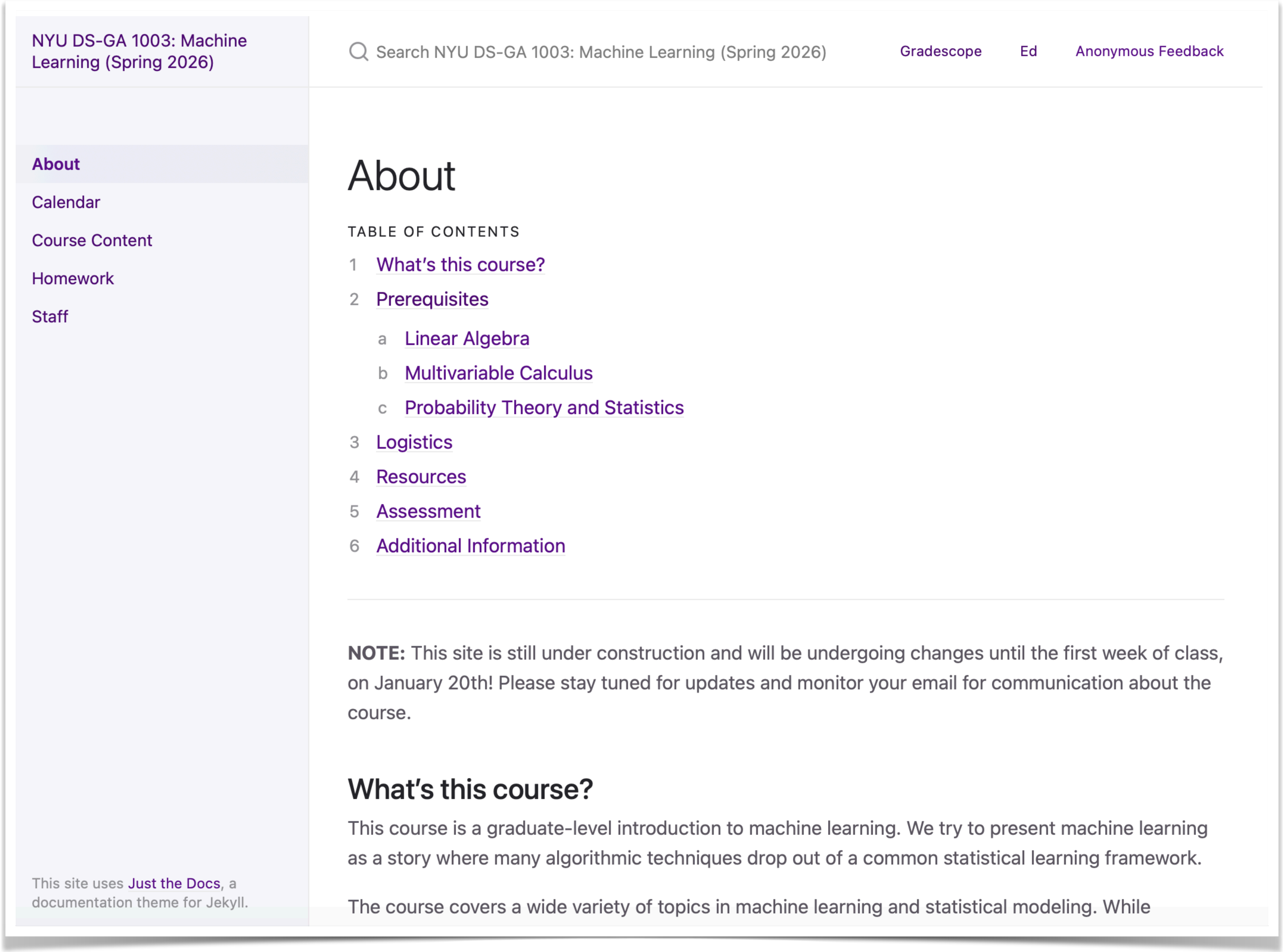
DS-GA 1003: Machine Learning

Lecture 1: Intro & Supervised Learning Framework

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

Outline

Course Website


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

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Gradescope Ed Anonymous Feedback

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

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.

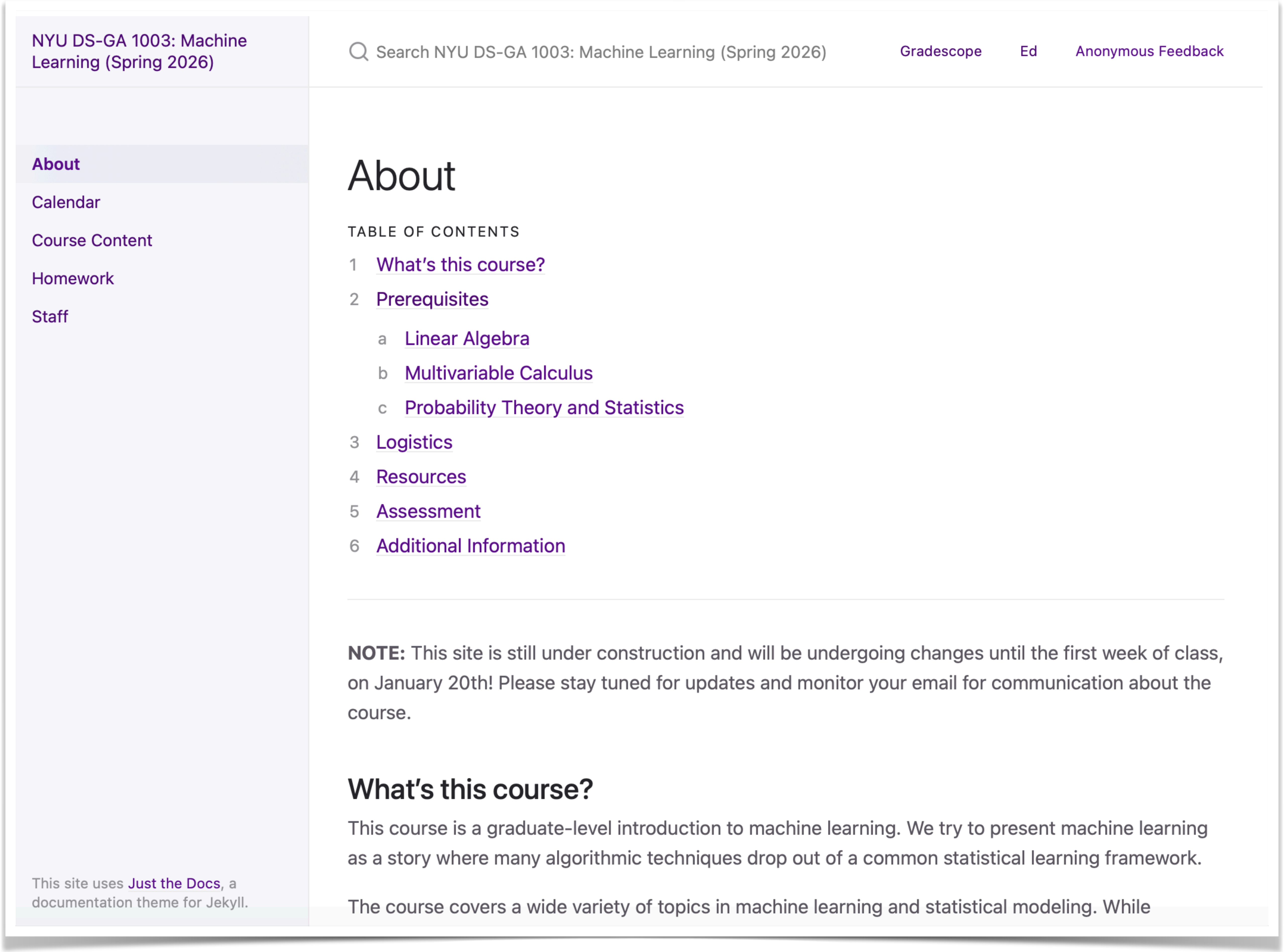
What's this course?

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.

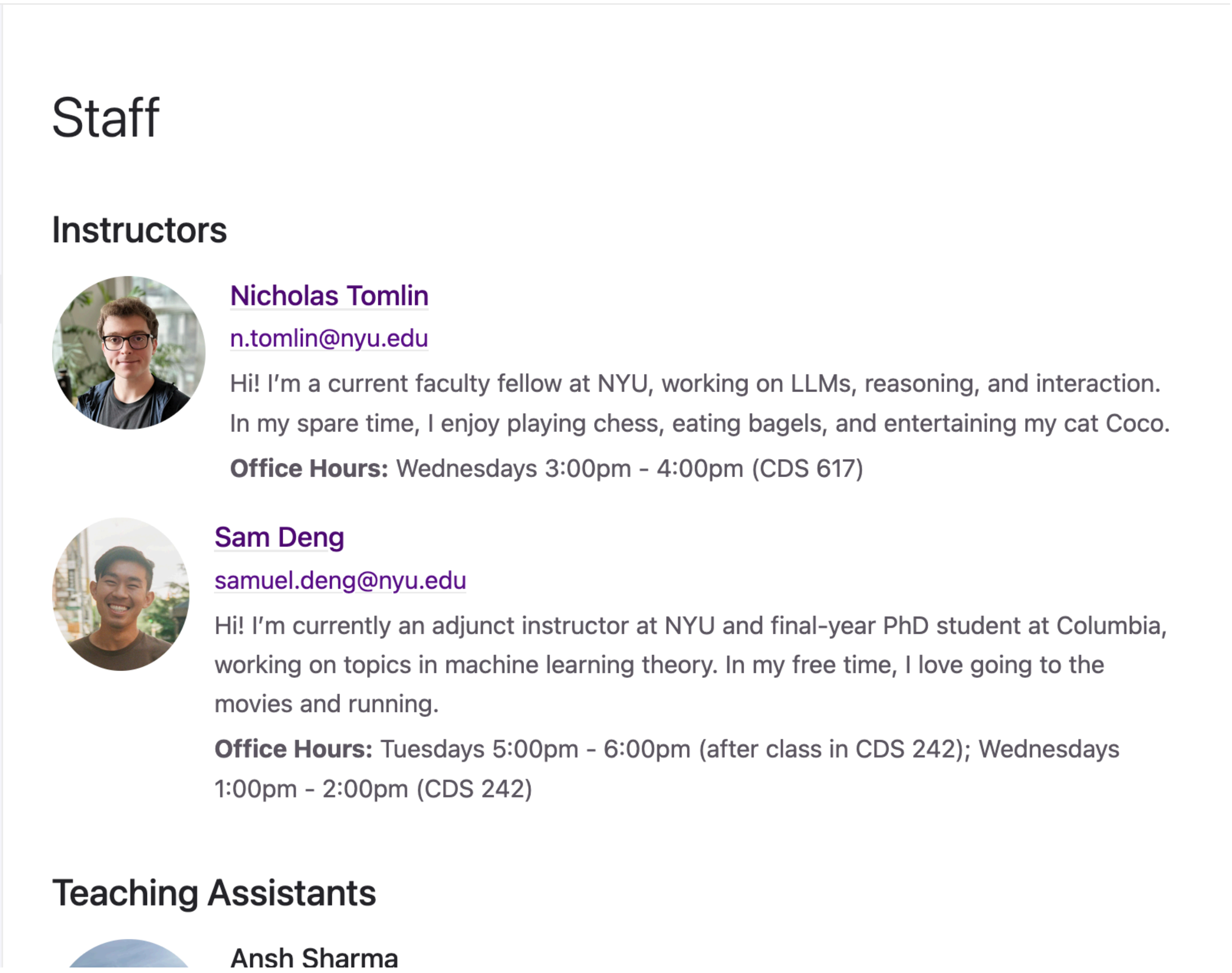
The course covers a wide variety of topics in machine learning and statistical modeling. While

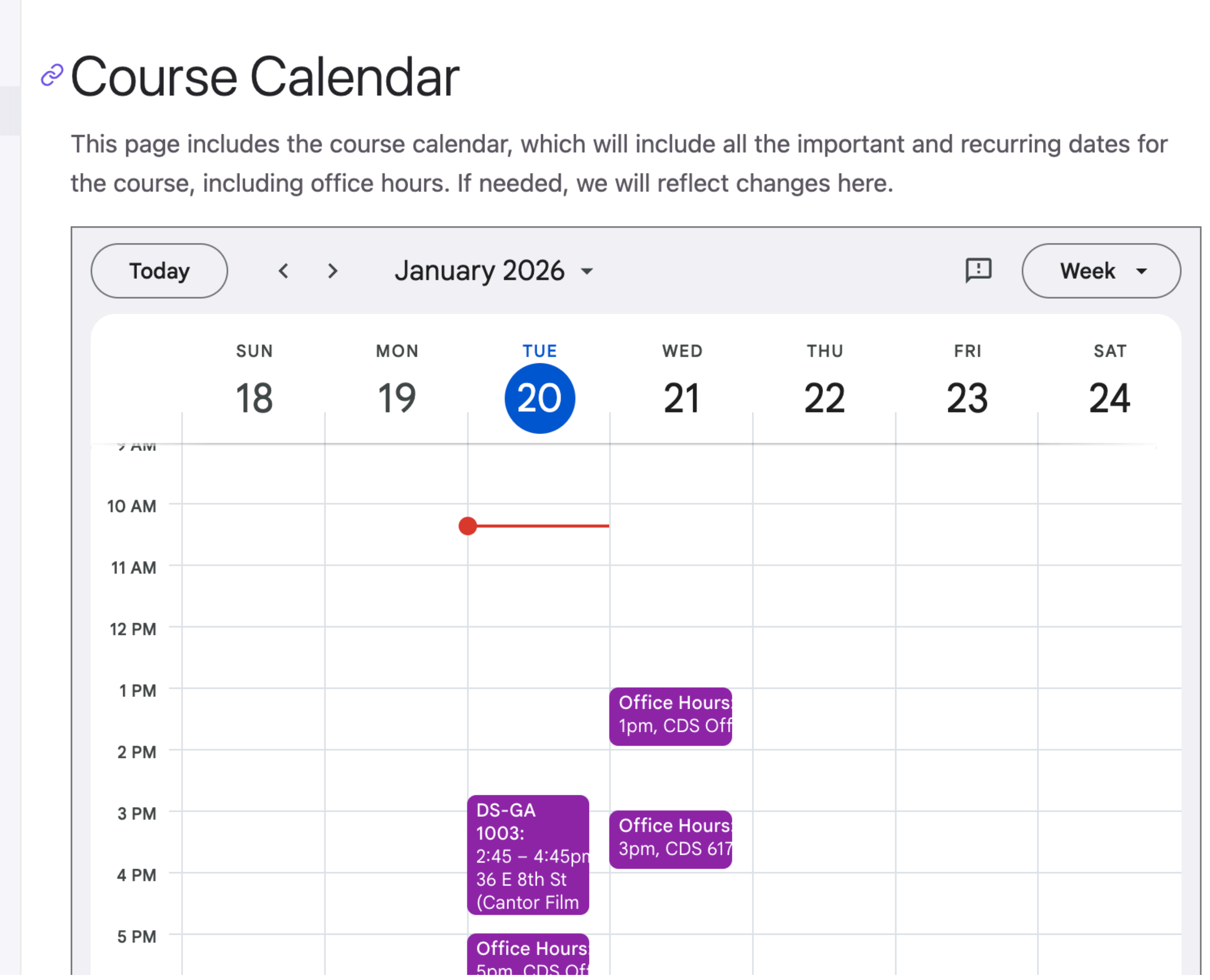
Course Website

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



Staff & Office Hours





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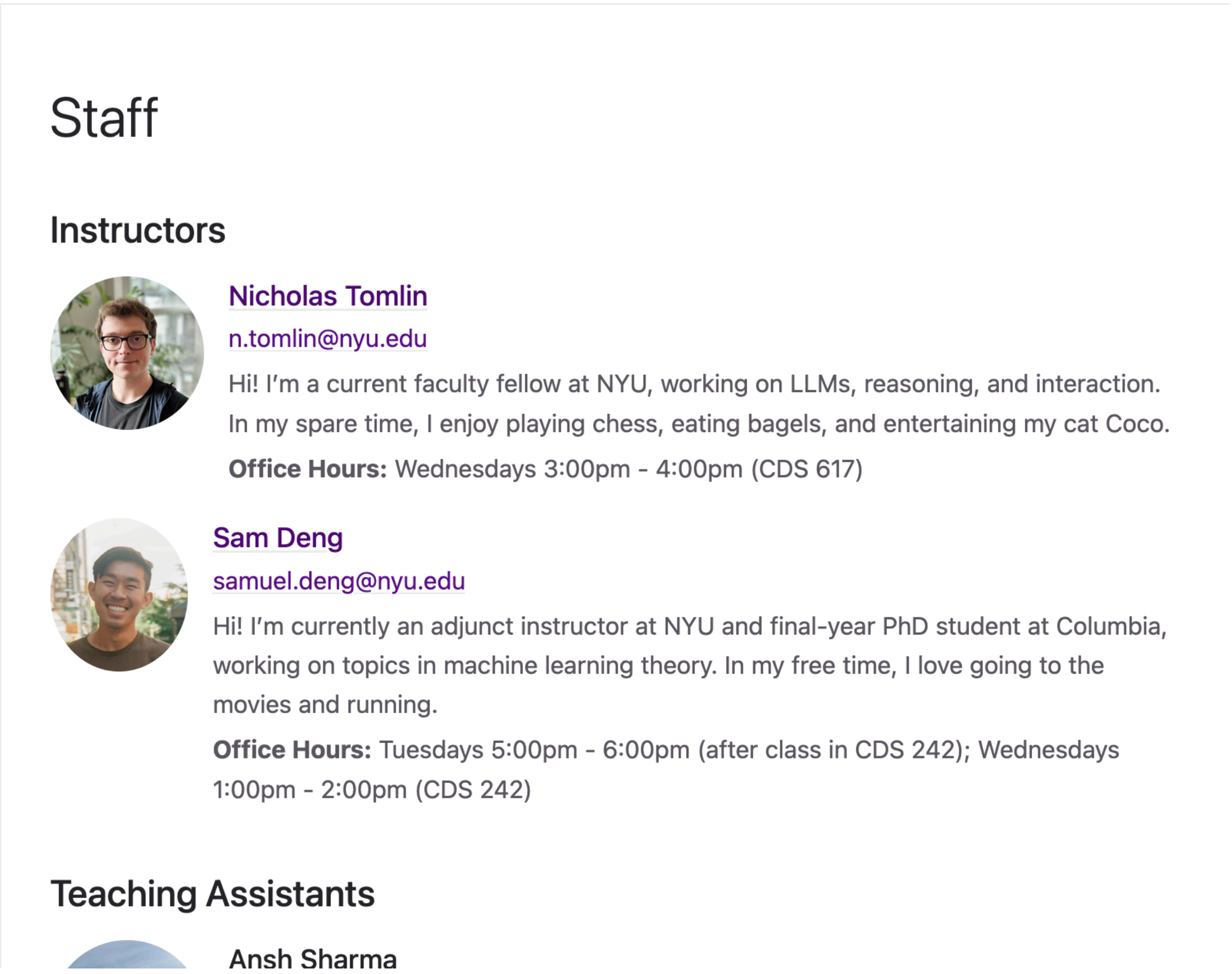

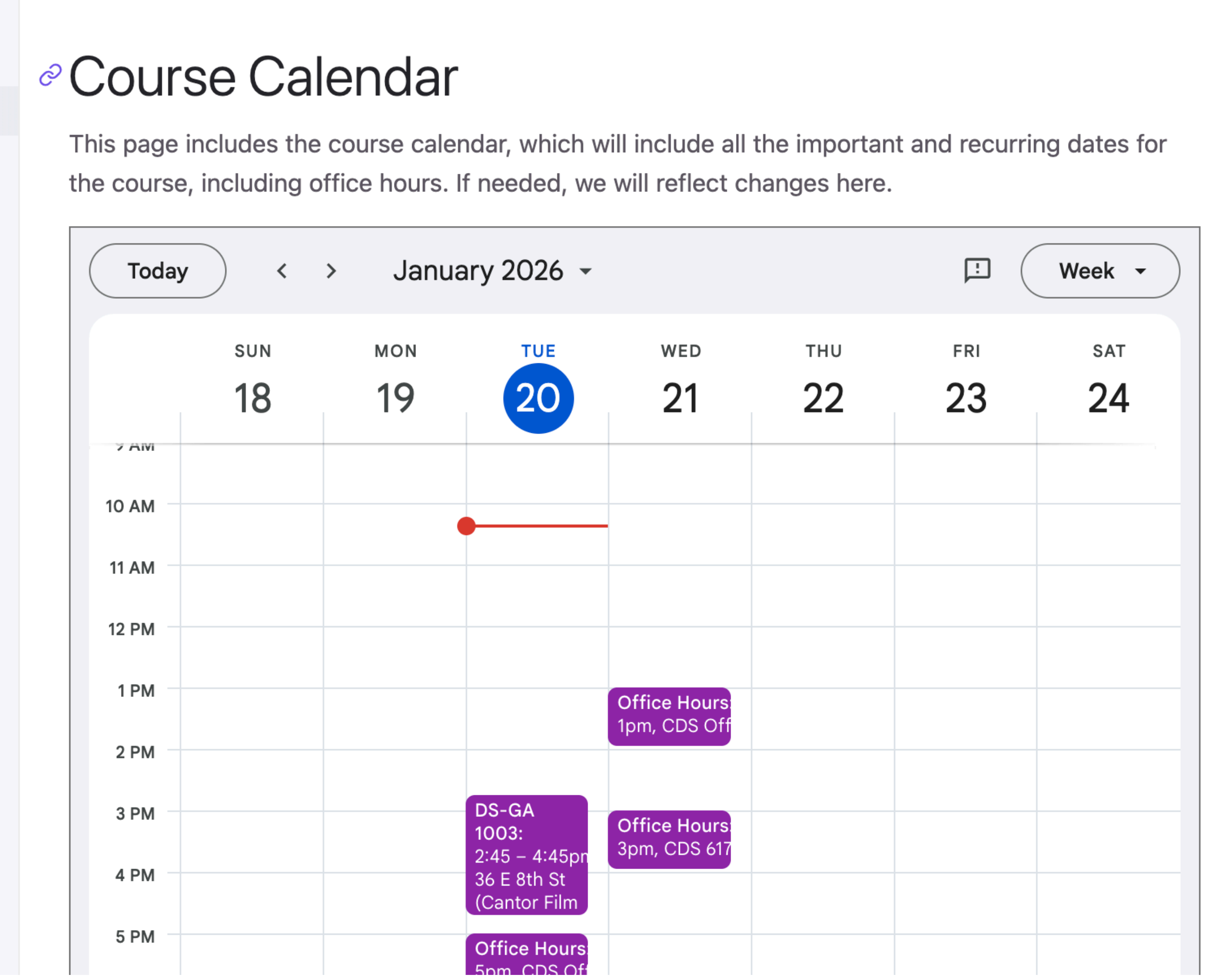

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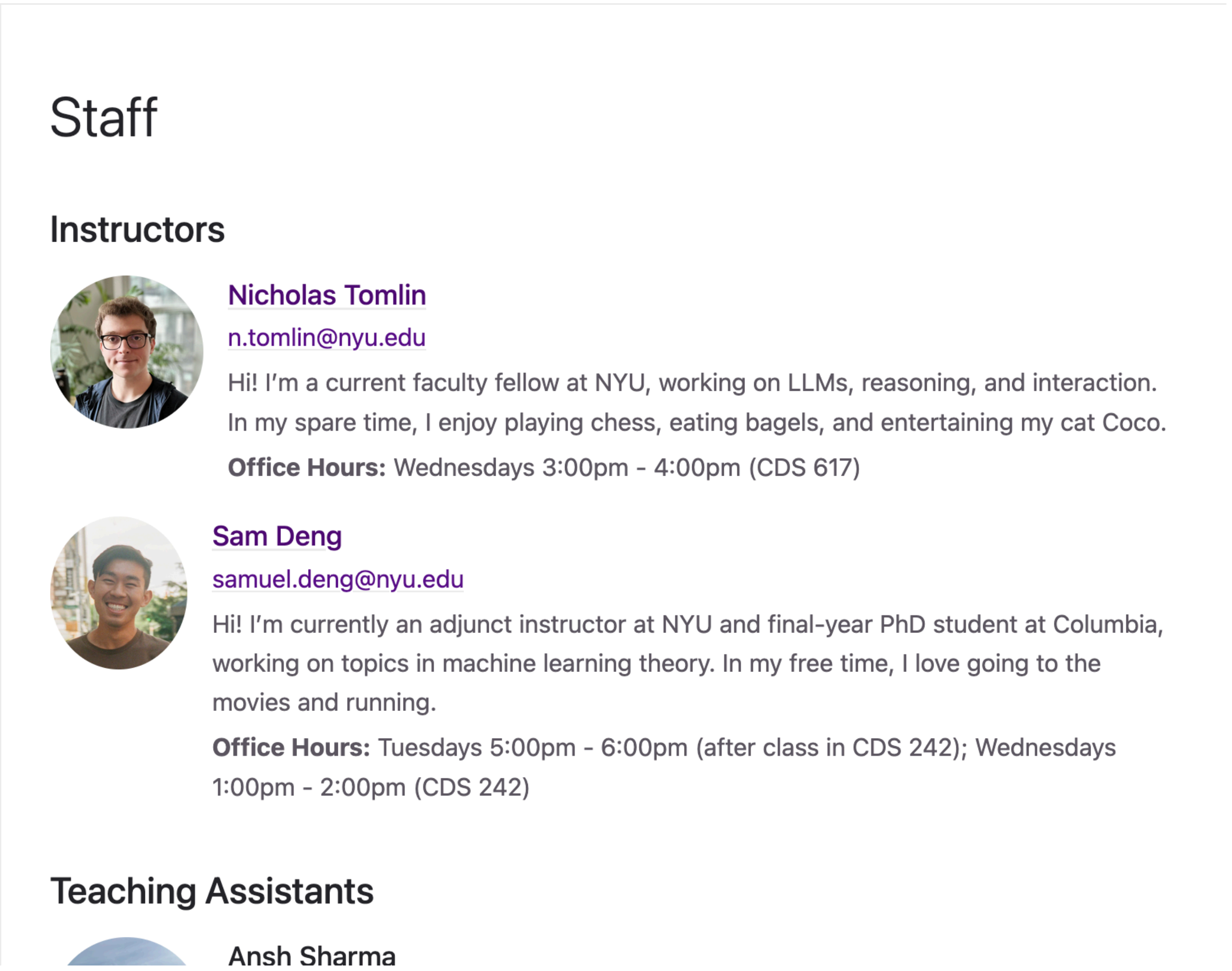

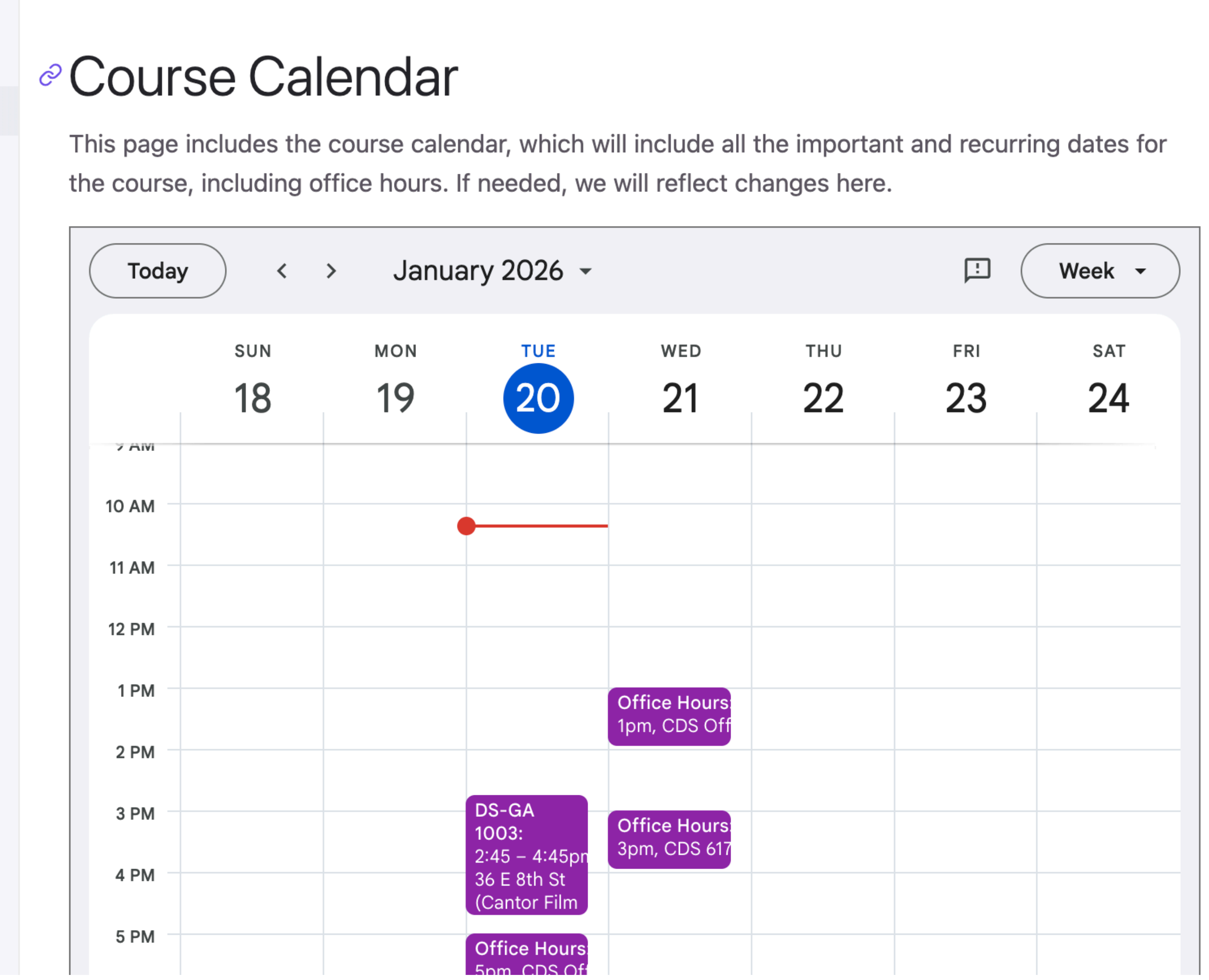

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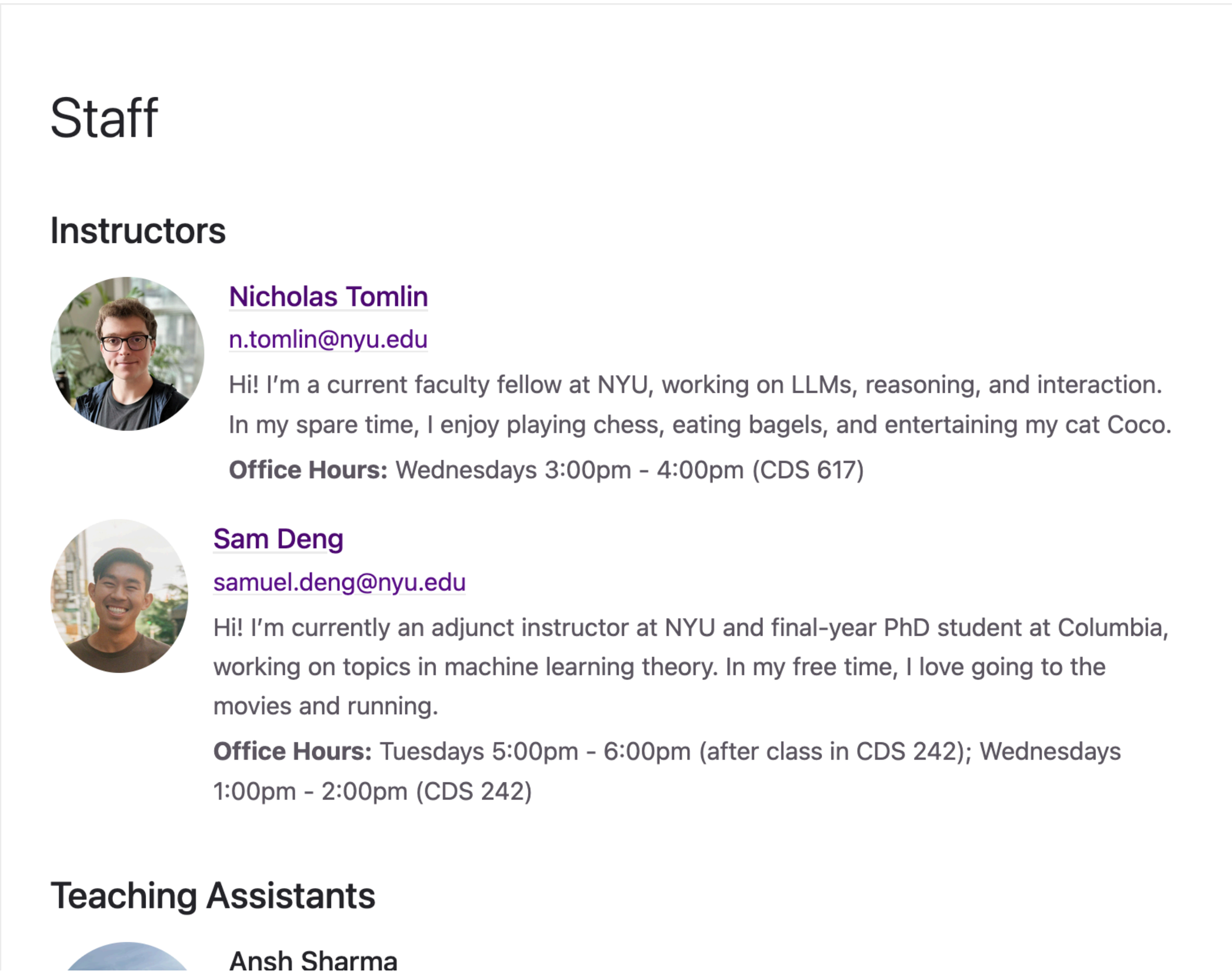

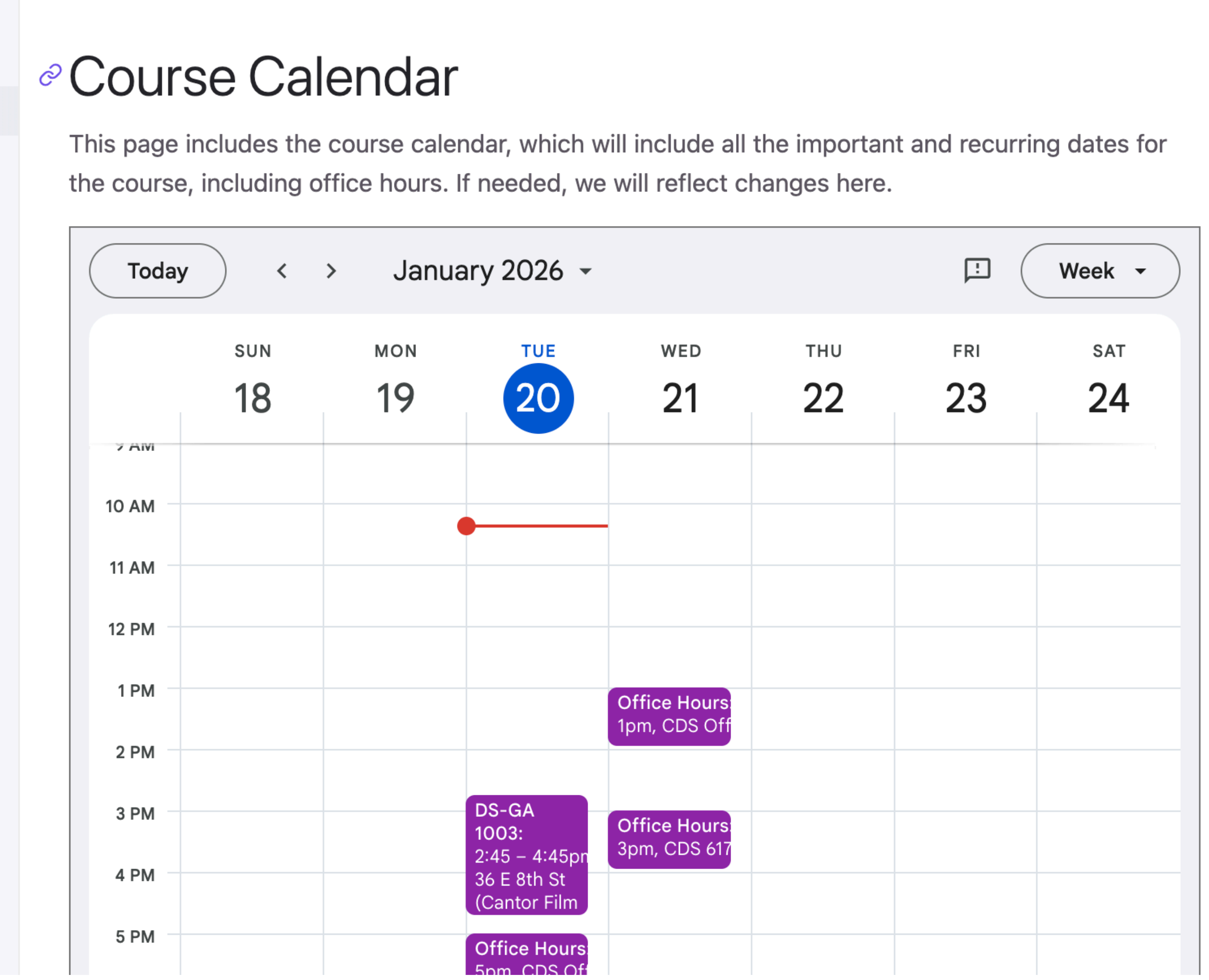

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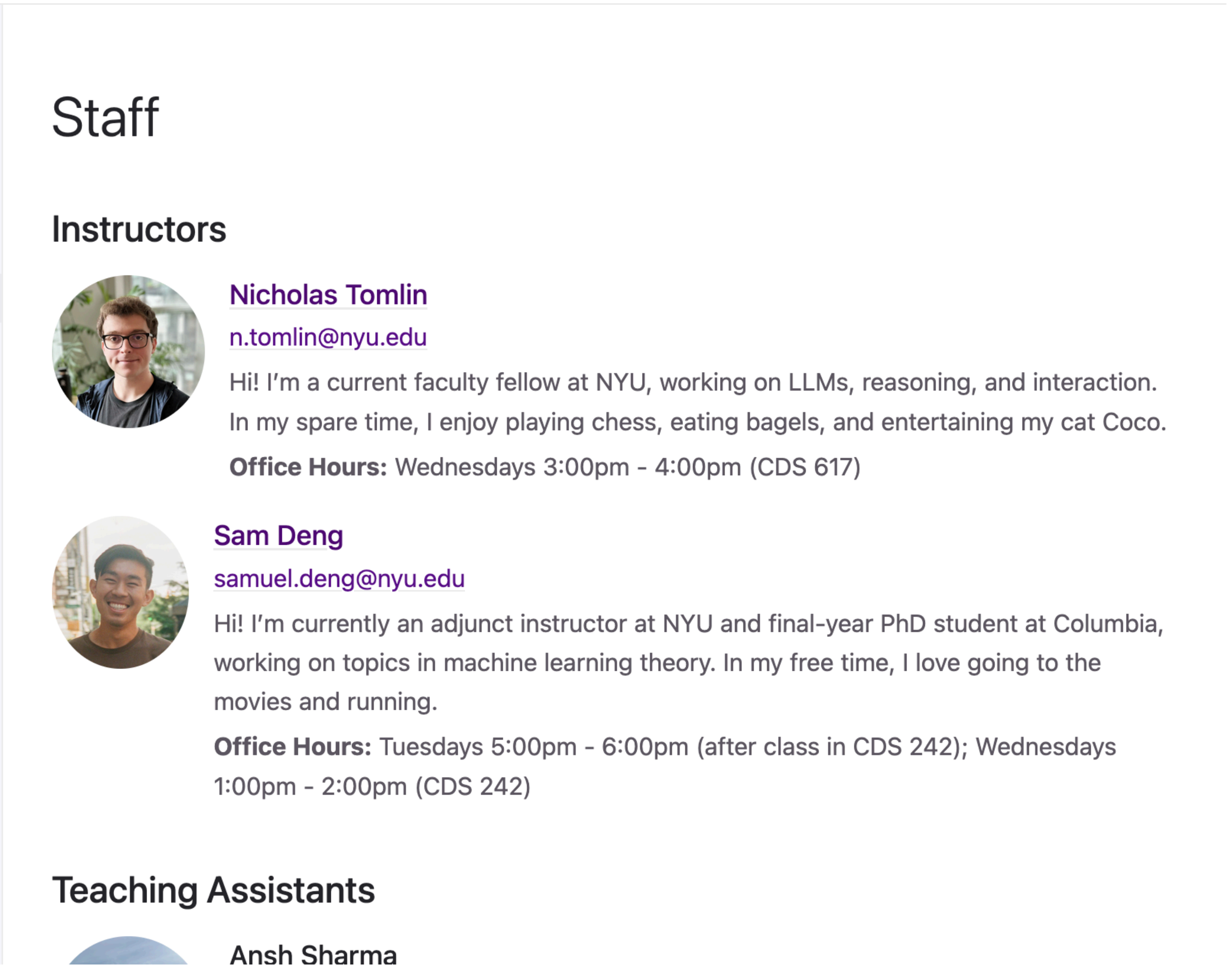

Staff

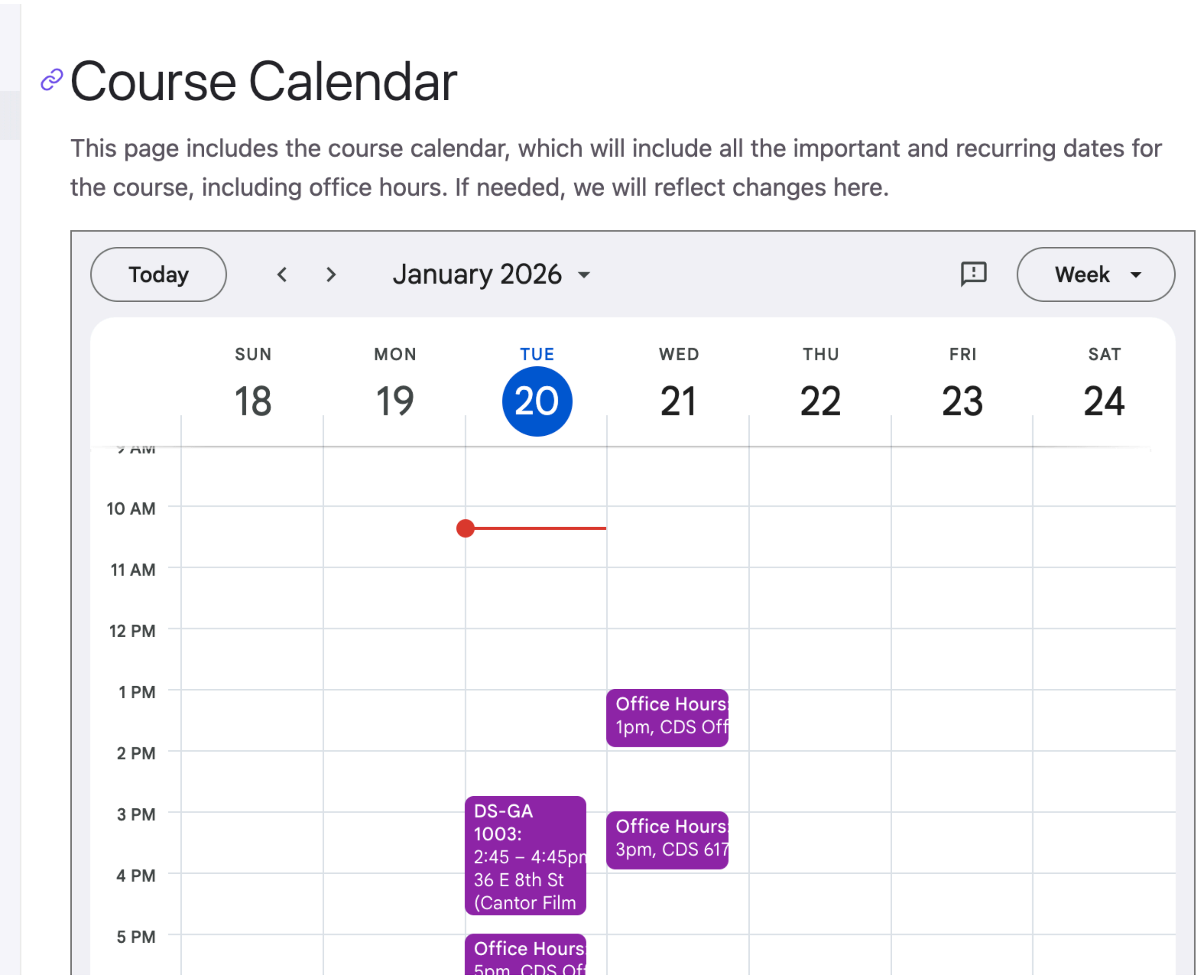
Instructors

Nicholas Tomlin
n.tomlin@nyu.edu
Hi! I'm a current faculty fellow at NYU, working on LLMs, reasoning, and interaction. In my spare time, I enjoy playing chess, eating bagels, and entertaining my cat Coco.
Office Hours: Wednesdays 3:00pm - 4:00pm (CDS 617)

Sam Deng
samuel.deng@nyu.edu
Hi! I'm currently an adjunct instructor at NYU and final-year PhD student at Columbia, working on topics in machine learning theory. In my free time, I love going to the movies and running.
Office Hours: Tuesdays 5:00pm - 6:00pm (after class in CDS 242); Wednesdays 1:00pm - 2:00pm (CDS 242)

Teaching Assistants

Ansh Sharma


Course Calendar

This page includes the course calendar, which will include all the important and recurring dates for the course, including office hours. If needed, we will reflect changes here.

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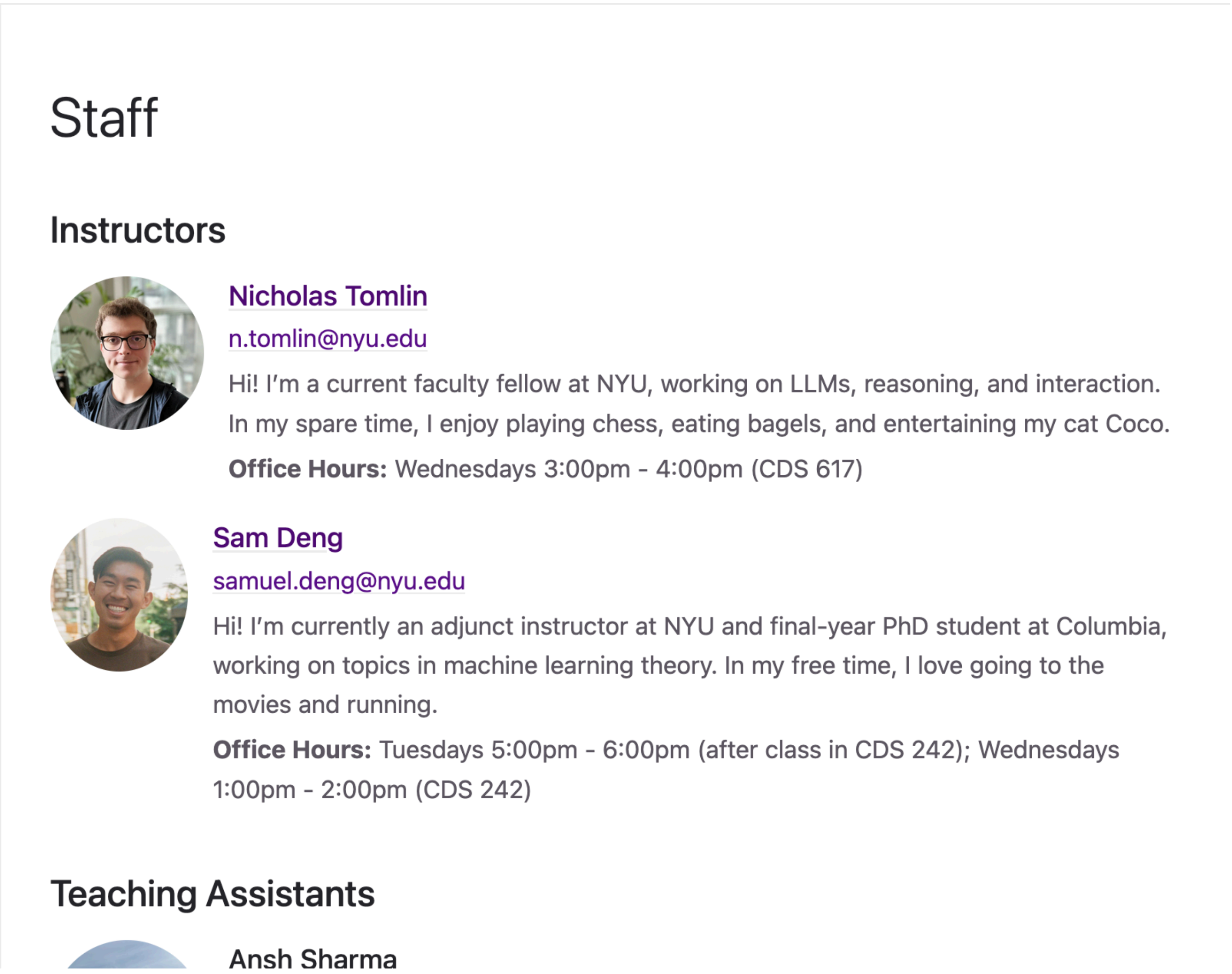

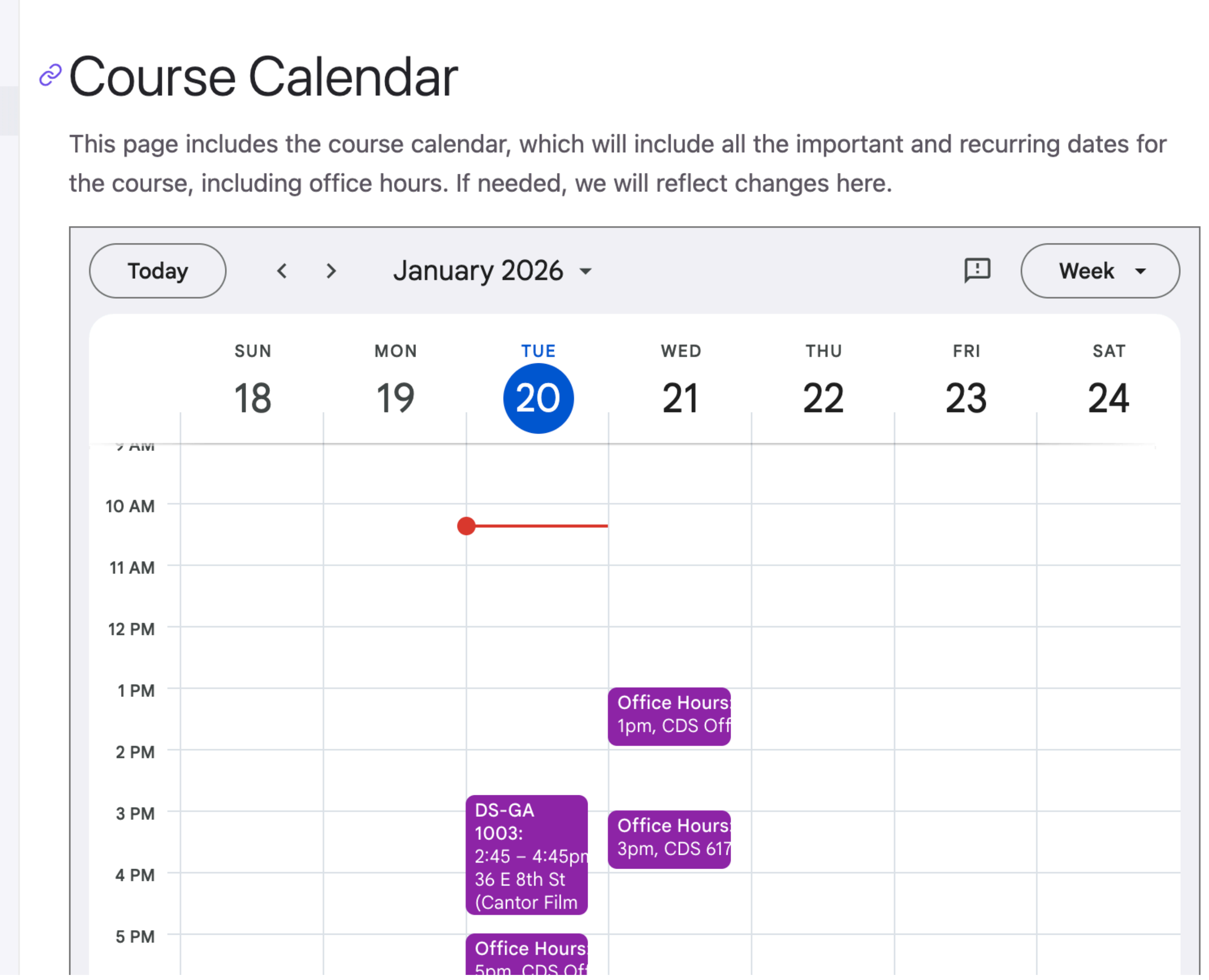

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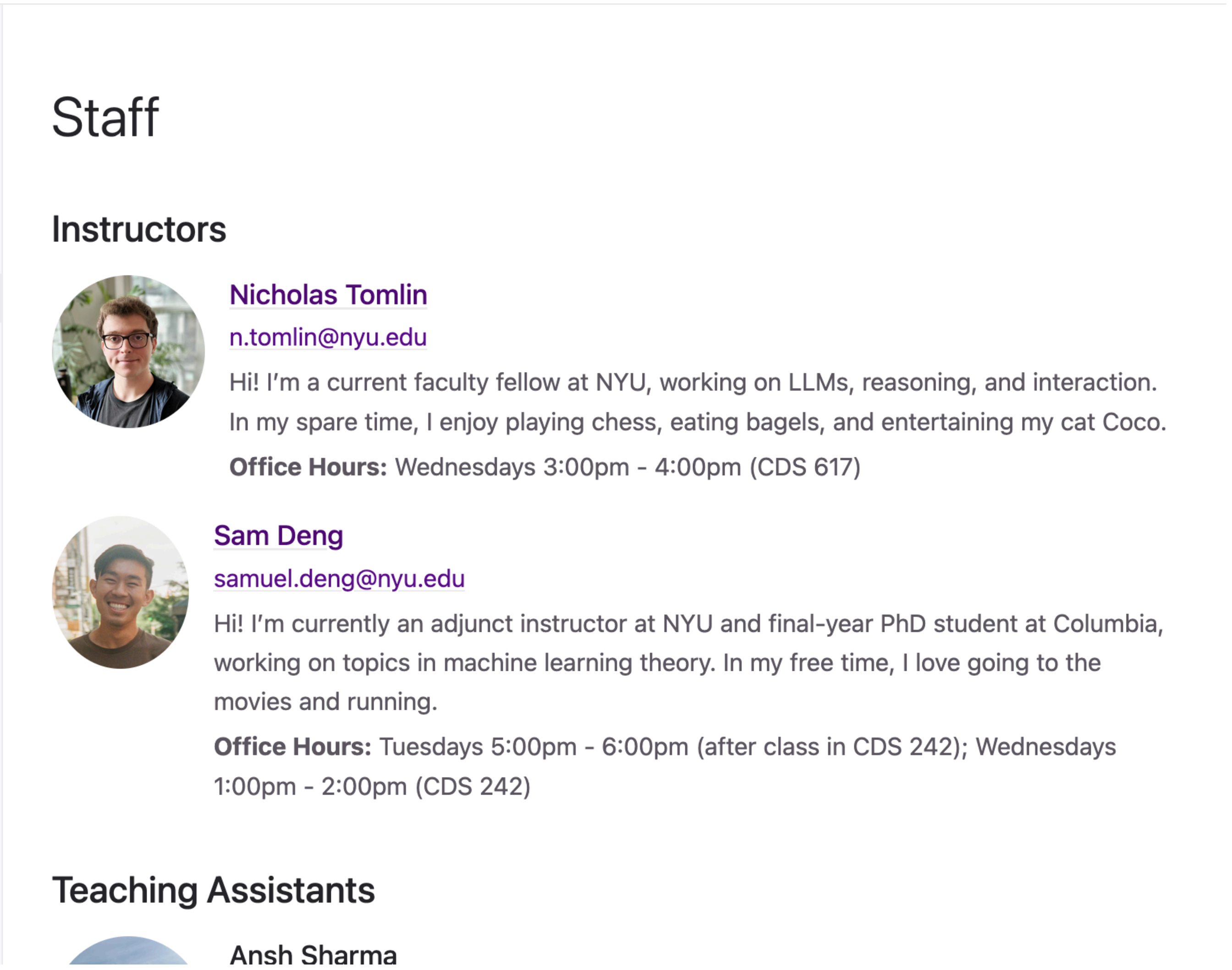

