Introduction to Machine Learning

Mengye Ren

NYU

September 3, 2024

Contents

Logistics

- Class webpage: https://nyu-cs2565.github.io/2024-fall
  - Course materials (lecture slides, homeworks) will be made available on the website
- Discussion / questions on CampusWire: https://campuswire.com/p/G4788841F

8275

https://campuswire.com/p/G4788841F

- Sign up to Gradescope to submit homework assignments (entry code **Z3PB2W**)
- Office Hour: Thursday 1:00-2:00 pm, Room 508, 60 Fifth Ave.

Logistics

Course Staff

- Instructor:
  - Mengye Ren (mr3182@nyu.edu)
- Graders:
  - Pavan Ravishankar (pr2248@nyu.edu)
  - Yilun Kuang (yk2516@nyu.edu)
- All course material, assignment, and exam related questions should be posted on CampusWire.
- Assignment regrade requests should be initiated on Gradescope. Further questions directed to the graders.
- I will only respond to administration related emails.

Assessment

- 4 assignments (40%)
- Midterm Exam (Oct 22) (30%)
- Final Project (30%)
- Extra credits (2%) answer other students' questions in a substantial and helpful way on Campuswire

100%

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 3 students (by Oct 22, after the midterm).
- Goals:
  - Find a problem and a dataset
  - Survey existing approaches, identify remaining challenges
  - Apply and design ML algorithms in real applications
  - Compare and analyze empirical performance
- Project proposal due Oct 29, 2024, 12PM (Noon)
- Last lecture: Project presentation
- Final report due Wednesday, Dec 13, 2024, 12PM (Noon)

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

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- 1 week: **Unsupervised** learning: **clustering** and **latent variable** models

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- 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."

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“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
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  - Given an **input** x,
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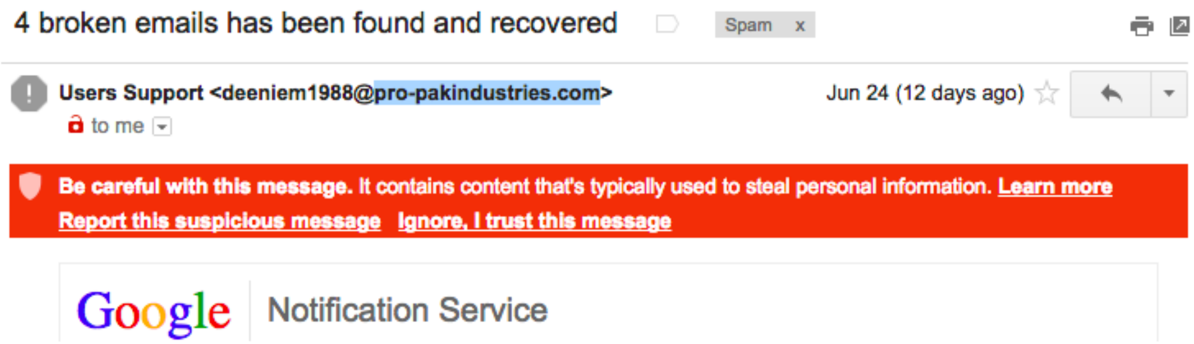
- Why might you want to use a learning algorithm?
  - hard to code up a solution by hand (e.g. vision, speech)
  - system needs to adapt to a changing environment (e.g. spam detection)
  - want the system to perform *better* than the human programmers
  - privacy/fairness (e.g. ranking search results)

Example: Spam Detection

Let's start with a few canonical examples.

