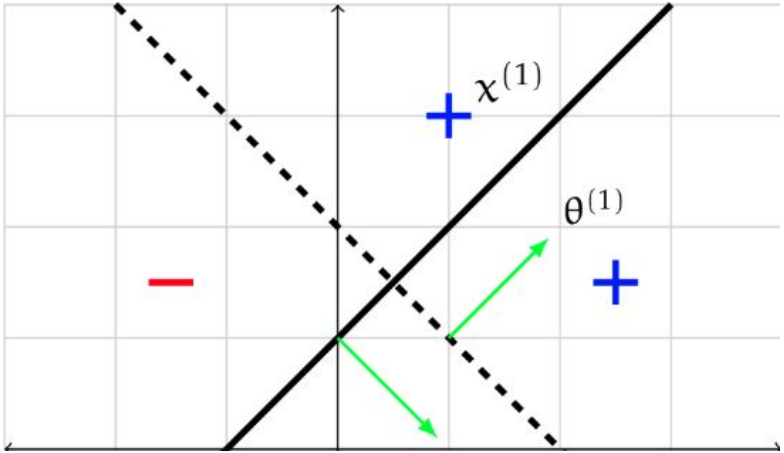
Fall 2023!

6.390

# Introduction to Machine Learning

https://introml.mit.edu




The 6.390 Instructor Team
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## Instructors

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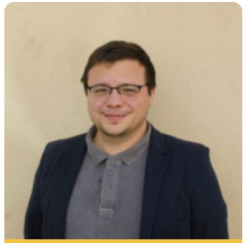

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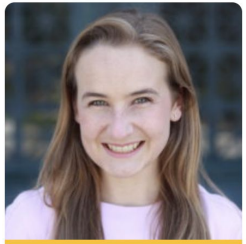
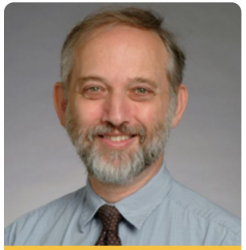


Tess Smidt



Peter Szolovits

**Course Assistant**

**Taylor Braun**

Logistical issues? Personal concerns?
We'd love to help out at 6.390-personal@mit.edu

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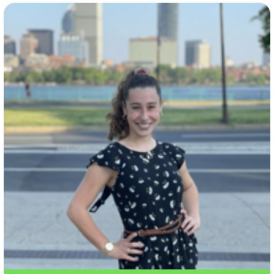

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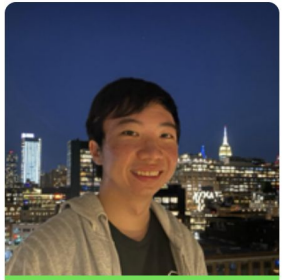

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Mimi Lohanimit

Helen Merker

Haley Nakamura

and ~50 awesome LAs!

# Course pedagogy:

A nominal week – mix of theory, concepts, and application to problems!

- **Exercises:** Released on Wed., due following Mon. 9AM
  Easy questions based on that week's notes reading (and viewing optional recorded lecture)
- **Recitation**: Monday, with attendance check-in
  Assumes you have read and done exercises; start on homework
- **Homework:** Releases Monday morning; due Wednesday (9 days later) at 11PM
  Harder questions: concepts, mechanics, implementations
- **Lab:** Wednesday, with attendance check-in (starting today)
  In-class empirical exploration of concepts
  Work with partner on lab assignment
  **Check-off** conversation with staff member

Office hours: **lots!** posted on website. Also use Piazza forum for help!

Exams:

- Midterm: *Wed, 25 Oct at 7:30pm-9:30pm*
- Final: scheduled by Registrar (posted in 3rd week). **Alert – might be as late as Dec 22!**

# Grading and collaboration (details on web)

Our **objective** (and we hope yours) is **for you to learn about machine learning**

- take responsibility for your understanding
- we will help!

**Formula:**

**exercises 5% + attendance 5% + homework 15% + labs 15% + midterm 25% + final 35%**

Lateness: 20% penalty per day, applied linearly (so 1 hour late is -0.83%)

Extensions:

- **20 one-day extensions** (move one assignment's deadline forward by one day) will be **applied automatically** at the end of the term in a way that is maximally helpful
- for medical or personal difficulties see $S^3$ & contact us at **`6.390-personal@mit.edu`**

Collaboration: don't cheat!

