

# Explanatory Notes for 6.390

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# CHAPTER 4

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## Classification

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### 4.0.1 Regression (Review)

In chapter 2, we handled the problem of **Regression**: taking in lots of data (stored as a **vector of real numbers**), and returning another single **real number**.

Remember that we used a  $(d \times 1)$  column vector for our data points  $x^{(i)}$ .

$$h_{reg} : \mathbb{R}^d \rightarrow \mathbb{R} \quad (4.1)$$

This was good for when we wanted to predict some **numeric** output: stock prices, height, life expectancy, and so on.

But, this isn't the **only** type of problem we might have to deal with.

## 4.1 Classification

### 4.1.1 Motivation: Putting things into classes

We don't *always* want a **real number** output: sometimes, we just have a different kind of question.

Often, it's more useful to, rather than give numeric values, instead sort things into **categories**, or what we will call **classes**.

#### Definition 1

A **class** is **set** of things that have something relevant in **common**.

**Example:** A beagle and a golden retriever could both be put in a **class** called "dog". This is useful if you just want to know whether you have a dog or not!

#### 4.1.2 What is classification?

This is the goal of **classification**: we want to take lots of **information**, and use them to **predict** what **class** a data point belongs in.

##### Definition 2

**Classification** is the **machine learning problem** of sorting items into different, **discrete** classes.

In this setting, we take **real-valued data**, stored in a  $(d \times 1)$  **vector**, and return one of our **classes**.

$$h : \mathbb{R}^d \rightarrow \{C_1, C_2, C_3, \dots C_n\}$$

Where  $\{C_1, C_2, C_3, \dots C_n\}$  are all **classes**. Sometimes, we call the value we return a **label** instead.

**Example:** Suppose you want to classify different **animals** as a bird, a mammal, or a fish. You are given (as input) 5 pieces of useful data to **classify** with.

As a refresher, the function notation here just says, "take in a  $d$ -dimensional vector, and output one of our  $n$  discrete classes."

$$h : \mathbb{R}^5 \rightarrow \{\text{Bird, Mammal, Fish}\} \quad (4.2)$$

**Classification** can be useful for lots of situations:

- **Deciding** which **action** to take in a difficult situation
- **Diagnosing** a patient, and determining the best **treatment**
- **Sort** information to be **processed** later
- And more!

Just like with regression, we can depict our **hypothesis** as the function

$$x \rightarrow [h] \rightarrow y \quad (4.3)$$

**Concept 3**

**Classification** is also **supervised**: meaning, you have **training** data  $\mathcal{D}_n$  with the **correct** answers given:

$$\mathcal{D}_n = \left\{ \left( x^{(1)}, y^{(1)} \right), \dots, \left( x^{(n)}, y^{(n)} \right) \right\}$$

In **unsupervised** problems, you're not told the "correct" answer and have to just guess one!

### 4.1.3 Important Facts about Classes

There's a few important things we should remember about classes moving forward.

- Classes are **discrete**: each class is a distinct "thing", **separate** from other classes.
  - This is unlike real numbers, which are **continuous**: you can **smoothly** transition between them.
- This isn't **always** true, but usually, classes are **finite**: there are only so many of them, which we write as  $n$ .
  - Meanwhile, there are **infinitely many** real numbers.
- These classes may not have a natural **order**: is there a correct way to order "[Bird, Mammal, Fish]"? Not really.
  - The real numbers are ordered, too.
- In some problems, you get to **decide** what classes you choose. Do you want to compare dogs vs. cats, mammals vs. fish, color of fur? What goes in different classes, or the same?
  - You can change units (lb vs kg), but you don't "decide" how the real numbers work.

**Concept 4**

**Classes** are

- **discrete**
- **finite** (usually)
- **not** necessarily **ordered**
- often **defined** based on your **needs**

#### 4.1.4 Binary Classification

So, how do we get **started**? Well, we want to create the **simplest** case, and maybe we can get the **general** idea.

**Two** is the **smallest** number of useful classes: often, this boils down to a **yes-or-no** question. Typically, we **represent** these two choices as  $+1$  and  $-1$ , respectively.

##### Definition 5

**Binary classification** is the **problem** of sorting elements into one of **two categories**.

Often, these categories are defined by a "**yes-or-no**" question.

$$h : \mathbb{R}^d \rightarrow \{-1, +1\}$$

**Example:** You could look at a person and say, "are they sick?" or, "is that a dog"? You can **classify** data in a binary way **based** on those questions.

#### 4.1.5 Classification Performance

And how do we measure how well this model is doing? The easiest way might be, "count the number of wrong guesses".

This is captured by **0-1 Loss**:

##### Definition 6

**0-1 Loss** is a way of measuring **classification** performance: if you get the **wrong** answer, you get a loss of **1**. If you're **right**, then **0** loss.

$$\mathcal{L}(g, a) = \begin{cases} 0 & \text{if } g = a \\ 1 & \text{otherwise} \end{cases}$$

This type of loss is as **simple** as we can get: similar to counting how many wrong answers you get on a **multiple-choice** test.

If we want to get our training error, we'll just average over the data points:

$$\mathcal{E}_n(h) = \frac{1}{n} \sum_{i=1}^n \begin{cases} 0 & \text{if } g_i = a_i \\ 1 & \text{otherwise} \end{cases}$$

Just like before, we care about **testing loss** more than **training loss**: we want our model to **generalize**.

This relies on our typical IID assumption from chapter 1.

$$\mathcal{E}(h) = \frac{1}{m} \sum_{i=n+1}^{n+m} \begin{cases} 0 & \text{if } g = a \\ 1 & \text{otherwise} \end{cases}$$

Next, we figure out what **model** we use to do our classification.

## 4.2 Linear Classifiers

If you wanted to break up your data into two parts (+1 and -1), how might you do it? Let's explore that question.

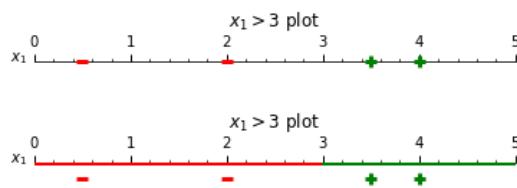
### 4.2.1 1-D Linear Classifiers

As usual, we'll start with the **simplest** case we can think of: 1-D. So, we only have one variable  $x_1$  to **classify** with.

The simplest version might be to just **split** our space in **half**: those above or below a certain **value**. This is our parameter,  $C$ .

$$x_1 > C \quad \text{or} \quad x_1 - C > 0 \quad (4.4)$$

**Example:** For the below data (where green gives positive and red gives negative), could classify positive as  $x_1 > 3$ .



We plot everything above  $x = 3$  as **positive**, and **negative** otherwise.

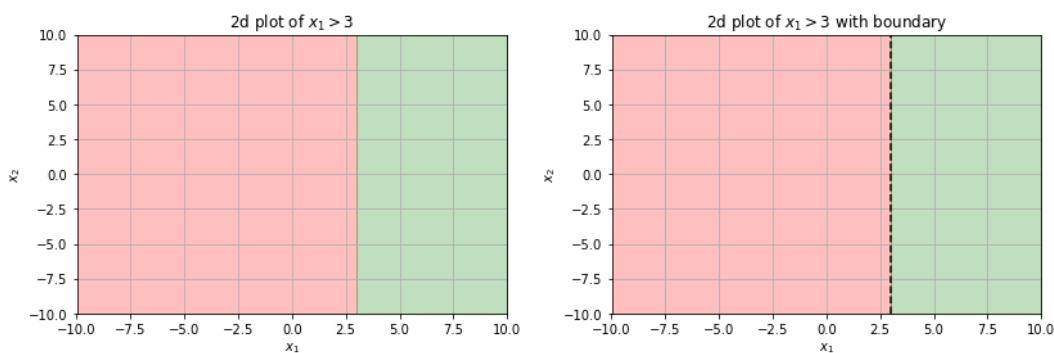
We could also call it  $\theta_0$ , in the spirit of our  $\theta$  notation for parameters.

$$x_1 + \theta_0 > 0 \quad (4.5)$$

### 4.2.2 1-D classifiers in 2-D

Let's add a variable and see how our classifier looks on a 2-D plot.

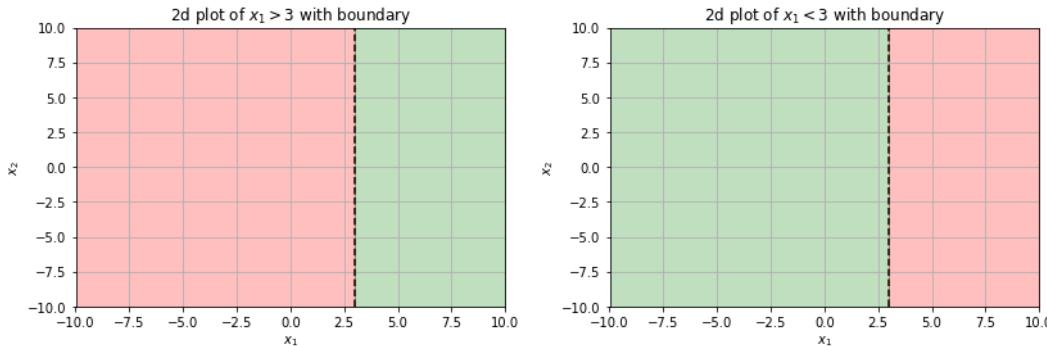
We'll omit the data points for now.



On the right, we've drawn the **dividing** line between our two regions.

Interesting - the **boundary** between positive and negative is defined by a **vertical line**.

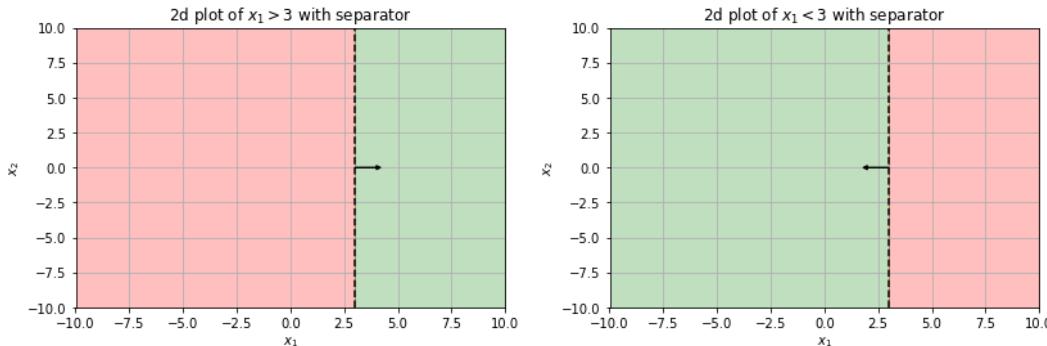
A vertical line is missing some information, though: compare  $x_1 > 3$  and  $x_1 < 3$ :



These two plots have the same line, but have their sides flipped.

So, we have a **line** that gives us the boundary, but we **also** need to include information about which way is the **positive** direction.

What tool best represents **direction**? We could use angles, but we haven't used that much so far. Instead, let's use a **vector** to **point** in the right direction.



Now, it's clear which plot is which, just using our **line** and **vector**!

The object that represents our classification is called a **separator**!

Since our variables are  $x_1$  and  $x_2$ , this is a separator in **input space**.

### Definition 7

A **separator** defines how we **separate** two different classes with our **hypothesis**.

It includes

- The **boundary**: the **surface** where we **switch** from one **class** to another.
- The **orientation**: a **description** of which **side** of the boundary is assigned to **which class**.

For example, let's take our specific separator from above.

### Concept 8

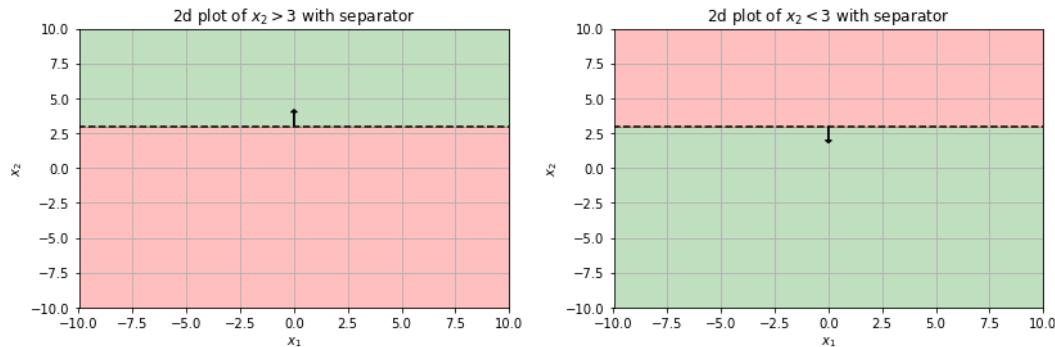
We can define our **1-D separator** using

- The **boundary** between the **positive** and **negative** regions: in 2-D input space, this looks like a vertical or horizontal **line**.
- A **vector** pointing towards whichever side is given a **+1 value**.

We call it "orientation" because you could imagine "flipping over" the space, so the positive and negative regions are swapped.

### 4.2.3 A second 1-D separator, and our problem

What if we use  $x_2$  to **separate** our data?

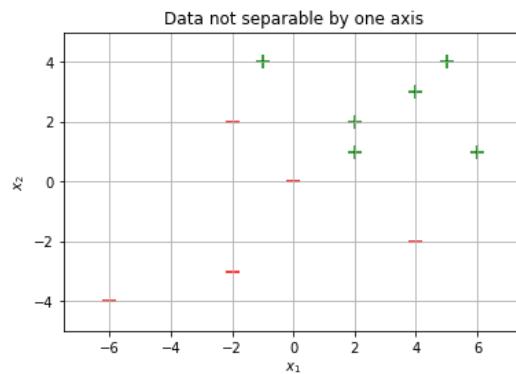


Instead of having a vertical separator, we have a **horizontal** one.