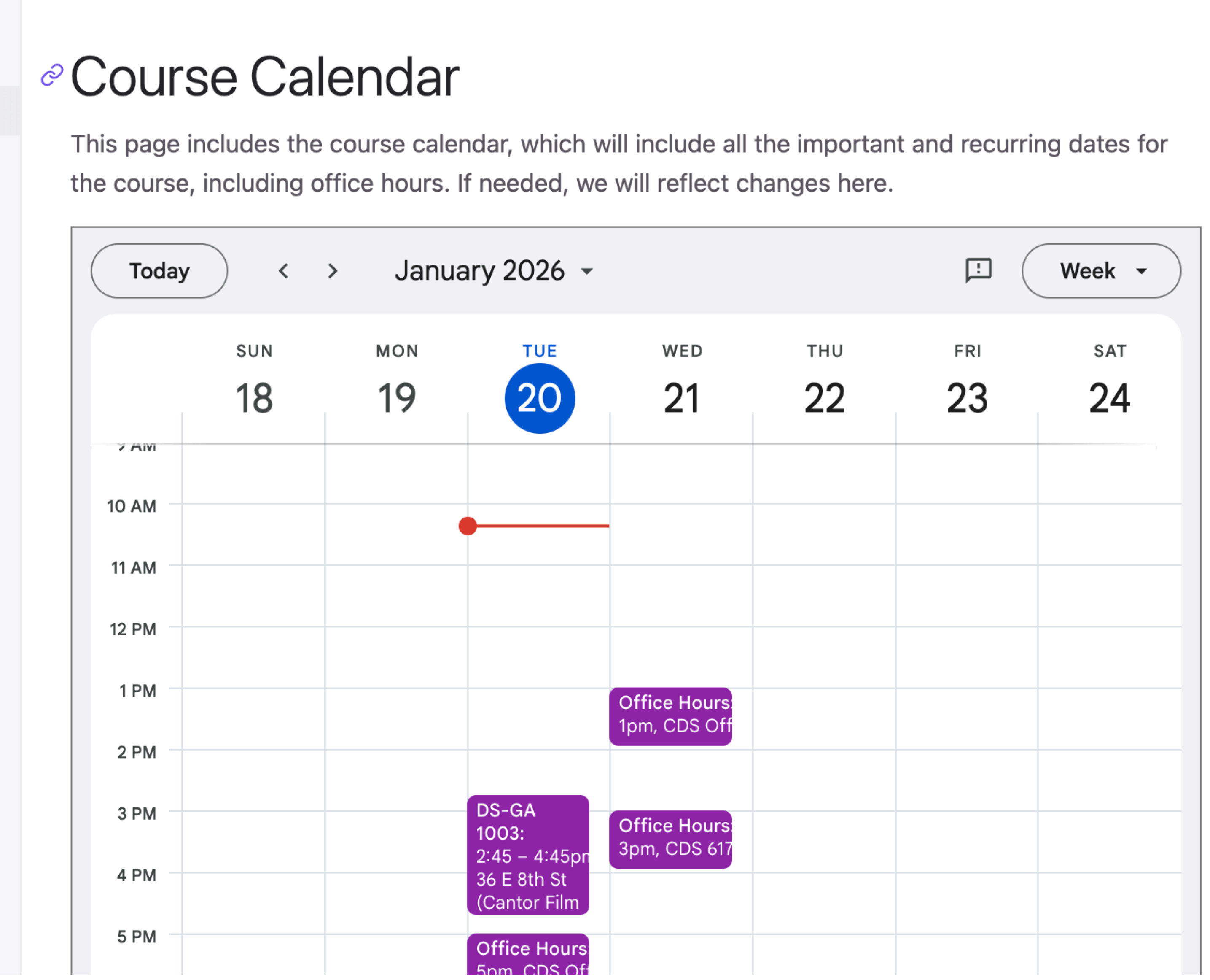

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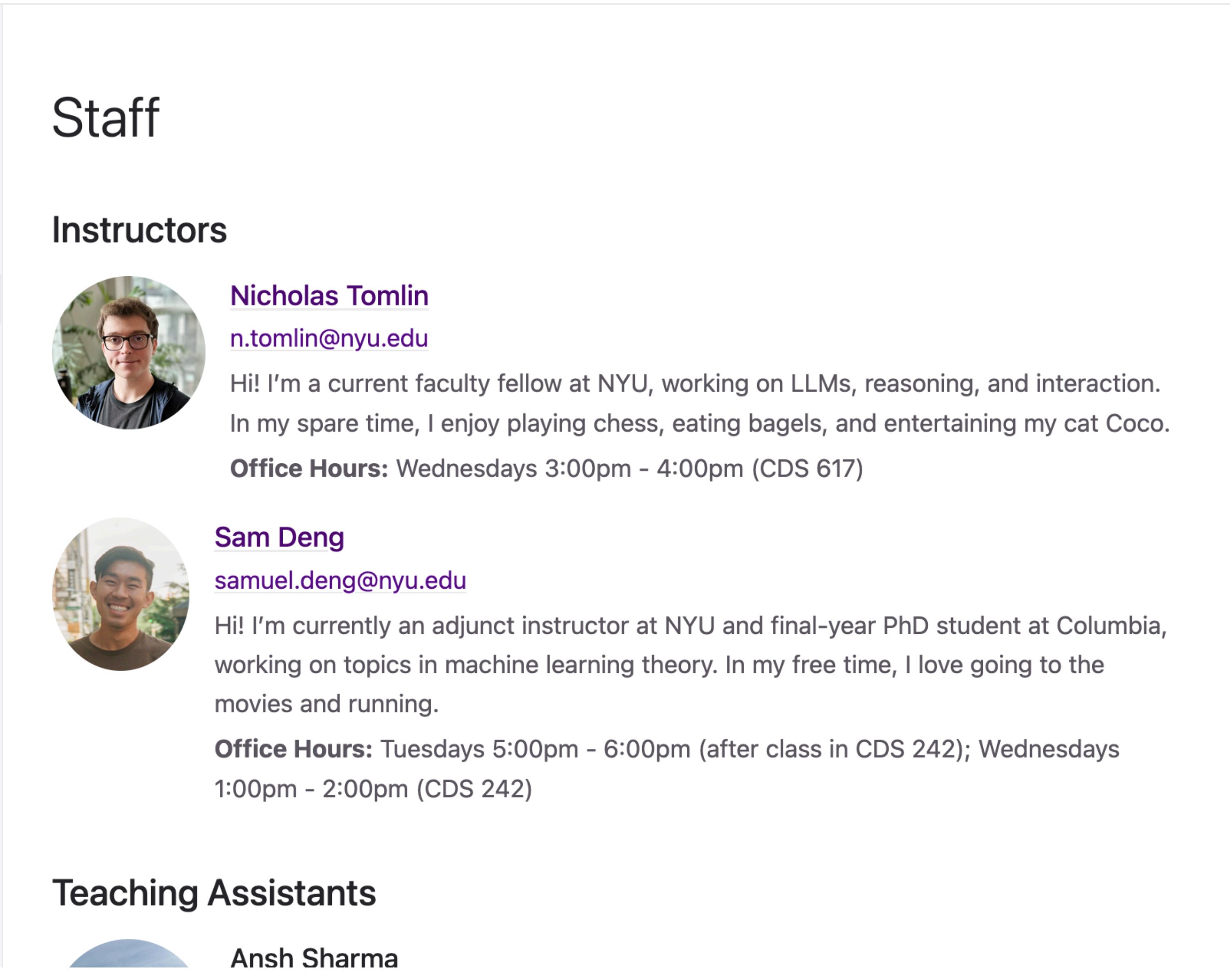
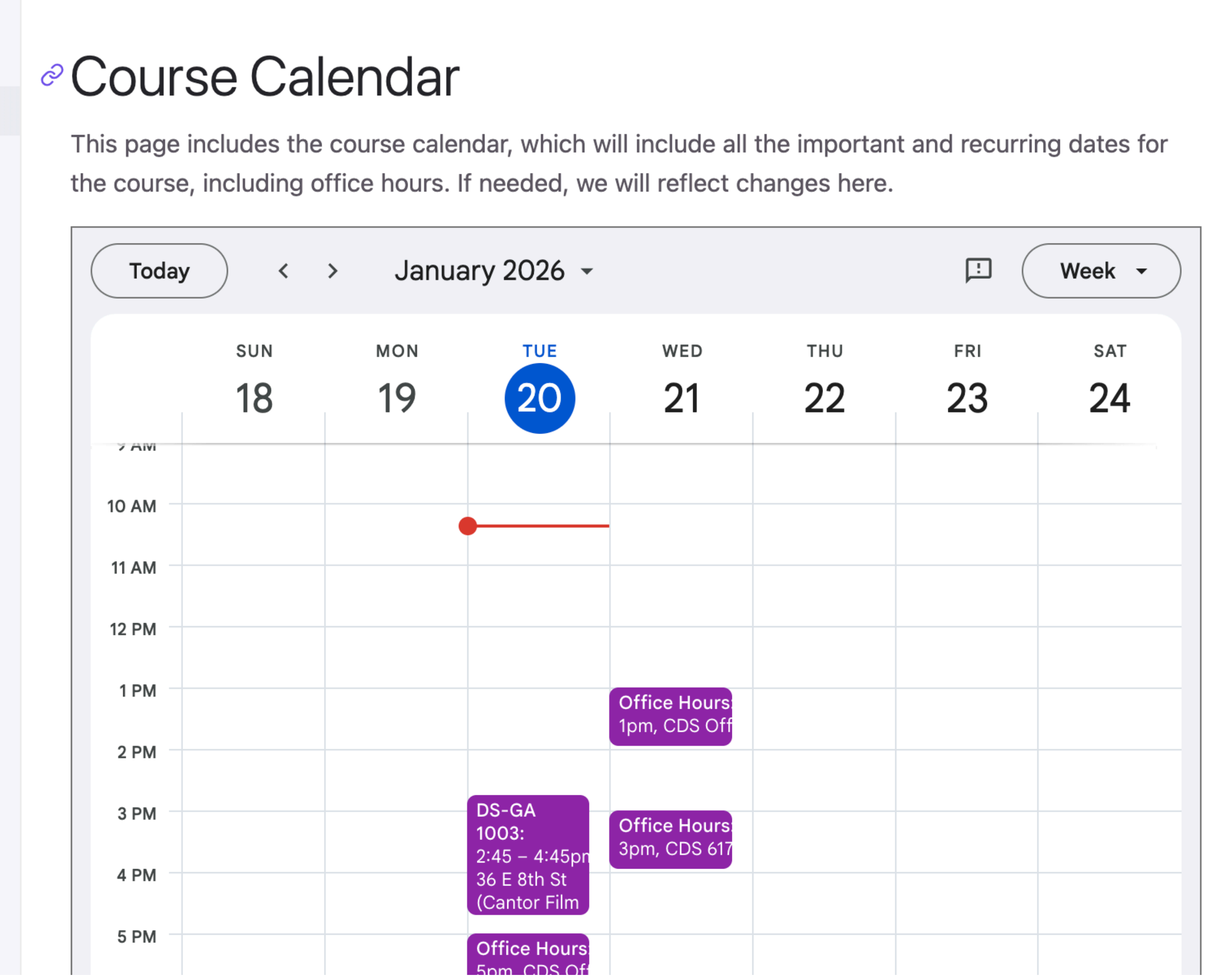
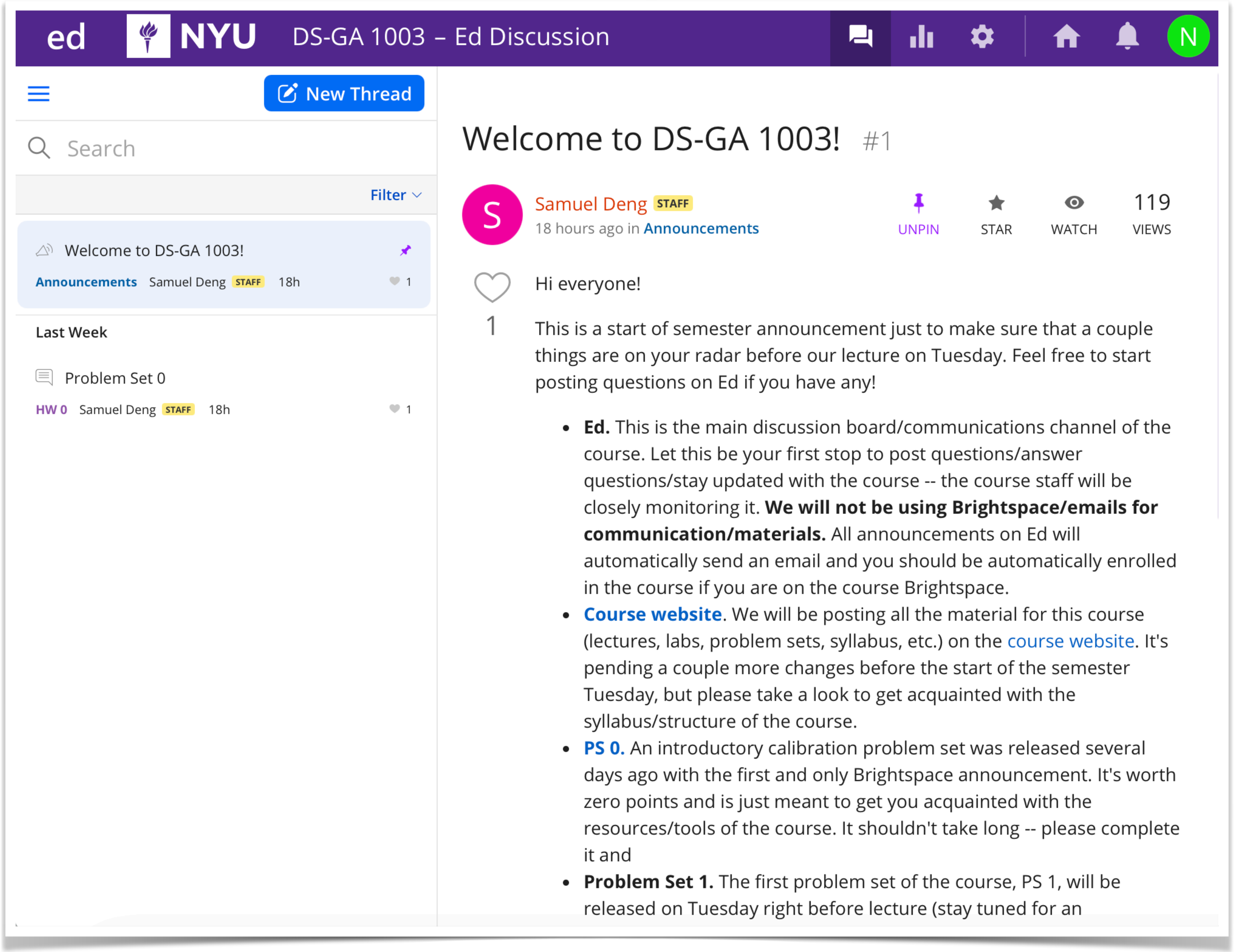
Nick's: Wed 3 - 4pm





EdStem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Hi everyone!
This is a start of semester announcement just to make sure that a couple things are on your radar before our lecture on Tuesday. Feel free to start posting questions on Ed if you have any!
Ed. This is the main discussion board/communications channel of the course. Let this be your first stop to post questions/answer questions/stay updated with the course -- the course staff will be closely monitoring it. We will not be using Brightspace/emails for communication/materials. All announcements on Ed will automatically send an email and you should be automatically enrolled in the course if you are on the course Brightspace.
Course website. We will be posting all the material for this course (lectures, labs, problem sets, syllabus, etc.) on the course website. It's pending a couple more changes before the start of the semester Tuesday, but please take a look to get acquainted with the syllabus/structure of the course.
PS 0. An introductory calibration problem set was released several days ago with the first and only Brightspace announcement. It's worth zero points and is just meant to get you acquainted with the resources/tools of the course. It shouldn't take long -- please complete it and
Problem Set 1. The first problem set of the course, PS 1, will be released on Tuesday right before lecture (stay tuned for an

EdStem

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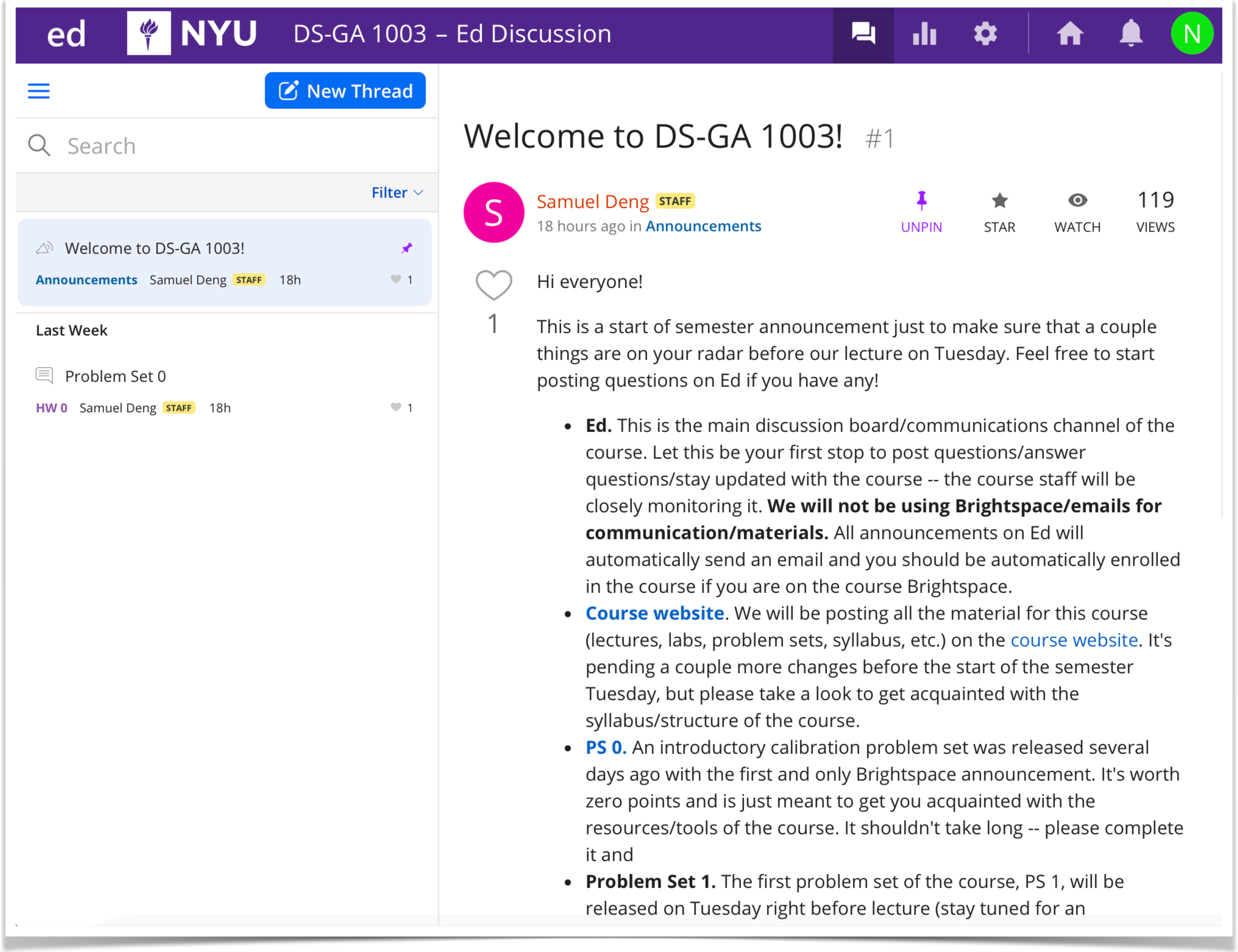

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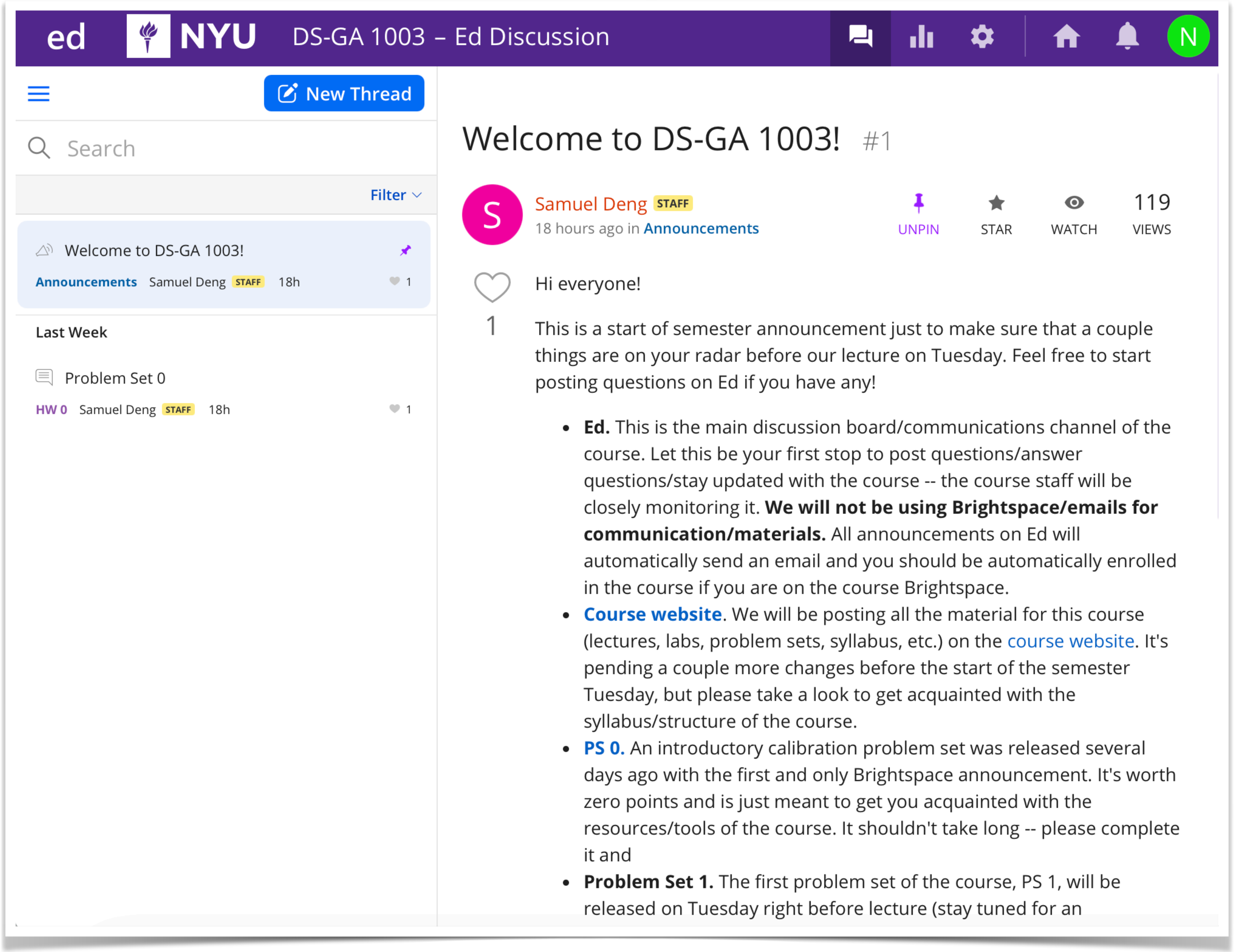

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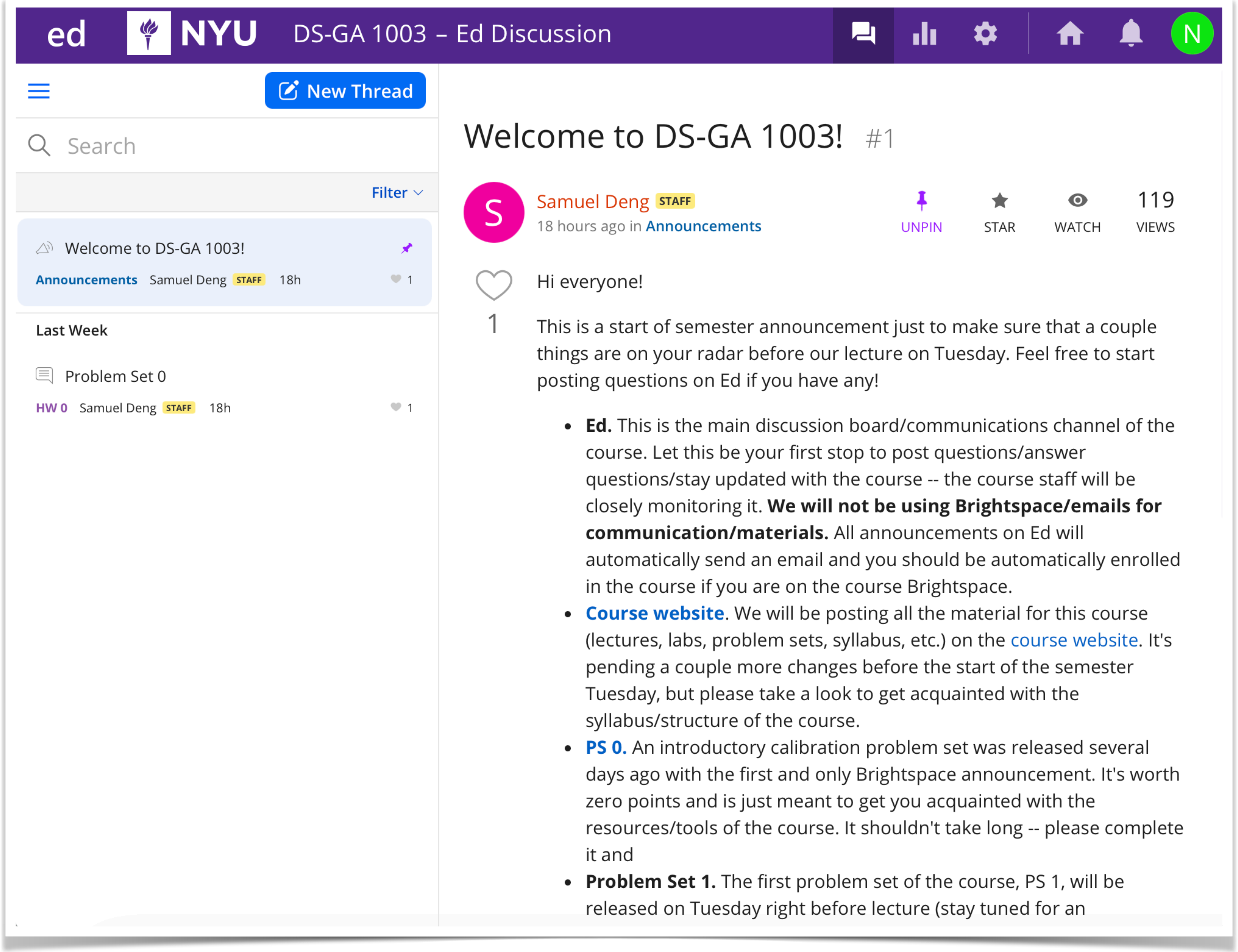

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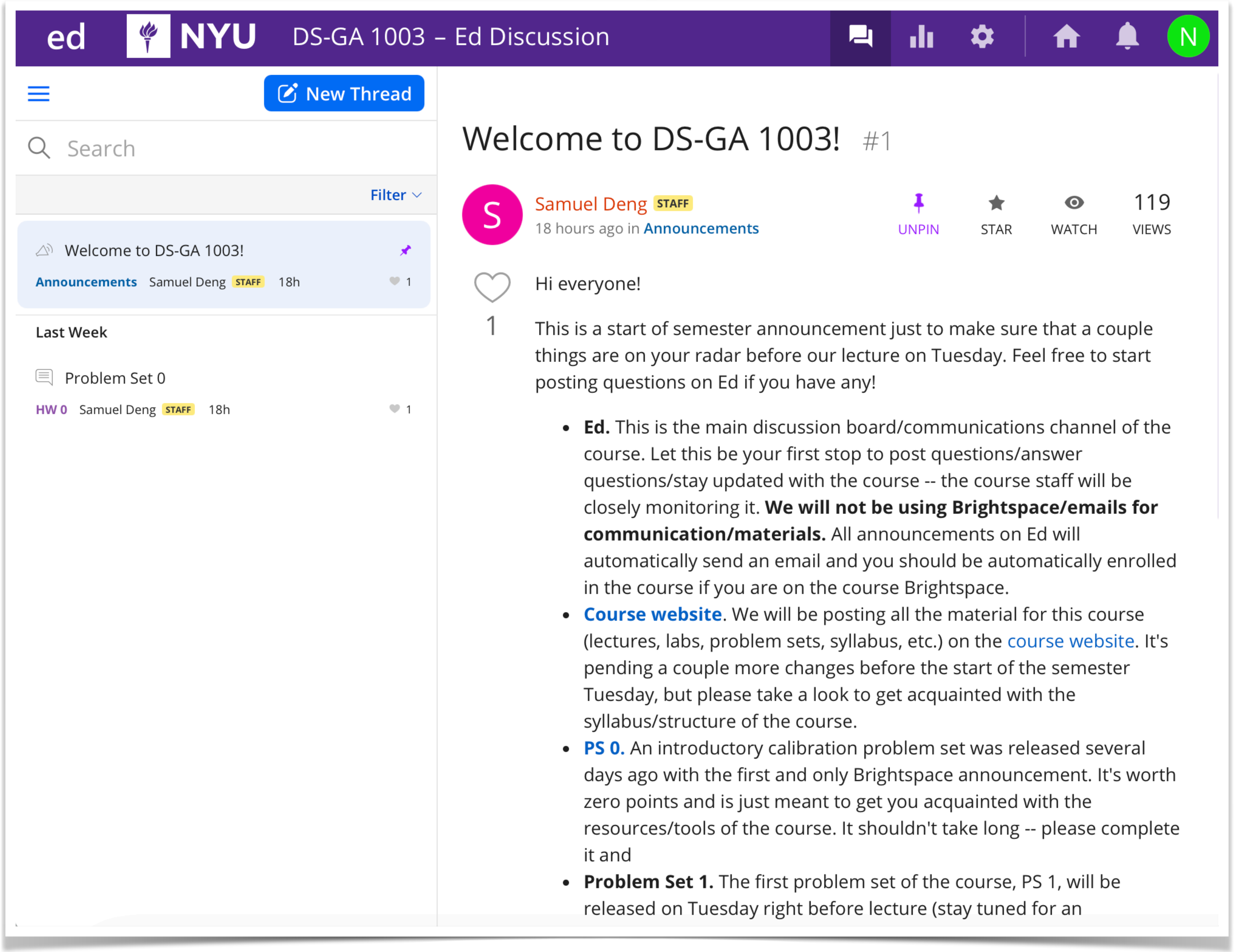

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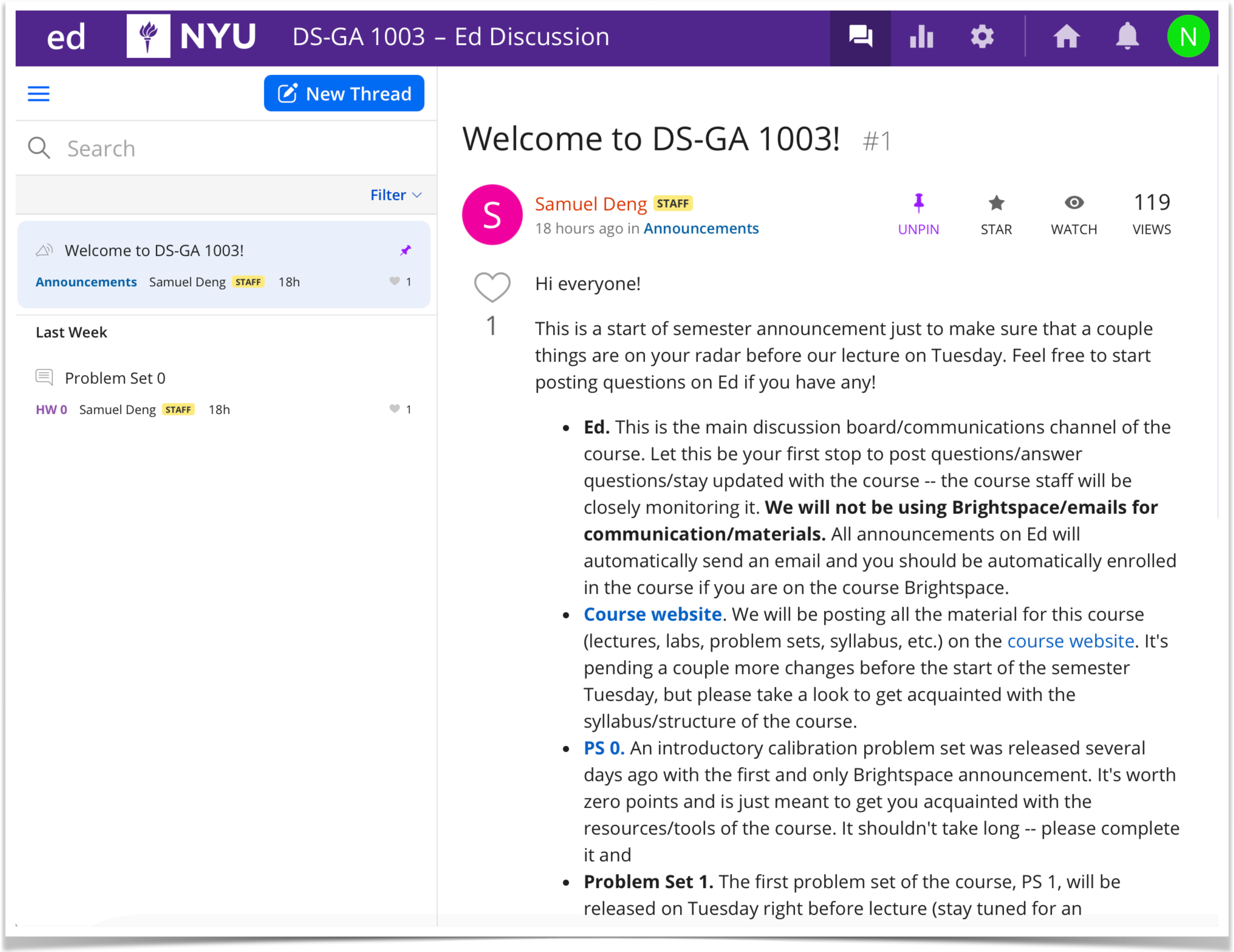

Grading Rubric

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Homeworks: 20%

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Midterm Exam: 35%

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Final Project: 35%

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Lab Attendance: 10%

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

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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

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

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- Groups formed for projects: Feb 28th

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- Final project submitted: May 8th

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

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- You can drop your lowest homework grade

Homeworks

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

Homeworks

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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	

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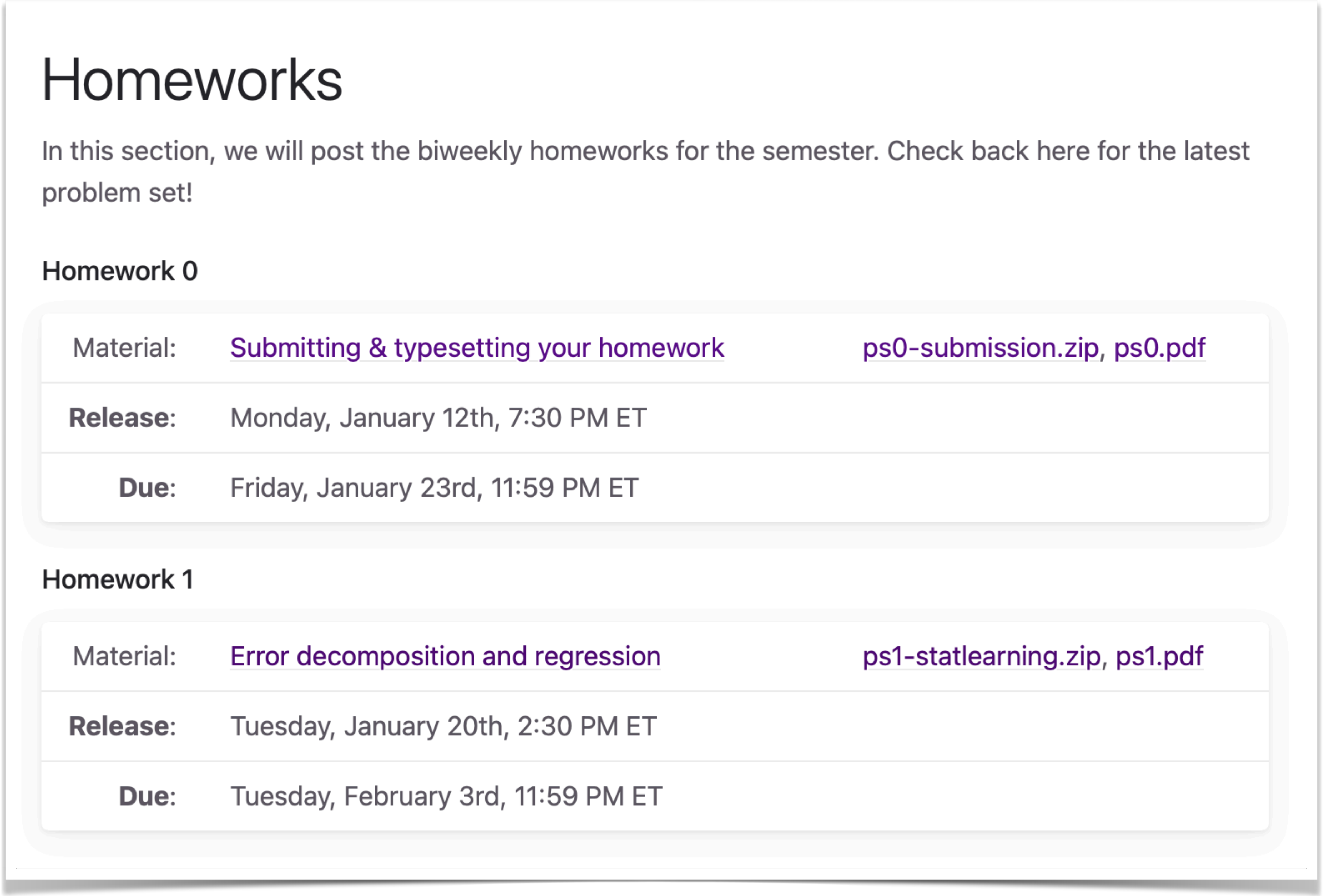

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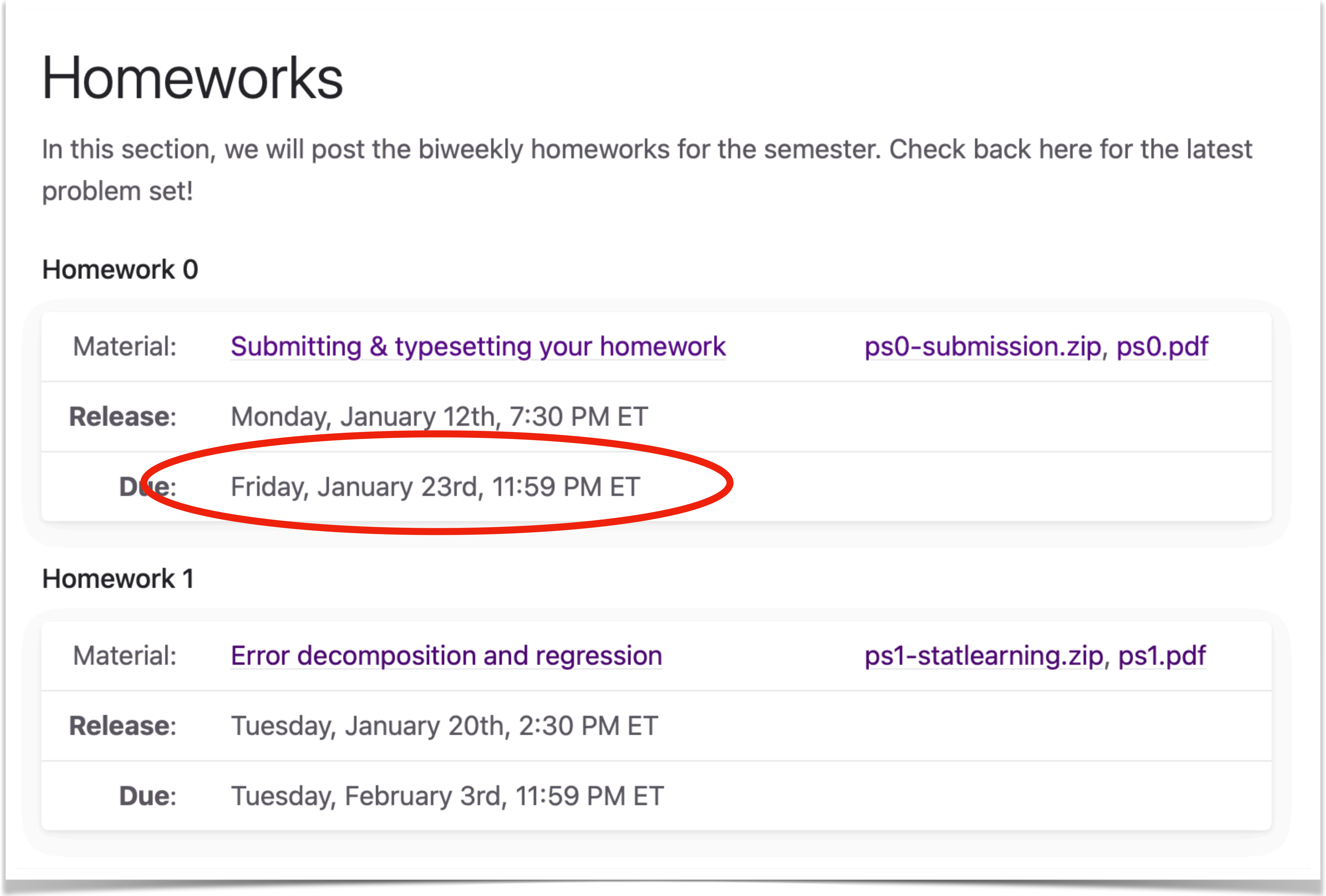

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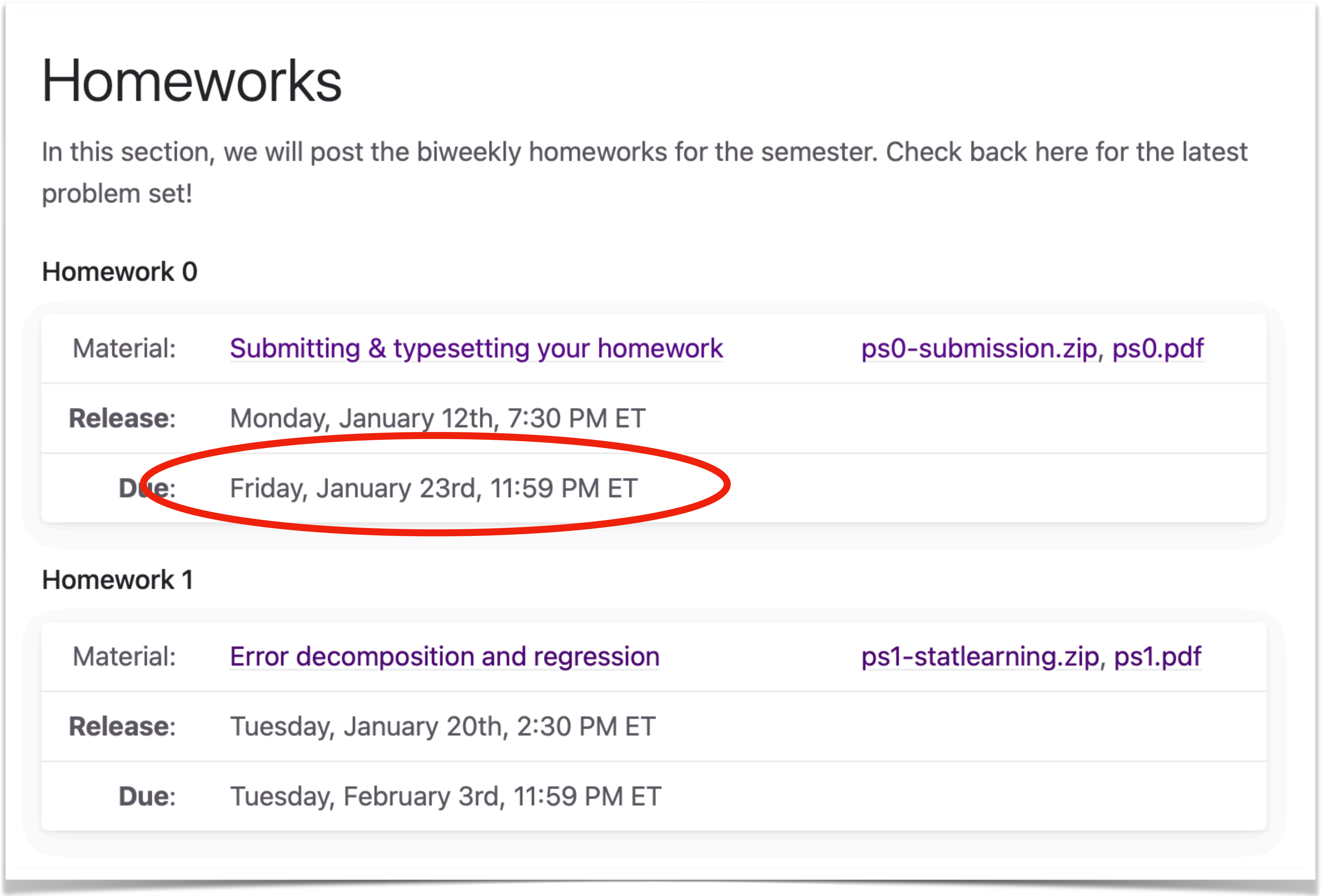

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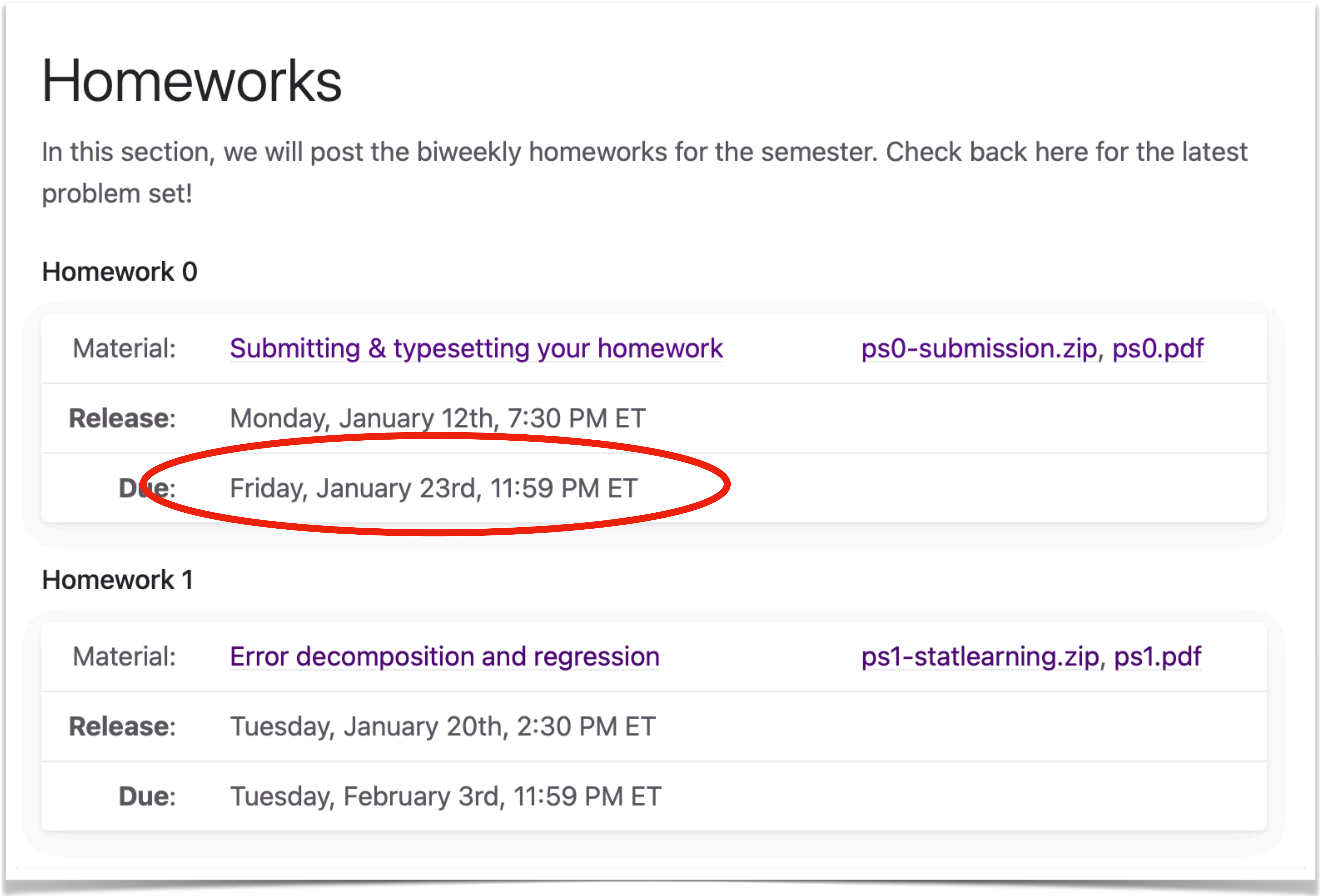

