CrossTALK: ML Crash Course

Q1 2025

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Agenda

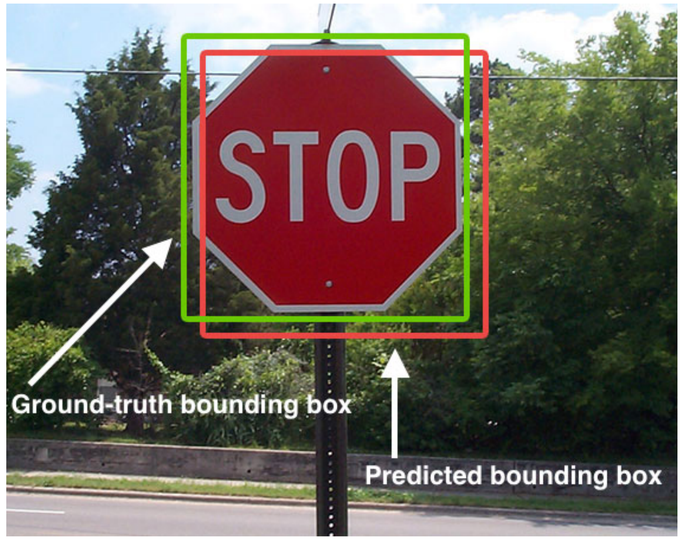
- The Story of A Single Bit
- Prediction, Learning, Conditional Prediction
- This Bootcamp

The Story of A Single Bit

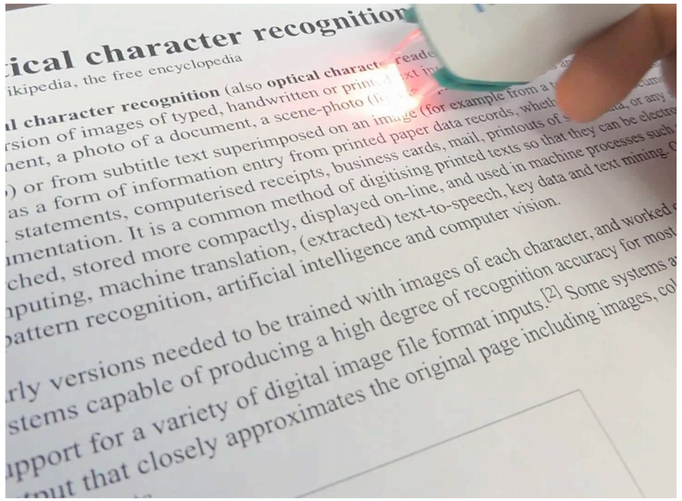
Machine learning: algorithms for prediction

For example,

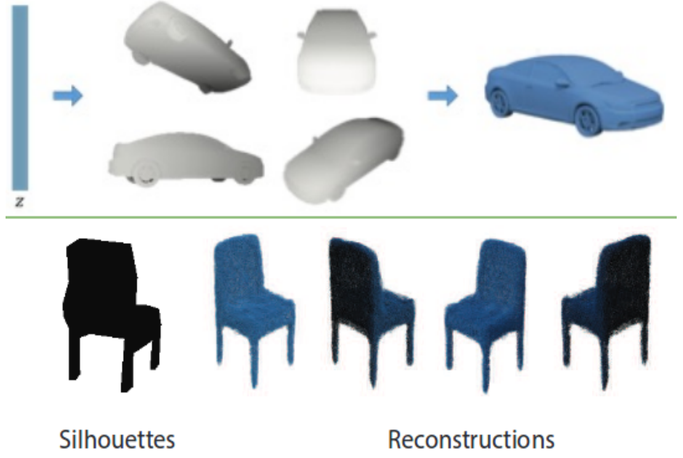
sign identification



optical character recognition

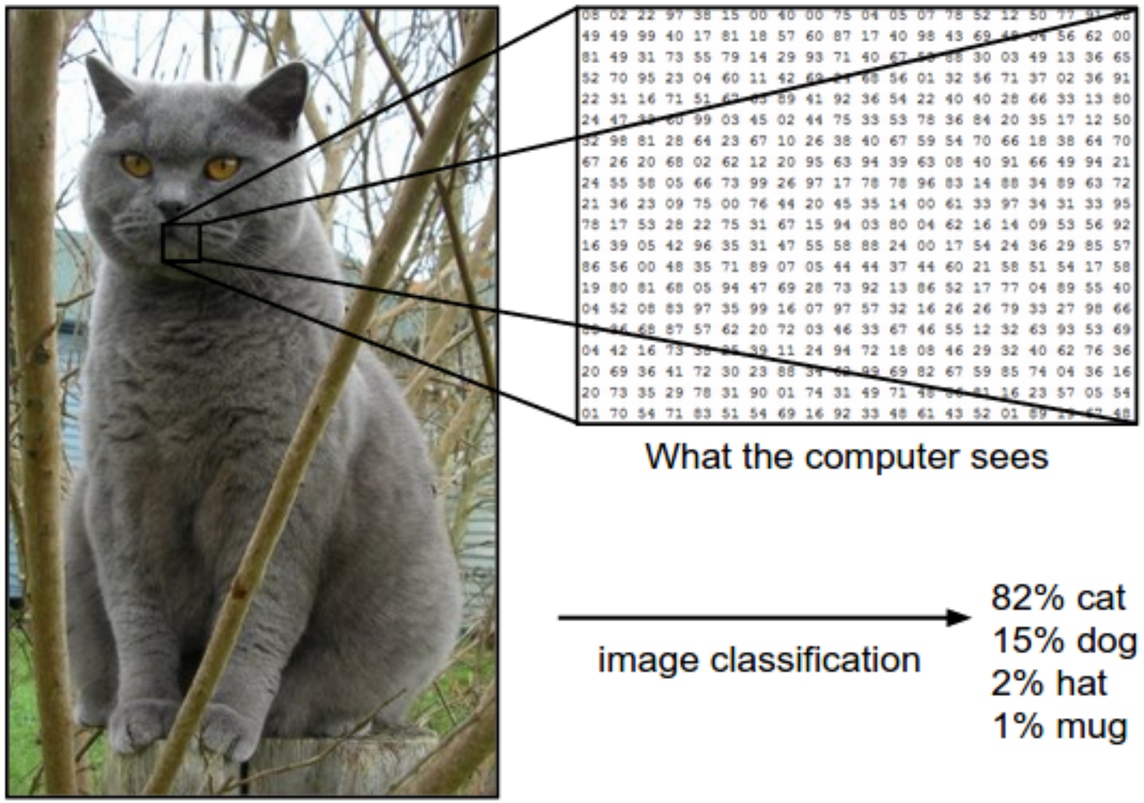


3d reconstructions



Data begins with a measurement

- A **measurement is an action that determines a property** of a system.
  - *E.g.*, silver halide crystals in film reducing to metallic silver determine light intensity.
- Stored measurements are data.
- In computers, we store data in a **digital representation.**
  - I*.e.*, a list of numbers.



Source: Andrej Karpathy

Bits

- More precisely, data is typically stored as sequences of 1s and 0s

$$(Y_1, Y_2, \ldots, Y_n) \in \{0,1\}^n$$

- I will tell you the story of a single bit of data, which is my story.
- What I am trying to highlight:
  - **Data is not an abstract thing.**
  - The processes that produce it are complex and also very personal.

A Single Bit

- 1987, I was born in Boston.
- 2016, MSc from UofT.
- 2019, a novel coronavirus spreads across the world.
- 2020, PhD from Oxford.
- 2020, I joined the faculty at UofT.
- 2022, I decided to stop being as cautious about COVID.

A Single Bit

- Let Y be the outcome of a rapid antigen test, 1 if positive, 0 o.w.
- 7 February 2022, the single bit that changed my life:

$$Y = 1$$

- Something to think about: what is the provenance of a bit?

