Introduction to Statistical Learning Theory

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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

Definition

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]

- Written English text [speech recognition]
- Probability that a picture contains an animal [computer vision]

- Probability distribution on the earth [storm tracking]
- Adjust accelerator pedal down by 1 centimeter [automated driving]

Evaluation Criterion

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

Examples of Evaluation Criteria

- Is classification correct?
- Does text transcription exactly match the spoken words?
    - Should we give partial credit? How?
- Is probability "well-calibrated"?

Real Life: Formalizing a Business Problem

- First two steps to formalizing a problem:
    1. Define the *action space* (i.e. the set of possible actions)
    2. Specify the evaluation criterion.
- Finding *the right formalization* can be an interesting challenge
- 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]
- Side Information [Various settings]

Examples of Inputs

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

Output / Outcomes

Inputs often paired with *outputs* or *outcomes*

Examples of outputs / outcomes

- 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

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: $\ell(a, y)$.

Note

- Outcome y is often **independent** of action a
- But this is **not always the case**:
  - URL recommendation
  - automated driving

Some Formalization

The Spaces

- $\mathcal{X}$: input space
- $\mathcal{Y}$: output space
- $\mathcal{A}$: action space

Decision Function

A **decision function** produces an action $a \in \mathcal{A}$ for any input $x \in \mathcal{X}$:

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

Loss Function

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

$$\begin{aligned} \ell: \quad \mathcal{A} \times \mathcal{Y} & \rightarrow \mathbf{R}^{\geqslant 0} \\ (a, y) & \mapsto \ell(a, y) \end{aligned}$$

Real Life: Formalizing a Business Problem

- First two steps to formalizing a problem:
  1. Define the *action space* (i.e. the set of possible actions)
  2. Specify the evaluation criterion.
- When a "stakeholder" asks the data scientist to solve a problem, she
  - may have an opinion on what the action space should be, and
  - hopefully has an opinion on the evaluation criterion, but
  - she really cares about your **producing a "good" decision function.**
- Typical sequence:
  1. Stakeholder presents problem to data scientist
  2. Data scientist produces decision function
  3. Engineer deploys "industrial strength" version of decision function

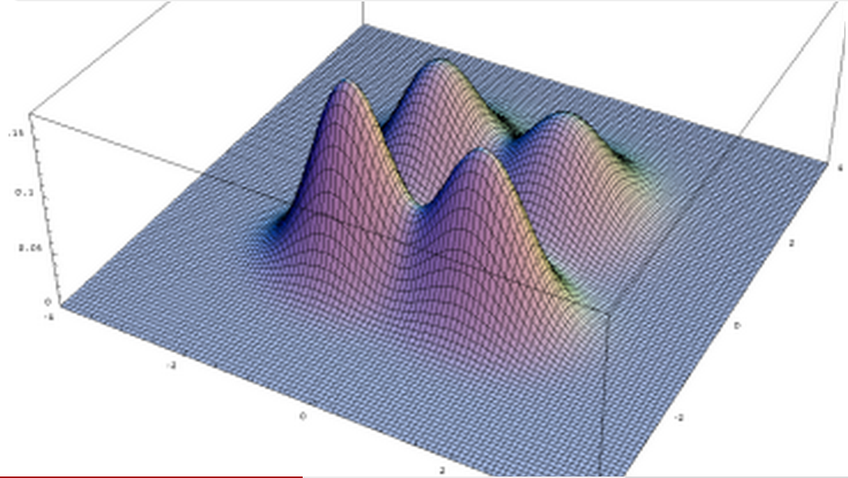
Evaluating a Decision Function

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

Setup for Statistical Learning Theory

Data Generating Assumption

All pairs $(X, Y) \in \mathcal{X} \times \mathcal{Y}$ are drawn i.i.d. from some **unknown** $P_{\mathcal{X} \times \mathcal{Y}}$.



The Risk Functional

Definition

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

$$R(f) = \mathbb{E}\ell(f(X), Y),$$

where the expectation taken is over $(X, Y) \sim P_{\mathcal{X} \times \mathcal{Y}}$.

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 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:

$$R(f^*) = \inf_f R(f),$$

where the infimum is taken over all measurable functions from $\mathcal{X}$ to $\mathcal{A}$.
The risk of a Bayes decision function is called the **Bayes risk**.

- A Bayes decision function is often called the "target function", since it's what we would ultimately like to produce as our decision function.

