Introduction to Machine Learning

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NYU

September 5, 2023

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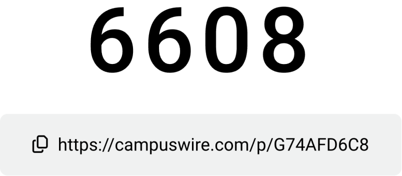
Logistics

- Class webpage: https://nyu-cs2565.github.io/2023-fall
    - Course materials (lecture slides, homeworks) will be made available on the website
- Discussion / questions on CampusWire: https://campuswire.com/p/G74AFD6C8



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https://campuswire.com/p/G74AFD6C8

- Sign up to Gradescope to submit homework assignments (entry code **RZJR36**)
- Office Hour: Tuesday 1:00-2:00 pm, Room 508, 60 Fifth Ave.

Logistics

Course Staff

- Instructor:
  - Mengye Ren (`mr3182@nyu.edu`)
- Graders:
  - Shreya Agarwal (`sa6981@nyu.edu`)
  - Jash Rathod (`jsr10000@nyu.edu`)
- All course material, assignment, and exam related questions should be posted on CampusWire
- I will only respond to administration related emails

Assessment

- 4 assignments (40%)
- Midterm Exam (Oct 24) (30%)
- Final Project (30%)
- Extra credits (2%) answer other students' questions in a substantial and helpful way on Campuswire

Homework

- Submit through Gradescope as a **PDF document**
- Late policy: You have 4 late days in total which can be used throughout the semester without penalty (see more details on website).
- You can discuss with other students on the homework assignments, but:
  - Write up the solutions and code on your own;
  - List the names of the students you discussed with.
- If your solution or code is substantially similar to other students then the incident will be reported to the University.

Final Project

- Groups of maximum three students.
- Goals:
  - Find or collect a dataset (can be related to your area of study/research)
  - Survey existing approaches
  - Apply a set of ML algorithms in real applications
  - Compare and analyze performance
- Project rubric will be posted.
- Project proposal due Friday, Oct 27, 2023, 11:59PM
- Last lecture: Project presentation
- Final report due Wednesday, Dec 15, 2023, 11:59PM

Prerequisites

- Multivariate Calculus: partial derivatives/gradient.
- Linear Algebra: vector/matrix manipulations, properties.
- Probability Theory: common distributions; Bayes Rule.
- Statistics: expectation, variance, covariance, median; maximum likelihood.
- Programming: Python, numpy

Course Overview and Goals

Syllabus (Tentative)

12 weeks of instruction + 1 week midterm exam + 1 week project presentation

- 2 weeks: introduction to **machine learning**, **optimization**
- 2 weeks: **Linear** methods for binary classification and regression (also **kernel methods)**
- 2 weeks: **Probabilistic models**, **Bayesian** methods
- 1 week: **Multiclass** classification and introduction to **structured prediction**
- 3 weeks: **Nonlinear** methods (**trees**, **ensemble** methods, and **neural networks**)
- 1 week: **Unsupervised** learning: **clustering** and **latent variable** models
- 1 week: **Reinforcement** learning
- More detailed schedule on the course website (still subject to change)

The high level goals of the class

- Our focus will be on the fundamental building blocks of machine learning
- Understand what kind of problems can ML help solve
- Accomodate different types of input, output, problem characteristics
- Understand the pros & cons of each method, understand the motivation why we choose one method over the other
- Fancy new methods are often combination of basic techniques
- Apply and develop ML algorithms in practical problems

The level of the class

- Many ML algorithms have been implemented in standard libraries (e.g. sklearn)
- Many people only know how to call these library functions.
- We will learn how to implement each ML algorithm **from scratch** using numpy alone, without any ML libraries.
- Once we have implemented an algorithm from scratch once, we will use the sklearn version.

Introduction to Machine Learning

What is learning?

"The activity or process of gaining knowledge or skill by studying, practicing, being taught, or experiencing something."