Prediction

Prediction

- **Could I have predicted whether I would test positive before the test?**
- Let's study this abstractly. At a high level, the set up is as follows.
  - We specify a **prediction *before*** observing the outcome. A prediction is a statement about a future event.
  - The **loss quantifies our error on average on random, unseen data.**

Bernoulli outcome with cross-entropy

A special case

- Represent the test outcome as a binary random variable $Y \in \{0,1\}$.
- We specify a prediction using a real number $q \in [0,1]$ to model the probability that $Y = 1$, i.e., $P(Y = 1)$.
- How do we score our prediction?

*The base of the logarithm does not change our discussion.

Bernoulli outcome with log-loss

A special case

- We can score our prediction for a specific outcome using the log-loss*,

$$\ell(Y, q) = -Y \log(q) - (1 - Y)\log(1 - q)\,.$$

- To capture how well we expect to do *in expectation* on an *unseen outcome*, we would like to use the **cross-entropy loss,**

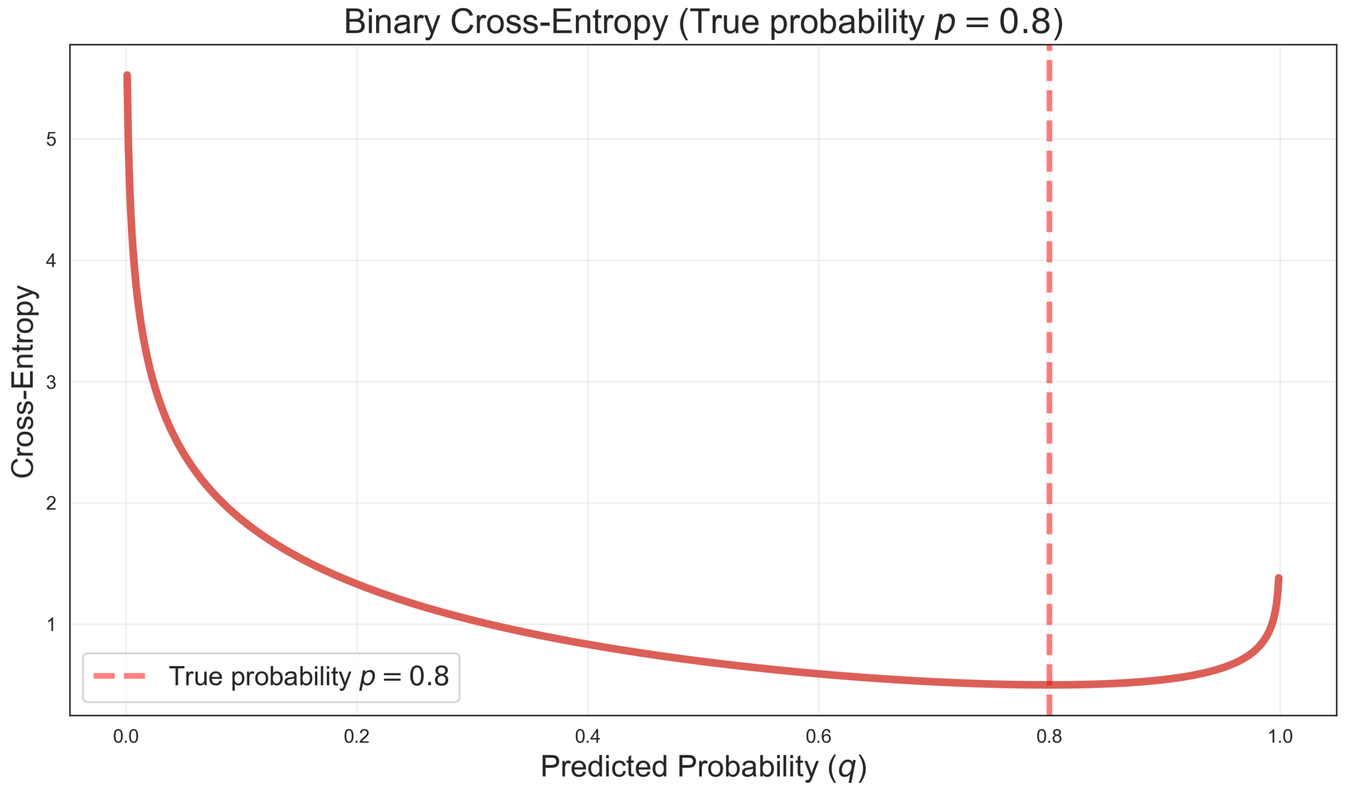
$$\ell(p, q) = -p \log(q) - (1 - p)\log(1 - q).$$

where $p = P(Y = 1)$.

*The base of the logarithm does not change our discussion.

Why is this a good choice for the loss?

p uniquely minimizes the cross-entropy



The prediction with the lowest risk is the true probability p.

Uncertainty

Motivating the cross-entropy

- You can think of the cross-entropy as quantifying the **"amount of uncertainty that is resolved when we observe an outcome Y given that I expected $P(Y = 1) = q$"**, which measures how surprised we are to observe its value.
- This reasoning can be formalized and you can show that the cross-entropy uniquely captures a certain **statistical notion of uncertainty**.

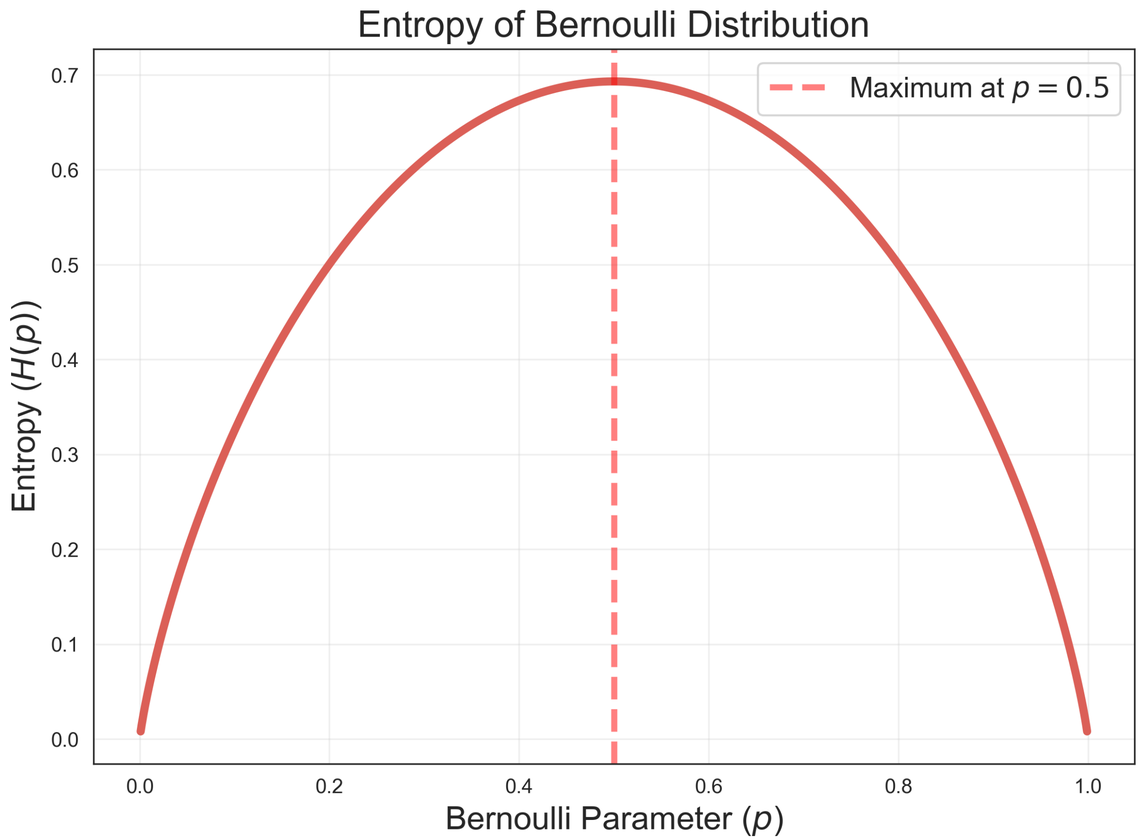
Entropy

the least surprised we could be

- The cross-entropy is minimized at $q = p$ and equals

$$-p\log(p) - (1-p)\log(1-p)$$

- Called the **entropy, which is the least surprised we could be**.
  - Most surprised at outcomes if $p = 0.5$ and least surprised if $p \in \{0,1\}$.