- **Input x:** Incoming email



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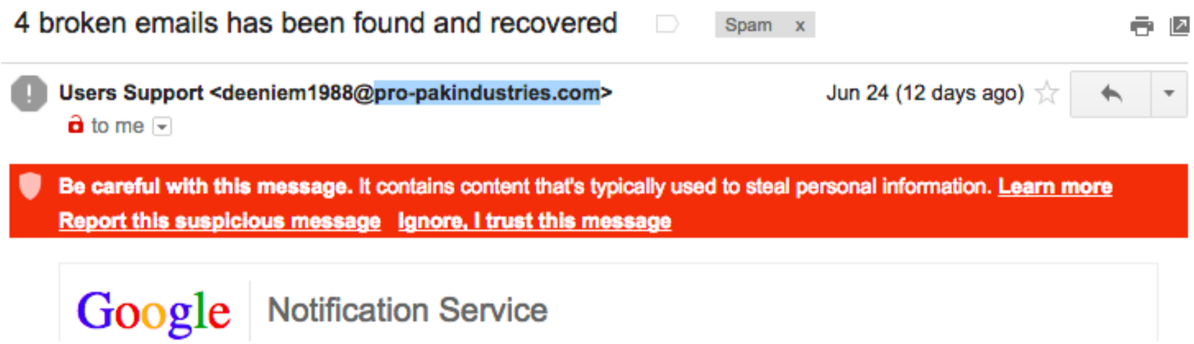

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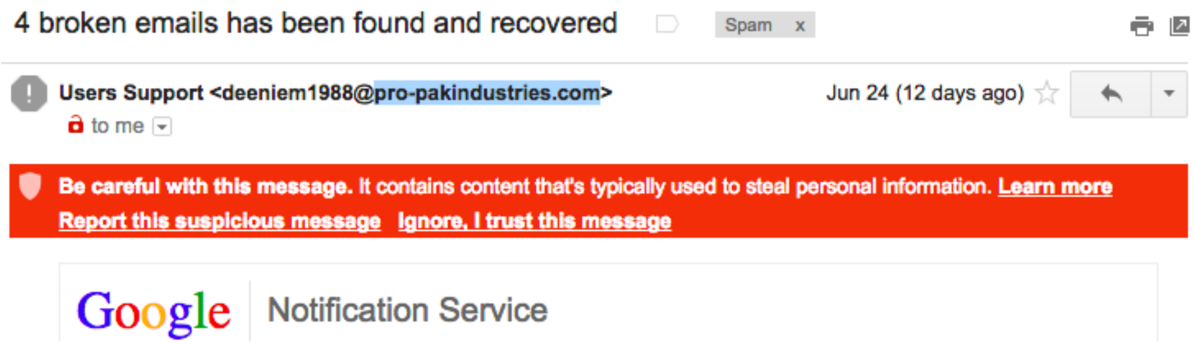

- **Output y:** "SPAM" or "NOT SPAM"
- This is a **binary classification** problem: there are two possible outputs.

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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

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- **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*.

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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

