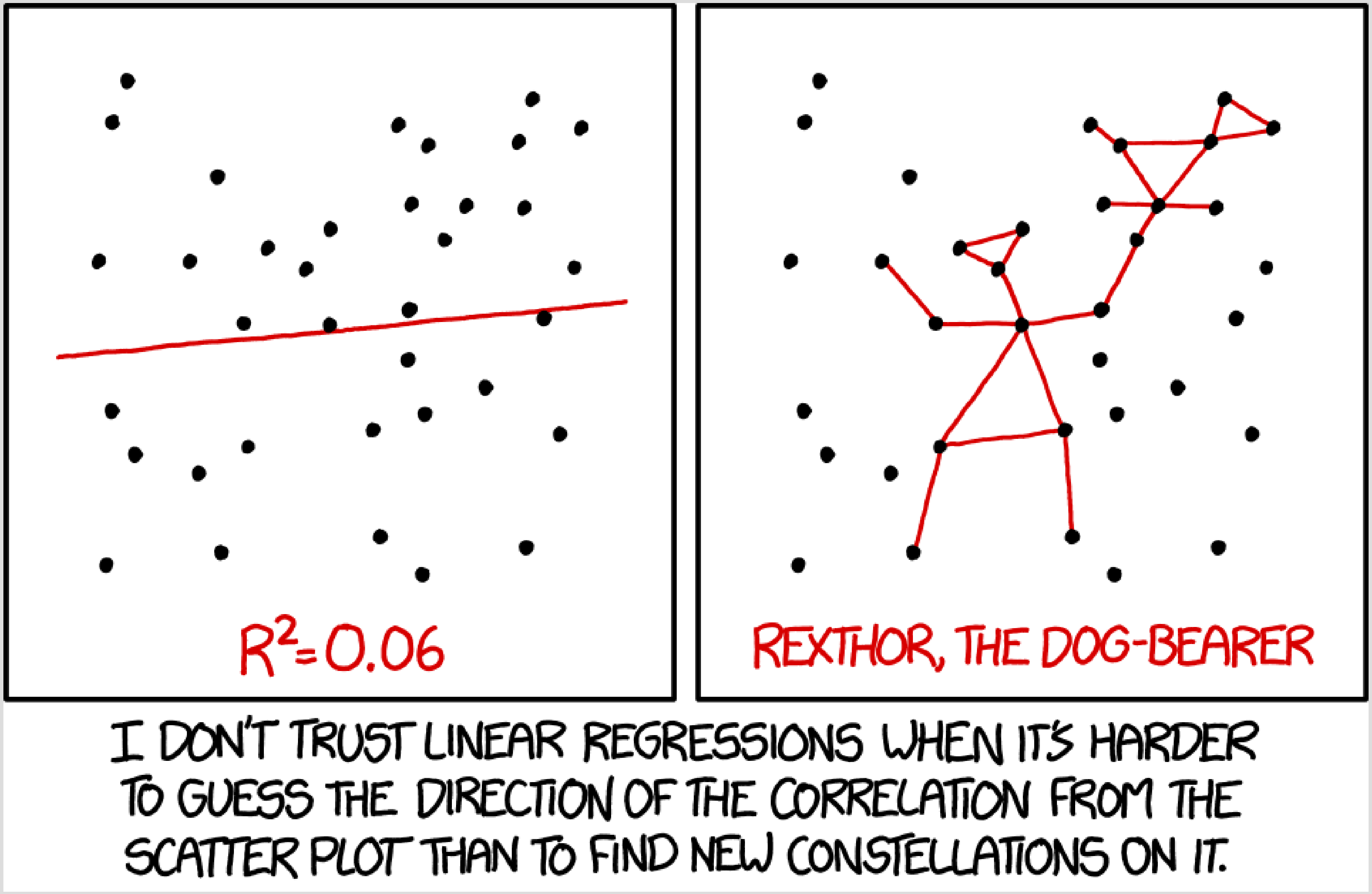
Linear Regression/Classification (Ch. 18.6-18.7)


$R^2 = 0.06$
REXTHOR, THE DOG-BEARER
I DON'T TRUST LINEAR REGRESSIONS WHEN IT'S HARDER TO GUESS THE DIRECTION OF THE CORRELATION FROM THE SCATTER PLOT THAN TO FIND NEW CONSTELLATIONS ON IT.