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Don’t use LLMs

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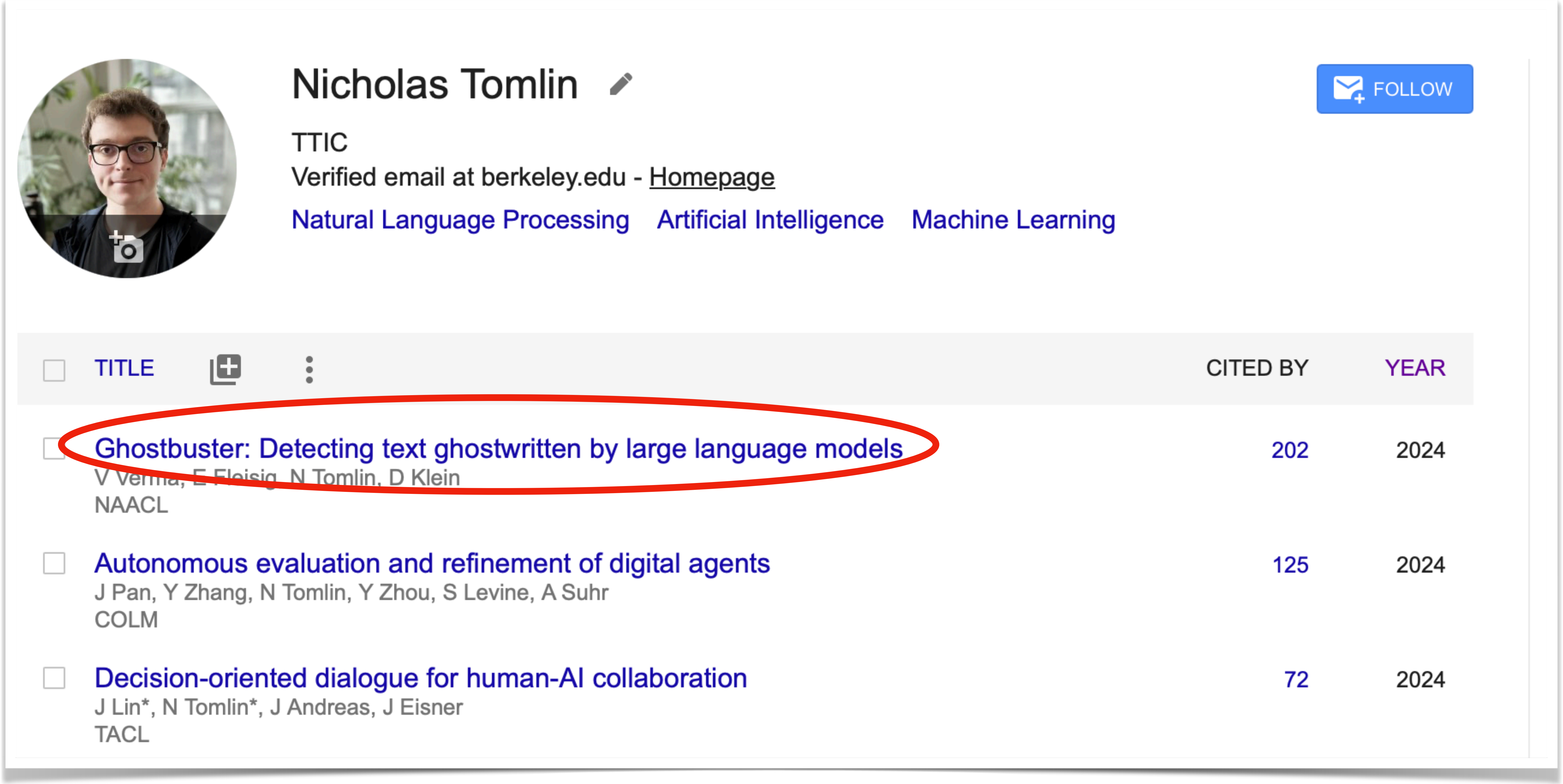
Nicholas Tomlin
FOLLOW
TTIC
Verified email at berkeley.edu - Homepage
Natural Language Processing
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Machine Learning
TITLE
CITED BY
YEAR
Ghostbuster: Detecting text ghostwritten by large language models
V Verma, E Fleisig, N Tomlin, D Klein
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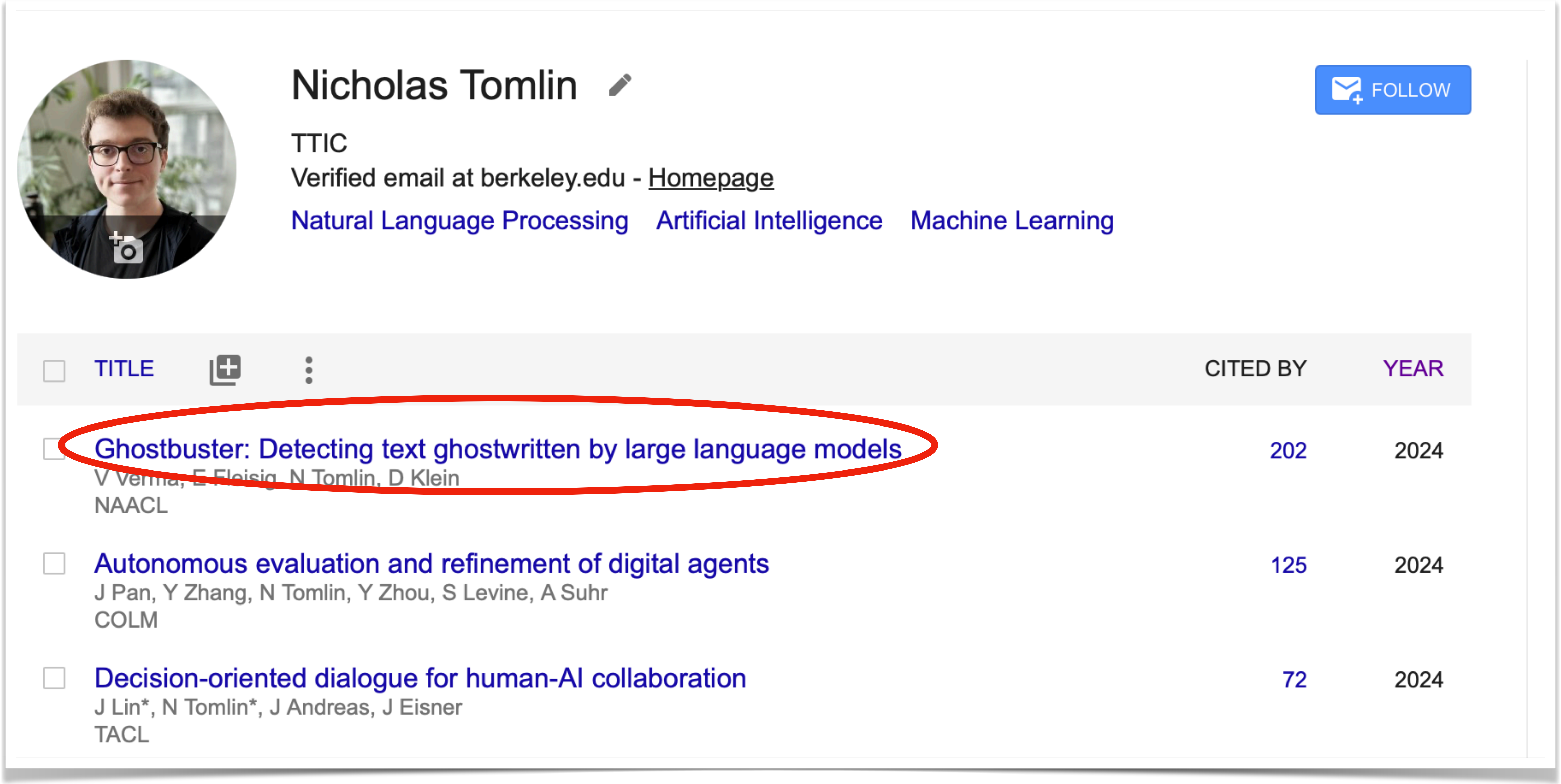

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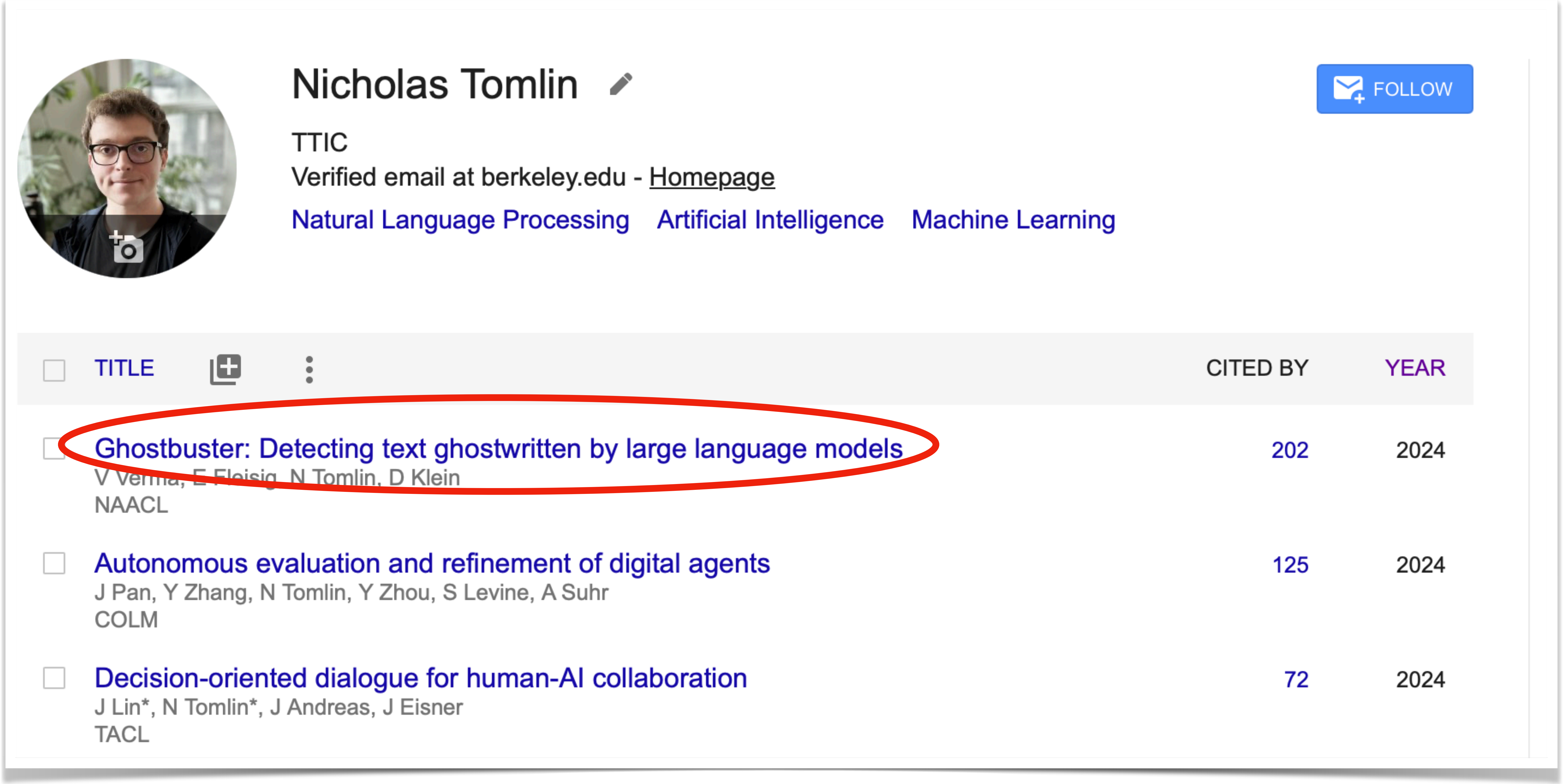

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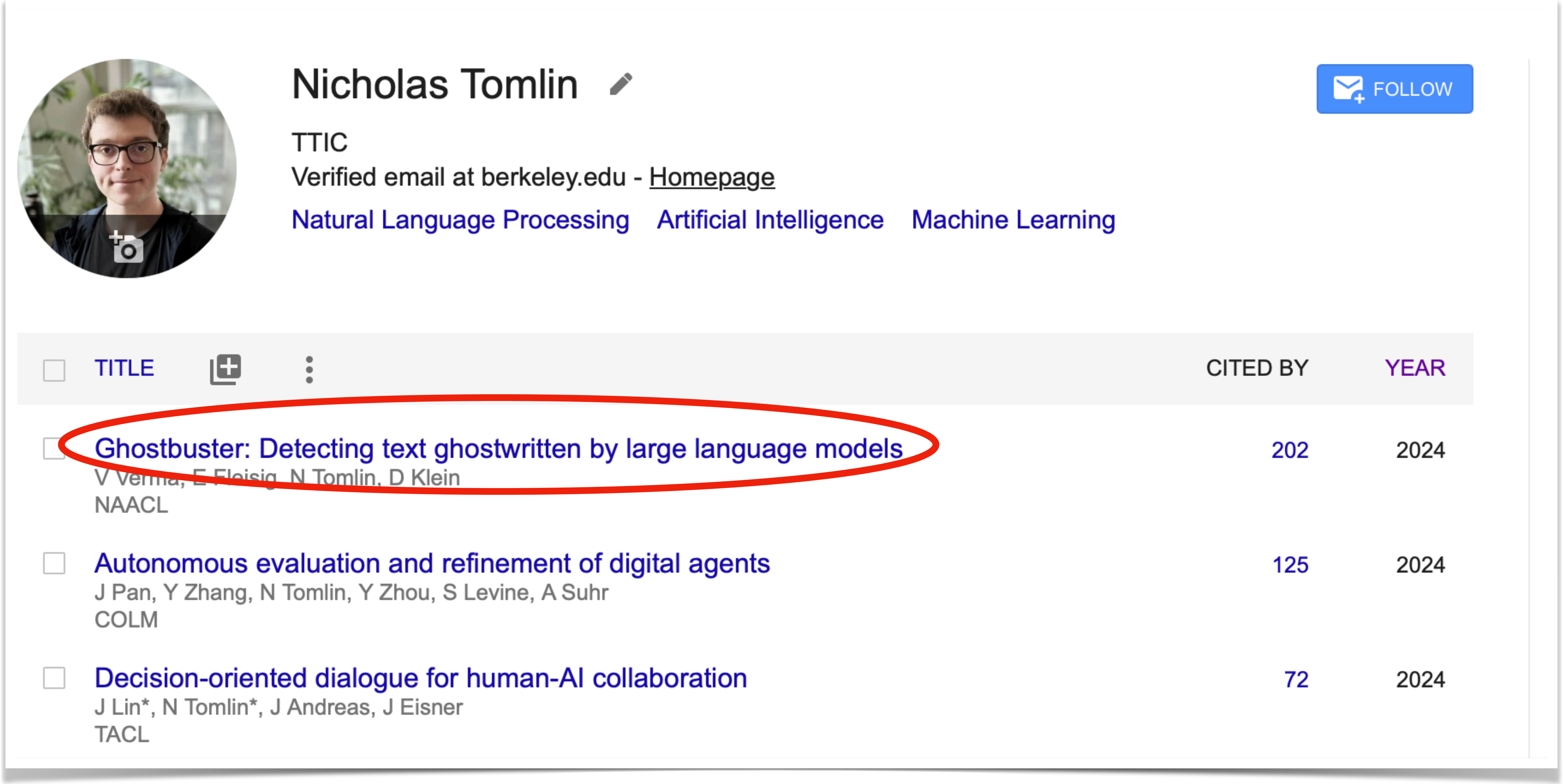

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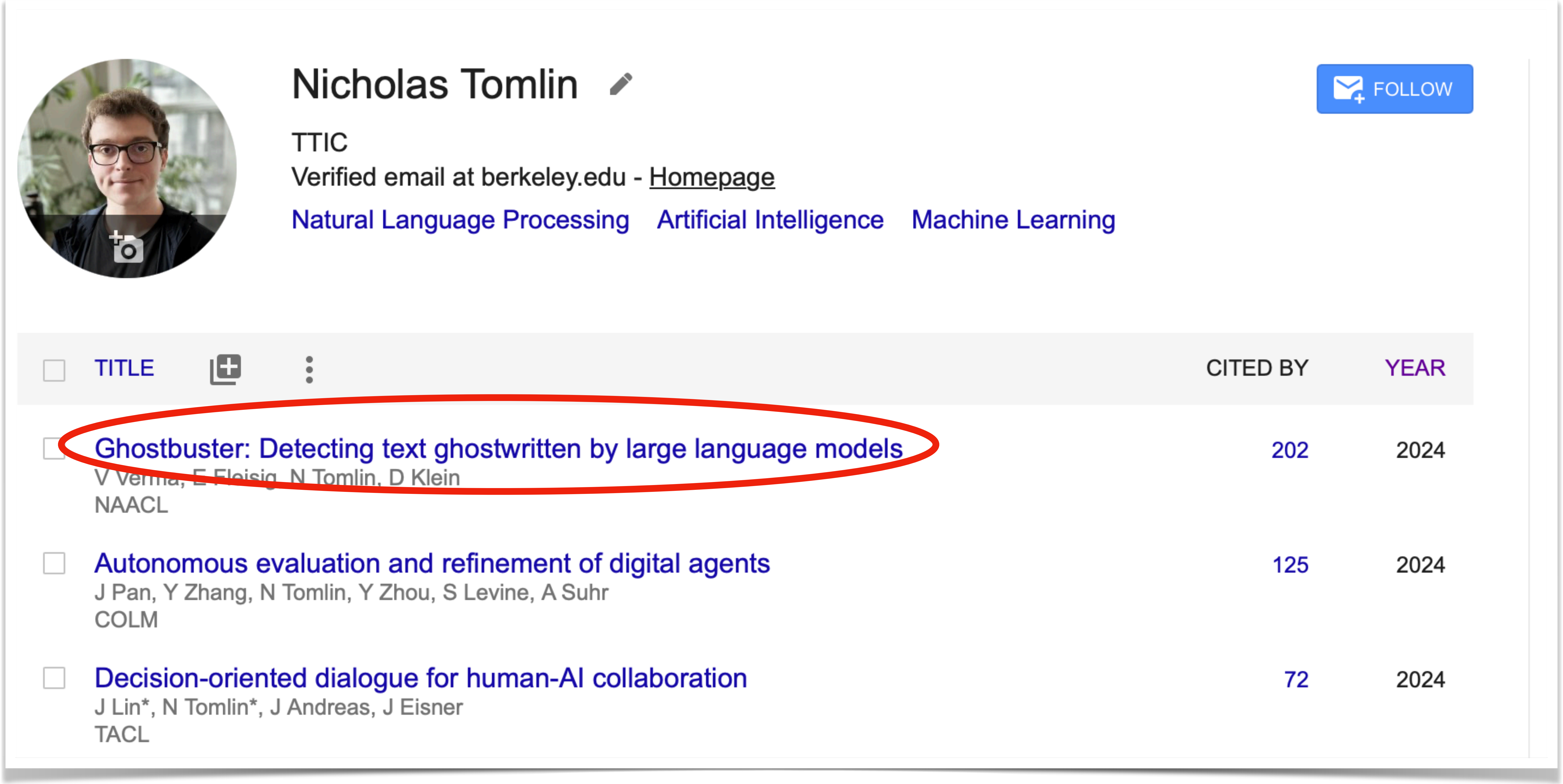
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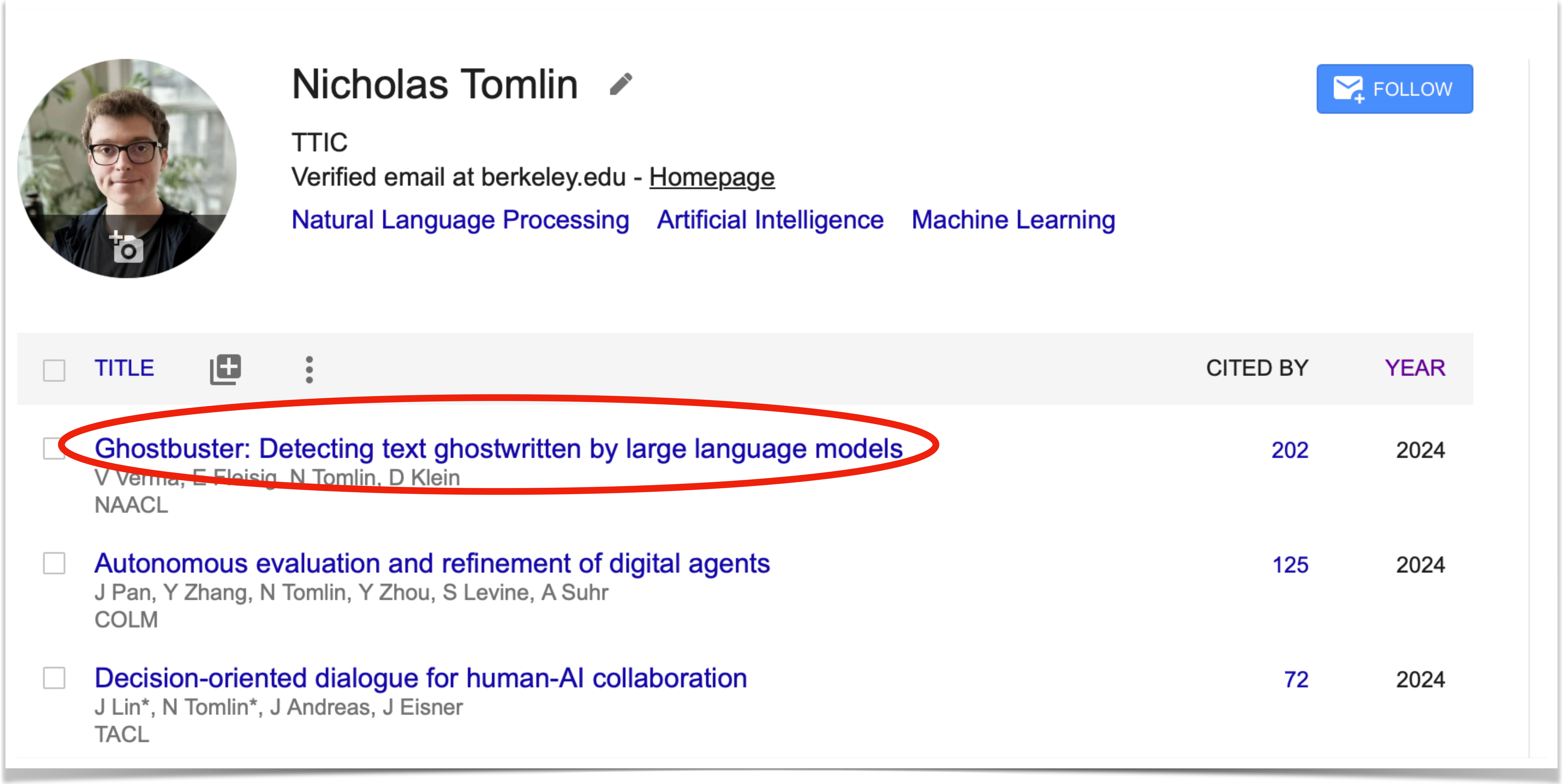

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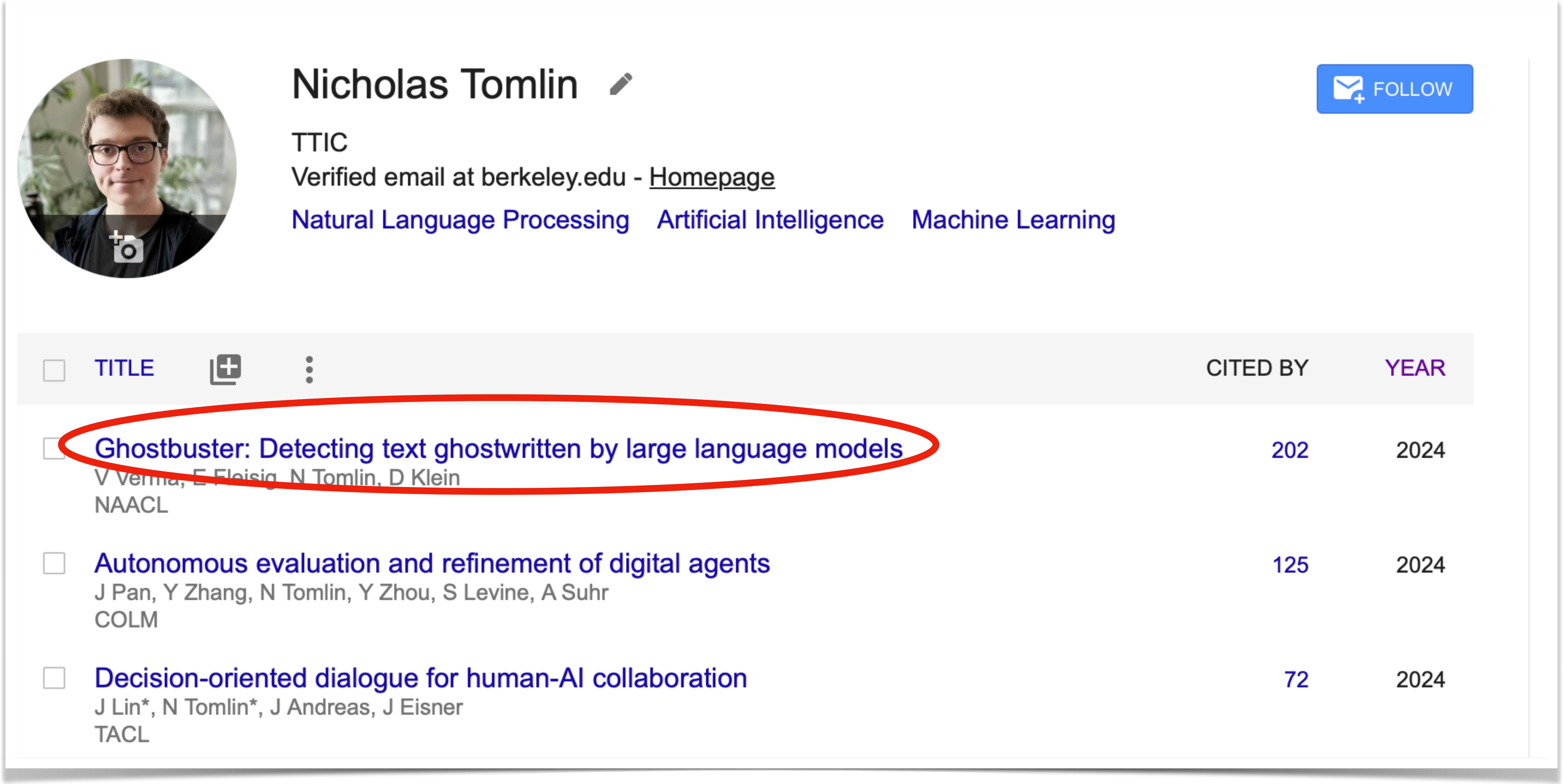

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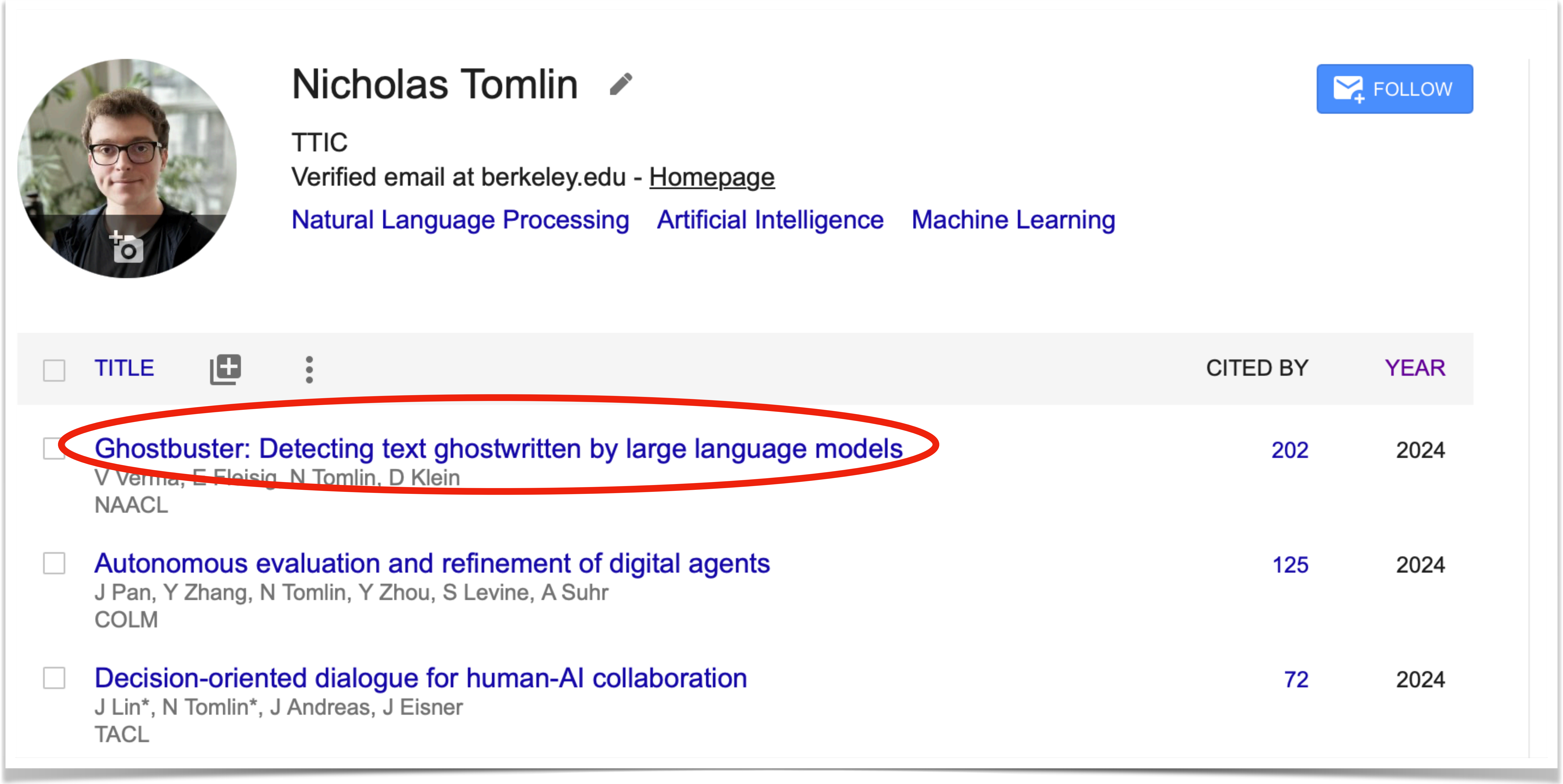

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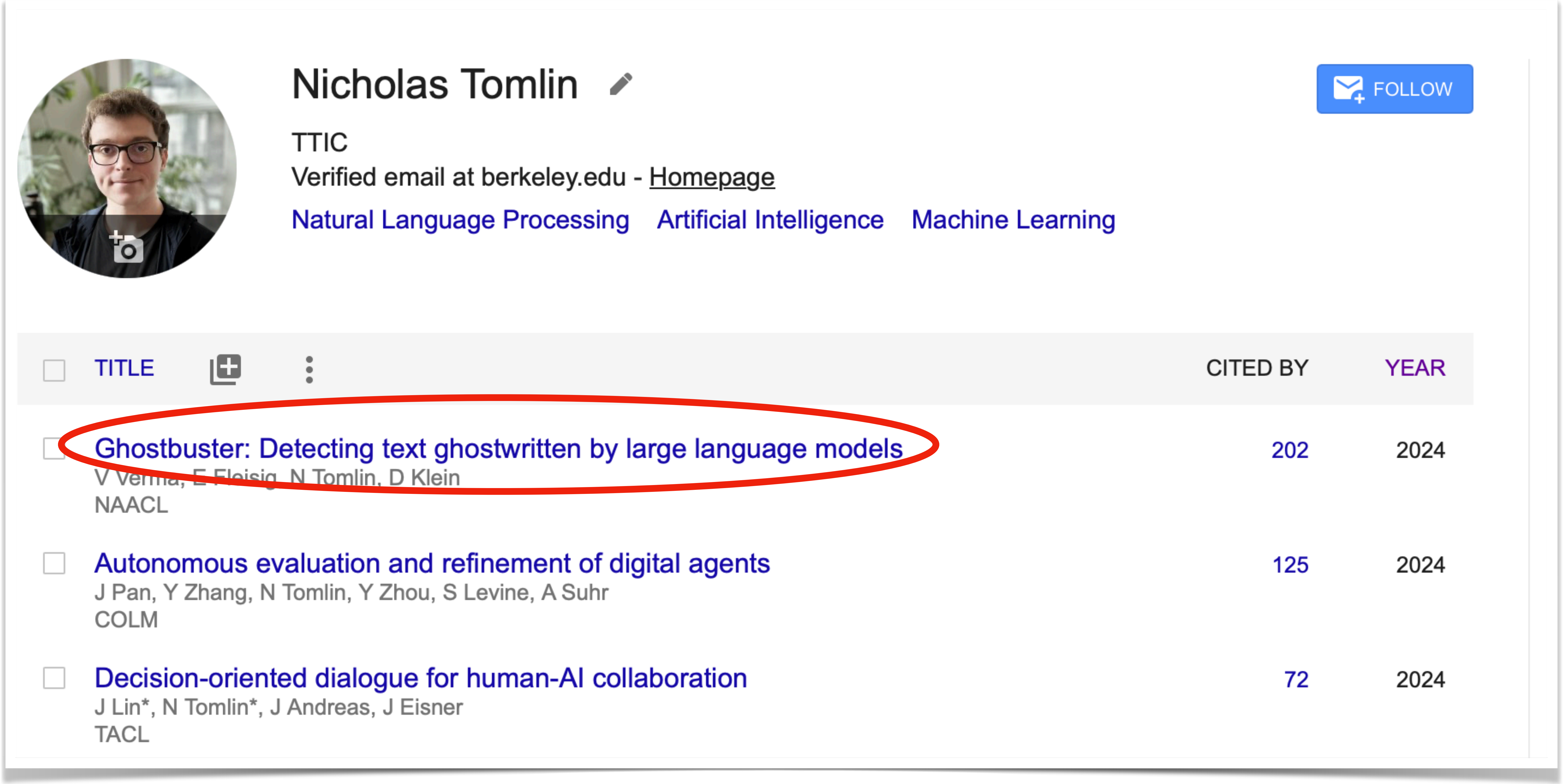

One exception: coding tools like Cursor and Claude Code are allowed if you are doing the "research track" for the final project. However, using LLMs for writing your final report is not allowed under either track.

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

Key dates and deadlines

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Jan 23rd: Homework 0 due

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

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Feb 28th: project groups formed

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Mar 10th: midterm, in-class

Should I take this class?

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Yes, if:

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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

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Currently: 154 students (max of 200)

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Priority order for registration:

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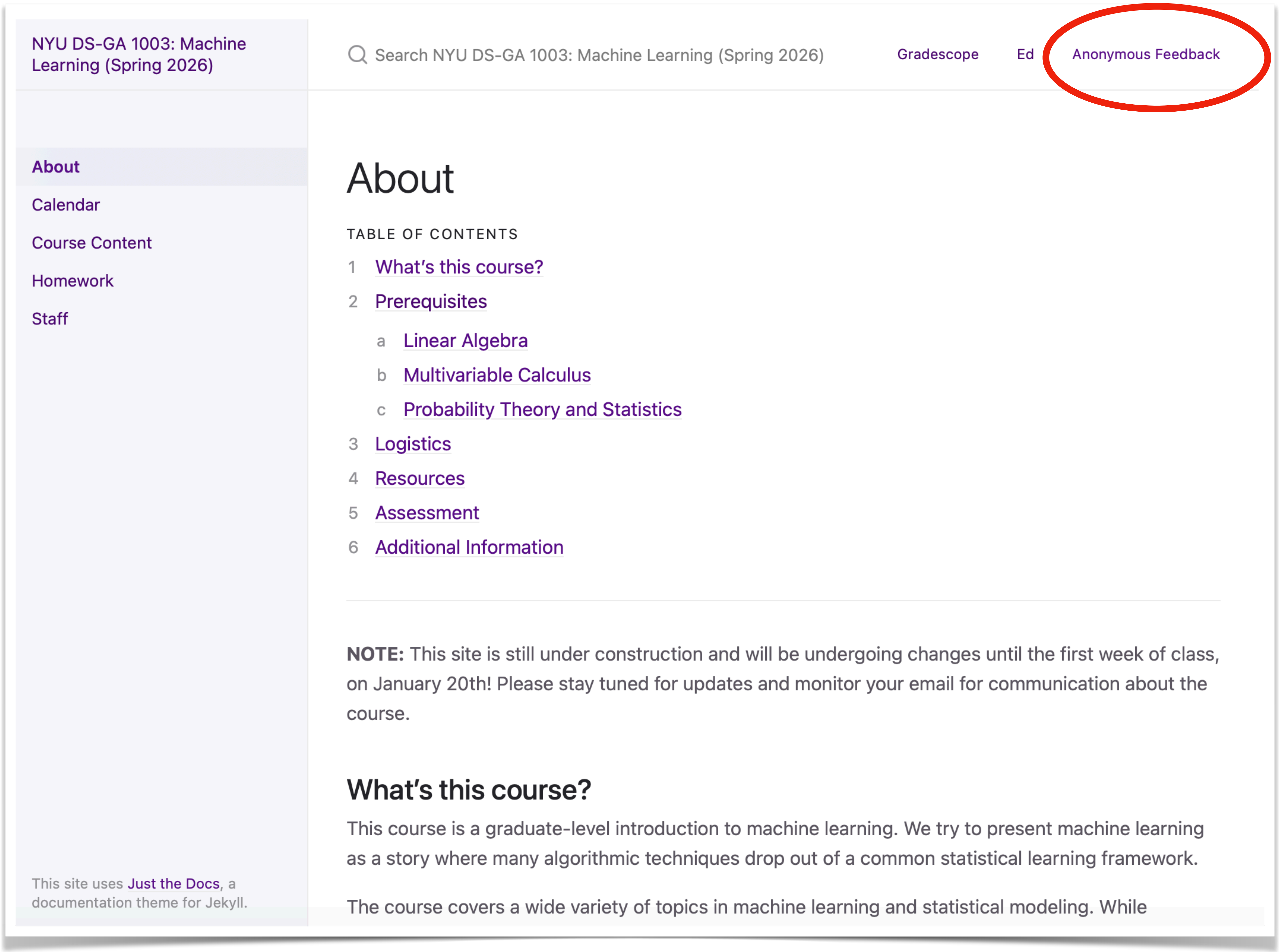
- MS students from other departments with appropriate prerequisites: registration should now be open. If you have issues, please contact cds-masters@nyu.edu

Anonymous Feedback



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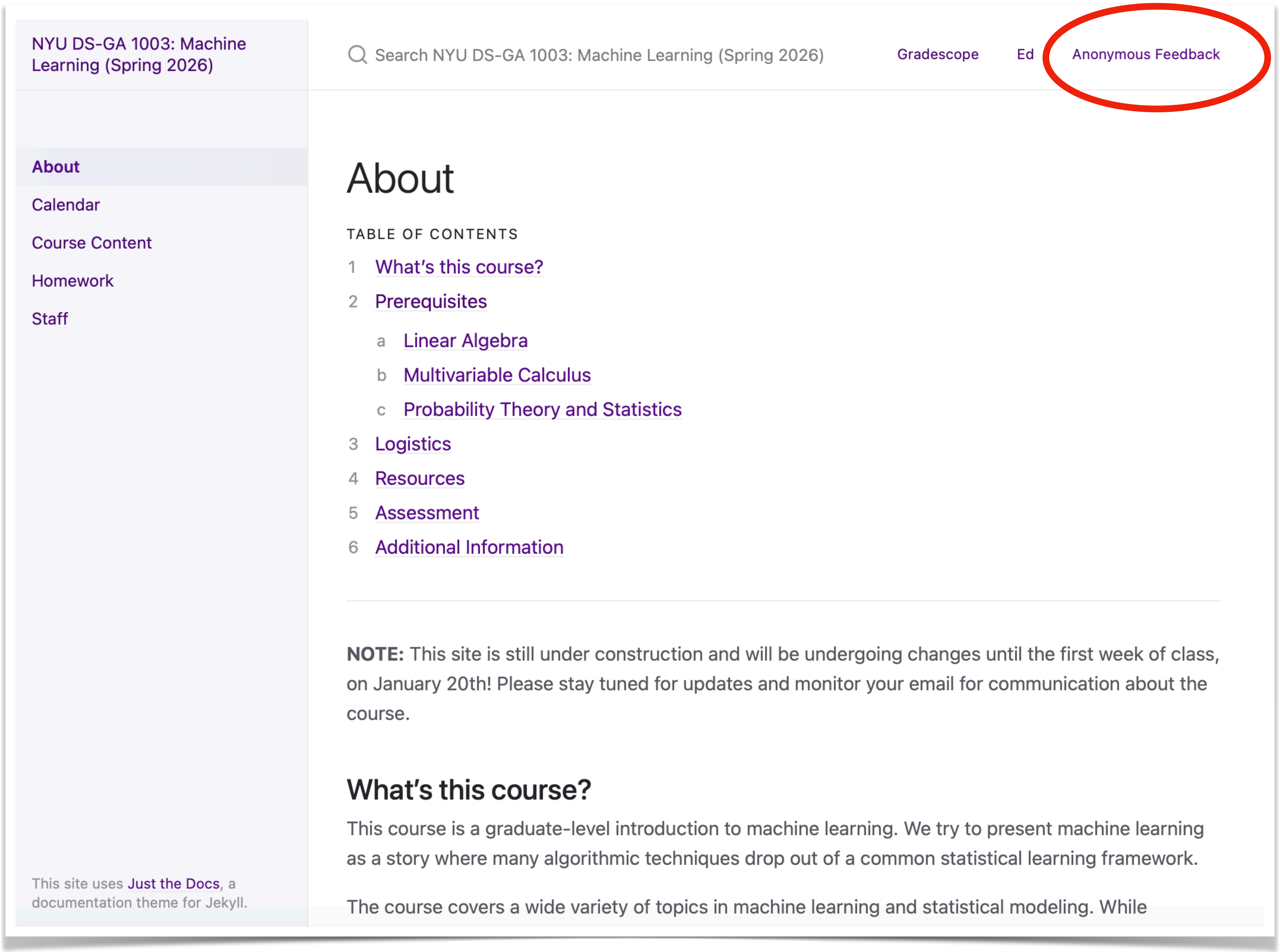

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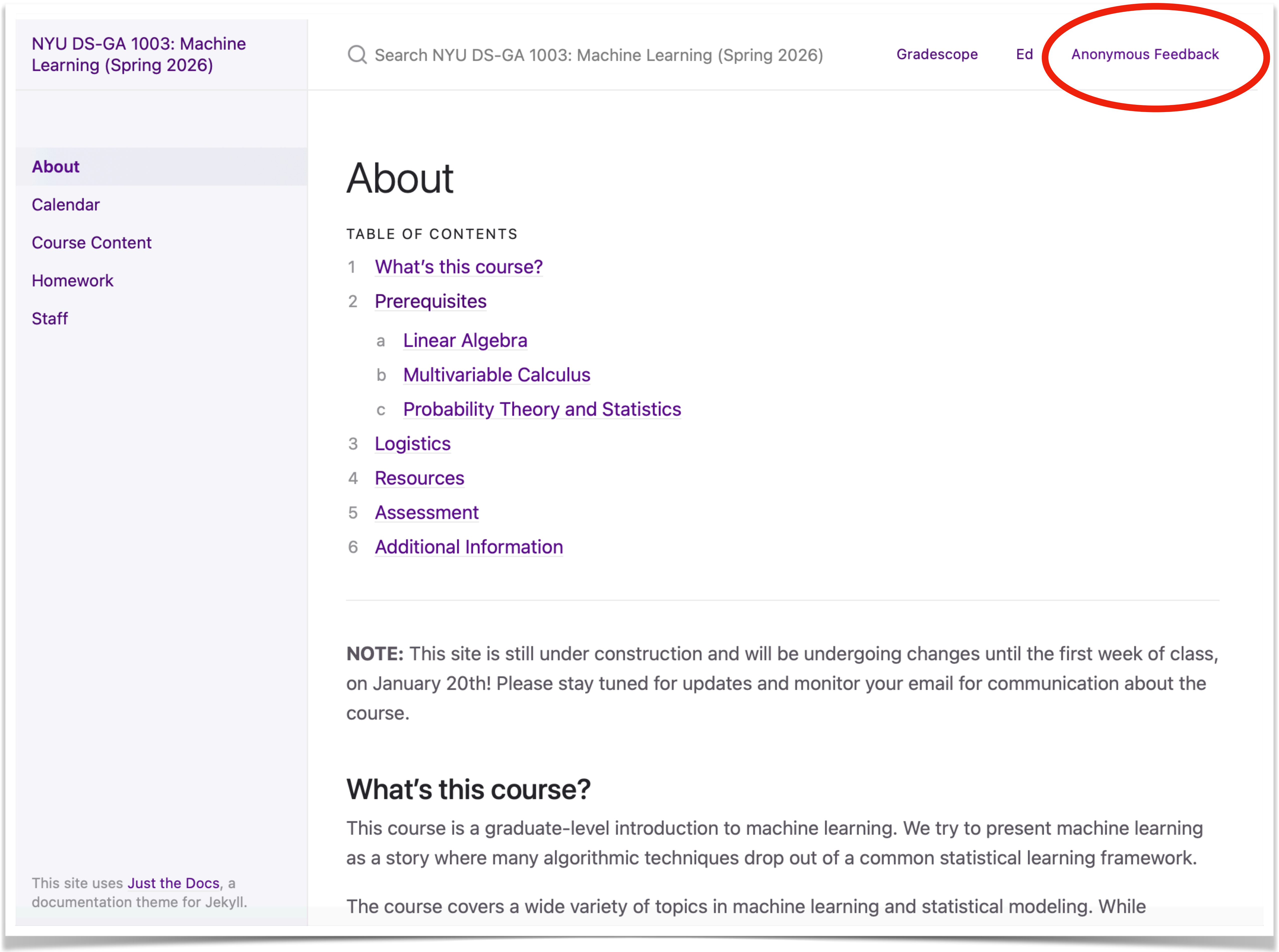
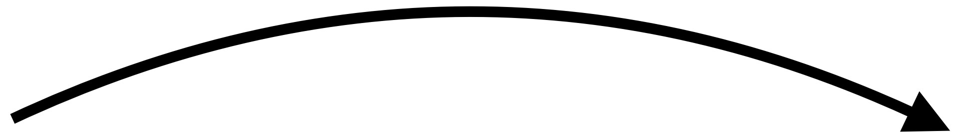


Outline

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

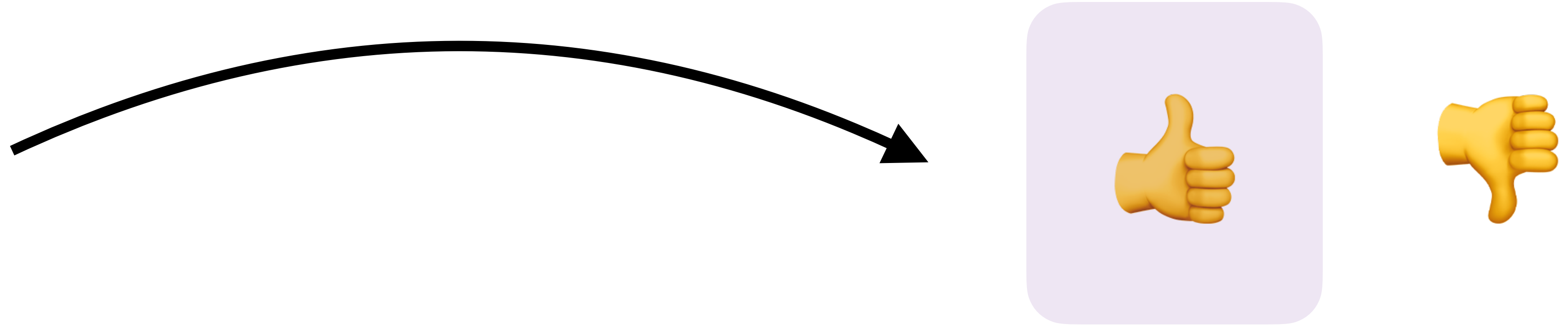
By Karin Langner-Bahmann, upload von Martin Bahmann - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=3020045



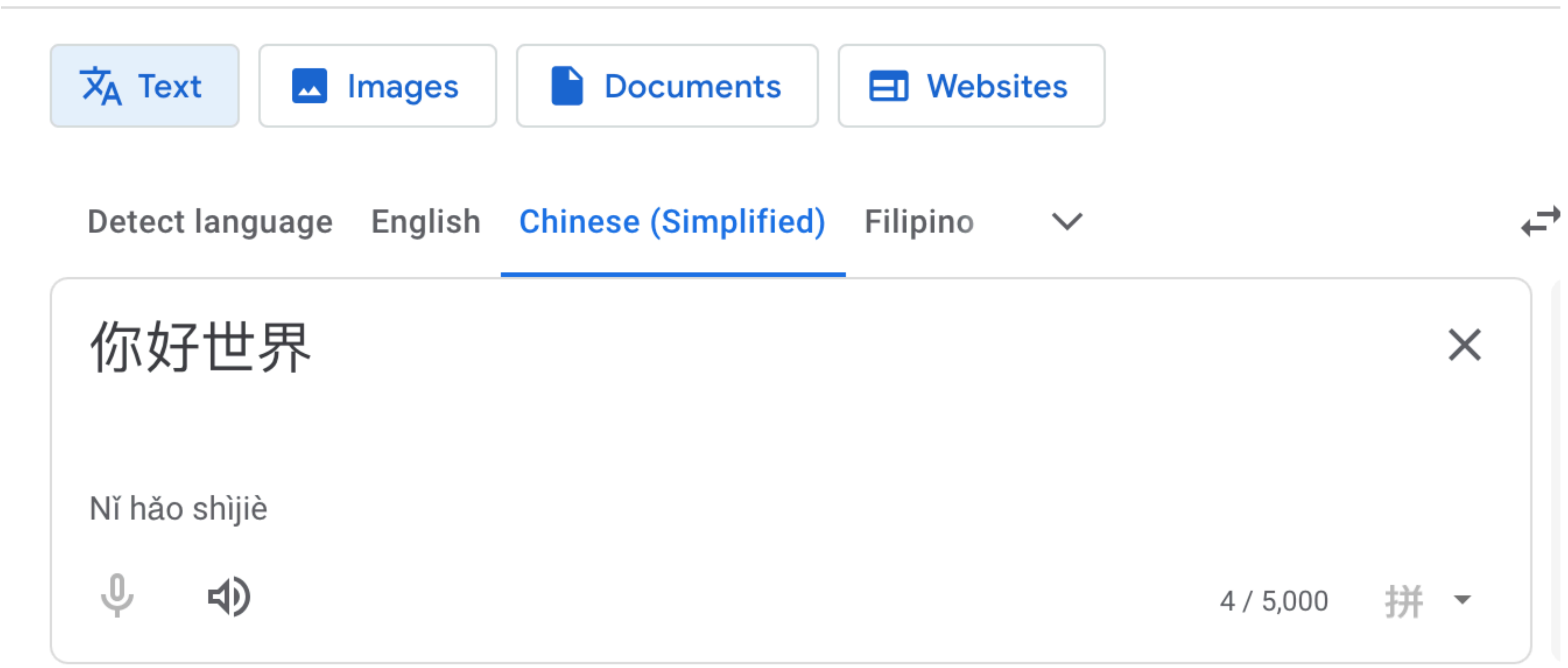
“Siamese”

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

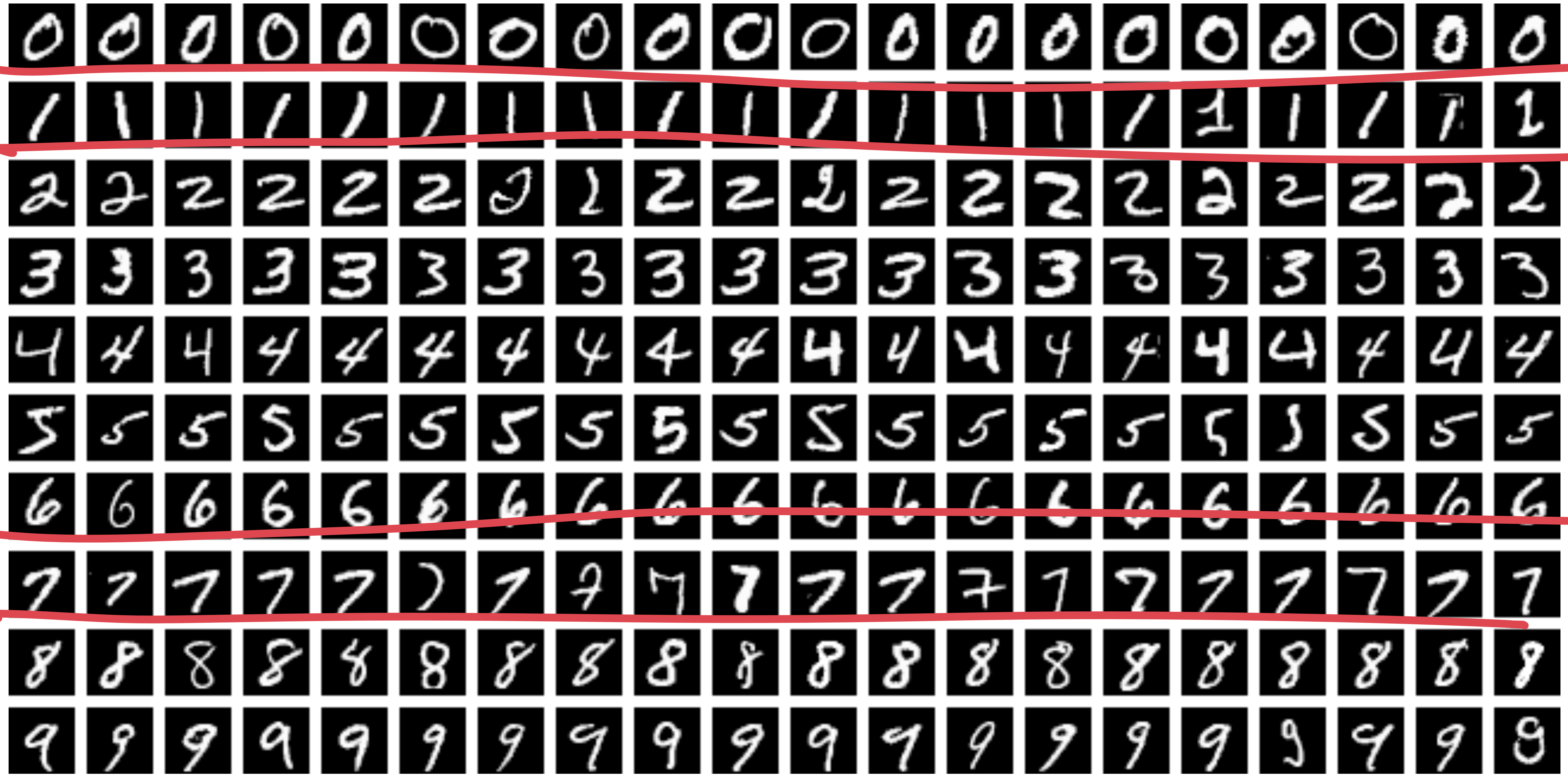
Many problems are difficult to "program by hand."