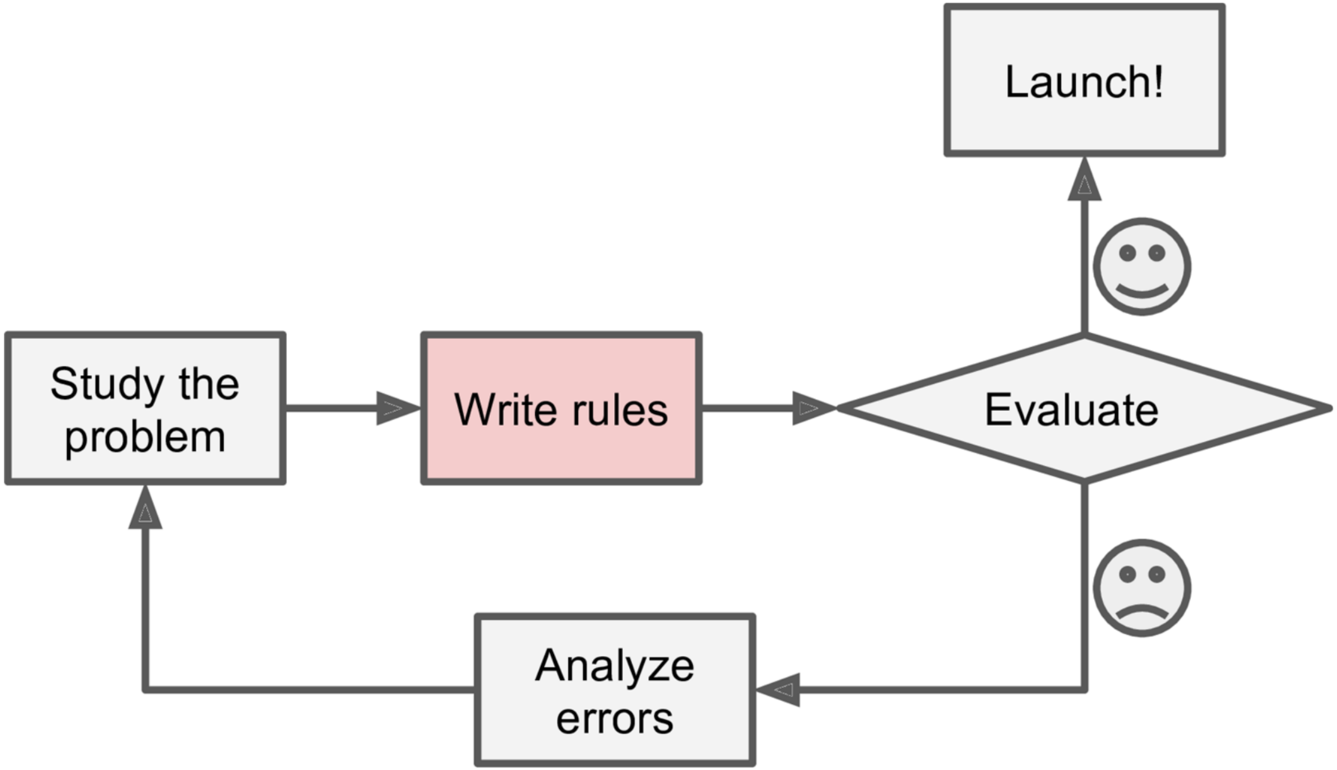

Fig 1-1 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

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- Leverage existing domain expertise.
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- Produce reliable answers for the scenarios that are included in the knowledge bases.

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- Don't naturally handle uncertainty.

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- We have the machine **learn** on its own from inputs and outputs (decisions).

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- 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. Cat detector
  - 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**.

Correct output

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.
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- 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