Merriam Webster dictionary

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

Tom Mitchell

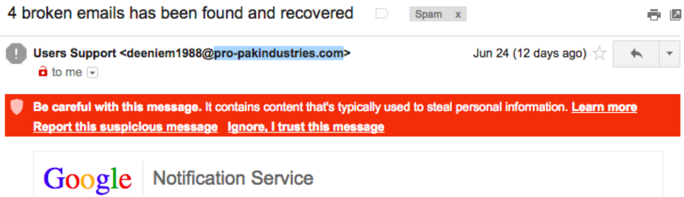
Machine learning as meta-programming

- For many problems, it's difficult to program the correct behavior by hand
  - recognizing people and objects
  - understanding human speech
- Machine learning approach: program an algorithm to automatically learn from data, or from experience, and output a program, typically to solve a prediction problem:
  - Given an **input** x,
  - **Predict** an **output** y.
- Why might you want to use a learning algorithm?
  - hard to code up a solution by hand (e.g. vision, speech)
  - system needs to adapt to a changing environment (e.g. spam detection)
  - want the system to perform *better* than the human programmers
  - privacy/fairness (e.g. ranking search results)

Example: Spam Detection

Let's start with a few canonical examples.

- **Input x:** Incoming email



4 broken emails has been found and recovered

Users Support <deeniem1988@pro-pakindustries.com>

to me

Jun 24 (12 days ago)

Be careful with this message. It contains content that's typically used to steal personal information. Learn more

Report this suspicious message Ignore, I trust this message

Google Notification Service

- **Output y:** "SPAM" or "NOT SPAM"
- This is a **binary classification** problem: there are two possible outputs.

Example: Medical Diagnosis

- **Input x:** Symptoms (fever, cough, fast breathing, shaking, nausea, ...)
- **Output y:** Diagnosis (pneumonia, flu, common cold, bronchitis, ...)
- A **multiclass classification** problem: choosing an output out of a *discrete* set of possible outputs.

How do we express uncertainty about the output?

- **Probabilistic classification** or **soft classification**:

$$\begin{aligned} \mathbb{P}(\text{pneumonia}) &= 0.7 \\ \mathbb{P}(\text{flu}) &= 0.2 \\ \vdots \quad & \quad \vdots \end{aligned}$$

Example: Predicting a Stock Price

- **Input x:** History of the stock's prices
- **Output y:** The price of the stock at the close of the next day
- This is called a **regression** problem (for historical reasons): the output is *continuous*.

Comparison to Rule-Based Approaches (Expert Systems)

Consider the problem of medical diagnosis.

1. Talk to experts (in this case, medical doctors).
2. Understand how the experts come up with a diagnosis.
3. Implement this process as an algorithm (a **rule-based system**): e.g., a set of symptoms $\rightarrow$ a particular diagnosis.
4. Use logical deduction to infer new rules from the rules that are stored in the knowledge base.

Rule-Based Approach

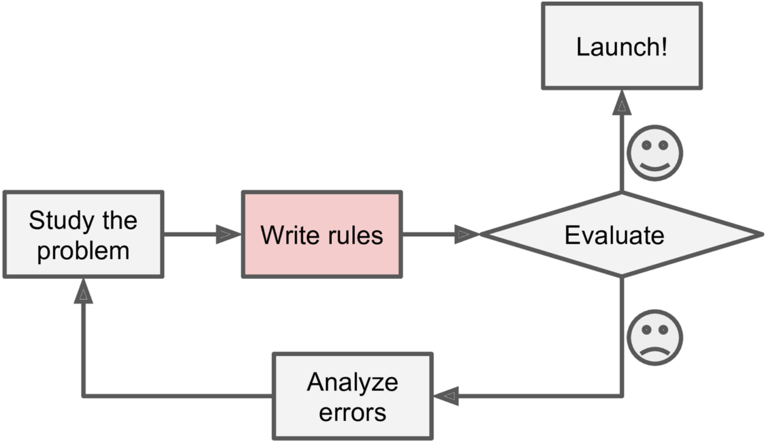


Fig 1-1 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

Advantages of Rule-Based Approaches

- Leverage existing domain expertise.
- Generally **interpretable**: We can describe the rule to another human
- Produce reliable answers for the scenarios that are included in the knowledge bases.