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”



Algorithm
1 if less white pixels
7 otherwise

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 multiclass classification problem, 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

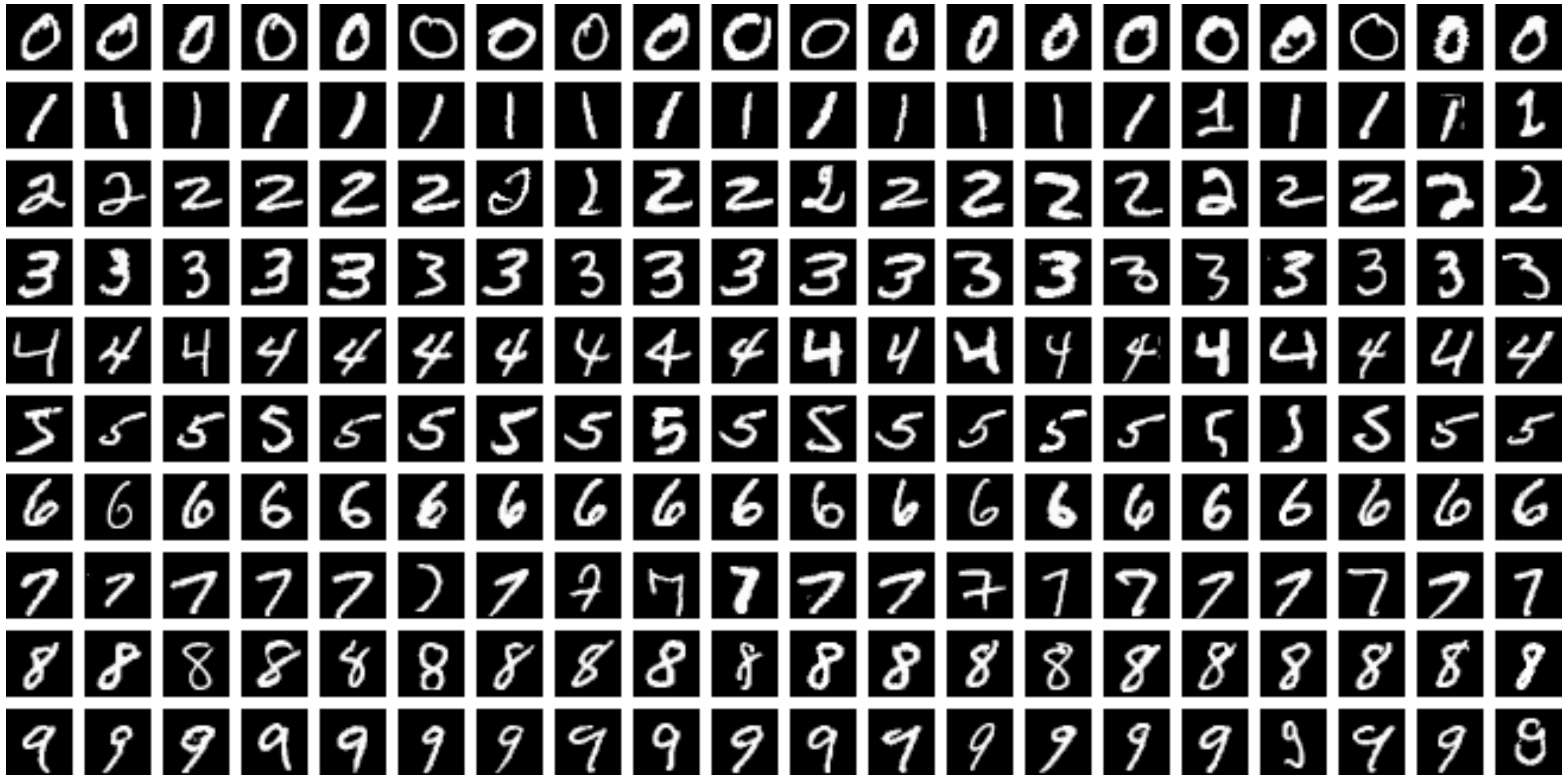
Given an input x, predict the output y.

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*.

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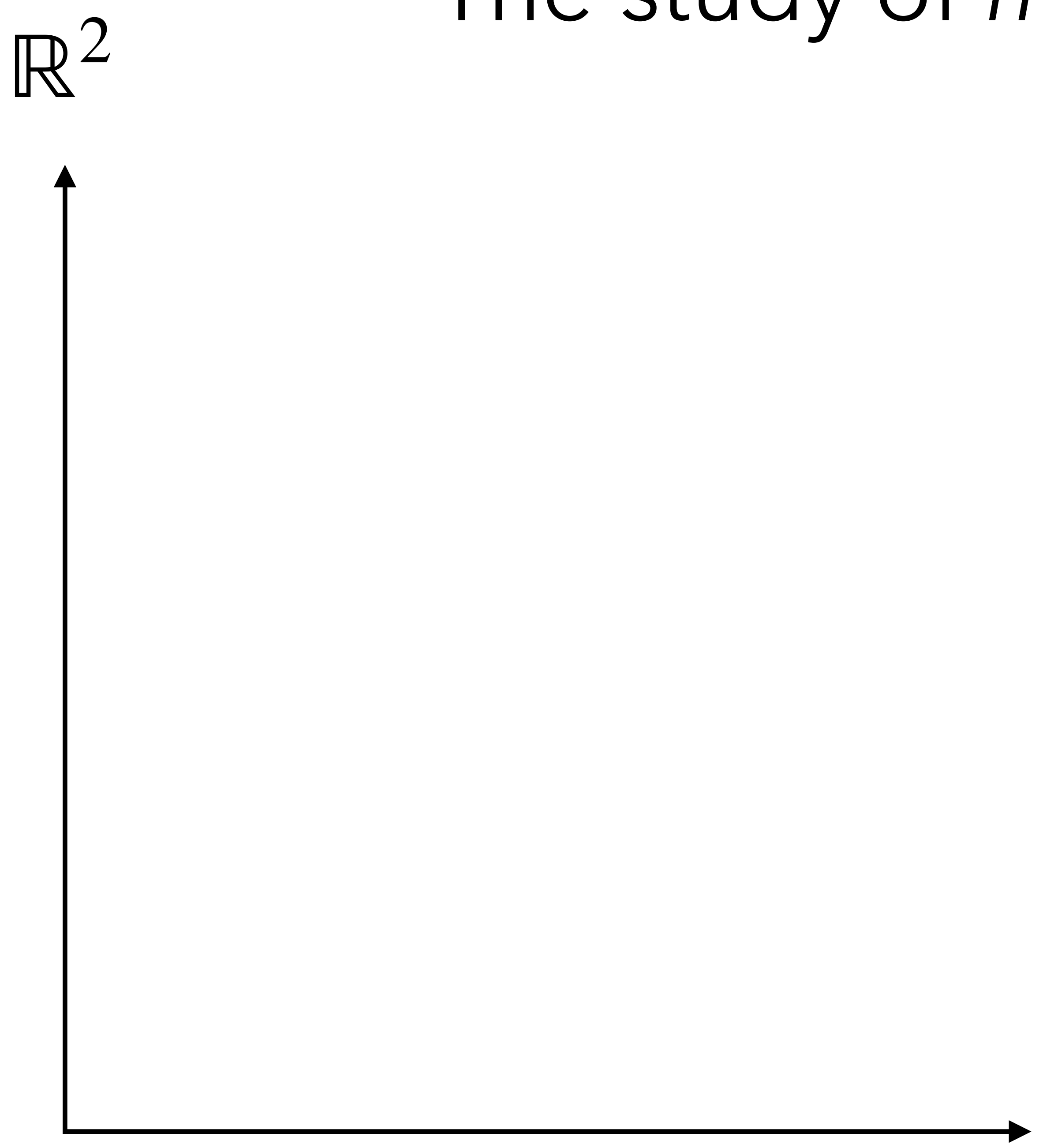

$\mathcal{X}$

$\mathcal{Y}$

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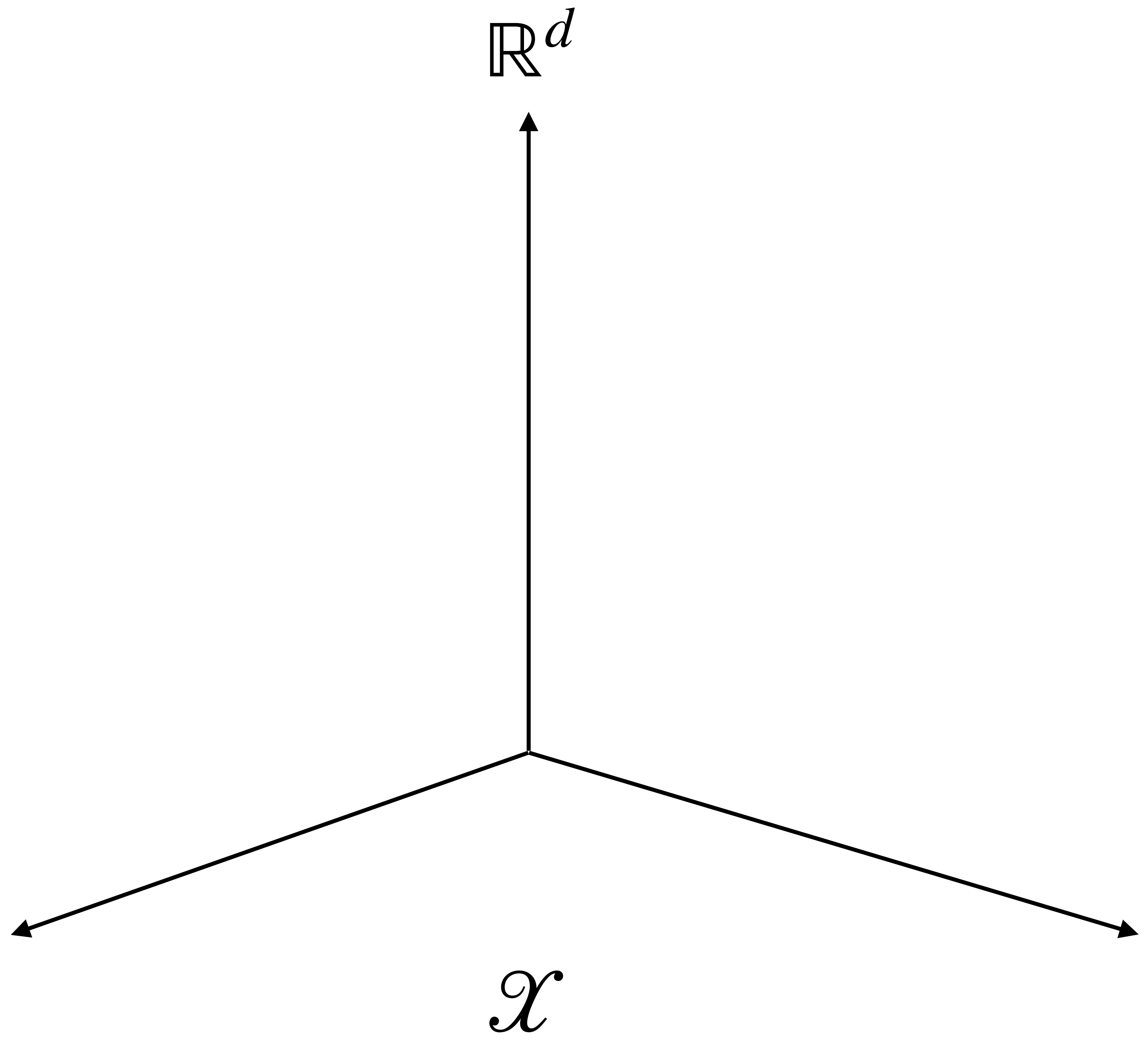

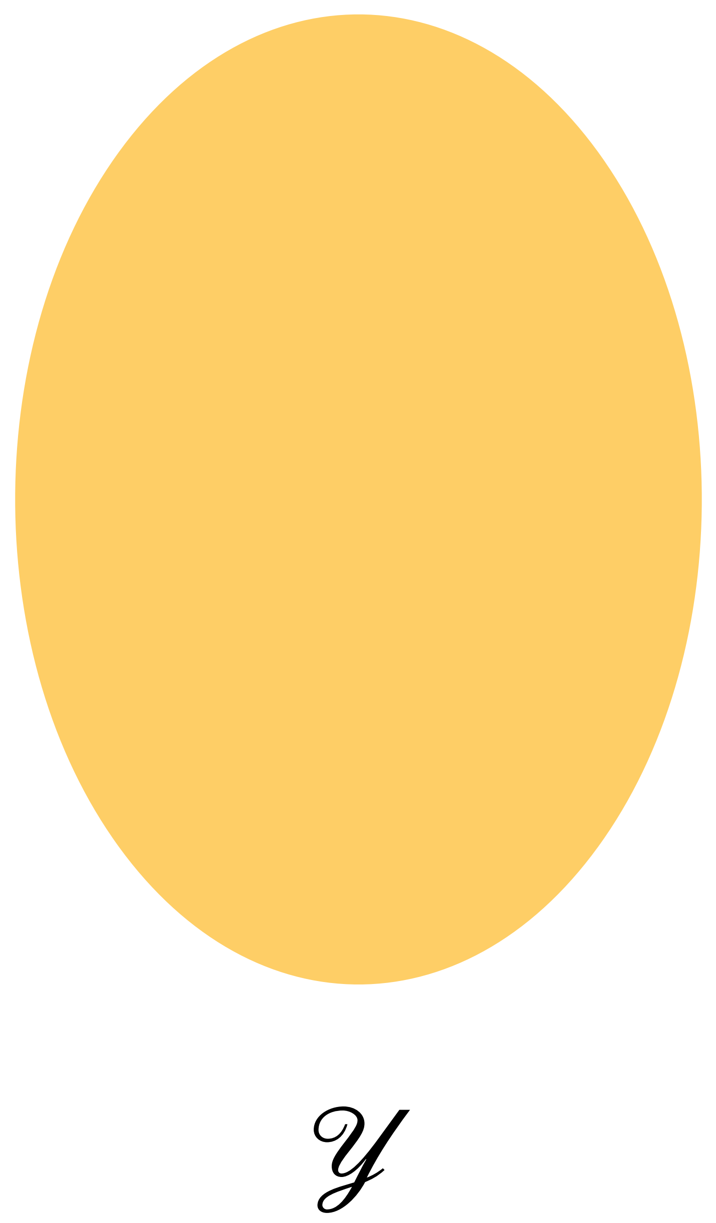

Supervised Machine Learning

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

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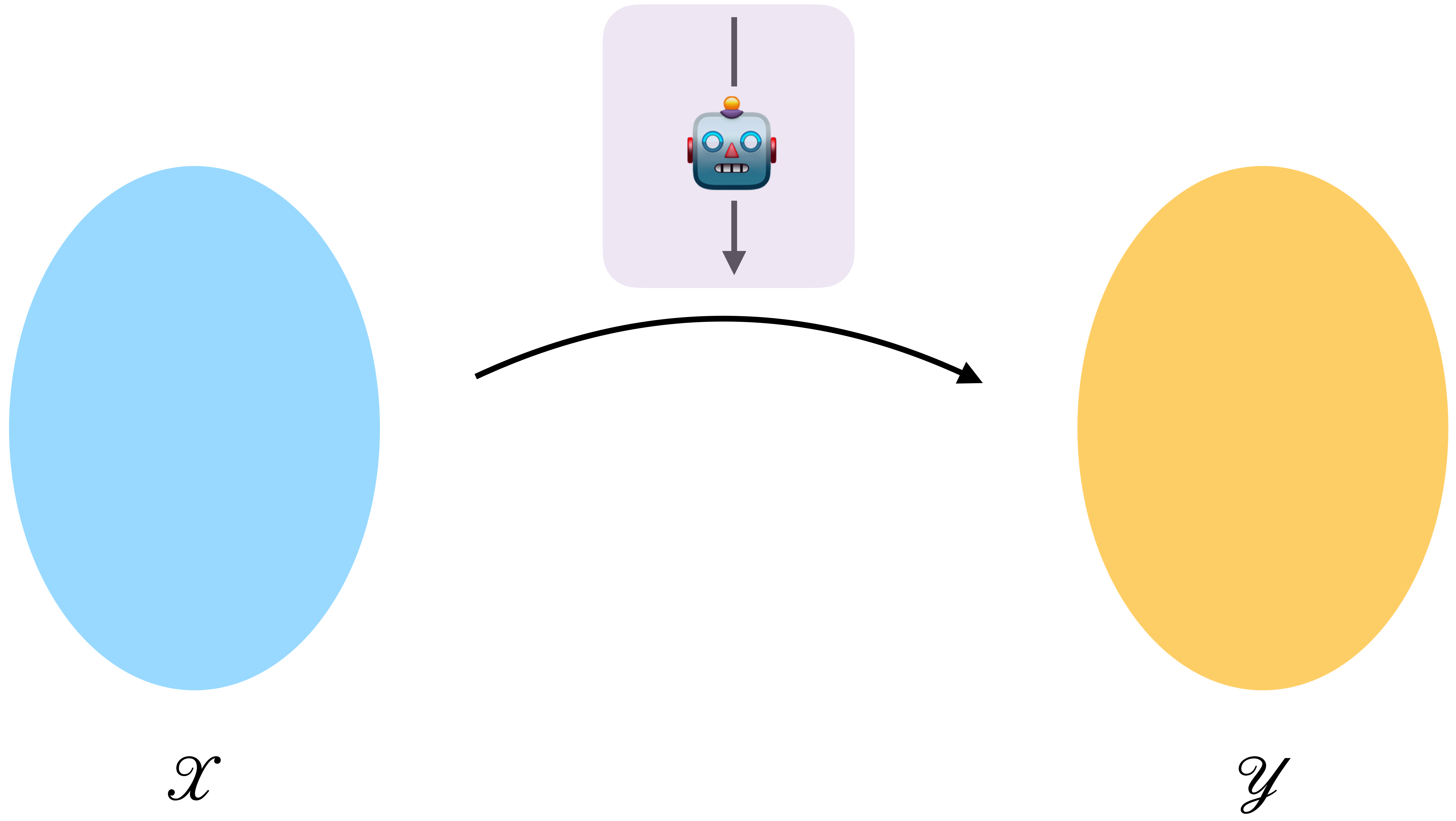

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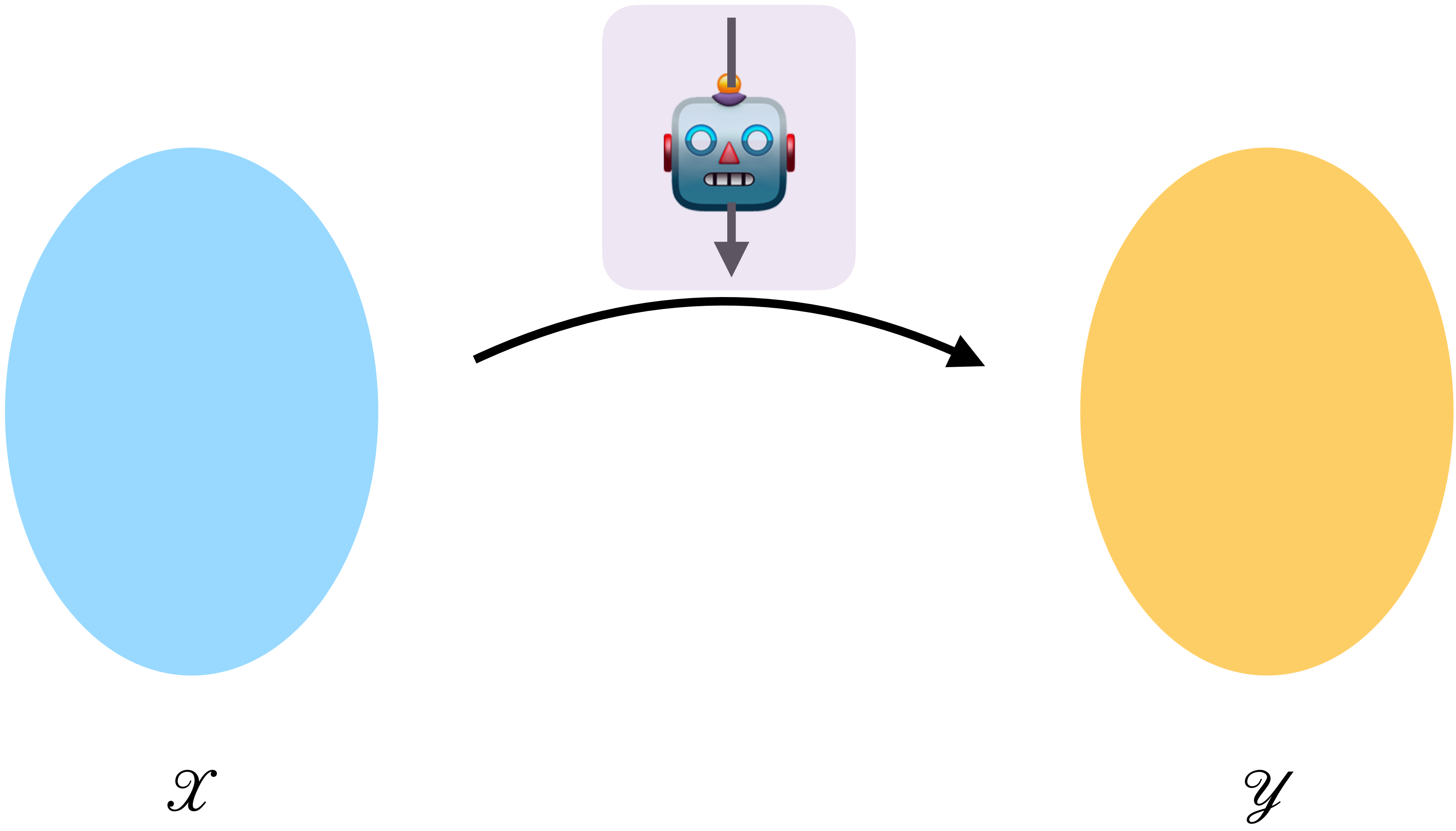

Supervised Learning

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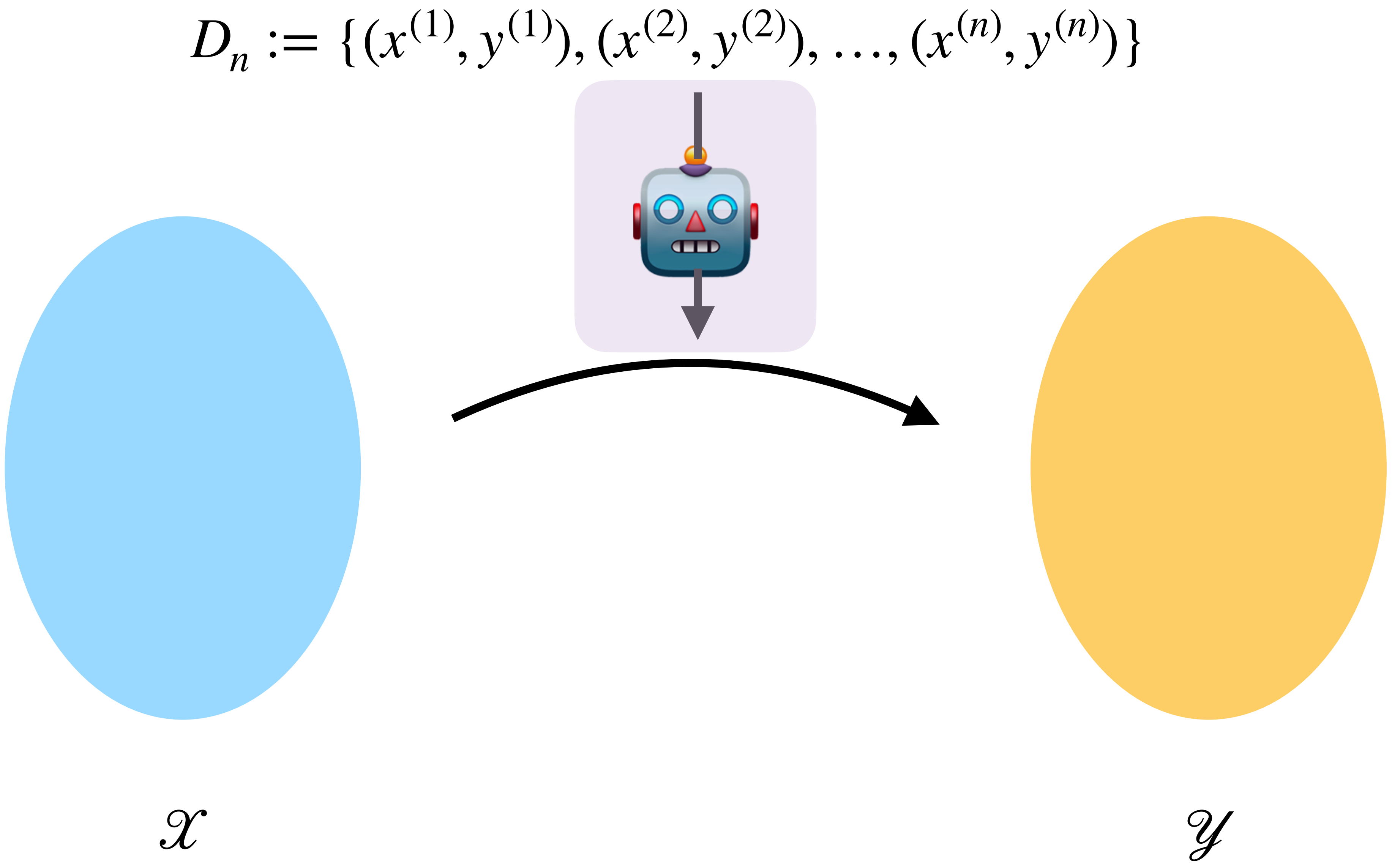

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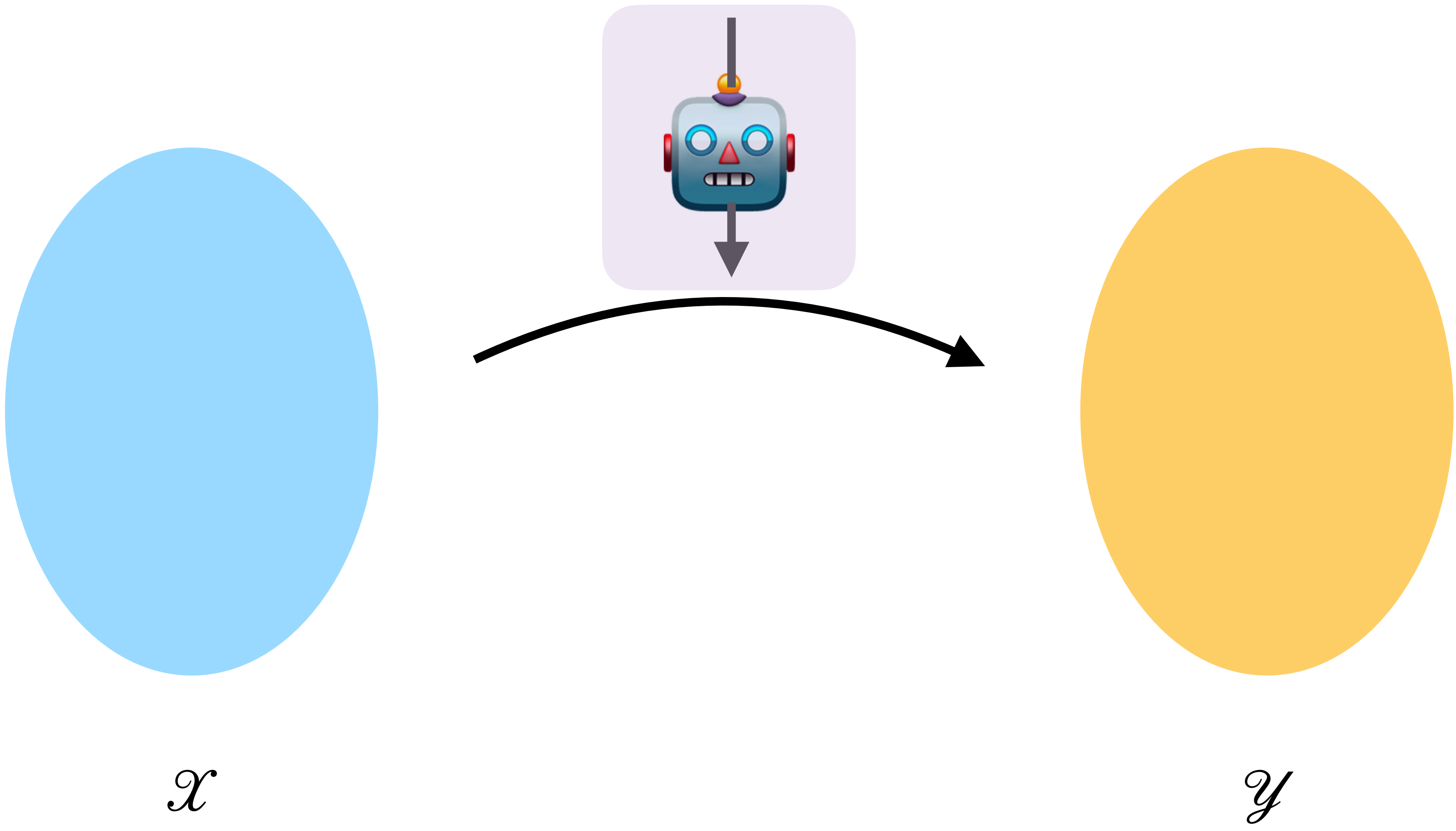

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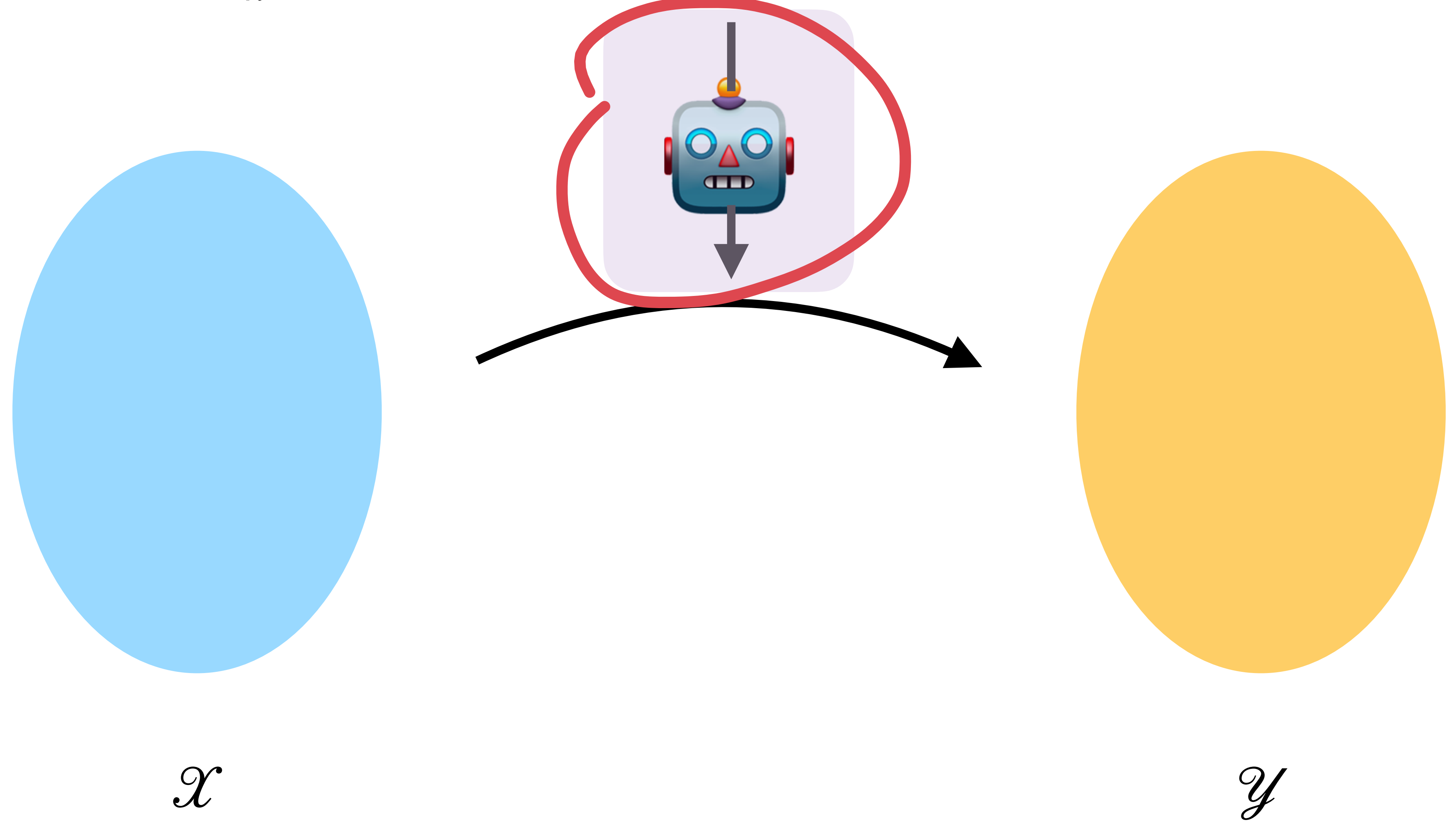

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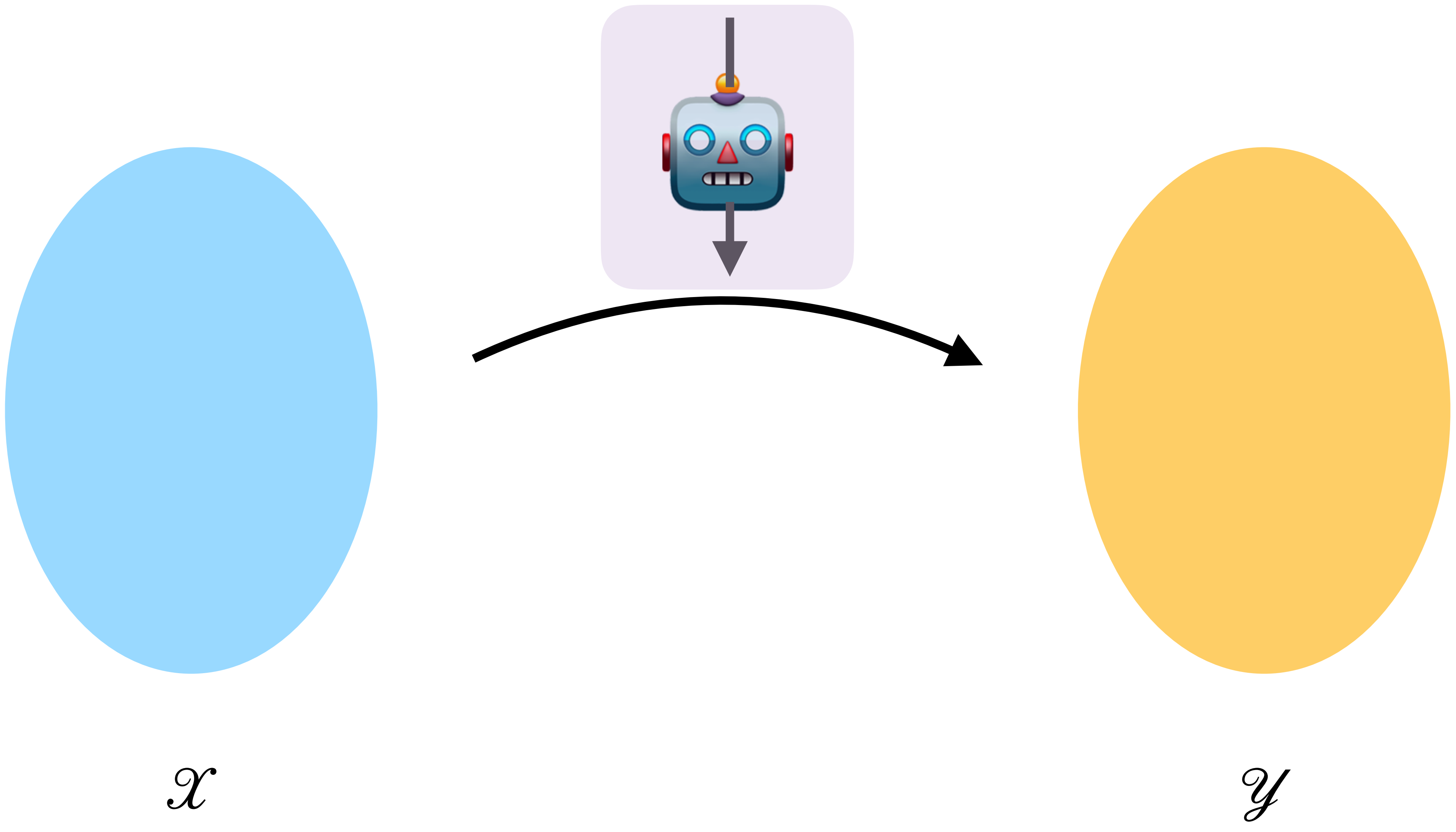

Supervised Learning

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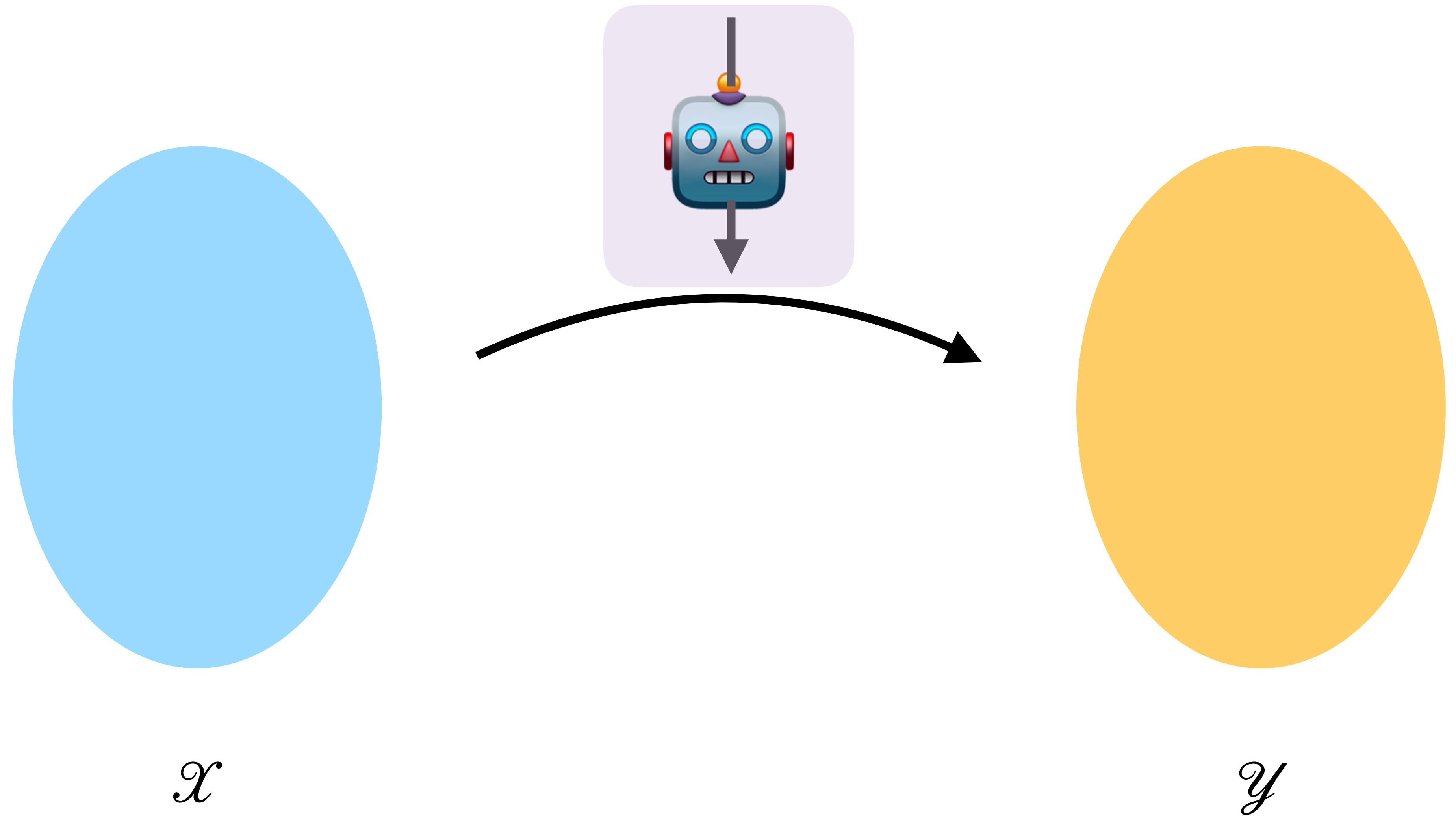

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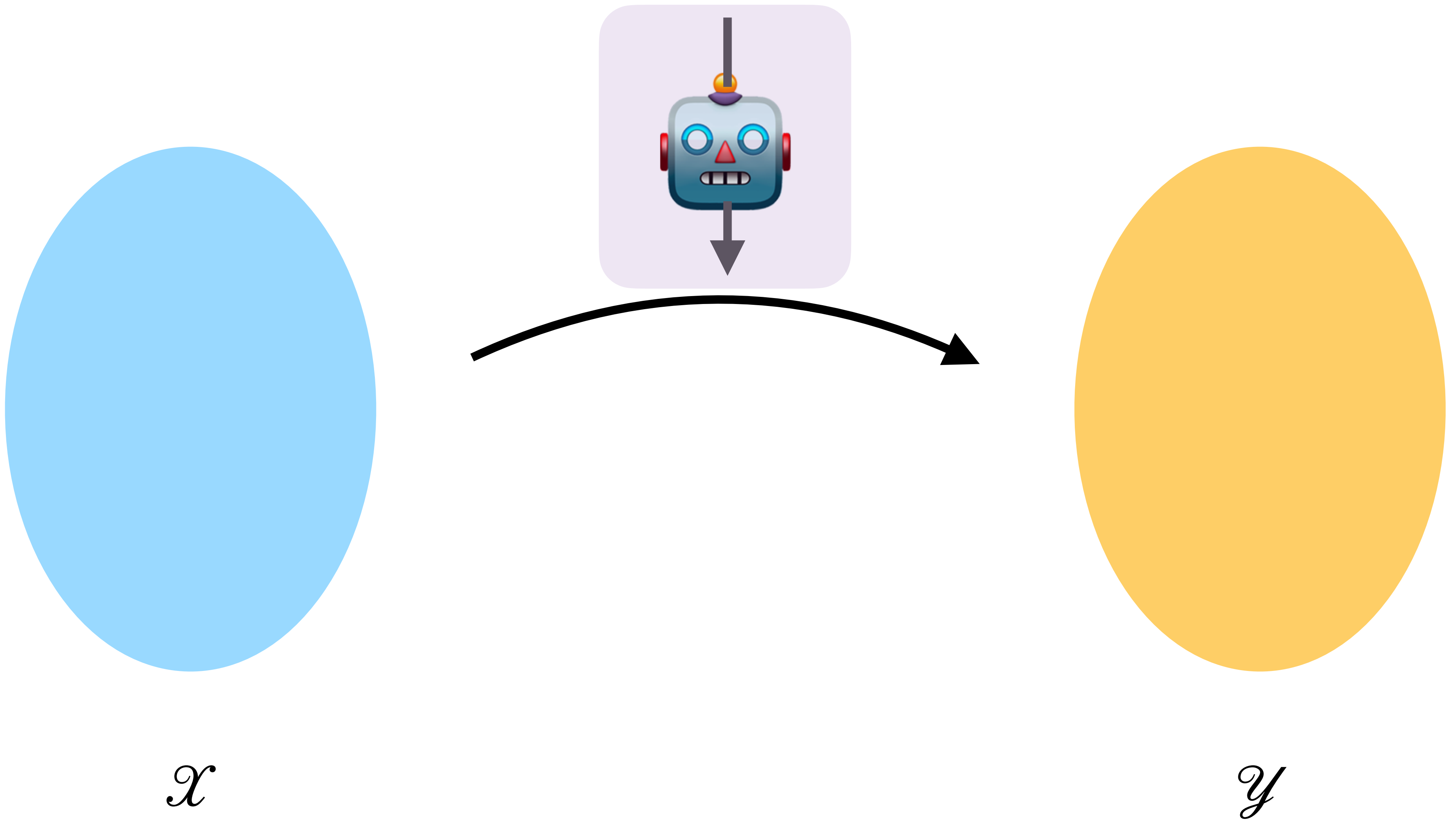

Supervised Learning

Basic Pipeline

② Unsupervised learning

③ Reinforcement learning

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**

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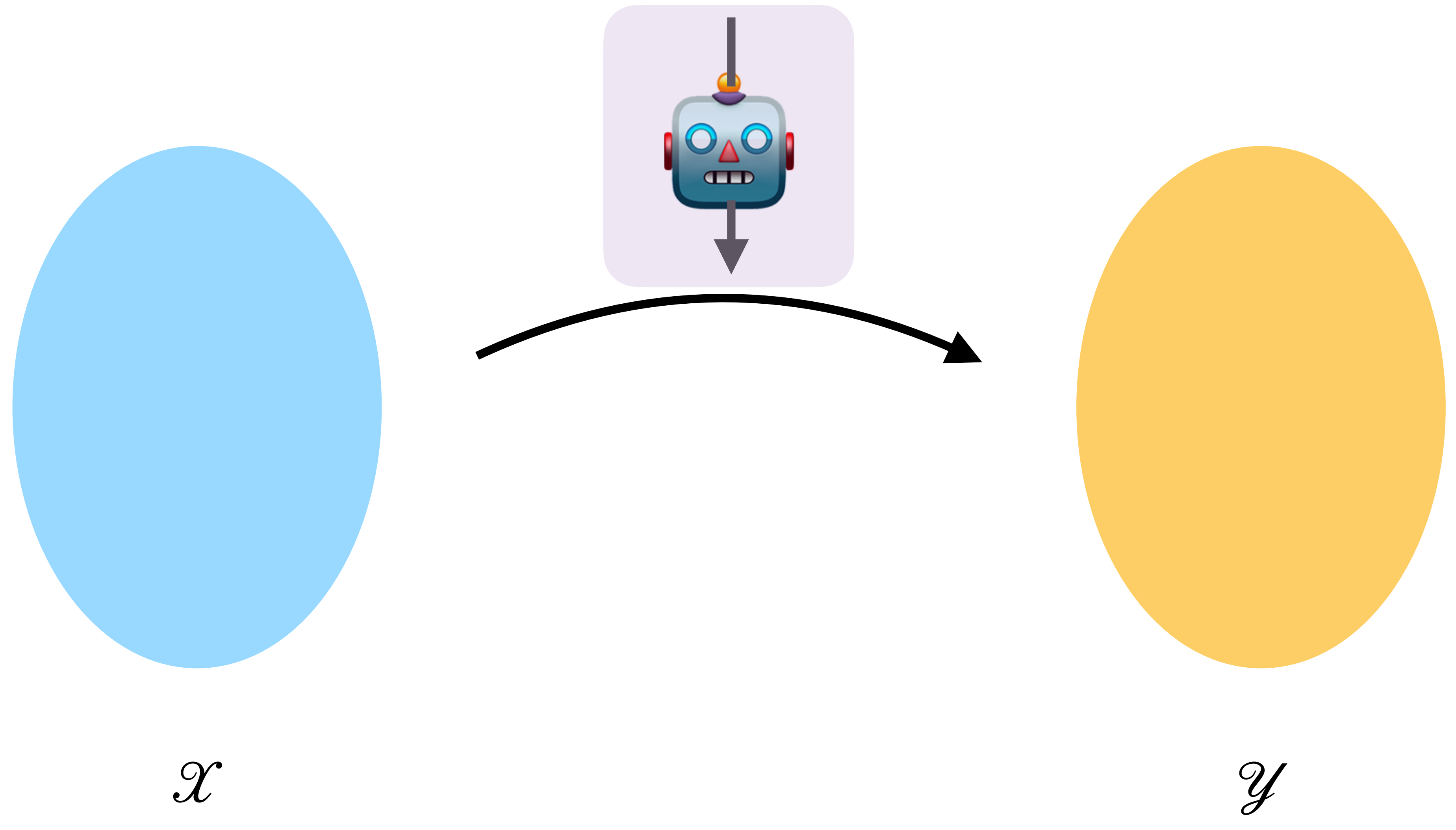

Outline

Inputs, Outcomes, and Evaluation

The Basic Prediction Problem

Inputs, Outcomes, and Evaluation

The Basic Prediction Problem

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

Inputs, Outcomes, and Evaluation

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Inputs, Outcomes, and Evaluation

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Inputs, Outcomes, and Evaluation

Input Space

Inputs, Outcomes, and Evaluation

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Inputs, Outcomes, and Evaluation

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

Inputs, Outcomes, and Evaluation

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

Inputs, Outcomes, and Evaluation

Action Space

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

Inputs, Outcomes, and Evaluation

Evaluation (Loss Functions)

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

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

Inputs, Outcomes, and Evaluation

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

Inputs, Outcomes, and Evaluation

Loss Function Examples

Inputs, Outcomes, and Evaluation

Loss Function Examples

Classification

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

Inputs, Outcomes, and Evaluation

Loss Function Examples

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

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

or, shorthand: $\ell(\hat{y}, y) := \mathbf{1}\{a \neq y\}$

indicator function.

Inputs, Outcomes, and Evaluation

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

Inputs, Outcomes, and Evaluation

The Basic Prediction Problem

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We will construct prediction functions to do this.

Hypothesis

Definition & Goal

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classifier

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Data Generating Distribution

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P(A, B) = P(A) P(B)

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

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$P(A, B) = P(A|B)P(B)$

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X is a random variable
→ F(X) is a random variable

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

Function

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Evaluation, Overall

Definition of Risk

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Evaluation, Overall

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

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 $\mathcal{X} \times \mathcal{Y}$?

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Summary of Characters So Far

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What's the smallest possible risk?

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$$\mathbb{E}[\ell(h(x),y)] = \int_{x,y} \ell(h(x),y)\, f(x,y)$$

$$\mathbb{E}[\ell(h(x),y)] = \sum_{x,y} \ell(h(x),y)\, \Pr(x,y)$$

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The risk of h^* is called the Bayes risk. → $R(h^*)$

Bayes Risk

Example: Binary Classification

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

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

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

$\mathcal{X} = \{1, 2, 3, 4\}$

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h that minimizes: $R(h) = \Pr(h(x) \neq y) = \mathbb{E}_X[\Pr(h(x) \neq y \mid X = x)]$

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

$= \Pr(X=1)\Pr(h(1) \neq y \mid X=1) + \dots + \Pr(X=4)\Pr(h(4) \neq y \mid X=4)$

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$=1$

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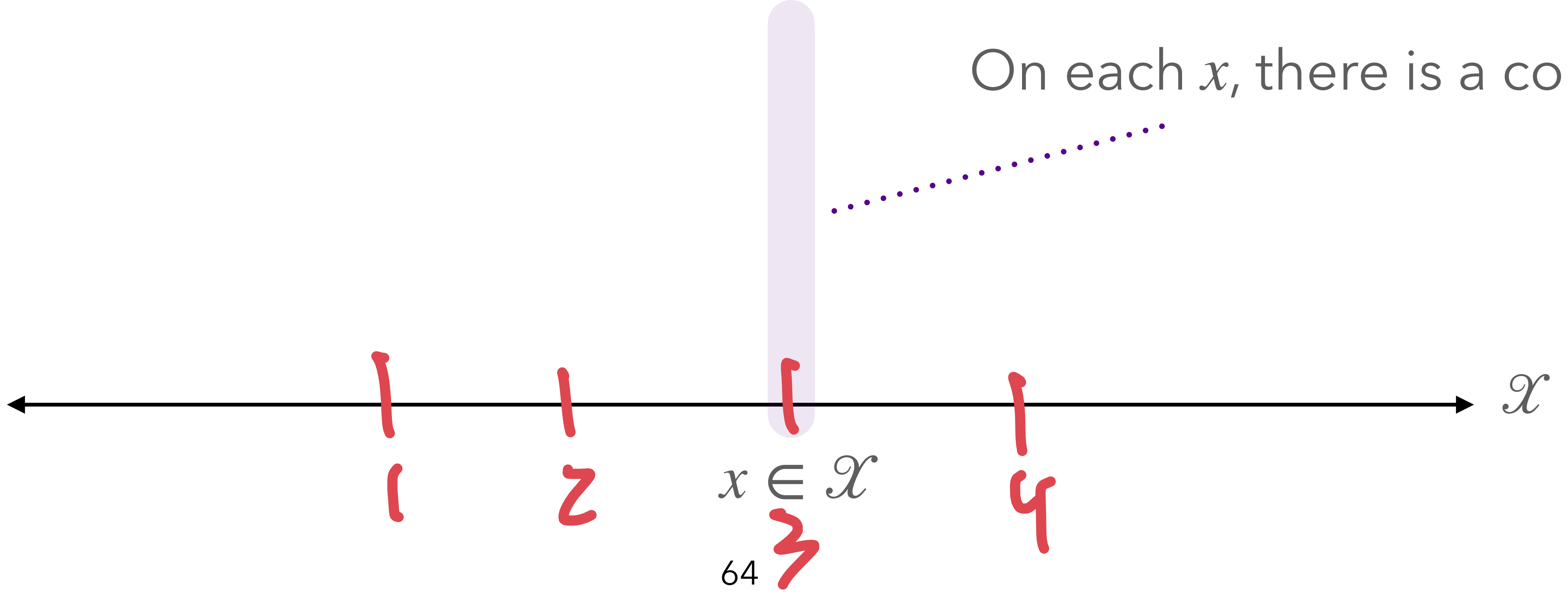
On each x, there is a conditional distribution $\Pr(y \mid x)$.