- Understand everything you turn in
- Coding and detailed derivations must be done by you
- See collaboration policy/examples on course web site

# Expected prerequisite background

**Things we expect you to know (we use these constantly, but don't teach them explicitly):**

**Programming (e.g. as in 6.1010[6.009] or 6.1210[6.006])**

- Intermediate Python, including classes
- Exposure to algorithms – ability to understand & discuss pseudo-code, and implement in Python

**Linear Algebra (e.g. as in 18.06, 18.C06, 18.03, or 18.700)**

- Matrix manipulations: transpose, multiplication, inverse etc.
- Points and planes in high-dimensional space
- (Together with calculus): taking gradients, matrix calculus

# Useful background

**Things it helps to have prior exposure to, but we don't expect (we use these in 6.390, but will discuss as we go):**

- numpy (Python package for matrix/linear algebra)
- pytorch (python package for modern ml models like deep neural networks)
- Basic discrete probability: random variables, independence, conditioning

# Heads-up for Next Week

- Attend your **assigned section** only starting Monday Sept. 11
- If you need to change your permanent section assignment, you will be able to self-switch, starting 5pm today; details on introml homepage

# Rest of Today

- Start our ML journey with an overview
- Form a group with those around you to complete the lab
- Ask questions by putting yourself in the help queue
- No worries if no introml.mit.edu access yet; great chance to know your neighbor (ask them to put you in the queue)

# What we're teaching: Machine Learning!

## Given:

- a **collection of examples** (gene sequences, documents, tree sections)
- an **encoding of those examples** in a computer (as vectors)

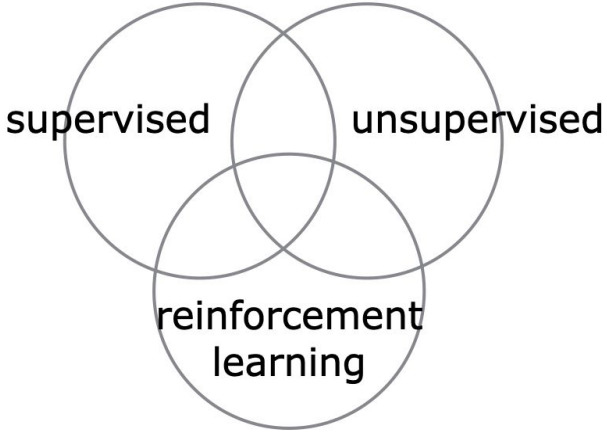
## Derive:

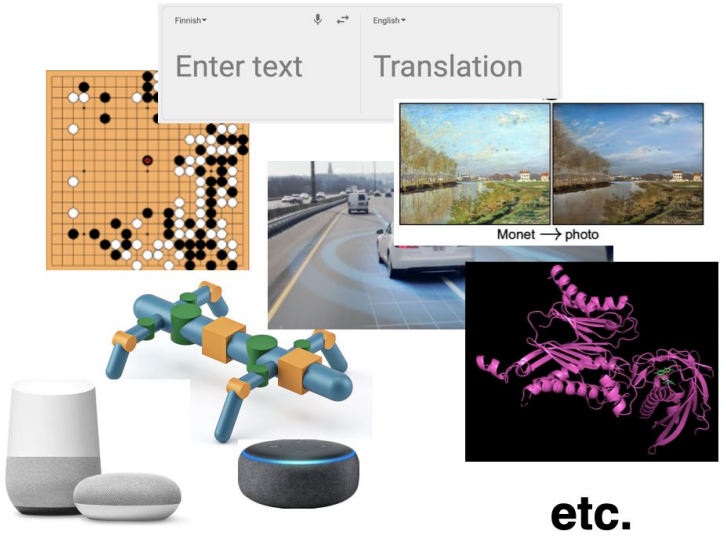
- a **computational model** (called a hypothesis) that describes relationships within and among the examples that is expected to characterize well new examples from that same population, to make good predictions or decisions

## A model might:

- **classify images** of cells as to whether they're cancerous
- **specify groupings (clusters)** of documents that address similar topics
- **steer** a car appropriately given lidar images of the surroundings