Limitations of Rule-Based Systems

- Labor intensive to build: experts' time is expensive.
- Rules work very well for areas they cover, but often do not **generalize** to unanticipated input combinations.
- Don't naturally handle uncertainty.

The Machine Learning Approach

- Instead of explicitly engineering the process that a human expert would use to make the decision...
- We have the machine **learn** on its own from inputs and outputs (decisions).
- We provide **training data**: many examples of (input x , output y) pairs, e.g.
    - A set of videos, and whether or not each has a cat in it.
    - A set of emails, and whether or not each one should go to the spam folder.
- Learning from training data of this form (inputs and outputs) is called **supervised learning**.

Machine Learning Algorithm

- A **machine learning algorithm** learns from the training data:
  - **Input**: Training Data (e.g., emails x and their labels y)
  - **Output**: A prediction function that produces output y given input x.
- The goal of machine learning is to find the "best" (to be defined) prediction function **automatically, based on the training data**
- The success of ML depends on
  - The availability of large amounts of data;
  - **Generalization** to unseen samples (the test set): just memorizing the training set will not be useful.

Machine Learning Approach

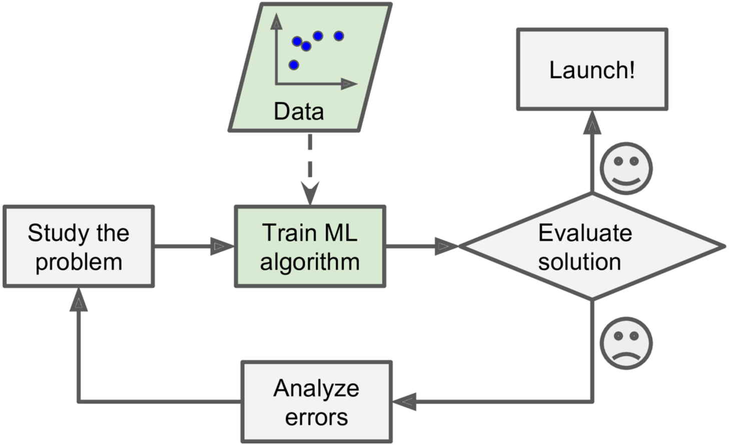


Fig 1-2 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

Key concepts

- The most common **ML problem types**:
  - Classification (binary and multiclass)
  - Regression
- **Prediction function**: predicts output y (e.g. spam or not?) given input x (e.g. email)
- **Training data**: a set of (input x, output y) pairs
- **Supervised learning algorithm**: takes training data and produces a prediction function
- Beyond prediction
  - **Unsupervised learning**: finding structures in data, e.g. clustering
  - **Reinforcement learning**: optimizing long-term objective, e.g. Go
  - **Representation learning**: learning good features of real-world objects, e.g. text

Core Questions in Machine Learning

Given any task, the following questions need to be answered:

- **Modeling**: What class of prediction functions are we considering?
- **Learning**: How do we learn the “best” prediction function in this class from our training data?
- **Inference**: How do we compute the output of the prediction function for a new input?

Relations to statistics

- It's similar to statistics...
  - Both fields try to uncover patterns in data
  - Both fields draw heavily on calculus, probability, and linear algebra, and share many of the same core algorithms
- But it's not statistics...
  - Stats is more concerned with **helping scientists and policymakers** draw good conclusions; ML is more concerned with **building autonomous agents**
  - Stats puts more emphasis on **interpretability and mathematical rigor**; ML puts more emphasis on predictive **performance, scalability, and autonomy**

Relations to AI

- Nowadays, “machine learning” is often brought up with “artificial intelligence” (AI)
- AI does not often imply a learning based system
  - Symbolic reasoning
  - Rule based system
  - Tree search
  - etc.
- Learning based system → learned based on the data → more flexibility, good at solving pattern recognition problems.