Recap
Prediction

- A prediction is a statement about a future event.
- We can predict random bits by specifying the probability of them being 1.
- The cross-entropy scores our surprise at observing the outcome.
- The optimal prediction under the cross-entropy is the true probability.

Learning

Learning

- To predict well, we want $P(Y = 1)$. **But how can we get this in practice?**
- **Learning is the study of procedures that estimate predictors from data.**
- When we do a good job of learning, i.e., we found a good predictor from a set of observations, we say that we have achieved good **generalization**.
- Returning to our Bernoulli example, we will study a simple learning algorithm.

Learning

A special case

- We observe a data set $\{Y_i\}_{i=1}^n$ for outcomes Y_i that are i.i.d. Bern(p).
  - *E.g.*, a set of COVID test outcomes from Toronto during the pandemic.
- Ideally we would minimize the cross-entropy to get p,

$$\min_{q \in [0,1]} \ell(p, q)$$

But there's a problem!

A special case

- So far we've been referring to the cross-entropy $\ell(p, q)$, but we don't actually have p!
- To get around this, we can approximate the cross-entropy with **the empirical cross-entropy**:

$$\frac{1}{n}\sum_{i=1}^{n} \ell(Y_i, q).$$

- Notice that $\frac{1}{n}\sum_i \ell(Y_i, q) \to \ell(p, q)$ by properties of random variables

Learning

A special case

- This motivates **empirical risk minimization**, which is the estimation procedure that finds

$$\min_{q \in [0,1]} \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, q)$$

- Given $\{Y_i\}_{i=1}^n$ i.i.d. Bern(p), the ERM w.r.t. the empirical cross-entropy is minimized by

$$\hat{p}_n = \frac{1}{n} \sum_{i=1}^{n} Y_i$$

Learning with cross-entropy

- Does $\hat{p}_n$ approach p as $n \to \infty$ in some sense?
- We can study this by studying the behaviour of **the excess cross-entropy**

$$\mathscr{E}(q) = \ell(p, q) - \ell(p, p)$$

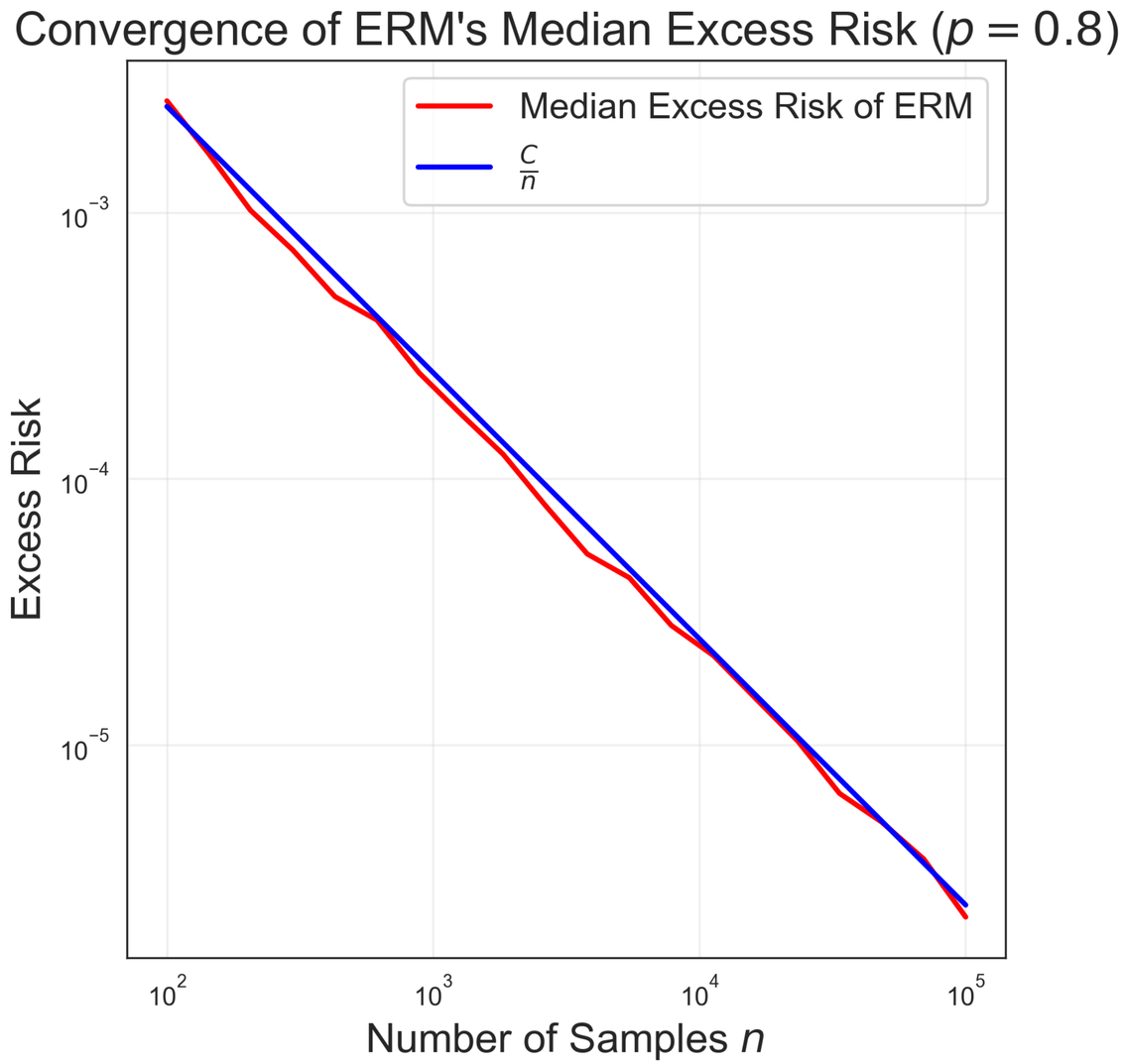
- Note two things:
  - $\mathscr{E}(q) \geq \mathscr{E}(p) = 0$ for all $q \in [0,1]$.
  - $\mathscr{E}(\hat{p}_n)$ **is a non-negative real-valued *random* variable.**

Learning convergence

- Let's study convergence in simulation (derivation in the Bernoulli case is a bit tricky).
- **Median converges like,**

$$\textbf{median}\left[\mathscr{E}(\hat{p}_n)\right] \to C/n$$

  - Typical rate for learning.
- **Key take-home: the more data we have, the better our predictions.**



Recap
Learning

- Learning is the study of procedures that estimate predictors from data.
- Empirical risk minimization tries to solve this by picking the predictor that minimizes the average loss on a data set.
- Predictors obtained from data are random because the data is random.
- We can study predictors by studying the excess loss, *i.e.*, the deviation of the expected loss from the best possible expected loss.
- When the excess loss is small, we have generalized.
- **The more data we have, the better we generalize.**

Conditional Prediction

Conditional prediction

- Could I have **predicted my test more accurately, if I had other measurements** about me?
  - Did anything in the last 37 years make $Y = 1$ more likely?
- Answer is **typically yes!**
- Let's study a special case of conditional prediction: **logistic regression**.