We get the same sort of plot along the **other axis**!

So, this is cool so far, but it's not a very **powerful** model: we can only handle a situation where the data is evenly divided by **one axis**.

And if that's the case, what's the point of our **other** variable?



There's no vertical or horizontal line we can use to split this space!

#### 4.2.4 The 2-D Separator: What vector do we use?

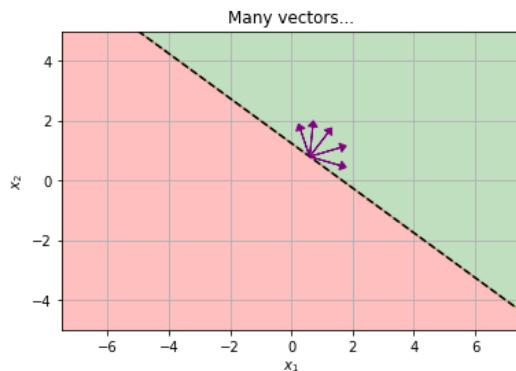
Just looking at our example, we might wonder, "well, if we can use **vertical** lines or **horizontal** lines, can't we just use a line in **another** orientation?"

It turns out, we **can**!



If we allow lines at an angle, we can classify all of our data correctly!

So, we've got our **boundary**. But we still need a vector to tell us which side is **positive**. But there are **many** possible vectors we could choose:



All of these vectors point towards the **correct** side of the plane. Is there a **best** one to use?

Above, we used the vector that was **vertical** or **horizontal**. This makes sense: if we're doing  $x_1 > 3$ , it seems reasonable to have the arrow **point** in the positive- $x_1$  direction.

But this vector also happened to be **perpendicular** to our **line**: this is the line's **normal vector**,  $\hat{n}$ . This vector has a couple nice properties:

- It is **unique**: in 2-D, there is only 1 **normal** direction. The opposite side is just  $-\hat{n}$ .
- It points directly **away** from the plane.
- If our plane is at the **origin**, any point with a **positive**  $\hat{n}$  component is on the **positive** side. This will be important later!

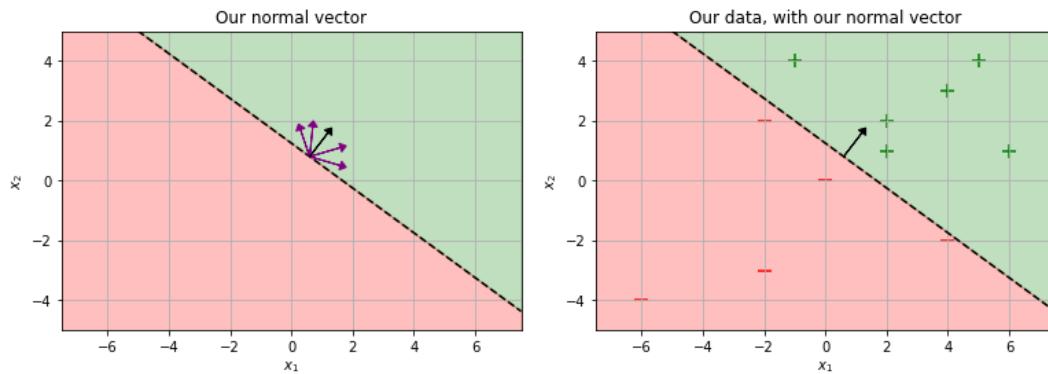
So, we have a **unique** vector that tells us which side is **positive**. Let's go with that!

### Concept 9

Every **line** in 2-D has a **unique normal vector** that can be used to **define** the **angle/direction** of the line.

The **direction** the vector is "facing" is also called the **orientation**.

Our normal vector for the above separator:



We can define our plane using the **normal vector**!

It's clear that this vector in some way is a **parameter**: if we change this vector, we get a different **orientation**, and a different **classifier**.

We have **represented** parameters in the past using  $\theta$ . We need **two** different  $\theta_k$ : one for the  $x_1$  component, another for the  $x_2$  component.

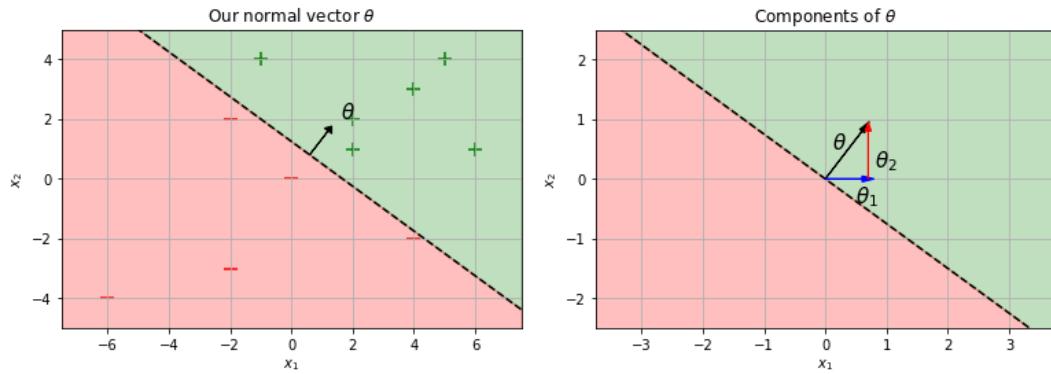
So, we'll use that.

### Notation 10

The vector  $\theta$  represents the **normal vector** to our line in 2D.

$$\hat{\theta} = \theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

We add this to our diagram:

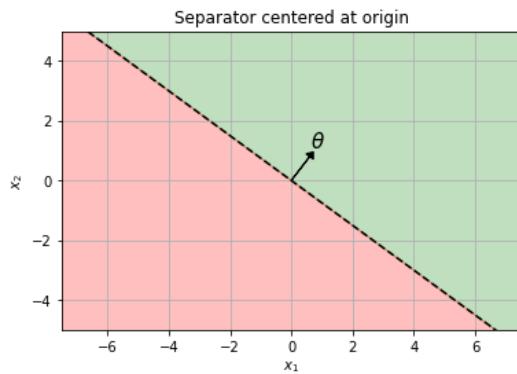


$\theta$  is our normal vector!

Nice work so far. The next question is: how do we describe this separator **mathematically**?

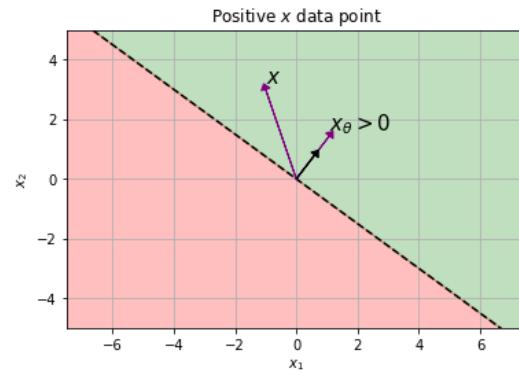
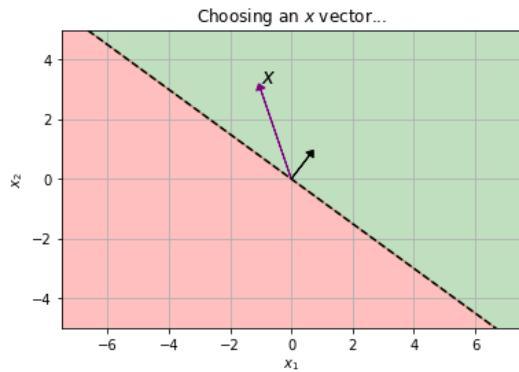
#### 4.2.5 2D Separator - Matching components

As always, we'll **simplify** the problem to make it more manageable: for now, we'll assume our **separator** is centered at the **origin**.

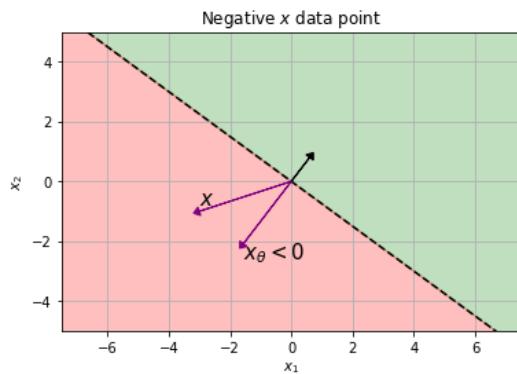


So, we have our vector,  $\hat{n}$ . As we mentioned above, anything on the **same** side as  $\hat{n}$  is **positive**, and anything on the **opposite** side is **negative**.

For a line on the origin, "On the same side of the line" can be interpreted as "has a positive  $\hat{n}$  component". We'll find that component next.



This vector has a **positive** component in the  $\theta$  direction.



This vector has a **negative** component in the  $\theta$  direction.

How do we represent "on the same side" mathematically? How do we **find** whether the component is **positive or negative**? We use the **dot product**.

#### 4.2.6 The Dot Product (Review)

How to calculate the dot product should be familiar to you, but we'll talk about some **intuition** that you may not be exposed to.

**Concept 11**

You can use the **dot product** between unit vectors to measure their "similarity": if two vectors are more **similar**, they have a **larger** dot product.

In the most clear cases, take unit vectors  $\hat{a}$  and  $\hat{b}$ :

- If they are in the **exact same** direction,  $\hat{a} \cdot \hat{b} = 1$
- If they are in the **exact opposite** direction,  $\hat{a} \cdot \hat{b} = -1$
- If they are **perpendicular** to each other,  $\hat{a} \cdot \hat{b} = 0$

Remember, **unit vectors** have a length of 1.

What about non-unit vectors?

These unit vectors are then scaled up by the **magnitude** of each of our vectors. Because magnitudes are **always positive**, the dot product sign doesn't change.

**Concept 12**

You can use the **dot product** between non-unit vectors to measure their "similarity" **scaled by their magnitude**.

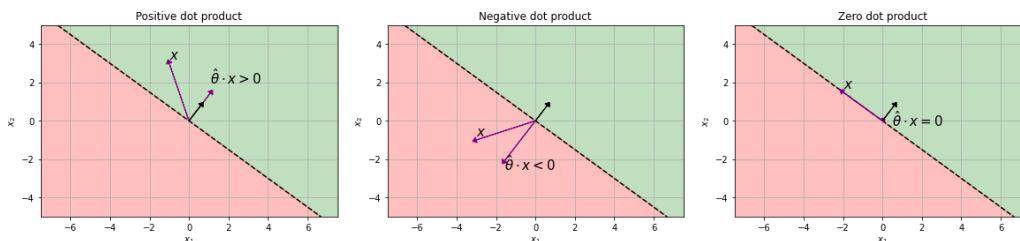
If two vectors are more **similar**, they have a **larger** dot product.

- If the vectors are **less** than  $90^\circ$  apart, they are more similar: they will share a **positive** component:  $\vec{a} \cdot \vec{b} > 0$
- If the vectors are **more** than  $90^\circ$  apart, they will share a **negative** component:  $\vec{a} \cdot \vec{b} < 0$
- If they are **perpendicular** ( $90^\circ$ ) to each other,  $\vec{a} \cdot \vec{b} = 0$

**4.2.7 Using the dot product**

So, the **sign** of the dot product is a useful tool. If a point is on the line, it is **perpendicular** to  $\theta$ , our **normal vector**.

So, if a point has a **positive** dot product, it is on the **same side** as  $\theta$ , and if it's **negative**, it's on the opposite side.



Our various dot products can show us where in the space we are.

So, we can classify things based on the **sign** of it. Written as an equation, we can define the sign function:

### Key Equation 13

For a **linear separator** centered on the **origin**, we can do **binary classification** using the hypothesis

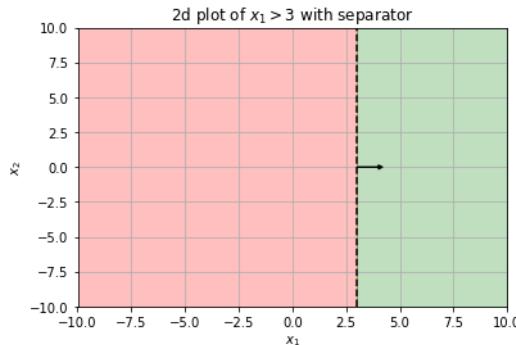
$$h(x; \theta) = \text{sign}(\theta \cdot x) = \begin{cases} +1 & \text{if } \theta \cdot x > 0 \\ -1 & \text{otherwise} \end{cases}$$

- Note that we assigned  $-1$  if  $\theta \cdot x = 0$ .
- This is an **arbitrary** convention: we could also have assigned  $+1$  for  $\theta \cdot x = 0$ .
- All that matters is to have a decision, and be consistent about it.

### 4.2.8 Introducing our offset

Now that we have handled the case where our linear separator is on the **origin**, we want to **shift** our separator **away** from it.

In our **1-D** case, we easily **shifted** away from the origin: any separator  $x_1 > C$  where  $C$  **isn't zero**, we shift by  $C$  units.



By making our inequality  $x_1 > 3$  **nonzero**, we moved away from the origin by 3 units!

We could make our inequality **nonzero**, then! That could move us **away** from the origin, just in a different **direction**.

Or, we could equivalently do this... Note:  $A \iff B$  means A and B are equivalent!

$$x_1 > 3 \iff x_1 - 3 > 0 \quad (4.6)$$

So, instead, we could just add a constant to our expression, which we will call  $\theta_0$ .