$\Pr(h(1) \neq y \mid X=1)$

$h(1)=1$: $\Pr(y=0 \mid X=1)$

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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

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Law of Large Numbers

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are all random variables…

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$$\hat{R}_n(h) = \frac{1}{n}\sum_{i=1}^{n} \underbrace{\ell(h(x^{(i)}), y^{(i)})}_{\text{Random variables}}. \approx \mathbb{E}[\ell(h(x), y)] = R(h)$$

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By the strong law of large numbers,

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

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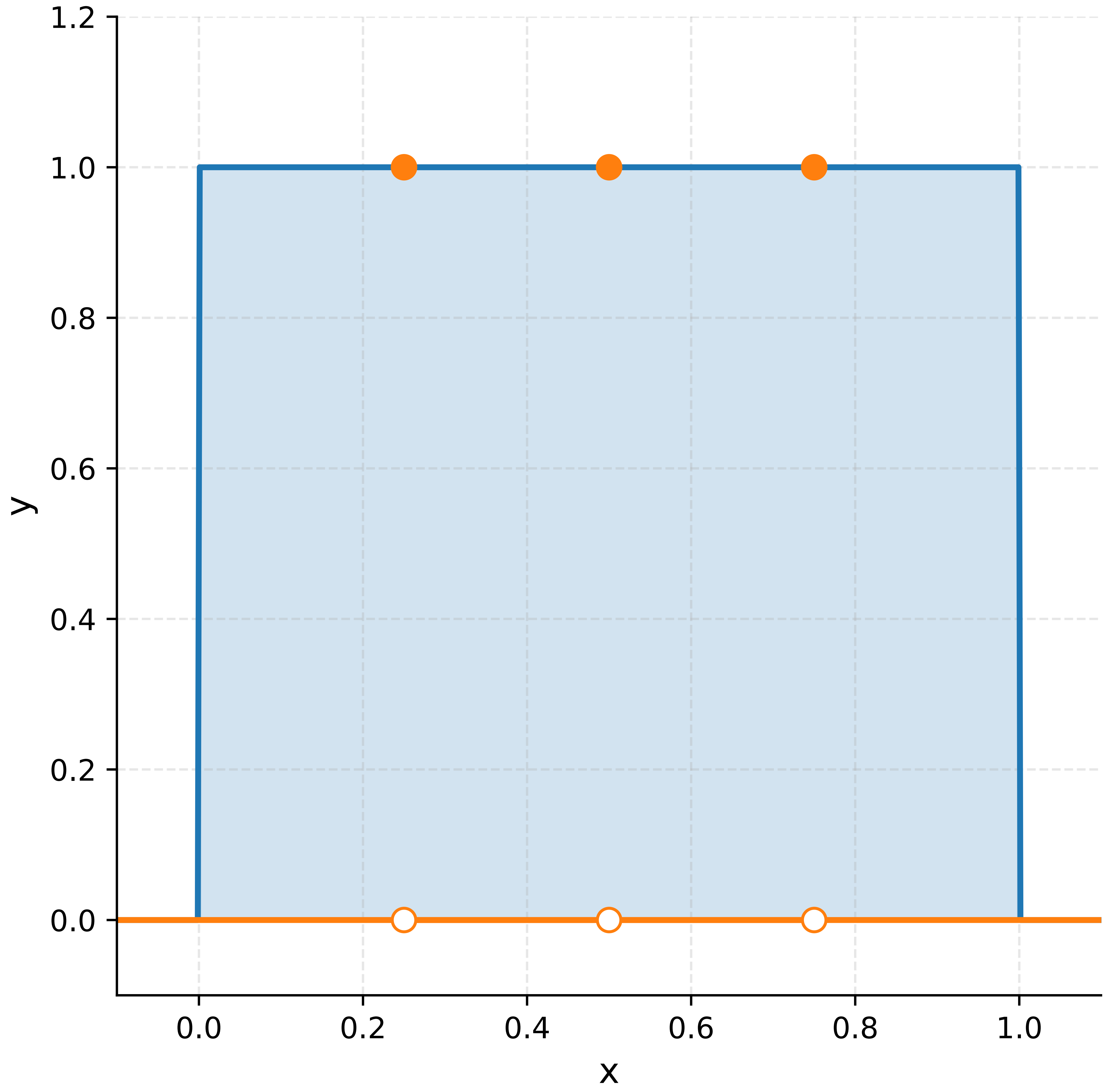
Example



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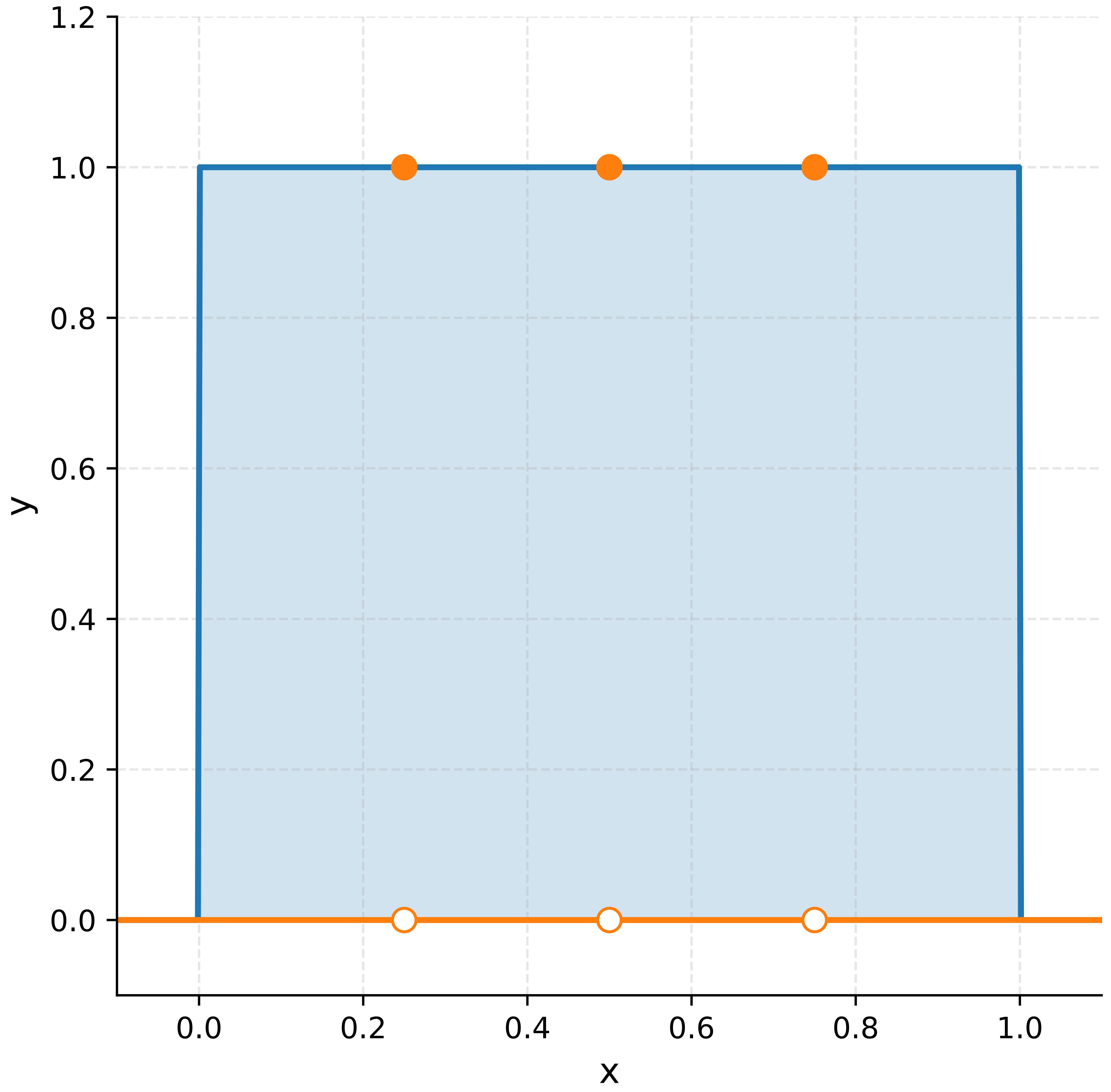

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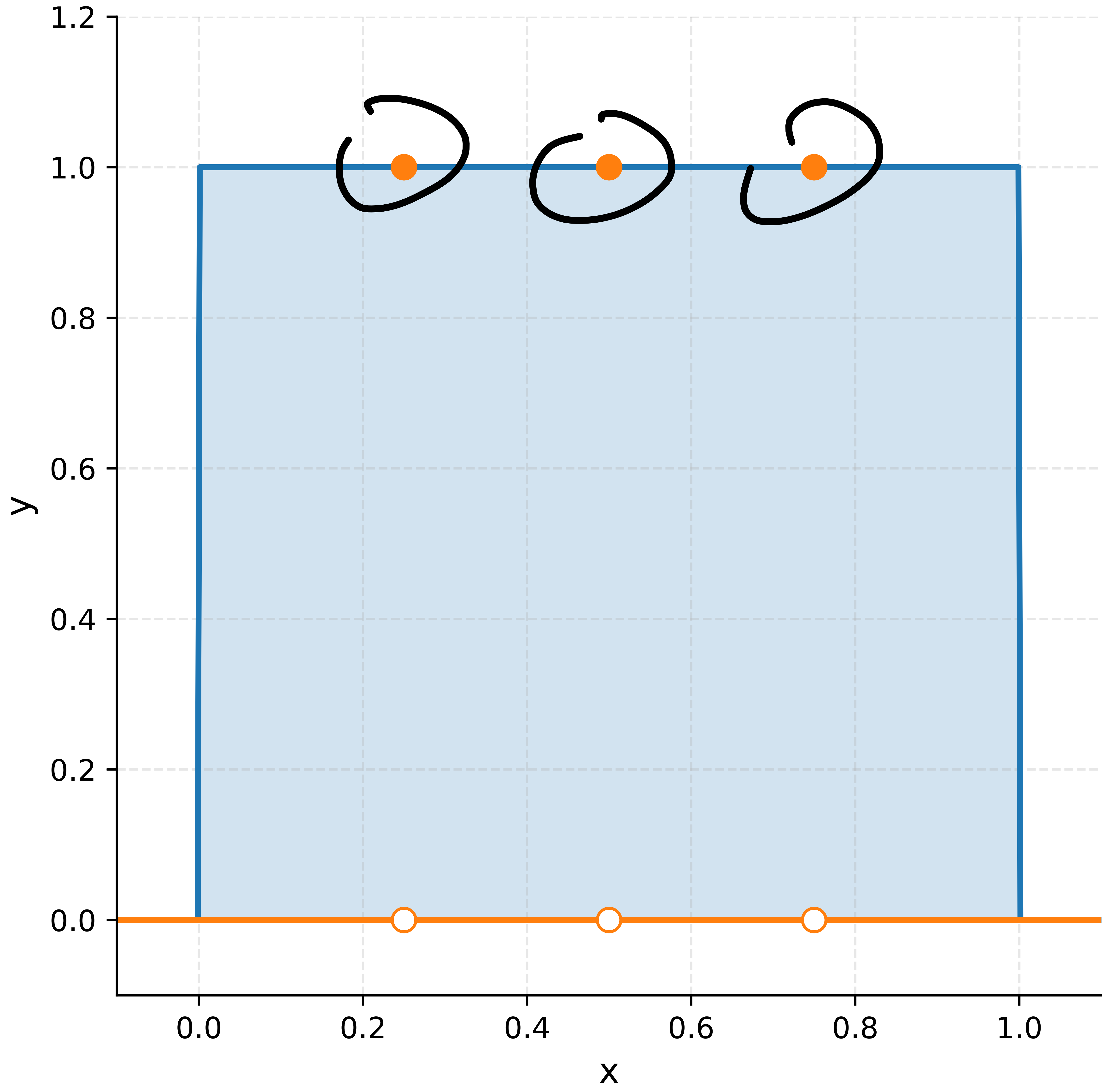
Draw i.i.d. sample of size $n = 3$:



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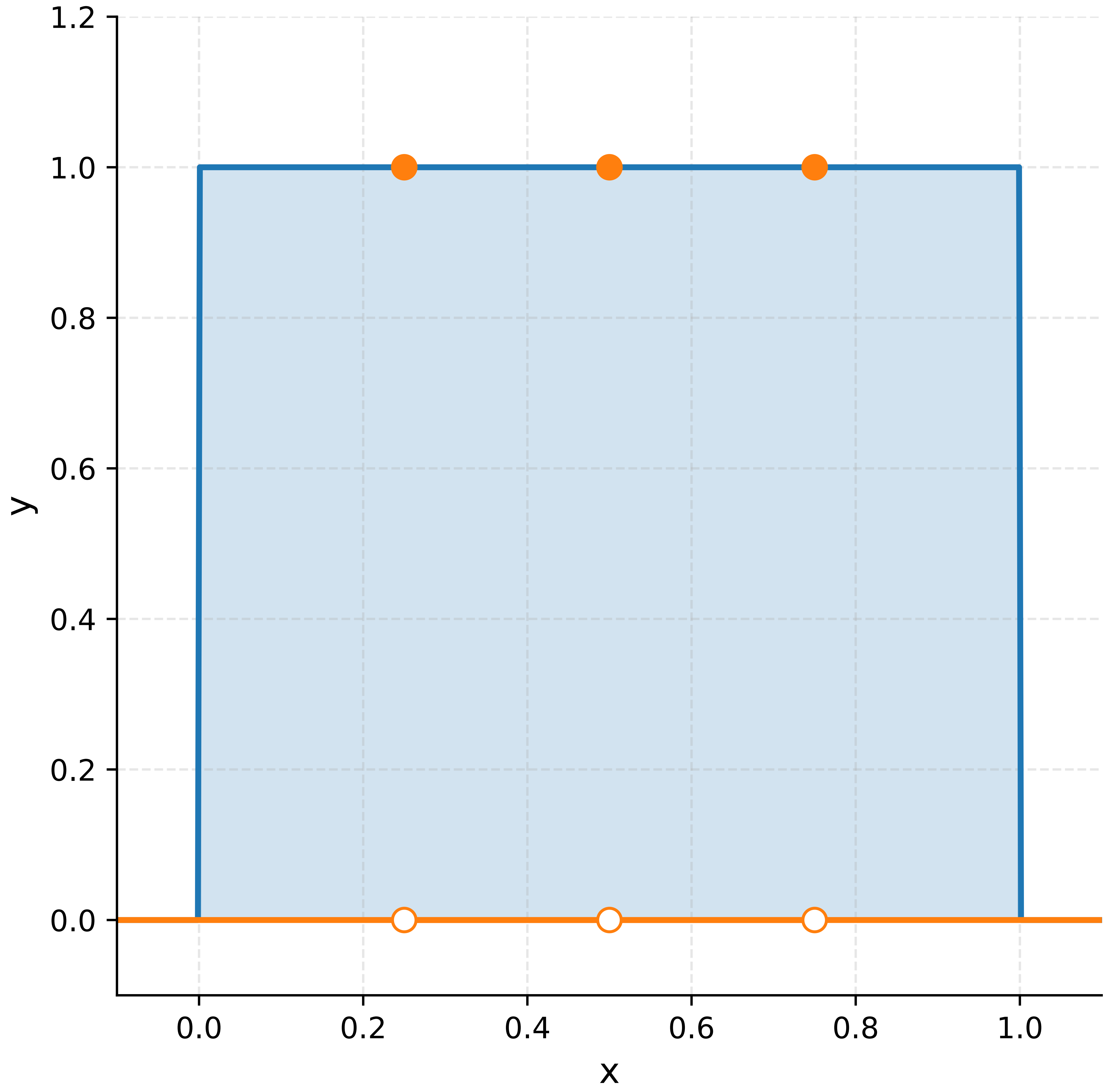

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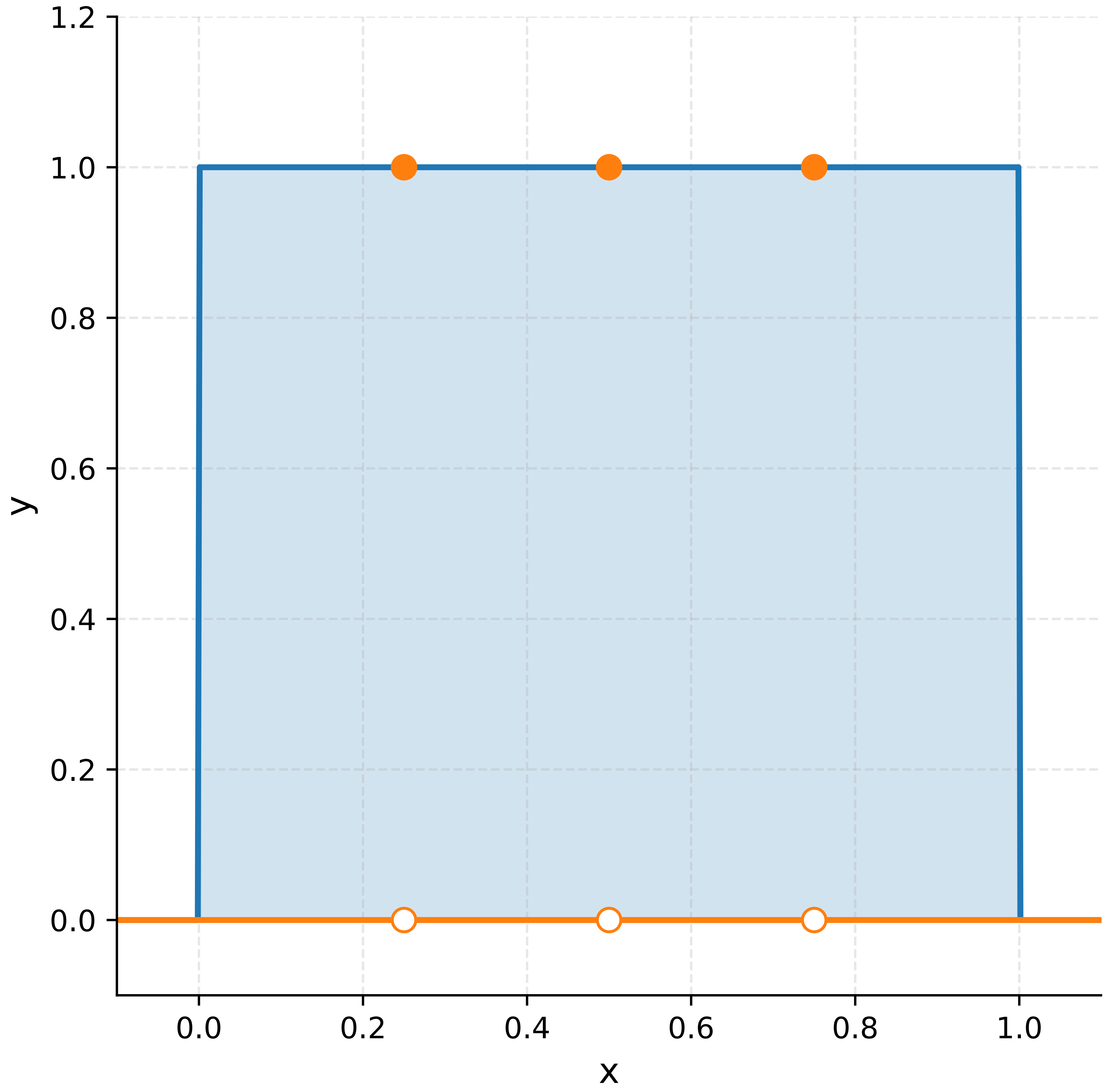

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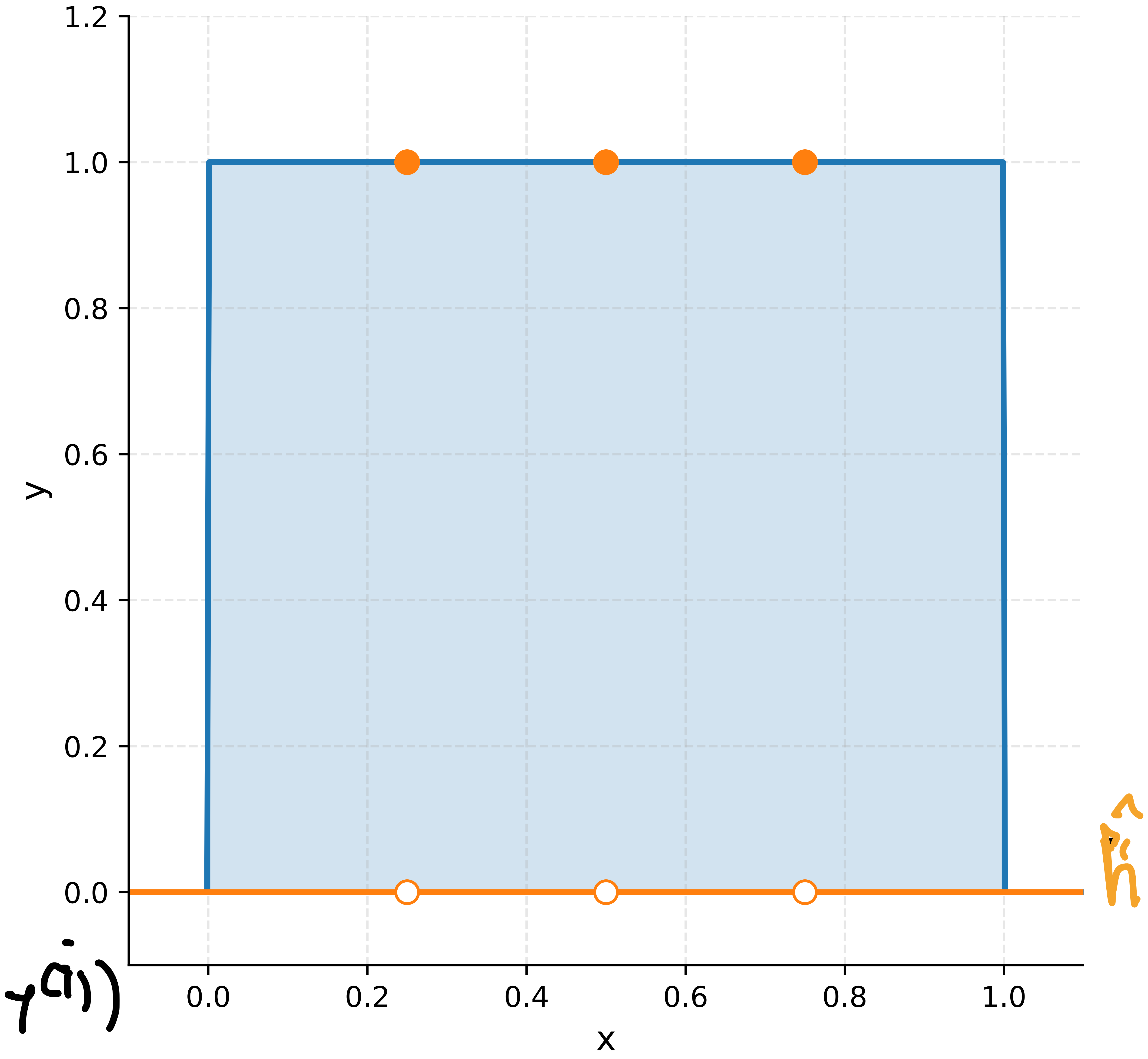

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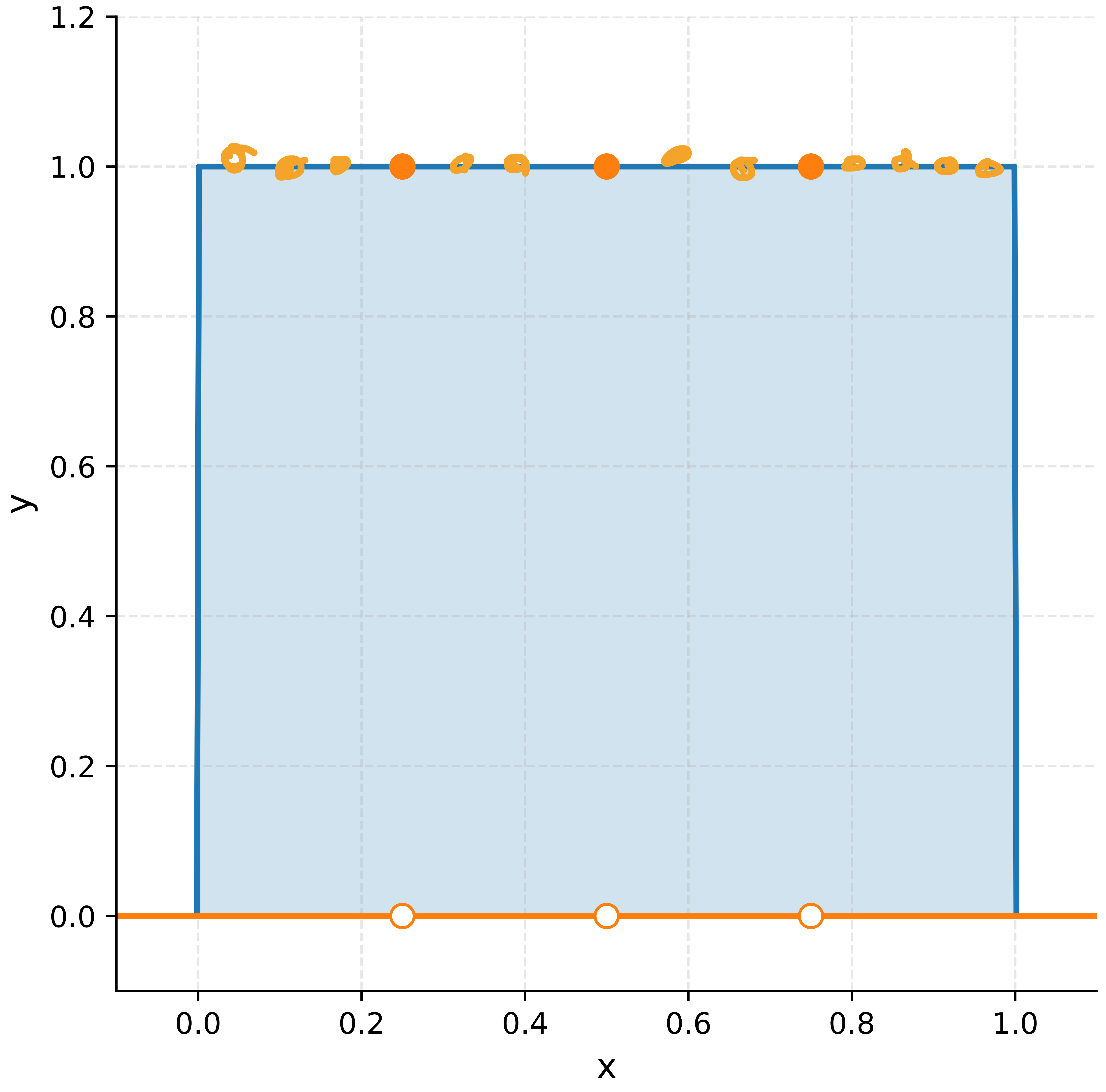

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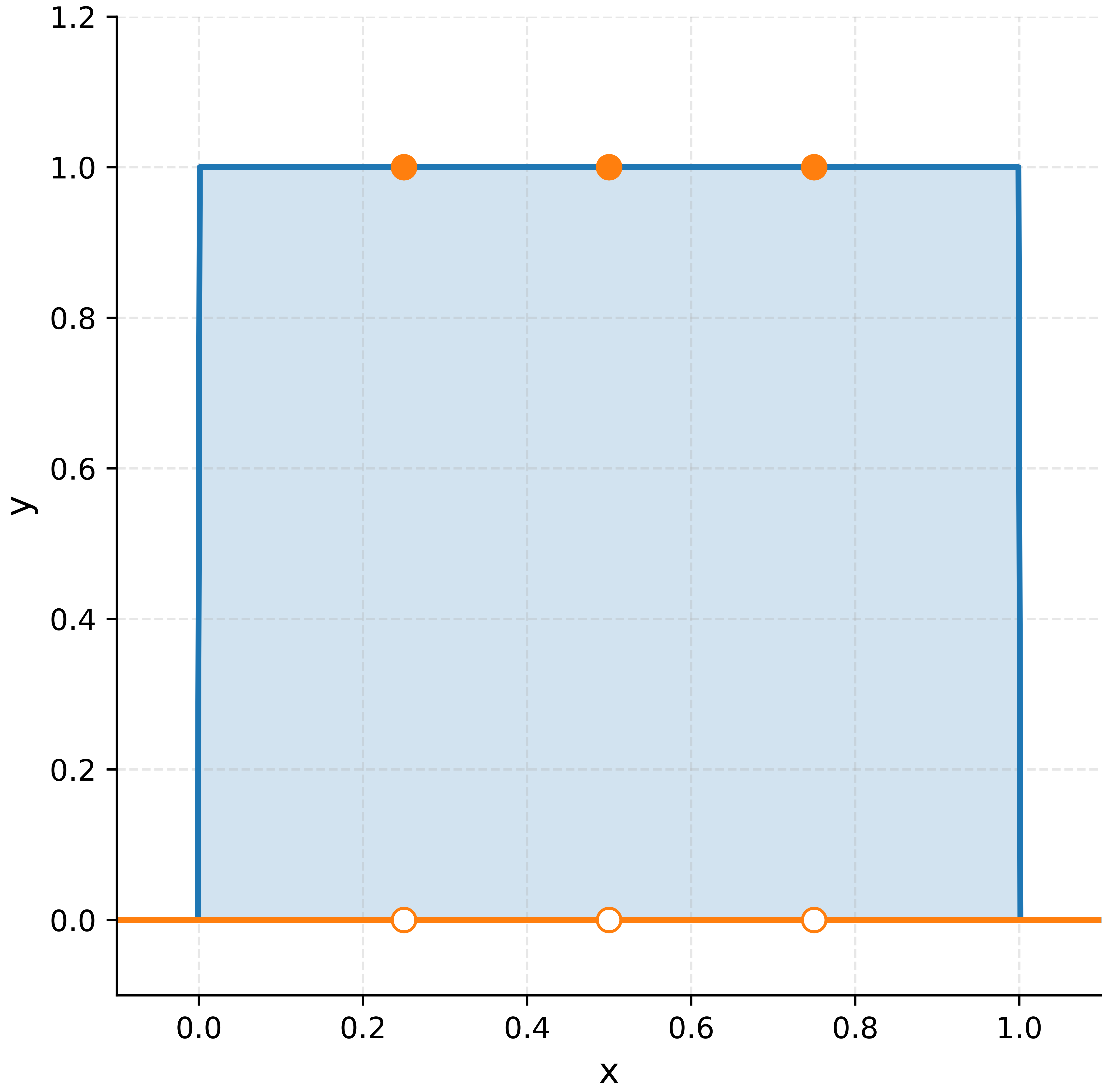
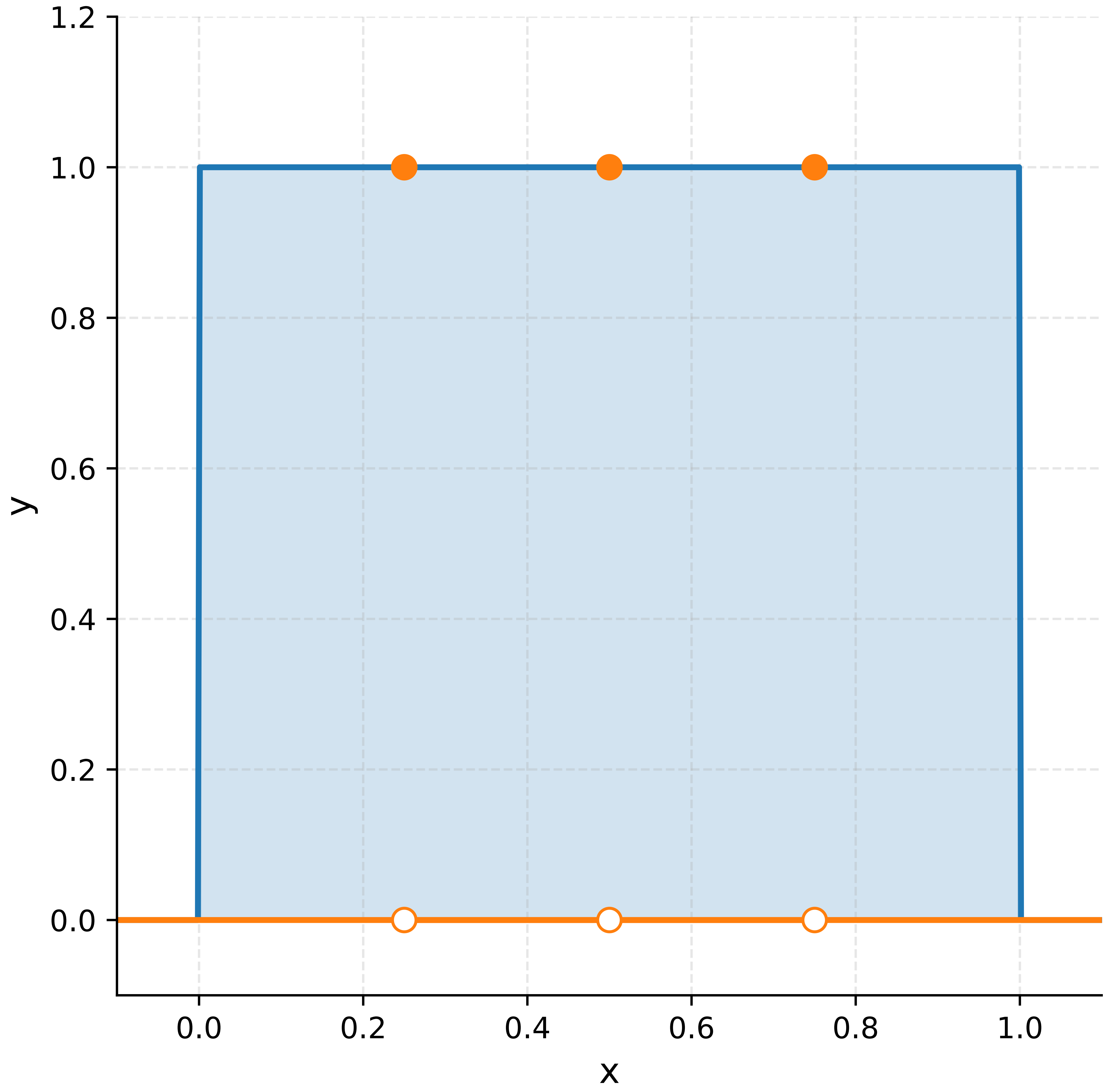


Empirical Risk Minimization

Example: Gap with true risk



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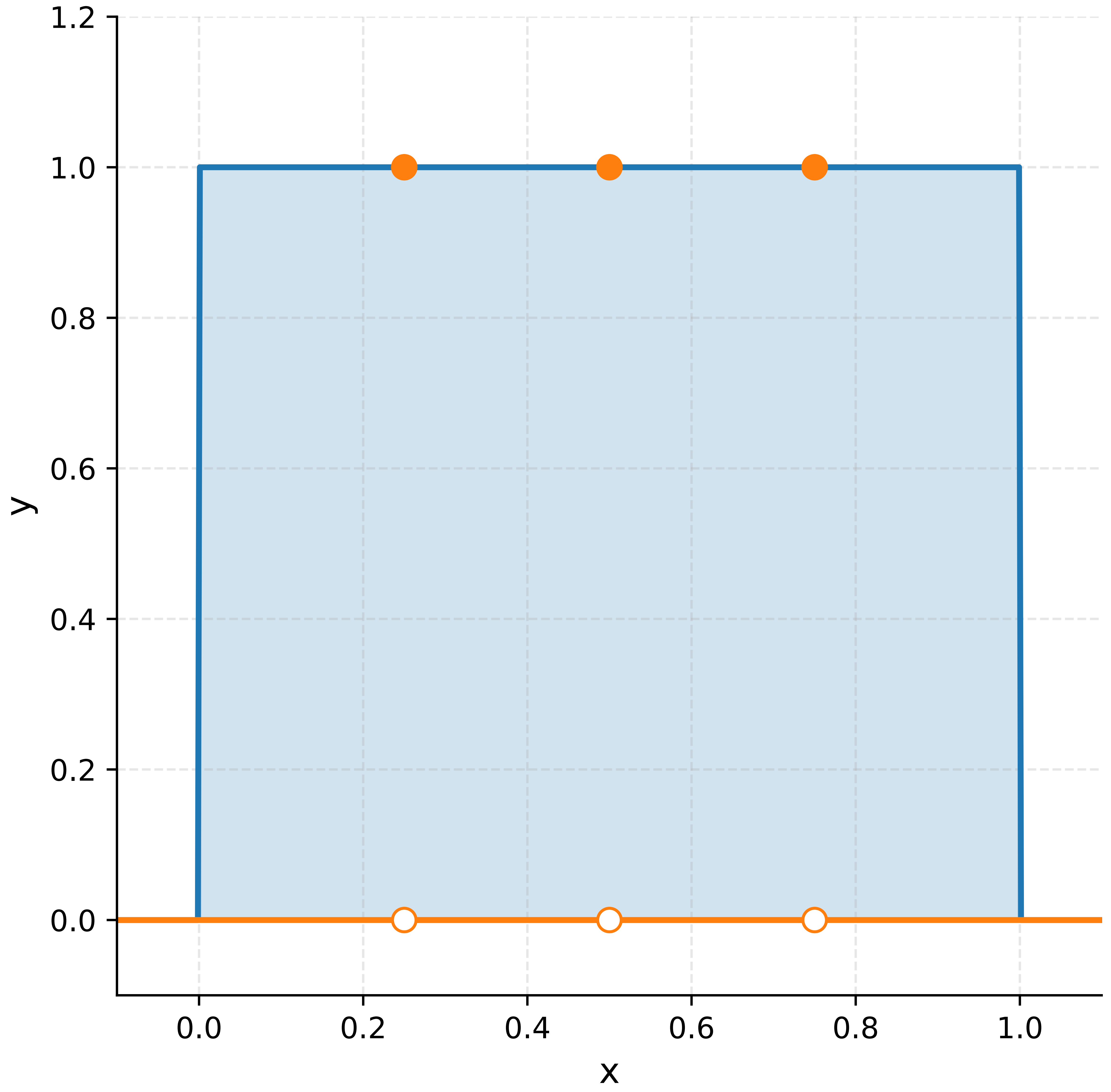

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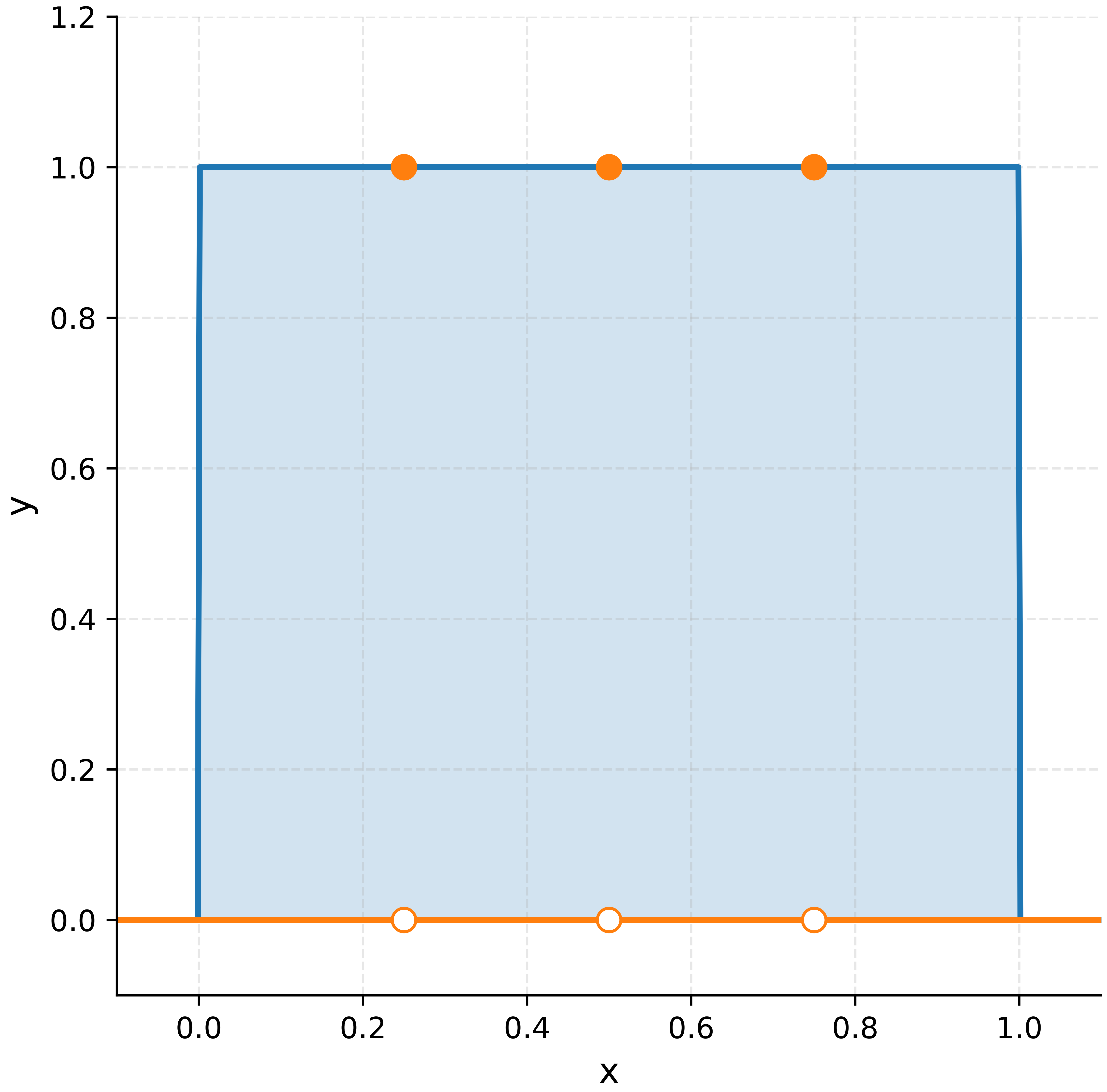

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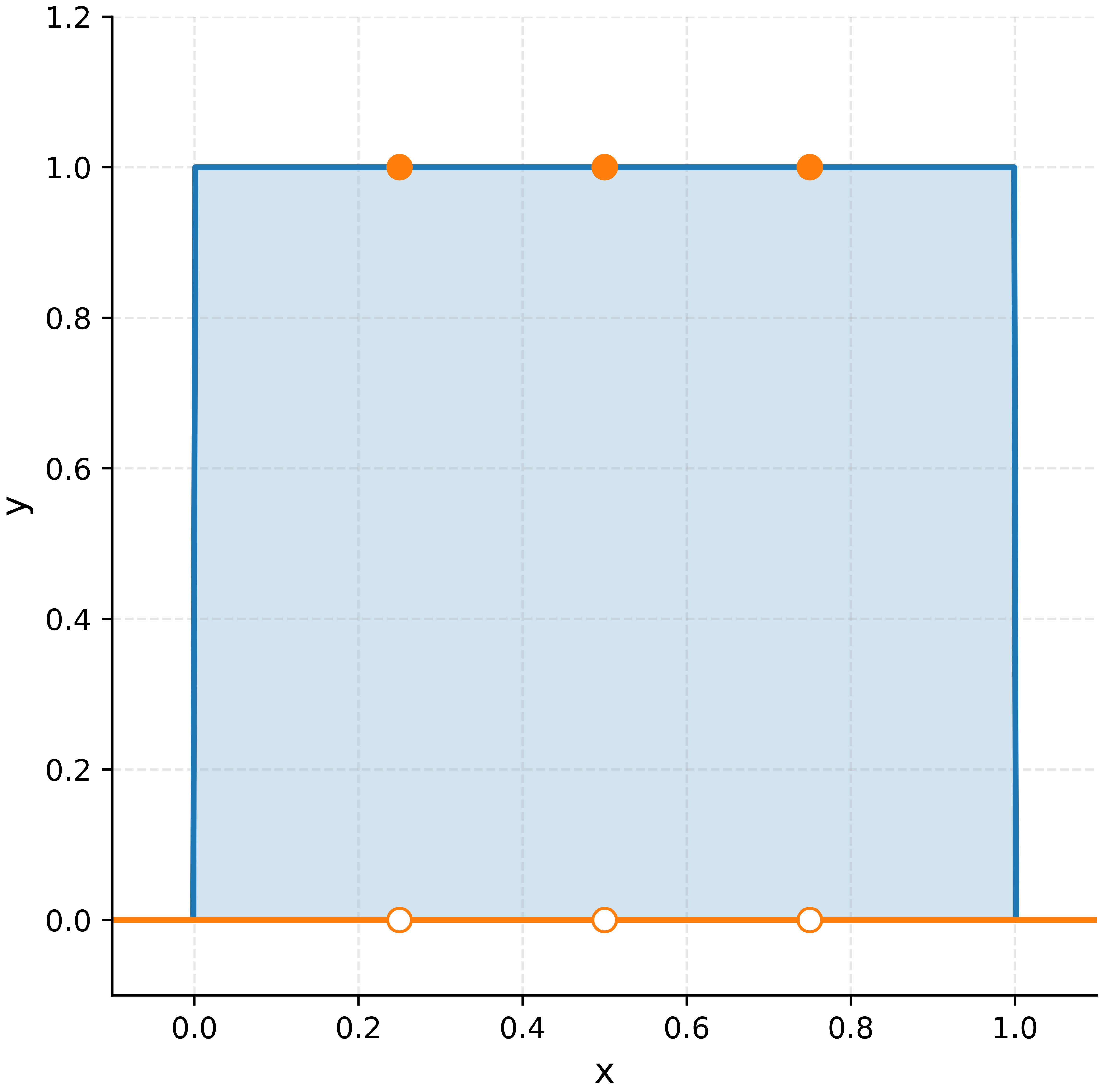

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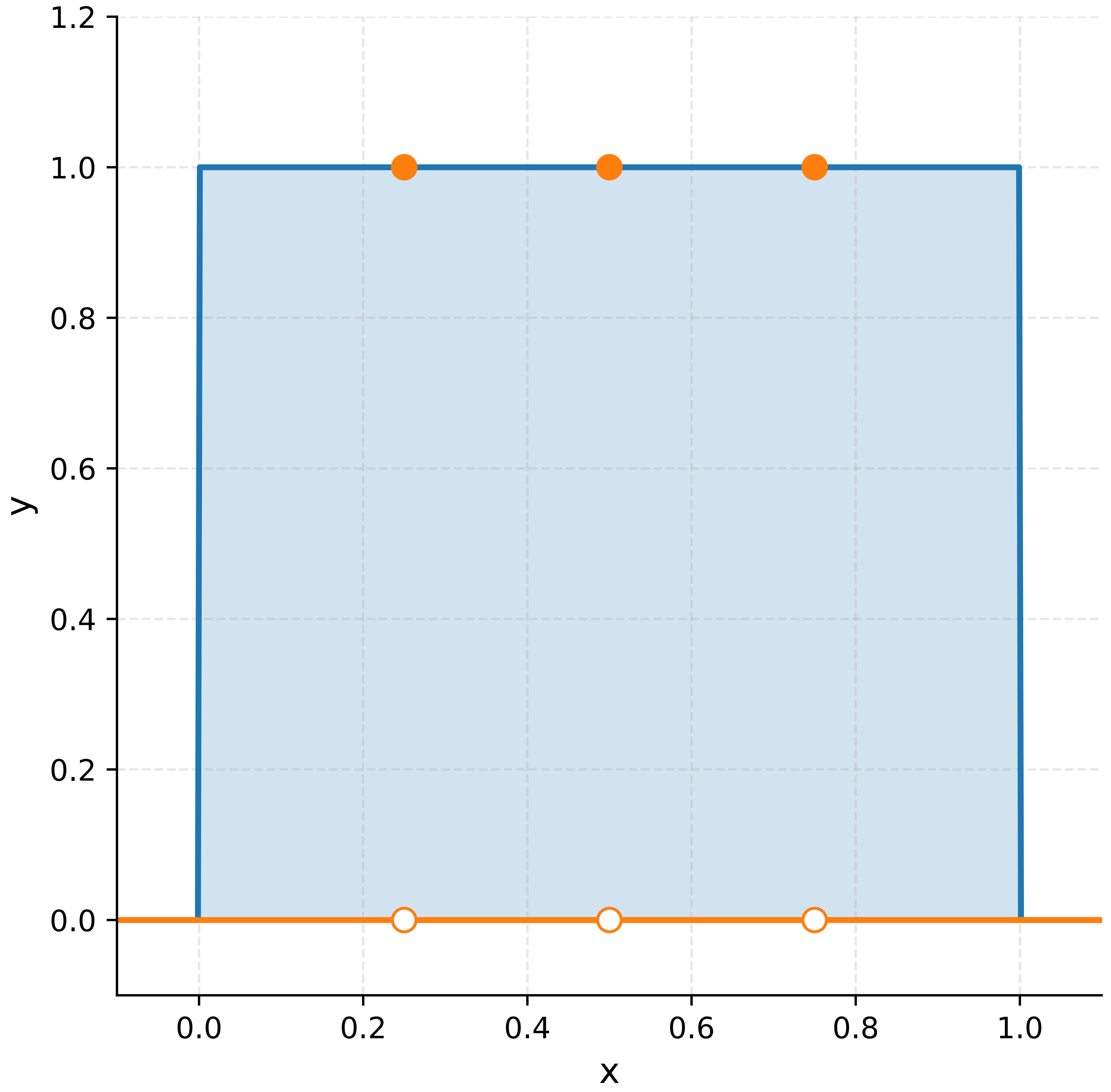

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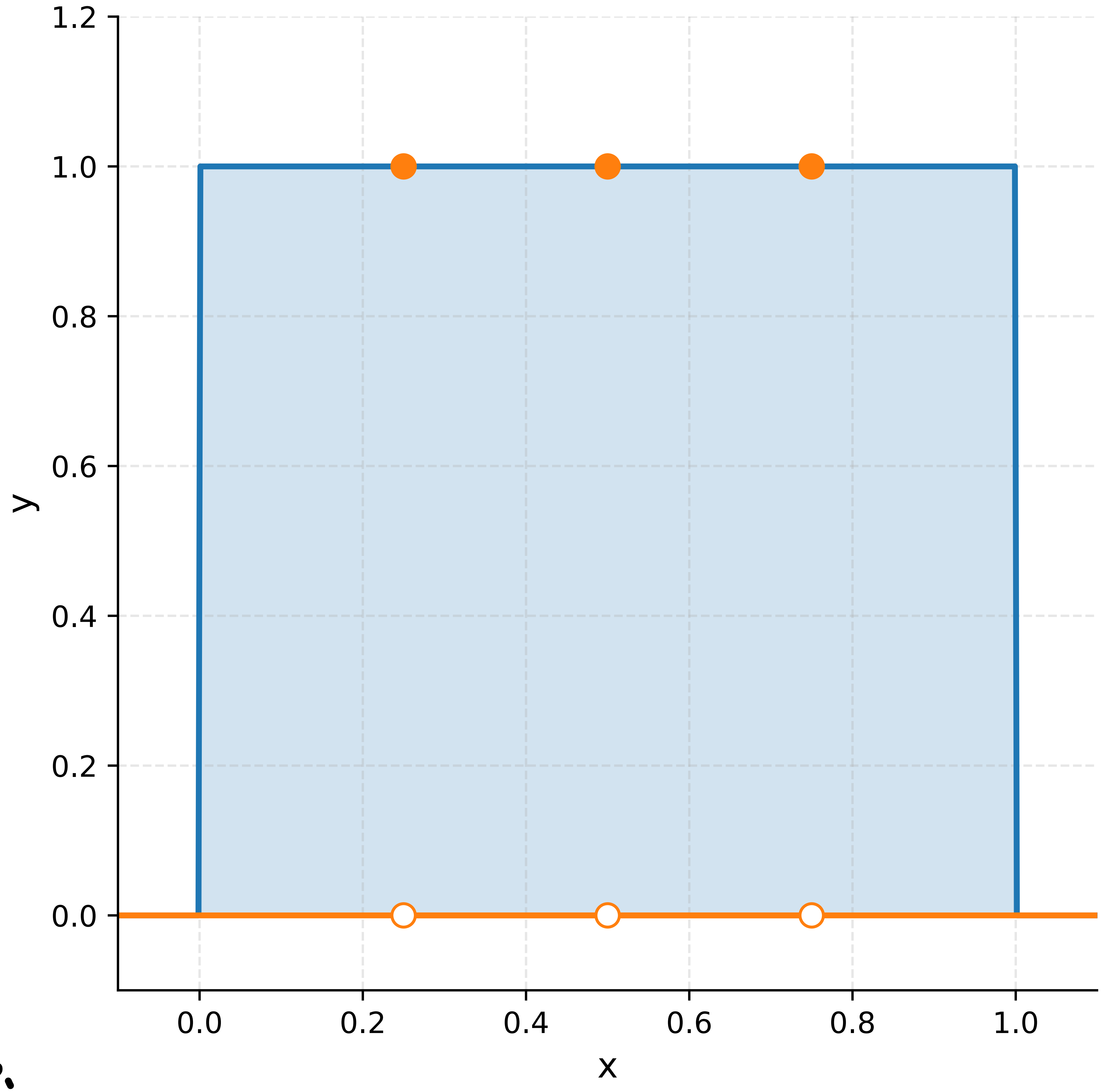
True risk under zero-one loss:

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

↓ Unif is continuous.



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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 $\mathcal{X}$!

