Explanatory Notes for 6.390

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The problem

Now, our goal is to create a **good model** for our problem, **binary classification**.

To do this, we can **try** using our 0-1 loss $\mathcal{L}$:

$$J(\theta, \theta_0) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}\left(\text{sign}(\theta^T x^{(i)} + \theta_0), y^{(i)}\right) \tag{1}$$

The **first** thing to note is that there isn't an easy **analytical** solution, no simple **equation**: $\text{sign}(u)$ isn't a function that we can explicitly **solve**, like we could for **linear regression**.

To be fair, this is true for most possible problems: most of them can't be solved analytically.

So, we refer to our other approach, **gradient descent**.

But in order to do that, we'll just need to get the **gradient**.

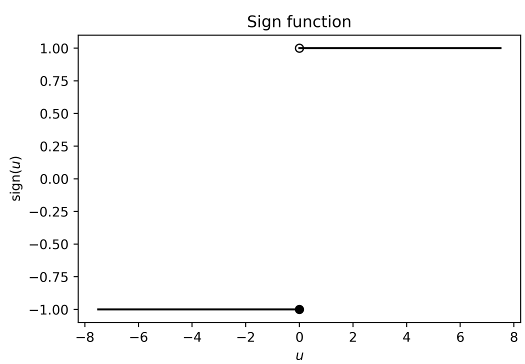
$$\nabla_\theta J = 0 \tag{2}$$

...Well that's not good.

Why not? Because we use our **gradient** to decide **how** to change θ, if the gradient is 0, we'll never **improve** θ at all!

The real problem: $\text{sign}(u)$ is flat

What's going on here? Let's look at the sign function:



Sign is a flat function! The slope is 0 everywhere, except $u = 0$, where it's **undefined**.

Well, that explains why we can't use the gradient: the function is **flat**.

Another way to say this is that our function doesn't **tell** us when we're **closer** to being right.

There's **no difference** between being **wrong** by 1 unit or being wrong by 10 units: you can't tell if you're getting **closer** to a correct answer.

And the **gradient** doesn't tell you which way to move in **parameter space** to further improve.

Remember, parameter space is what we move through as we change our parameter vector θ.

In fact, the best way we know how to approach this kind of problem takes **exponential** time: it takes exponentially **longer** to solve based on our **number** of data points.

That's way too **slow**. So, we'll have to come up with a **better** function: something to **replace** $\text{sign}(u)$, that still serves the same role.

Concept 1

The **sign function** is difficult to optimize, because it isn't **smooth**: not only is the slope undefined at 0, it is 0 everywhere else.

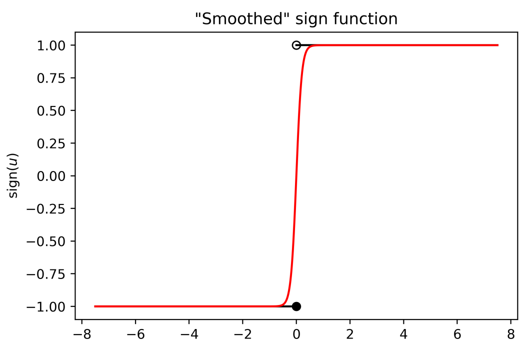
This causes two problems:

- We can't tell whether one **hypothesis** is **closer** to being **correct**, if it has gotten **better**, unless its accuracy has increased.
  - This makes it harder to **improve**.
- We can't indicate how **certain** we are in our answer: $\text{sign}(u)$ is **all-or-nothing**: we choose one class, with no information about how **confident** we are in our choice.
  - Knowing how **uncertain** we are can be **helpful**, both for **improving** our machine and also **judging** the choices or machine makes.

So, we need to explore a **new** approach: we'll **replace** $\text{sign}(u)$ with something else.

The sigmoid function

So, what do we **replace** sign with? We like the way sign **works** (choosing between two different classes based on a **threshold**), so maybe we want a **smoother** version of it.