We'll also switch out  $\theta \cdot x = \theta^T x$ .

### Key Equation 14

A general **linear separator** can do **binary classification** using the hypothesis

$$h(x; \theta) = \text{sign}(\theta^T x + \theta_0) = \begin{cases} +1 & \text{if } \theta^T x + \theta_0 > 0 \\ -1 & \text{otherwise} \end{cases}$$

- Again, we assigned  $-1$  if  $\theta \cdot x = 0$ .
- Again, this choice is **arbitrary**. Consistency is what matters most.

Notice that this looks very similar to what we did in regression! We'll get into that in a bit.

First, a quick look at the components of our equation:

### Concept 15

For **binary classification**,  $\theta$  and  $\theta_0$  entirely **define** our **linear separator**.

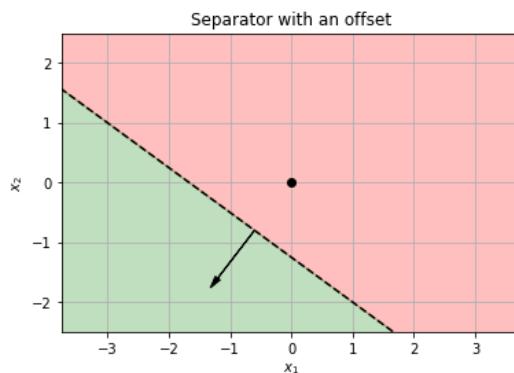
- $\theta$  gives us the **orientation** of our line.
- $\theta_0$  **shifts** that line around in **space**.

### 4.2.9 How does the offset affect our classifier?

So, how exactly does our offset  $\theta_0$  affect our **classifier**? Well, we mark our classifier with our **normal vector** and the **boundary**.

Our **normal vector** is entirely captured by  $\theta$ : it's unchanged by  $\theta_0$ .

What about our **boundary**? We have its **orientation**, but we don't know where it has **shifted** to.



Note that the origin has been marked.

Well, let's use our equation: if your formula is positive, you get +1. If your formula is negative, you get -1.

The **boundary** line is between positive and negative: it's at **zero**.

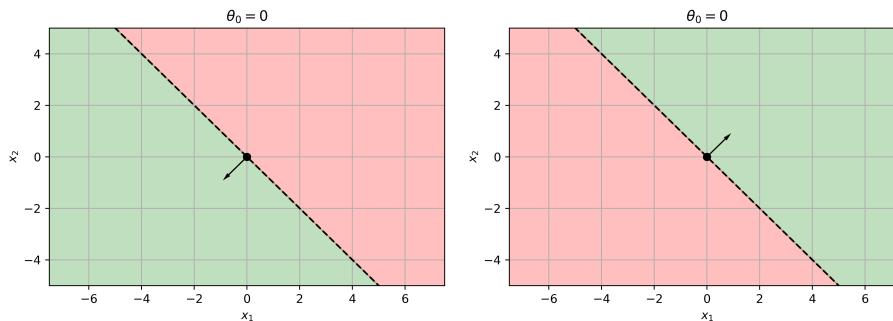
$$\theta^T x + \theta_0 = 0 \iff \theta^T x = -\theta_0 \quad (4.7)$$

We'll break the effects of  $\theta_0$  into three cases: \_\_\_\_\_

For each, we'll show a boundary, and a **flipped** version of that boundary.

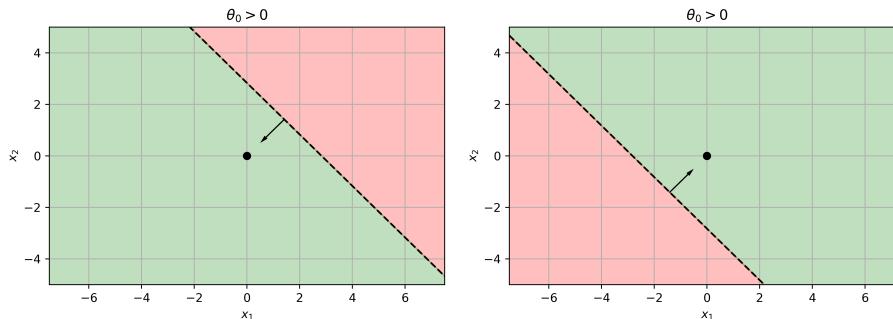
Note: the below statements are true no matter what  $\theta$  we choose!

- If  $\theta_0 = 0$ , then  $x = (0, 0)$  is **on the line**.
  - Without an **offset**, our line goes through the **origin**.



The boundary is on the origin.

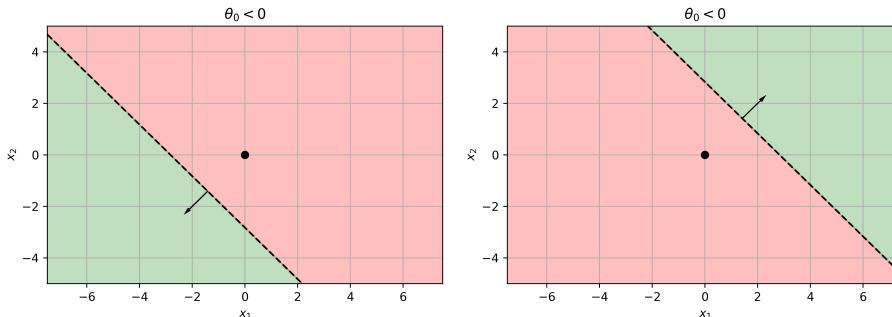
- If  $\theta_0 > 0$ , then the **origin** is in the **positive** region.
  - That means the positive region is "larger": some space that was negative, is positive.
  - The boundary line has moved in the  $-\theta$  direction.



If we have a **positive** constant, it's "easier" to get a positive **result**: more positive space.

- If  $\theta_0 < 0$ , then the **origin** is in the **negative** region.

- That means the positive region is "smaller": some space that was positive, is negative.
- The boundary line has moved in the  $+θ$  direction.



If we have a **negative** constant, it's "harder" to get a positive **result**: more negative space.

This can be a bit confusing, so we'll summarize:

#### Concept 16

The **sign** of our  $\theta_0$  and the **direction** we move away from the origin are **opposite**.

If  $\theta_0 > 0$  (positive), our boundary moves in the  $-θ$  **direction**.

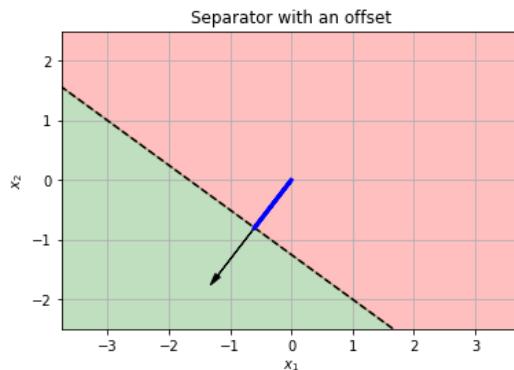
If  $\theta_0 < 0$  (negative), our boundary moves in the  $+θ$  **direction**.

This gives us a general idea of how the offset affects it, but what is the **exact** effect of  $\theta_0$  on the line?

We'll focus on one point on the line: the **closest point to the origin**. We want to look at this **point** because it's **unique**.

Points that aren't unique are hard to keep track of!

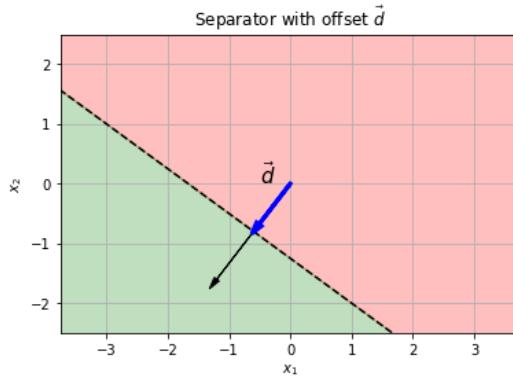
#### 4.2.10 Distance from the Origin to the Plane



Notice that the **shortest** path from the origin to the line is **parallel** to  $θ$ !

So, we can think of our **line** as having been **pushed** in the  $\theta$  direction. This **matches** what we did for 1-D separators:  $x_1 > 3$  was moved in the  $x_1$  direction.

So, we'll take the closest point on the line,  $\vec{d}$ . The **magnitude**  $d$  will give us the **distance** that the separator has been **shifted**.



Since  $\vec{d}$  is in the direction of  $\theta$ , the direction can be captured by the unit vector  $\hat{\theta}$ . Let's take a look at that:

$$\theta = \|\theta\| \hat{\theta} \quad (4.8)$$

Remember, a vector is direction (unit vector) times magnitude (scalar).

$$\vec{d} = d \hat{\theta} \quad (4.9)$$

They're in the same **direction**, so they have the same **unit vector**  $\hat{\theta}$ .

$\vec{d}$  is on the **line**, so it satisfies:

We'll use  $\theta \cdot \vec{d}$  instead of  $\theta^\top \vec{d}$  here.

$$\theta \cdot \vec{d} + \theta_0 = 0 \quad (4.10)$$

We can plug our equations 4.8 and 4.9, where we've separated magnitude from unit vector:

$$\underbrace{(\|\theta\| \hat{\theta})}_{\theta} \cdot \underbrace{(d \hat{\theta})}_{\vec{d}} + \theta_0 \quad (4.11)$$

We can move the scalars  $\|\theta\|$  and  $d$  out of the way of the dot product:

$$\|\theta\| d (\hat{\theta} \cdot \hat{\theta}) + \theta_0 \quad (4.12)$$

We know that  $\hat{\theta} \cdot \hat{\theta} = 1$ :

$$\|\theta\| d + \theta_0 = 0 \quad (4.13)$$

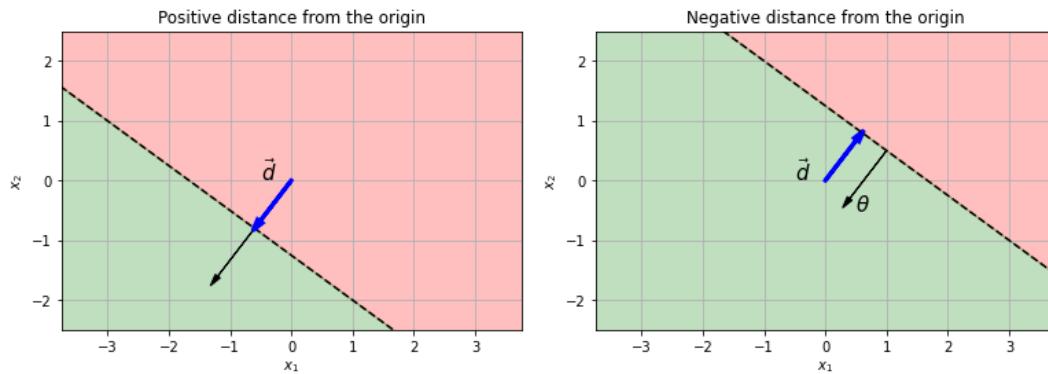
And now, we just solve for d:

### Concept 17

The **distance** d from the **origin** to our **linear separator** is

$$d = \frac{-\theta_0}{\|\theta\|} \quad (4.14)$$

A "negative" distance means  $\vec{d}$  (the vector from the origin to the line) is pointed in the opposite direction of  $\theta$ .



Notice, again, that this agrees with our **earlier** thought: the sign of  $\theta_0$  is the opposite ( $-1$ ) of the  $\theta$  direction we move in.

#### 4.2.11 Extending to higher dimensions

We've now fully conquered the 2D problem! Now, we can move up in **dimensions**.

In terms of equations, the answer is simple, just like it is for regression: just add more terms to  $\theta$ .

**Key Equation 18**

A general d-dimensional **linear separator** can do **binary classification** using the hypothesis

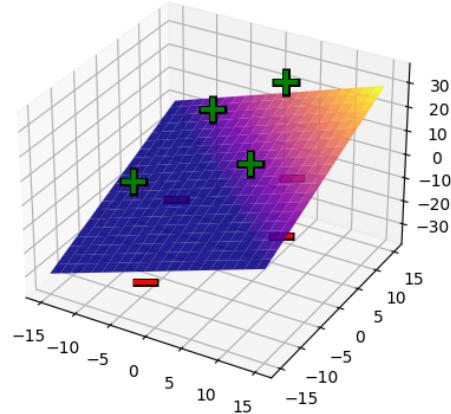
$$h(x; \theta) = \text{sign}(\theta^T x + \theta_0) = \begin{cases} +1 & \text{if } \theta^T x + \theta_0 > 0 \\ -1 & \text{otherwise} \end{cases}$$

Where

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_d \end{bmatrix} \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

What about how it looks? Well, if we have 3 input variables, our line turns into a **plane**:

Classification in 3D



Notice the green + signs are "above" the plane, while the red - signs are "below" the plane.

Just like with regression, this is when we introduce the **hyperplane**:

**Concept 19**

Our  $n$ -dimensional **linear separator** solution to the **binary classification** problem **splits** our space into two **halves**: a positive and a negative half.

The **surface** that **splits** space like this is a  $(n - 1)$ -dimensional **hyperplane**.

The hyperplane is **oriented**: there is a **normal** vector  $\theta$  which defines the **orientation** of the hyperplane, and which side is **positive**.

It also has an **offset** term  $+\theta_0$ , that slides it in the  $-\theta$  direction **away** from the origin.

- $\theta_0$  can be any real number, but the shift will always be in the opposite direction.