add data
clean data
improve algorithm

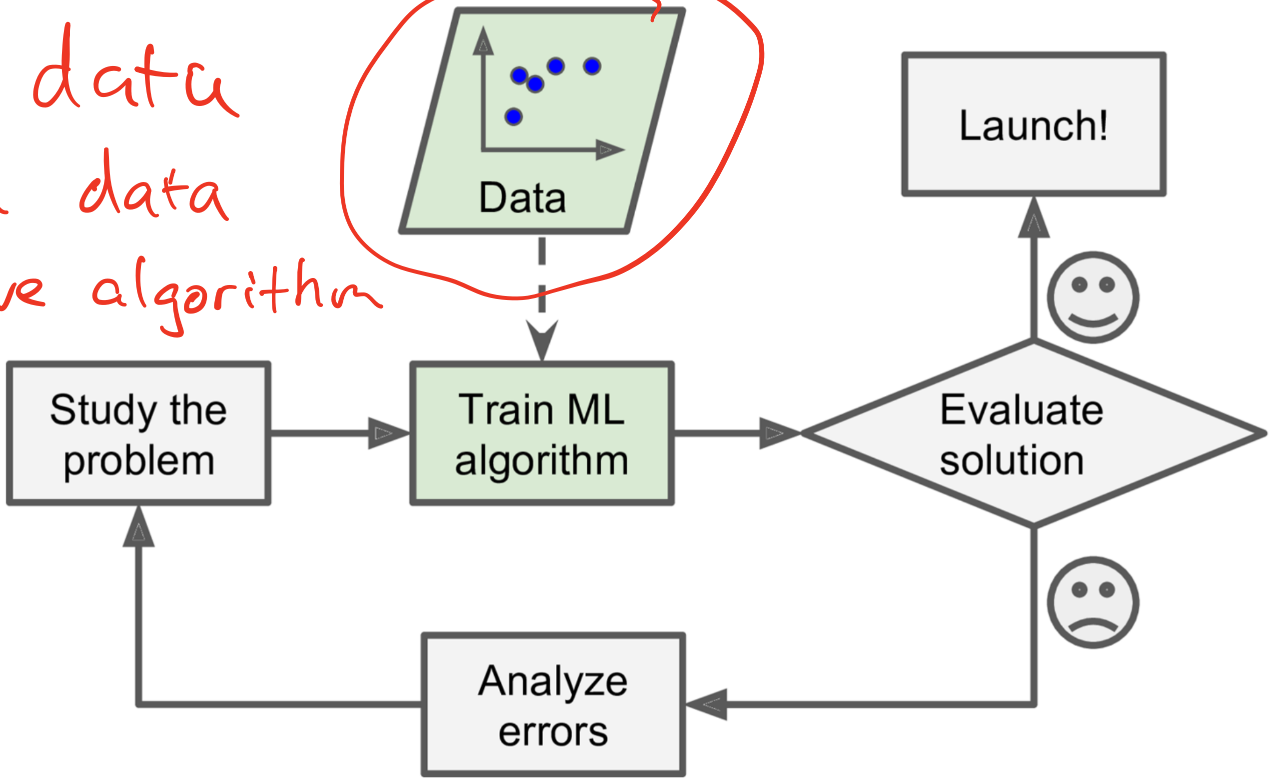

Fig 1-2 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

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  - **Representation learning**: learning good features of real-world objects, e.g. text

Core Questions in Machine Learning

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Linear function

$\boxed{y = W \cdot x}$

$\mathbb{R}^D$ input $\in \mathbb{R}^D$

(0, 0)
(0, 1)
(0.5, 0.5)

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- **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

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- 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**

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- Learning based system $\rightarrow$ learned based on the data $\rightarrow$ more flexibility, good at solving pattern recognition problems.

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  - An entire multitasking system (vision, language, motor control, etc.)
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- Machines may borrow ideas from biological systems (e.g. neural networks).

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- 1957 — Perceptron algorithm (implemented as a circuit!)
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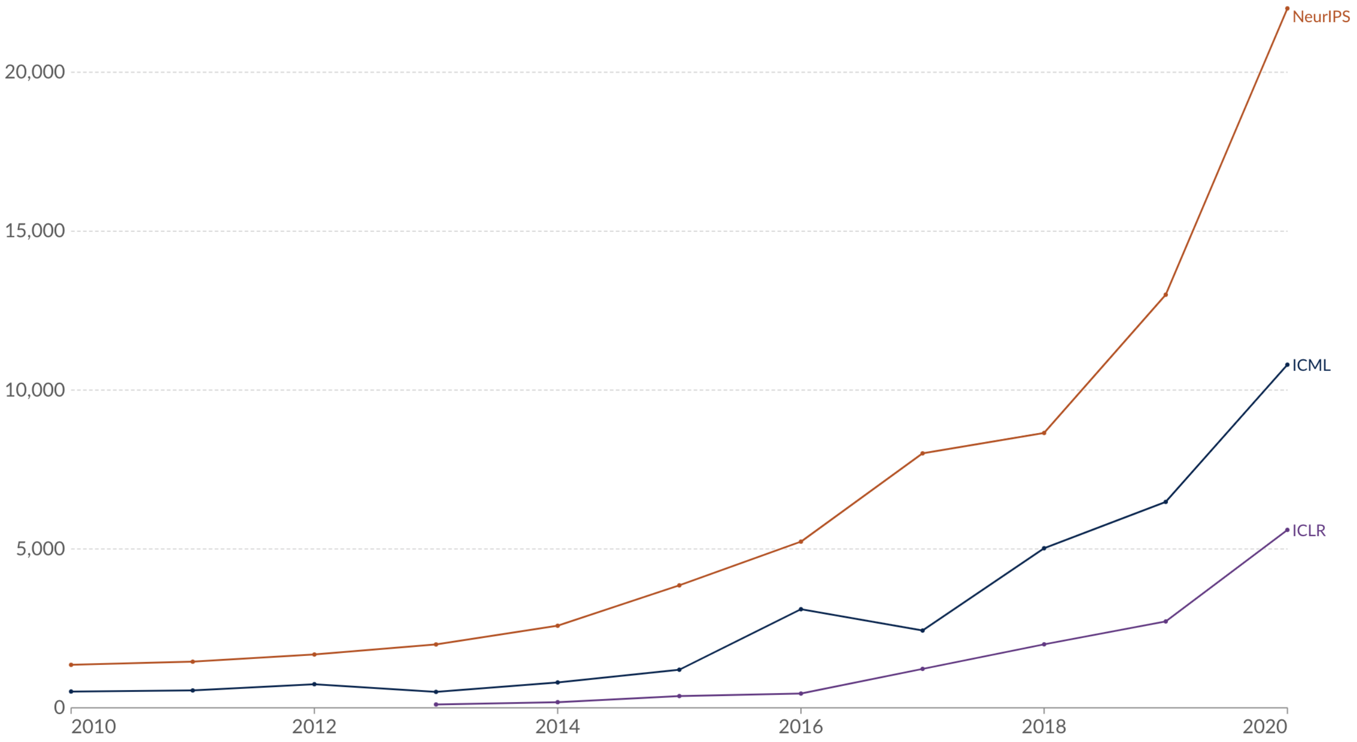
  - 2022 — ChatGPT, chatbot, general intelligence