Relations to human learning

- It is tempting to imagine machine learning as a component in AI just like human learning in ourselves.
- Human learning is:
  - Very data efficient
  - An entire multitasking system (vision, language, motor control, etc.)
  - Flexible to adapt new skills
  - Takes at least a few years :)
- For serving specific purposes, machine learning doesn't have to look like human learning in the end.
- Machines may borrow ideas from biological systems (e.g. neural networks).

History of machine learning

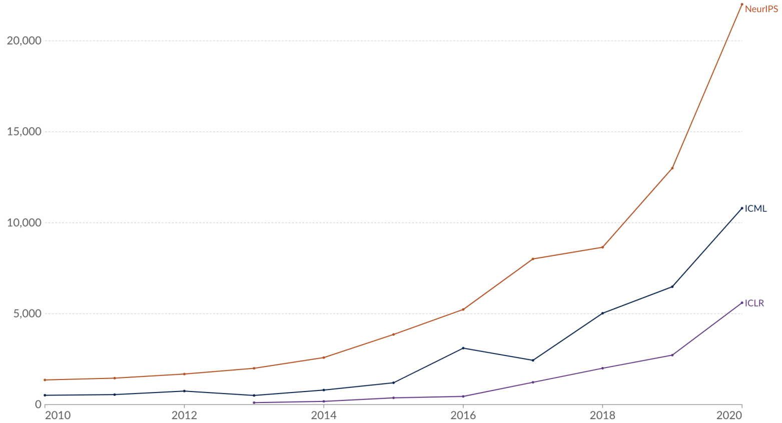
- 1957 — Perceptron algorithm (implemented as a circuit!)
- 1959 — Arthur Samuel wrote a learning-based checkers program that could defeat him
- 1969 — Minsky and Papert's book *Perceptrons* (limitations of linear models)
- 1980s — Some foundational ideas
  - Connectionist psychologists explored neural models of cognition
  - 1984 — Leslie Valiant formalized the problem of learning as PAC learning
  - 1988 — Backpropagation (re-)discovered by Geoffrey Hinton and colleagues
  - 1988 — Judea Pearl's book *Probabilistic Reasoning in Intelligent Systems* introduced Bayesian networks
- 1990s — the "AI Winter", a time of pessimism and low funding

History of machine learning

- A lot of practical ML algorithms were invented in the 90s: CNNs, SVMs, boosting, etc.
- 2000s — applied AI fields (vision, NLP, etc.) adopted ML
- 2010s — deep learning
  - 2010–2012 — neural nets smashed records in speech-to-text and object recognition
  - Increasing adoption by the tech industry, many downstream problems
  - 2014 — GANs and generative AI
  - 2016 — AlphaGo defeated the human Go champion
  - 2018–2020 — AlphaFold predicts protein structure
  - 2022 — ChatGPT, chatbot, general intelligence

History of machine learning

Top ML conferences attendance over year:



Supervised Learning Setup

ML problems

In supervised learning problems, we generally need to:

- Make a decision:
  - Move email to spam folder?
- Take an action:
  - In a self-driving car, make a right turn
  - Reject the hypothesis that $\theta = 0$ (classical statistics)
- Produce some output:
  - Whose face is it in the image?
  - The Hindi translation of a Japanese input sentence
- Predicting where a storm will be in an hour (what forms of output are possible here?)

Outcome

Inputs are often paired with **labels**.

Examples of labels

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

Evaluation Criterion

Finding "optimal" outputs, under various definitions of optimality.

Examples of Evaluation Criteria

- Is the classification correct?
- Does the transcription exactly match the spoken words?
  - Should we give partial credit (for getting only some of the words right)? How?
- How far is the storm from the predicted location? (If we're producing a point estimate)
- How likely is the storm's actual location under the predicted distribution? (If we're doing density prediction)

Typical Sequence of Events

Many problem domains can be formalized as follows:

1. Observe input x.
2. Predict an output $\hat{y}$.
3. Observe label y.
4. Evaluate output in relation to the label.

Formalization

Prediction Function

A **prediction function** gets input $x \in \mathcal{X}$ and produces an output $y \in \mathcal{Y}$.