For any dimensional input, we can use hyperplanes as separators.

#### 4.2.12 IMPORTANT: A difference between regression and classification

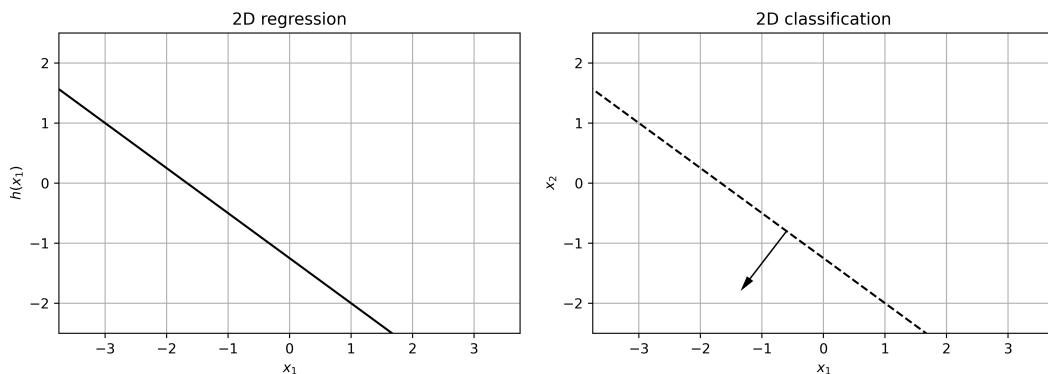
Here is an important misconception that comes up between regression and classification.

Both functions use the equation

$$\theta^T x + \theta_0 \quad (4.15)$$

So, one might think of them as interchangeable.

However, they are **not**. Why is that?



These two plots look almost the same, but represent completely different things!

Notice that these two plots are **both** plotted in 2-D, and both have a **line** plotted. But, they **aren't** as **similar** as they look.

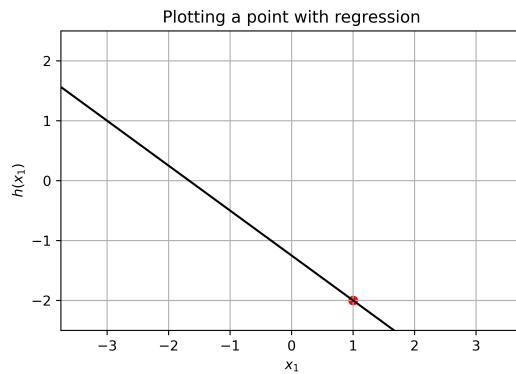
Notice, for example, that the regression plot has **only**  $x_1$ , while the classification plot has  $x_1$  **and**  $x_2$ .

The reason why? The **output**.

- In **regression**, the output is a **real number**: every point on that line represents an input  $x_1$ , and an output  $h(x_1)$ .
  - This plot can only contain **one** input variable: the **second** axis is reserved for the **output!**
- In **classification**, the output is **binary**. So, that line represents only the **values** where the output is  $h(x) = 0$ .
  - This plot can contain **two** input variables:  $x_1$  and  $x_2$ . Rather than **displaying** the output, we only show one **slice** of the output: the  $h(x) = 0$  slice.

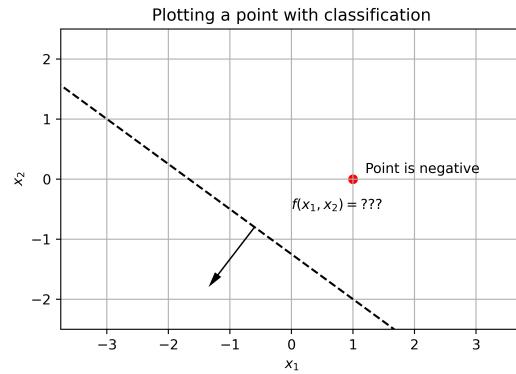
If we think in terms of  $f(x) = \theta^T x + \theta_0$ , we can compare them directly.

The regression plot shows the exact value on the y-axis. If we want to know what  $f(x_1 = 1)$  looks like, we can check the plot: we just get  $f(1) = -2$ .



We have one input, and we get the exact value of our output. We only plot values on the line.

But the classification plot **doesn't!** We aren't given the value of  $\theta^T x + \theta_0$  at  $x = (1, 0)$ : we just know that it's **negative**.



We have two inputs, and we **don't** get the exact output. We can plot inputs anywhere in space.

If we wanted to know the exact value of our 2-D classification, we would need to view it as a plane in 3-D space.

This is the trade-off between these two plots: one gives more information about the **output**, and the other allows for more inputs in a **lower-dimensional** visualization.

### Clarification 20

**Regression** and **classification** plots that look the same, have **different functions**:

When looking at the output of  $f(x) = \theta^T x + \theta_0$ ,

- A **regression** plot gives the **exact numeric**  $f(x)$ .
- A **classification** plot only shows where  $f(x) = 0$ , and the sign of  $f(x)$  elsewhere.

In short:

Regression adds the whole **y number line**, classification only shows  $y = 0$ . This saves **one dimension of space**.

~~~~~

When plotting  $d$  inputs,

- A **regression** plot uses a  **$d+1$**  dimensions ( $d$ -dim hyperplane) to plot: +1 dimension for the **output axis**.
  - **Example:** You have one input dimension,  $d = 1$ . You need to plot the **input and output**: you'll be plotting it on a 2D plane.
  - However, on that 2D plane, you'll plot a **line**: despite existing in 2D space, a line is a 1-d hyperplane.
- A **classification** plot only needs  **$d$**  dimensions (( $d-1$ )-dim hyperplane): we don't need an output axis, because we only plot  **$y = 0$** .
  - **Example:** You have three input dimensions,  $d = 3$ . You'll be plotting every combination of **three inputs** that gives  **$y = 0$** : you'll be plotting it in 3D space.
  - However, in 3D space, you'll plot a **plane**: despite existing in 3D space, a plane is 2-d hyperplane.

**Notation 21**

A  $(d - 1)$ -dimensional hyperplane is a  $d$ -dimensional **separator**.

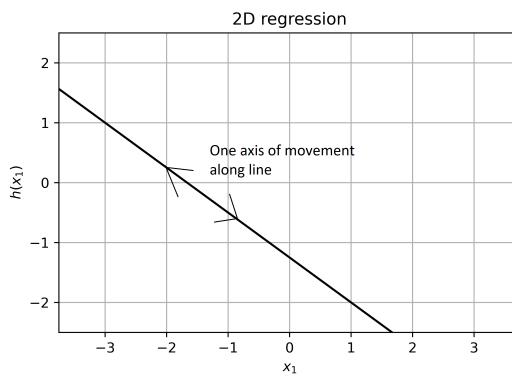
That's because it's **splitting** the  $d$ -dimensional space in half.

- **Example:** A **line** (1-dim) splits the **plane** (2-dim) in half.
- So, it separates the two halves of 2-d space.

Why do we need  $d + 1$  dimensions to plot a  $d$ -dimensional **hyperplane**? Because the hyperplane doesn't fill the whole space.

Here's an example: a **line** in 2-D space is a 1-D **hyperplane**: we have only **one axis** we can move on the line.

It's a 1-d object "embedded" in 2-d space.



Our plot is 2-D, but we can only move along one axis on our line!

- Notice that our line does not fill up the whole space: that's why it's a lower dimension.
- You need 2 dimensions to see **where** the line is, but the line itself is only 1-d.

Because of these differences,  $\theta$  also acts differently:

**Clarification 22**

$\theta$  appears differently in 2-D regression and classification:

- In **2-D regression**,  $\theta$  is the **slope** of the line

$$h(x) = \theta x + \theta_0$$

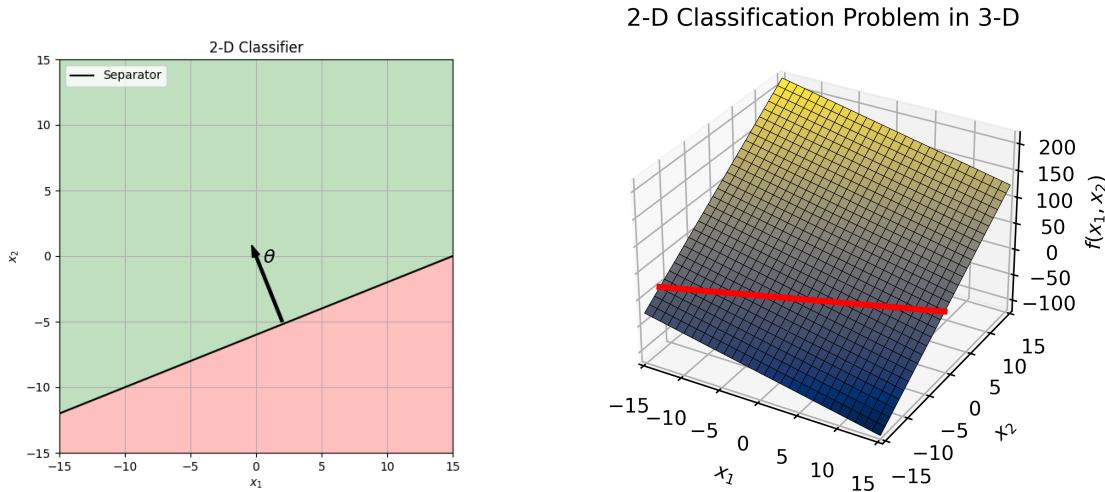
- In **2-D classification**,  $\theta$  is the **normal vector** of the line

$$\theta = \theta^T x + \theta_0$$

### 4.2.13 3d plot of 2d separator

For additional understanding, you might view the full output of  $\theta^T x + \theta_0$ , before we simplify the output to  $\{-1, +1\}$ .

The below plot "reveals" the 3rd dimension (output of  $h(x)$ ) that the classification plot usually hides.



We can **compare** what we usually see (left plot) to an **alternate** version that shows the 3rd dimension (right plot). These are the **same classifier**!

We mentioned before that, if we wanted to show the exact value of  $f(x)$  for our 2-D classifier, we'd need a 3-D plot (just like for regression).

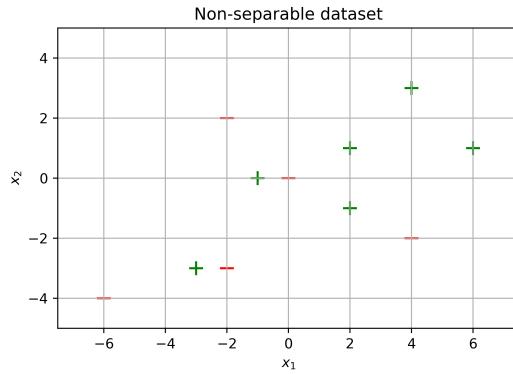
So here, we've done **exactly** that: the **height** is the output of  $h(x)$ .

But, because we don't **care** about the **exact** output in classification, we usually only graph the plane containing the **red line**: where  $f(x_1, x_2) = 0$ .

This shows how we're taking a 2D slice ( $f(x) = 0$ ) out of a 3-D plot (full hyperplane), to **save** on one dimension of **plotting**.

### 4.2.14 Separable vs Non-separable data

One more consideration: **not all** data can be correctly **divided** by a linear separator!



There's no line we could draw through this data to **separate** the points from each other.

If we can, we call it **linearly separable**.

**Definition 23**

A **dataset** is **linearly separable** if you can **perfectly** classify it with a **linear classifier**.

A couple common reasons for data to not be linearly separable:

- A positive and negative data point have the exact **same position** in input space.
- Two points on either **side** of a point with opposite classification:  $+ - +$  or  $- + -$ , for example.

Very often, real-world datasets **can't** linearly separated, because of **complexities** in the real world, or random **noise**.

But, sometimes, we can **almost** linearly separate it: we get very high **accuracy**. In those cases, it may be **fine** to use a linear separator: we might risk **overfitting** if we use a more complex model.

- Still, if a dataset is not **linearly separable**, or at least **high-accuracy** with a linear separator, that could mean we need a **richer** hypothesis class.
- We'll get into ways to make a **richer** class in the **next** chapter: **feature transformations**.

What is "high enough accuracy"? Depends on what you need it for!

Remember: a "richer" or more "expressive" hypothesis class is one that can create more hypotheses that our current one can't!

## 4.3 Linear Logistic Classifiers

### 4.3.1 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  $\mathcal{L}$ :

$$J(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(\text{sign}(\theta^T x^{(i)} + \theta_0), y^{(i)}) \quad (4.16)$$

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**.

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

First, we need to compute the **gradient**.

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

$$\nabla_{\theta} J = 0 \quad (4.17)$$

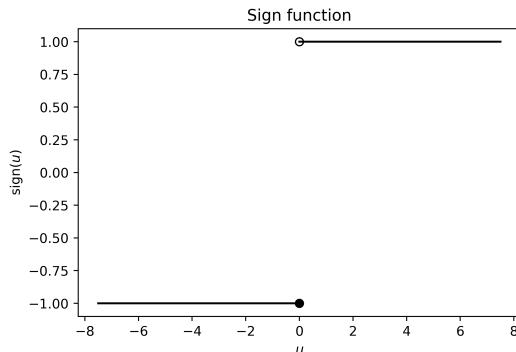
...Well that's not good.

Why not? Because we use our **gradient** to decide **how** to change  $\theta$ .

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

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

If the gradient is 0,  $\theta$  never changes, and we never **improve**  $\theta$  at all!



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.

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.

Remember, parameter space is what we move through as we change our parameter vector  $\theta$ .

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 24

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.

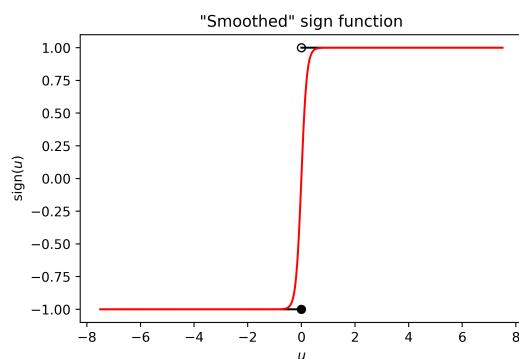
This causes two problems:

- 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 our machine makes.

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

#### 4.3.3 The sigmoid function

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

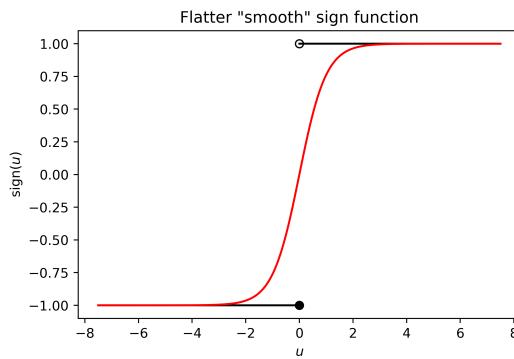


The red line shows a "smoother" sign function, that mostly behaves the same, while solving our problem.

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

We could also make it less steep:

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



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 25

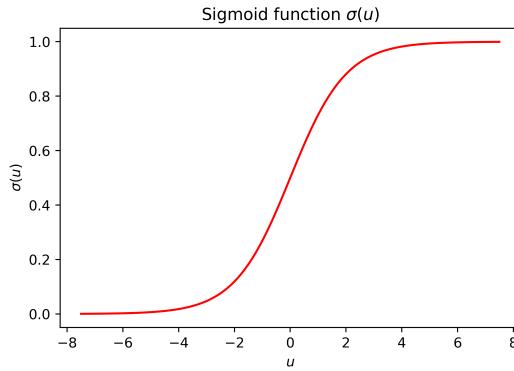
The **sigmoid** function

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

...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:



### 4.3.4 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 26

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

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

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

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

### 4.3.5 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 27

**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:

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

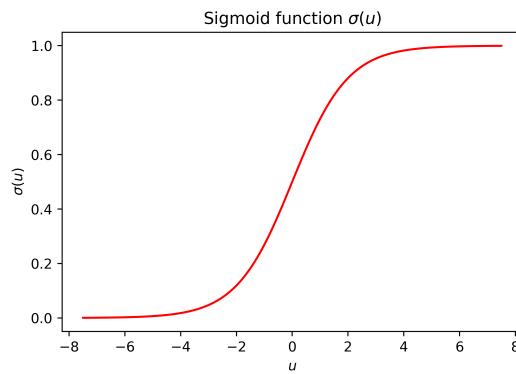
We have a problem, though: **logistic regression** is a... **regression** function. It takes in a real **vector**, and outputs a real **number**:  $\mathbb{R}^d \rightarrow \mathbb{R}$ .

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

#### 4.3.6 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  $u(x) = 0$ .

What happens to  $\sigma$  if  $u = 0$ ?

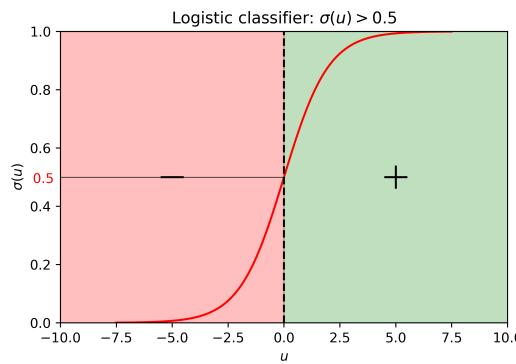


If we go to  $u = 0$  on the x-axis, we find  $\sigma = .5$  on the y-axis.

We get  $\sigma(u = 0) = 0.5$ . So, we could use that as our classification:  $\sigma(u) > 0.5$ .

$$u > 0 \iff \sigma(u) > 0.5 \quad (4.18)$$

If we want to plot the positive and negative regions:



But, we don't necessarily always want to use  $\sigma = 0.5$  as our boundary:

**Example:** Imagine if you wanted to **classify** whether someone needs a **test** for a disease. Classify  $-1$  if we test them,  $+1$  if we don't.

Let's say you got  $\sigma(u) = 0.6$ , so you're only 60% sure they **don't** need it. You'd classify that as  $\sigma(u) > 0.5$ : they're assigned "**no test**".

If the disease is life-threatening, and the test is cheap, then a 40% chance could justify getting the test.

- Whether or not they **should** get that test isn't usually decided by whether the chance is greater than 50%: that's a pretty **arbitrary** number.
- In real life, the **certainty** you want depends on the situation.

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

How expensive is the test? How bad is it, if we don't catch the disease now? Etc.

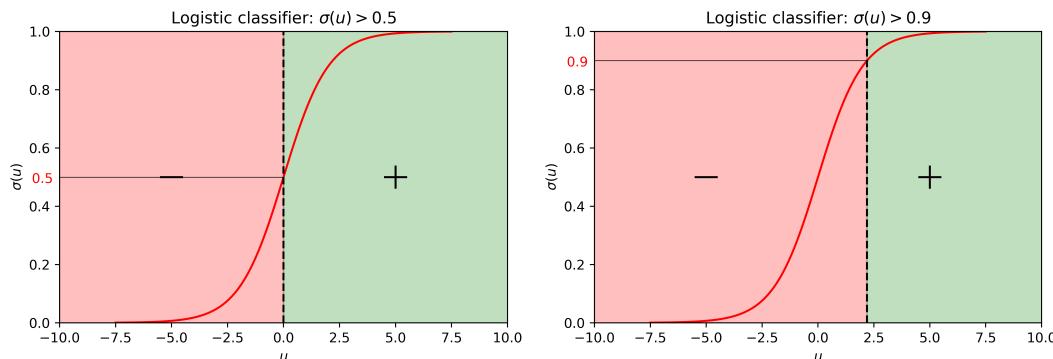
### Definition 28

The **prediction threshold**  $\sigma_{\text{thresh}}$  is the value where you go from **negative** classification to **positive**.

Our **default** value is a threshold of 0.5, but our threshold can be **anywhere** in the range

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

**Example:** If  $\sigma_{\text{thresh}} = 0.9$ , we would see:



We switch from a 0.5 threshold (left) to a 0.9 threshold (right).

In this example, more things will be negatively classified.

#### 4.3.7 Linear Logistic Classifier

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

**Key Equation 29**

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

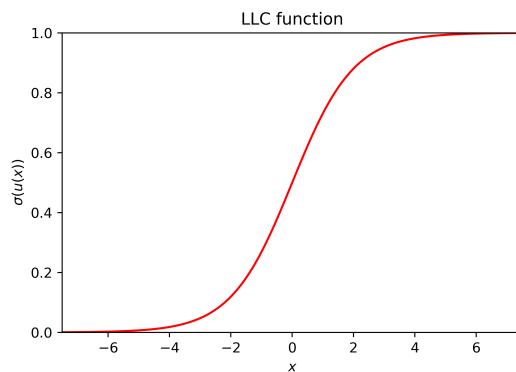
$$u = \theta^T x + \theta_0 \quad \sigma(u) = \frac{1}{1 + e^{-u}}$$

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

### 4.3.8 Modifying our sigmoid

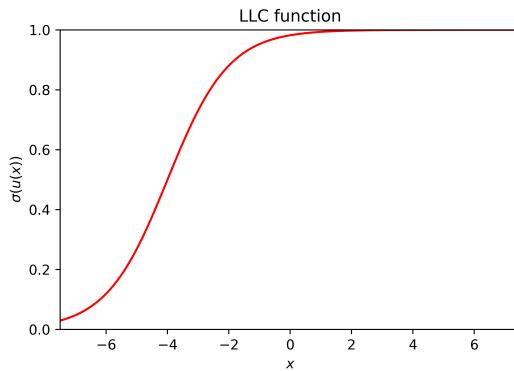
What happens when you modify the **parameters** of an LLC? Let's find out.

We'll use a 1-D input: our variables will be  $\theta$  (scalar) and  $\theta_0$ :  $\theta x + \theta_0$



Our baseline LLC:  $u(x) = 1x + 0$

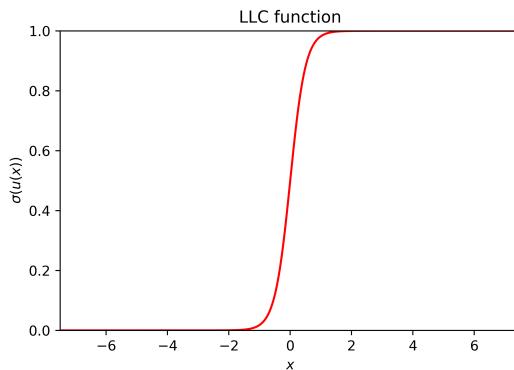
What if we shift by increasing  $\theta_0$ ?



Our shifted LLC:  $u(x) = 1x + 4$ .  $\theta_0$  shifts us along the x-axis!

Just like in linear regression, it **shifts** us in the **opposite** direction: if  $\theta_0$  is **positive**, we shift in the **negative** direction, and vice versa.

What if we increase the magnitude of  $\theta$ ?



Our new LLC:  $u(x) = 4x$ . Increasing  $\theta$  makes our function steeper!

Making the magnitude of  $\theta$  larger makes our function **change** faster.

- This makes some sense: if  $\theta$  (linear slope of  $u(x)$ ) makes  $u(x)$  **change** faster, it will make  $\sigma(u)$  change faster **too**.

You can combine these changes as well: you can shift your LLC with  $\theta_0$ , and also make it steeper/less steep by changing magnitude of  $\theta$ .

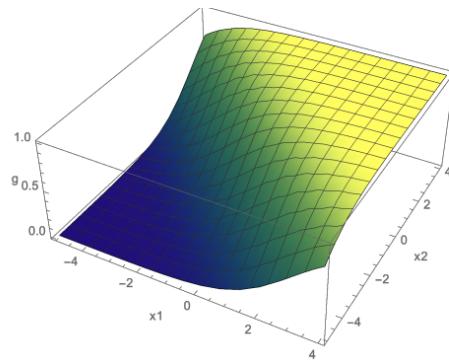
### Concept 30

When working with **sigmoids**, you can **transform** them using your **parameters**:

- A higher **magnitude**  $\|\theta\|$  makes the slope **steeper**, and answers more **confident**.
- **Increasing**  $\theta_0$  **shifts** the sigmoid in the  $-\theta$  **direction**, and vice versa.

### 4.3.9 Viewing our sigmoid in 3D

Let's quickly take a look at a sigmoid in 3D, with two inputs:



As you can see, you get mostly the same shape: if you look at it from the side, it's exactly the same, in fact! Just stretched out into 3D.

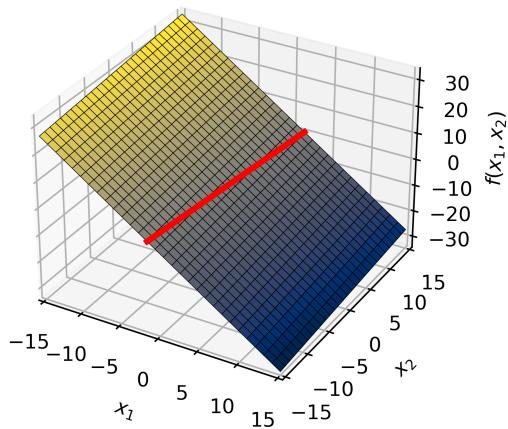
### 4.3.10 LLCs and LCs have the same boundary

One more important thing to note: noticed that we set  $\sigma_{\text{thresh}} = 0.5$ , because that was when  $u(x) = 0$ .

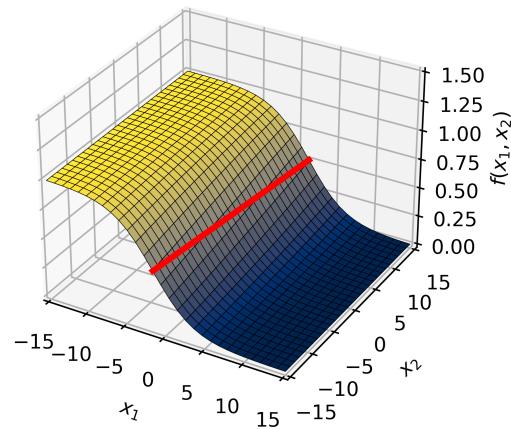
$$u = 0 \iff \sigma(u) = 0.5 \quad (4.19)$$

This means that, if our threshold is 0.5, then the boundary of our LLC should look exactly the same as if it were LC: the only difference is the values that we *can't* see:

2-D Classification Problem in 3-D



2-D Classification Problem in 3-D



Despite having different shapes in 3D, they both create 2-D **linear** classifiers: on the left,  $u(x) = 0$ , and on the right,  $\sigma(u) = .5$ .

One way to think about this difference is that while one may be logistic, they are both

**linear:** they both create the same **linear separator**.

The main benefit of switching to LLC is that  $\sigma(u)$  has a useful **gradient**, while  $\text{sign}(u)$  does **not**, so we can do **gradient descent**.

- Even if we adjust our threshold  $\sigma_{\text{thresh}}$ , that will simply shift the linear classifier.

The probability interpretation is also more appropriate: we usually aren't fully confident in our answers.

### Concept 31

**LLCs** (Linear Logistic Classifiers) and **LCs** (Linear Classifiers) both create a **linear hyperplane separator** in  $d - 1$  dimensional **space**.

If the **threshold value** is 0.5, then they have the **exact same** separator.

- This is because the **same set of inputs**  $x$  that cause  $u(x) = 0$ , will also cause  $\sigma(u(x)) = 0.5$ .
- So, if  $u(x) = 0$  (LC) creates a hyperplane, then  $\sigma(u(x)) = 0.5$  (LLC) will, too.

### 4.3.11 Learning LLCs: Loss Functions

Now that we have fully **built up** LLCs, we can start trying to **train** our own.

In order to do that, we need a way to **evaluate** our hypotheses: a **loss function**.

Earlier in the chapter, we tried **0-1 Loss**:

$$\mathcal{L}_{01}(\mathbf{h}(\mathbf{x}; \Theta), y) = \begin{cases} 0 & \text{if } y = \mathbf{h}(\mathbf{x}; \Theta) \\ 1 & \text{otherwise} \end{cases}$$

But, this **loss** function has the same problem our **sign** function did: it isn't **smooth**!

- It's a **discrete** function based on our **discrete classes**: so, it won't have a smooth **gradient** we can do **descent** on.

For our **sign** function, we switched to the **sigmoid** function, which measures in terms of **probabilities**: this gave us some **smoothness** to our classification.

Could we do the same here?

### 4.3.12 Building our new loss function

So, the **output** of our sigmoid  $\sigma(u)$  is a **probability**: it tells us, "how **likely** do we think a point is to be in class +1?"

We want a loss function

$$\mathcal{L}(g, y) \tag{4.20}$$

That considers two facts: the **correct** answer  $y$ , and how likely we **expected** +1 to be,  $g = \sigma(u)$ .

### Notation 32

For our **loss function**, rather than using  $\hat{y} \in \{-1, +1\}$ , we switch to **probabilities**:  $y \in \{0, 1\}$ .

$$\hat{y} \in \{-1, +1\} \rightarrow y \in \{0, 1\}$$

That way,  $\sigma(u)$  and  $y$  **match**:

$$y \in \{0, 1\} \quad g \in (0, 1)$$

Both represent "the chance that  $\hat{y} = +1$ ".  $\sigma(u)$  makes a prediction, while  $y$  uses the known result:

- If  $\hat{y} = +1$ , there's a **100% chance** that  $\hat{y} = +1$ .
  - So, the "true" output is  $y = 100\% = 1$
- If  $\hat{y} = -1$ , there's a **0% chance** that  $\hat{y} = +1$ .
  - So, the "true" output is  $y = 0\% = 0$

In this problem, it's easier to think in terms of "goodness" of the result. We'll use a "goodness" function  $G(g, y)$ .

- We want the "true" and "predicted" probabilities to be as close as possible.
  - If the correct answer is  $y = 1$ , then we want  $g = \sigma(u)$  to be **high**.
  - If the correct answer is  $y = 0$ , we want  $g = \sigma(u)$  to be **low**.

To get the loss function, we just take the negative of it later.

We represent this as

$$G(g, y) = \begin{cases} g & \text{if } y = 1 \\ 1 - g & \text{else } (y = 0) \end{cases} \quad (4.21)$$