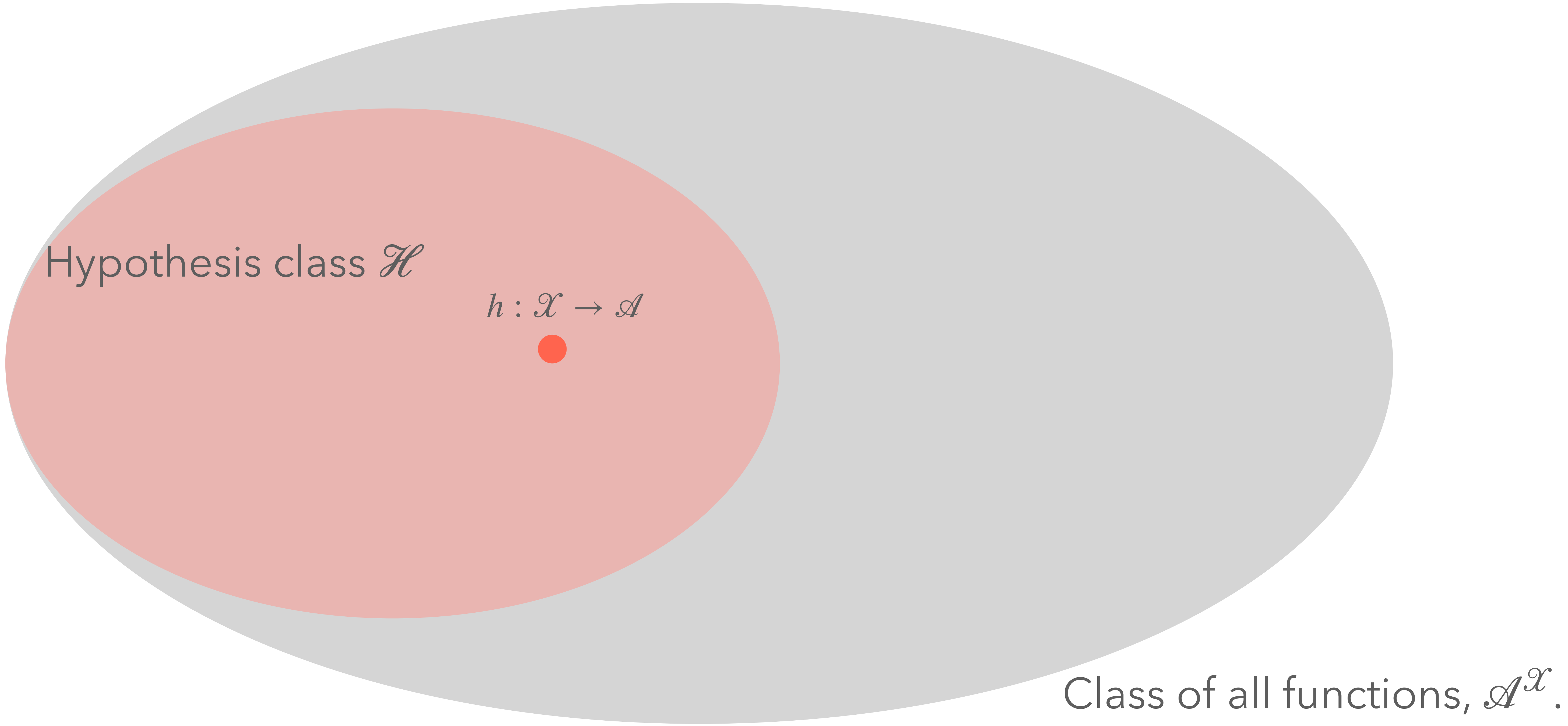
Outline

Hypothesis Class

Definition

A = {0, 1}

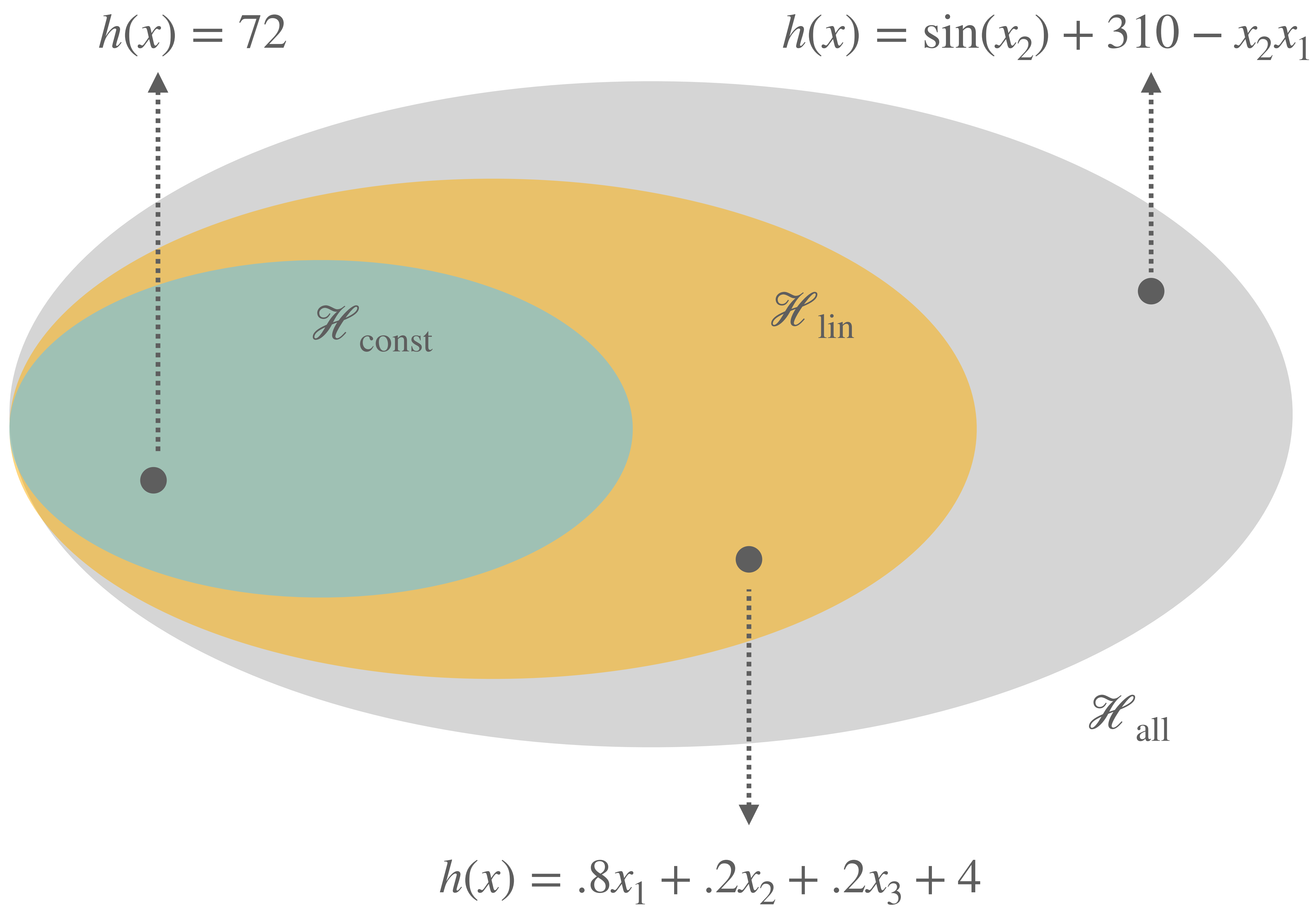
A hypothesis class is a set of functions $\mathscr{H} \subseteq \mathscr{A}^{\mathscr{X}}$ where we will search for h.



Hypothesis Class

Example

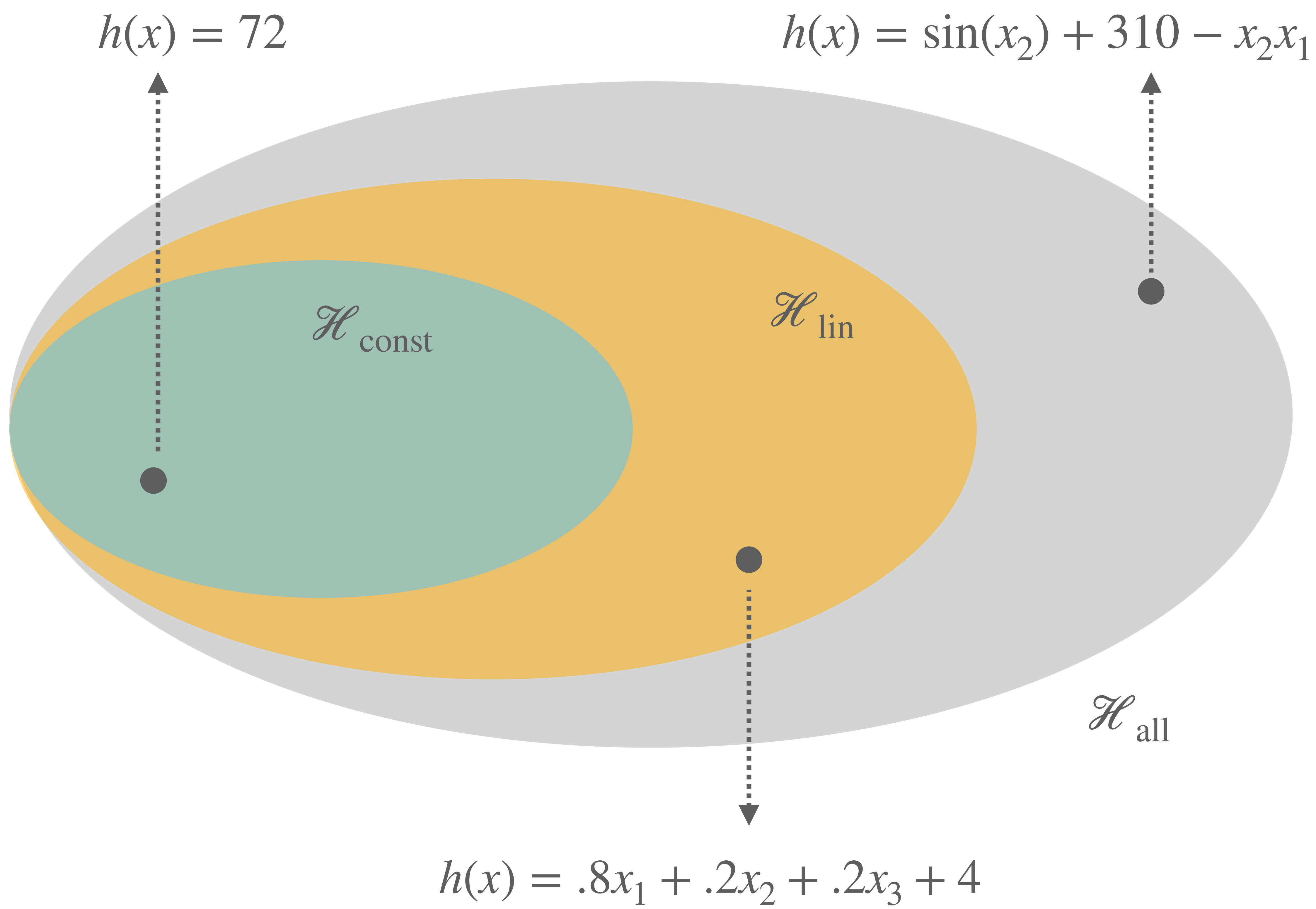
$h: \mathcal{X} \rightarrow \{0,1\}$



Hypothesis Class

Example

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



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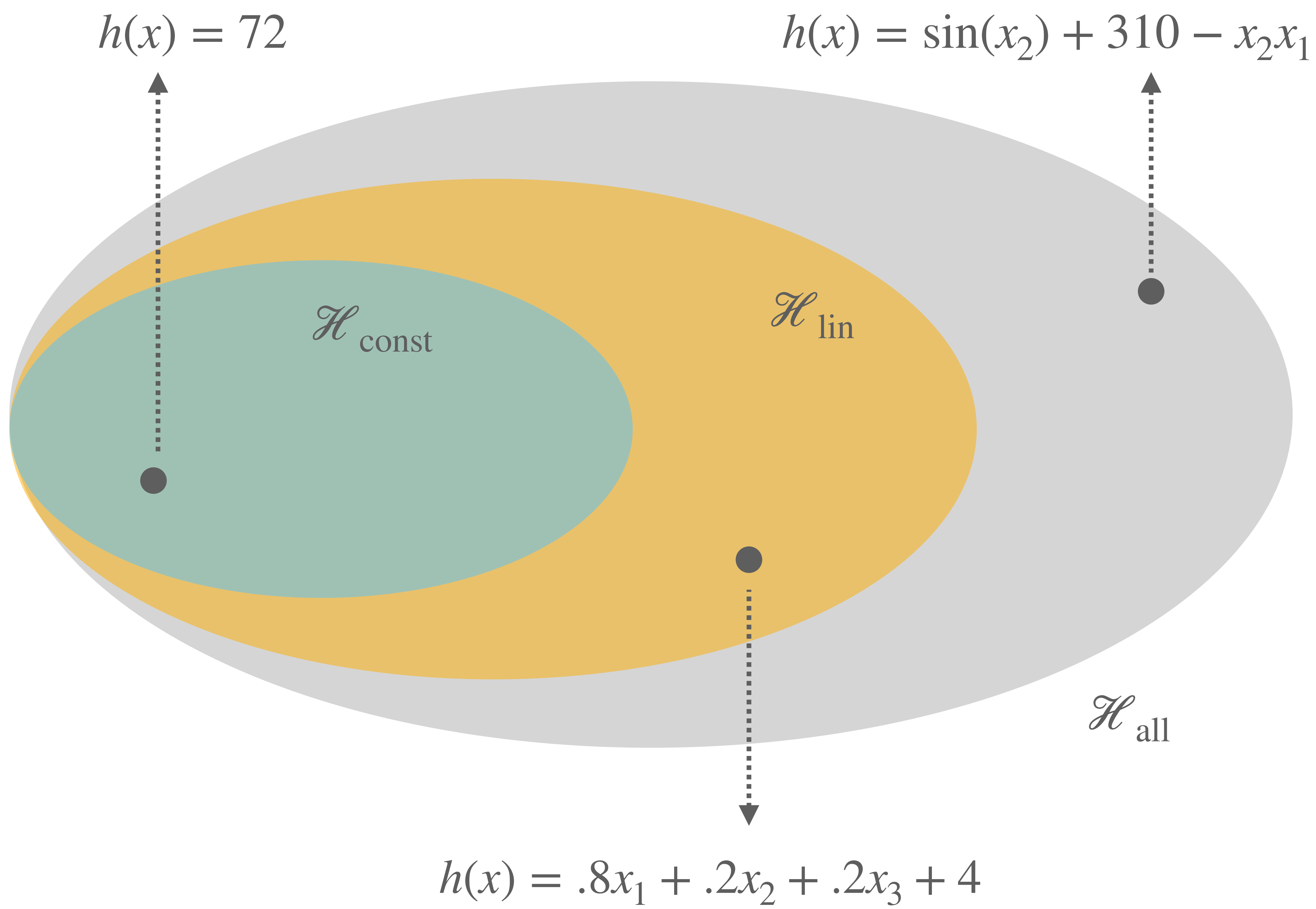

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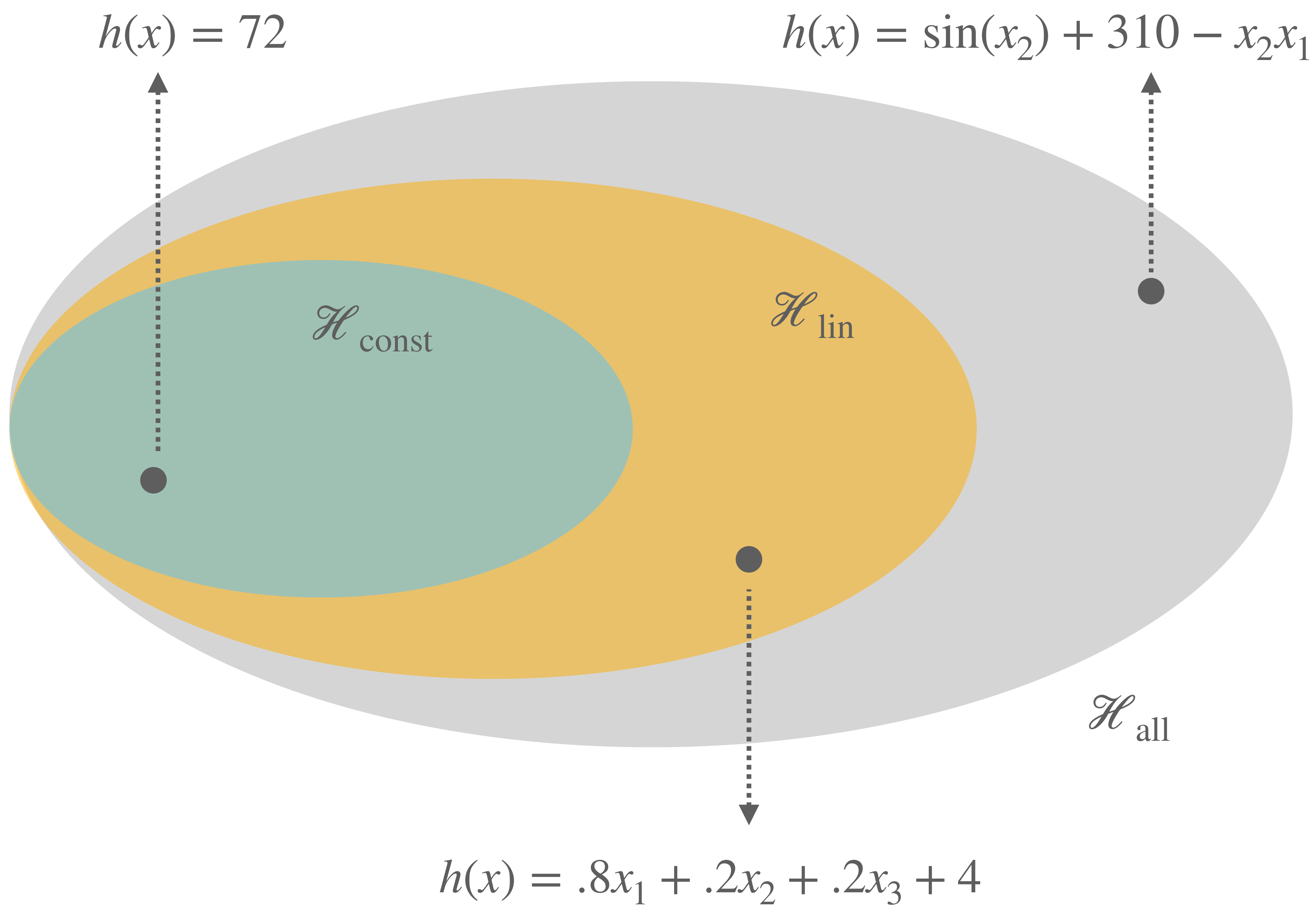

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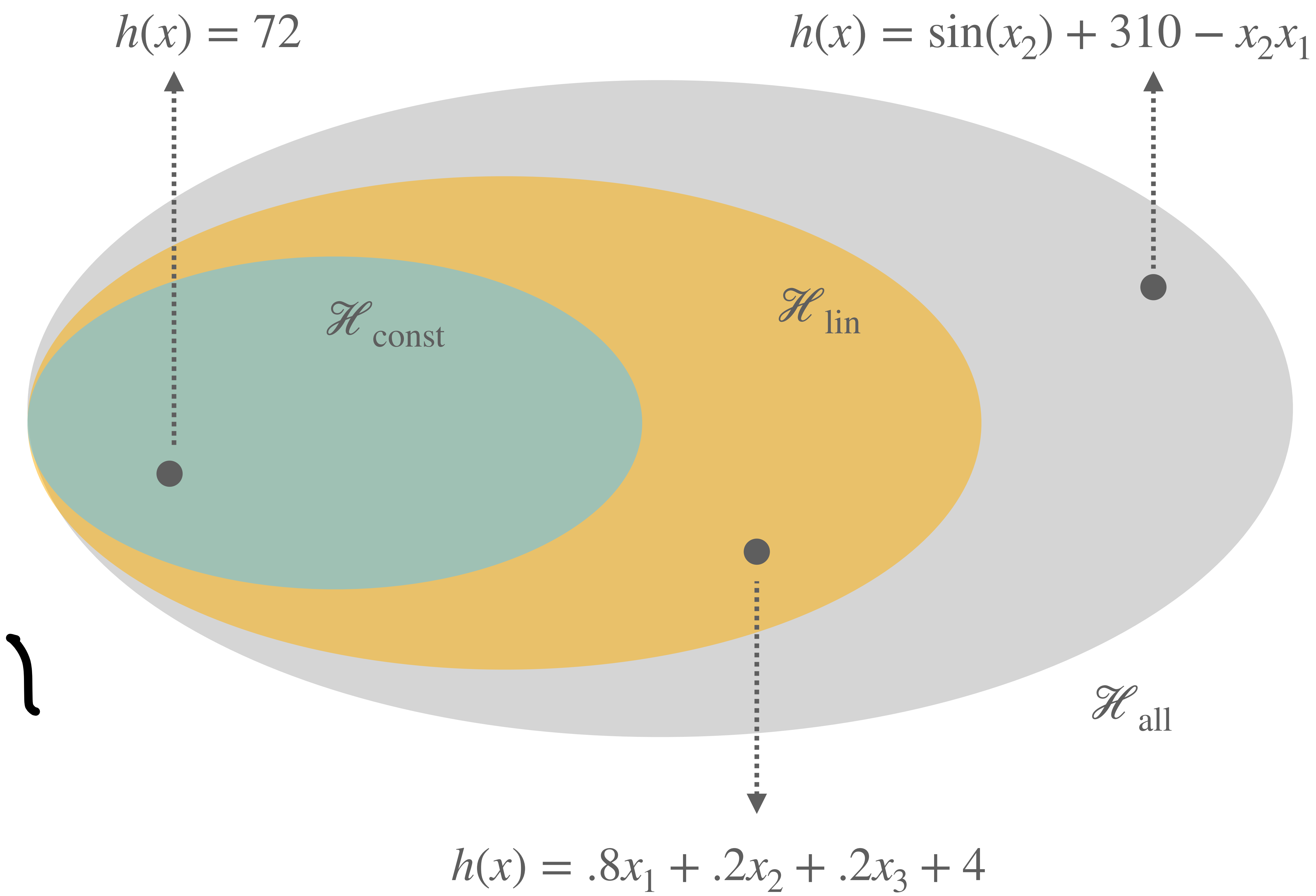
Possible hypothesis classes:

$\mathscr{H}_{\text{const}} = \{x \mapsto b : b \in \mathbb{R}\}$ h(x) = 1



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

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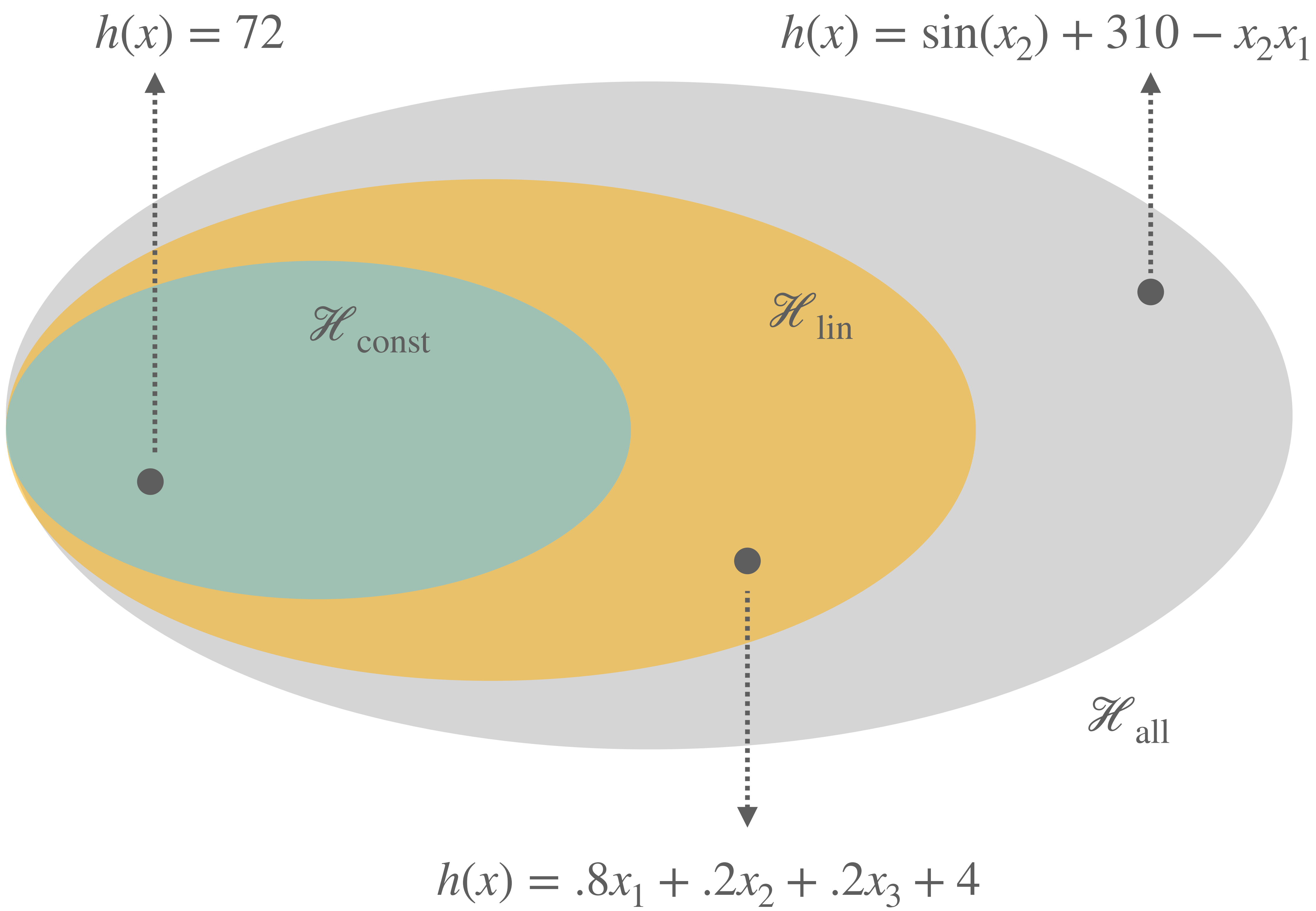

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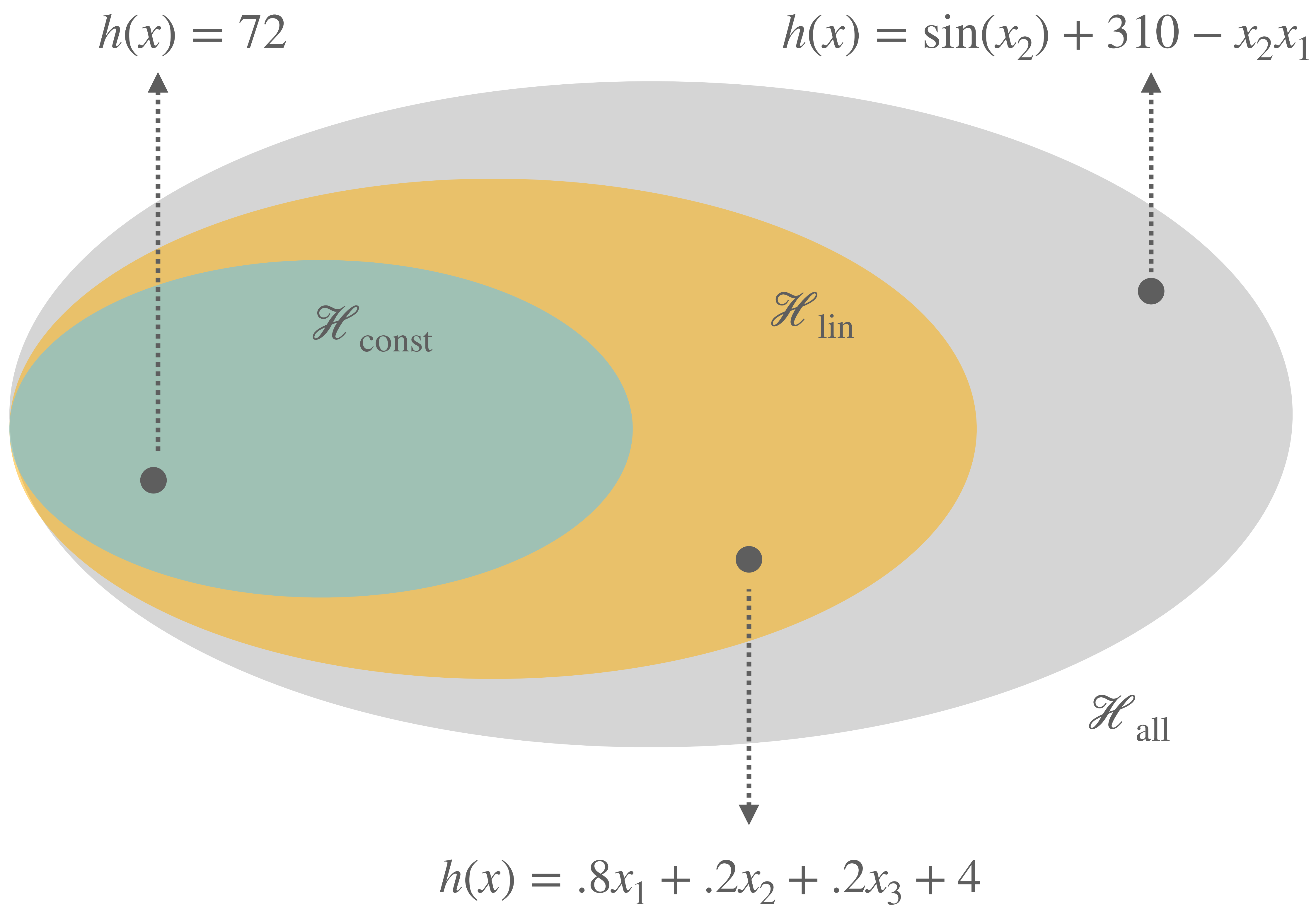
$$\mathscr{H}_{\text{all}} = \{\mathbb{R}^3 \mapsto \mathbb{R}\}$$



Empirical Risk Minimization

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

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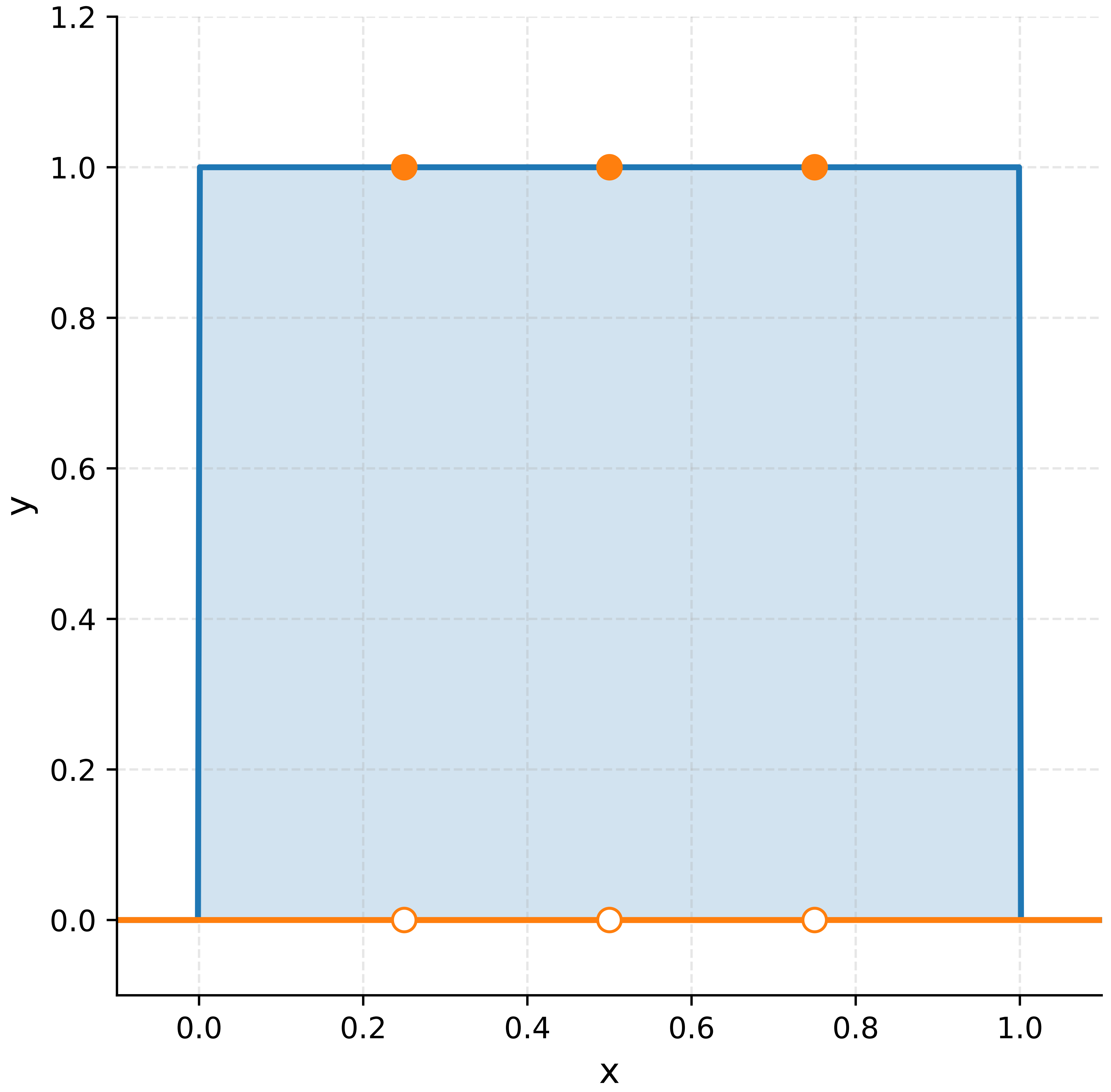
$$\hat{h}(x) = \begin{cases} 1 & \text{if } x \in \{0.25, 0.5, 0.75\} \\ 0 & \text{otherwise} \end{cases}$$

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 $\mathscr{H}$ is a function $\hat{h}$ satisfying

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

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

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

true Risk

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

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

Outline

Course Overview and Logistics

Introduction to Machine Learning

Statistical Learning Setup

Statistical Learning: Bayes Risk

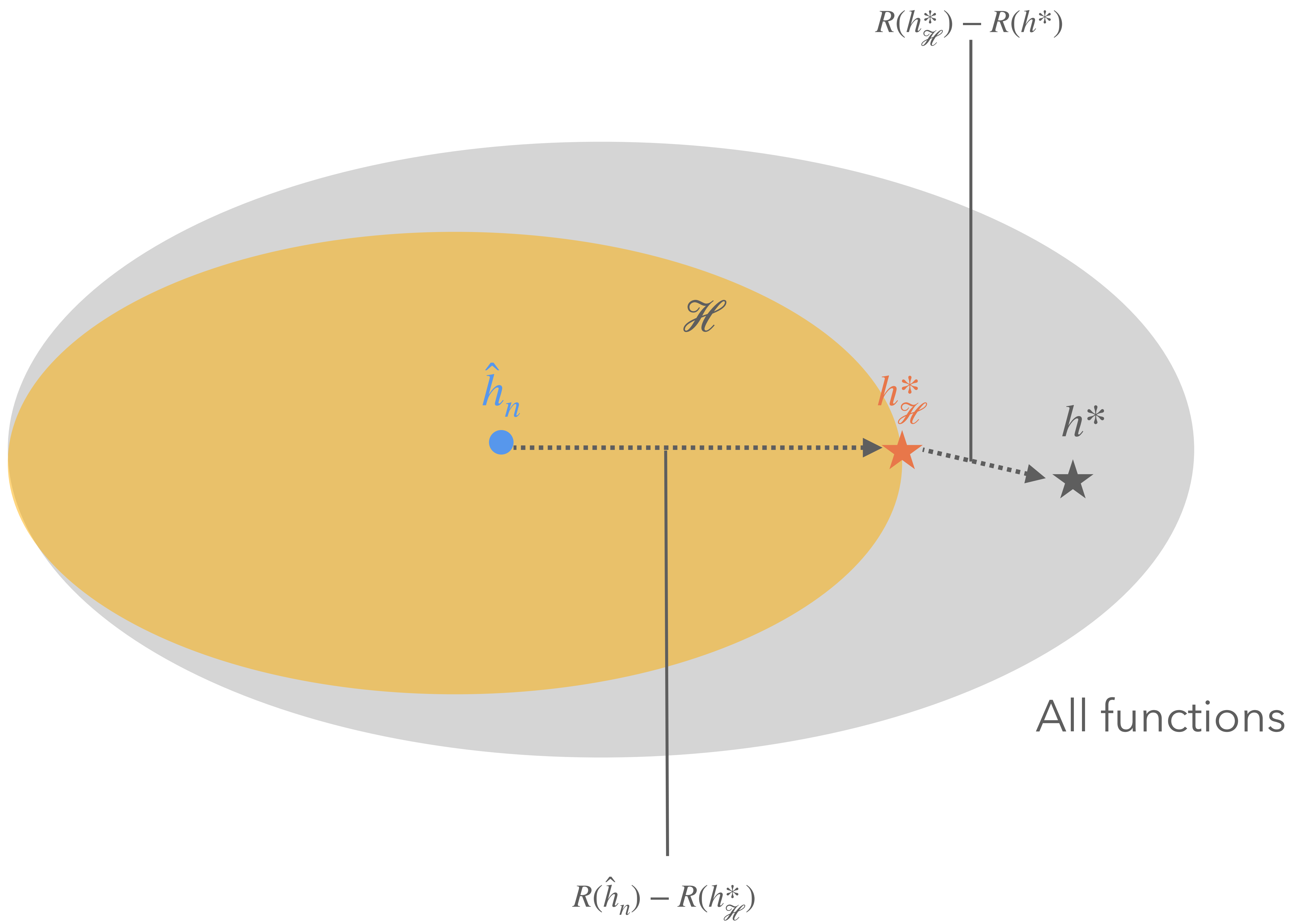
Statistical Learning: Empirical Risk and ERM

Statistical Learning: Hypothesis Class

Excess Risk Decomposition and Three Types of Error

Excess Risk

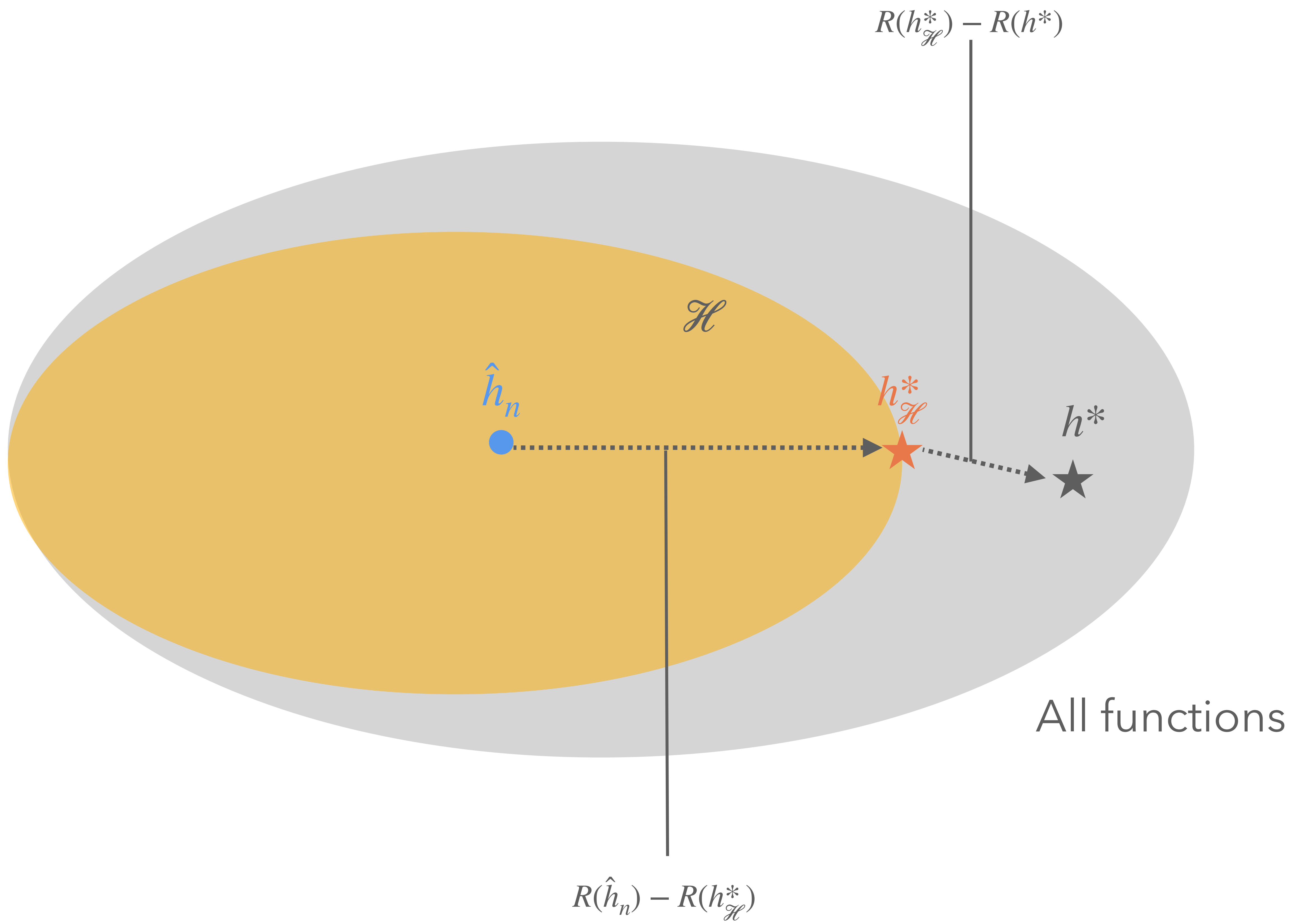
Definition



Excess Risk

Definition

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



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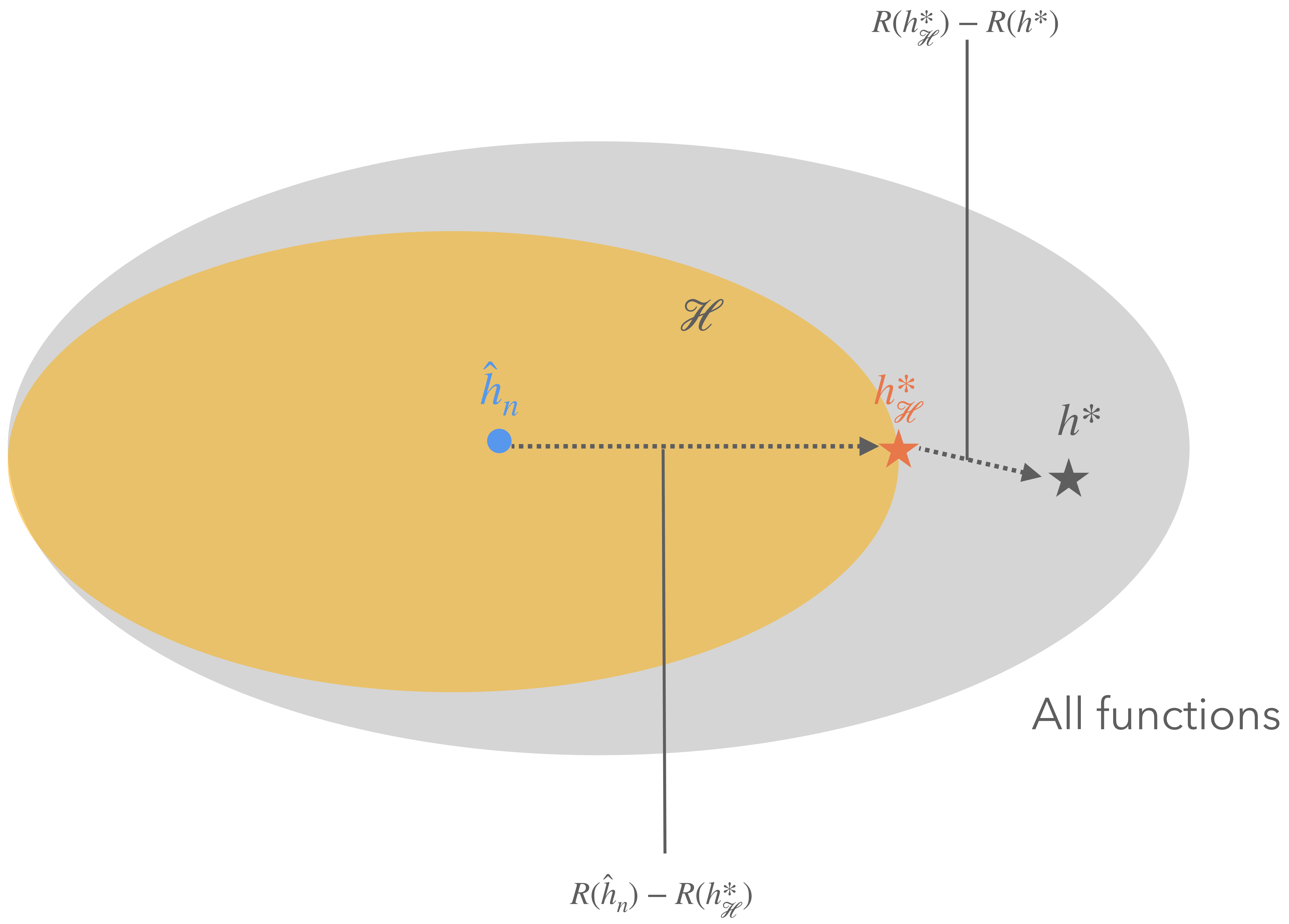

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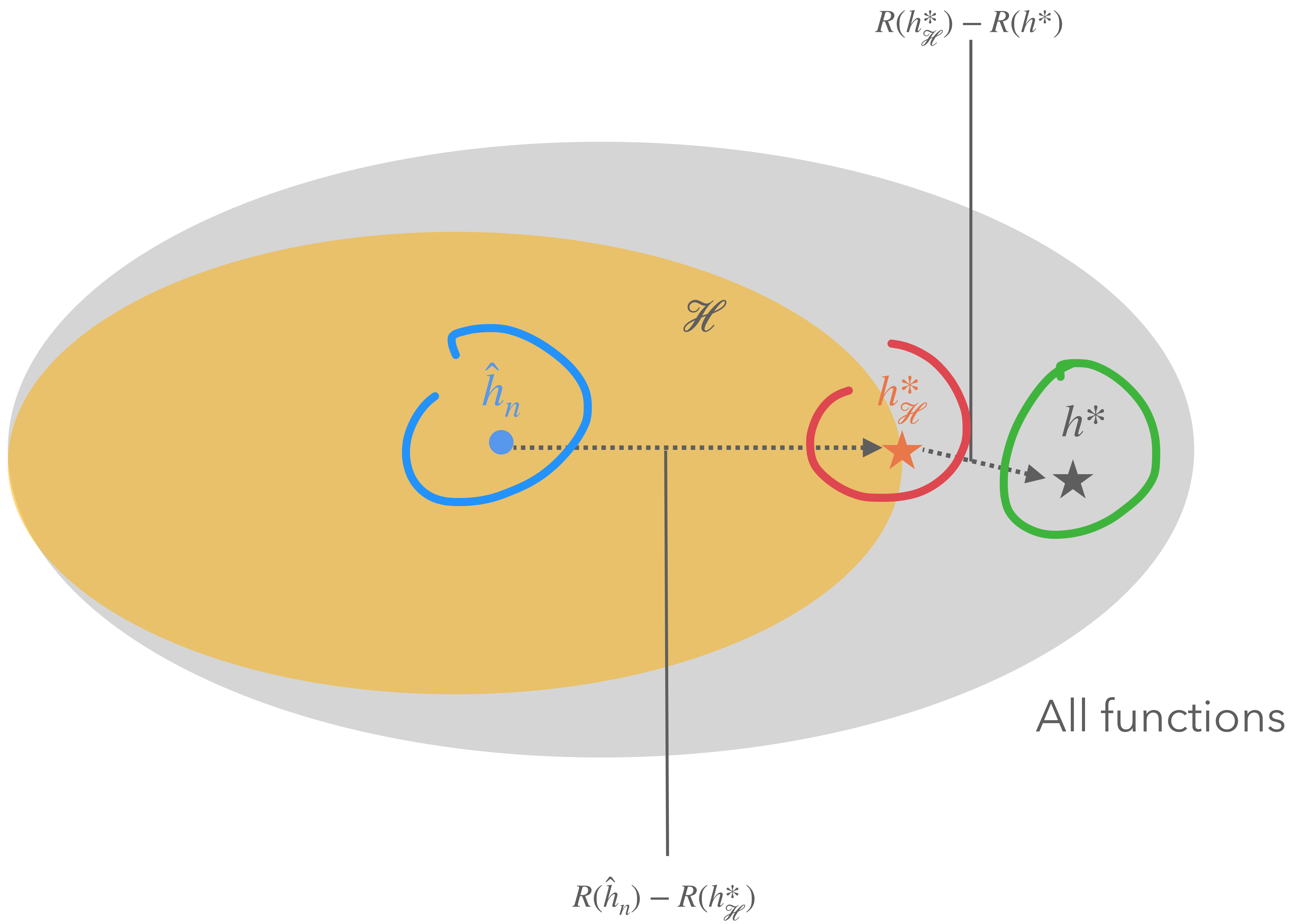

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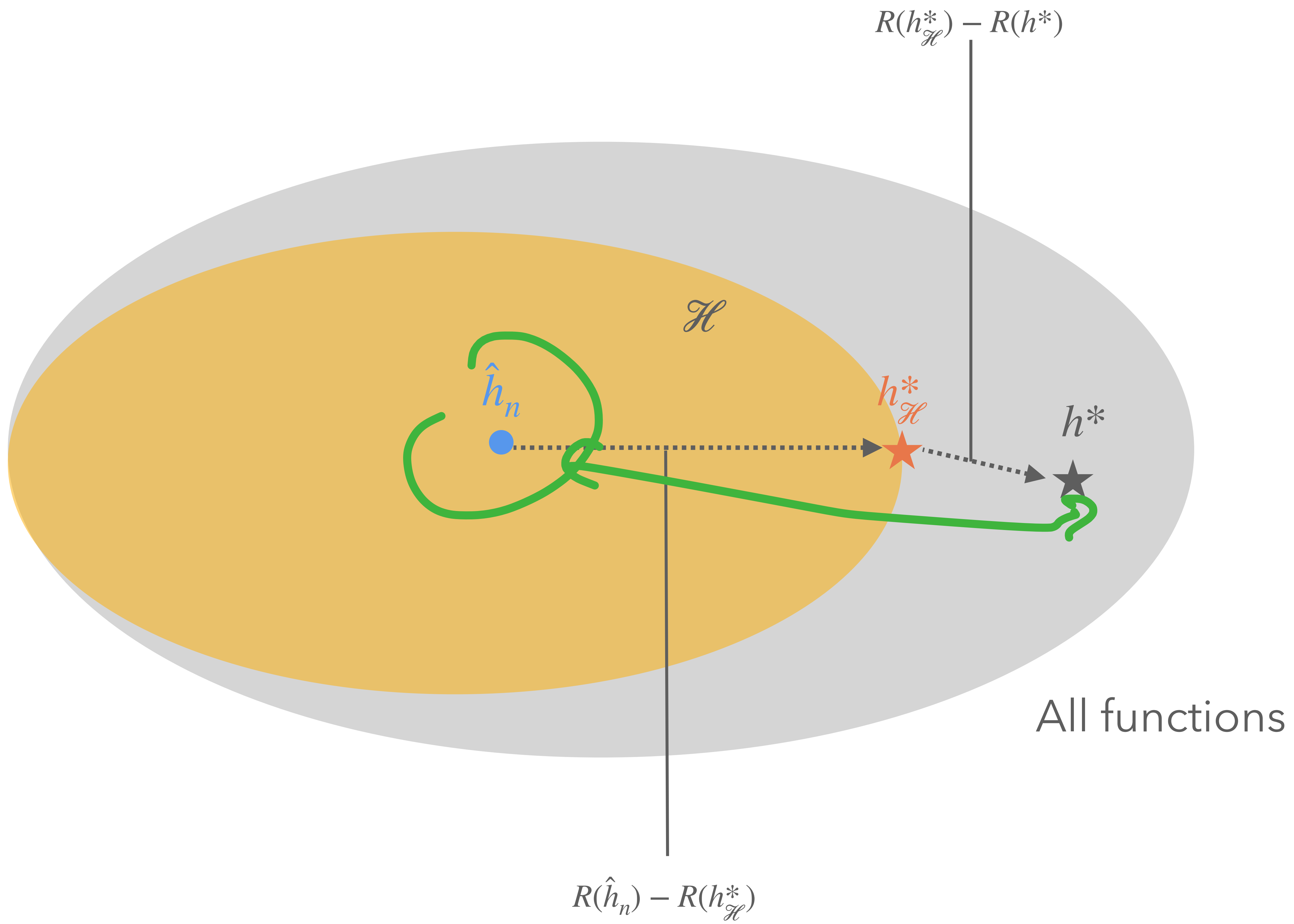
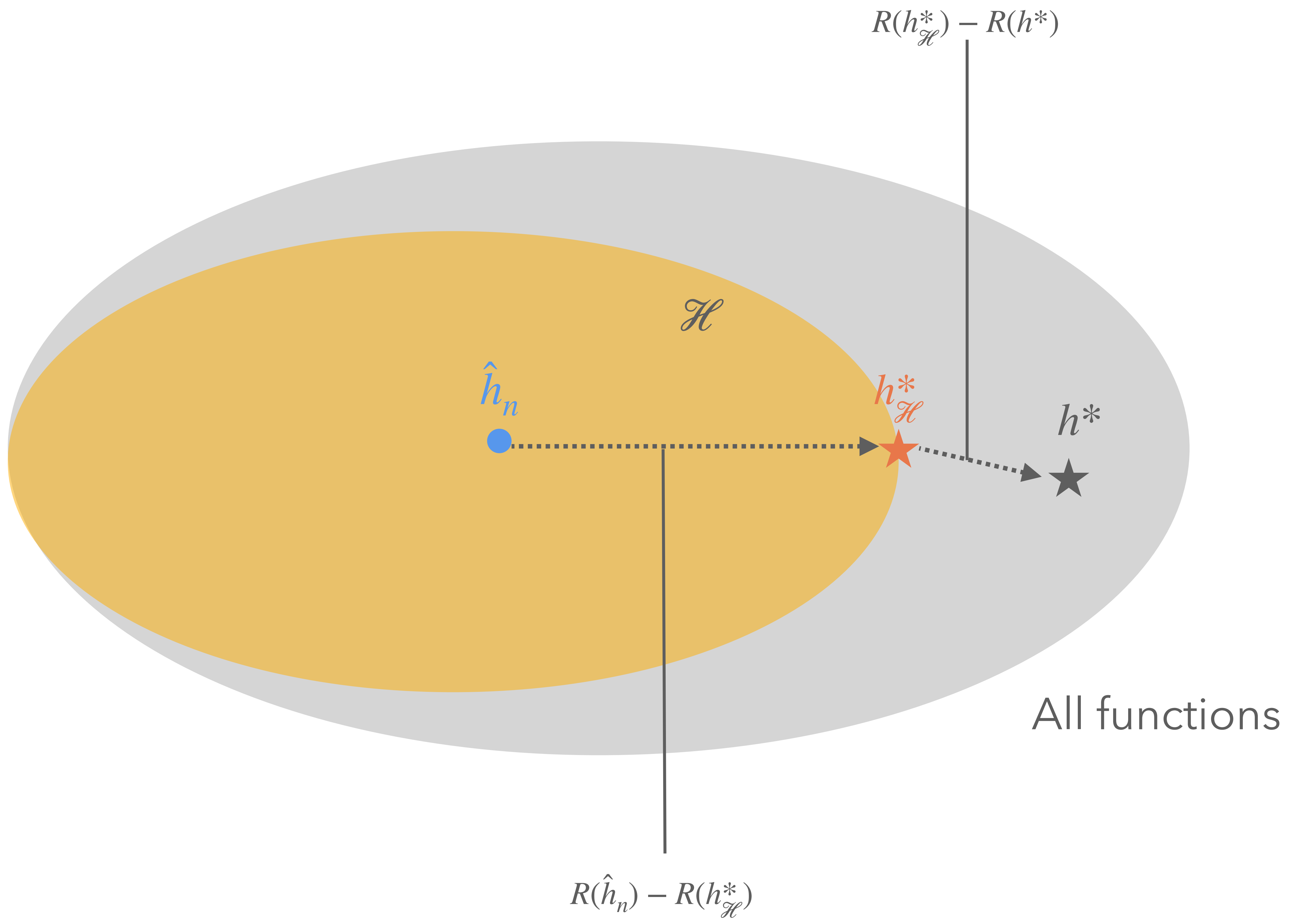


