DS-GA 1003: Machine Learning

Lecture 1: Intro & Supervised Learning Framework

Slides adapted from material from David Rosenberg's version of DS-GA 1003.

Outline

Course Overview and Logistics

Introduction to Machine Learning

Statistical Learning Setup

Statistical Learning: Bayes Risk

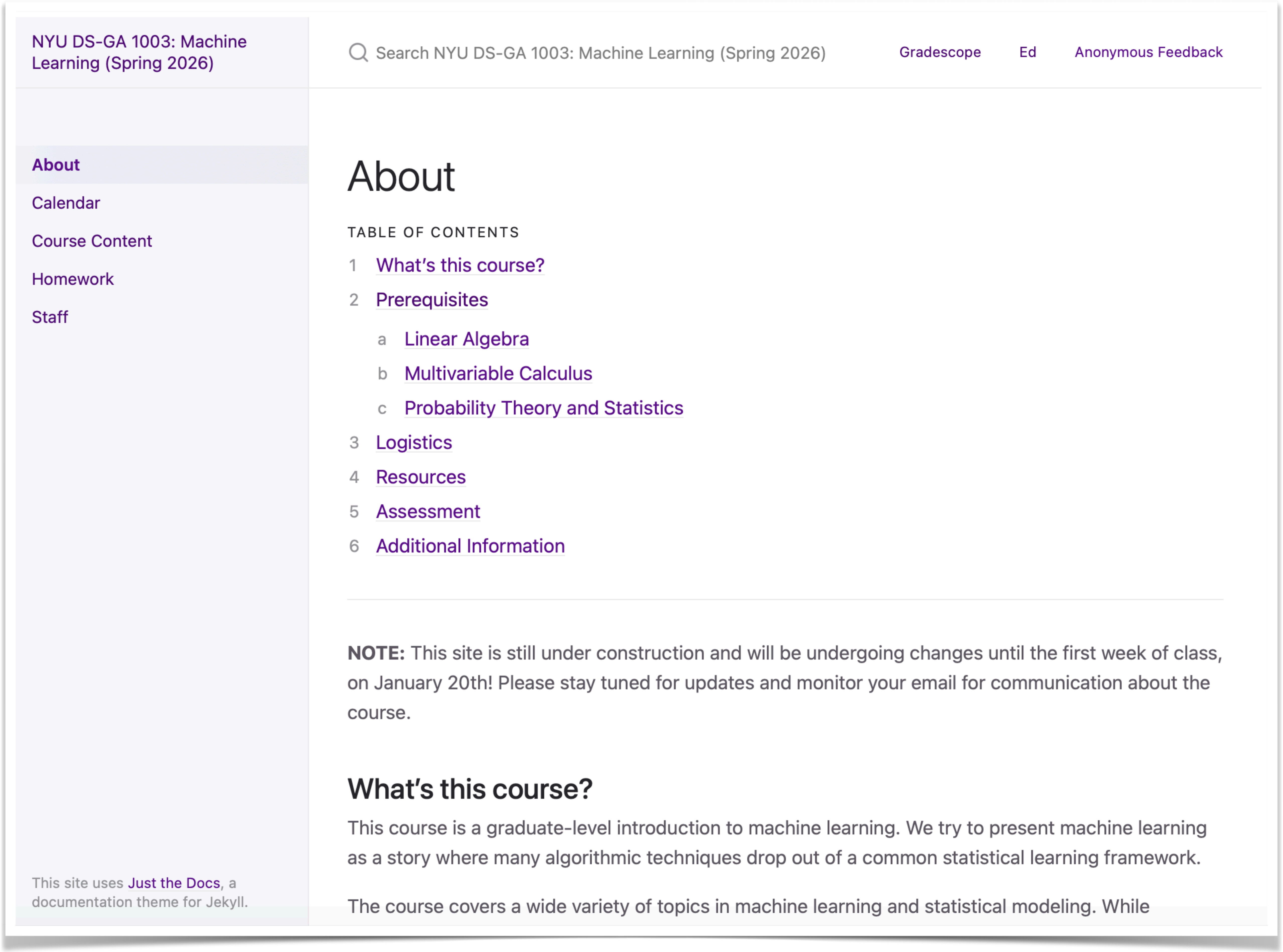
Statistical Learning: Empirical Risk and ERM

Statistical Learning: Hypothesis Class

Excess Risk Decomposition and Three Types of Error

Course Website

https://nyu-dsga-1003.github.io/sp26/



NYU DS-GA 1003: Machine Learning (Spring 2026)

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Gradescope Ed Anonymous Feedback

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About

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NOTE: This site is still under construction and will be undergoing changes until the first week of class, on January 20th! Please stay tuned for updates and monitor your email for communication about the course.

What's this course?

This course is a graduate-level introduction to machine learning. We try to present machine learning as a story where many algorithmic techniques drop out of a common statistical learning framework.

The course covers a wide variety of topics in machine learning and statistical modeling. While

This site uses Just the Docs, a documentation theme for Jekyll.

Staff & Office Hours

8 course staff teaching assistants.

Check the **Staff** page: https://nyu-dsga-1003.github.io/sp26/staff/

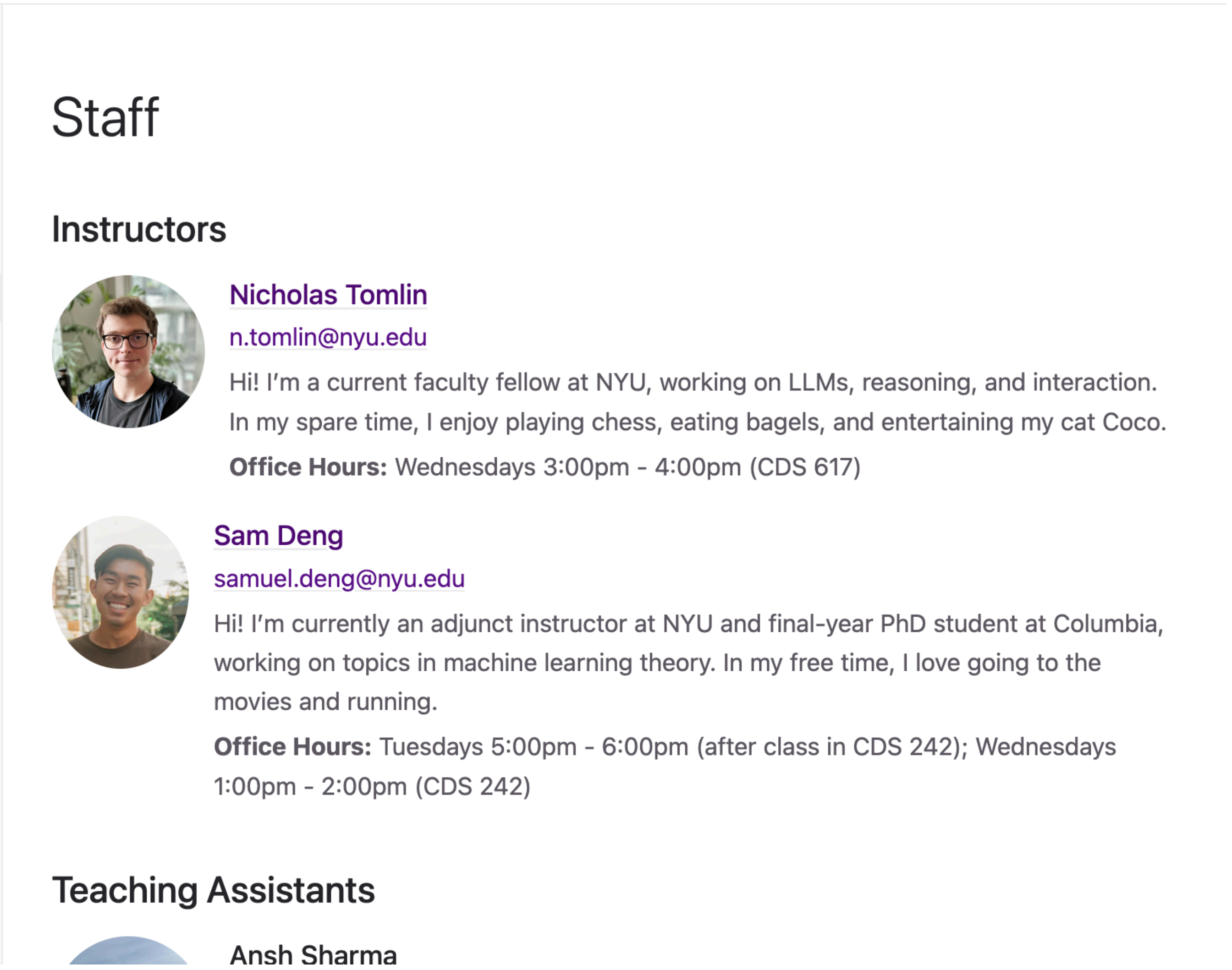
Office hours available every day of the week!

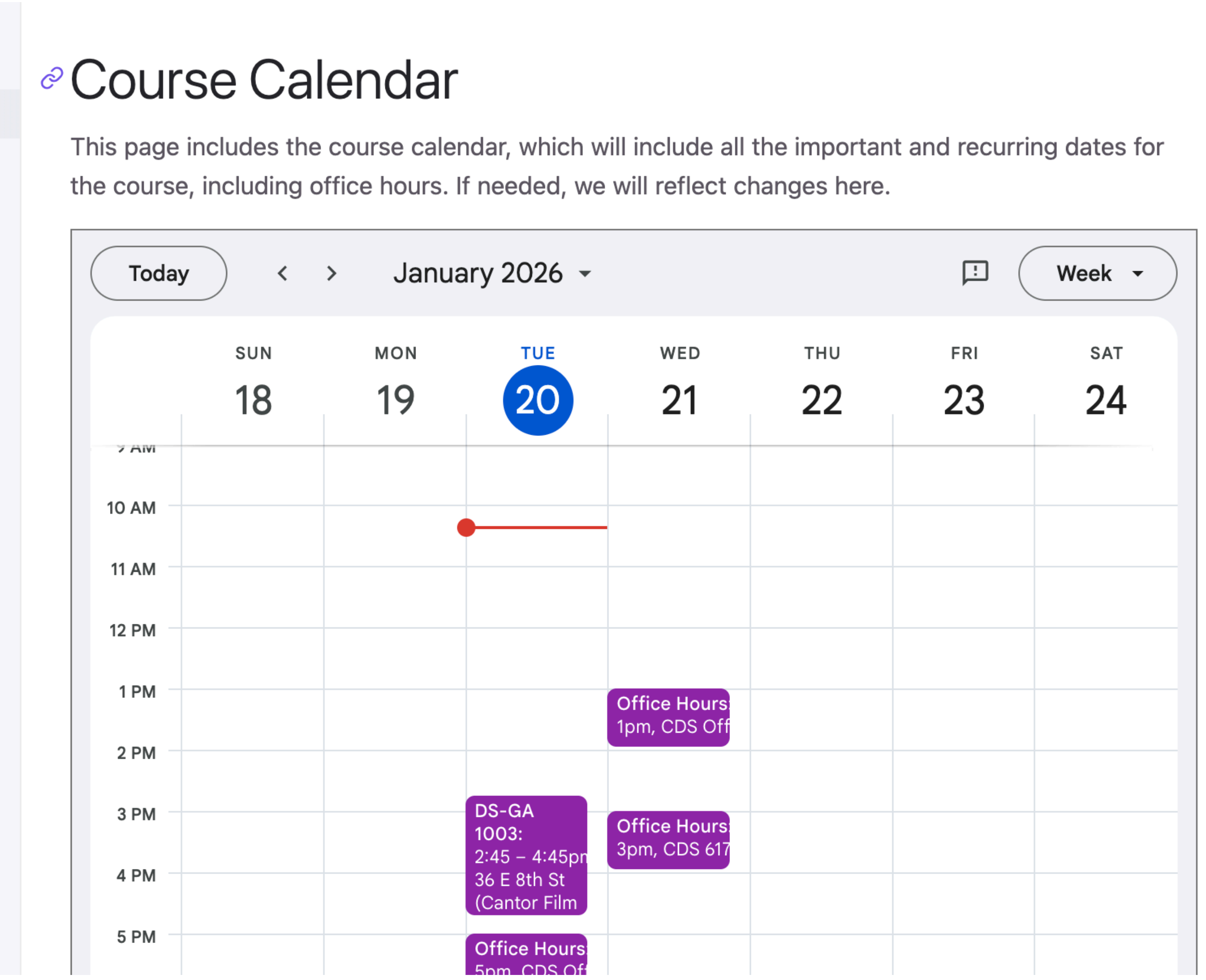
Check the **Calendar** page: https://nyu-dsga-1003.github.io/sp26/calendar/

Strongly welcome and encouraged to come to office hours!

Sam's: Tues 5 - 6pm; Wed 1 - 2pm

Nick's: Wed 3 - 4pm





EdStem

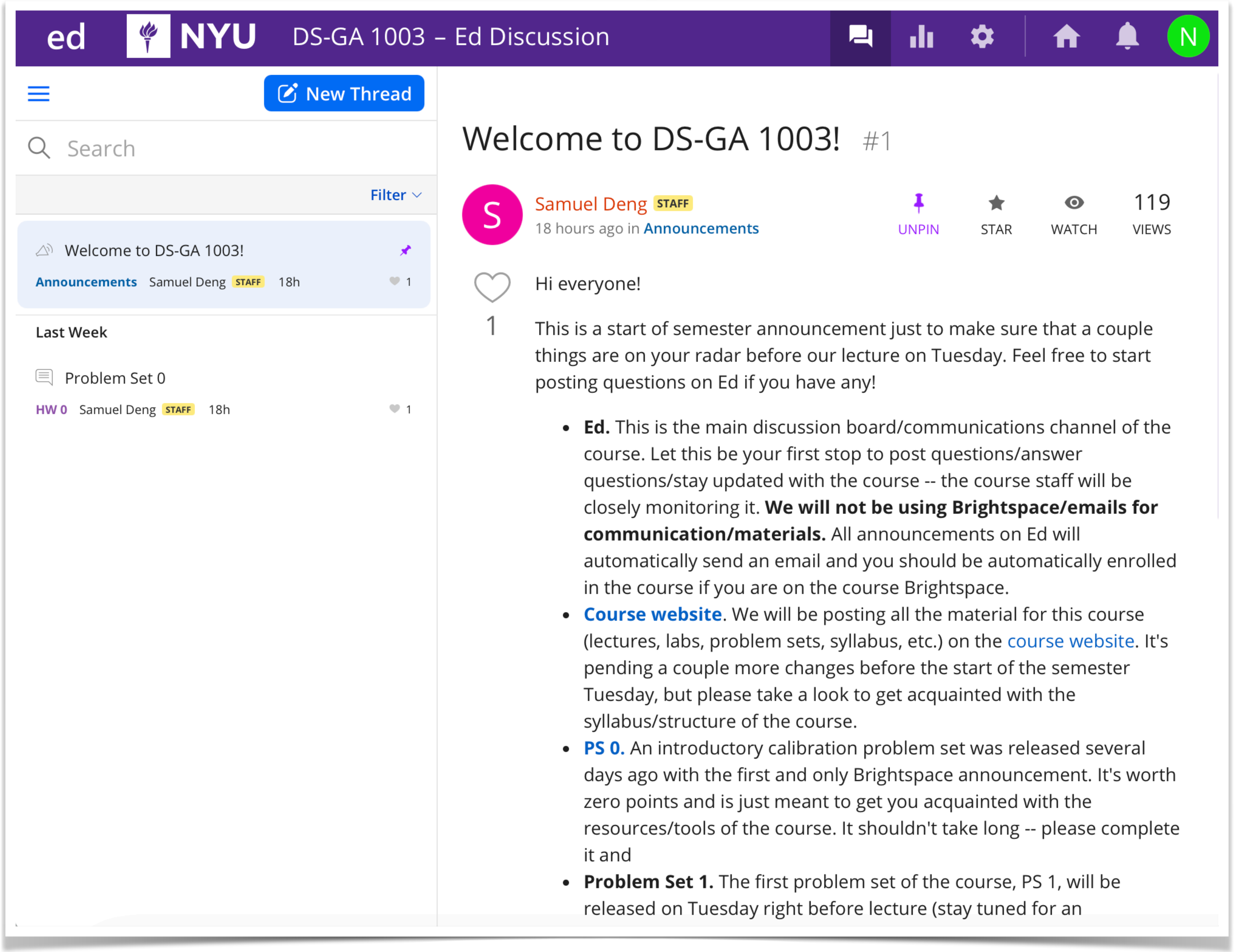
We'll use Ed for all course communications!

By default, please make your questions <u>public</u>; if you have a question, it's likely many other people do too!

If necessary (e.g., if your question reveals the answer to a homework question), post <u>privately</u>

Only email the instructors as a last resort. We are flooded with emails!

<u>*We are not using Brightspace!*</u>



Grading Rubric

Homeworks: 20%

Midterm Exam: 35%

Final Project: 35%

Lab Attendance: 10%

Course Format

Lectures: Tuesdays, 2:45-4:45PM, 36 E 8th St (Cantor Film Ctr) Room 200

Labs (mandatory!): Thursday, 7:10-8PM, 238 Thompson St (GCASL) Room C95

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Lectures:

- Weeks 1-11: “classical ML” (gradient descent, regularization, SVMs, etc.)
- Weeks 12-16: “applied ML” (neural nets, generative models, LLMs, etc.)
- We’ll do our best to post lecture slides and other relevant materials before class!
- Lectures will be recorded (on Brightspace), but we strongly recommend in-person attendance

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Lab grading policy:

- There are 12 labs in total
- You must attend 10+ labs to receive full credit for lab attendance
- You can receive 1 point of extra credit for each additional lab you attend

Midterm

The midterm will be held in-class on Tuesday, March 10th, from 2:45-4:45PM.