**Remark (Optional) 33**

This loss function can be interpreted as, "if we had a  $g$  chance of picking +1, how often would we have been right?"

- If  $y = 1$ , then we want +1. The chance of choosing +1 is  $g$ .
- If  $y = 0$ , then we want -1. The chance of choosing -1 is  $1 - g$ .

0-1 loss works the same way for a non-random model (one that picks the larger odds every time): what's percentage of the data we get right.

As we mentioned, we'll need to take the negative of this later to get the "loss" function.

### 4.3.13 Loss Function for Multiple Data Points

Now, how do we consider **multiple** data points? Well, let's think in terms of **probability**: guessing each point is a separate **event**.

We *could* add or **average** our guesses. But, since we're working with **probabilities**, there's a natural way to **combine** them: multiple events **occurring** at the same time.

Before, we asked, "how likely were we to be **right**?" for **one** data point. We could **extend** this question to, "how likely are we to get **every** question right?"

Well, each question we get right is an **independent** event  $E_i$ . If we want two independent events to **both** happen, we have to **multiply** their probabilities.

**Key Equation 34**

The probability of two independent events A and B happening at the same time is

$$P\{A \text{ and } B\} = P\{A\} * P\{B\}$$

So if we want **all** of them, we just multiply:

$$P\{E_{\text{all}}\} = P\{E_1\} * P\{E_2\} * \dots * P\{E_n\} \quad (4.22)$$

Written using pi notation, and also  $g^{(i)}$  for multiple data points: \_\_\_\_\_

$$P\{E_{\text{all}}\} = \prod_{i=1}^n P\{E_i\} = \prod_{i=1}^n \begin{cases} g^{(i)} & \text{if } y^{(i)} = 1 \\ 1 - g^{(i)} & \text{if } y^{(i)} = 0 \end{cases} \quad (4.23)$$

Pi notation is described in the prerequisites chapter! The short version: instead of adding terms with  $\sum$ , you multiply with  $\prod$ .

### 4.3.14 Simplifying our expression - Piecewise

Our piecewise function is a bit **annoying**, though: is there a way to **simplify** it so that it doesn't have to be **piecewise**?

Our goal is to **combine** our two piecewise cases into a **single** equation. That means one of them needs to **cancel out** whenever the other is true.

Well, let's see what we have to **work** with.

Our **two** cases happen when  $y = 0$  or  $y = 1$ : these are **nice** numbers! Why? Because of the **exponent** rules for these two:

- $c^0 = 1$ : an exponent of 0 outputs 1: a factor of 1 in a product might as well **not be there**. It has been effectively **cancelled** out.
- $c^1 = c$ : an **exponent** of 1 leaves the factor **unaffected**.

So, let's consider the **first** case,  $g$ . we can use  $\textcolor{red}{g}^y$ : if  $y = 1$ , it's **unaffected**. If  $y = 0$ , the term is **removed**.

We want the **opposite** for  $1-g$ . We can **swap** 1 and 0 by doing  $1-y$ . This gives us  $(1-\textcolor{red}{g})^{1-y}$ .

For one data point:

$$P\{E\} = \underbrace{\textcolor{blue}{g}^y}_{y=1} \underbrace{(1-\textcolor{red}{g})^{1-y}}_{y=0} \quad (4.24)$$

We've gotten rid of the piecewise function! Let's add back in the product:

$$P\{E_{all}\} = \prod_{i=1}^n P\{E_i\} = \prod_{i=1}^n \textcolor{red}{g}^{(i)} \textcolor{blue}{y}^{(i)} (1-\textcolor{red}{g}^{(i)})^{1-\textcolor{blue}{y}^{(i)}} \quad (4.25)$$

Looks pretty ugly, but we'll work on that.

### 4.3.15 Getting rid of the product

Our exponents look pretty **ugly**. Can we do something about that?

- More important than ugliness: **products** are also pretty unpleasant: we can't use **linearity!**

Linearity uses **addition** between variables. What sort of **function** could change a **product** into a **sum**?

Linearity makes lots of problems easy to work with, so we try to keep it.

Well, we could **list** out different basic functions, to see which ones connect sums and products. It turns out, one **interesting** function is

$$\overbrace{\log ab}^{\text{product}} = \overbrace{\log a + \log b}^{\text{sum}} \quad (4.26)$$

Aha! If we take the **log** of our function, we can turn a **product** into the **sum**!

$$\overbrace{\log \left( \prod_{i=1}^n p_i \right)}^{\text{product}} = \overbrace{\sum_{i=1}^n \log(p_i)}^{\text{sum}} \quad (4.27)$$

Plugging in  $p_i = P\{E_i\}$ :

$$\sum_{i=1}^n \log \left( g^{(i)y^{(i)}} (1 - g^{(i)})^{1-y^{(i)}} \right) \quad (4.28)$$

The below equation looks complicated, but all we've done is swap the product for a sum!

We can also separate our two **factors**,  $g^y$  and  $(1 - g)^{1-y}$ .

$$\sum_{i=1}^n \left( \log(g^{(i)y^{(i)}}) + \log((1 - g^{(i)})^{1-y^{(i)}}) \right) \quad (4.29)$$

And finally, we can remove the **exponents**:

$$\sum_{i=1}^n \left( y^{(i)} \log g^{(i)} + (1 - y^{(i)}) \log(1 - g^{(i)}) \right) \quad (4.30)$$

### Concept 35

Our **negative log likelihood** (NLL) comes from a couple steps:

- Use  $y \in \{0, 1\}$  instead of  $y \in \{-1, +1\}$  so that  $y$  and  $g$  have **matching** outcomes.
- Get the **chance** the model is right on every **guess**: a **product**.
- Use **exponents** to convert the **piecewise** expression into a single **equation**.
- Take the **log** of our expression to switch from a **product** to a **sum**.
- Take the **negative** to get the **loss** rather than the "goodness" of our function.

### 4.3.16 Negative Log Likelihood

Remember, at the **beginning**, we said that we need to take the **negative**: our function represents how **good** our function is, but we want the **loss**.

With this, our function is in its final form:

**Key Equation 36**

We can get the loss of our **linear logistic classifier (LLC)** using the **negative log likelihood (NLL)** loss function

$$\mathcal{L}_{\text{nll}}(\mathbf{g}^{(i)}, \mathbf{y}^{(i)}) = -\left( \mathbf{y}^{(i)} \log \mathbf{g}^{(i)} + (1 - \mathbf{y}^{(i)}) \log (1 - \mathbf{g}^{(i)}) \right)$$

Or,

$$-\left( (\text{answer}) \log(\text{guess}) + (1 - \text{answer}) \log(1 - \text{guess}) \right)$$

Our total loss is

$$\sum_{i=1}^n \mathcal{L}_{\text{nll}}(\mathbf{g}^{(i)}, \mathbf{y}^{(i)}) \quad (4.31)$$

Finally, we add our **regularizer**:

$$J_{\text{lr}}(\theta, \theta_0; \mathcal{D}) = \frac{1}{n} \sum_{i=1}^n \left( \mathcal{L}_{\text{nll}}(\mathbf{g}^{(i)}, \mathbf{y}^{(i)}) \right) + \lambda \|\theta\|^2 \quad (4.32)$$

**Key Equation 37**

The full **objective function** for **LLC** is given as

$$J_{\text{lr}}(\theta, \theta_0; \mathcal{D}) = \frac{1}{n} \sum_{i=1}^n \left( \mathcal{L}_{\text{nll}}(\sigma(\theta^T \mathbf{x} + \theta_0), \mathbf{y}^{(i)}) \right) + \lambda \|\theta\|^2$$

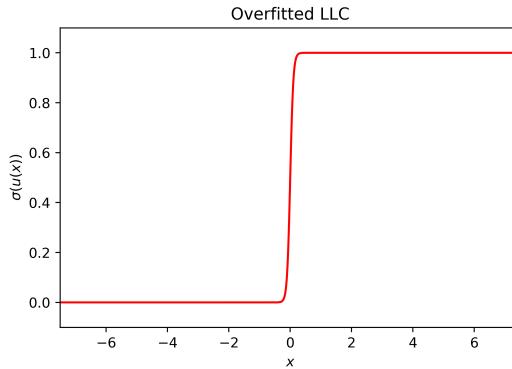
Using our **loss** function  $\mathcal{L}_{\text{nll}}$ , and our **logistic** function  $\sigma(u)$ .

### 4.3.17 LLCs and overfitting

In chapter 2, we reduced **overfitting** by limiting the **magnitude** of  $\theta$  using

$$R(\theta) = \lambda \|\theta\|^2 \quad (4.33)$$

In this chapter, it's more clear why reducing **magnitude** reduces **overfitting**. Let's see what happens when  $\theta$  is very **large**:

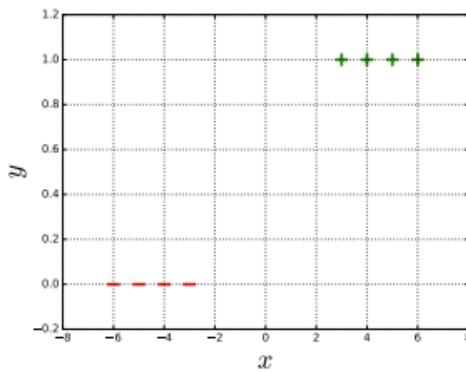


Our "squished" LLC:  $u(x) = 20x$ .

This function starts looking more and more like the **sign** function. This means we very, **very quickly** go from **confident** in one answer, to confident in another.

- If we go from  $x = -0.5$  to  $x = +0.5$ , we go from "incredibly sure of  $-1$ " to "incredibly sure of  $+1$ ".
- That's a small change in input, for a big chance in confidence!

This sort of certainty isn't always appropriate: consider the below example.



In this case, you definitely want to separate the left and right side. Our  $\theta = 20$  separator above, would work just fine.

- But, is it **appropriate**? Let's try to use our model to predict new data.
- If you give that model  $x = 0.5$ , then our model believes  $\hat{y} = +1$  with .99995 confidence.
- When our closest data point to 0 is at  $\pm 3$ , that's unreasonably high certainty.

In other words, the model could create a very sensitive boundary, without having enough data to justify it: this could be a sign of **overfitting**.

Why would we train such an extreme model? Is this even a problem we have to worry about?

It's more serious than you'd expect: we can see why, by consider how our loss function works: here's an excerpt from earlier.

- We want the "true" and "predicted" probabilities to be as close as possible.
  - If the correct answer is  $y = 1$ , then we want  $g = \sigma(u)$  to be **high**.
  - If the correct answer is  $y = 0$ , we want  $g = \sigma(u)$  to be **low**.

The short version: we want to maximize our confidence in the correct answer. This is directly coded into our loss function, and all of the variations.

We just discussed that increasing  $\theta$  will increase your confidence in the answer. So, this loss function encourages our model to make  $\theta$  larger and larger!

So, we need to prevent  $\theta$  from **growing** to an unreasonably high value. Thus, we **penalize** a large  $\|\theta\|$ .

This means we're **penalizing** the machine's **overconfidence** in its answer, so that it **generalizes** better.

### Concept 38

In **classification**, the **regularizer** follows the form

$$R(\theta) = \lambda \|\theta\|^2$$

Regularization in this form reduces **overfitting** to our data by

- Making the **transition** between classifications less **sharp**, when it shouldn't be so **certain** of the boundary.
- It also prevents our model from becoming **overly confident** in its answer.

## 4.4 Gradient Descent for Logistic Regression

### 4.4.1 Summary

Now, we have developed all the tool we need to do binary classification with LLC:

- A **linear** model that lets us combine our **input** variables into a single, predictive **number**:

$$u(x) = \theta^T x + \theta_0 \quad (4.34)$$

- A **logistic** model that turns this **number** into a **probability** of a classification,

$$\sigma(u) = \frac{1}{1 + e^{-u}} \quad (4.35)$$

- A **threshold value** we use to determine how to use this **probability** to **classify**:

$$h(x; \theta) = \begin{cases} +1 & \text{if } \sigma(u(x)) > \sigma_{\text{thresh}} \\ 0 & \text{otherwise} \end{cases} \quad (4.36)$$

- A **loss function** NLL we use to evaluate the **quality** of our **classifications**:

$$\mathcal{L}_{\text{nll}}(g^{(i)}, y^{(i)}) = - \left( y^{(i)} \log g^{(i)} + (1 - y^{(i)}) \log (1 - g^{(i)}) \right)$$

- And an **objective function** we can **optimize** and reduce our **loss**:

$$J_{\text{lr}}(\theta, \theta_0; \mathcal{D}) = \lambda \|\theta\|^2 + \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\text{nll}}(g^{(i)}, y^{(i)}) \quad (4.37)$$

We have everything we need to do optimization.

### 4.4.2 The problem: Gradient Descent

We want to do **gradient descent** to minimize  $J_{\text{lr}}$

$$J_{\text{lr}}(\theta, \theta_0) = R(\theta) + \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\text{nll}}(g^{(i)}, y^{(i)}) \quad (4.38)$$

We want repeatedly **adjust** our model  $\Theta = (\theta, \theta_0)$  to improve  $J_{\text{lr}}$ . To do that, we want the gradients for  $\theta$  and  $\theta_0$ . Let's start with  $\theta$ .

$$\nabla_{\theta} J_{\text{lr}} = \frac{\partial J_{\text{lr}}}{\partial \theta} \quad (4.39)$$

First,  $J_{\text{lr}}$  has **two** terms, so we'll separate them.

$$\nabla_{\theta} J_{lr} = \frac{\partial R}{\partial \theta} + \frac{1}{n} \sum_{i=1}^n \frac{\partial \mathcal{L}_{NLL}}{\partial \theta}(g^{(i)}, y^{(i)}) \quad (4.40)$$

The regularization term is pretty easy, because we did it last chapter:

$$\frac{\partial R}{\partial \theta} = 2\lambda\theta \quad (4.41)$$

But what about our first term?

### 4.4.3 Getting the gradient: Chain Rule

Now, we just need to do

$$\frac{\partial \mathcal{L}_{NLL}}{\partial \theta}(g, y) \quad (4.42)$$

With our  $\mathcal{L}_{NLL}$  term, we run into an issue: how do we take the **derivative**? The function is very, very deeply **nested**. In our case:

$x$  **affects**  $u(x)$ .  $u(x)$  **affects**  $\sigma(u)$ .  $\sigma(u) = g$  **affects**  $\mathcal{L}_{NLL}(g, y)$ , which finally **affects**  $J(\theta, \theta_0)$ .

How do we represent this **chain** of functions? With the **chain rule**:

This next line is a generic chain rule: not specific to our problem.

$$\frac{\partial A}{\partial C} = \frac{\partial A}{\partial B} \cdot \frac{\partial B}{\partial C} \quad (4.43)$$

So, we'll build up a **chain rule** for our needs. We'll use  $g = \sigma(u)$ .

$$\frac{\partial \mathcal{L}_{NLL}}{\partial \theta} = \frac{\partial \mathcal{L}_{NLL}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial \theta} \quad (4.44)$$

Sigma contains  $u$ , so we'll add that to the chain:

$$\frac{\partial \mathcal{L}_{NLL}}{\partial \theta} = \frac{\partial \mathcal{L}_{NLL}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial u} \cdot \frac{\partial u}{\partial \theta} \quad (4.45)$$

This is our full **chain rule**!

#### Key Equation 39

The **gradient** of **NLL** can be calculated using the **chain rule**:

$$\frac{\partial \mathcal{L}_{NLL}}{\partial \theta} = \frac{\partial \mathcal{L}_{NLL}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial u} \cdot \frac{\partial u}{\partial \theta} \quad (4.46)$$

### 4.4.4 Getting our individual derivatives

We can take the derivative of each of these objects. First, let's look at  $\mathcal{L}_{NLL}$

$$\mathcal{L}_{\text{NLL}}(\sigma, y) = - \left( y \log \sigma + (1 - y) \log (1 - \sigma) \right)$$

And we'll use  $\frac{d}{dx} \log(x) = \frac{1}{x}$

$$\boxed{\frac{\partial \mathcal{L}_{\text{NLL}}}{\partial \sigma} = - \left( \frac{y}{\sigma} - \frac{1-y}{1-\sigma} \right)} \quad (4.47)$$

Now, we look at  $\sigma(u)$ :

$$\sigma(u) = \frac{1}{1 + e^{-u}} \quad (4.48)$$

If we take the derivative, we can get:

$$\frac{\partial \sigma}{\partial u} = \frac{-e^{-u}}{(1 + e^{-u})^2} \quad (4.49)$$

Which we can rewrite, conveniently, as

Try this yourself if you're curious!

$$\boxed{\frac{\partial \sigma}{\partial u} = \sigma(1 - \sigma)} \quad (4.50)$$

Finally, our last derivative:

$$u = \theta^T x + \theta_0 \quad (4.51)$$

$$\boxed{\frac{\partial u}{\partial \theta} = x} \quad (4.52)$$

#### 4.4.5 Simplifying our chain rule

So, now, we can put together our chain rule:

$$\frac{\partial \mathcal{L}_{\text{NLL}}}{\partial \theta} = \frac{\partial \mathcal{L}_{\text{NLL}}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial u} \cdot \frac{\partial u}{\partial \theta} \quad (4.53)$$

Plug in the derivatives:

$$\frac{\partial \mathcal{L}_{\text{NLL}}}{\partial \theta} = - \left( \frac{y}{\sigma} - \frac{1-y}{1-\sigma} \right) \cdot \sigma(1 - \sigma) \cdot x \quad (4.54)$$

Simplify:

$$\frac{\partial \mathcal{L}_{\text{NLL}}}{\partial \theta} = ((1 - \mathbf{y})\sigma - \mathbf{y}(1 - \sigma)) \cdot \mathbf{x} \quad (4.55)$$

And finally, we sum the terms. We can do the  $\theta_0$  gradient at the same time: the only difference is that  $\frac{\partial u}{\partial \theta_0} = 1$ , instead of  $x$ .

#### Key Equation 40

The **gradients** of NLL for gradient descent are

$$\nabla_{\theta} \mathcal{L}_{\text{NLL}} = (\sigma - \mathbf{y})\mathbf{x}$$

$$\frac{\partial \mathcal{L}_{\text{NLL}}}{\partial \theta_0} = (\sigma - \mathbf{y})$$

We can plug this into  $J_{\text{lr}}$ :

$$\nabla_{\theta} J_{\text{lr}} = \frac{1}{n} \sum_{i=1}^n \left( (\mathbf{g}^{(i)} - \mathbf{y}^{(i)}) \mathbf{x}^{(i)} \right) + 2\lambda\theta \quad (4.56)$$