Logistic regression

A special case

- **Let $X \in \mathbb{R}^d$ be a random vector of other measurements called "features".**
  - E.g., my age as a number, my location as coordinates, etc.
- Seeing $X = x$ **may inform us about** Y and make $Y = 1$ more predictable.
  - I.e., $P(Y = 1 \mid X = x)$ may have less entropy than $P(Y = 1)$.
- To take advantage of this, we can build **conditional predictions of Y given X**.
  - Logistic regression is a special case!

Logistic regression

A special case

- **Logistic regression:** predict $P(Y = 1 \mid X)$ with a sigmoid function that depends linearly on X:

$$q(X) = \sigma(\sum_{i=1}^{d} w_i X_i)$$

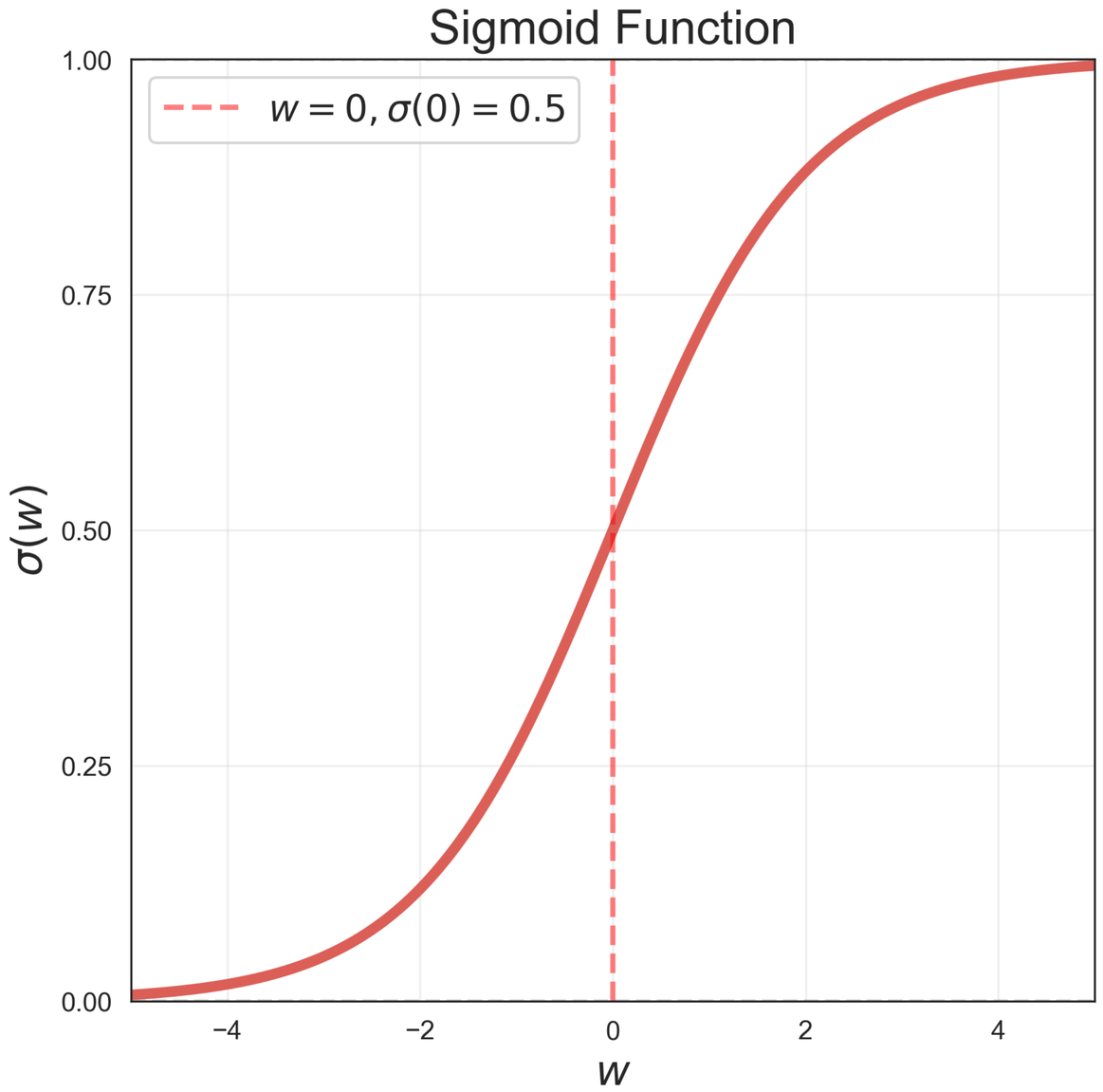
where $\sigma(t) = \frac{1}{1 + \exp(-t)}$ is the sigmoid and $w \in \mathbb{R}^d$ **are called parameters**.

- The params. plus the rule for computing the prediction is called **the model**.

Logistic regression

Intuition

- This is a generalization of the Bernoulli prediction case we considered.
  - Take $X \equiv 1$ to be constant.
  - Then $q(1) = \sigma(w)$ where $w \in \mathbb{R}$.
  - Can represent any $q \in (0,1)$ this way.