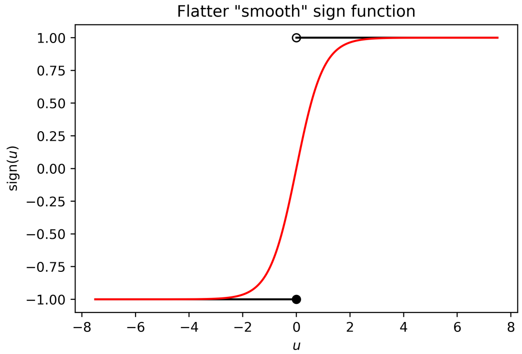


The red line shows a "**smoother**" sign function, that mostly behaves the same, while solving our problem.

This solves **one** of our two problems: the **gradient** is **nonzero**.

It's hard to see visually, but the function is **smooth**, and the slope is nonzero **everywhere**!

We could also make it less steep:



So, we need a **function** that accomplishes this. It turns out there are **several** that work: $\tanh u$, for example.

For our purposes, we'll use the following function:

Definition 2

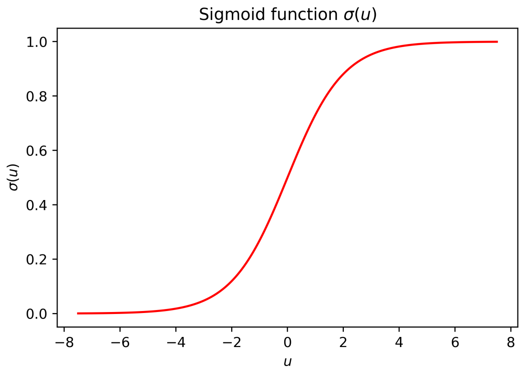
The **sigmoid** function

$$\sigma(u) = \frac{1}{1 + e^{-u}} \tag{3}$$

...is a nonlinear function that we use to **compute** the output of our **classification** problem.

It is also called the **logistic** function.

The function looks like this:



Sigmoid as a probability

Something you may **notice** is that $\sigma(x)$ is always between 0 and 1. But before, $\text{sign}(x)$ was **always** between -1 and +1. Why would we use *this* function?

Because going between 0 and 1 has a different advantage: we can interpret it as a **probability**.

Your **value** of $\sigma(u)$ can be stated as, "what does the machine think is the **probability** we **classify** this data point as +1".

And, on the **flip** side, $1 - \sigma(u)$ is the **probability** we **classify** as -1.

This solves the second problem we mentioned **earlier**: we can indicate how **confident** the machine is in its answer!

Concept 3

The output of the **sigmoid function** $\sigma(u(x))$ gives the **probability** that the data point x is classified **positively**.

$$\sigma(u) = \mathbf{P}\{x \text{ is classified } +1\}$$

$$1 - \sigma(u) = \mathbf{P}\{x \text{ is classified } -1\}$$

Note that this works because $\sigma(u) \in (0, 1)$.

Logistic Regression

So, we've seen the benefits of switching from $\text{sign}(u)$ to $\sigma(u)$. So we'll do that:

We're using $u(x) = \theta^T x + \theta_0$

Key Equation 4

Logistic Regression is a **modification** of **linear regression**.

$$h(x; \theta) = \sigma(\theta^T x + \theta_0)$$

where

$$\sigma(u) = \frac{1}{1 + e^{-u}}$$

It outputs the **probability** of a **positive** classification.

If we **plug** this in, we get this slightly ugly expression:

$$h(x; \theta) = \frac{1}{1 + e^{-(\theta^T x + \theta_0)}}$$

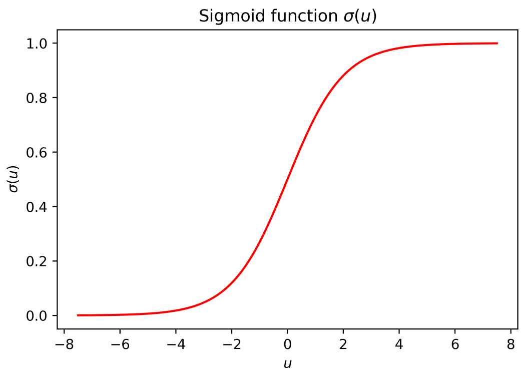
We have a problem, though: **logistic regression** is a... **regression** function. It takes in a real **vector**, and outputs a real **number**: $\mathbb{R}^d \to \mathbb{R}$.