IMPORTANT: Please make sure you are available at this time as we will not be able to offer makeup midterms! If you have a conflict, then you should consider not taking this course.

Final Project

Form groups of 2-3 students and write an 8-page paper:

- Track 1: Applied ML - choose a real-world problem, identify how and why machine learning could be helpful, and find or collect a relevant dataset for the problem. Then, establish baselines and compare performance of many different ML techniques learned in class.

- Track 2: Research - identify a gap in the literature for an ML topic of interest, and then propose and execute experiments to address the gap. Then, write a NeurIPS/ICML/ICLR-style paper.

Key dates:

- Groups formed for projects: Feb 28th

- Project proposal (~2 pages): March 31st

- Final project submitted: May 8th

Homeworks

Seven homeworks, plus Homework 0 (“Submitting and typesetting your homework”)

You will have roughly two weeks to complete each homework once it is assigned

Late policy:

- You have 6 late days in total across the semester; if you want to submit 1-2 days late but have already used your late days, you will incur a 20% grade penalty per day
- However, you can use a maximum of 2 late days per homework. Gradescope will close 48 hours after the assignment deadline
- You can drop your lowest homework grade

Homeworks

1. Regression & Statistical Learning
2. Regularization & GD
3. Linear Classification & SVM
4. MLE & Conditional Probability Models
5. Decision/RFs & Boosting
6. NNs
7. Generative Models & RL

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Homeworks

In this section, we will post the biweekly homeworks for the semester. Check back here for the latest problem set!

Homework 0

Material:	Submitting & typesetting your homework	ps0-submission.zip, ps0.pdf
Release:	Monday, January 12th, 7:30 PM ET	
Due:	Friday, January 23rd, 11:59 PM ET	

Homework 1

Material:	Error decomposition and regression	ps1-statlearning.zip, ps1.pdf
Release:	Tuesday, January 20th, 2:30 PM ET	
Due:	Tuesday, February 3rd, 11:59 PM ET	

Homeworks

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LLM Policy

Don't use LLMs

LLM Policy

You are not allowed to use LLMs like ChatGPT or Cursor for homework or final projects

LLMs are great! But there's a growing body of evidence that LLMs can harm learning

Using LLMs on homeworks may leave you unprepared for the midterm exam

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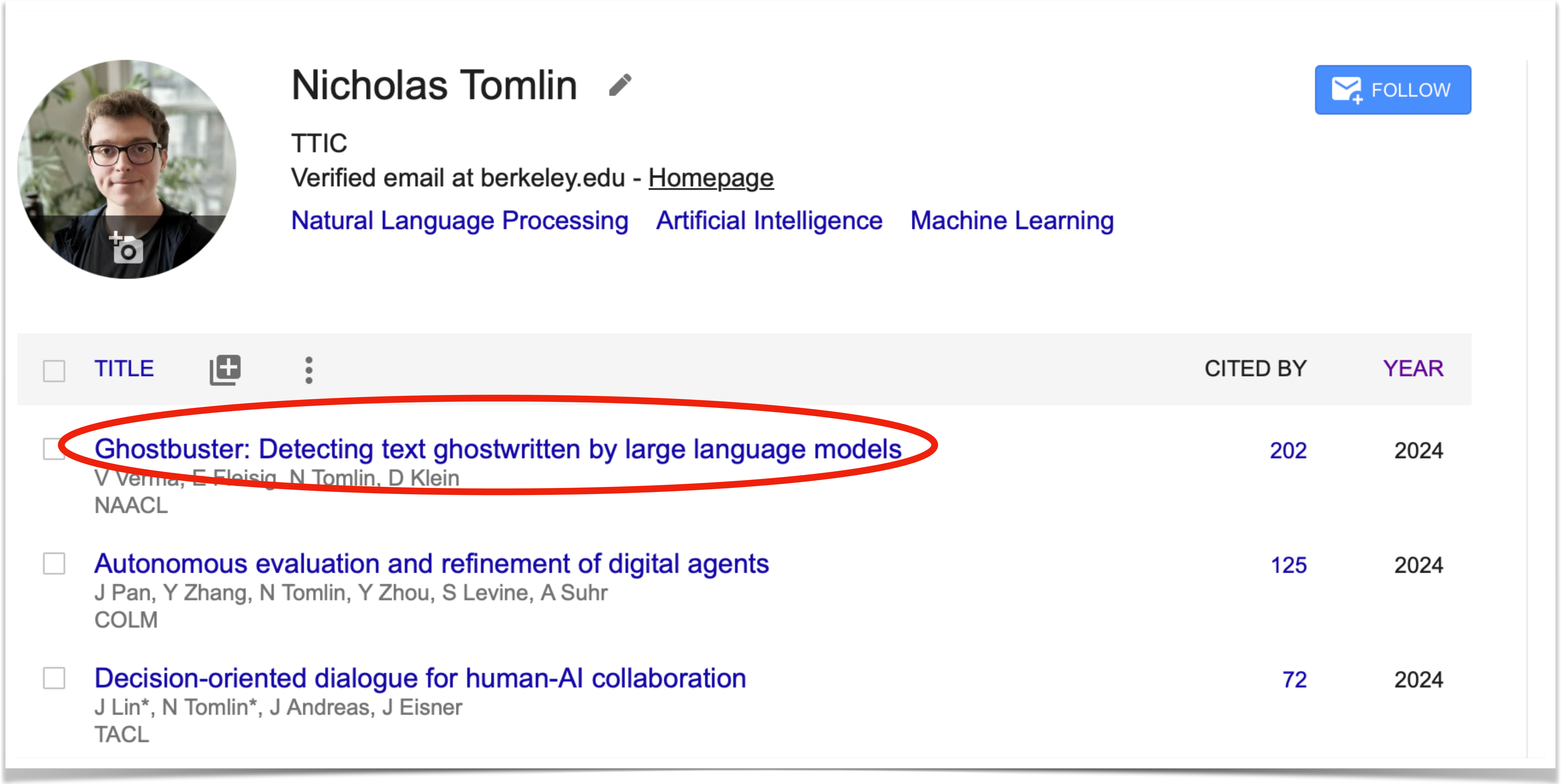

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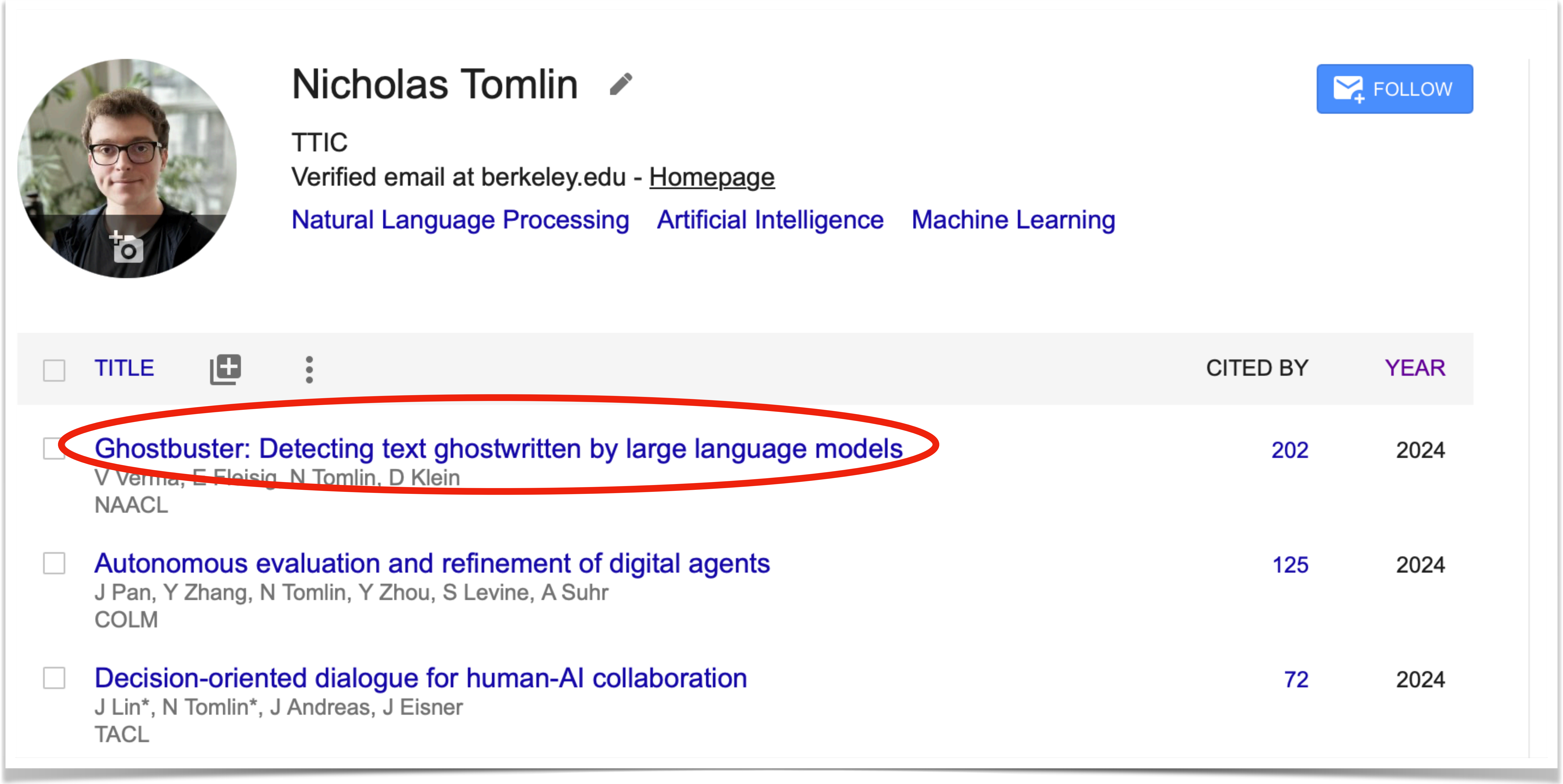

One exception: coding tools like Cursor and Claude Code are allowed if you are doing the "research track" for the final project. However, using LLMs for writing your final report is not allowed under either track.

Accommodations

If you need accommodations for the midterm or have accessibility concerns, please contact the Moses Center for Disabilities: mosescsd@nyu.edu

If there are things we can do to help accommodate, let us know.

Key dates and deadlines

Jan 23rd: Homework 0 due

Feb 2nd: last day to add/drop classes on Albert

Feb 3rd: Homework 1 due

Feb 28th: project groups formed

Mar 10th: midterm, in-class

Should I take this class?

Yes, if:

- You are a CDS MS or PhD student
- You have familiarity with linear algebra, calculus, and basic programming
- You have taken DS-GA 1001 and DS-GA 1002
- You are available on Tuesday, March 10th from 2:45-4:45PM

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If you think you have equivalent experience but haven't met the prerequisites: please email us your transcript and relevant course syllabi and we can review your waiver request

Enrollment priority

Currently: 154 students (max of 200)

Priority order for registration:

- Data science graduate students (MS and PhD)
- Non-data science PhD students: please ask your advisor to reach out to Tina Lam (tina.lam@nyu.edu) to request your enrollment in this course
- MS students from other departments with appropriate prerequisites: registration should now be open. If you have issues, please contact cds-masters@nyu.edu

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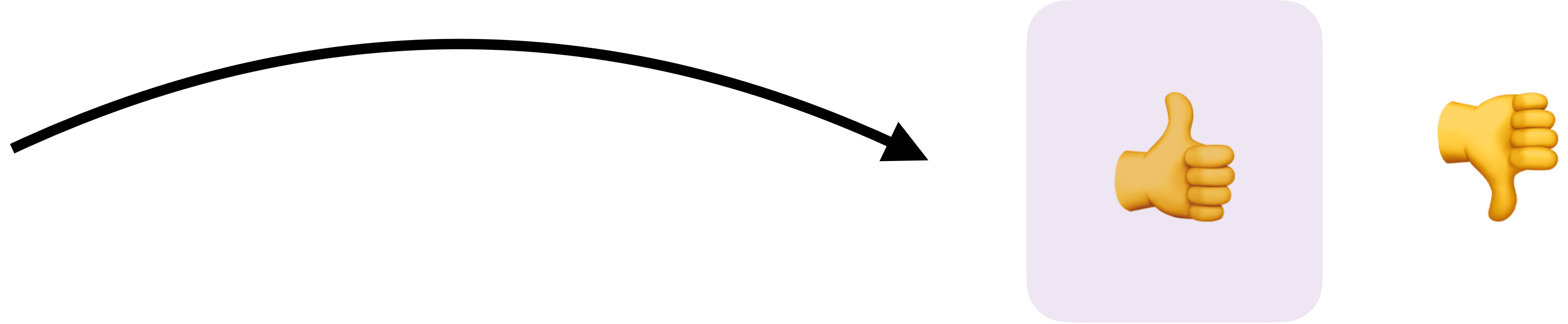
Given a dataset of photos of cats, predict the breed of a cat.

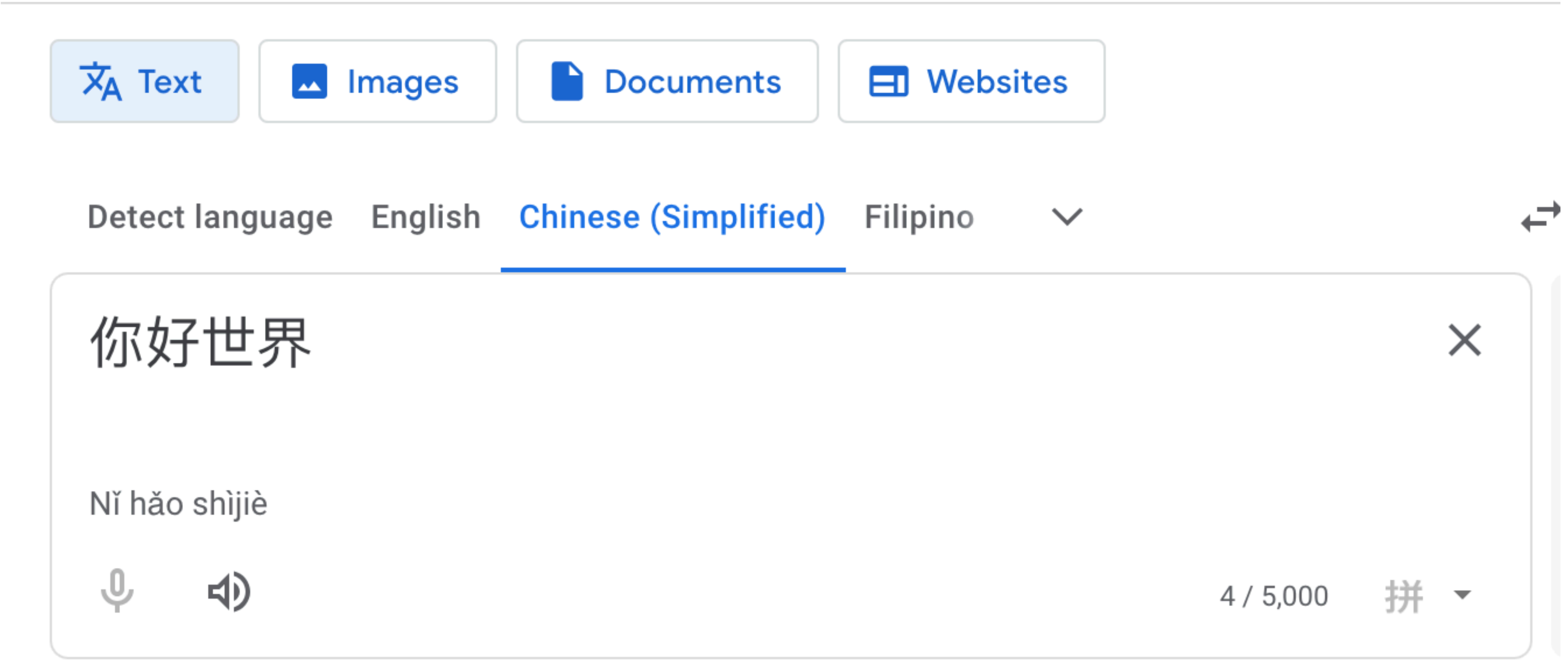
“Siamese”

Given a dataset of music listeners and songs, predict whether a user likes a song.



By https://open.spotify.com/album/26ZV7BuCkdY3INkETgEJ0e?si=-5kn-WvIQsesSQGof-BD3w, Fair use, https://en.wikipedia.org/w/index.php?curid=4897516

Given a written Chinese sentence, return the English translation.



"Hello world"

Given a dataset of meteorological measurements, forecast the temperature.

humidity	wind (mph)	cloud cover	month	pressure (in)
33%	7	2	march	29

81

Given a written English text passage, predict the ("most probable") next word.

It is a truth universally acknowledged, that a single man in possession of a good

...fortune, must be in want of a wife.

— *Jane Austen, Pride and Prejudice* (1813)

That's the famous opening line — would you like me to continue the paragraph, or do a short literary analysis of why this sentence is so iconic?