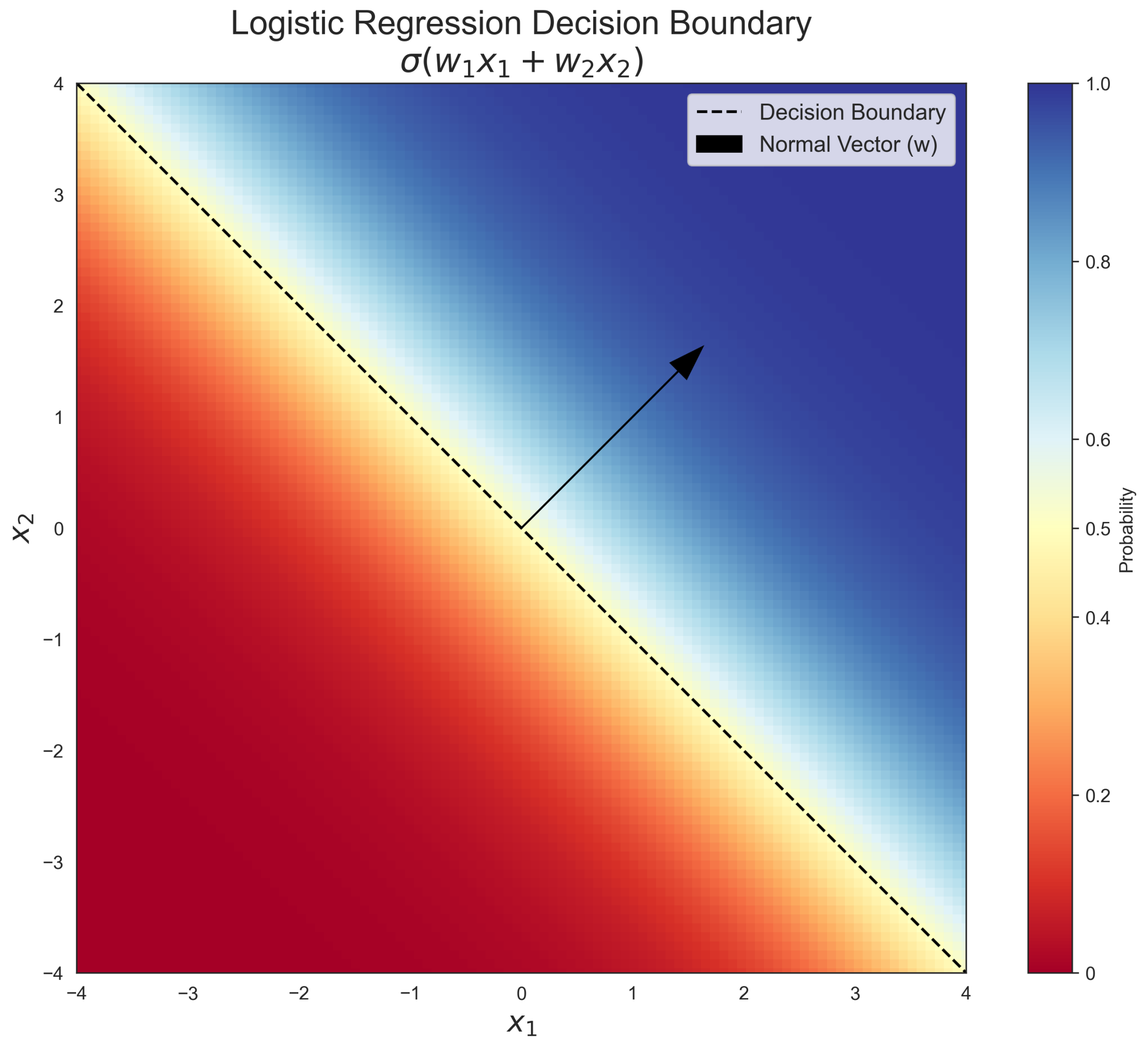
Logistic regression

Intuition

- The set of x where $\sigma(w^\top x) = 0.5$ is the hyperplane

$$\{x \in \mathbb{R}^d : w^\top x = 0\}$$

- **w separates our predictions.**
  - As x travels along w, our prediction that $Y = 1$ increases towards 1.
  - As x travels along $-w$, our prediction that $Y = 1$ decreases towards 0.



Logistic regression

Which *w* should we pick?

- How do we get w^*? As before, it is common to **optimize the conditional cross-entropy:**

$$\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(Y_i, \sigma(w^\top X_i)) \text{ where } (X_i, Y_i) \text{ are i.i.d. as } (X, Y)$$

Logistic regression

Which *w* should we pick?

- Optimizing is harder than the Bernoulli case: (i) sometimes there's no minimizer, (ii) when there is a minimizer, it's not always unique, and (iii) even if it's unique, there's often no closed form!
- Out of scope to study, let's assume there exists a unique minimizer of the empirical risk, $\hat{w}_n^*$.
- How can we find the $\hat{w}_n^*$? **Gradient descent is one choice!**

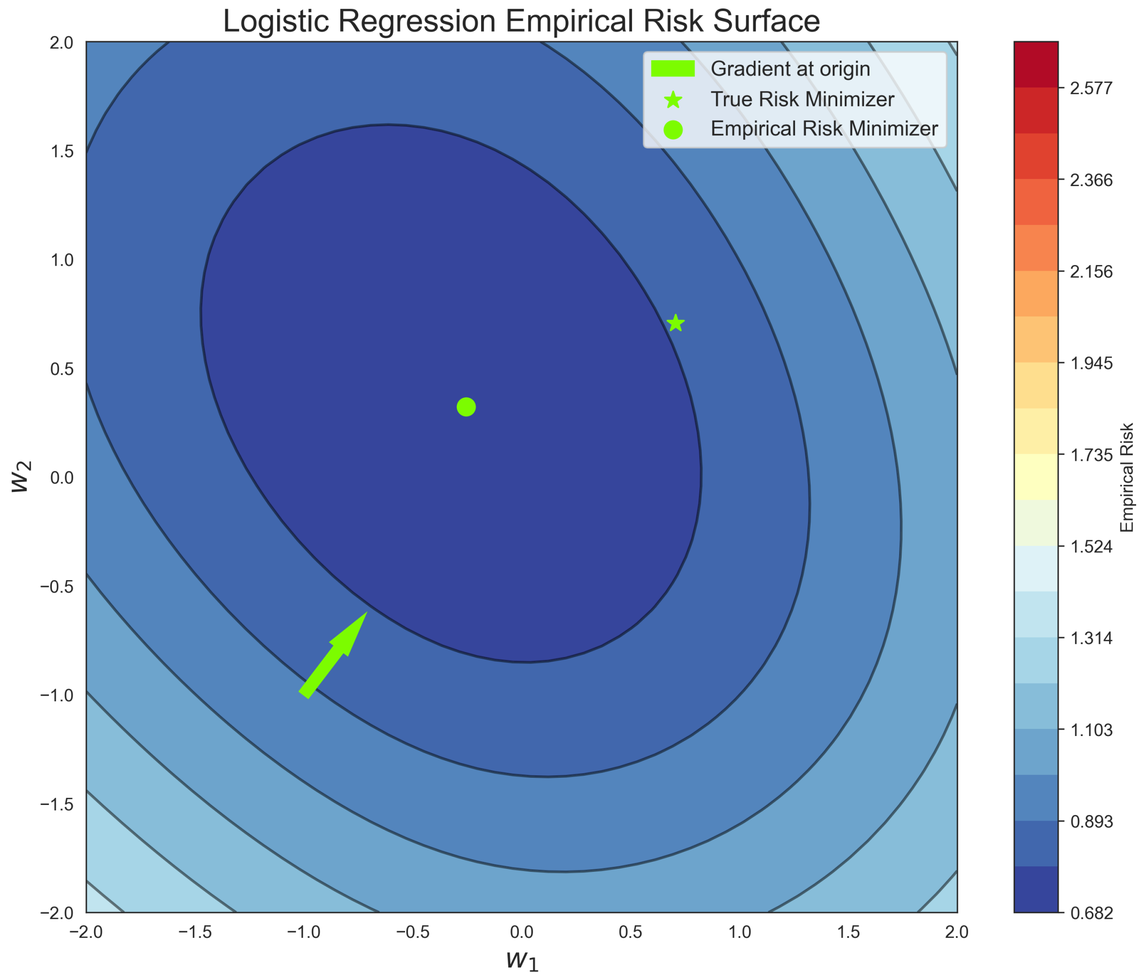
Gradient descent

Intuition

- The **gradient of the empirical cross-entropy** is the vector of partial derivatives,

$$\nabla \hat{R}_n(w) = \left(\frac{\partial \hat{R}_n}{\partial w_j} \right)_{j=1}^{d}$$

- **The negative gradient is the direction of greatest instantaneous descent on the surface of $\hat{R}_n(w)$.**