We can't use this to do **classification**, where want $\mathbb{R}^d \to \{-1, +1\}$!

Prediction Threshold

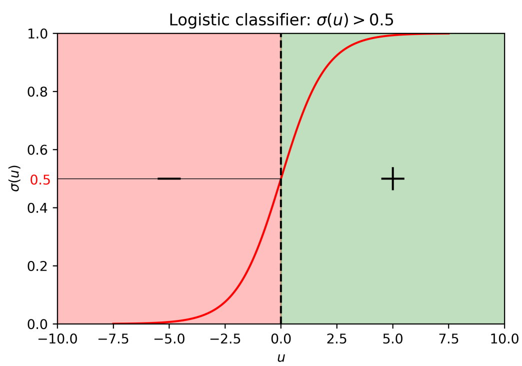
When we were just using $u(x) = \theta^T x + \theta_0$, we classified data points by saying whether $u(x) > 0$. Our boundary was $u(x) = 0$.

We can't quite do that here, because $\sigma(u) = 0$ is **impossible**: $\sigma(u)$ is **always** greater than 0.



$\sigma(u)$ approaches 0 as u approaches $-\infty$, but it never reaches it.

Well, what happens when $u(x) = 0$? We get $\sigma(0) = .5$. So, we could use that as our classification: $\sigma(u) > .5$



But, we don't necessarily always want to use .5:

Example: Imagine if you wanted to **classify** whether someone needs **life-saving** treatment. Classify -1 if sick (they need it), $+1$ if healthy (they don't).

Let's say you got $\sigma(u) = .6$, so you're only 60% sure they **don't** need it. You'd classify that as $\sigma(u) > .5$: they're '**healthy**'.

Even so, you probably shouldn't **refuse** someone treatment that's 40% likely to **save** their life. We might not want to use $\sigma(u) > .5$ after all.

We call the **boundary** between positive and negative the **prediction threshold**.

Definition 5

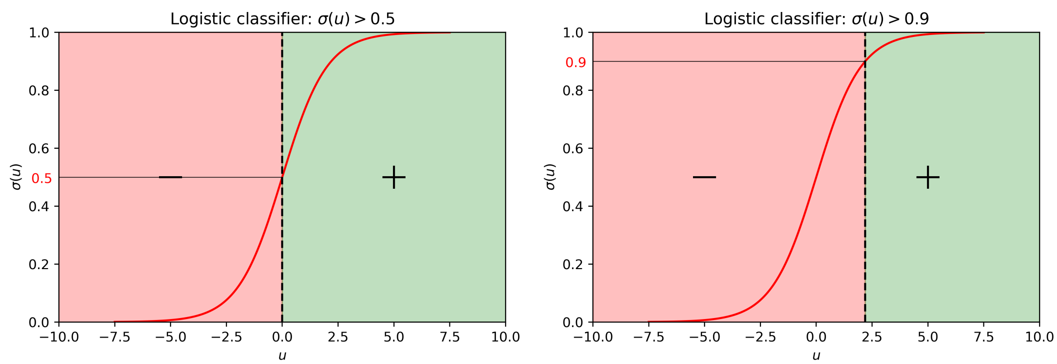
The **prediction threshold** σ_{thresh} is the value where you go from **negative** classification to **positive**.

In general, we say

Our **default** value is a threshold of .5, but our threshold can be **anywhere** in the range

$$0 < \sigma_{\text{thresh}} < 1$$

Example: If $\sigma_{\text{thresh}} = .9$, we would see:



We switch from a .5 threshold to a .9 threshold.

Linear Logistic Classifier

This finally gives us our **linear logistic classifier** (LLC)

Key Equation 6

The **linear logistic classifier** is a **binary** classifier of the form

$$h(x;\theta) = \begin{cases} +1 & \text{if } \sigma(u(x)) > \sigma_{\text{thresh}} \\ -1 & \text{otherwise} \end{cases}$$

where

$$u = \theta^T x + \theta_0 \qquad\qquad \sigma(u) = \frac{1}{1+e^{-u}} \tag{4}$$

We call it linear because of the linear inner function $u(x)$, and logistic because of the outer function $\sigma(u)$.