Excess Risk

Decomposition



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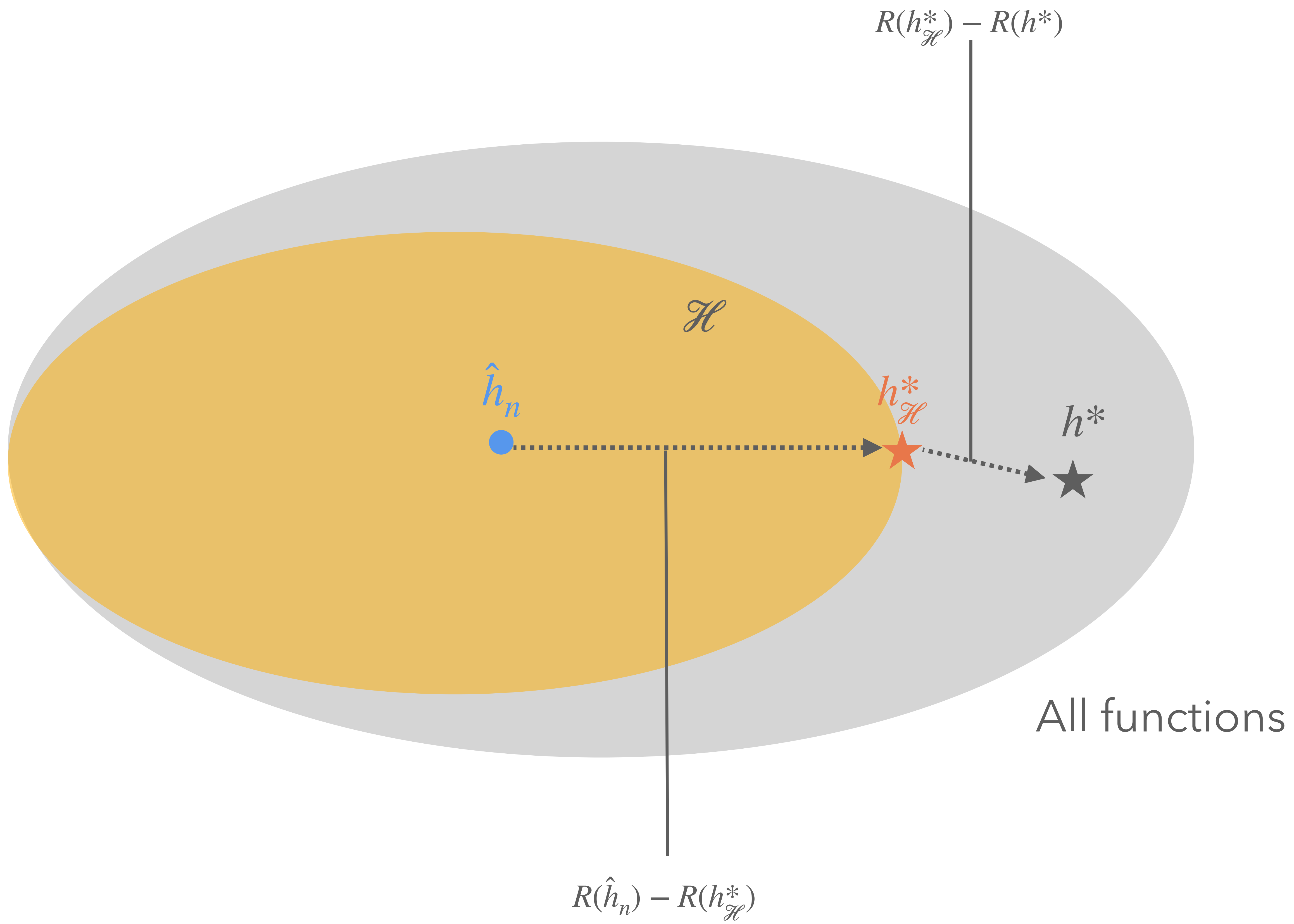

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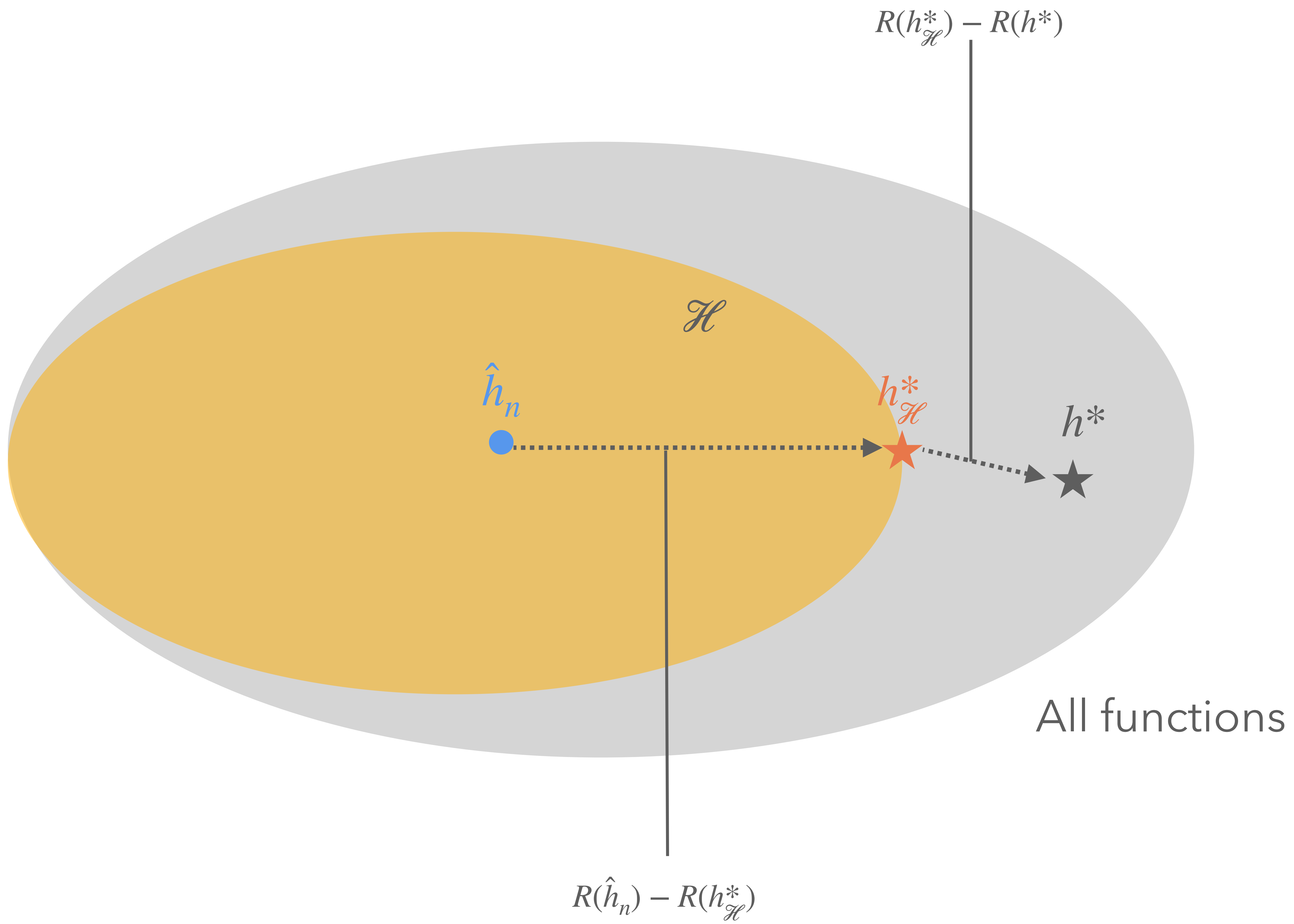

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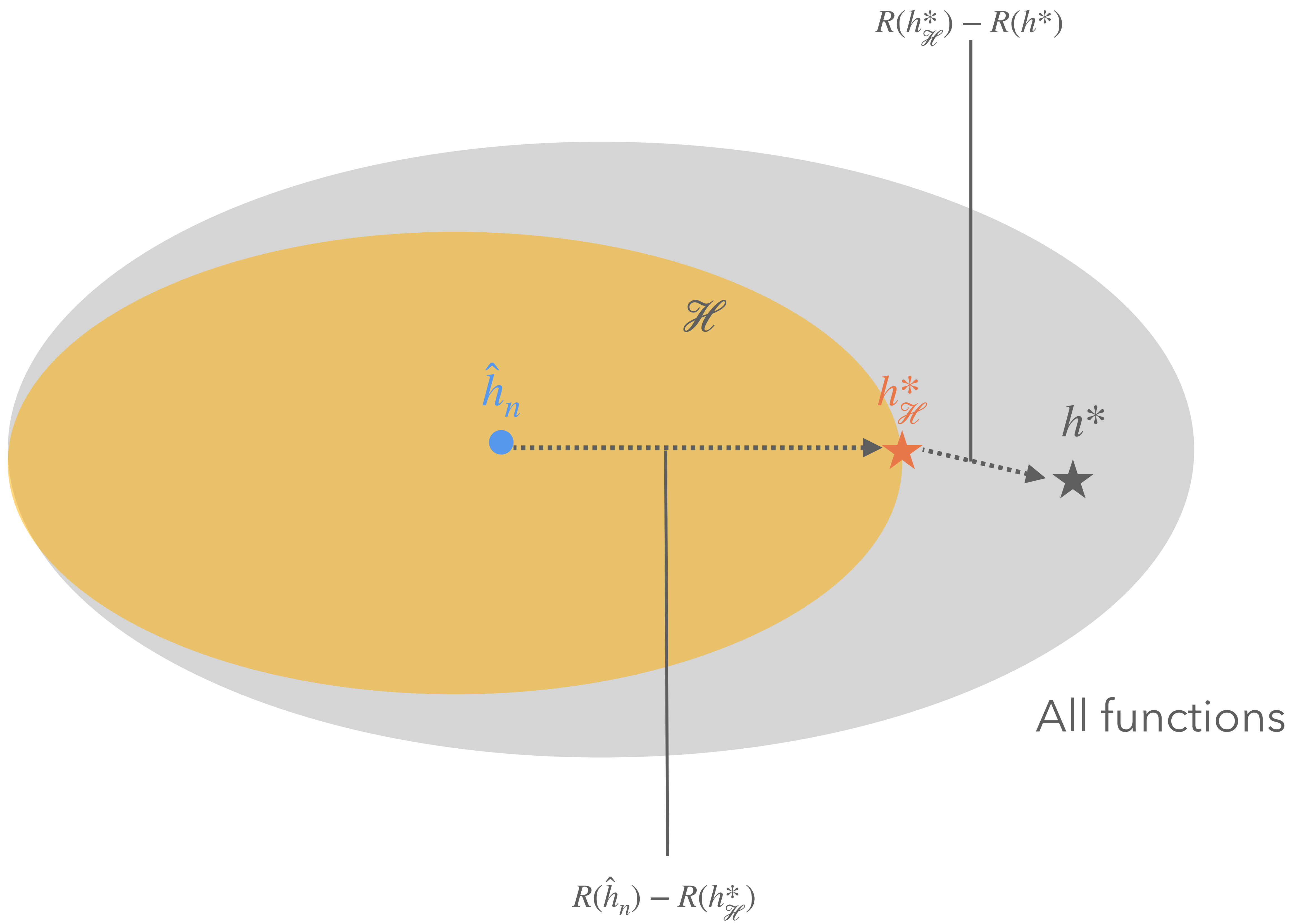

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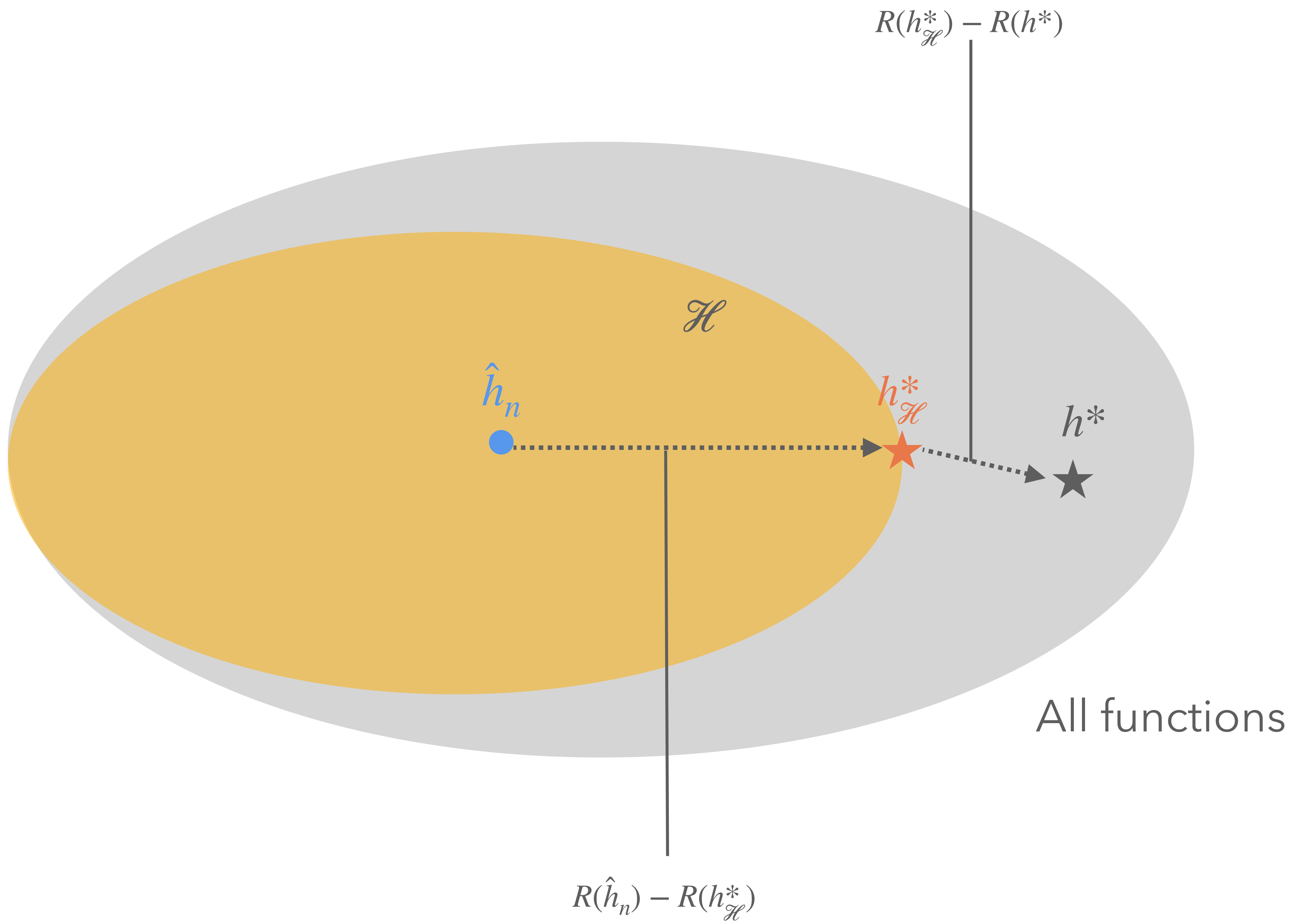

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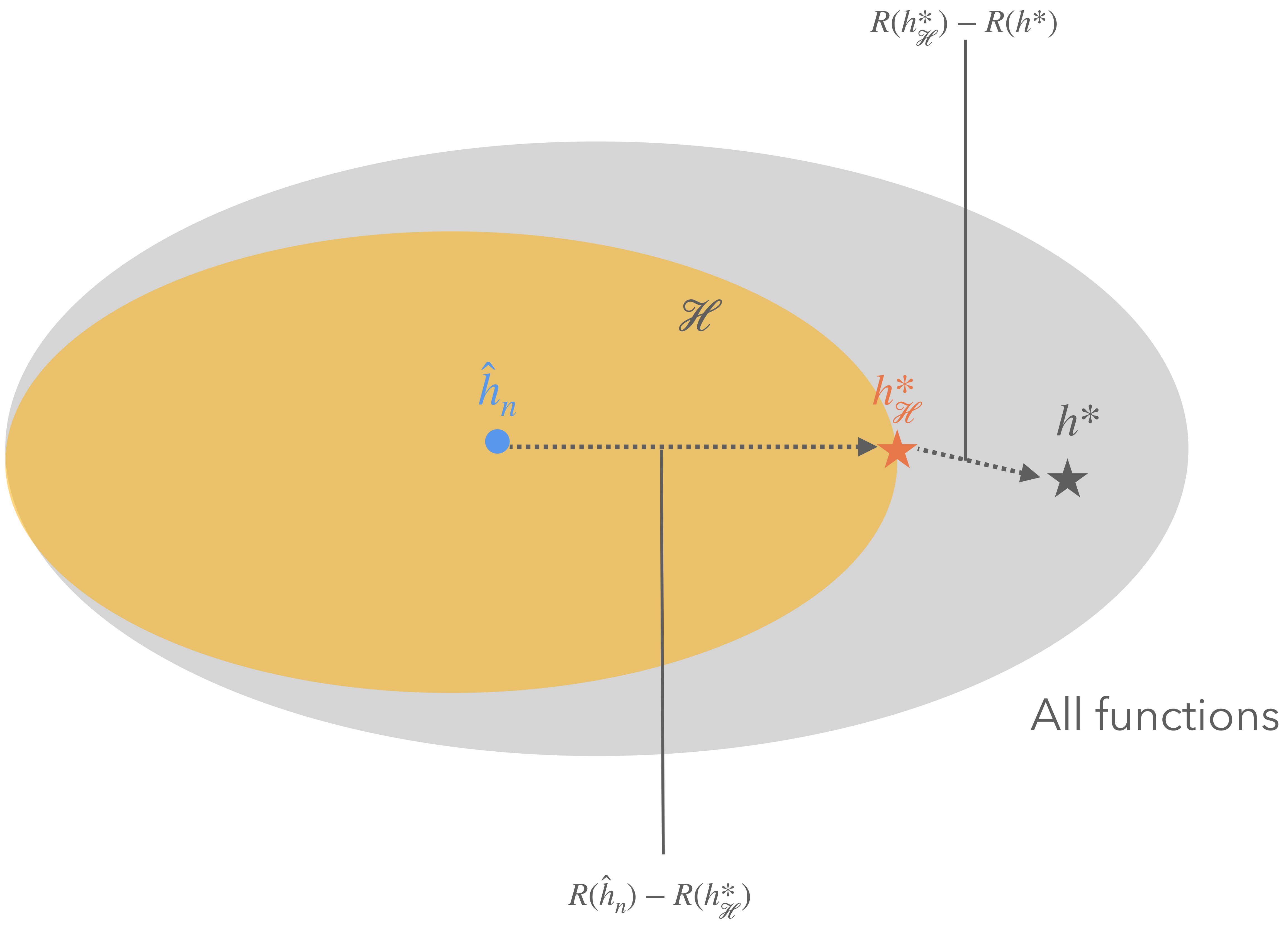
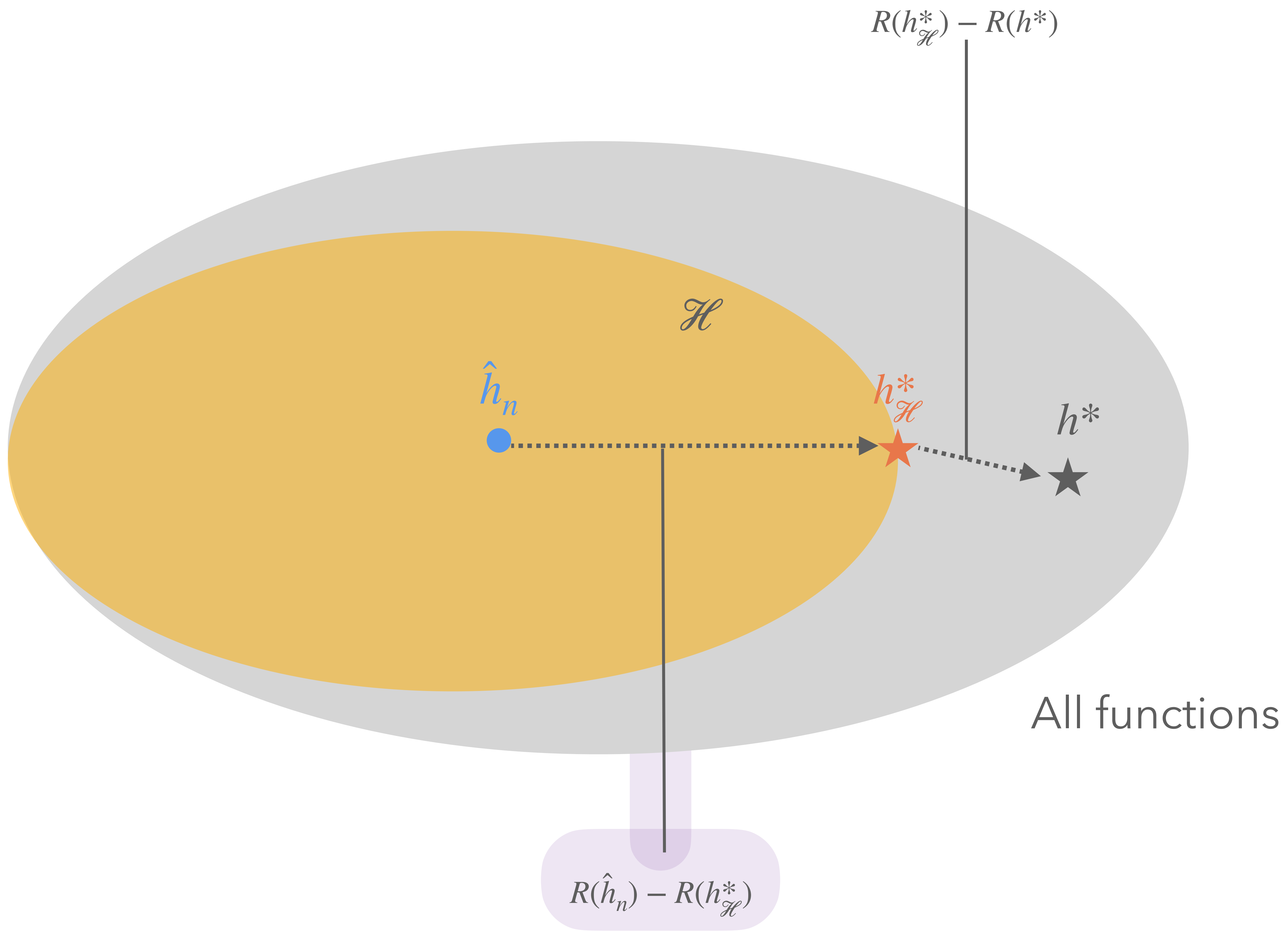
Estimation error is from using finite training as a proxy for risk (a generalization issue).

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



Estimation Error

Details

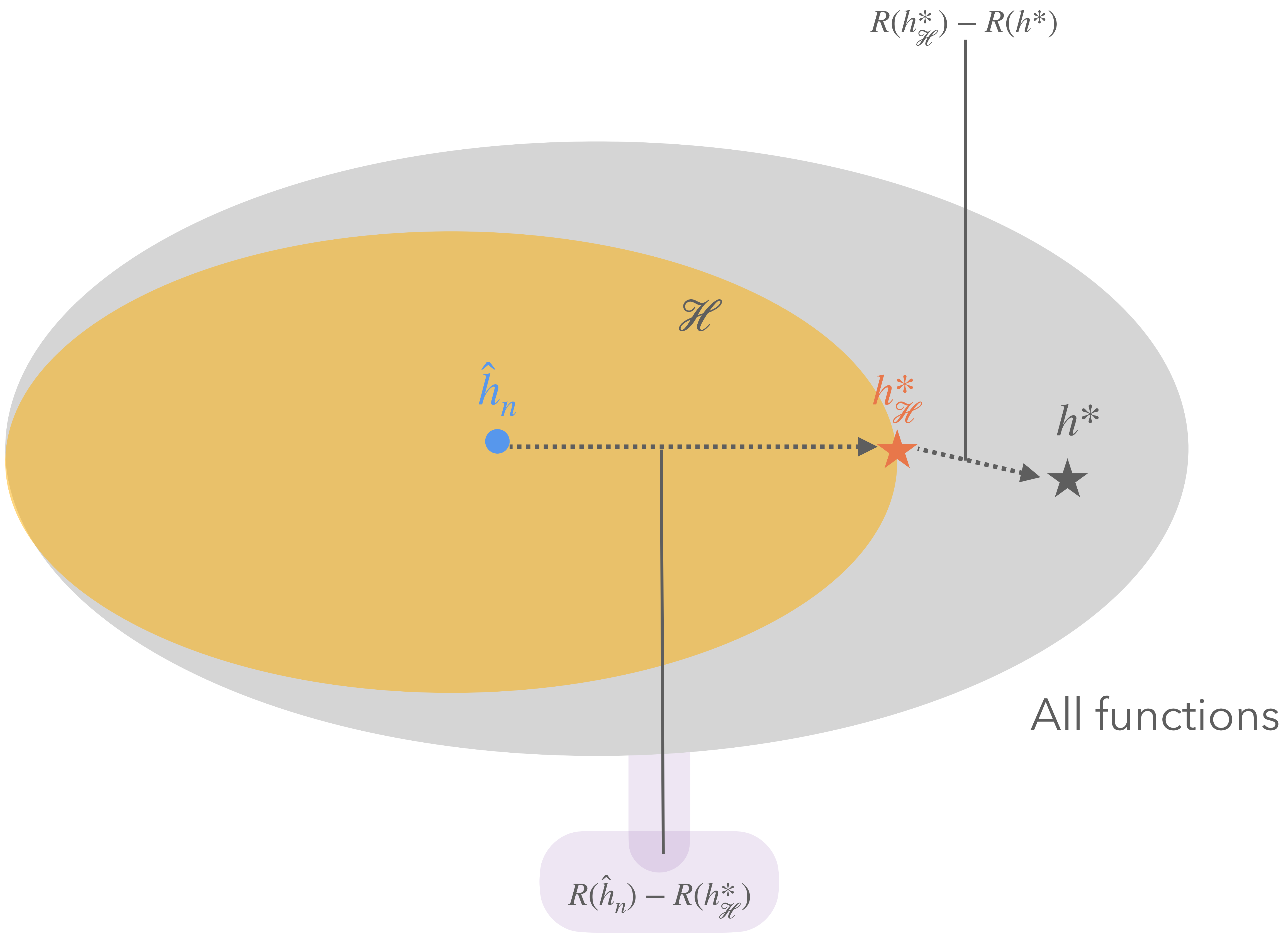


Estimation Error

Details

Function of random variables

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



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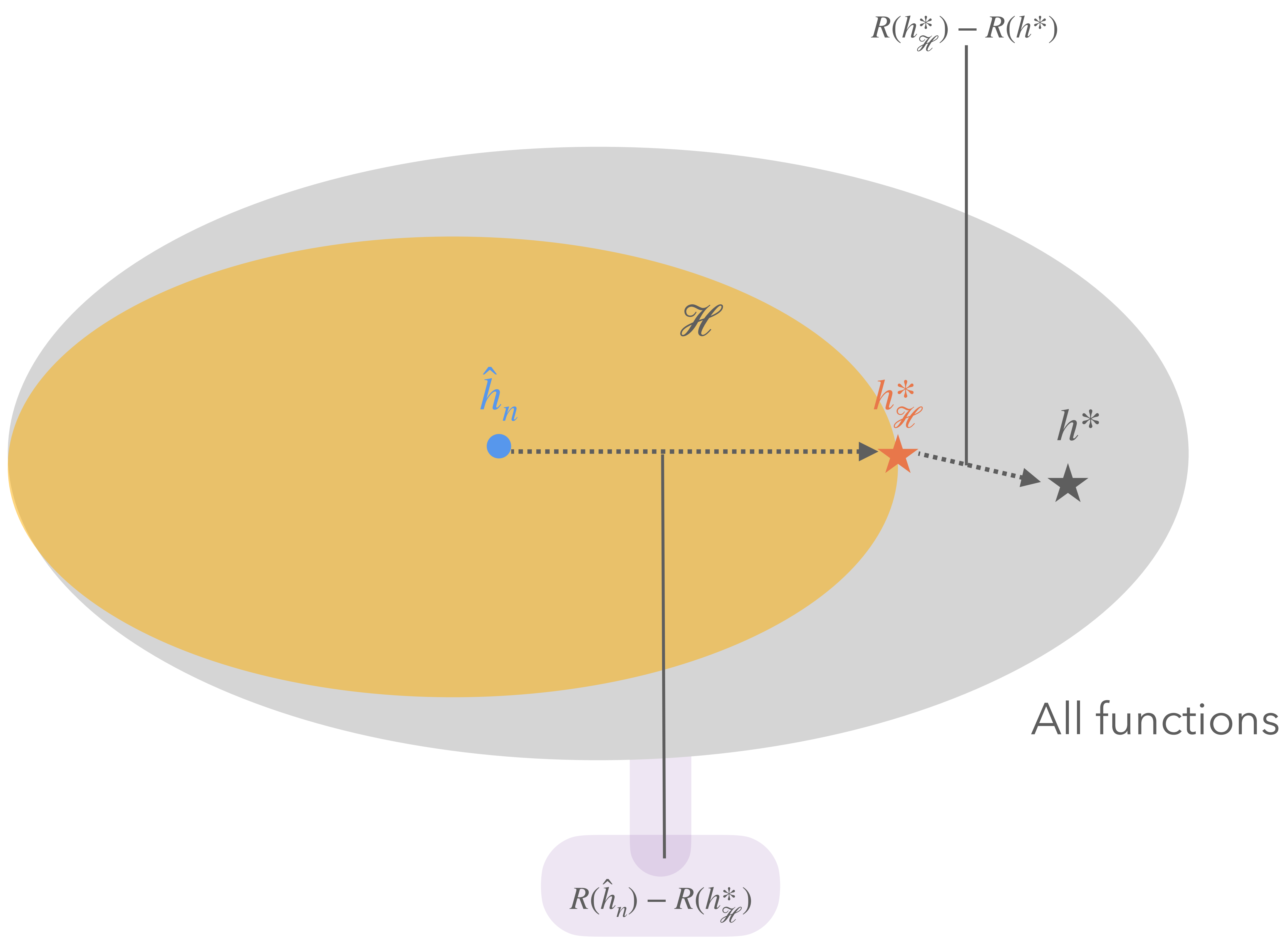

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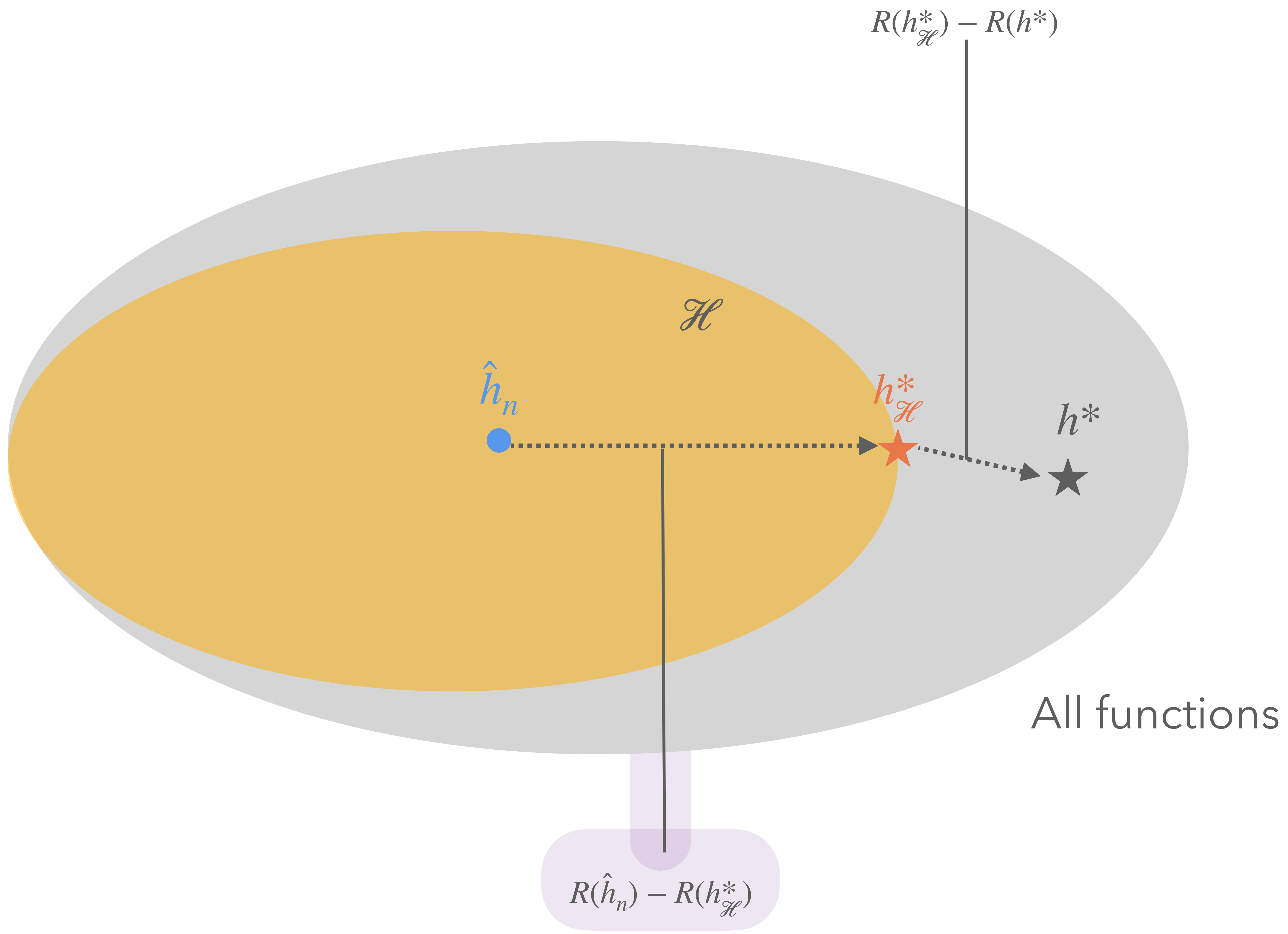

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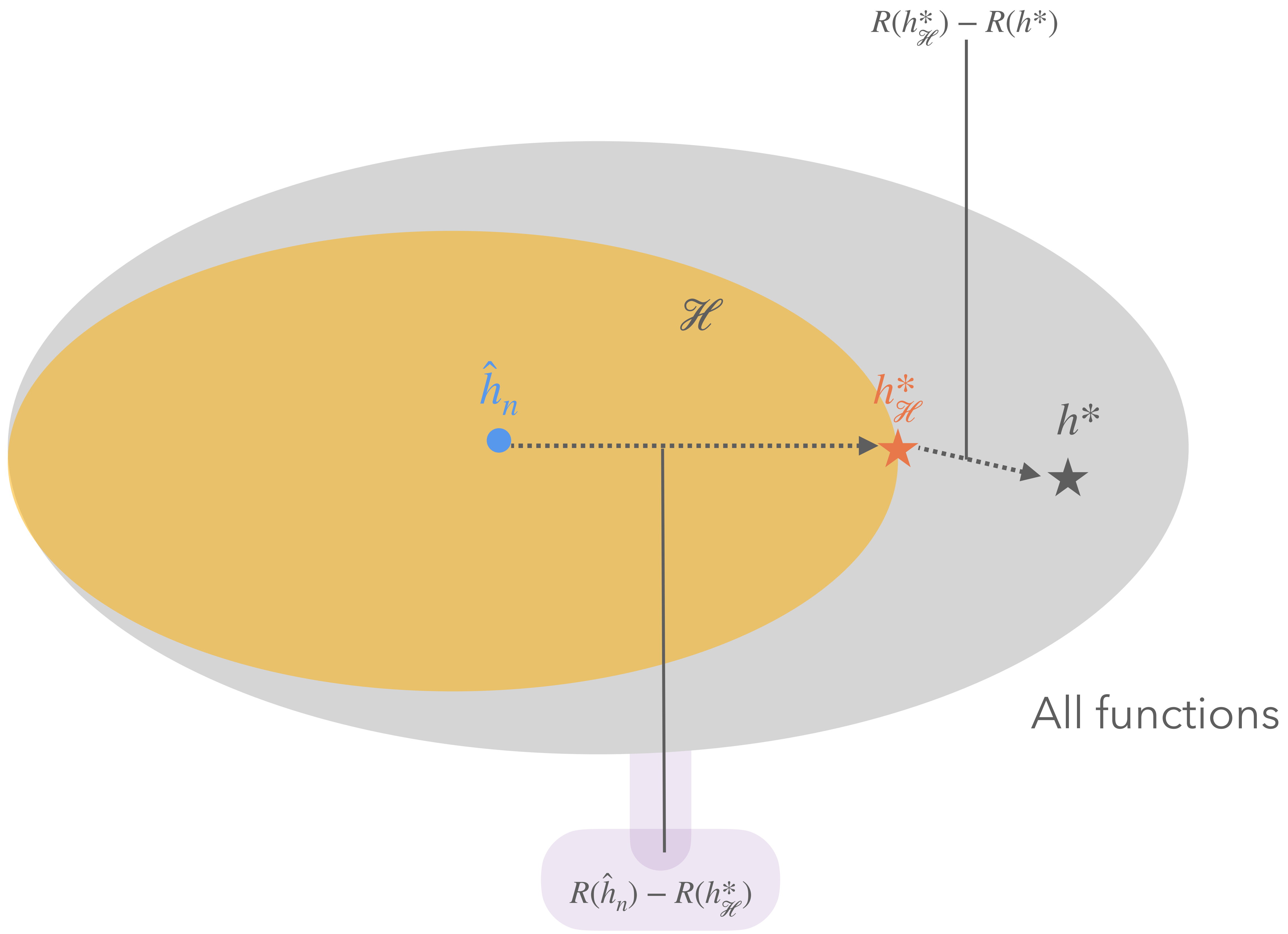

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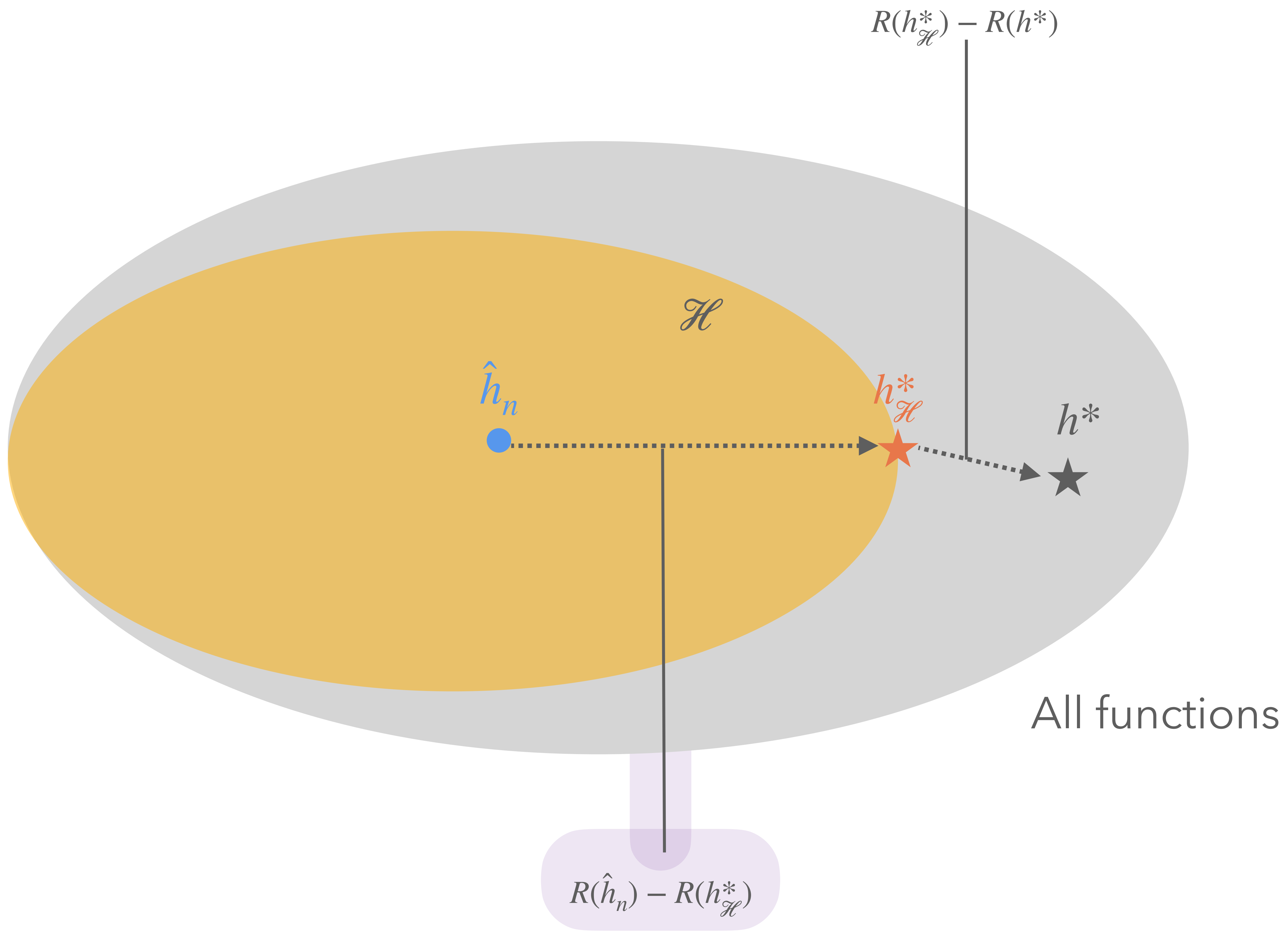
Very rough intuition: a "variance" term.



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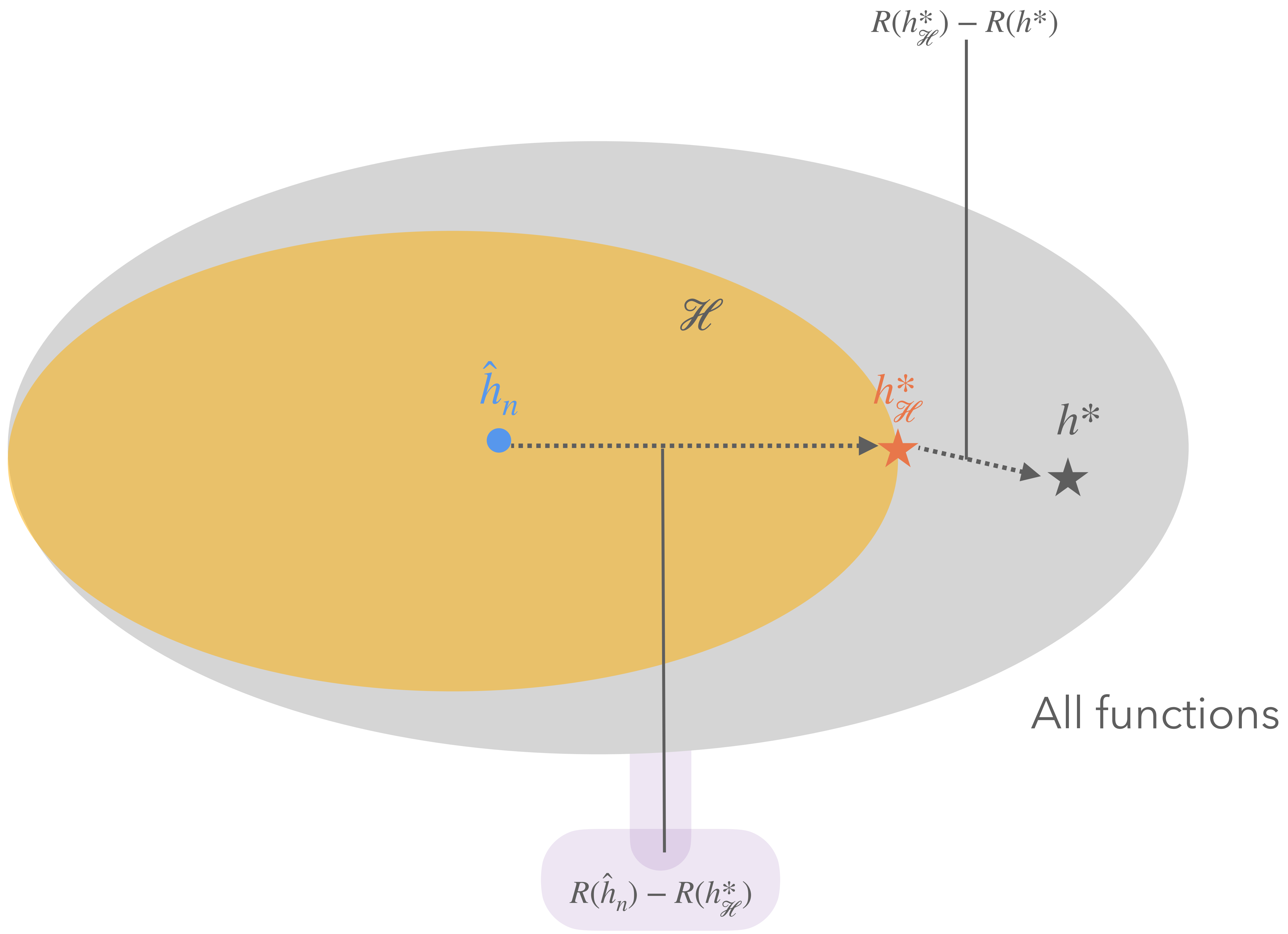
We expect that estimation error *increases* with *larger $\mathcal{H}$*.

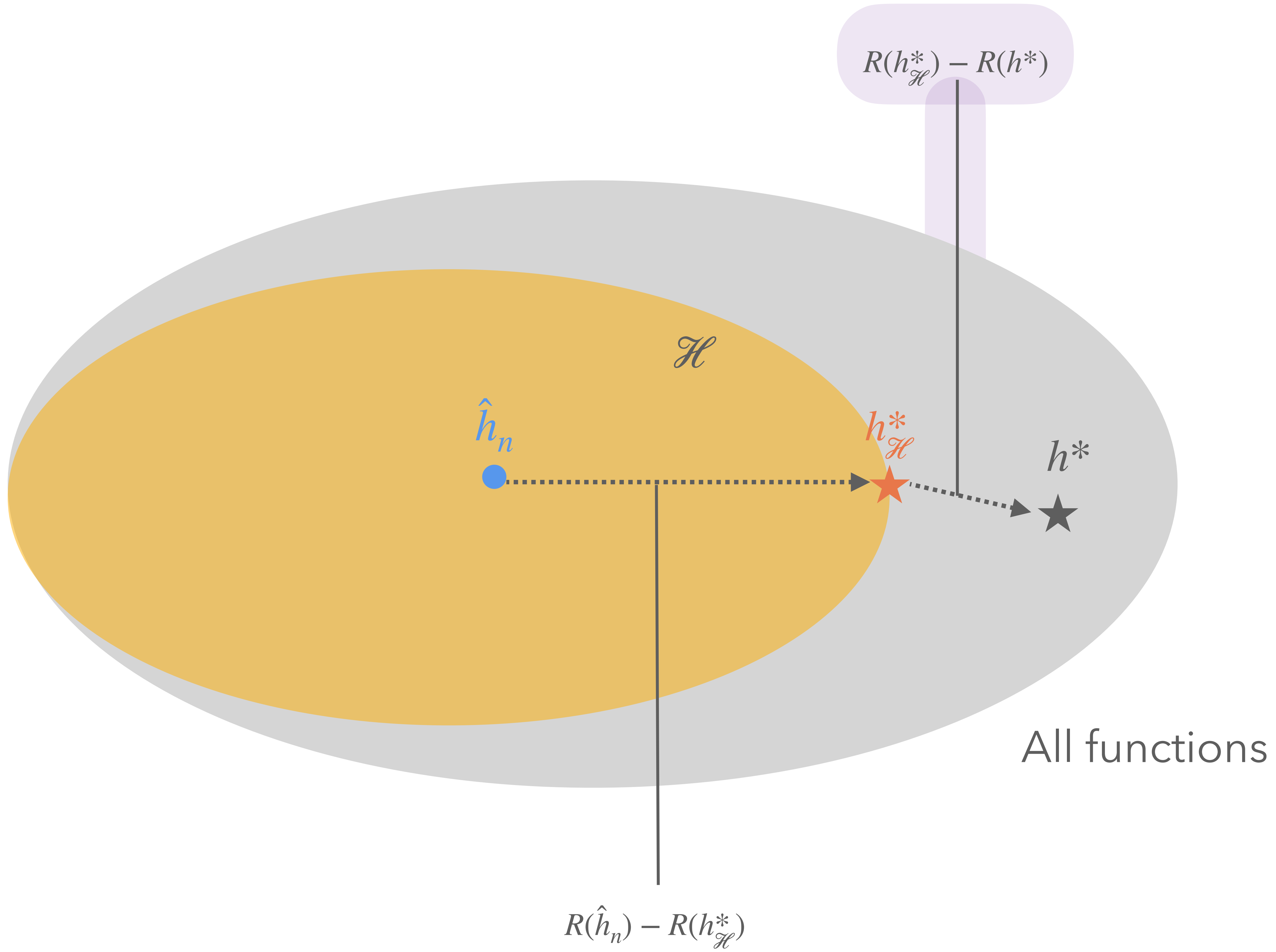
Very rough intuition: a "variance" term.



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

Approximation Error

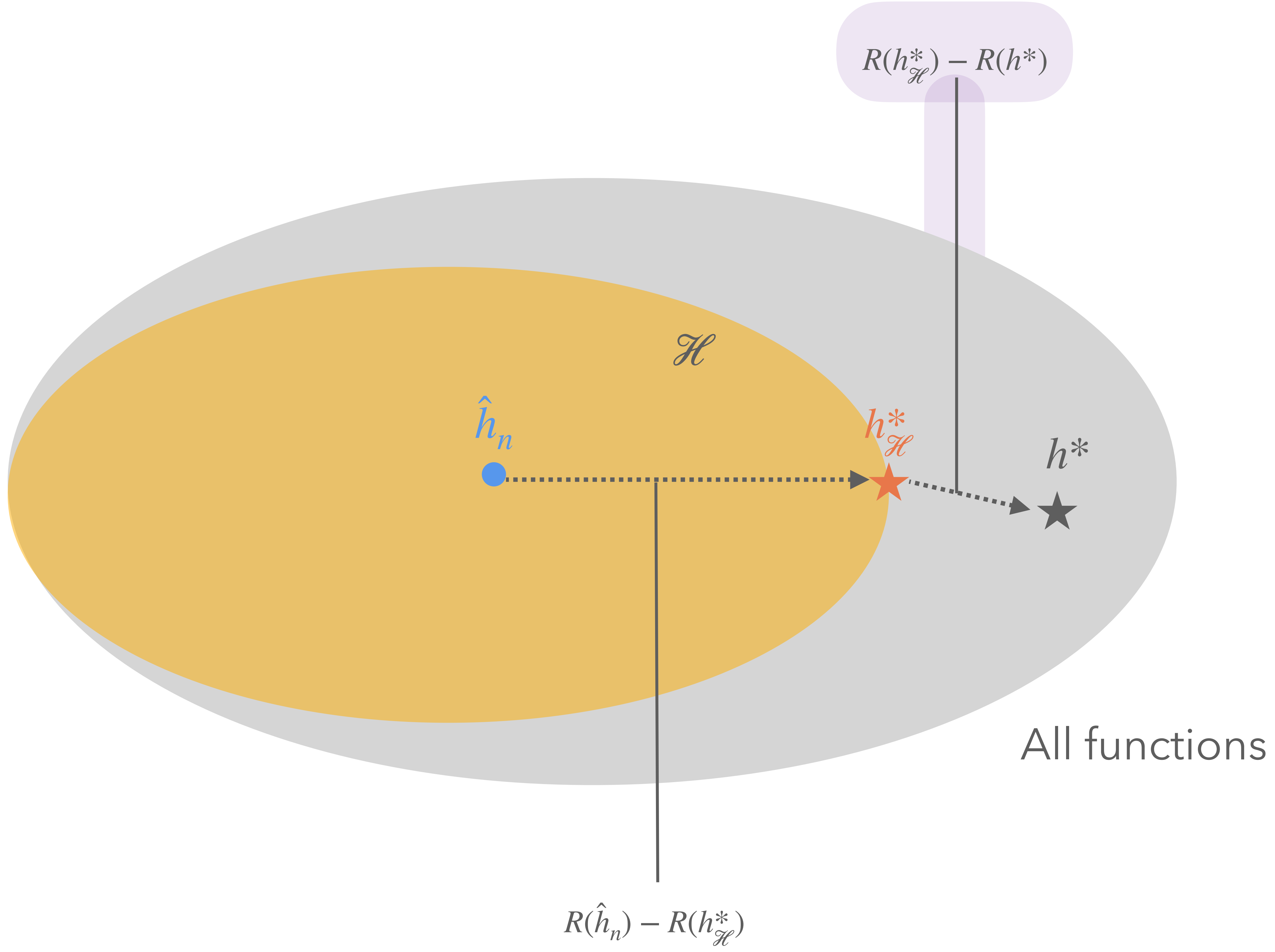
Details



Approximation Error

Details

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



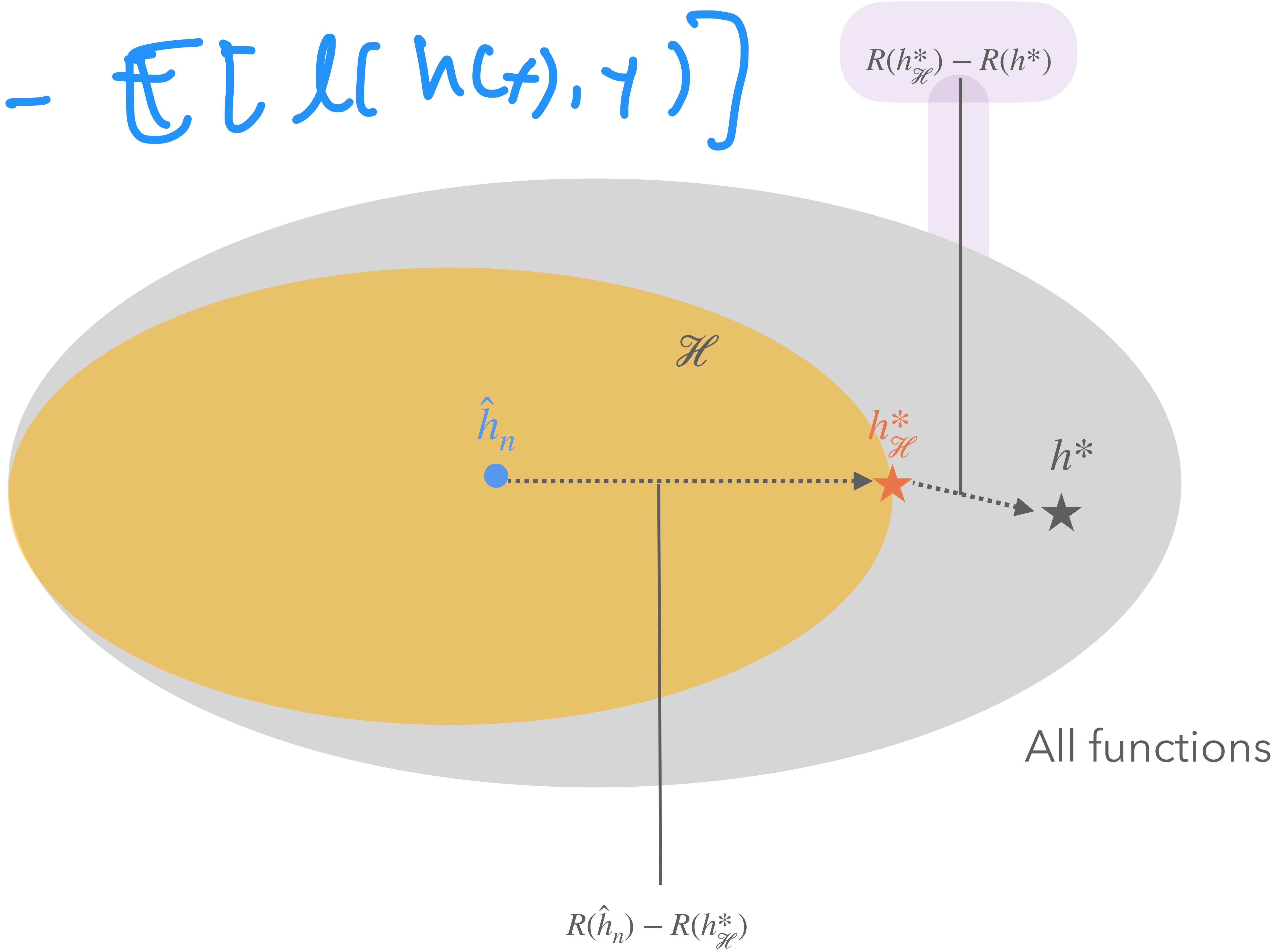
Approximation Error

Details

$\mathbb{E}[\ell(h^*(x), y)] - \mathbb{E}[\ell(h(x), y)]$

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)?