"fortune"

“Traditional Programs” vs. Machine Learning

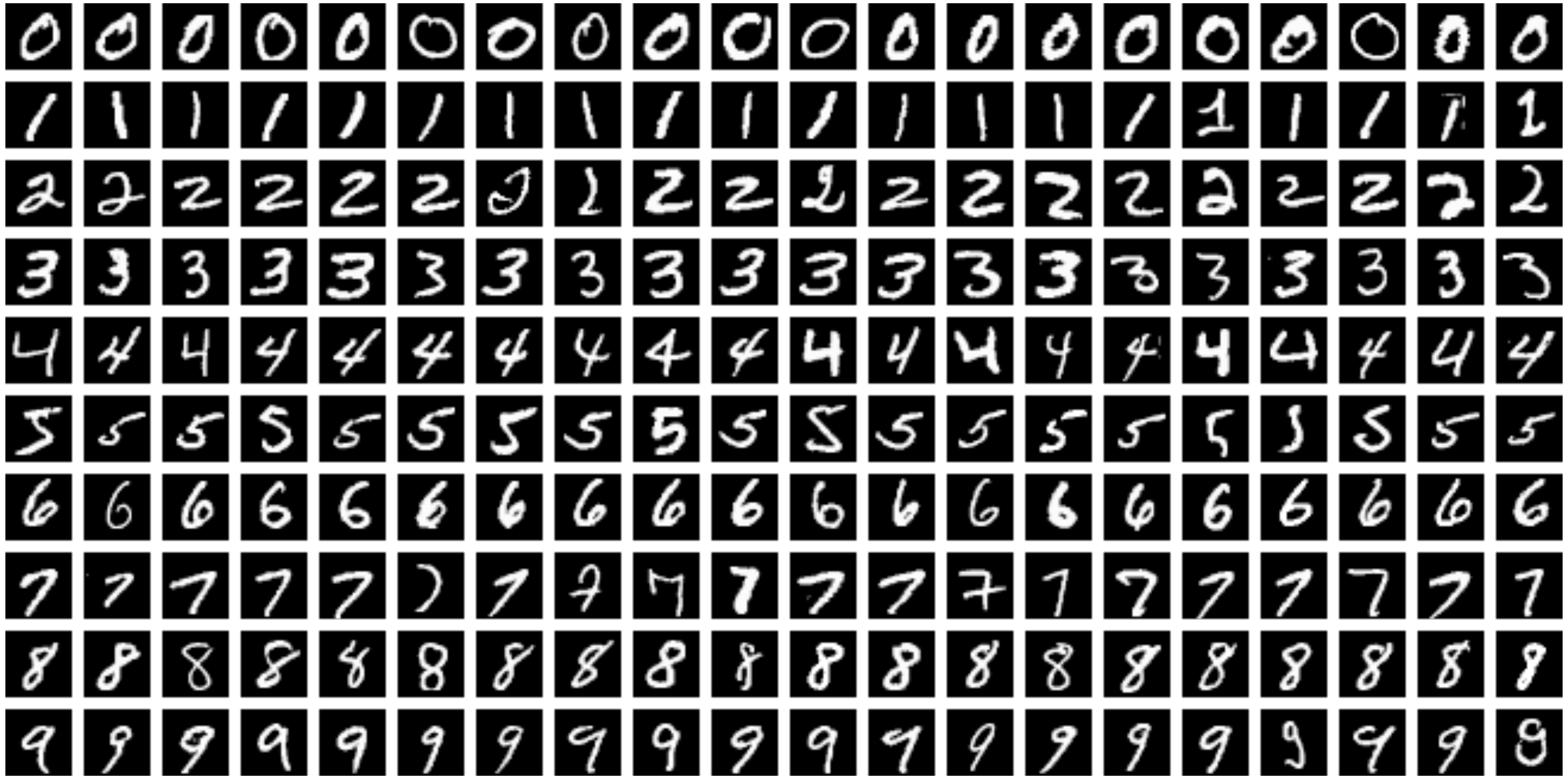
Many problems are difficult to “program by hand.”

Image recognition, language processing, product recommendation, etc.

Machine learning approach: construct an algorithm that learns automatically from data or experience, and output a program, typically to solve a prediction problem:

Given an input x, predict the output y.

“Traditional Programs”



Suppose we want to classify handwritten digits (example: **MNIST dataset**).

How would you handwrite code to distinguish between digits?

Example: Image Classification

Binary Classification

Given an input x, predict the output y.

Input x: 1000x1000 pixel image of a cat or dog.

Output y: “CAT” or “DOG”

This is a binary classification problem, where y is one of two possible outputs.

Example: Medical Diagnosis

Multiclass Classification

Given an input x, predict the output y.

Input x: Symptoms of an individual patient (*fever, cough, nausea…*)

Output y: Diagnosis (*pneumonia, flu, cold, bronchitis, …*)

This is a <u>multiclass classification problem</u>, where y is from a *discrete* set of possible outputs.

$$\Pr(\text{pneumonia}) = 0.7$$

$$\Pr(\text{flu}) = 0.1$$

$$\vdots$$

Example: Stock Price Prediction

Regression

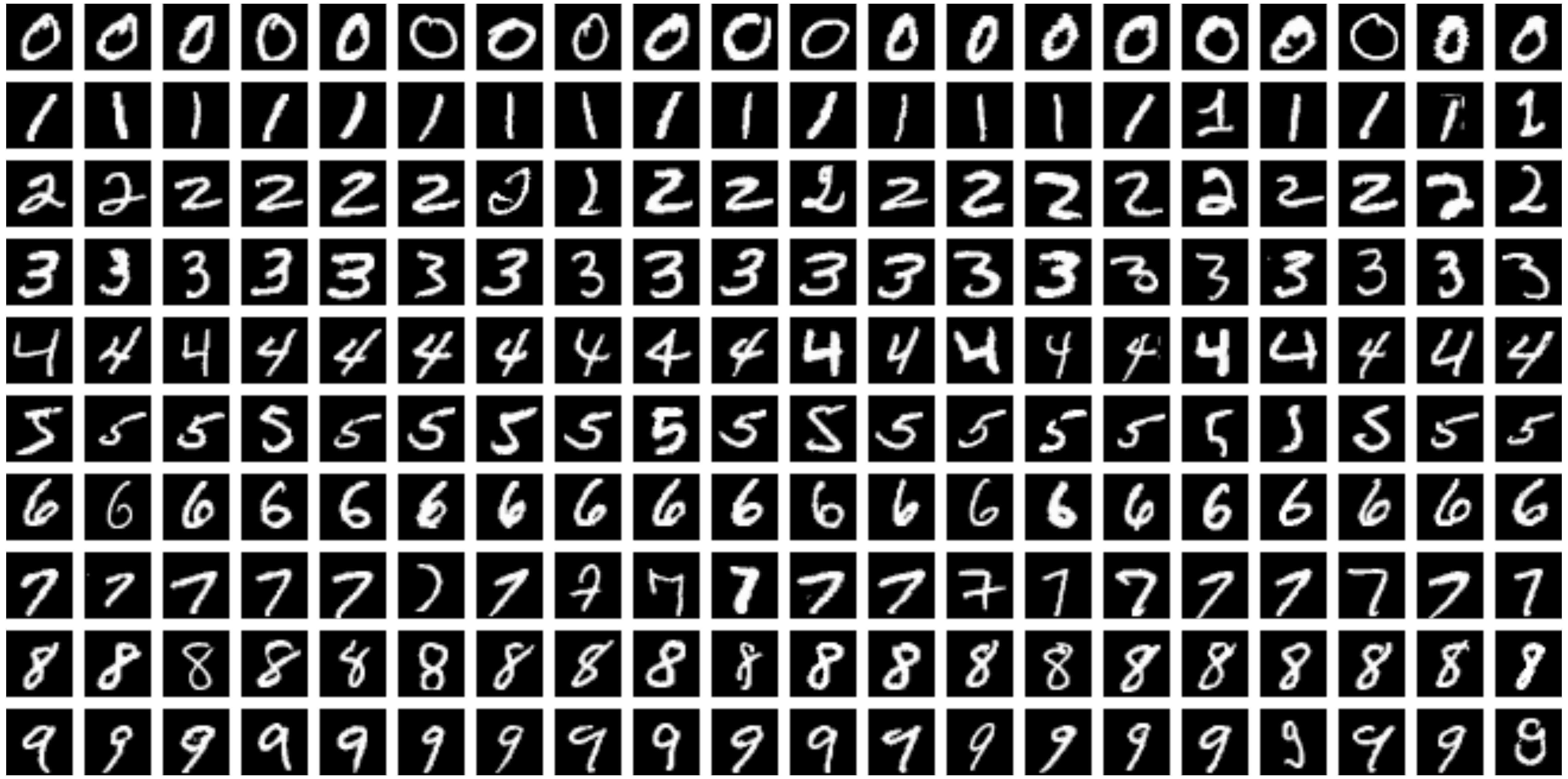
Given an input x, predict the output y.

Input x: History of stock prices, volume of stock.

Output y: Price of a stock at the close of the next day.

This is a regression problem, where y is a *continuous* output.

Machine Learning Approach



Suppose we want to classify handwritten digits (example: **MNIST dataset**).

Gather a labeled dataset of inputs and outputs.

Use this data to "automatically" find the best rule for classifying digits.

Supervised Machine Learning

A Definition

$$D_n := \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$$

The study of *making predictions* from *data*.

$\mathscr{X}$ $\mathscr{Y}$

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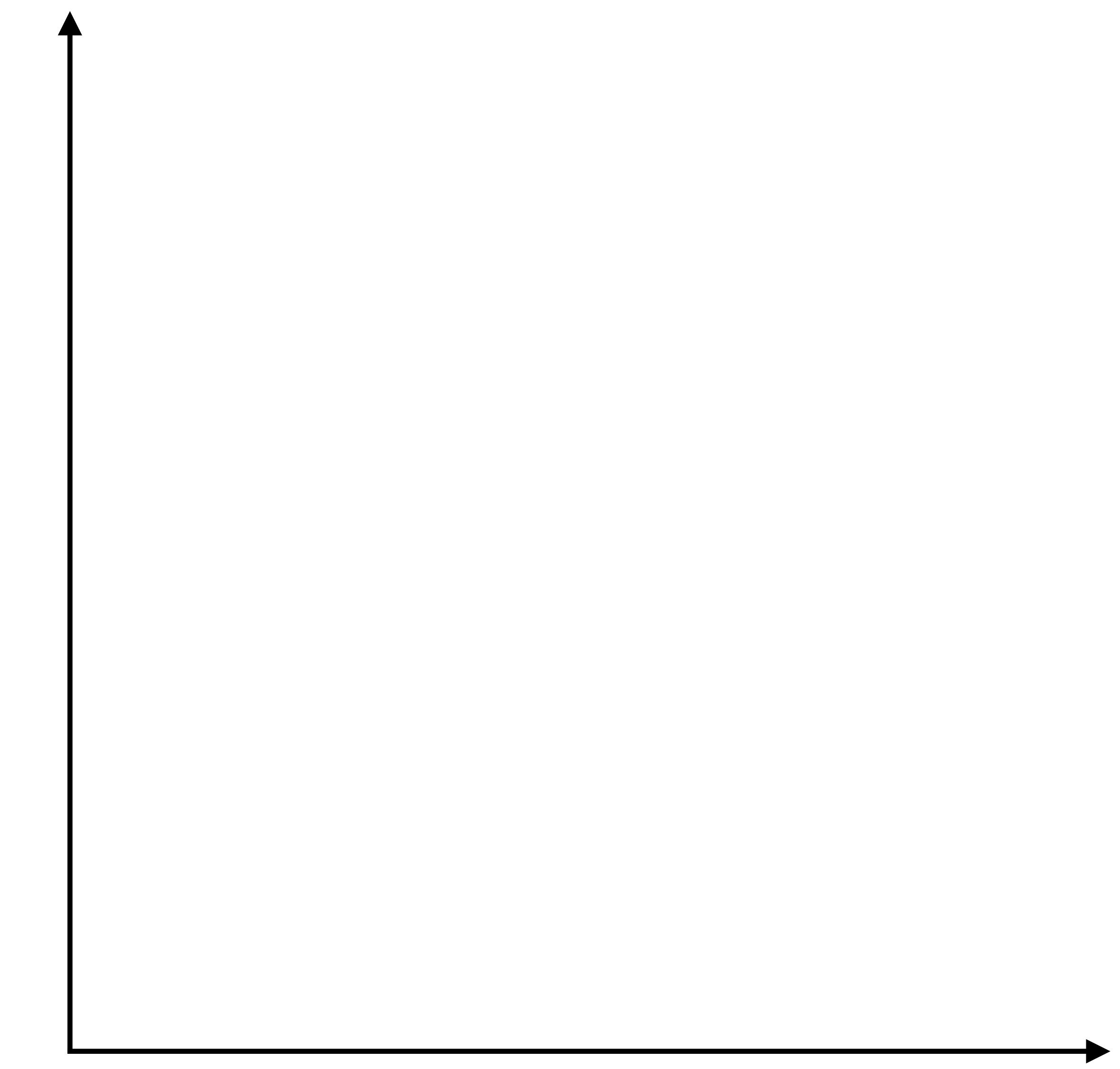
$\mathbb{R}^2$



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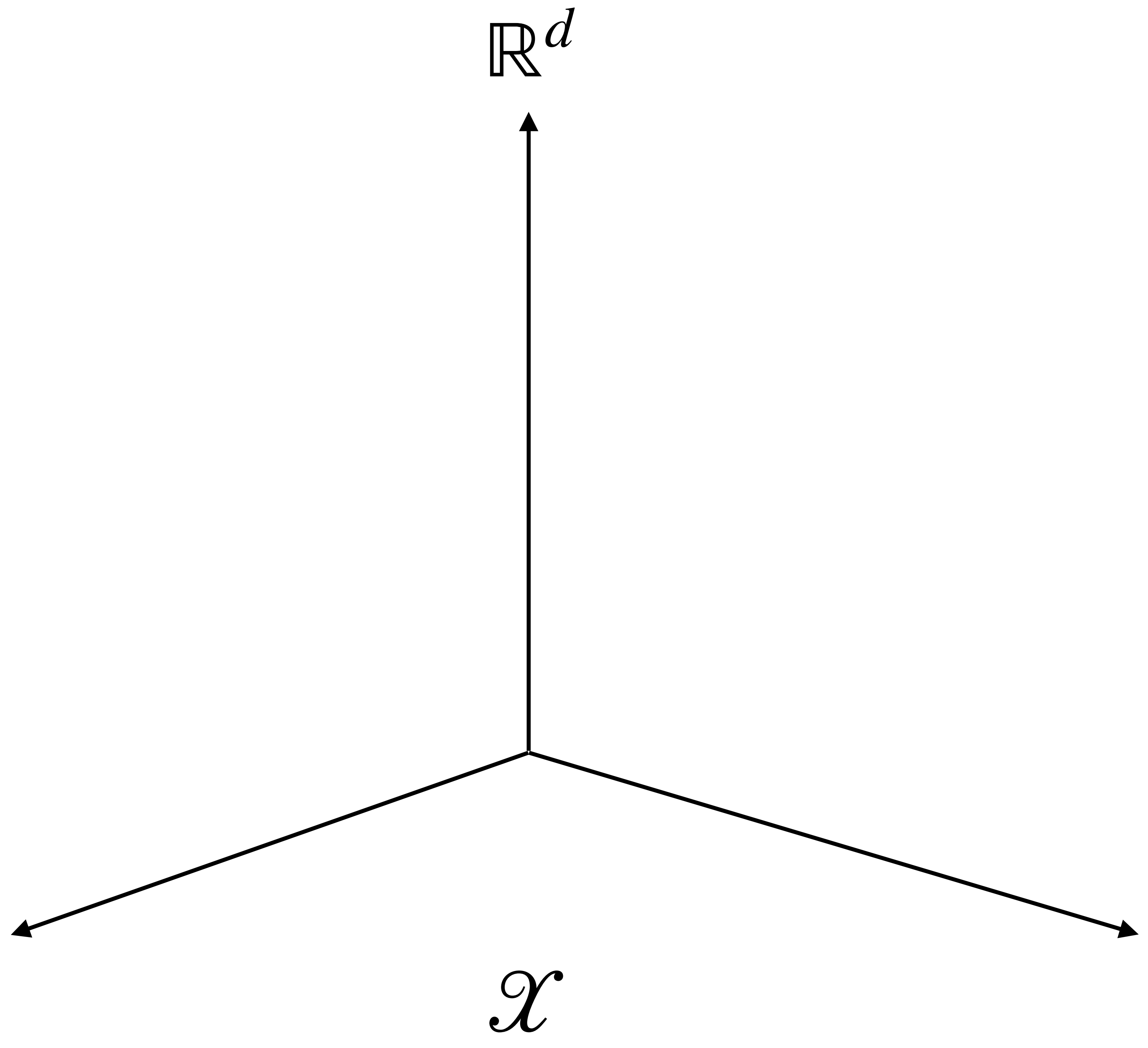