# Very roughly, ML can be categorized into



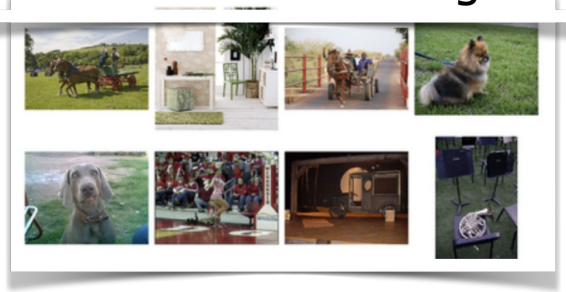




(the categorization can be refined, e.g. there are active learning, semi-supervised, selective, contrastive, few-shot, inverse reinforcement learning… )

[Slides adapted from 6.790]

# Supervised learning

**Goal:** correctly classify so far unseen test images



Goal: predict to what degree a drug candidate binds to the intended target protein (based on a dataset of already screened molecules against the target)

- Learning a machine translation system from pairs of sentences

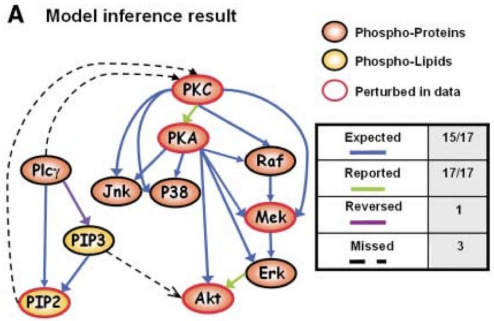
| **Spanish (input)** | **English (output)** |
|---|---|
| Aquí tienes un bolígrafo | Here's a pen |
| Las conferencias de ML son divertidas | ML conferences are fun |
| Todo el mundo debería estudiar AI | Everyone should study AI |
| ... | ... |

[Slides adapted from 6.790]

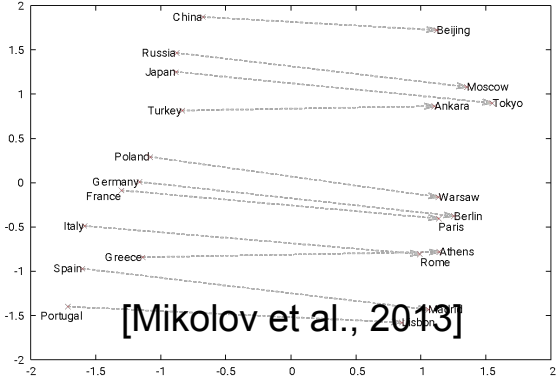
# Unsupervised learning

dimensionality reduction, embedding

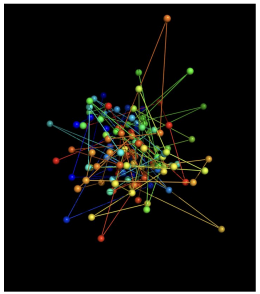
dependency /causal structure

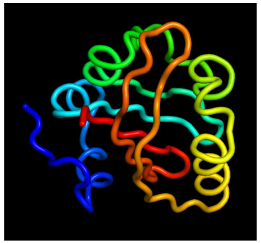



[Sachs et al 05]




[Mikolov et al., 2013]

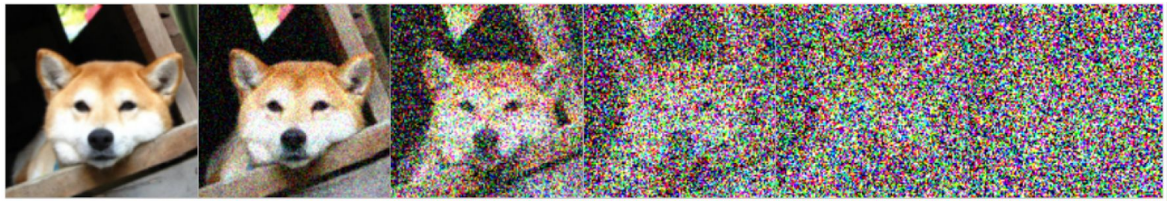




[courtesy of Jason Yim]

Over 3D protein structures, etc.