One comment we didn't make: remember that  $R(\theta)$  won't show up in the  $\theta_0$  derivative!

$$\frac{\partial J_{\text{lr}}}{\partial \theta_0} = \frac{1}{n} \sum_{i=1}^n (\mathbf{g}^{(i)} - \mathbf{y}^{(i)}) \quad (4.57)$$

We can use this to do **gradient descent**!

$$\theta_{\text{new}} = \theta_{\text{old}} - \eta \nabla_{\theta} J_{\text{lr}}(\theta_{\text{old}}) \quad (4.58)$$

In  $\theta^{(t)}$  notation:

$$\theta^{(t)} = \theta^{(t-1)} - \eta \left( \nabla_{\theta} J_{\text{lr}}(\theta^{(t-1)}) \right) \quad (4.59)$$

$$\theta_0^{(t)} = \theta_0^{(t-1)} - \eta \left( \frac{\partial J_{\text{lr}}(\theta^{(t-1)})}{\partial \theta_0} \right) \quad (4.60)$$

- This chain-rule approach will return when we do Neural Networks in a later chapter.

## 4.5 Handling Multiple Classes

Now, we have developed a **binary** classifier, using logistic regression. But, many (almost all) problems have **more than two classes!**

**Example:** Different animals, genres of movies, sub-types of disease, etc.

### 4.5.1 Approaches to multi-class classification

So, we need to a way to do **multi-classing**. Consider two main approaches:

- Train many binary classifiers on different **classes** and **combine** them into a single model.
  - There are several ways to **combine** these **classifiers**. We won't go over them here, but some **names**: OVO (one-versus-one), OVA (one-versus-all).
- Make **one** classifier that handles the multi-class problem by itself.
  - This model will be a **modified** version of **logistic regression**, using a variant of NLL.

The **latter** approach is what we will use in this **next** section.

### 4.5.2 Extending our Approach: One-Hot Encoding

Rather than being **restricted** to classes 0 and 1, we'll have **k distinct classes**. Our **hypothesis** will be

$$h : \mathbb{R}^d \rightarrow \{C_1, C_2, C_3, \dots, C_k\}$$

Where  $C_i$  is the  $i^{\text{th}}$  class. Meaning, we want to **output** one of those  $k$  **classes**.

Because we'll be using our computer to do **math** to get the **answer**, we need to represent this with **numbers**. Before, we would simply **label** with 0 or 1.

- We could return  $\{1, 2, 3, 4, 5, \dots, k\}$  for each **label**. But this is **not a good idea**: it implies that there's a natural **order** to the classes, which isn't necessarily true.
- If we don't **actually** think  $C_1$  is **closer** to  $C_2$  than to  $C_5$ , we probably shouldn't represent them with numbers that are **closer** to each other.

Instead, each class needs to be a **separate** variable. We can store them in a **vector**:

$$\begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_k \end{bmatrix} \quad (4.61)$$

So, our **label** will be

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix} \quad (4.62)$$

In binary classification, we used 0 or 1 to indicate whether we fit into one **class**. So, that's how we'll do each class: 0 if our data point is **not** in this class, 1 if it **is**.

This approach is called **one-hot encoding**.

#### Definition 41

**One-hot encoding** is a way to represent **discrete** information about a data point.

Our  $k$  classes are stored in a length- $k$  column **vector**. For **each** variable in the vector,

- The value is **0** if our data point is **not in that class**.
- The value is **1** if our data point is **in that class**.

In one-hot encoding, items are **never** labelled as being in **two** classes at the **same time**.

**Example:** Suppose that we want to classify **furniture** as table, bed, couch, or chair.

$$\begin{bmatrix} \text{table} \\ \text{bed} \\ \text{couch} \\ \text{chair} \end{bmatrix} \quad (4.63)$$

For each class:

$$y_{\text{chair}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \quad y_{\text{table}} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad y_{\text{couch}} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad y_{\text{bed}} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad (4.64)$$

### 4.5.3 Probabilities in multi-class

So, we now know our **problem**: we're taking in a data point  $x \in \mathbb{R}^d$ , and **outputting** one of the classes as a **one-hot vector**.

So, now that we know what sorts of data we're **expecting**, we need to decide on the formats of our **answer**.

We'll be returning a vector of length- $k$ : **one** for each **class**. When we were doing **binary** classification, we estimated the **probability** of the positive class.

So, it should make sense to do the same **here**: for each class, we'll return the estimated **probability** of our data point being in that class.

$$g = \begin{bmatrix} P\{x \text{ in } C_1\} \\ P\{x \text{ in } C_2\} \\ \vdots \\ P\{x \text{ in } C_k\} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_k \end{bmatrix} \quad (4.65)$$

We need one **additional** rule: the probabilities need to **add up to one**: we should assume our point ends up in some class or **another**.

$$g_1 + g_2 + \dots + g_k = \sum_i g_i = 1 \quad (4.66)$$

#### Concept 42

The different terms of our **multi-class** guess  $g_i$  represent the **probability** of our data point being in class  $C_i$ .

Because we should assume our data point is in **some** class, all of these probabilities have to **add** to 1.

Let's be careful, though: this is only true for probabilities within a single data point.

**Example:** Suppose you have two animals (data points).

- It's impossible for the first animal to be **both** 90% cat and 90% dog.
- *But*, there's no issue with the first animal being 90% cat and the second animal being 90% dog.

**Clarification 43**

It's only true that all of the probabilities for the **same data point** need to add to 1.

If you have  $P\{\text{class 1}\}$  for one data point and  $P\{\text{class 2}\}$  for another data point, those **aren't related**.

So, we want to scale our values so they add to 1: this is called **normalization**. How do we do that?

Well, let's say each class gets a **value** of  $r_i$ , before being **normalized**. For now, let's ignore how we got  $r_i$ , just know that we have it.

To make the total 1, we'll **scale** our terms by a factor  $C$ :

$$C(r_1 + r_2 + \dots + r_k) = C \left( \sum_{i=1}^k r_i \right) = 1 \quad (4.67)$$

We can get our factor  $C$  just by dividing:

$$C = \frac{1}{\sum r_i} \quad (4.68)$$

We've got our desired  $g_i$  now!

$$g = \begin{bmatrix} r_1 / \sum r_i \\ r_2 / \sum r_i \\ \vdots \\ r_k / \sum r_i \end{bmatrix} \quad (4.69)$$

#### 4.5.4 Turning sigmoid multi-class

Now, we just need to compute  $r_i$  terms to plug in. To do that, we'll see how we did it using sigmoid:

$$g = \sigma(u) = \frac{1}{1 + e^{-u}} \quad (4.70)$$

This function is 0 to 1, which is good for being a probability.

Just for our convenience, we'll switch to positive exponents: all we have to do is multiply by  $e^u/e^u$ .

Negative numbers are easy to mess up in algebra.

$$g = \frac{e^u}{e^u + 1} \quad (4.71)$$

We'll think of **binary** classification as a **special case** of **multi-class** classification. The above probability could be thought of as  $g_1$ : the probability for our first class.

**Concept 44**

**Binary classification** is a **special** case of **multi-class** classification with only **two** classes.

So, we can use it to figure out the **general** case.

So, what was our **second** probability,  $1 - g$ ? This will be our second class,  $g_2$ .

$$g_2 = 1 - g = \frac{1}{1 + e^u} \quad (4.72)$$

This follows an  $r_i / (\sum r_i)$  format! The numerators (1 and  $e^u$ ) add to **equal** the denominator ( $1 + e^u$ ).

$$g = \begin{bmatrix} e^u / (e^u + 1) \\ 1 / (e^u + 1) \end{bmatrix} = \begin{bmatrix} r_1 / (r_1 + r_2) \\ r_2 / (r_1 + r_2) \end{bmatrix} \quad (4.73)$$

How do we **extend** this to **more** classes? Well, 1 and  $e^u$  are **different** functions: this is a problem. We want to be able to **generalize** to many  $r_i$ .

How do they make them **equivalent**? We could say  $1 = e^0$ . So, we could treat both terms as **exponentials**!

$$g_1 = \frac{e^u}{e^u + e^0} \quad g_2 = \frac{e^0}{e^u + e^0} \quad (4.74)$$

What if we want more classes? We just need more exponentials! They'll fit into the pattern from  $e^u$  and  $e^0$ :

$$g_i = \frac{r_i}{\sum r_j} = \frac{e^{u_i}}{\sum e^{u_j}} \quad (4.75)$$

Now, we have a template for expanding into higher dimensions!

### 4.5.5 Our Linear Classifiers

What are each of those  $u_i$  terms? When we were doing **binary classification**, we used a **linear regression** function to help generate the probability:

$$u(x) = \theta^T x + \theta_0 \quad (4.76)$$

Remember that  $u(x)$  is not a probability yet: we use a sigmoid to turn it *into* a probability.

Now, we want multiple probabilities. So, we create multiple different functions  $u_i$ :  $k$  different linear regression models  $(\theta, \theta_0)$ . We'll represent each vector as  $\theta_{(i)}$ .

$$\theta_{(1)} = \begin{bmatrix} \theta_{1(1)} \\ \theta_{2(1)} \\ \vdots \\ \theta_{d(1)} \end{bmatrix} \quad \theta_{(2)} = \begin{bmatrix} \theta_{1(2)} \\ \theta_{2(2)} \\ \vdots \\ \theta_{d(2)} \end{bmatrix} \quad \theta_{(k)} = \begin{bmatrix} \theta_{1(k)} \\ \theta_{2(k)} \\ \vdots \\ \theta_{d(k)} \end{bmatrix} \quad (4.77)$$

Each of these models could be seen as a "different perspective" of our data point: what about that data point is **prioritized** (large  $\theta_i$  magnitudes), and how do we **bias** the result ( $\theta_0$ )?

This "perspective" we call  $\theta_{(i)}$  will tell us if our data point is "closer" to the **class** it represents

$$u_1(x) = \theta_{(1)}^T x + \theta_{0(1)} \quad u_2(x) = \theta_{(2)}^T x + \theta_{0(2)} \quad u_k(x) = \theta_{(k)}^T x + \theta_{0(k)} \quad (4.78)$$

These equations allow us to directly compute each  $u_i$ .

- Intuitively, if  $u_i(x)$  is **larger than**  $u_j(x)$ , then our data point  $x$  is **more similar to** class  $i$  than class  $j$ .

In the last section, we emphasized that we can only use  $\sum p_i = 1$  for the probabilities of a **single** data point. Based on this, we'll focus on only one data point.

#### Clarification 45

In this section,  $x$  represents only **one data point**  $x^{(i)}$ .

Softmax treats each data point **individually**, so it's easier to not group them together.

Having all these separate equations for  $\theta_i$  is tedious. Instead, we can combine them all into a  $(d \times k)$  **matrix**.

$$\theta = \begin{bmatrix} \theta_{(1)} & \theta_{(2)} & \cdots & \theta_{(k)} \end{bmatrix} = \begin{bmatrix} \theta_{1(1)} & \theta_{1(2)} & \cdots & \theta_{1(k)} \\ \theta_{2(1)} & \theta_{2(2)} & \cdots & \theta_{2(k)} \\ \vdots & \vdots & \ddots & \vdots \\ \theta_{d(1)} & \theta_{d(2)} & \cdots & \theta_{d(k)} \end{bmatrix} \quad (4.79)$$

k classes, so we need k classifiers. We'll stack them side-by-side like how we stacked multiple data points to create X.

And our constants,  $\theta_0$ , in a  $(k \times 1)$  matrix:

$$\theta_0 = \begin{bmatrix} \theta_{0(1)} \\ \theta_{0(2)} \\ \vdots \\ \theta_{0(k)} \end{bmatrix} \quad (4.80)$$

**Concept 46**

We can combine **multiple classifiers**  $\Theta_{(i)} = (\theta_{(i)}, \theta_{0(i)})$  into large **matrices**  $\theta$  and  $\theta_0$  to compute **multiple** outputs  $u_i$  at the **same** time.

This will put all of our terms into a  $(1 \times k)$  vector  $u$ .

$$u(x) = \theta^T x + \theta_0 = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_k \end{bmatrix} \quad (4.81)$$

Which creates a deceptively simple formula: this is one of the perks of matrix multiplication!

### 4.5.6 Softmax

We now have all the pieces we need.

- Our **linear regression** for each class:

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_k \end{bmatrix} = \theta^T x + \theta_0 \quad (4.82)$$

- The **exponential** terms, to get **logistic** behavior

$$r_i = e^{u_i} \quad (4.83)$$

- The **averaging** to get the probabilities to add to 1:

$$g = \begin{bmatrix} r_1 / \sum r_i \\ r_2 / \sum r_i \\ \vdots \\ r_k / \sum r_i \end{bmatrix} \quad (4.84)$$

And so, our multiclass function is...

**Definition 47**

The **softmax function** allows us to calculate the probability of a point being in each class:

$$g = \begin{bmatrix} e^{u_1} / \sum e^{u_i} \\ e^{u_2} / \sum e^{u_i} \\ \vdots \\ e^{u_k} / \sum e^{u_i} \end{bmatrix}$$

Where

$$u_i(x) = \theta_{(i)}^T x + \theta_{0(i)} \quad (4.85)$$

If we are forced to make a **choice**, we choose the class with the **highest probability**: we return a **one-hot encoding**.

### 4.5.7 NLLM

One loose end left to tie up: our **loss function**. We need to evaluate our hypothesis, and be able to improve it.

For **binary classification**, we did **NLL**:

$$\mathcal{L}_{\text{nll}}(g, y) = - \left( y \log g + (1 - y) \log (1 - g) \right)$$

How do we make this work in **general**? Well, we want to make our two terms have a **similar** form, so we can generalize to more classes.

- $g$  and  $1 - g$  are both **probabilities**: we can think of them as  $g_1$  and  $g_2$ , respectively.
  - If  $g = g_1$ , then we would expect  $y = y_1$ .
  - Similarly,  $1 - g = g_2$  pairs with  $1 - y = y_2$ .

$$\mathcal{L}_{\text{nll}}(g, y) = - \left( y_1 \log g_1 + (y_2) \log (g_2) \right)$$

They have the **same** format now! Much tidier. And it tracks: when one **label** is correct, the other term is  $y_j = 0$ , and **vanishes**.

Does this **generalize** well? It turns out it does: with **one-hot encoding**, the correct label is **always**  $y_j = 1$ , and the incorrect labels are **all**  $y_j = 0$ .

So, we'll write it out:

#### Key Equation 48

The **loss** function for **multi-class** classification, **Negative Log Likelihood Multiclass (NLLM)**, is written as:

$$\mathcal{L}_{\text{NLLM}}(\mathbf{g}, \mathbf{y}) = - \sum_{j=1}^k y_j \log(g_j)$$

Because of **one-hot encoding** for  $y$ , all terms except one have  $y_j = 0$ , and thus **vanish**.

Using all of these functions, we can finally do gradient descent on our multi-class classifier. However, we won't go through that work in these notes.

#### 4.5.8 A side comment: Sigmoid vs. Softmax

Let's jump back to softmax real quick and clarify something.

Usually, we expect to use **softmax** if we have **more than 2** classes, because that's what we built it for.

- However, this isn't always the case – there's another aspect of softmax we haven't focused on:
- **Softmax** represents  $k$  different classes/events. These classes are assumed to be **mutually exclusive**: you can't be in multiple at the same time.

In other words, the classes of softmax are **disjoint**.

#### Definition 49

If two events are **disjoint**, they **can't** happen at the **same time**.

If  $n$  events are **disjoint**, only **one** of them can happen at a time.

**Example:** We usually wouldn't classify an animal as both a cat and a dog: it's either one or the other.

When events are disjoint, their probabilities are separate:

**Concept 50**

If two events are **disjoint**, then they have **separate** probabilities: there's no overlap. Since  $P\{A \cap B\} = 0$ , we can say:

$$P\{A \cup B\} = P\{A\} + P\{B\}$$

If we have **every** event and they're all **disjoint**, then their probabilities sum to 1.

$$\sum_i p_i = 1 \quad (4.86)$$

**Example:** If the weather options are rain, cloudy, and sunny, and you have to only choose one, you should expect that:

$$P\{\text{Rain}\} + P\{\text{Cloudy}\} + P\{\text{Sunny}\} = 1 \quad (4.87)$$