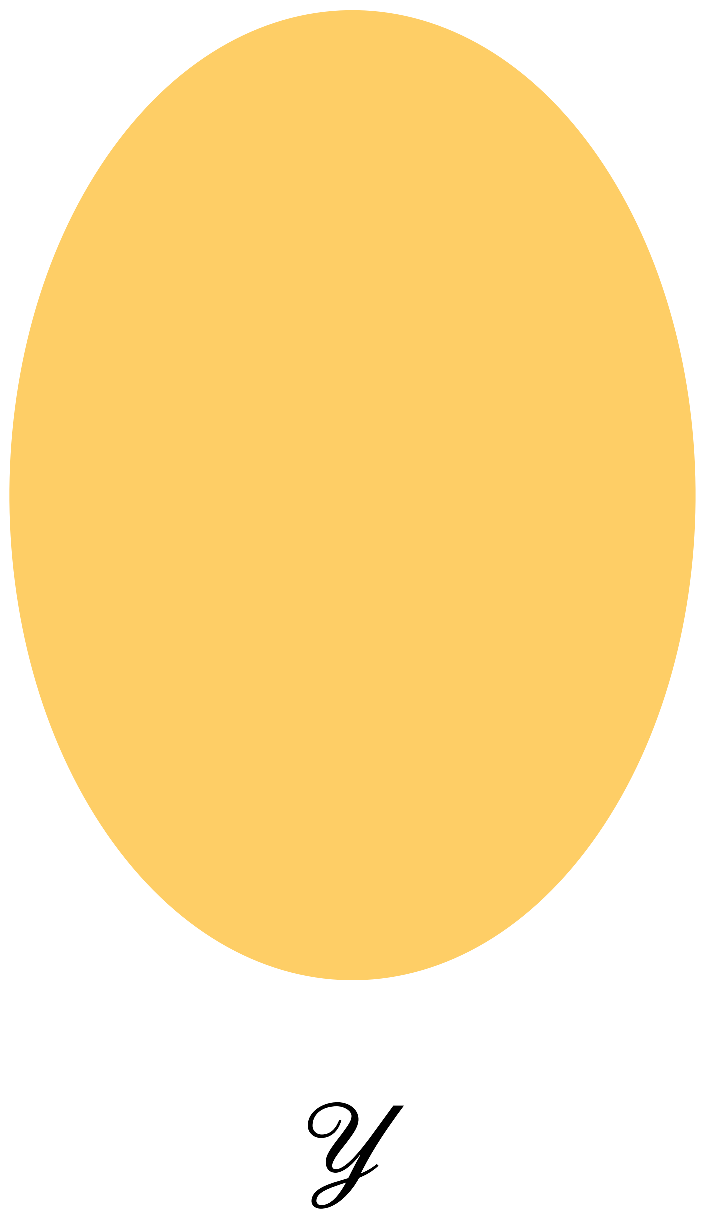

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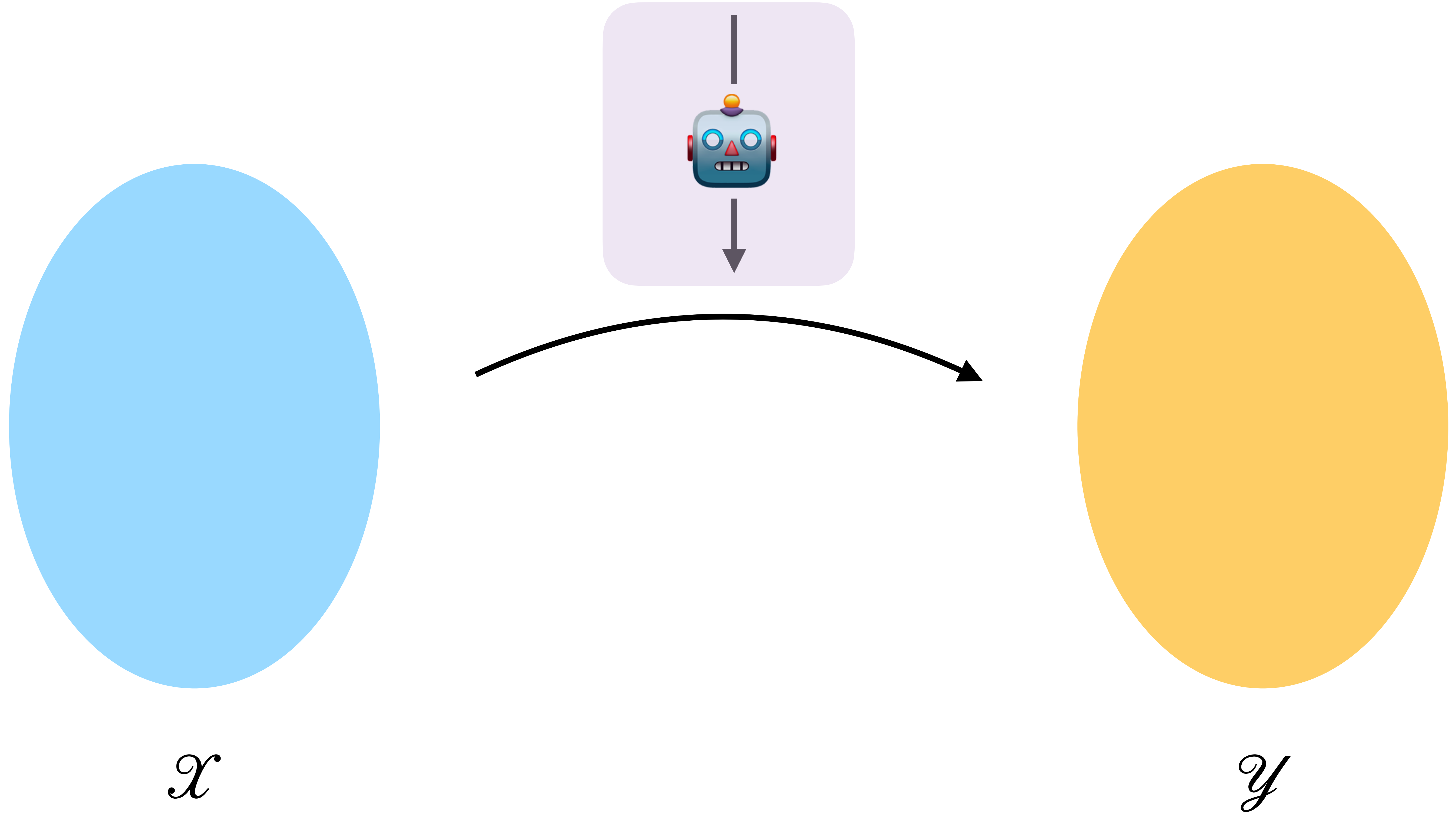


Supervised Learning

Basic Pipeline

1. Collect training dataset, a collection of labeled input-output pairs.

2. Decide on the template of the hypothesis mapping that will map inputs to actions.

Representation

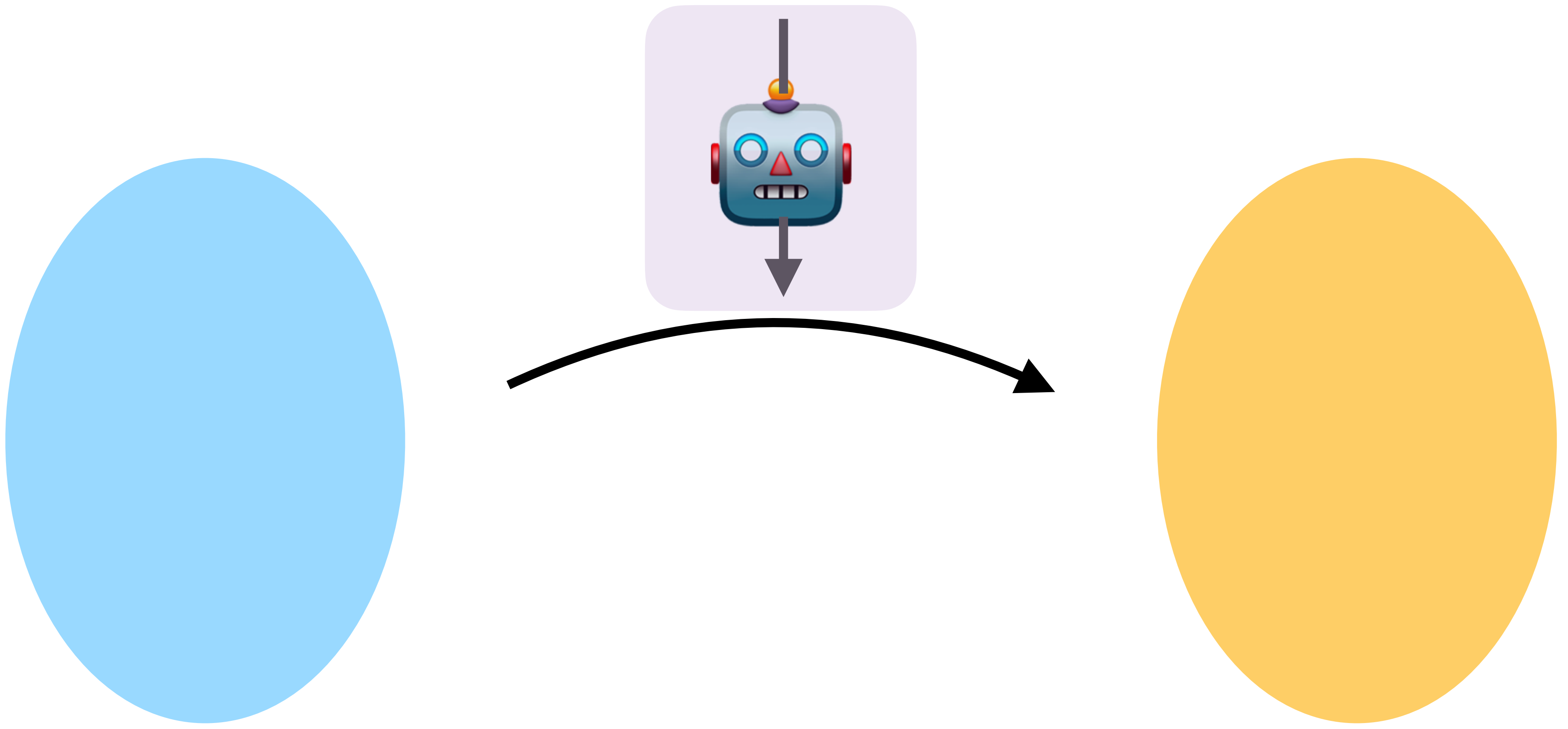
3. A learning algorithm takes the labeled training data as input and outputs a hypothesis.

Optimization

4. The hypothesis predicts on new, unseen data which we hope it does well on, under a notion of loss.

Generalization

$$D_n := \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$$



$\mathcal{X}$ $\mathcal{Y}$

Outline

Inputs, Outcomes, and Evaluation

The Basic Prediction Problem

The “template” of the problems we care about follow this structure:

1. Observe an input $x \in \mathcal{X}$.
2. Take an action $a \in \mathcal{A}$.
3. Observe the true outcome $y \in \mathcal{Y}$.
4. Evaluate the actions in relation to the outcome.

Inputs, Outcomes, and Evaluation

Input Space

$\mathcal{X}$ is the input space (aka feature space), where $x \in \mathcal{X}$ is an input.

In many cases, $\mathcal{X} = \mathbb{R}^d$, d-dimensional Euclidean space.

Example: Measurements in an individual's medical exam (height, weight, BP, etc.)

Example: Pixels in a 1,024x1,024 image.

Example: Words in a document of English text.

The task of finding good features for a task is known as feature engineering.

Neural networks (latter half of semester) can be seen as "automated feature engineers."

Inputs, Outcomes, and Evaluation

Outcome Space

$\mathcal{Y}$ is the outcome space (aka label space), where $y \in \mathcal{Y}$ is outcome/label.

In many cases, $\mathcal{Y}$ can be encoded as a single number.

Example: $\mathcal{Y} = \{-1, +1\}$ (e.g. yes/no, cat/dog, etc.) in binary classification.

Example: $\mathcal{Y} = \{1,2,\ldots,k\}$ (e.g. English word, breed of cat, etc.) in multiclass classification.

Example: $\mathcal{Y} = \mathbb{R}$ (e.g. day's temperature, stock price, etc.) in regression.

Inputs, Outcomes, and Evaluation

Action Space

$\mathcal{A}$ is the action space, where $a \in \mathcal{A}$ is an action.

Generic term for what is produced by our system (in many cases, a **prediction**).

In many cases, we will set $\mathcal{A} = \mathcal{Y}$.

Example: Produce a $-1/1$ classification (binary classification).

Example: Reject hypothesis that $\theta = 0$ (classical statistics).

Example: Prediction of storm location in 3 hours.

Example: Written English text (image captioning, speech recognition, translation).

Inputs, Outcomes, and Evaluation

Evaluation (Loss Functions)

A loss function $\ell : \mathscr{A} \times \mathscr{Y} \to \mathbb{R}$ measures the "badness" of action a with respect to $y \in \mathscr{Y}$.

$$(a, y) \mapsto \ell(a, y)$$

By convention, smaller loss is better, and loss is usually non-negative.

Inputs, Outcomes, and Evaluation

Loss Function Examples

Example. $\mathscr{Y} = \{-1, +1\}$ or $\mathscr{Y} = \{1, \ldots, k\}$ and $\mathscr{A} = \mathscr{Y}$. A reasonable loss is zero-one loss.

$$\ell(a, y) = \begin{cases} 1 & \text{if } a \neq y \\ 0 & \text{otherwise} \end{cases} \qquad \text{or, shorthand: } \ell(\hat{y}, y) := \mathbf{1}\{a \neq y\}$$

Example. $\mathscr{Y} = \mathbb{R}$ and $\mathscr{A} = \mathscr{Y}$. A reasonable loss is the squared loss.

$$\ell(\hat{y}, y) = (a - y)^2.$$

Inputs, Outcomes, and Evaluation

The Basic Prediction Problem

The "template" of the problems we care about follow this structure:

1. Observe an input $x \in \mathcal{X}$.
2. Take an action $a \in \mathcal{A}$.
3. Observe the true outcome $y \in \mathcal{Y}$.
4. Evaluate the actions in relation to the outcome.

We will construct prediction functions to do this.

Hypothesis

Definition & Goal

A hypothesis (aka predictor/prediction function) is a function $h : \mathcal{X} \to \mathcal{A}$ that takes inputs/features x and maps to an action $h(x)$.

The loss of action a in context of y: $\ell(a, y)$

The loss of action $h(x)$ in context of y: $\ell(h(x), y)$

Goal. Turn our prediction problem into an *optimization problem*.

Question: How do we evaluate a prediction function h *as a whole*?

Data Generating Distribution

Definition & Goal

$\ell(h(x), y)$ is the quality of h for a single (x, y).

But how can we evaluate h over *all* of $\mathcal{X} \times \mathcal{Y}$?

We will assume that there exists a data-generating distribution $P_{\mathcal{X}\times\mathcal{Y}}$ over $\mathcal{X} \times \mathcal{Y}$.

Any input/output pair (x, y) is assumed generated i.i.d. (independent and identically distributed) from $P_{\mathcal{X}\times\mathcal{Y}}$ (this is the i.i.d. assumption).

In machine learning, $P_{\mathcal{X}\times\mathcal{Y}}$ is assumed to be unknown!

Data Generating Distribution

Considering what is random

🛑 and consider: *What is random in this problem?*

Input/output pairs (x, y) are random variables from joint distribution $P_{\mathcal{X}\times\mathcal{Y}}$.

The inputs x are random variables from marginal distribution $P_{\mathcal{X}}$.

For any given x, the y are random variables from the conditional distribution $P_{\mathcal{Y}|x}$.

For a fixed hypothesis h, the loss $\ell(h(x), y)$ is a random variable

Evaluation, Overall

Definition of Risk

$\ell(h(x), y)$ is the quality of h for a single (x, y).

But how can we evaluate h over *all* of $\mathcal{X} \times \mathcal{Y}$?

The risk of a hypothesis $h : \mathcal{X} \to \mathcal{A}$ is the expected loss of h over $P_{\mathcal{X} \times \mathcal{Y}}$:

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

Our ultimate goal will typically be to minimize this quantity!

Statistical Learning Setup

Summary of Characters So Far

1. Observe an input $x \in \mathcal{X}$.
2. Predict an action $a \in \mathcal{A}$.
3. Observe the true outcome $y \in \mathcal{Y}$.
4. Evaluate the actions in relation to the outcome.

$\mathcal{X}$ is the input space (e.g. $\mathbb{R}^d$, pixels, words).

$\mathcal{Y}$ is the output space (e.g. $\{0,1\}$ or $\mathbb{R}$).

$\mathcal{A}$ is the action space (e.g. prediction of y, some decision).

$h : \mathcal{X} \to \mathcal{A}$ is a hypothesis to generate action $h(x)$.

Evaluate h with loss function $\ell : \mathcal{A} \times \mathcal{Y} \to \mathbb{R}$.

$\ell(h(x), y)$ evaluates h on (x, y).

$R(h) = \mathbb{E}_{(x,y)\sim P_{\mathcal{X}\times\mathcal{Y}}}[\ell(h(x), y)]$ is risk of h.

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Minimizing Risk

What's the smallest possible risk?

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

Our ultimate goal will typically be to minimize this quantity!

Bayes Risk

Definition

The Bayes hypothesis $h^*: \mathscr{X} \to \mathscr{A}$ is a function that achieves the *minimal risk* among all possible functions

$$h^* \in \arg\min_h R(h)$$

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

The risk of h^* is called the Bayes risk.

Bayes Risk

Example: Binary Classification

Binary classification: $\mathscr{Y} = \{0,1\}$ and $\mathscr{A} = \{0,1\}$.