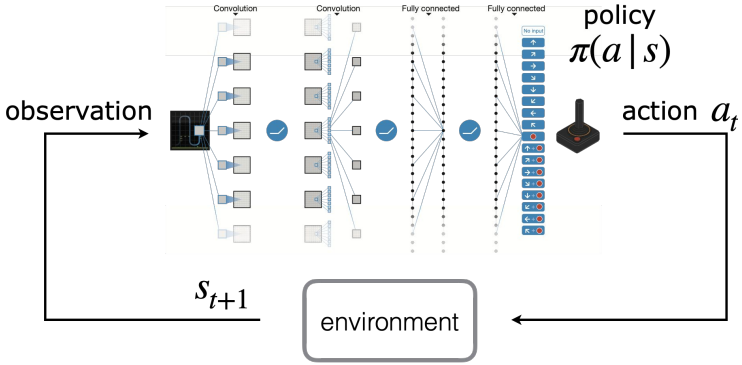
de-noising diffusion models over images

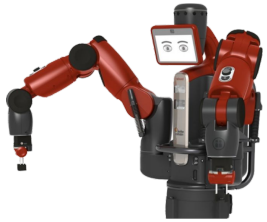


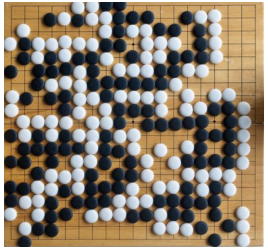
[image from Rissanen et al 2022]

[Slides adapted from 6.790]

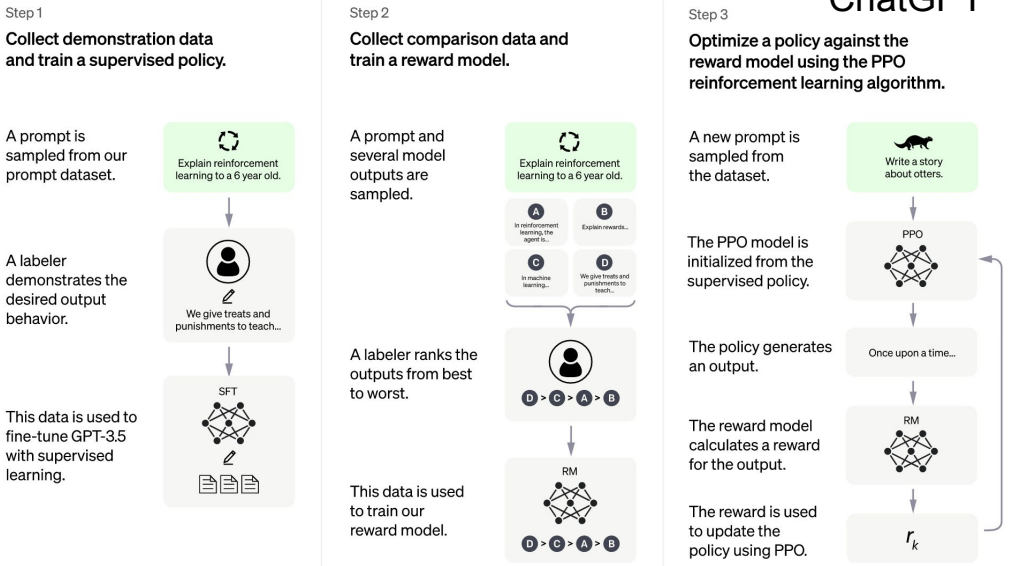
# Reinforcement learning

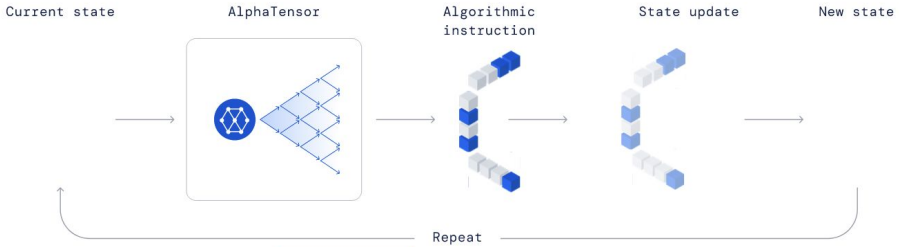




ChatGPT




Single-player game played by AlphaTensor, where the goal is to find a correct matrix multiplication algorithm. The state of the game is a cubic array of numbers (shown as grey for 0, blue for 1, and green for -1), representing the remaining work to be done.