Loss Function

A **loss function** evaluates the output $\hat{y}$ in the context of the true outcome y.

Evaluating a Prediction Function

Goal: Find the optimal prediction function.

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

- The loss function ℓ evaluates a *single* output
- How do we evaluate the prediction function *as a whole*?

Loss Function

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 $P_{\mathcal{X} \times \mathcal{Y}}$.

One common desideratum is to have a 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 $f : \mathcal{X} \to \mathcal{Y}$ 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 $P_{\mathcal{X}\times\mathcal{Y}}$.

- 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** $f^* : \mathcal{X} \to \mathcal{Y}$ 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 $\mathcal{Y}$.

- 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: $\mathcal{Y} = \{1, \ldots, k\}$
- 0-1 loss:

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

- 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.

- The Bayes prediction function returns the most likely class:

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

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** $P_{\mathcal{X}\times\mathcal{Y}}$.
- One thing we can do in ML/statistics/data science is **estimate** it:

Assume we have sample data:

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

- We draw 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.

The Empirical Risk

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 $f : \mathcal{X} \to \mathcal{Y}$ 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

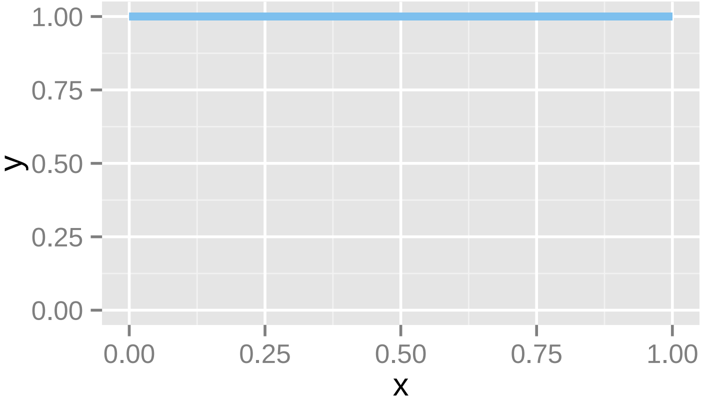
$$\hat{f} \in \arg\min_{f} \hat{R}_n(f),$$

where the minimum is taken over all functions $f : \mathcal{X} \to \mathcal{Y}$.

- In an ideal world we'd want to find the risk minimizer.
- Is the empirical risk minimizer close enough?
- In practice, we always only have a finite sample...

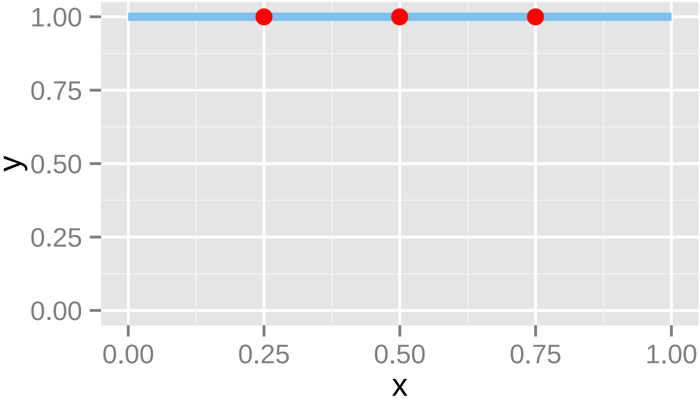
Empirical Risk Minimization

- $P_{\mathcal{X}} = \text{Uniform}[0,1]$, $Y \equiv 1$ (i.e. Y is always 1).
- A plot of $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$:



Empirical Risk Minimization

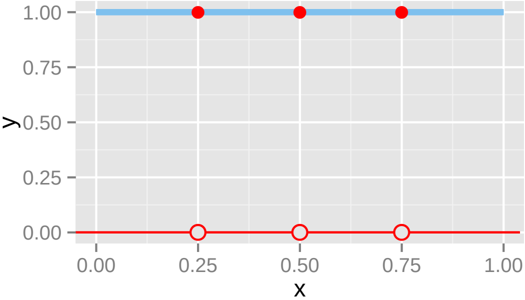
$P_{\mathcal{X}} = \text{Uniform}[0,1]$, $Y \equiv 1$ (i.e. Y is always 1).