Zero-one loss: $\ell(\hat{y}, y) = \mathbf{1}\{\hat{y} \neq y\} := \begin{cases} 1 & \hat{y} \neq y \\ 0 & \text{otherwise} \end{cases}$ (when $\mathscr{A} = \mathscr{Y}$, use $\hat{y} \in \mathscr{A}$ as shorthand)

$$R(h) = \mathbb{E}[\mathbf{1}\{\hat{y} \neq y\}] = 1 \cdot \Pr(h(x) \neq y) + 0 \cdot \Pr(h(x) = y)$$

$$\implies R(h) = \Pr(h(x) \neq y).$$

Therefore, the Bayes hypothesis returns the most likely label:

$$h^*(x) = \begin{cases} 1 & \text{if } \Pr(y = 1 \mid x) \geq 1/2 \\ 0 & \text{otherwise} \end{cases}$$

Bayes Risk

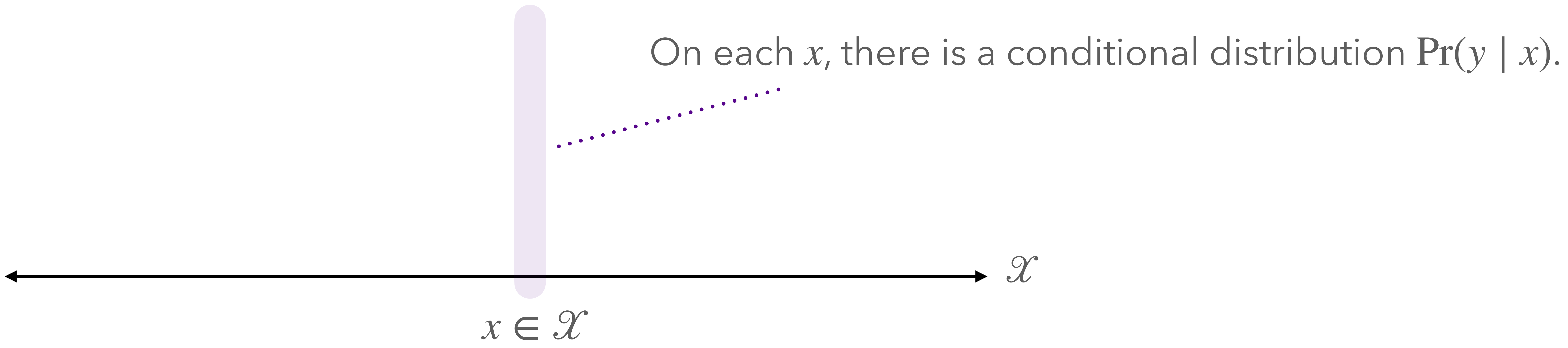
Example: Binary Classification

$$\implies R(h) = \Pr(h(x) \neq y).$$

Therefore, the Bayes hypothesis returns the most likely label:

$$h^*(x) = \begin{cases} 1 & \text{if } \Pr(y = 1 \mid x) \geq 1/2 \\ 0 & \text{otherwise} \end{cases}$$

Minimizing $R(h)$ over every possible function allows us to define h^* "pointwise" for $x \in \mathcal{X}$.



Bayes Risk

Example: Squared Loss Regression

Regression: $\mathscr{Y} = \mathbb{R}$ and $\mathscr{A} = \mathbb{R}$.

Squared loss: $\ell(a, y) = (a - y)^2$

$$R(h) := \mathbb{E}[(h(x) - y)^2]$$

Can show that the Bayes hypothesis is:

$$h^*(x) = \mathbb{E}[y \mid x]$$

Bayes Risk

Example: Binary Classification

$$\implies R(h) = \Pr(h(x) \neq y).$$

Therefore, the Bayes hypothesis returns the most likely label:

$$h^*(x) = \begin{cases} 1 & \text{if } \Pr(y = 1 \mid x) \geq 1/2 \\ 0 & \text{otherwise} \end{cases}$$

Problem: We don't know what $P_{\mathscr{X}\times\mathscr{Y}}$ is in a machine learning problem!

Minimizing Risk

What's the smallest possible risk?

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

Our ultimate goal will typically be to minimize this quantity!

Problem: We don't know what $P_{\mathcal{X}\times\mathcal{Y}}$ is in a machine learning problem!

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Minimizing Risk

What's the smallest possible risk?

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

Our ultimate goal will typically be to minimize this quantity!

Problem: We don't know what $P_{\mathcal{X}\times\mathcal{Y}}$ is in a machine learning problem!

But we assume that we have a dataset of i.i.d. samples:

$$D_n := \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$$

Law of Large Numbers

Reminder

If $z_1, \ldots, z_n$ are i.i.d. random variables with expected value $\mathbb{E}[z]$, then

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} z_i = \mathbb{E}[z], \text{ with probability 1.}$$

If $D_n = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$ is drawn i.i.d. from $P_{\mathcal{X}\times\mathcal{Y}}$, then for a fixed $h : \mathcal{X} \to \mathcal{A}$ and $\ell : \mathcal{A} \times \mathcal{Y} \to \mathbb{R}$,

$$\ell(h(x^{(1)}), y^{(1)}), \ldots, \ell(h(x^{(n)}), y^{(n)})$$

are all random variables…

Empirical Risk

Definition

Let $D_n := \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$ be drawn i.i.d. from $P_{\mathcal{X}\times\mathcal{Y}}$.

The empirical risk of $h : \mathcal{X} \to \mathcal{A}$ with respect to D_n is

$$\hat{R}_n(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}).$$

By the strong law of large numbers,

$$\lim_{n\to\infty} \hat{R}_n(h) = R(h) \text{ almost surely.}$$

But, in practice, we only have a finite sample.

Empirical Risk Minimization

Definition

The empirical risk of $h : \mathcal{X} \to \mathcal{A}$ with respect to D_n is

$$\hat{R}_n(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}).$$

The empirical risk minimizer (ERM) (over all functions $h : \mathcal{X} \to \mathcal{A}$) is a function $\hat{h}$ satisfying

$$\boxed{\hat{h} \in \operatorname*{arg\,min}_h \hat{R}_n(h).}$$

Is this a good proxy?

In an ideal world, we want the Bayes hypothesis:

$$\boxed{h^* \in \operatorname*{arg\,min}_h R(h).}$$

Empirical Risk Minimization

Example

$P_{\mathscr{X}} = \mathrm{Unif}([0,1])$ and $Y = 1$ always.

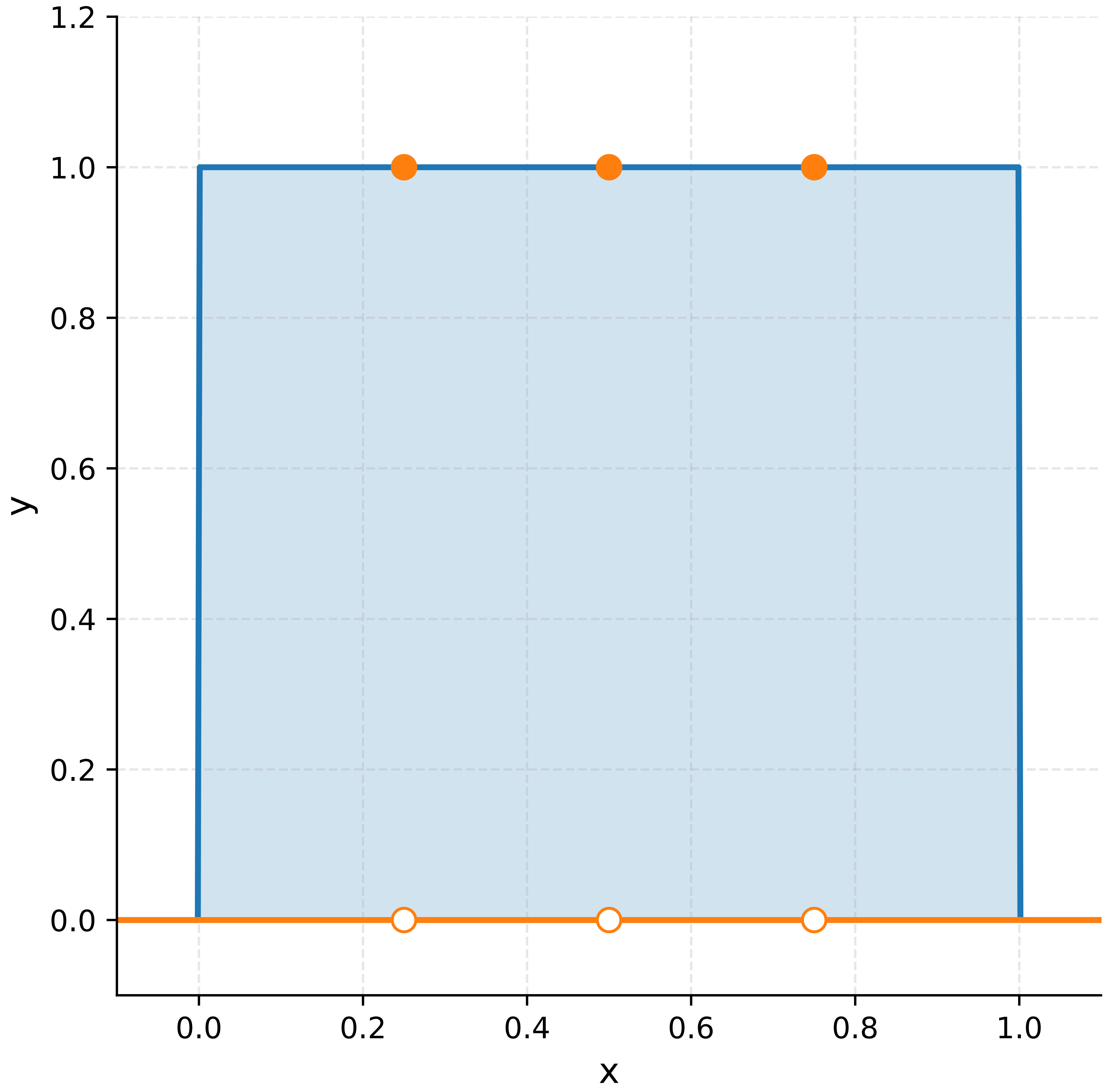
Draw i.i.d. sample of size $n = 3$:

$$D_n = \{(0.25,1), (0.5,1), (0.75,1)\}.$$

Under $\ell(\hat{y}, y) = \mathbf{1}\{\hat{y} \neq y\}$ (zero-one loss):

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

This is an ERM.



Empirical Risk Minimization

Example

$P_{\mathcal{X}} = \mathrm{Unif}([0,1])$ and $Y = 1$ always.

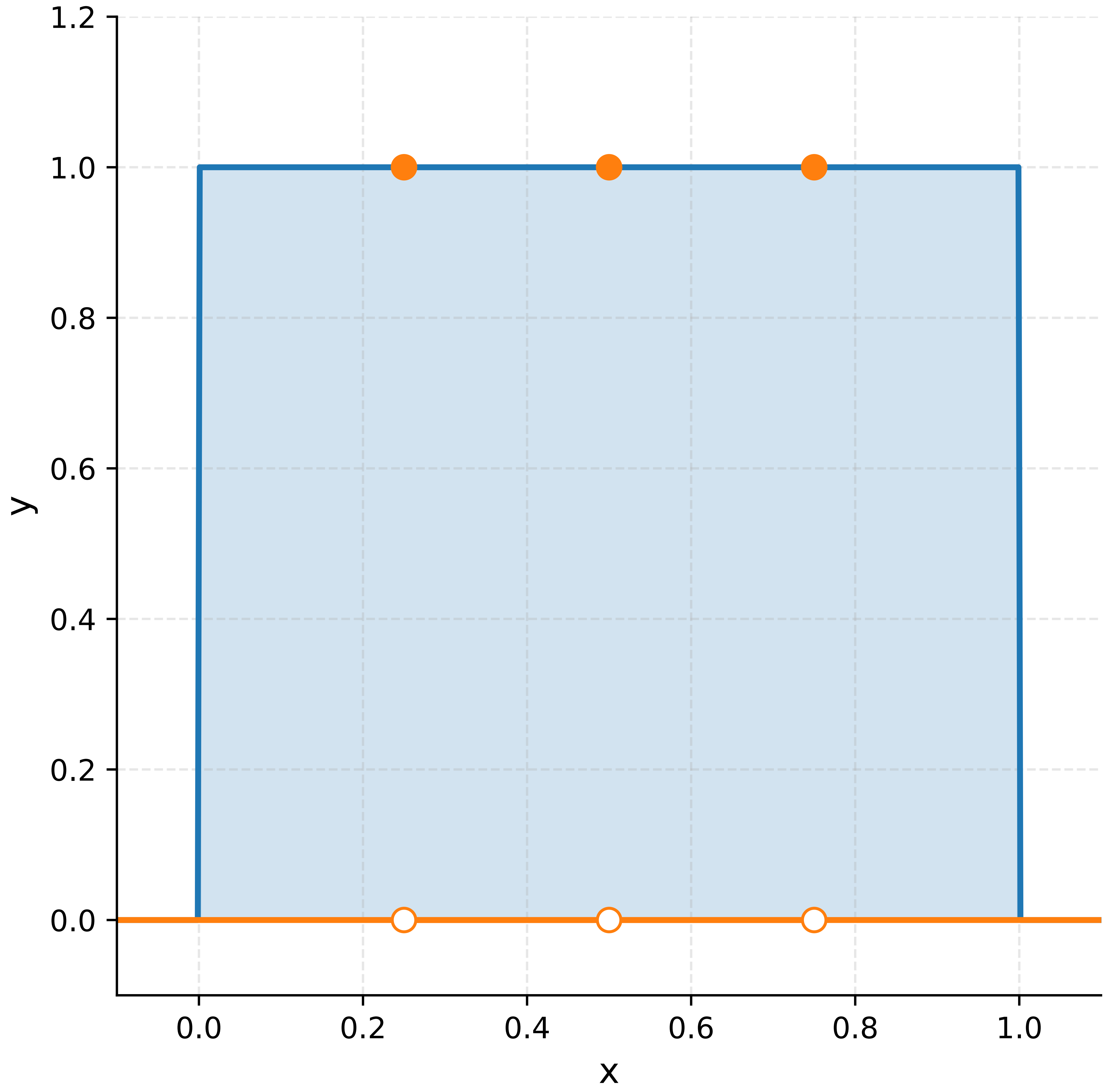
Draw i.i.d. sample of size $n = 3$:

$$D_n = \{(0.25,1), (0.5,1), (0.75,1)\}.$$

Under $\ell(\hat{y}, y) = (\hat{y} - y)^2$ (squared loss):

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

This is an ERM.



Empirical Risk Minimization

Example: Gap with true risk

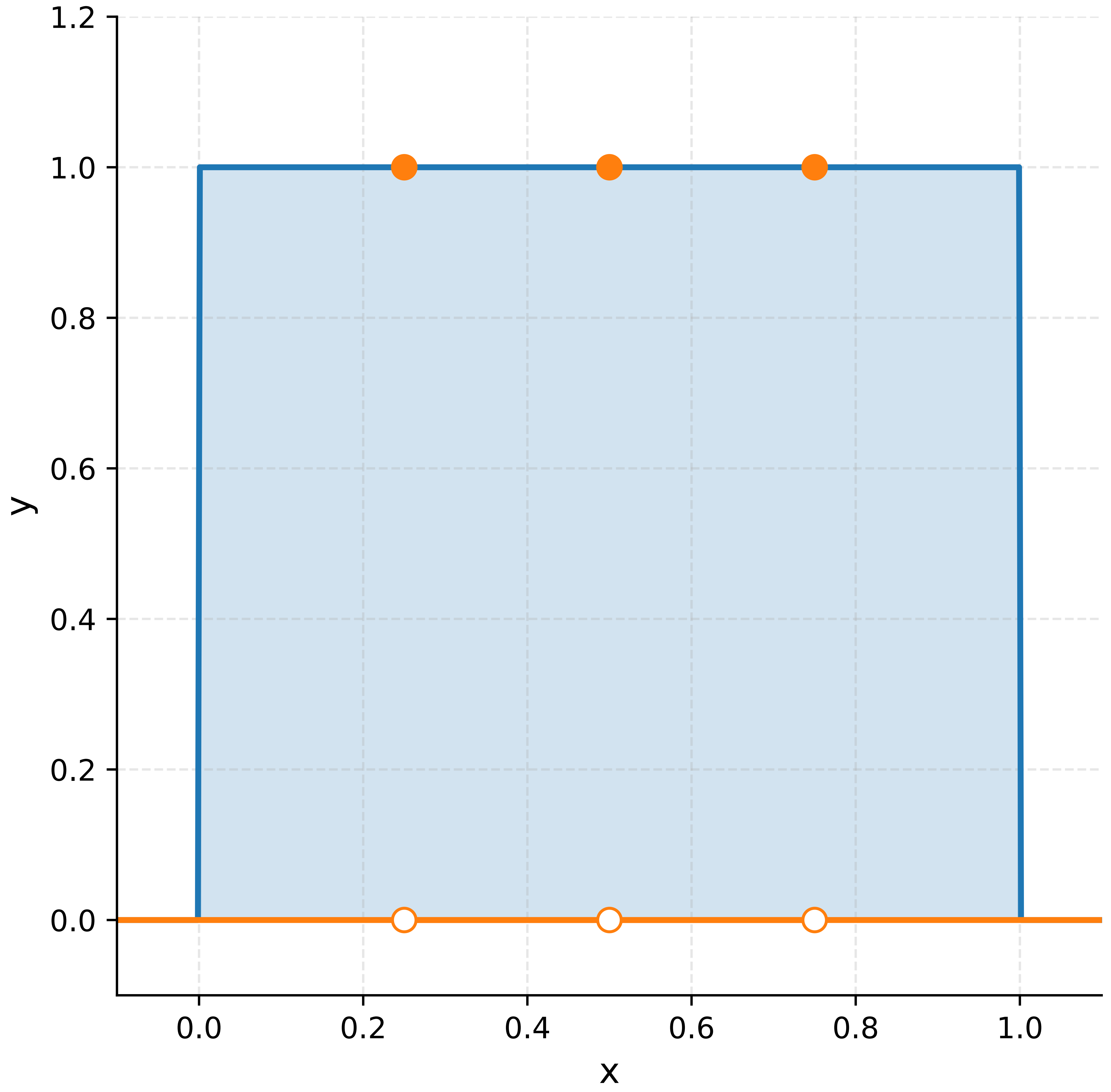
$$\hat{h}(x) = \begin{cases} 1 & \text{if } x \in \{0.25, 0.5, 0.75\} \\ 0 & \text{otherwise} \end{cases}$$

Empirical risk under zero-one loss:

$$\hat{R}_n(\hat{h}) = \frac{1}{3} \sum_{i=1}^{3} \mathbf{1}\{\hat{h}(x^{(i)}) \neq y^{(i)}\} = 0$$

True risk under zero-one loss:

$$R(\hat{h}) = \mathbb{E}[\mathbf{1}\{\hat{h}(x) \neq y\}] = \Pr(\hat{h}(x) \neq y) = 1$$



Empirical Risk Minimization

What went wrong?

$$D_n = \{(0.25,1), (0.5,1), (0.75,1)\}$$

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

This failed spectacularly because $\hat{h}$ just *memorized* the data.