[Slides adapted from 6.790]

# Machine learning (ML): why & what

- **What is ML?** Roughly, a set of methods for making predictions and decisions from data.
- **Why study ML?** To apply; to understand; to evaluate; to create!
- **Notes:** ML is a tool with pros & cons

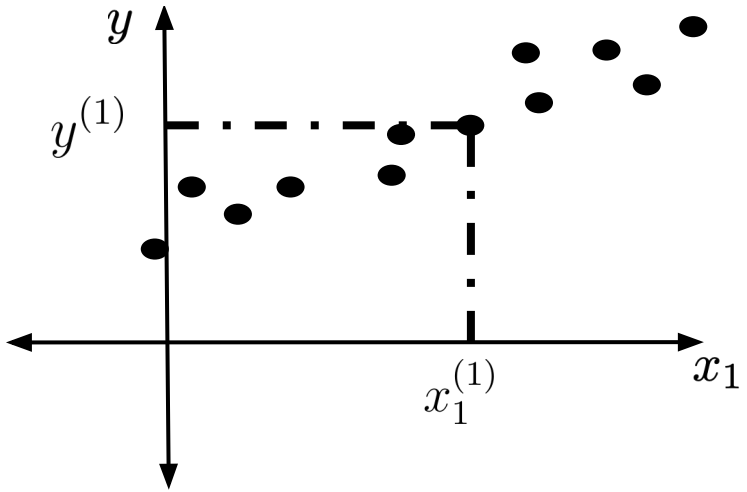
- **What do we have?** Data! And Computation!
- **What do we want?** To make predictions on new data!
- **How do we learn to make those decisions?**
  - The topic of this course!

# What do we have?

- There are many different problem classes in ML
  - We will first focus on an instance of supervised learning known as **regression**.

**(Training) data**

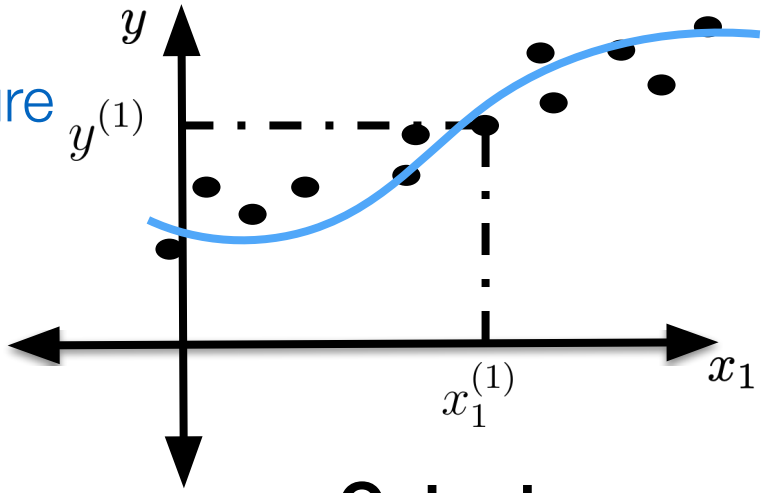
- *n* training data points
- For data point $i \in \{1, \dots, n\}$
  - Feature vector $x^{(i)} = (x_1^{(i)}, \dots, x_d^{(i)})^\top \in \mathbb{R}^d$
  - Label $y^{(i)} \in \mathbb{R}$
- Training data $\mathcal{D}_n = \{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$



# What do we want?

We want a "good" way to label new feature vectors

- How to label? Learn a hypothesis
- We typically consider a class of possible hypotheses