~~~~~  
But this only makes sense **if** events can't happen at the same time.

- In some situations, multiple classes/events can happen at the same time! They might even be **independent**.
- **Example:** There might be  $k$  different people we could find in an **image**. But, there can be multiple people in the **same** image!

So, it doesn't always make sense to assume that each event is **mutually exclusive**.

- If our events are not mutually exclusive, then we **shouldn't use softmax**.

The solution: for each class, find the **probability** for that class, vs. the **absence** of that class.

- This brings us back to binary classification: we just use **one sigmoid per class**.

**Clarification 51**

**Softmax** is used when each of our  $k$  classes is **disjoint** (mutually exclusive).

- However, if they aren't, then we **can't use softmax**.

~~~~~  
If our classes are independent, we can use  $k$  **sigmoid** functions: one for each of our  $k$  classes. We're using **binary classification** on each class separately.

- The  $i^{\text{th}}$  sigmoid tells us how likely the **data point** is to be in the  $i^{\text{th}}$  class.

**Example:** We might have an algorithm figuring out which **products** a customer might want. They might want **multiple**, so we can't treat them as disjoint.

In this case, each product is a class, and we determine the result based on the matching sigmoid

What happens if the events aren't disjoint, but they also aren't independent? You need a more complex model.

## 4.6 Prediction Accuracy and Validation

We've been working in **probabilities**, but in the end, the goal is usually to make a **decision** or **prediction**: which class do we pick?

In general, we just pick the class we predict with the **highest** probability.

And in practice, we often don't care about how close we were to right - we just care about how often we **were** right.

So, we use **accuracy**.

### Definition 52

The **accuracy**  $A$  of our model is the **percentage** of the time we get the **right** answer.

We can write this as

$$A(h; D) = 1 - \frac{1}{n} \sum_{i=1}^n \mathcal{L}(h(x^{(i)}), y^{(i)})$$

Where  $\mathcal{L}$  is 0-1 loss (**counting** the number of **wrong** answers)

Or, "one minus how often we get the answer **wrong**".

## 4.7 Terms

- Class
- Classification
- Label
- Binary Classification
- 0-1 Loss
- Linear Classifier
- Separator
- Orientation
- Boundary
- Normal Vector
- Dot Product (Conceptual)
- Linear Separator
- Sign Function
- Hyperplane
- Separability
- Non-separable data
- Sigmoid Function
- Logistic Regression
- Prediction Threshold
- Linear Logistic Classifier (LLC)
- Negative Log Likelihood (NLL)
- Multi-class Classification
- One-Hot Encoding
- Normalization
- Softmax Function
- Negative Log Likelihood Multi-Class (NLLM)
- Accuracy