In ML, we want our hypotheses to **generalize** from training data to new data.

In order to do this, we need to smooth things out:

Model how information is structured in input space $\mathcal{X}$ to unobserved parts of $\mathcal{X}$!

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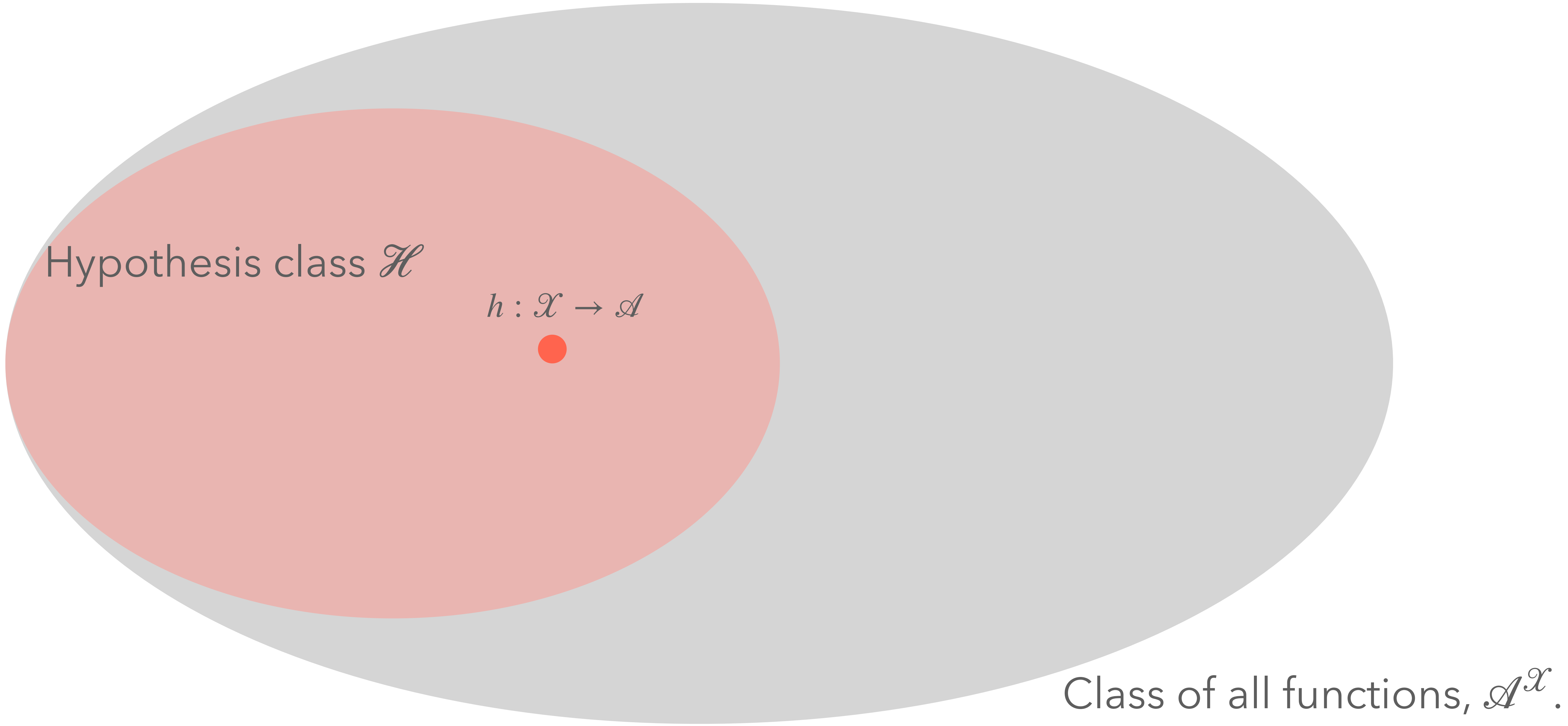
Hypothesis Class

Definition

A hypothesis class is a set of functions $\mathscr{H} \subseteq \mathscr{A}^{\mathscr{X}}$ where we will search for h.



Hypothesis Class

Example

$\mathscr{X} = \mathbb{R}^3$, with $x \in \mathscr{X}$ encoded as
$x = (\text{midterm}, \text{hours studied}, \text{hours slept})$.

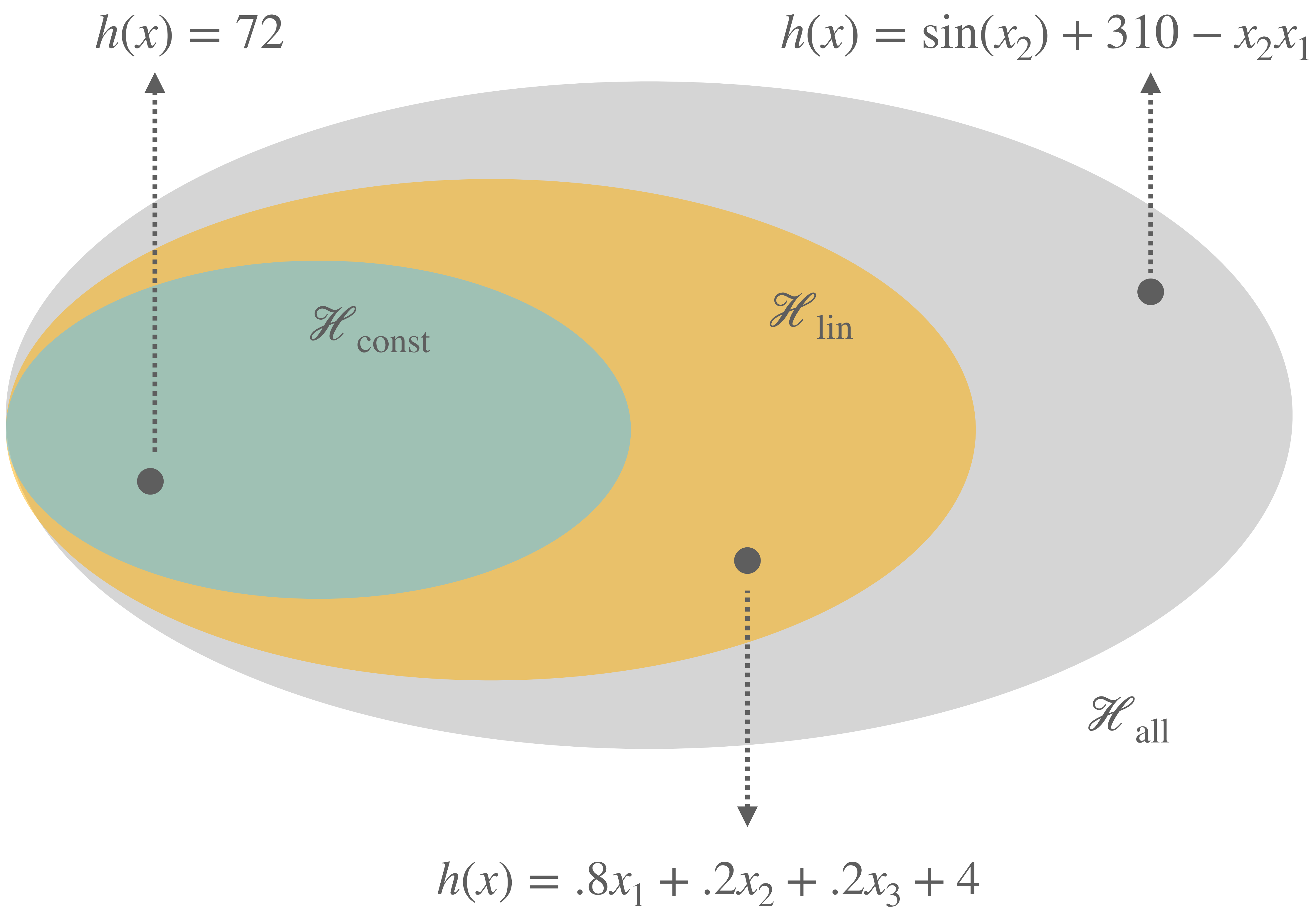
$\mathscr{A} = \mathbb{R}$, where $a \in \mathscr{A}$ is final exam score.

Possible hypothesis classes:

$$\mathscr{H}_{\text{const}} = \{x \mapsto b : b \in \mathbb{R}\}$$

$$\mathscr{H}_{\text{lin}} = \{x \mapsto w^\top x + b : w \in \mathbb{R}^3, b \in \mathbb{R}\}$$

$$\mathscr{H}_{\text{all}} = \{\mathbb{R}^3 \mapsto \mathbb{R}\}$$



Empirical Risk Minimization

Example: $\mathscr{H}_{\text{const}}$

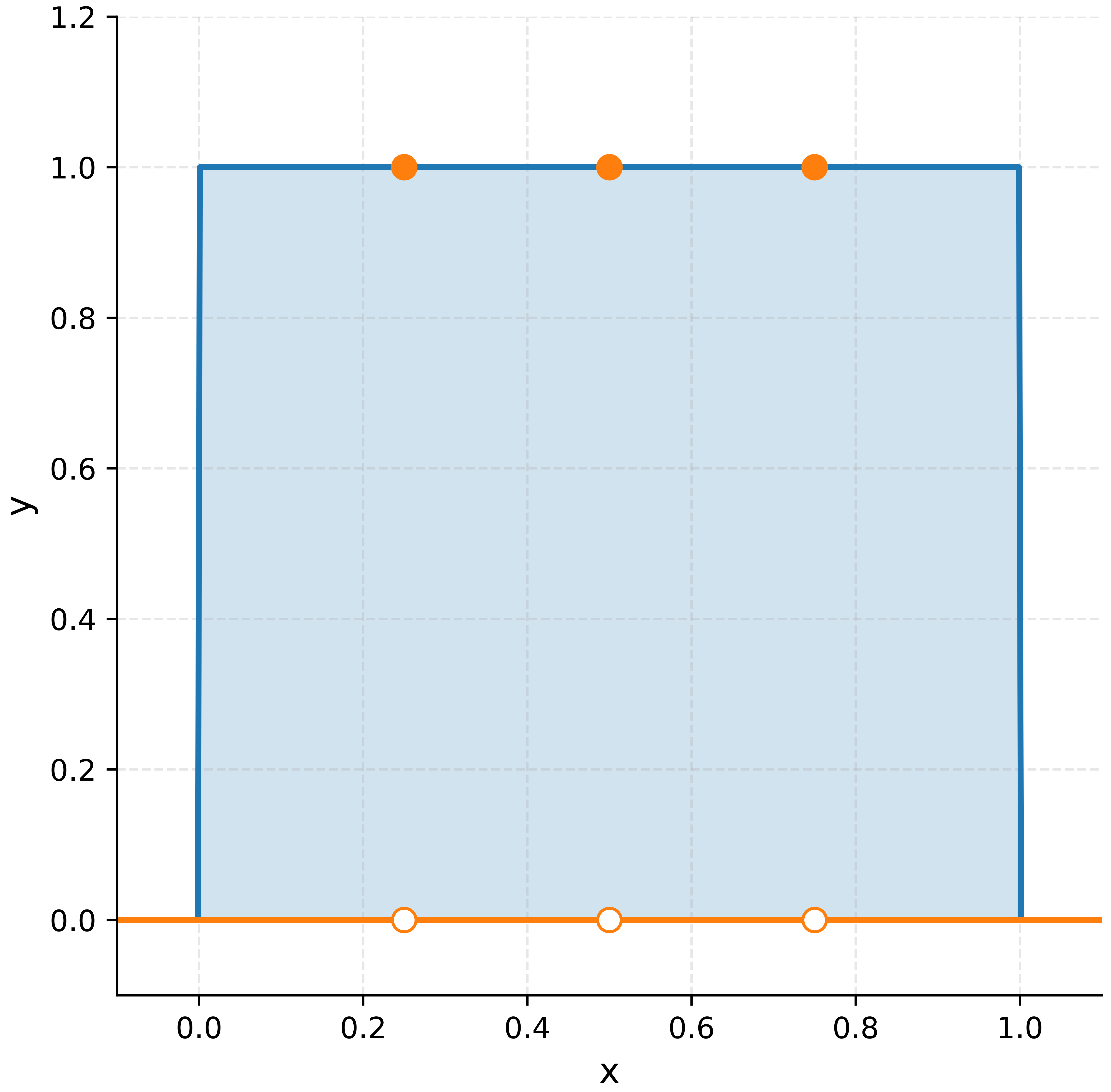
$P_{\mathscr{X}} = \text{Unif}([0,1])$ and $Y = 1$ always.

$$D_n = \{(0.25,1), (0.5,1), (0.75,1)\}.$$

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

ERM over $\mathscr{H}_{\text{const}} = \{x \mapsto b : b \in \mathbb{R}\}$:

$$\hat{h}(x) = 1$$



Hypothesis Class

Definition

A hypothesis class is a set of functions $\mathscr{H} \subseteq \mathscr{A}^{\mathscr{X}}$ where we will search for h.

Fixed *before* the learning process.

Encodes assumptions about the relationship of x to y.

Should be easy to work with (i.e. we have efficient algorithms to search over $\mathscr{H}$).

Risk Minimization

With a hypothesis class

The empirical risk minimizer (ERM) in $\mathcal{H}$ is a function $\hat{h}$ satisfying

$$\hat{h} \in \arg\min_{h \in \mathcal{H}} \hat{R}_n(h).$$

The risk minimizer in $\mathcal{H}$ is a function $\hat{h}$ satisfying

$$h^*_{\mathcal{H}} \in \arg\min_{h \in \mathcal{H}} R(h)$$

The Bayes hypothesis h^* is a function with *minimal risk* among all functions

$$h^* \in \arg\min_{h} R(h)$$

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Excess Risk

Definition

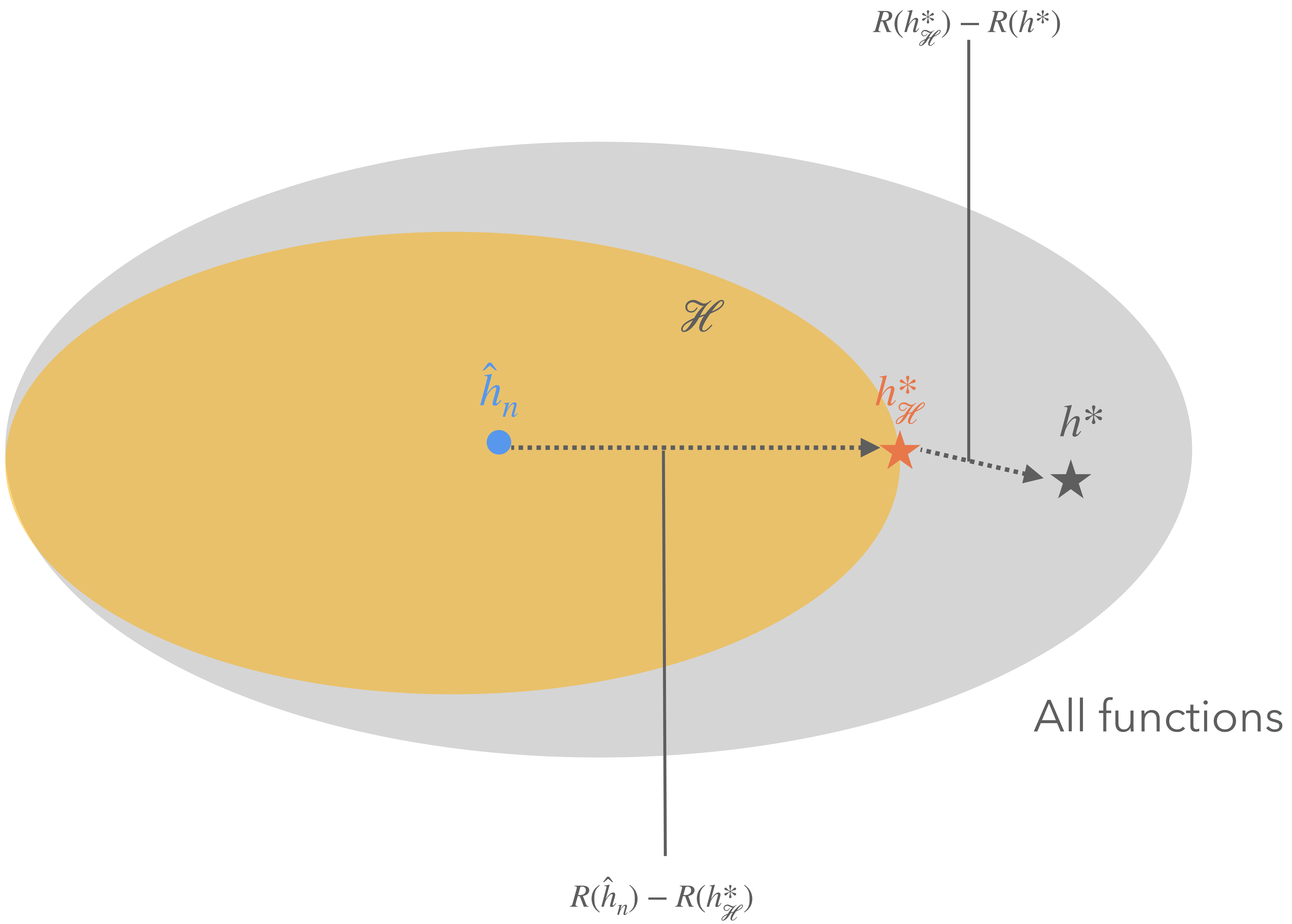
$$h^* \in \operatorname*{argmin}_{h} \underbrace{\mathbb{E}_{(x,y)\sim P_{\mathcal{X}\times\mathcal{Y}}}\left[\ell(h(x), y)\right]}_{R(h)}$$

$$h^*_{\mathcal{H}} \in \operatorname*{argmin}_{h\in\mathcal{H}} \underbrace{\mathbb{E}_{(x,y)\sim P_{\mathcal{X}\times\mathcal{Y}}}\left[\ell(h(x), y)\right]}_{R(h)}$$

$$\hat{h}_n \in \operatorname*{argmin}_{h\in\mathcal{H}} \underbrace{\frac{1}{n}\sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)})}_{\hat{R}_n(h)}$$