Example 1: Least Squares Regression

- spaces: $\mathcal{A} = \mathcal{Y} = \mathbf{R}$
- square loss:

$$\ell(a,y) = \frac{1}{2}(a-y)^2$$

- mean square risk:

$$\begin{aligned} R(f) &= \frac{1}{2}\mathbb{E}\left[(f(X)-Y)^2\right] \\ &= \frac{1}{2}\mathbb{E}\left[(f(X)-\mathbb{E}[Y|X])^2\right] + \frac{1}{2}\mathbb{E}\left[(Y-\mathbb{E}[Y|X])^2\right] \end{aligned}$$

- target function:

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

Example 2: Multiclass Classification

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

$$\ell(a, y) = 1(a \neq y)$$

- risk is misclassification error rate

$$\begin{aligned} R(f) &= \mathbb{E}\left[1(f(X) \neq Y)\right] \\ &= \mathbb{P}(f(X) \neq Y) \end{aligned}$$

- target function is the assignment to the most likely class

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

But we can't compute the risk!

- Can't compute $R(f) = \mathbb{E}\ell(f(X), Y)$ because we **don't know** $P_{\mathcal{X}\times\mathcal{Y}}$.
- Can we estimate $P_{\mathcal{X}\times\mathcal{Y}}$ from data?
- Under assumptions (e.g. comes from a parametric family), yes.
    - We'll come back to these approaches later in the course.
- Otherwise, we'll typically face a **curse of dimensionality**,
    - making $P_{\mathcal{X}\times\mathcal{Y}}$ very difficult ot estimate

A Curse of Dimensionality

The "volume" of space grows exponentially with the dimension.

Histograms

- Construct histogram for $X \in [0,1]$ with bins of size 0.1
  - That's 10 bins.
  - About 100 observations would be a good start for estimation.
- Constuct histogram for $X \in [0,1]^{10}$ with hypercube bins of side length 0.1
  - That's 10^{10} =10 billion bins.
  - About 100 billion observations would be a good start for estimation...

Takeaway Message

To estimate a density in high dimensions, you need additional assumptions.

The Empirical Risk Functional

Can we estimate $R(f)$ without estimating $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$?

Assume we have sample data

Let $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ be drawn i.i.d. from $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$.

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.

That's a start...

Empirical Risk Minimization

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

Definition

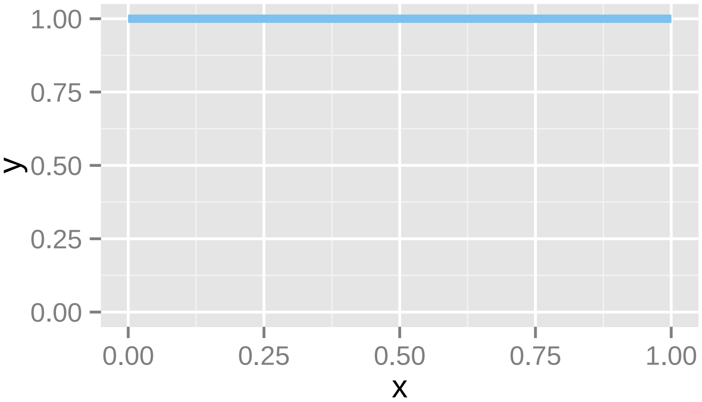
A function $\hat{f}$ is an **empirical risk minimizer** if

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

where the minimum is taken over all [measurable] functions.

Empirical Risk Minimization

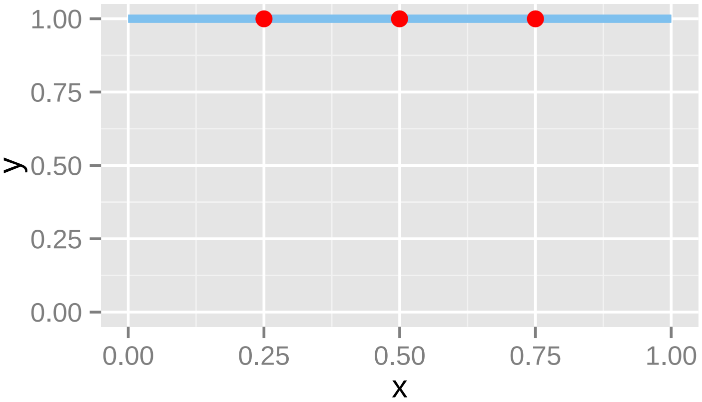
$P_{\mathcal{X}} = \text{Uniform}[0,1]$, $Y \equiv 1$ (i.e. Y is always 1).