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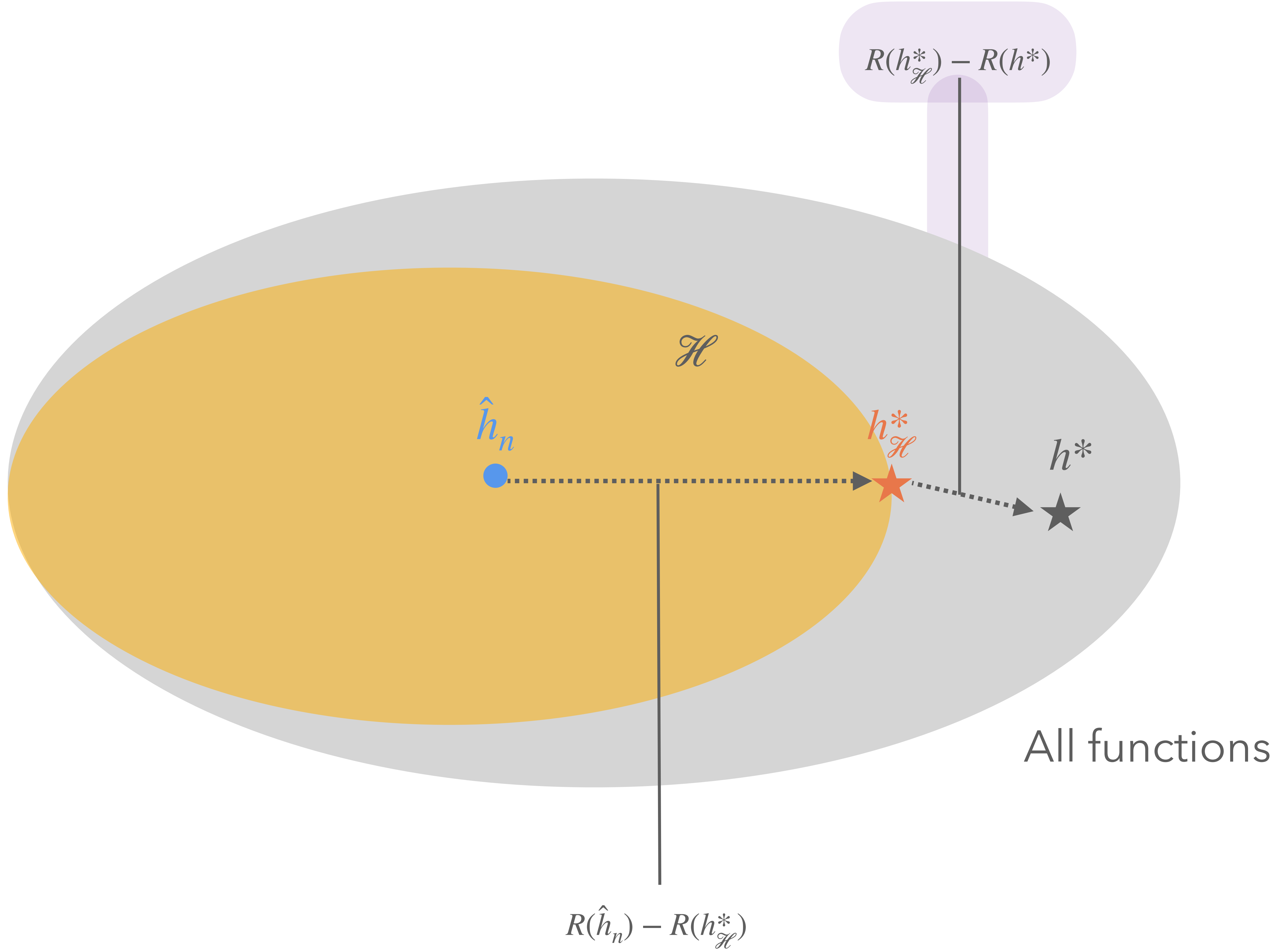
Typically, approximation error *<u>decreases</u>* with *<u>larger $\mathcal{H}$</u>*.



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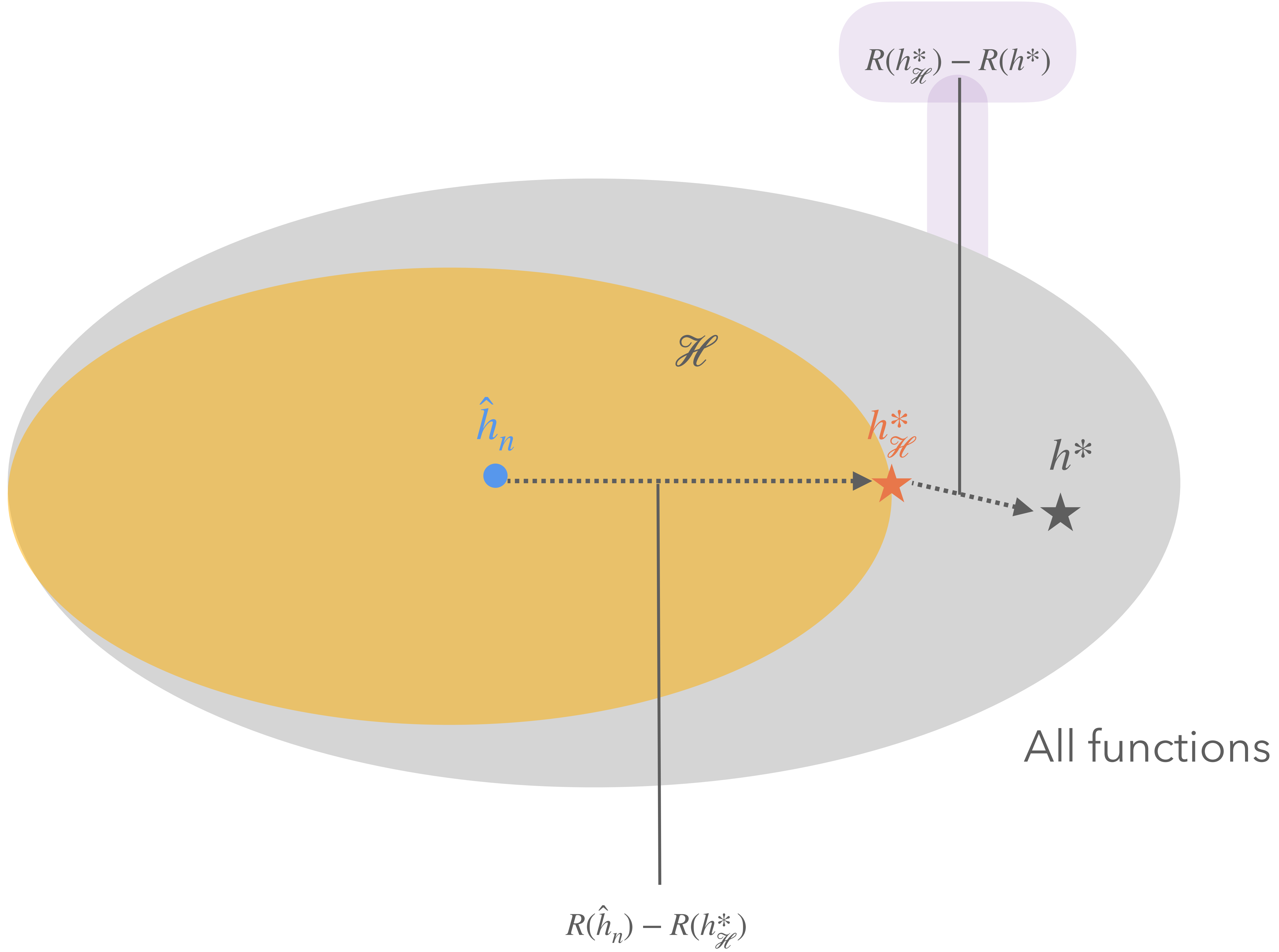
Details

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* $\mathcal{H}$.

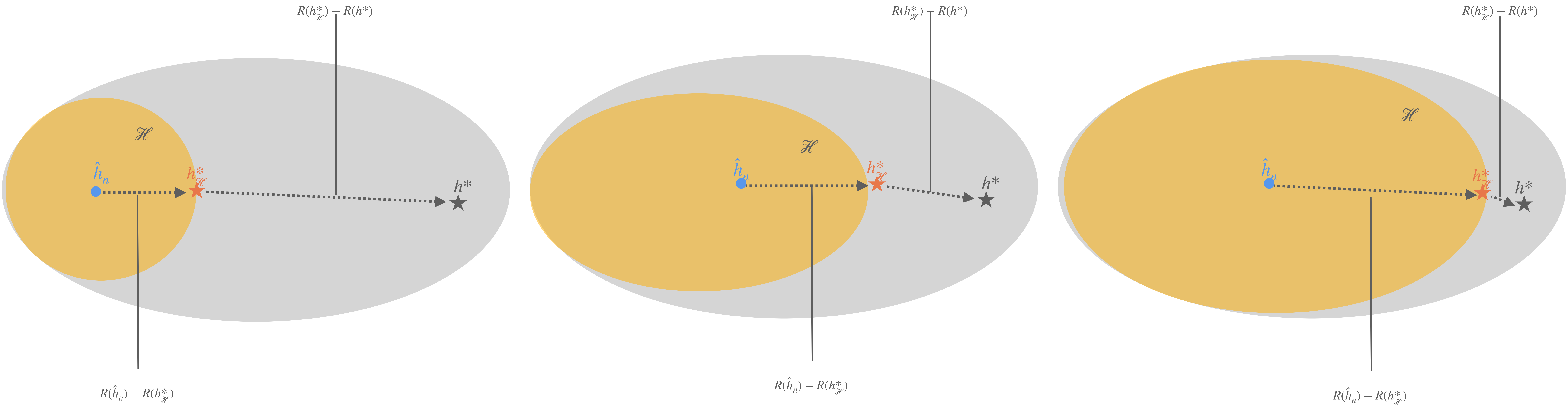
Very rough intuition: a "bias" term.



Excess Risk

Intuition: Size of $\mathscr{H}$

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



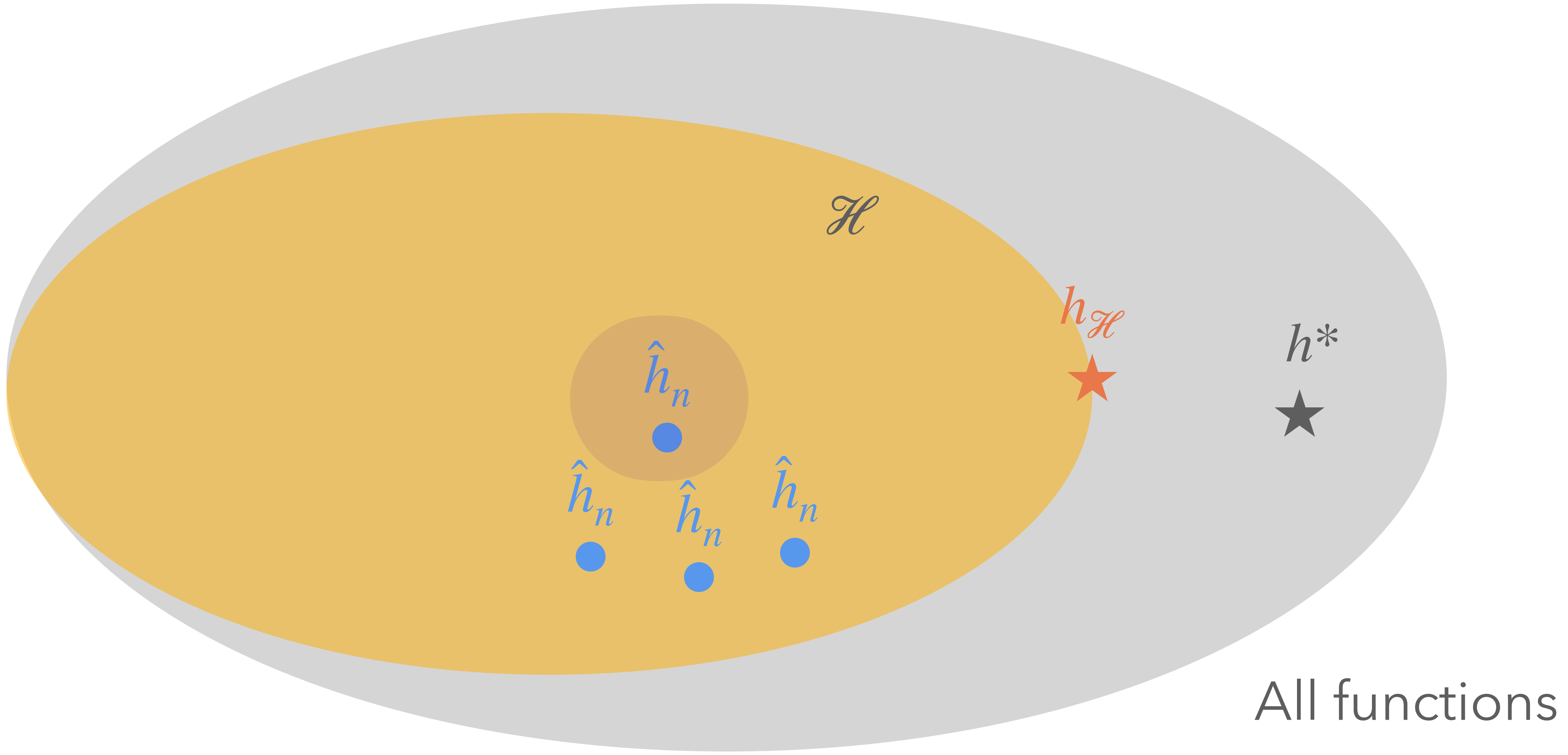
Optimization Error

Details

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

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

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



Optimization Error

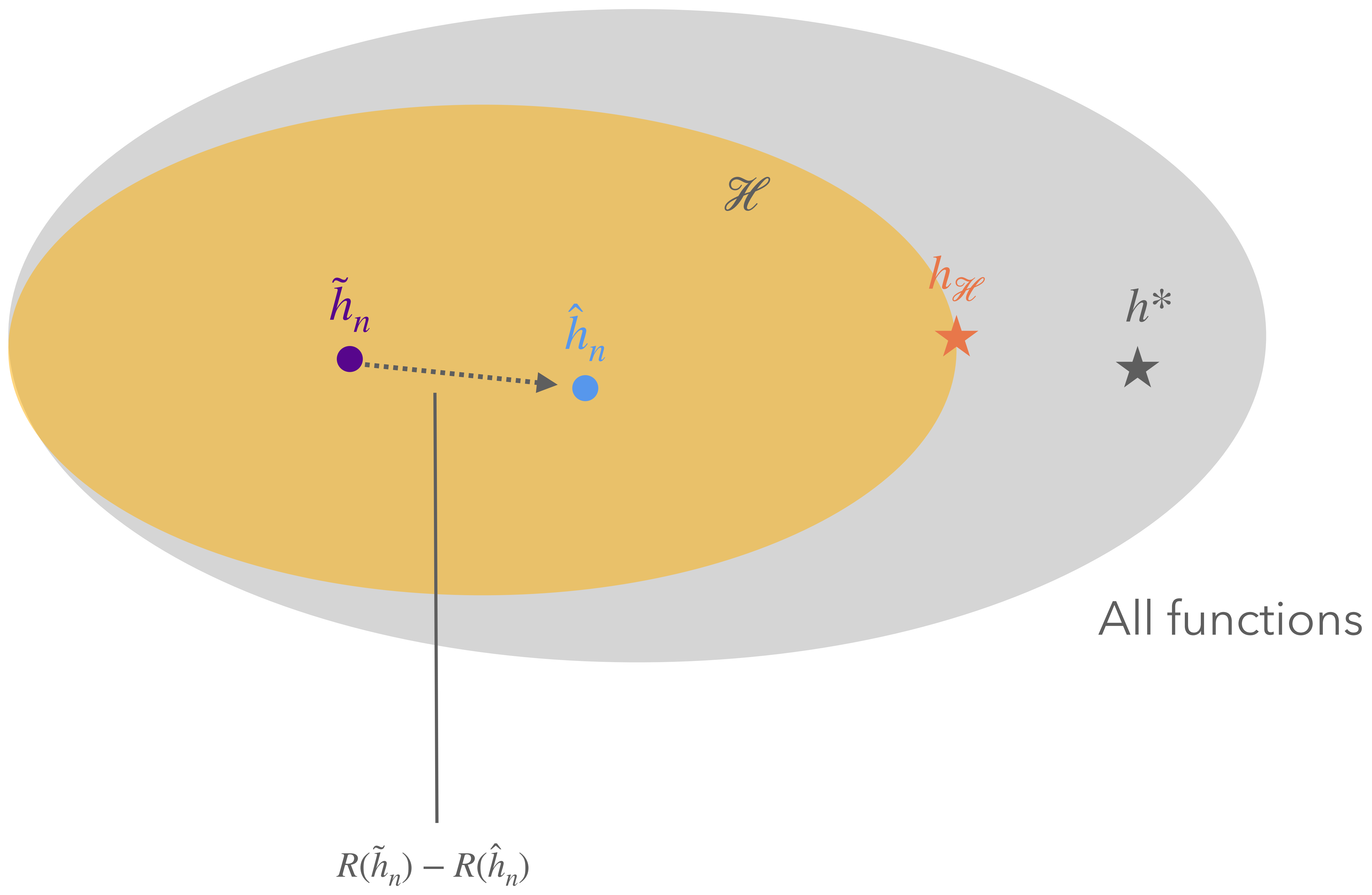
Details

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

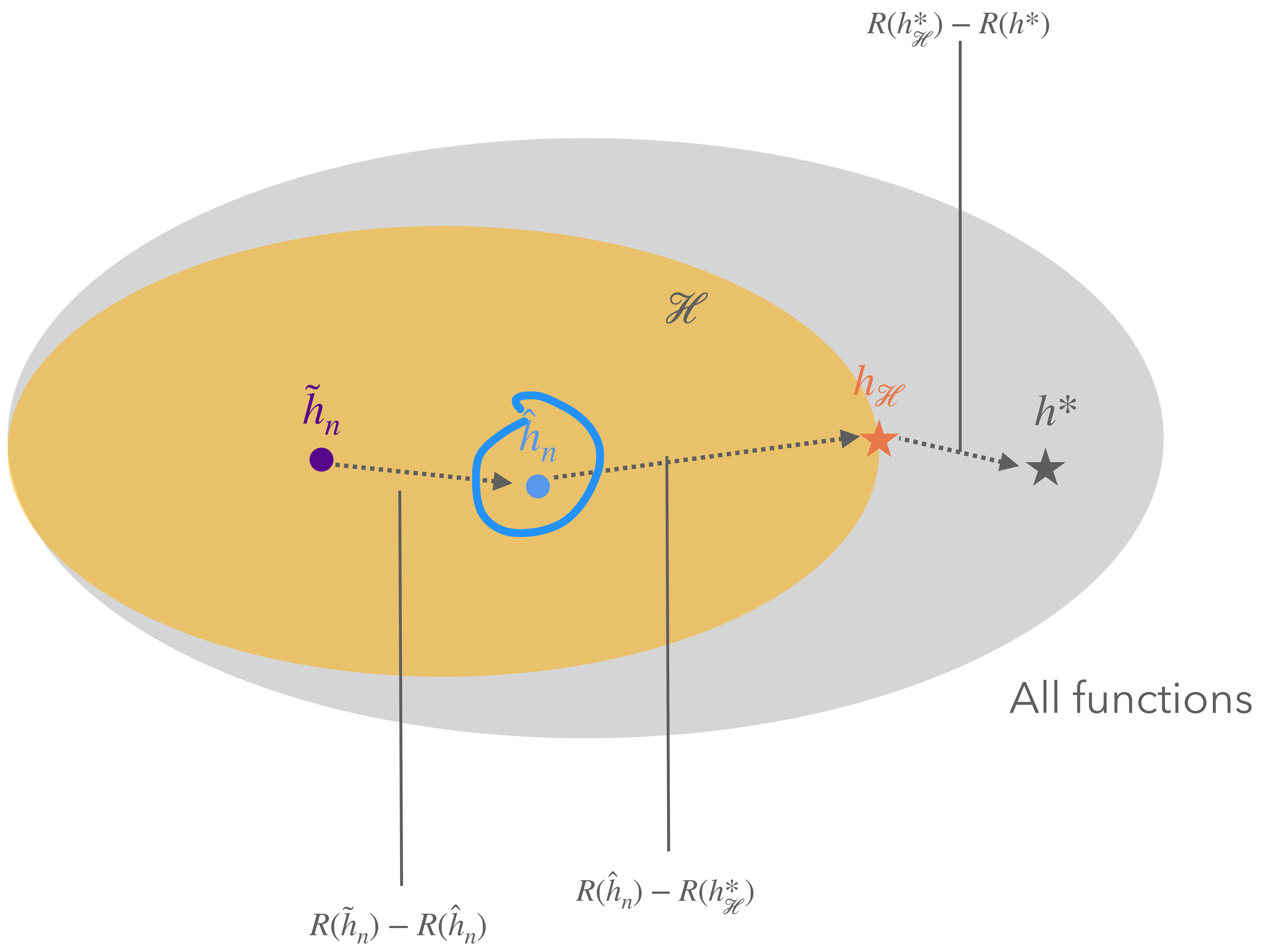
Full Decomposition

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

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

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

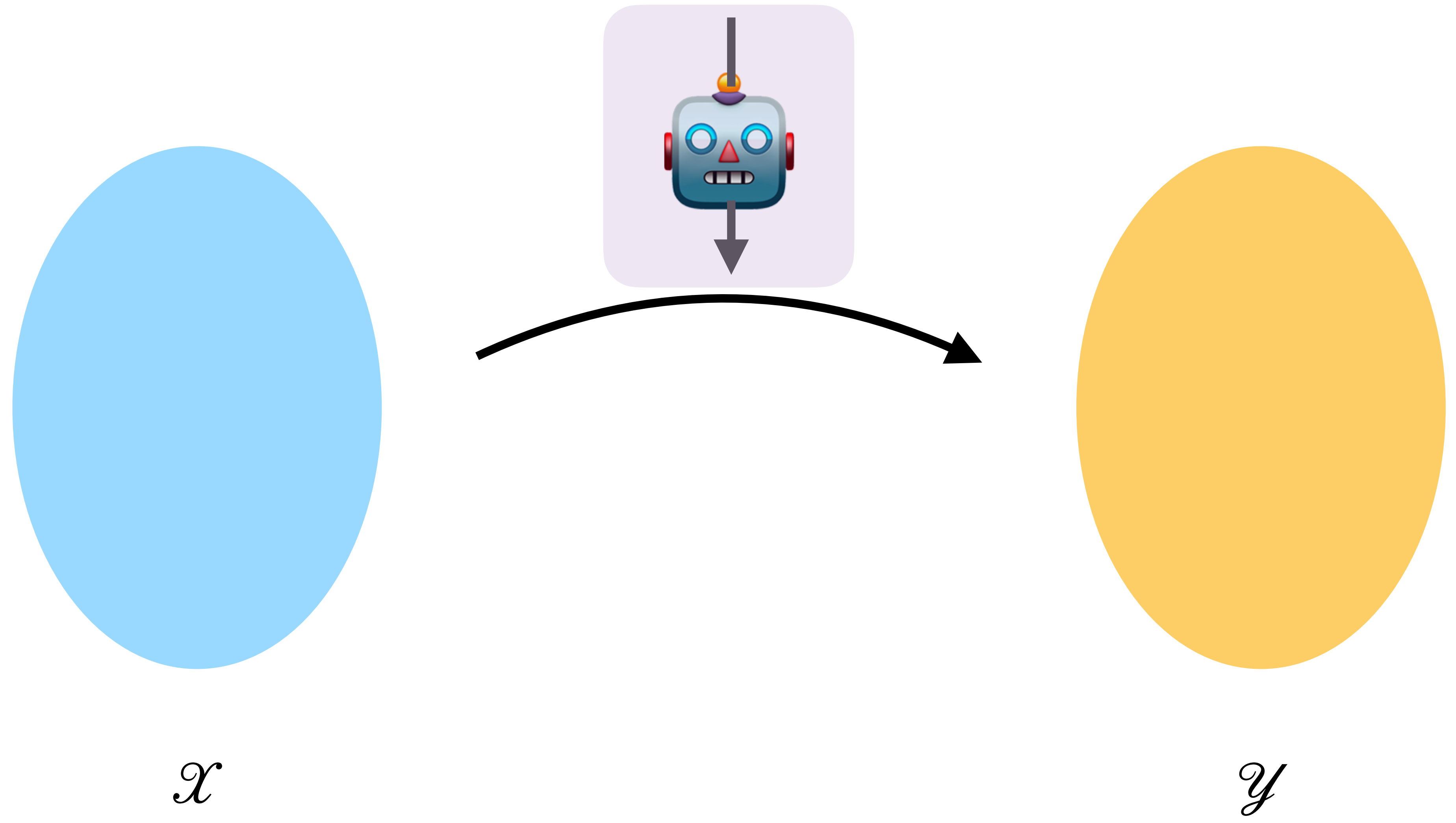
$$\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathscr{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathscr{H}}) - R(h^*)}_{\text{approx. error}}$$



Supervised Learning

Basic Pipeline

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



Supervised Learning

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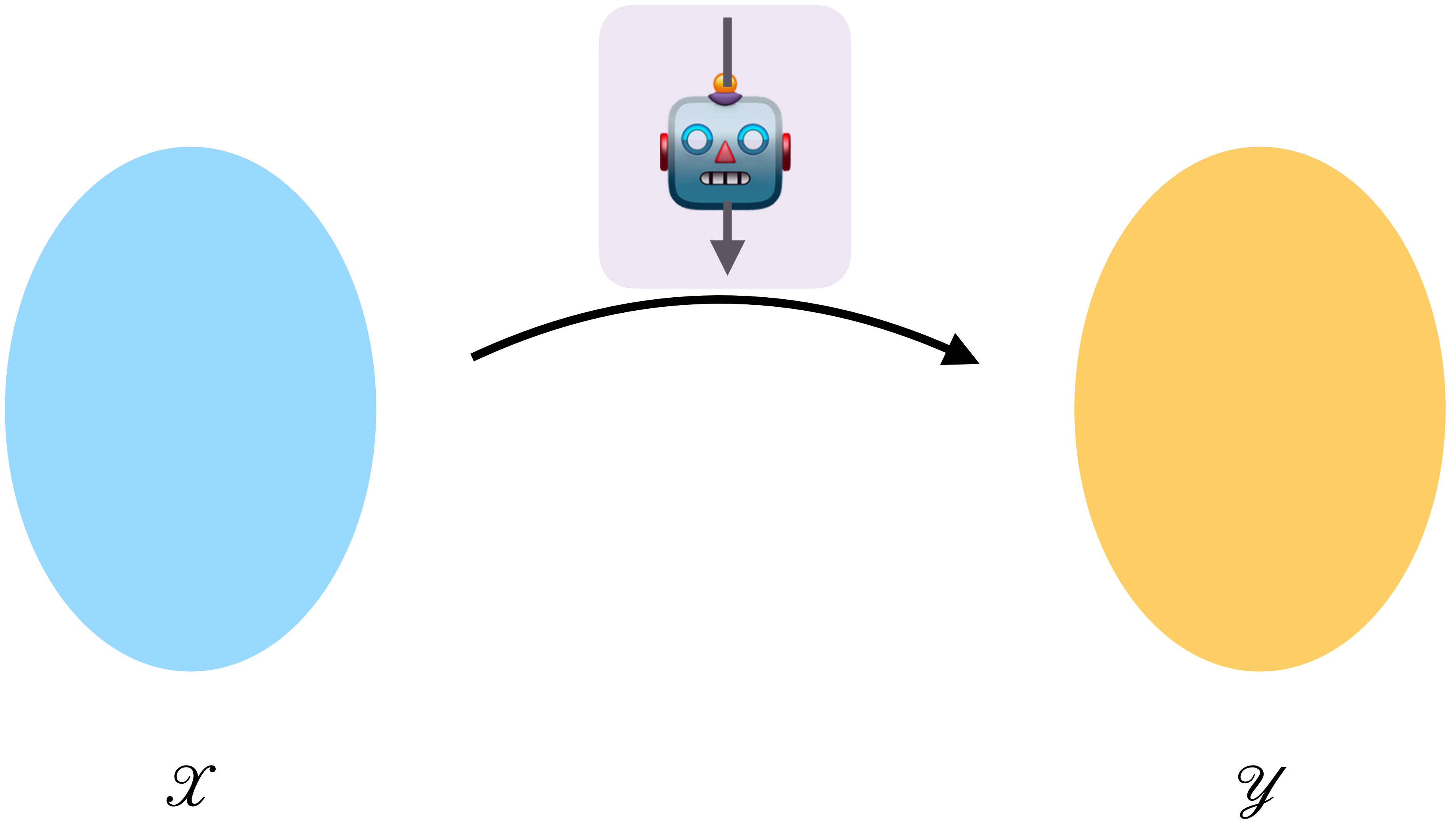

Supervised Learning

Basic Pipeline

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

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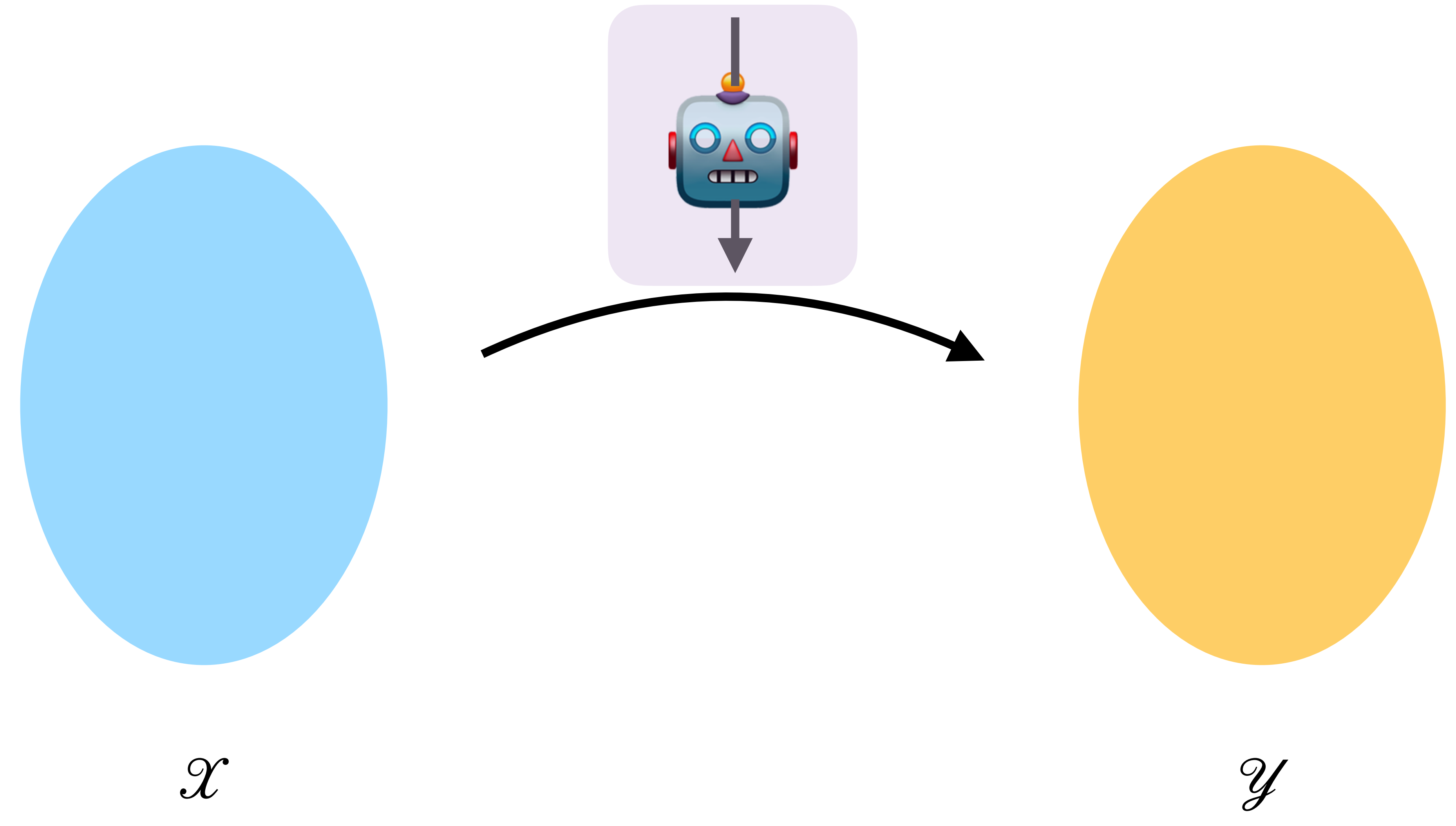

Supervised Learning

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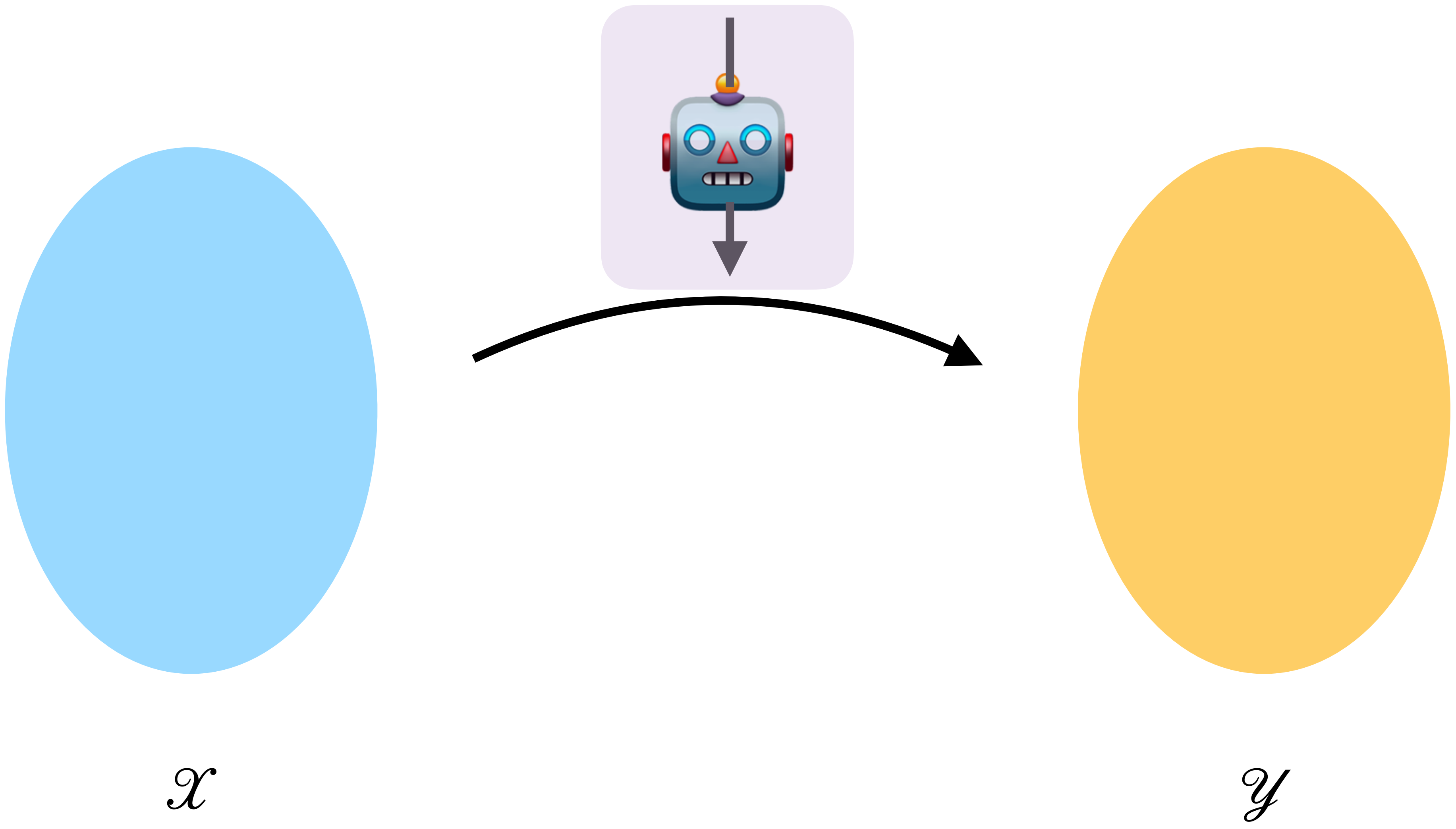

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4. The hypothesis predicts on new, unseen data which we hope it does well on, under a notion of loss.

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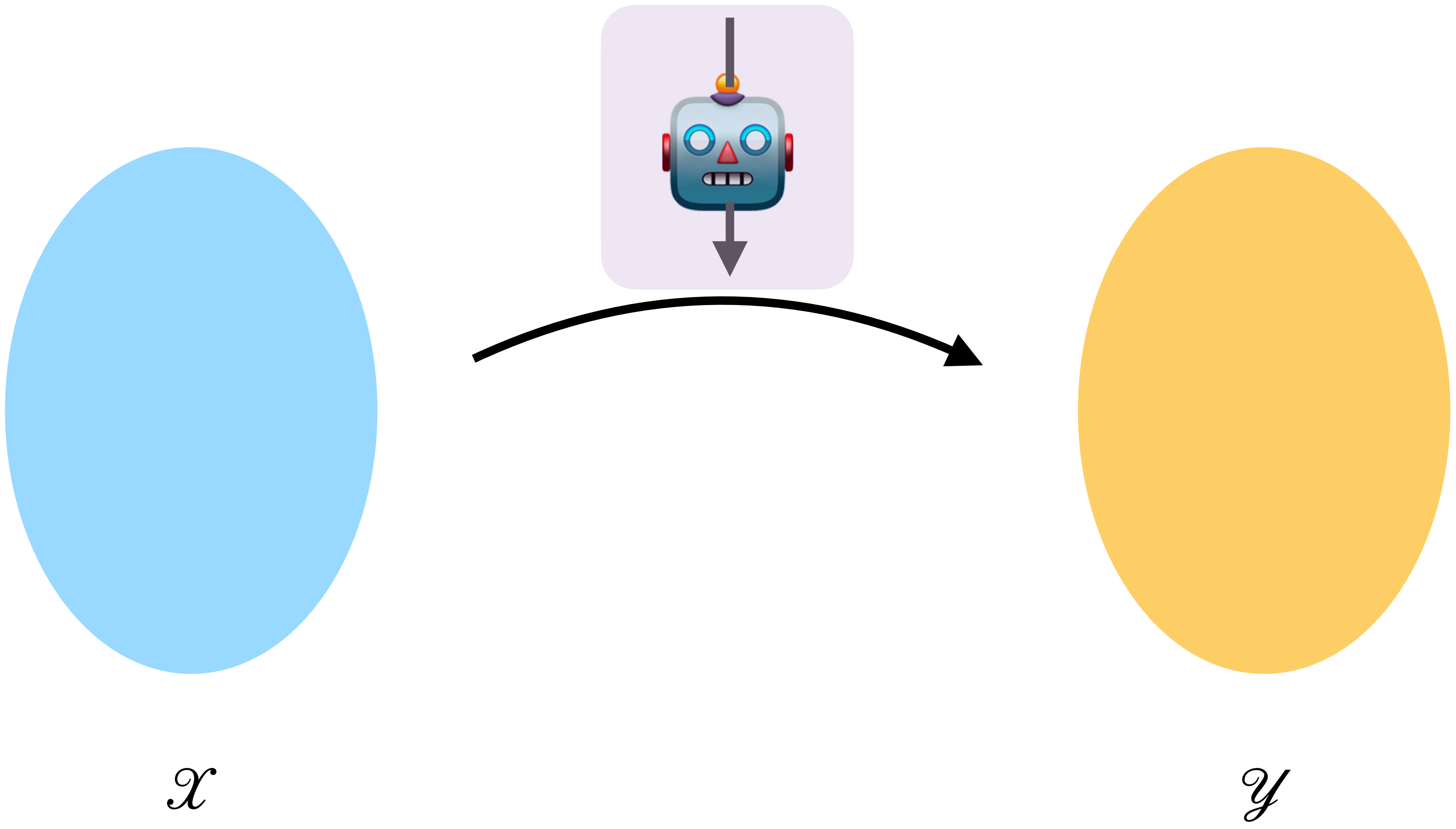

Supervised Learning

Basic Pipeline

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

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Representation

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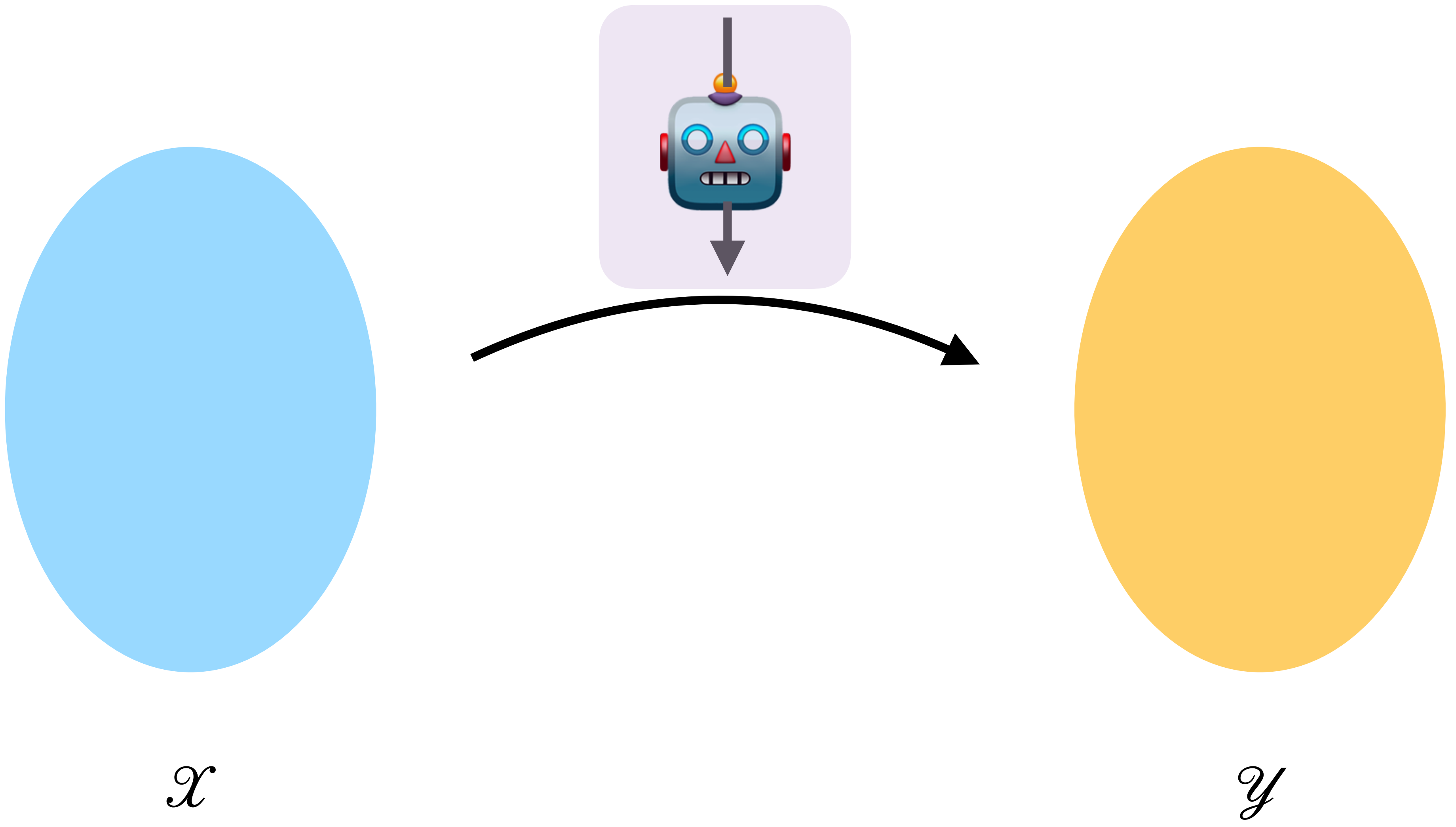

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Optimization

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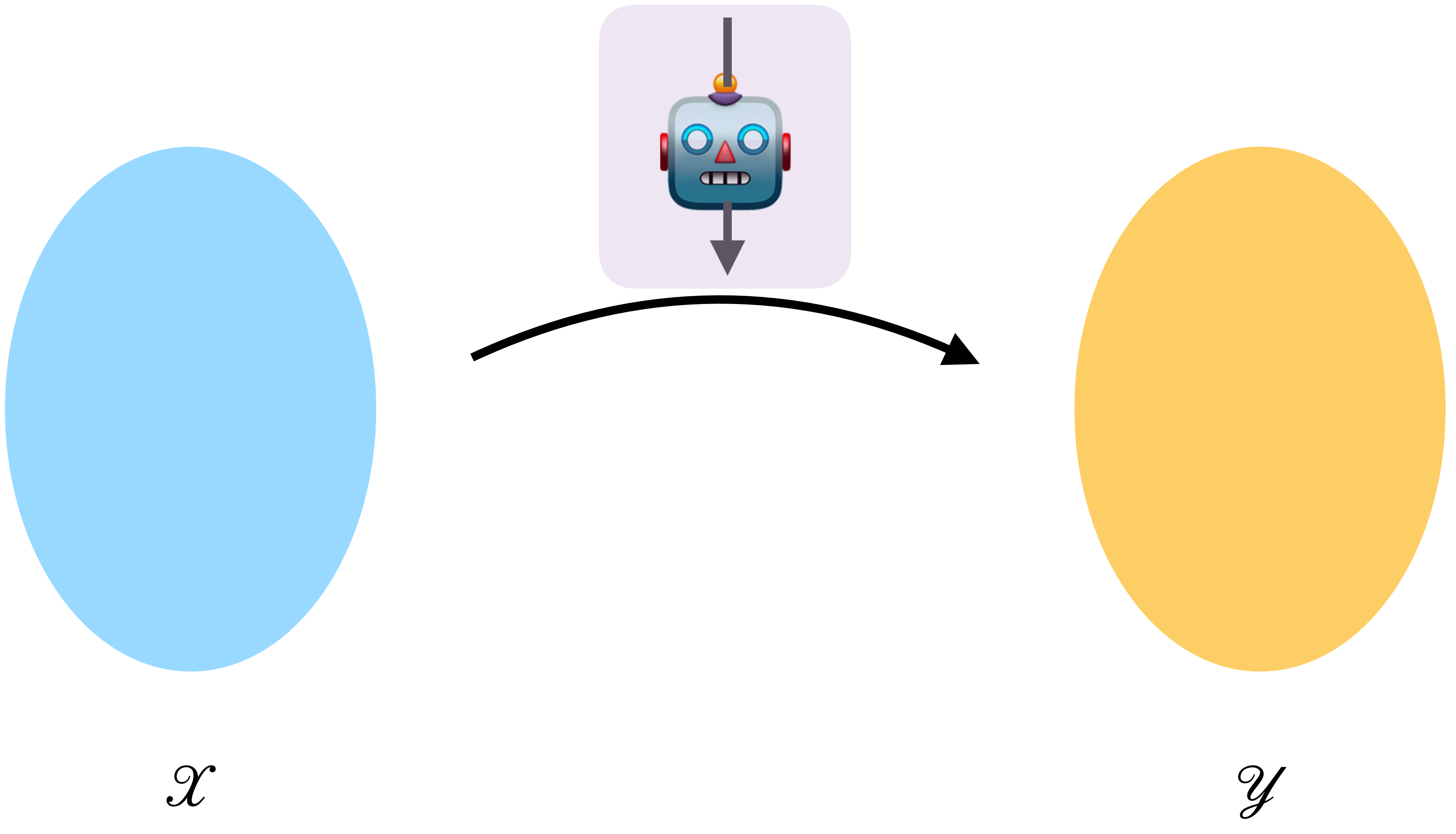


Supervised Learning

Basic Pipeline

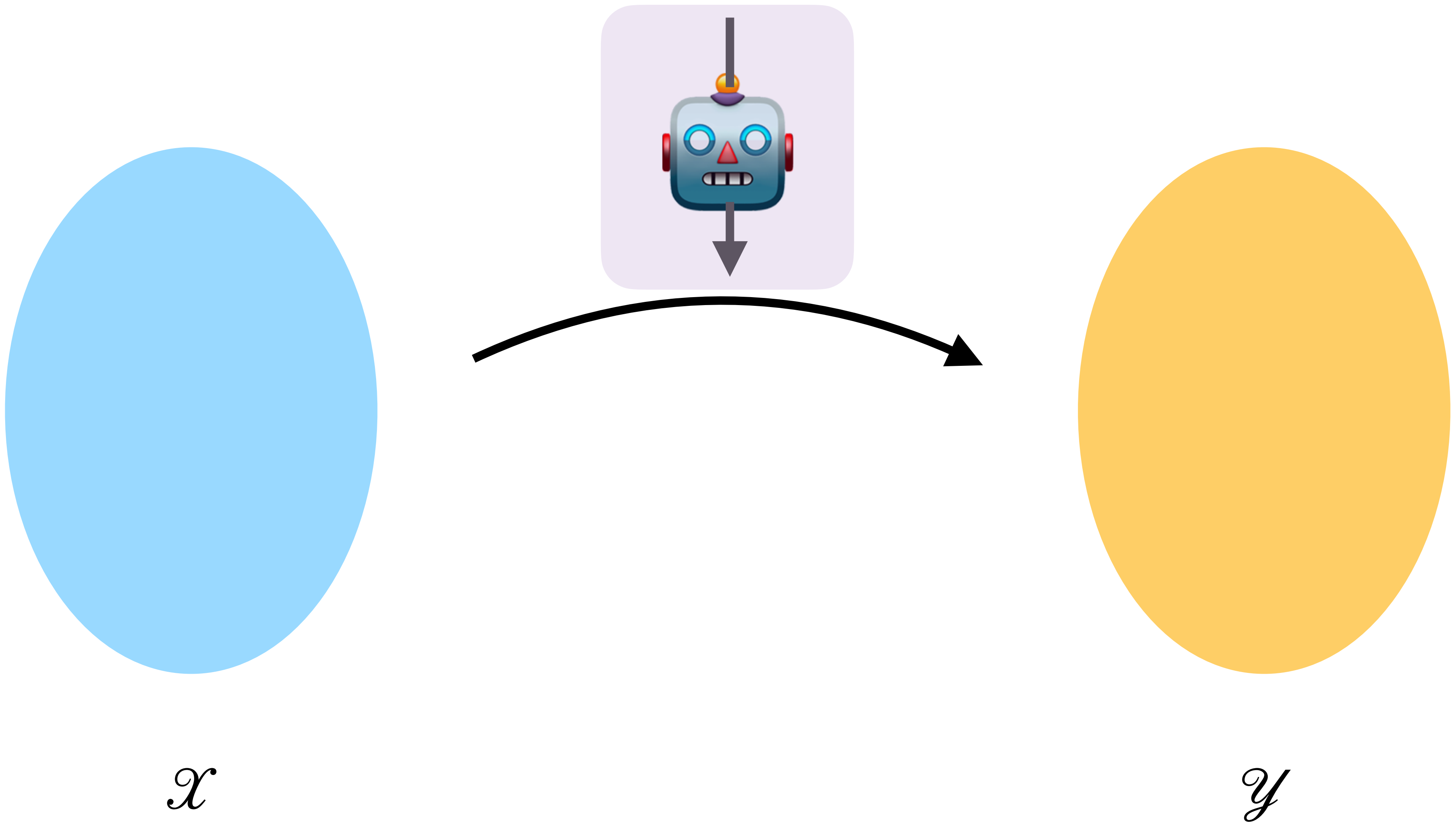
1. Collect training dataset, a collection of labeled input-output pairs.

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**

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



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 $\tilde{h}_n$:

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

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

Optimization | Generalization | Representation

Three Main Questions

Representation, Optimization, and Generalization

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

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

Optimization Generalization Representation

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

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

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

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Summary of the Problem

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

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

The Main Cast

Summary of the Problem

$$\Pr(h(x) \neq y) = \mathbb{E}\left[\Pr(h(x) \neq y \mid X = x)\right]$$

$h^*(x) = 1 \rightarrow \Pr(1 \neq y \mid X = x) = \Pr(y = 0 \mid X = x)$

$= 1 - \Pr(y = 1 \mid X = x) = 0.3$

0.7

0.3

$h^*(x) = 0 \rightarrow \Pr(0 \neq y \mid X = x) = \Pr(y = 1 \mid X = x) = 0.7$

$0.3 = 0.3$

$0.6 =$

The Main Cast

Summary of the Problem

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

The Main Cast

Summary of the Problem

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

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

The Main Cast

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

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

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

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

The Main Cast

Summary of the Problem

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Summary of the Problem

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

The Main Cast

Summary of the Problem

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

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

The Main Cast

Summary of the Problem

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

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

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

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

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