History of machine learning

Top ML conferences attendance over year:



Supervised Learning Setup

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- Predicting where a storm will be in an hour (what forms of output are possible here?)

Outcome

target
Correct output
ground truth

provided by human "labeler"

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? "Accuracy" 90%.
- 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. $\hat{y}$, y

Formalization

Prediction Function

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

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Loss Function

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

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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.

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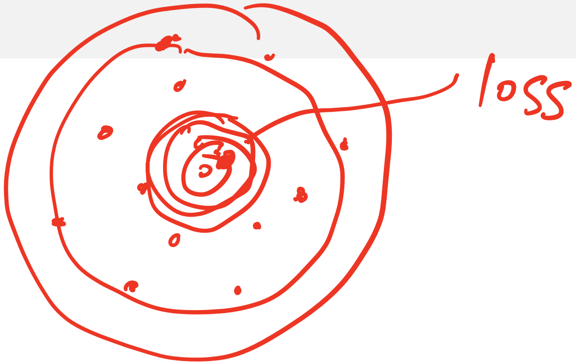
- The loss function ℓ evaluates a *single* output
- How do we evaluate the prediction function *as a whole*?

Loss Function



Define a space where the prediction function is applicable

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

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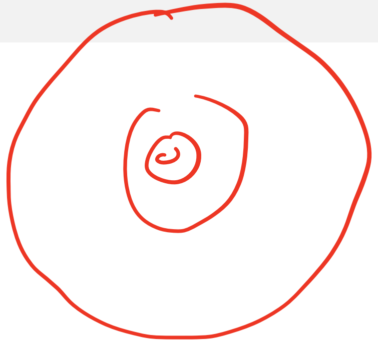

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One common desideratum is to have a prediction function $f(x)$ that "does well on average":

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

How can we formalize this? f input true output

predicted out

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 $\boxed{P_{\mathcal{X} \times \mathcal{Y}}}$, we cannot compute the expectation.

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- 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:

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

$P_{X \times Y}$

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:

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

Example: Multiclass Classification

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

$$\ell(\hat{y}, y) = \mathbb{1}[\underbrace{\hat{y} \neq y}_{\text{incorrectness}}] := \begin{cases} 1 & \text{if } \hat{y} \neq y \\ 0 & \text{otherwise.} \end{cases}$$

- Risk:

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

inaccuracy.

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!

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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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- 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

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

  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

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

vs. $\mathbb{E}$

true risk.

