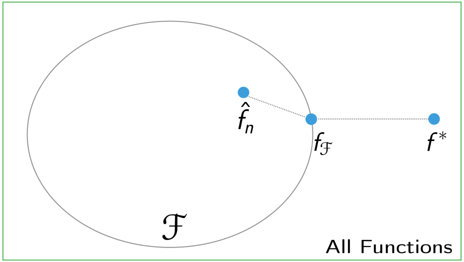
$$\hat{f}_n \in \underset{f \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

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

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

Excess Risk Decomposition

Error Decomposition



$$f^* = \arg\min_f \mathbb{E}[\ell(f(x), y)]$$

$$f_{\mathcal{F}} = \arg\min_{f \in \mathcal{F}} \mathbb{E}[\ell(f(x), y)]$$

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

- **Approximation Error** (of $\mathcal{F}$) $= R(f_{\mathcal{F}}) - R(f^*)$
- **Estimation error** (of $\hat{f}_n$ in $\mathcal{F}$) $= R(\hat{f}_n) - R(f_{\mathcal{F}})$

Excess Risk Decomposition for ERM

Definition

The **excess risk** compares the risk of f to the Bayes optimal f^*:

$$\textbf{Excess Risk}(f) = R(f) - R(f^*)$$

- Can excess risk ever be negative?

The excess risk of the ERM $\hat{f}_n$ can be decomposed:

$$\begin{aligned}
\textbf{Excess Risk}(\hat{f}_n) &= R(\hat{f}_n) - R(f^*) \\
&= \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}.
\end{aligned}$$

Approximation Error

Approximation error $R(f_{\mathcal{F}}) - R(f^*)$ is

- a property of the class $\mathcal{F}$
- the penalty for restricting to $\mathcal{F}$ (rather than considering all possible functions)

Bigger $\mathcal{F}$ mean *smaller* approximation error.

Concept check: Is approximation error a random or non-random variable?

Estimation Error

Estimation error $R(\hat{f}_n) - R(f_{\mathcal{F}})$

- is the performance hit for choosing f using finite training data
- is the performance hit for minimizing empirical risk rather than true risk

With *smaller* $\mathcal{F}$ we expect *smaller* estimation error.

Under typical conditions: "With infinite training data, estimation error goes to zero."

Concept check: Is estimation error a random or non-random variable?

ERM in Practice

- We've been cheating a bit by writing "argmin".
- In practice, we need a method to find $\hat{f}_n \in \mathcal{F}$.
- For nice choices of loss functions and classes $\mathcal{F}$, we can get arbitrarily close to a minimizer
  - But takes time – is it worth it?
- For some hypothesis spaces (e.g. neural networks), we don't know how to find $\hat{f}_n \in \mathcal{F}$.

Optimization Error

- In practice, we don't find the ERM $\hat{f}_n \in \mathcal{F}$.
- We find $\tilde{f}_n \in \mathcal{F}$ that we hope is good enough.
- **Optimization error:** If $\tilde{f}_n$ is the function our optimization method returns, and $\hat{f}_n$ is the empirical risk minimizer, then

$$\text{Optimization Error} \; = \; R(\tilde{f}_n) - R(\hat{f}_n).$$

- Can optimization error be negative? Yes!
- But

$$\hat{R}(\tilde{f}_n) - \hat{R}(\hat{f}_n) \geqslant 0.$$

Error Decomposition in Practice

- Excess risk decomposition for function $\tilde{f}_n$ returned by algorithm:

$$\begin{aligned}\textbf{Excess Risk}(\tilde{f}_n) &= R(\tilde{f}_n) - R(f^*)\\ &= \underbrace{R(\tilde{f}_n) - R(\hat{f}_n)}_{\text{optimization error}} + \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}\end{aligned}$$

- Concept check: It would be nice to have a concrete example where we find an $\tilde{f}_n$ and look at it's error decomposition. Why is this usually impossible?
- But we could constuct an artificial example, where we know $P_{\mathcal{X}\times\mathcal{Y}}$ and f^* and $f_{\mathcal{F}}$...

ERM Overview

- Given a loss function $\ell : \mathcal{A} \times \mathcal{Y} \to R$.
- Choose hypothesis space $\mathcal{F}$.
- Use an optimization method to find ERM $\hat{f}_n \in \mathcal{F}$:

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

- Data scientist's job:
  - choose $\mathcal{F}$ to balance between approximation and estimation error.
  - as we get more training data, use a bigger $\mathcal{F}$