The excess risk of h is how far h is from h^*:

$$R(h) - R(h^*).$$



Excess Risk

Decomposition

The excess risk of h is how far h is from h^*:

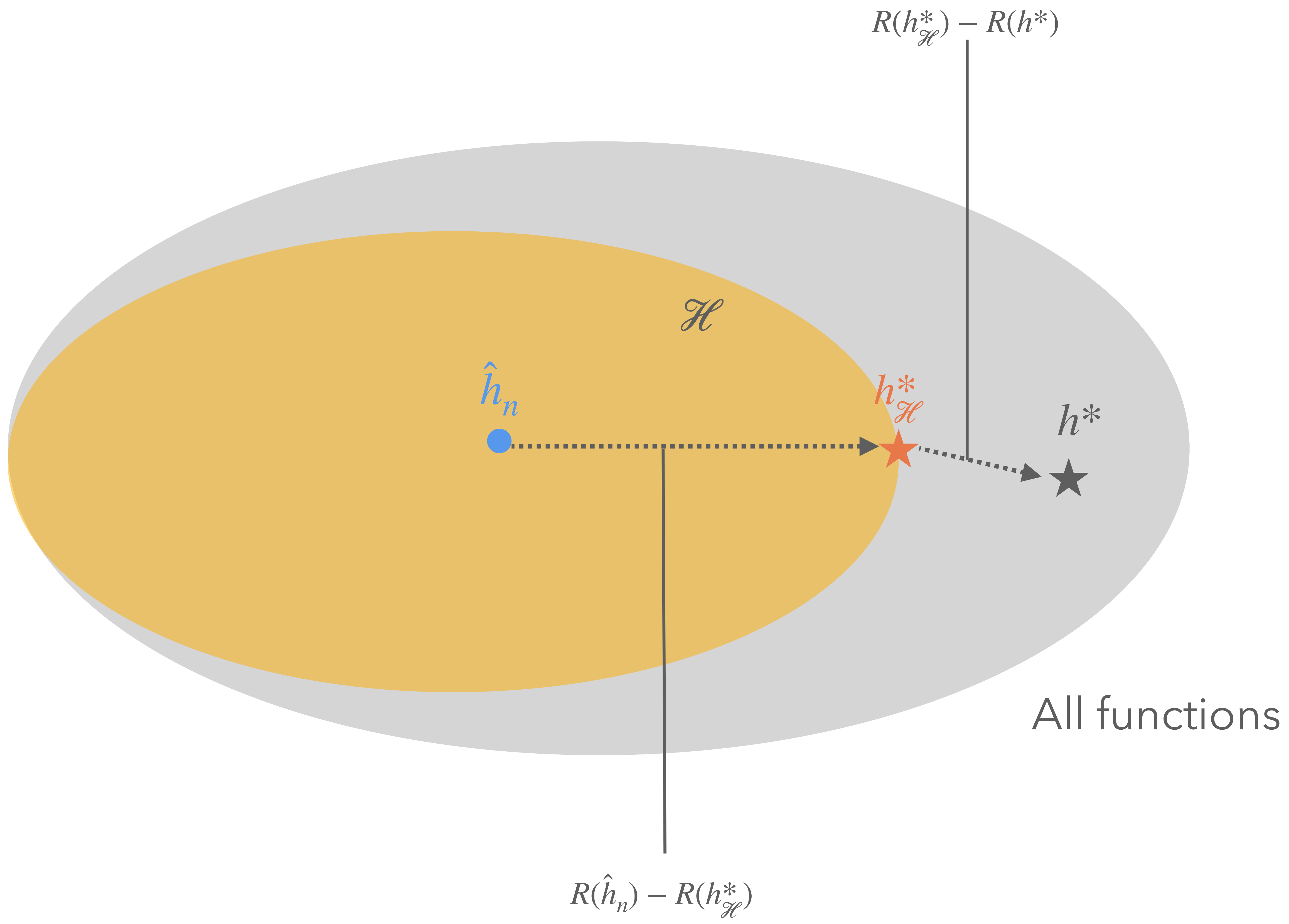
$$R(h) - R(h^*).$$

Excess risk of ERM $\hat{h}_n$:

$$R(\hat{h}_n) - R(h^*) = \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathcal{H}}) - R(h^*)}_{\text{approx. error}}$$

Estimation error is from using finite training as a proxy for risk (a generalization issue).

Approximation error is from our choice of class $\mathcal{H}$ (a representation issue).



Estimation Error

Details

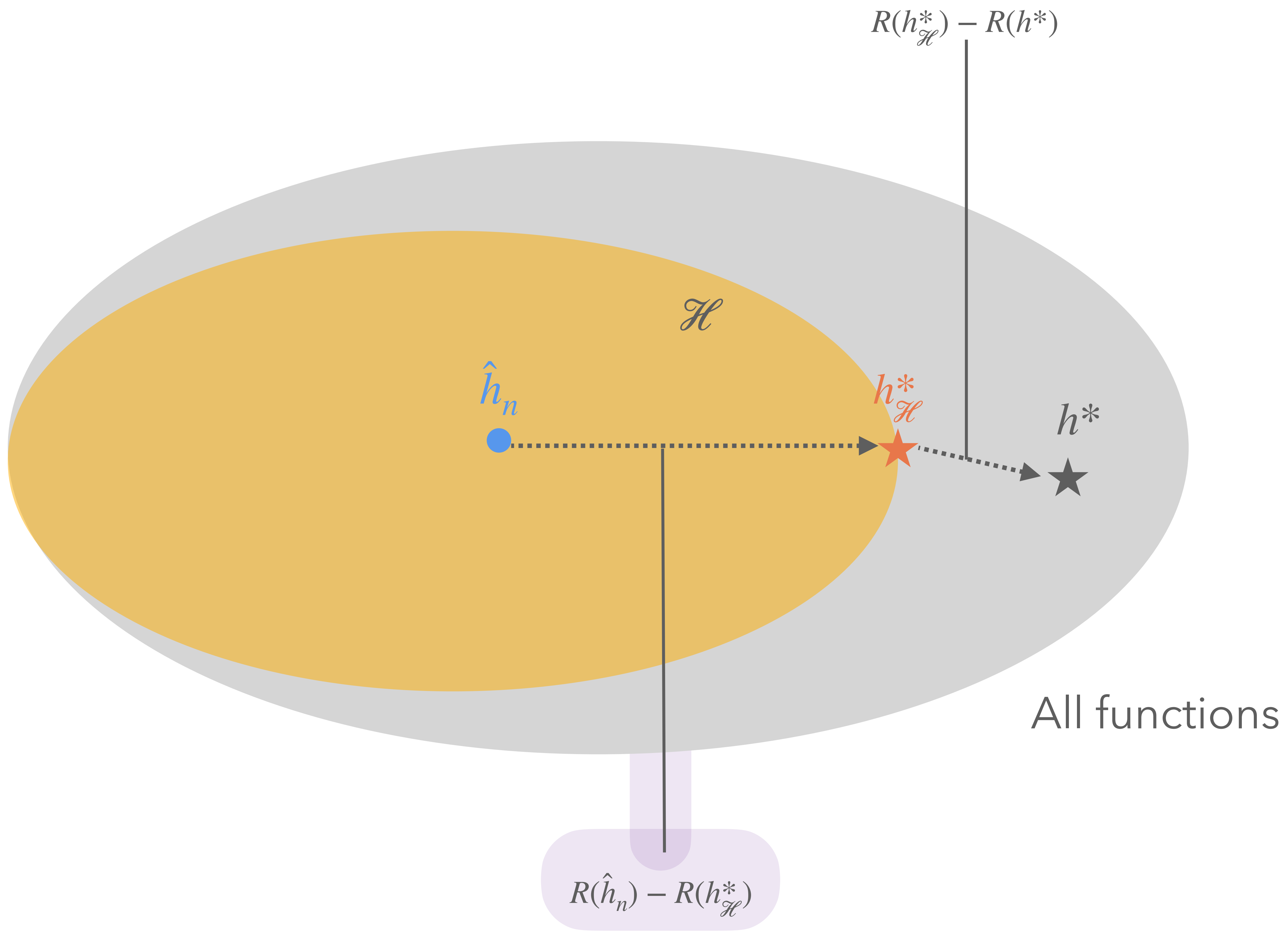
The <u>estimation error</u> $R(\hat{h}_n) - R(h^*_{\mathcal{H}})$ is the error incurred by using a finite sample D_n to obtain $\hat{h}_n$.

This is a random variable (why)?

Typically, when $n \to \infty$ (infinite training data), the estimation error goes to zero.

We expect that estimation error *<u>increases</u>* with *<u>larger $\mathcal{H}$</u>*.

Very rough intuition: a "variance" term.



We will come back to the tension this has with modern machine learning practice!

Approximation Error

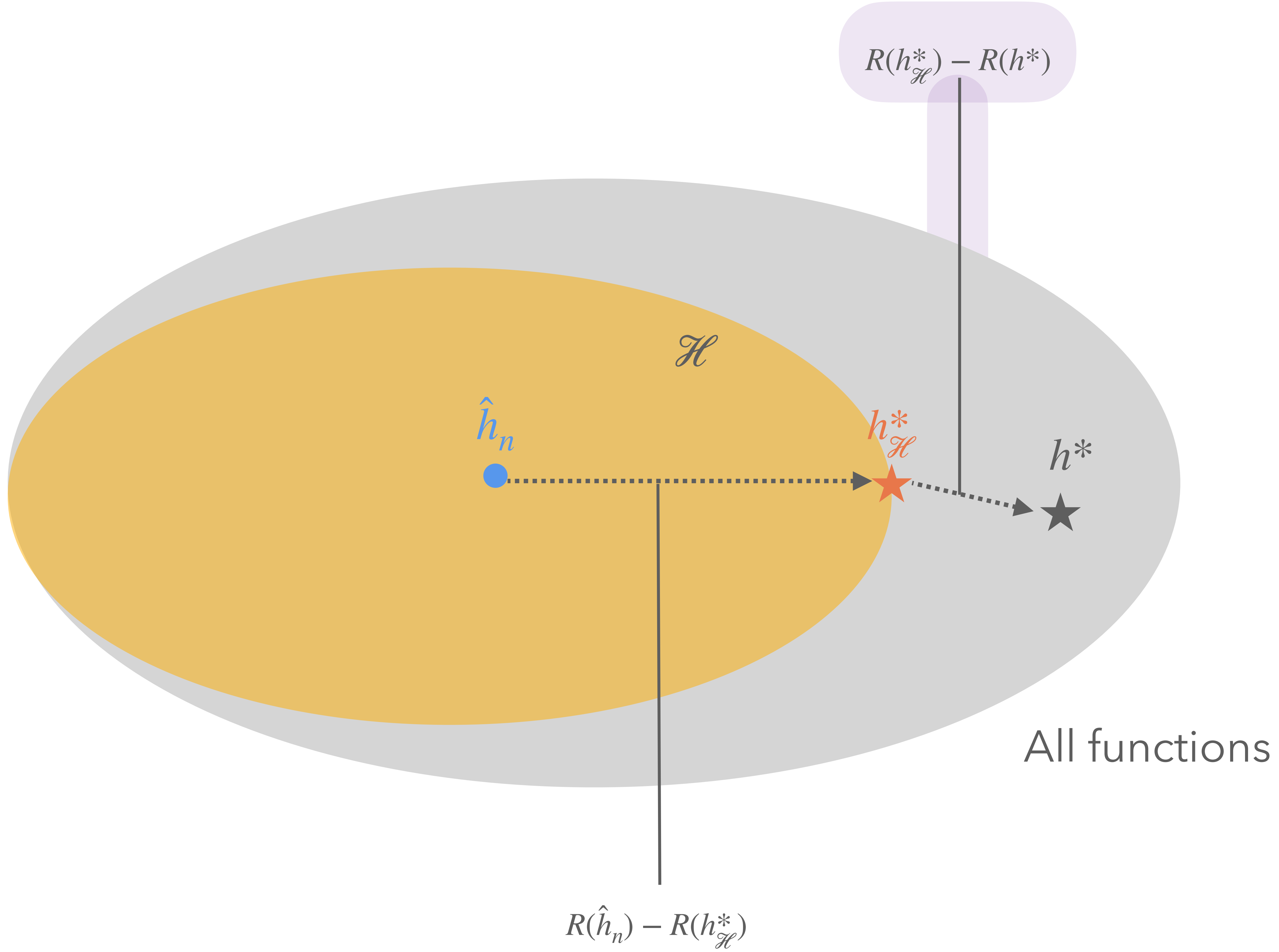
Details

The approximation error $R(h^*_{\mathcal{H}}) - R(h^*)$ is the error incurred by restricting to $\mathcal{H}$.

This is not a random variable (why)?

Typically, approximation error *decreases* with *larger* $\mathcal{H}$.

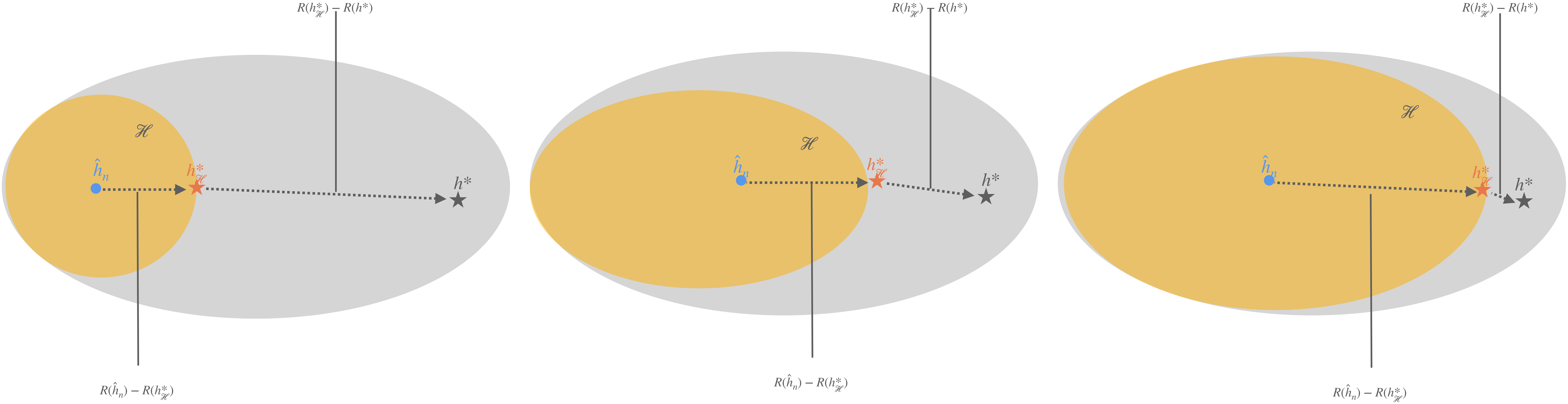
Very rough intuition: a "bias" term.



Excess Risk

Intuition: Size of $\mathscr{H}$

$$R(\hat{h}_n) - R(h^*) = \underbrace{R(\hat{h}_n) - R(h^*_{\mathscr{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathscr{H}}) - R(h^*)}_{\text{approx. error}}$$



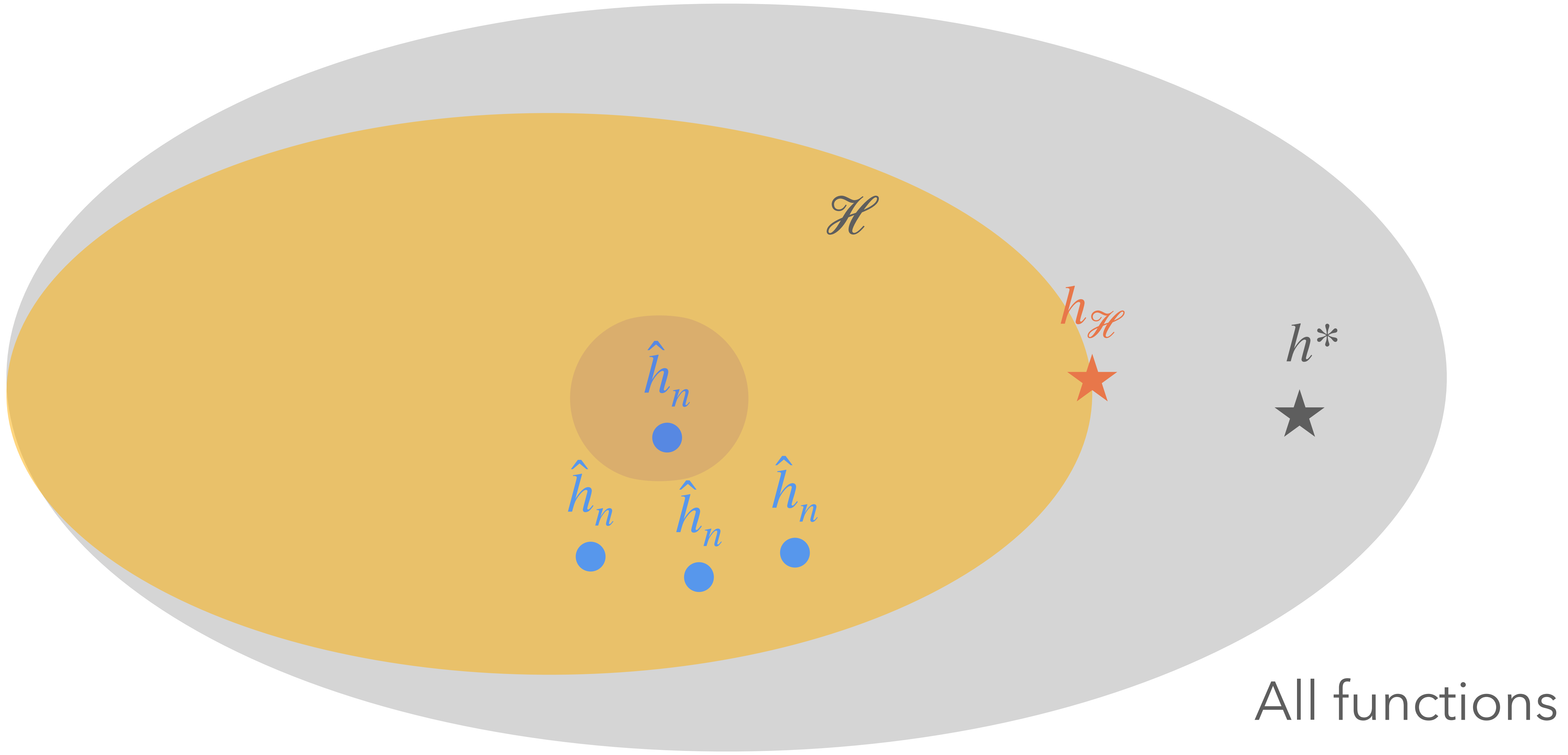
Optimization Error

Details

But how do we search for a hypothesis that minimizes empirical risk?

$$\hat{h}_n \in \boxed{\underset{h \in \mathcal{H}}{\operatorname{argmin}}} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)})}_{\hat{R}_n(h)}$$

To search for one of them, we run a learning algorithm which typically uses a well-defined optimization procedure.