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

Empirical Risk Minimization

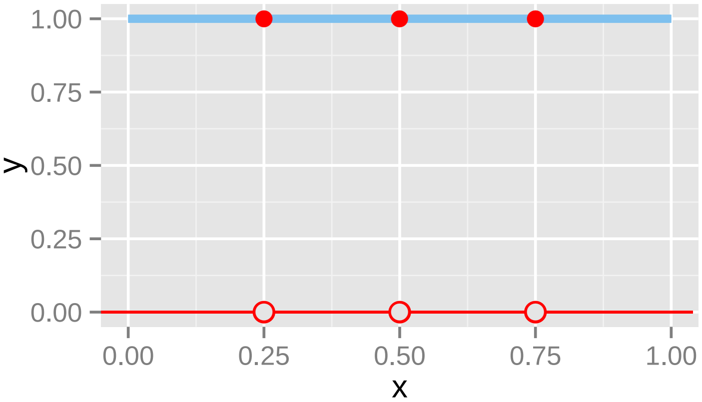
$P_{\mathcal{X}} = \text{Uniform}[0,1]$, $Y \equiv 1$ (i.e. Y is always 1).



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

Empirical Risk Minimization

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



Under square loss or 0/1 loss: Empirical Risk = 0. Risk = 1.

Empirical Risk Minimization

- 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.

Aside: Notation for Function Spaces

Notation

Let $\mathcal{C}^{\mathcal{D}}$ denote the set of all functions mapping from $\mathcal{D}$ [the domain] to $\mathcal{C}$ [the codomain].

Hypothesis Spaces

Definition

A **hypothesis space** $\mathcal{F} \subset \mathcal{A}^{\mathcal{X}}$ is a set of decision functions we are considering as solutions.

Hypothesis Space Choice

- Easy to work with.
- Includes only those functions that have desired "smoothness"

Constrained Empirical Risk Minimization

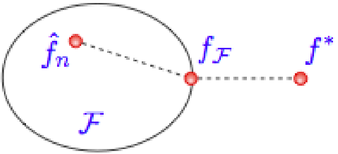
- Hypothesis space $\mathcal{F} \subset \mathcal{A}^{\mathcal{X}}$, a set of functions mapping $\mathcal{X} \to \mathcal{A}$
- **Empirical risk minimizer** (ERM) in $\mathcal{F}$ is $\hat{f} \in \mathcal{F}$, where

$$\hat{R}(\hat{f}) \quad = \quad \inf_{f \in \mathcal{F}} \hat{R}(f) = \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(X_i), Y_i).$$

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

$$R(f_{\mathcal{F}}^{*}) = \inf_{f \in \mathcal{F}} R(f) = \inf_{f \in \mathcal{F}} \mathbb{E}\ell(f(X), Y)$$

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

Error Decomposition

Definition

The **excess risk** of f is the amount by which the risk of f exceeds the Bayes risk

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

This is a more general expression of the bias/variance tradeoff for mean squared error:

- Approximation error = "bias"
- Estimation error = "variance"

Approximation Error

- Approximation error is a property of the class $\mathcal{F}$
- It's our penalty for restricting to $\mathcal{F}$ rather than considering all measurable functions
  - Approximation error is the minimum risk possible with $\mathcal{F}$ (even with infinite training data)
- *Bigger* $\mathcal{F}$ mean *smaller* approximation error.

Estimation Error

- *Estimation error*: The performance hit for choosing f using finite training data
  - *Equivalently*: It's the hit for not knowing the true risk, but only the empirical risk.
- *Smaller* $\mathcal{F}$ means *smaller* estimation error.
- *Under typical conditions:* "With infinite training data, estimation error goes to zero."
  - Infinite training data solves the *statistical* problem, which is not knowing the true risk.]

Optimization Error

- Does unlimited data solve our problems?
- There's still the *algorithmic* problem of *finding* $\hat{f}_n \in \mathcal{F}$.
- For nice choices of loss functions and classes $\mathcal{F}$, the algorithmic problem can be solved (to any desired accuracy).
    - Takes time! Is it worth it?
- **Optimization error:** If $\tilde{f}_n$ is the function our optimization method returns, and $\hat{f}_n$ is the empirical risk minimizer, then the optimization error is $R(\tilde{f}_n) - R(\hat{f}_n)$
- NOTE: May have $R(\tilde{f}_n) < R(\hat{f}_n)$, since $\hat{f}_n$ may overfit more than $\tilde{f}_n$!

ERM Overview

- Given a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbf{R}^{\geqslant 0}$.
- Choose hypothesis space $\mathcal{F}$.
- Use an algorithm (an optimization method) to find $\hat{f}_n \in \mathcal{F}$ minimizing the empirical risk:
$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(X_i), Y_i).$$
- (So, $\hat{R}(\hat{f}) = \min_{f \in \mathcal{F}} \hat{R}(f)$).
- Data scientist's job: choose $\mathcal{F}$ to optimally balance between approximation and estimation error.