**Input**:
Feature vector


**Output**:
Label

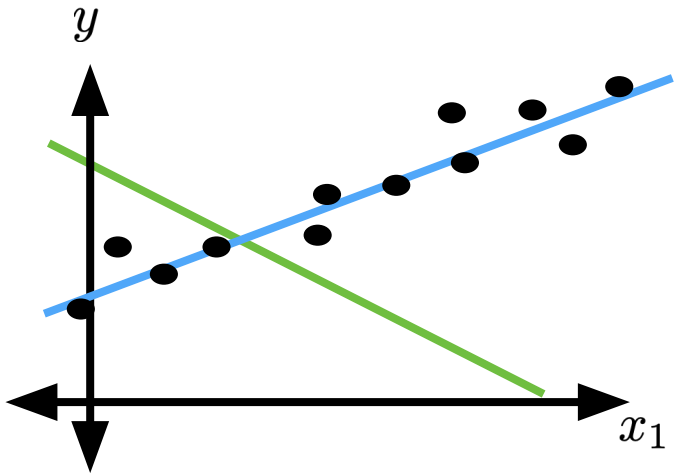
how well our hypothesis labels new feature vectors depends largely on how expressive the hypothesis class is

# What do we want?

We may consider the class of linear regressors:

- Hypotheses take the form:

$$h(x; \underbrace{\theta, \theta_0}_{\text{parameters to learn } \Theta}) = \theta^\top x + \theta_0$$

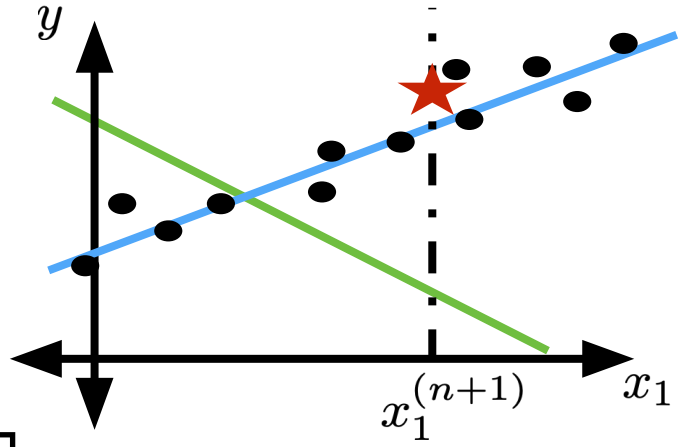



- What we really want is to generalize to **future data**!
- What we don't want:
  - Model does not capture the input-output relationship (e.g., not enough data) —> Underfitting
  - Model too specific to training data —> Overfitting

# How good is a hypothesis?

**Hopefully predict well on future data**

- How good is a regressor at one point?
  - Quantify the error using a loss function, $\mathcal{L}(g, a)$
  - Common choice: squared loss:




$$\mathcal{L}(g, a) = (g - a)^2$$

g: guess,
a: actual

- Training error:

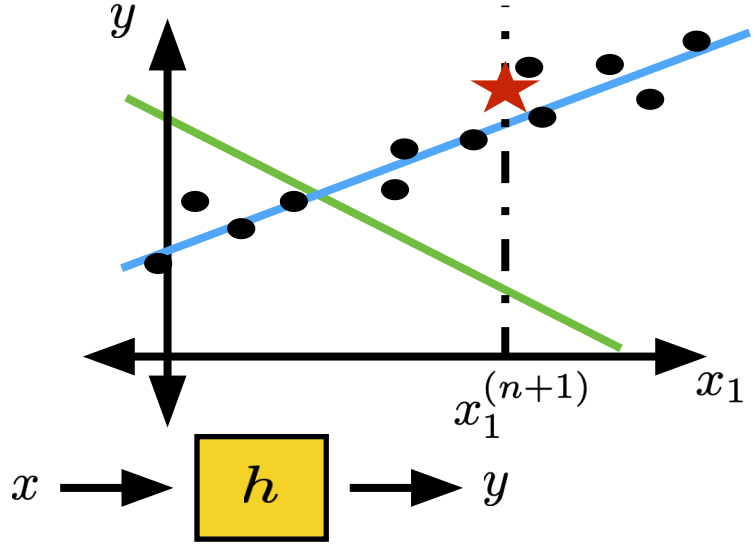
$$\mathcal{E}_n(h; \Theta) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}\left(h(x^{(i)}; \Theta), y^{(i)}\right)$$

- Validation or Test error (***n'*** new points):

$$\mathcal{E}(h) = \frac{1}{n'} \sum_{i=n+1}^{n+n'} \mathcal{L}\left(h(x^{(i)}), y^{(i)}\right)$$

# How do we learn?

- Have data; have hypothesis class
- Want to choose (learn) a good hypothesis (a set of parameters)




What we want:

How to get it:
(Next week!)