Optimization Error

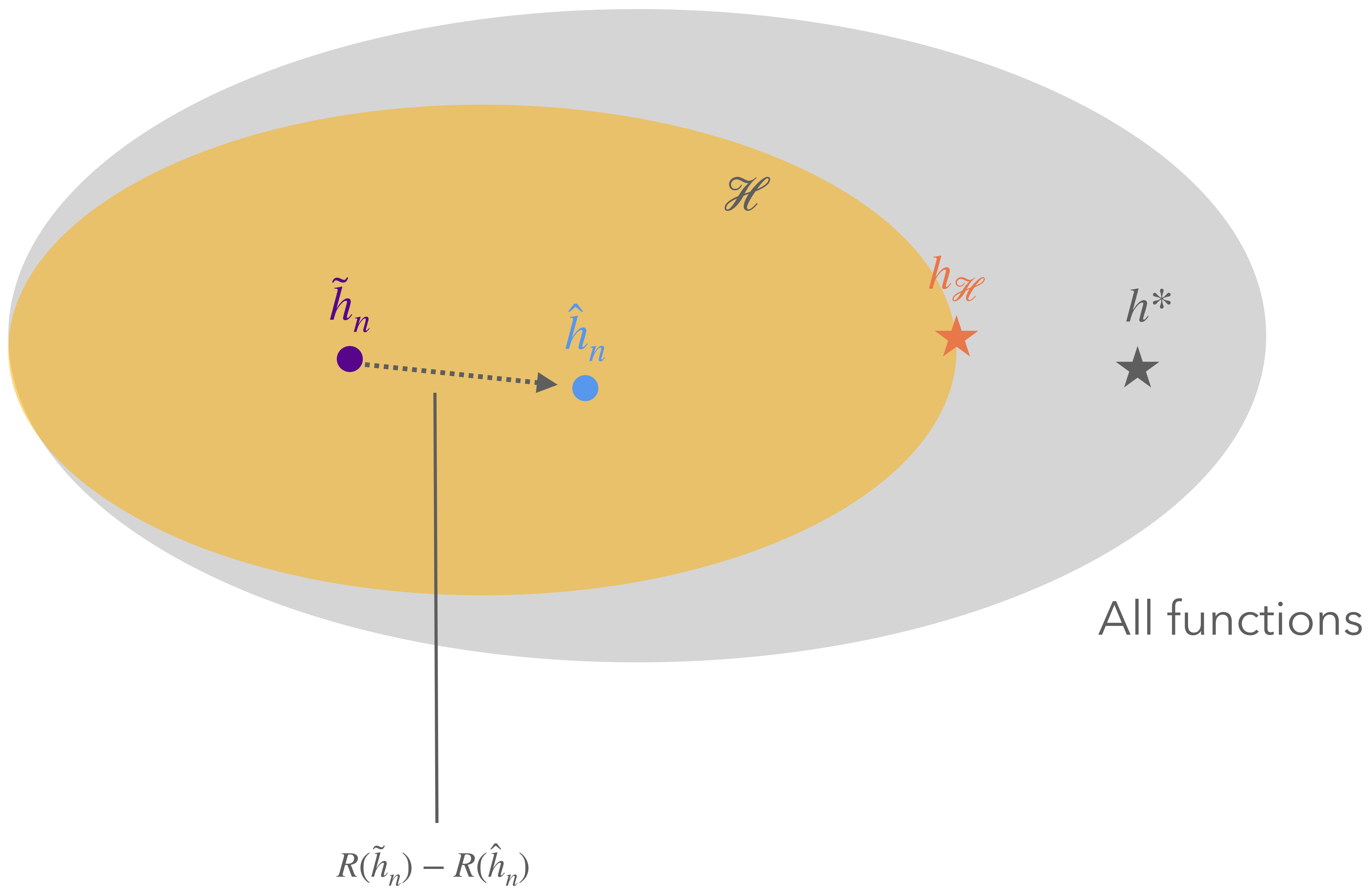
Details

We might not find the ERM $\hat{h}_n \in \mathscr{H}$.

We instead find $\tilde{h}_n \in \mathscr{H}$ via an algorithm, typically through optimization.

The optimization error is the gap between $\tilde{h}_n$ (which our algorithm returns) and $\hat{h}_n$ (the ERM):

$$R(\tilde{h}_n) - R(\hat{h}_n).$$



Excess Risk

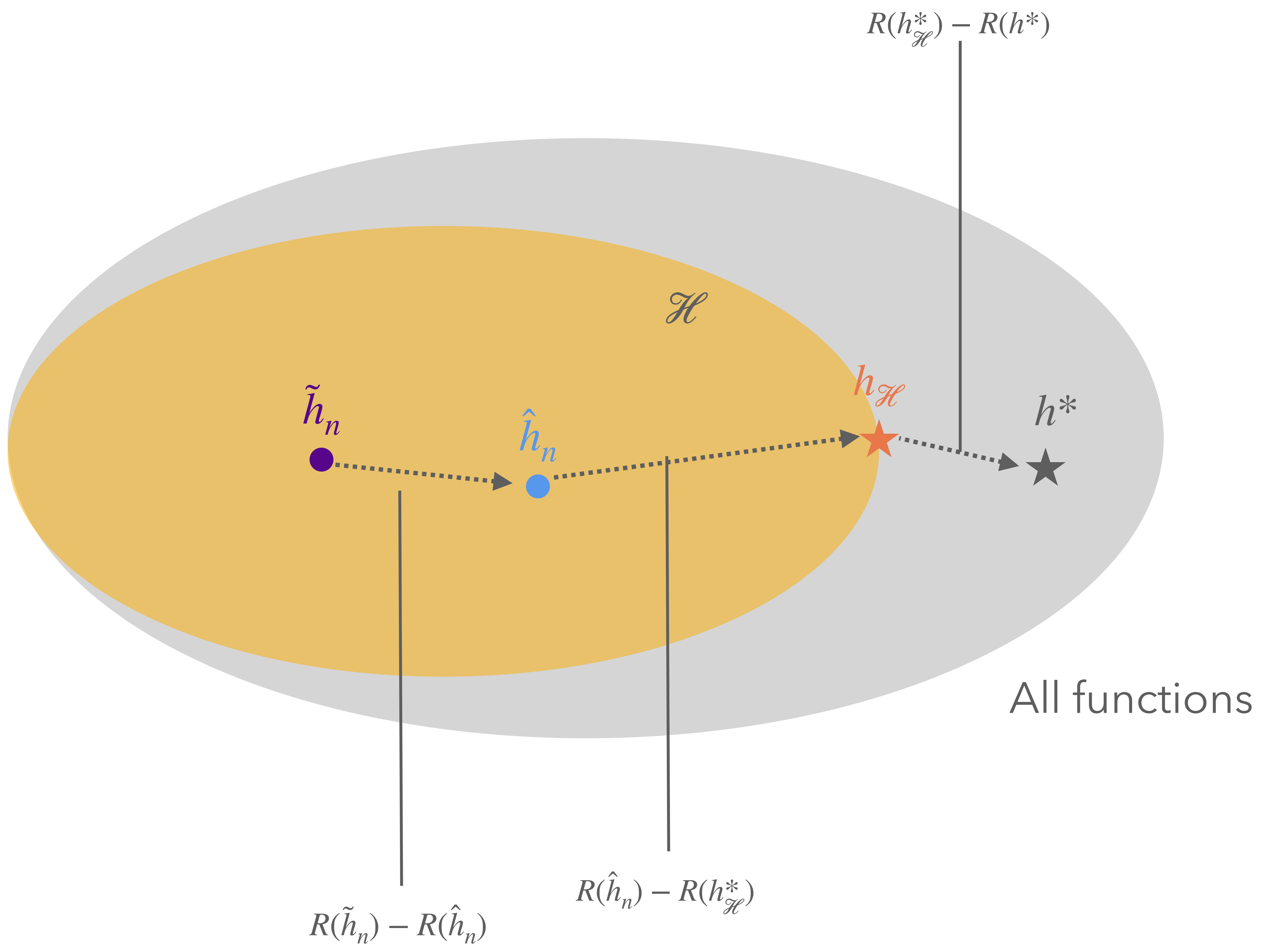
Full Decomposition

We receive $\tilde{h}_n$ from an algorithm.

Excess risk of $\tilde{h}_n$:

$$R(\tilde{h}_n) - R(h^*) =$$

$$\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathscr{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathscr{H}}) - R(h^*)}_{\text{approx. error}}$$



Supervised Learning

Basic Pipeline

1. Collect training dataset, a collection of labeled input-output pairs.

2. Decide on the template of the hypothesis mapping that will map inputs to actions.

Representation

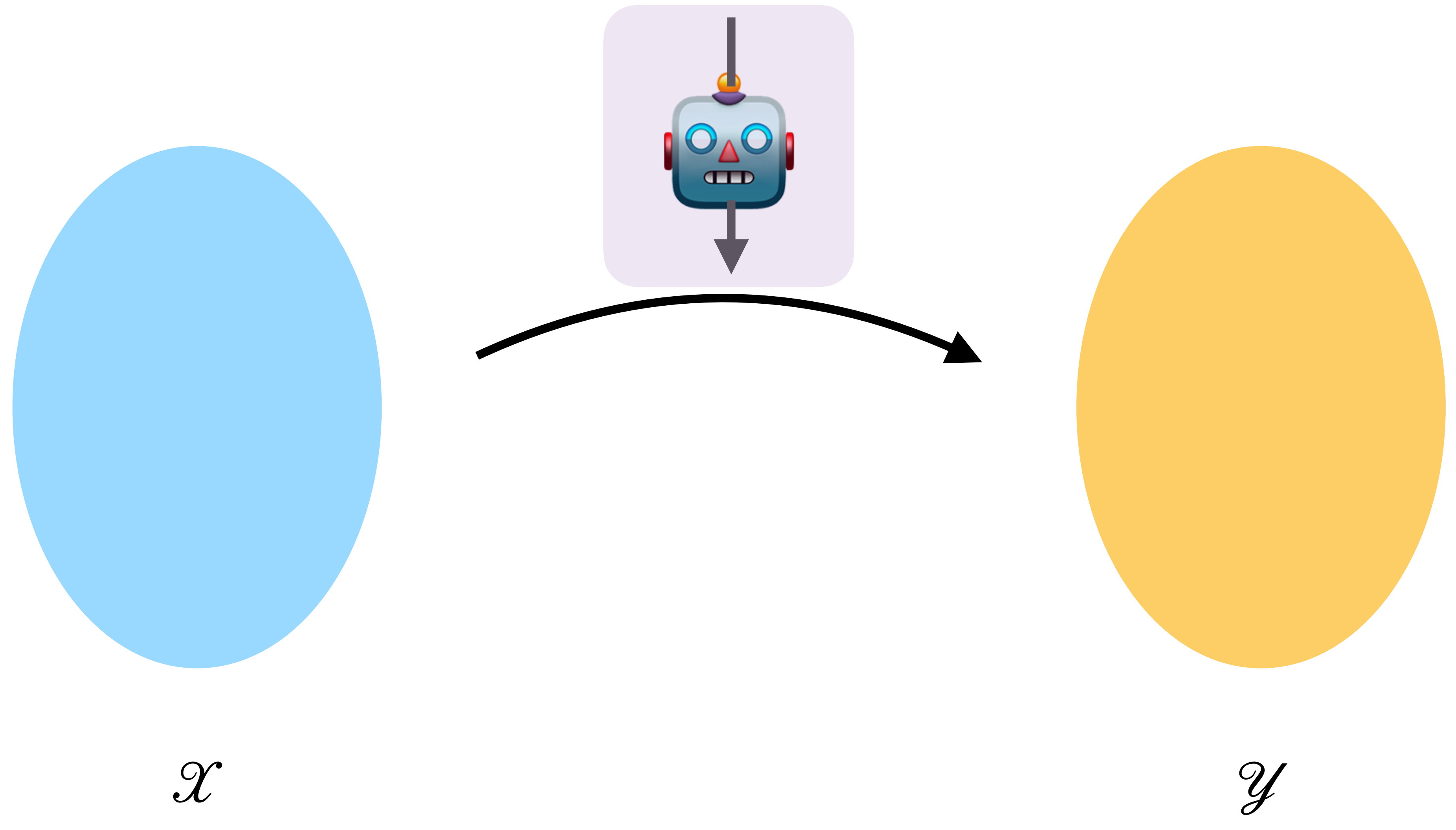
3. A learning algorithm takes the labeled training data as input and outputs a hypothesis.

Optimization

4. The hypothesis predicts on new, unseen data which we hope it does well on, under a notion of loss.

Generalization

$$D_n := \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$$



Supervised Learning

Excess Risk Formalization

1. Collect training dataset, a collection of labeled input-output pairs.

2. Decide on the template of the hypothesis mapping that will map inputs to actions. — Representation

3. A learning algorithm takes the labeled training data as input and outputs a hypothesis. — Optimization

4. The hypothesis predicts on new, unseen data which we hope it does well on, under a notion of loss. — Generalization

We receive $\tilde{h}_n$ from an algorithm.

Excess risk of $\tilde{h}_n$:

$$R(\tilde{h}_n) - R(h^*) =$$

$$\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathcal{H}}) - R(h^*)}_{\text{approx. error}}$$

Optimization — Generalization — Representation

Three Main Questions

Representation, Optimization, and Generalization

$$R(\tilde{h}_n) - R(h^*) =$$

$$\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathcal{H}}) - R(h^*)}_{\text{approx. error}}$$

Optimization Generalization Representation

Representation: *Which hypothesis class $\mathcal{H}$ best models the relationship of $\mathcal{X}$ to $\mathcal{A}$?*

Generalization: *How well can we extrapolate from training data to new, unseen data?*

Optimization: *How can we efficiently and accurately solve the ERM optimization problem?*

The Main Cast

Summary of the Problem

Examples from input space $\mathcal{X}$ and output space $\mathcal{Y}$; unknown distribution $P_{\mathcal{X}\times\mathcal{Y}}$ over $\mathcal{X} \times \mathcal{Y}$.

Action space $\mathcal{A}$ as the output (often, a *prediction*) of learned hypothesis/predictor.

We evaluate actions with a loss function $\ell : \mathcal{A} \times \mathcal{Y} \to \mathbb{R}$.

Goal: Find a hypothesis $h : \mathcal{X} \to \mathcal{A}$ to minimize the risk $R(h) := \mathbb{E}[\ell(h(x), y)]$.

We can approximate risk with the empirical risk over sample $D_n = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$:

$$\hat{R}_n(h) := \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}).$$

The Main Cast

Summary of the Problem

Goal: Find a hypothesis $h : \mathcal{X} \to \mathcal{A}$ to minimize the risk $R(h) := \mathbb{E}[\ell(h(x), y)]$.

We can approximate risk with the empirical risk over sample $D_n = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$.

Choose a hypothesis class $\mathcal{H}$ and find the empirical risk minimizer $\hat{h}_n \in \mathcal{H}$:

$$\hat{h}_n \in \operatorname*{argmin}_{h \in \mathcal{H}} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)})}_{\hat{R}_n(h)}$$

Or find $\tilde{h}_n$ that approximates $\hat{h}_n$ well.

The Main Cast

Summary of the Problem

<u>Goal:</u> Find a hypothesis $h : \mathcal{X} \to \mathcal{A}$ to minimize the risk $R(h) := \mathbb{E}[\ell(h(x), y)]$.

Overall quality (excess risk) of our produced $\tilde{h}_n$:

$$R(\tilde{h}_n) - R(h^*) = \underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathcal{H}}) - R(h^*)}_{\text{approx. error}}$$

Choose $\mathcal{H}$ that balances approximation error and estimation error.

With more data, estimation error typically decreases, can use bigger $\mathcal{H}$.

Produce $\tilde{h}_n$ via an algorithm that (approximately and efficiently) minimizes empirical error.

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