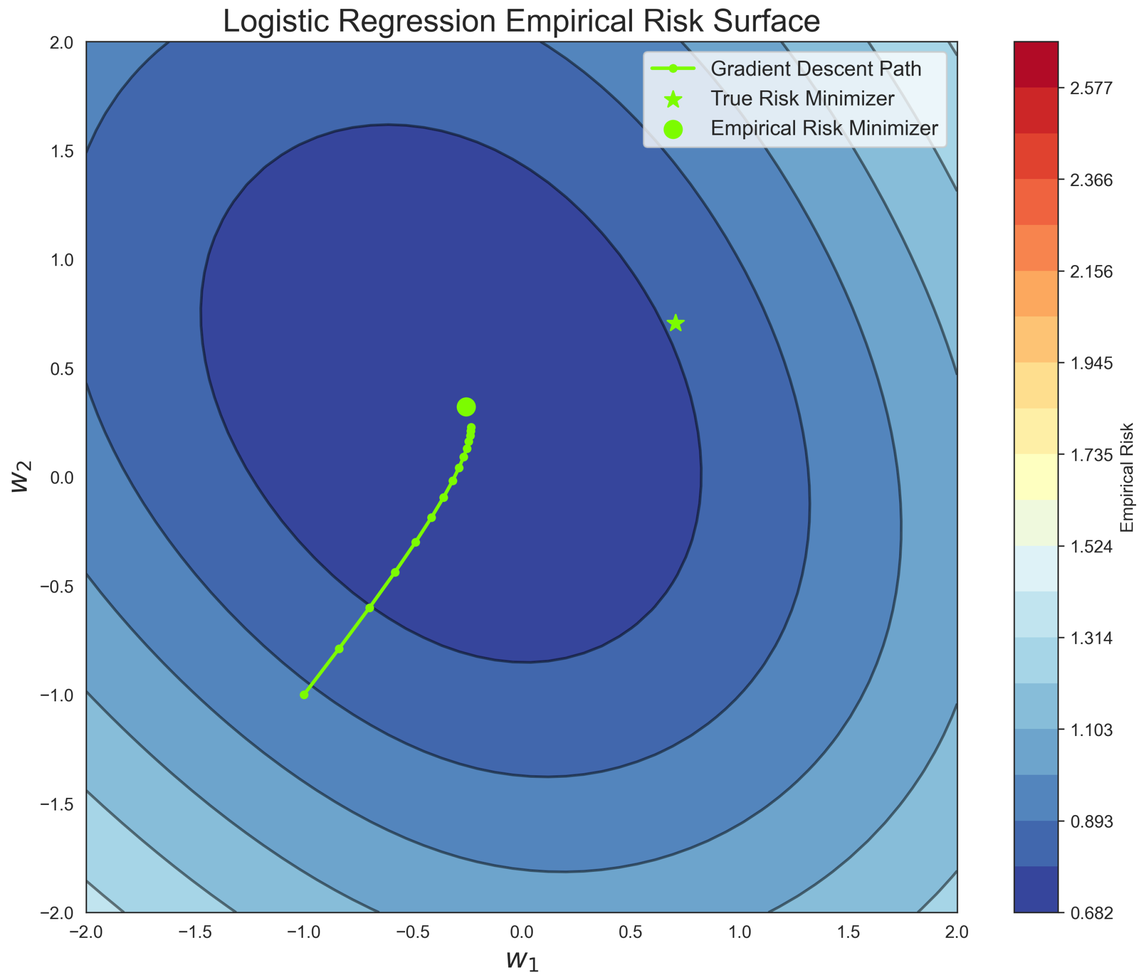
Gradient descent

Intuition

- The gradient descent algorithm iteratively **follows the gradient:**

$$w^{(t+1)} = w^{(t)} - \eta \nabla \hat{R}_n(w^{(t)})$$

for some step-size $\eta > 0$.



Gradient descent

Intuition

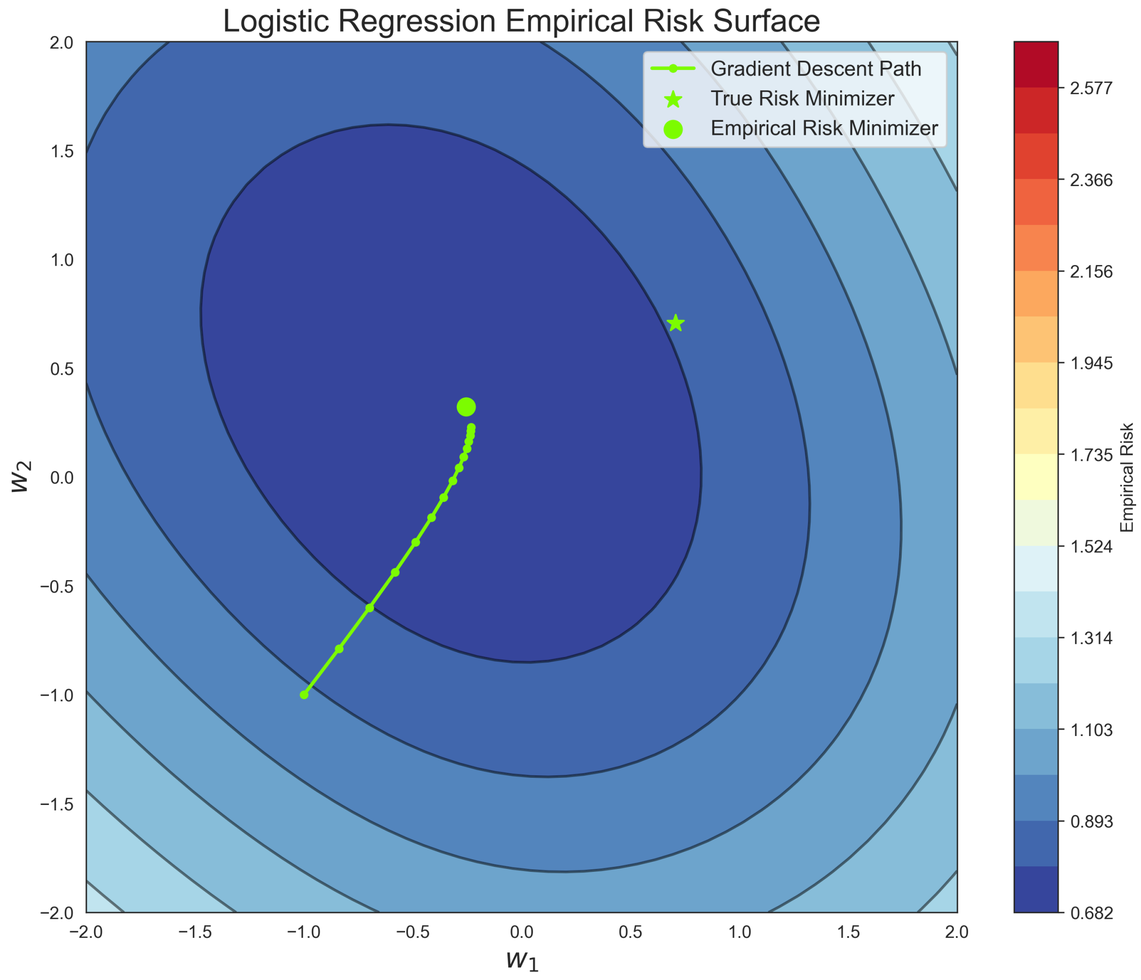
- In our setting, we have

$$w^{(t)} \to \hat{w}_n^*$$

for small η because the empirical risk is *smooth* and *convex*.

  - Technical terms that are out of scope for us.

- Optimization is another very large, very deep field (also out of scope).



Logistic regression

How well does ERM perform in this case?

- Does $\hat{w}_n^*$ approach the best possible w^* in expectation as $n \to \infty$ in some sense?
- Classical result (see Ostrovskii and Bach, 2020): under mild smoothness conditions, the *expected loss on a held out data point behaves like*

$$\frac{d}{2n} + o(n^{-1}) \text{ as } n \to \infty$$

- **Key take-home: the more data we have, the better our predictions, BUT the more parameters, the worse our predictions.**

Recap

Conditional Prediction

- Observing more measurements can sometimes improve predictions.
- We can compute conditional predictions with parametric models like logistic regression.
- In general, finding the ERM of parametric models is challenging and we often resort to iterative optimization algorithms like gradient descent.
- **Rule of thumb: learning in parametric models improves with data and deteriorates with parameter count.**

This Bootcamp

Quick admin

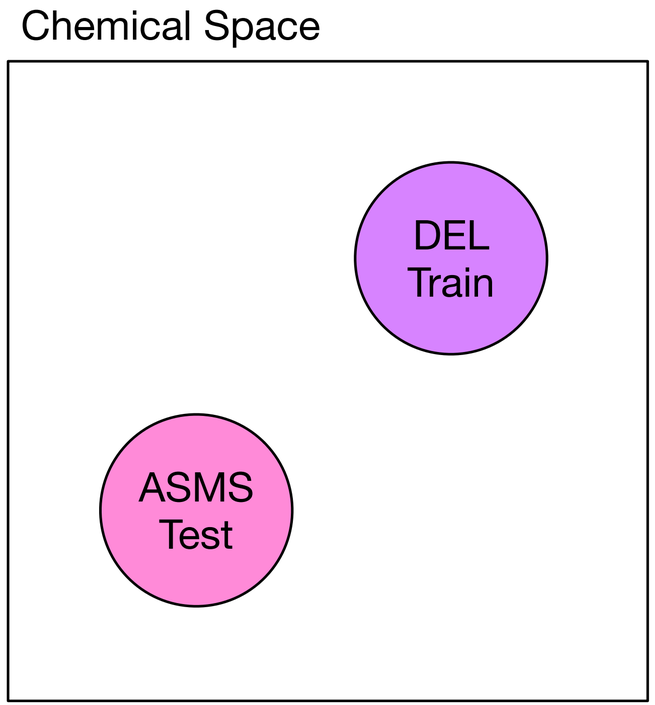
- You should have your teams already.
- Schedule:
  - Today: wrap up the lectures (hopefully)
  - March 3: hackathon, first model submission
  - March 6: wrap-up hackathon