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

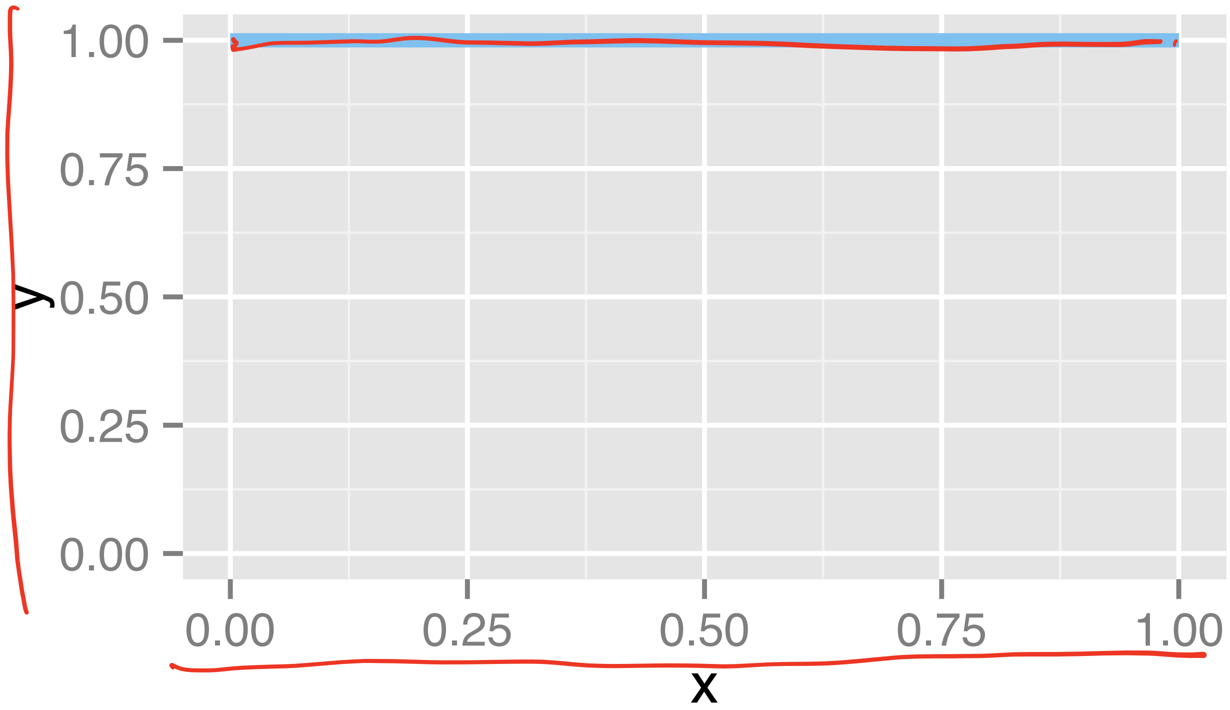
$$\hat{f} \in \arg\min_{f} \hat{R}_n(f),$$