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).

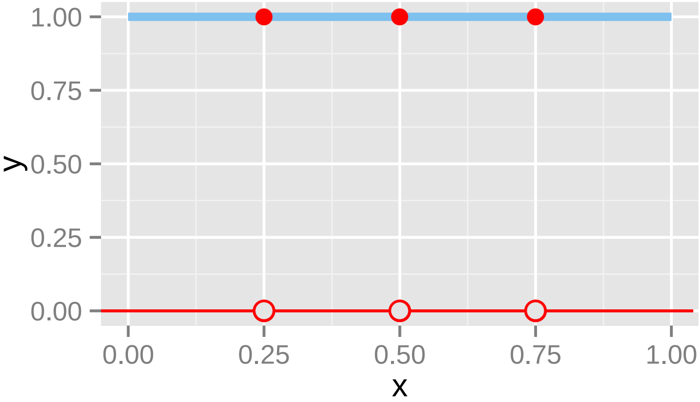


A proposed prediction function:

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

Empirical Risk Minimization

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



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

Empirical Risk Minimization

- In this case, ERM led to a function f that just memorized the data.
- How can we improve **generalization** from the training inputs to new inputs?
- We 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 is **constrained ERM**:
  - Instead of minimizing empirical risk over *all* prediction functions,
  - We constrain our search to a particular subset of the space of functions, called a **hypothesis space**.

Hypothesis Spaces

Definition

A **hypothesis space** $\mathcal{F}$ is a set of prediction functions $\mathcal{X} \to \mathcal{Y}$ that we consider when applying ERM.

Desirable properties of a hypothesis space:

- Includes only those functions that have the desired "regularity", e.g. smoothness, simplicity
- Easy to work with (e.g., we have efficient algorithms to find the best function within the space)

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

Constrained Empirical Risk Minimization

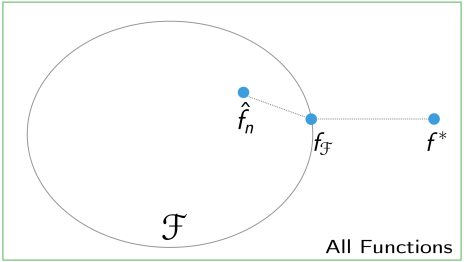
- Given a hypothesis space $\mathcal{F}$, a set of prediction functions mapping $\mathcal{X} \to \mathcal{Y}$,
- An **empirical risk minimizer** (ERM) in $\mathcal{F}$ is a function $\hat{f}_n$ such that

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

- A **risk minimizer** in $\mathcal{F}$ is a function $f_{\mathcal{F}}^* \in \mathcal{F}$ such that

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

Excess Risk Decomposition



$$f^* = \underset{f}{\arg\min}\, \mathbb{E}\left[\ell(f(x), y)\right]$$

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

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

- **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:

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

- There is a tradeoff between estimation error and approximation error

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

- What have we been glossing over by writing "argmin"?
- In practice, we need a method to find $\hat{f}_n \in \mathcal{F}$: this can be very difficult!
- For nice choices of loss functions and classes $\mathcal{F}$, we can get arbitrarily close to the exact minimizer
    - But that takes time – is it always 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

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

Error Decomposition in Practice

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

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

- How would we address each type of error?

ERM Overview

- Given a loss function ℓ,
- Choose a hypothesis space $\mathcal{F}$.
- Use an optimization method to find an empirical risk minimizer $\hat{f}_n \in \mathcal{F}$:

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

- Or find a $\tilde{f}_n$ that comes close to $\hat{f}_n$
- The machine learning scientist's job:
  - Choose $\mathcal{F}$ that balances approximation and estimation error.
  - As we get more training data, we can use a bigger $\mathcal{F}$.