Quick admin

- You have a **training set** of pairs (X, Y_{DEL}) where X is some chemical representation and Y is a binary outcome of hit / no hit on a DEL screen for WDR91.
  - Ben covered chemical representations.
- Your models will be **tested on a separate library** of compounds by according to how many ASMS hits against WDR91 they can find.
  - We release the test inputs.
  - You submit predictions.
  - We report your performance on the test labels without releasing the labels.

The challenge

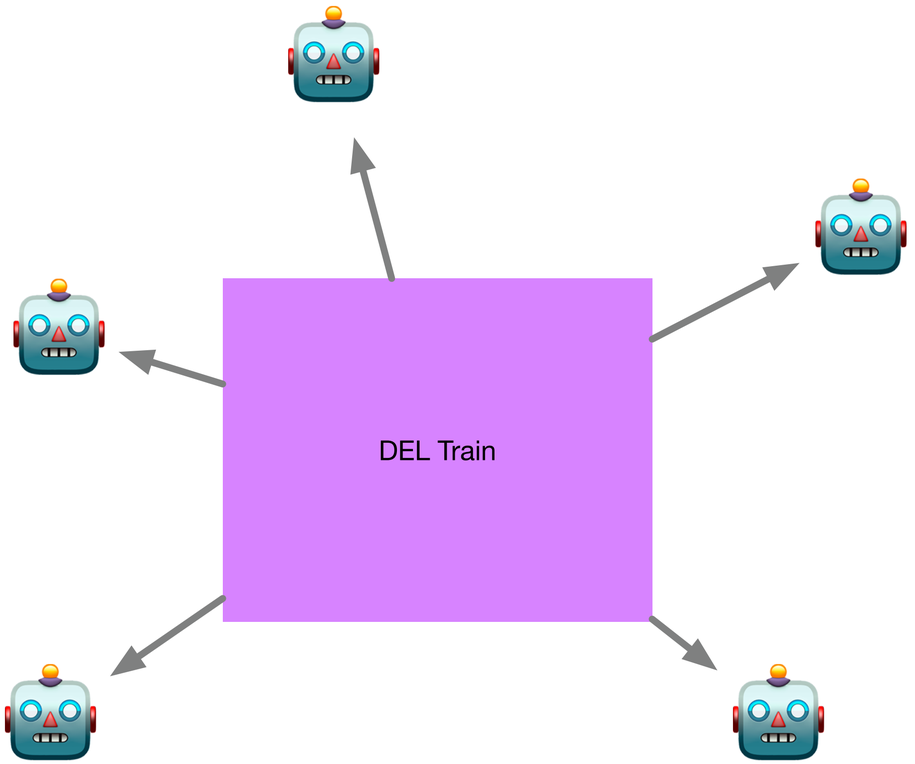
- You are facing two challenges:
    1. The test compounds look very different from training compounds.
    2. The test labels are from a different assay.
- 1. is probably a harder challenge.



The challenge

More generally

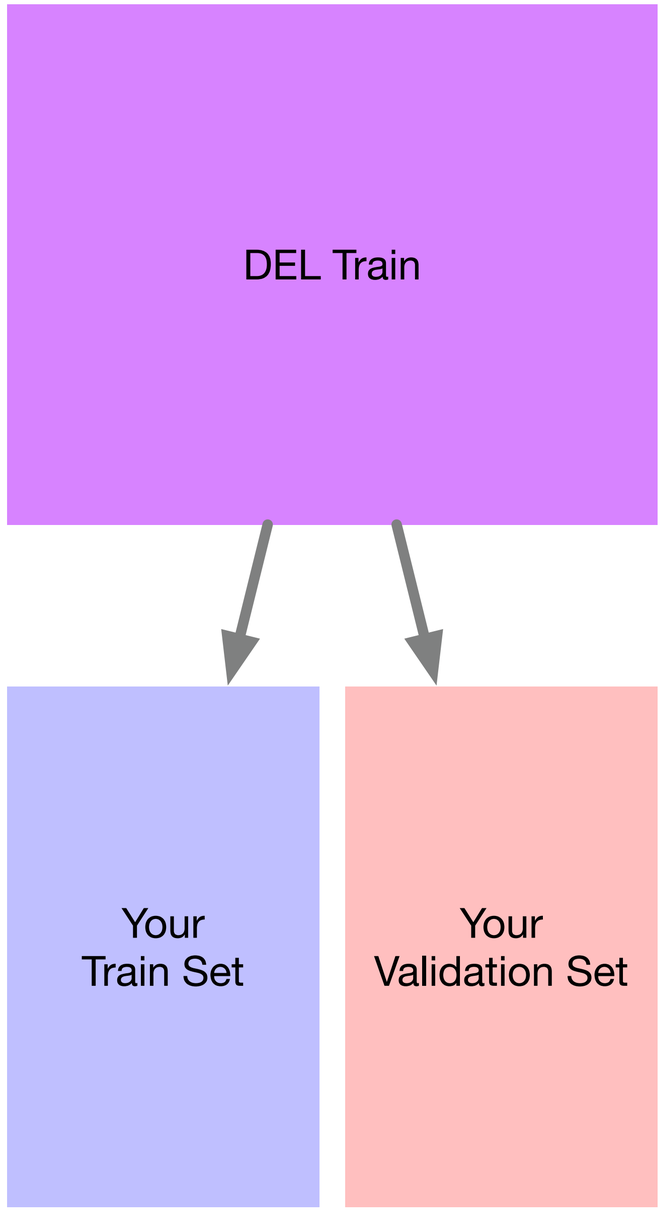
- You will be faced with a bunch of choices when you develop your model.
- Then your model will be assessed by metrics on the test set that we report back to you.
- How do you make those choices?



Which model do I pick???

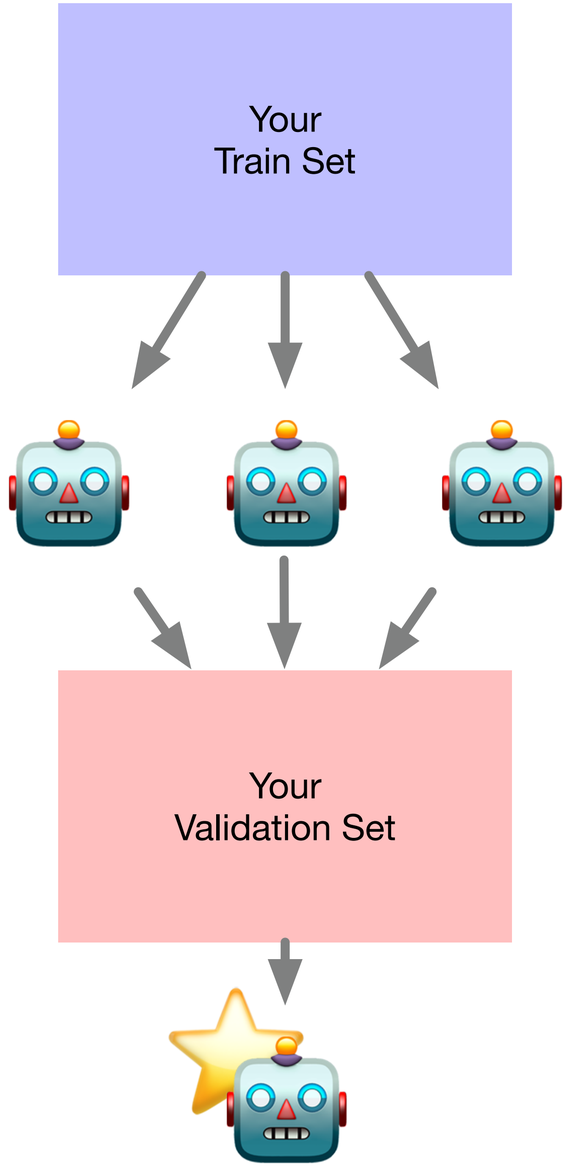
Validation sets

- You have full access to the DEL training set.
- You can mimic the testing set up by splitting the train data into a training set and **a validation set**.