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



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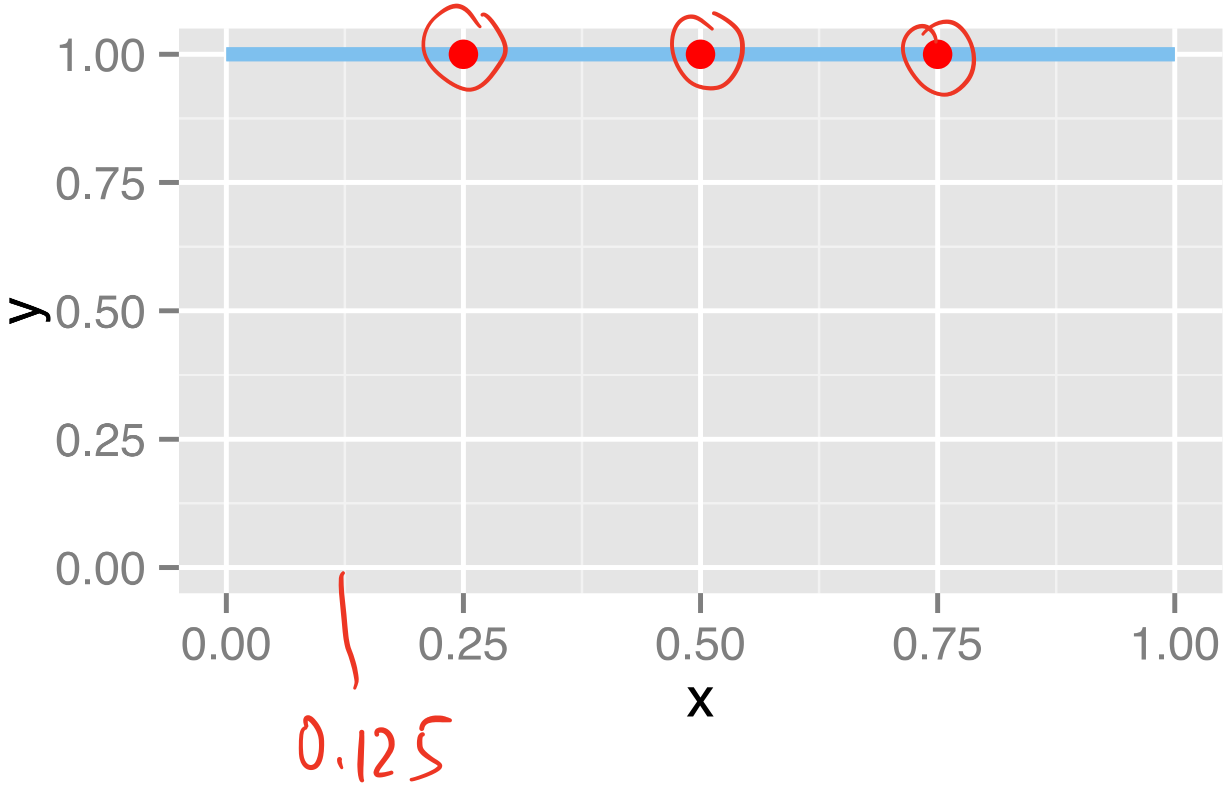

A sample of size 3 from $\mathcal{P}_{\mathcal{X}\times\mathcal{Y}}$.

Empirical Risk Minimization

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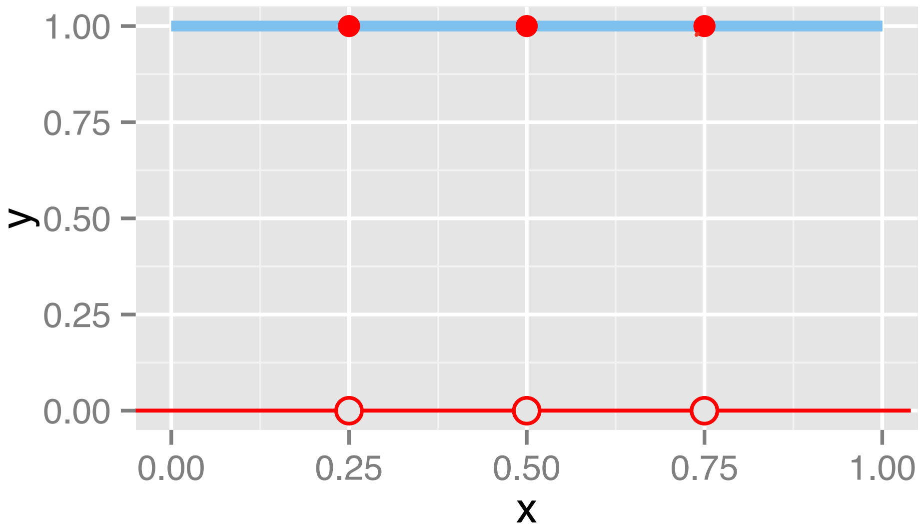

A proposed prediction function:

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

Empirical Risk Minimization

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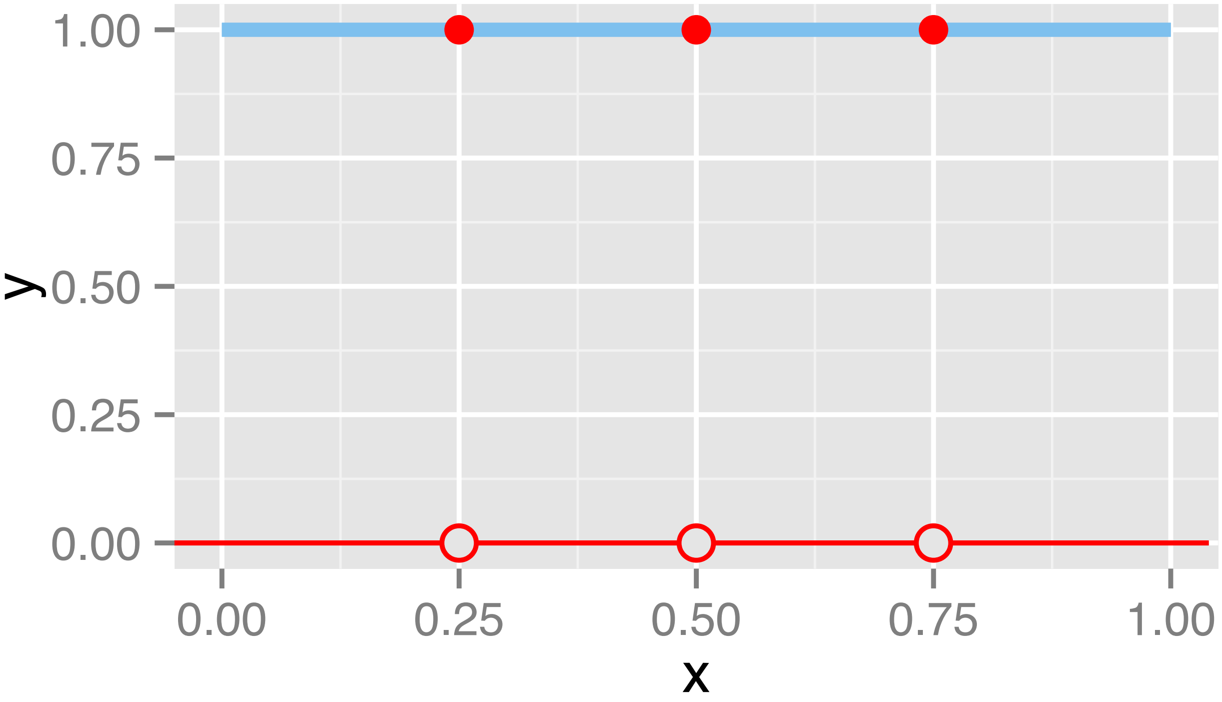


Under either the square loss or the 0/1 loss, $\hat{f}$ has Empirical Risk = 0 and Risk = 1.

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

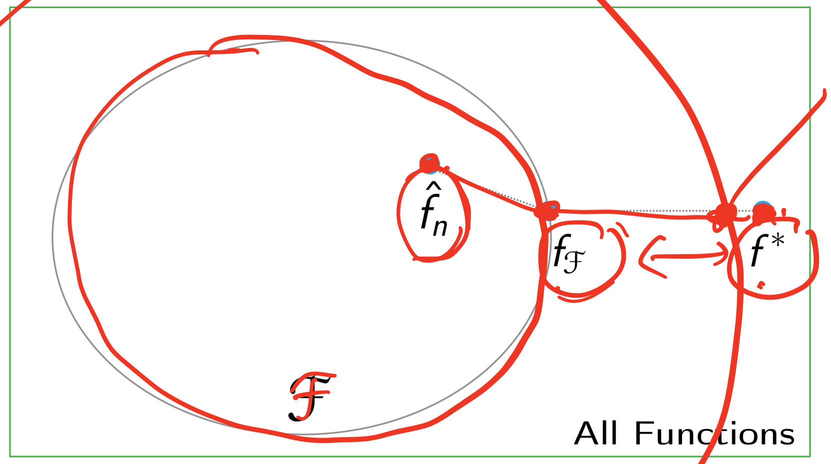
- Given a hypothesis space $\mathcal{F}$, a set of prediction functions mapping $\mathcal{X} \to \mathcal{Y}$,
- An **empirical risk minimizer** (ERM) in $\mathcal{F}$ is a function $\hat{f}_n$ such that

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

- 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



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

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

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

- **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?

func bigger smaller

approx ↓ ↑

est ↑ ↓

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?

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- 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

Output of optimization.

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

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

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- 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 $\mathcal{F}$.