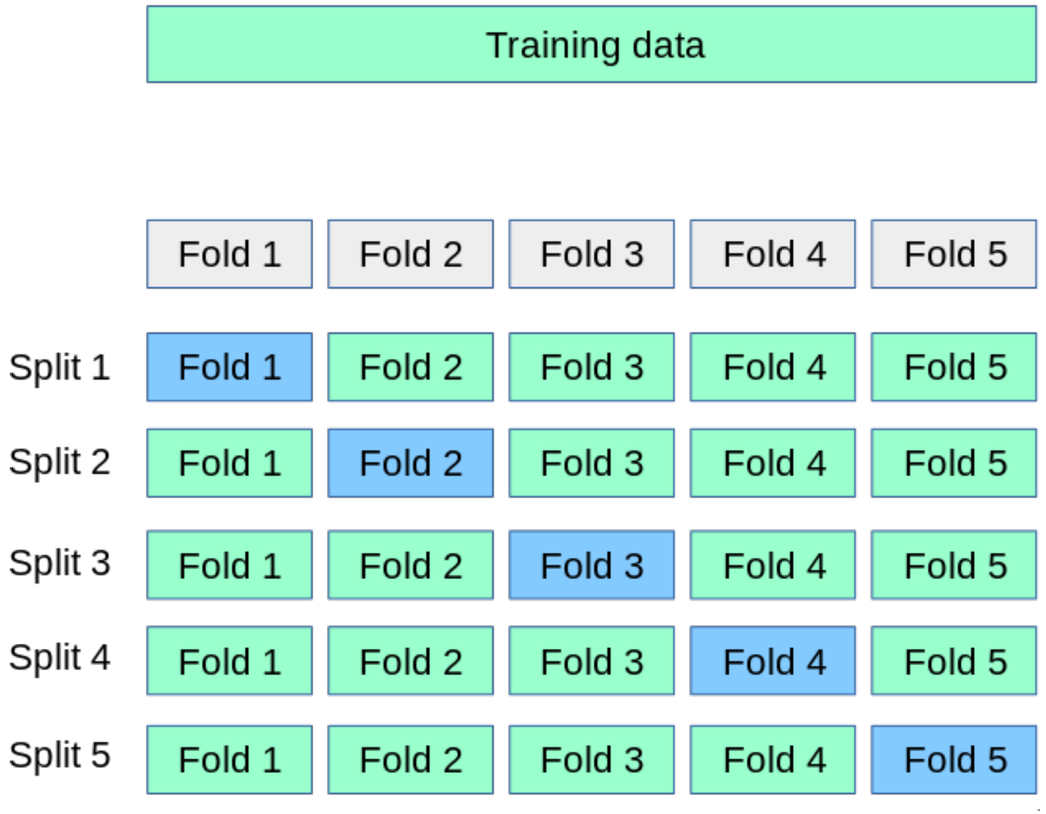
Validation sets

- The basic idea:
  - Train models on the train set
  - Pick the model that performs best on the validation set (according to your favourite metric).
- **Question: what is the best validation set if I want to pick a model that performs well on the CrossTALK test?**



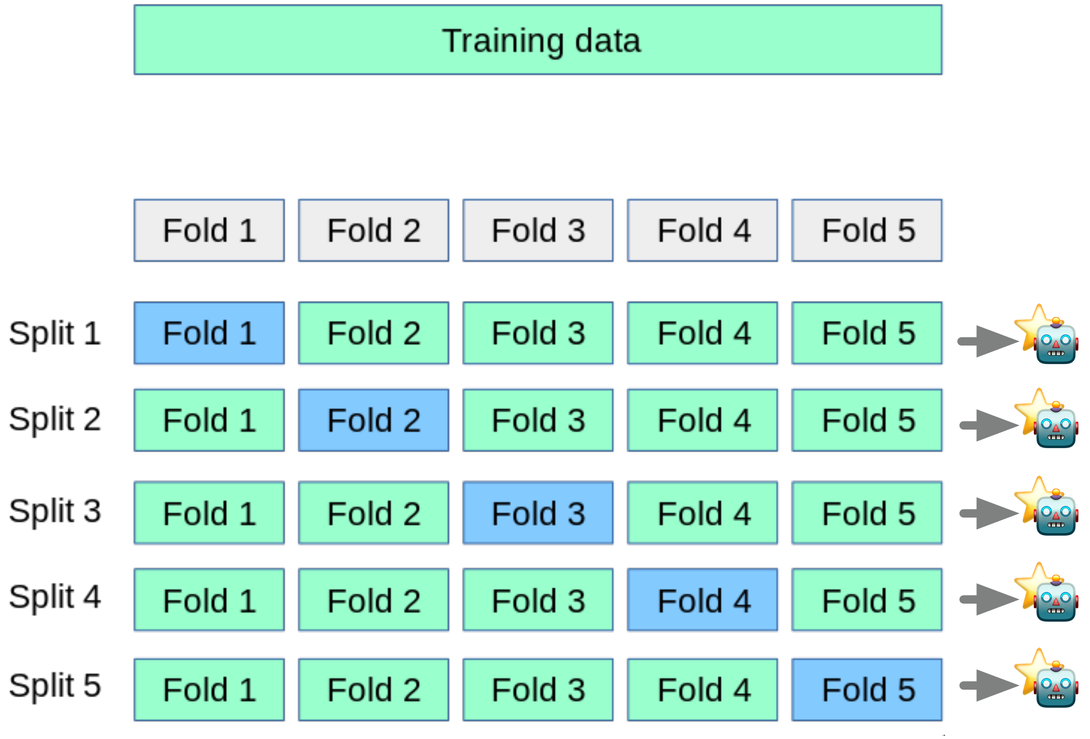
Cross-validation

- Sometimes we don’t have enough data to split into test and train.
- Cross-validation is one way to make better use of your data to help you make model choices.
- Split training data into K folds and each fold takes a turn as the validation set.



Cross-validation

- Many ways to use cross-validation.
- For example, if you're trying to check whether model A is better than model B.
- Train model A and B on all folds and average their performance on the validation sets. The one that does better on average is probably better.



Parting thoughts

- Machine learning is a vast and deep field
- There are a lot of approaches you can take to this problem
- Key questions:
  - How similar is your training loss to the testing loss?
  - How similar is your validation loss to the testing loss?
  - How similar is your validation set to the test set?
  - How challenging is your validation split as compared to the test split?

Parting thoughts

- Some approaches you might consider
  - Training losses that are less similar to cross-entropy and more similar to the ranking metrics that you'll be tested on
    - E.g., https://github.com/google/rax
  - Designing validation sets that mimic the kind of shift that you will be tested on
    - E.g., https://proceedings.mlr.press/v202/klarner23a.html

Thanks!