Linear Regression

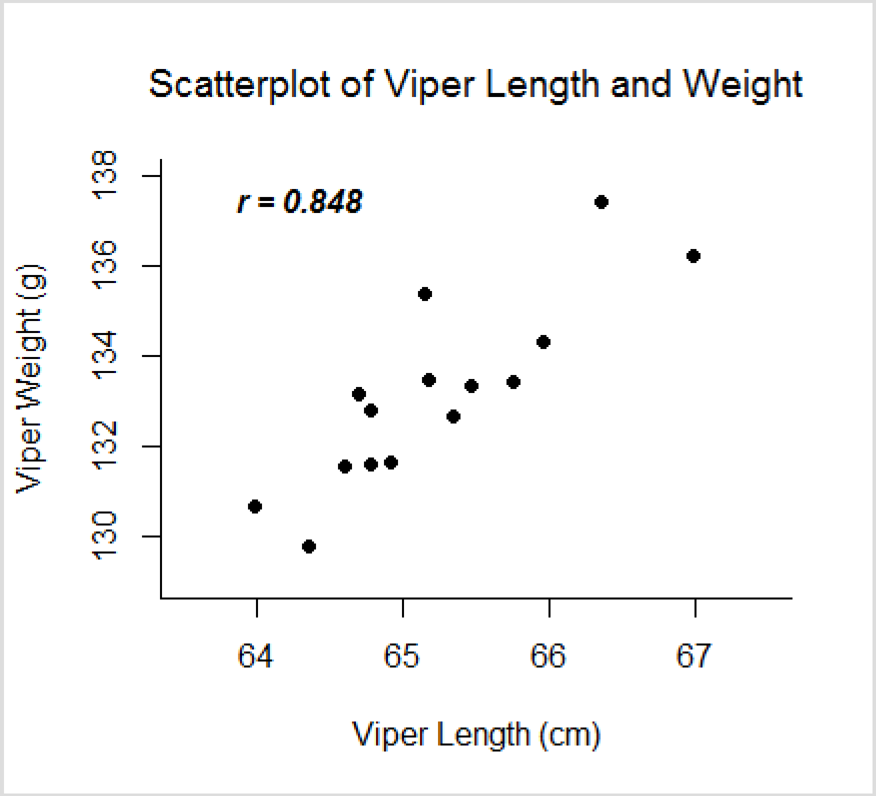
Let’s move away from decision trees (yay!) and talk about more general learning

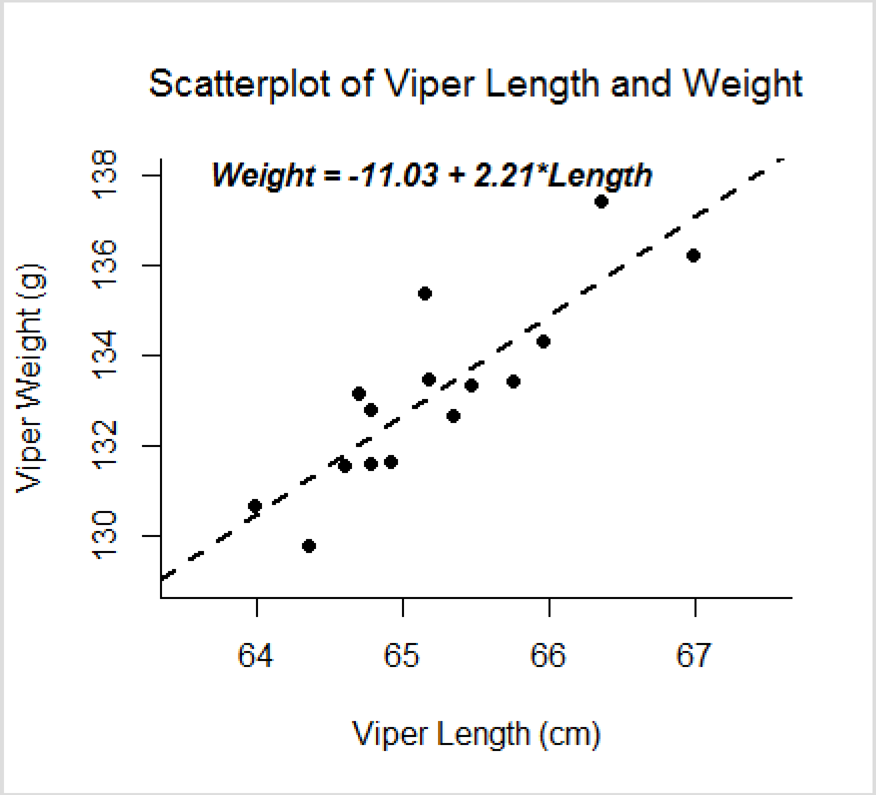
Today we will look at regression a bit (as I have been ignoring it mostly)

This is a concept that you may have encountered before, but not in the context of learning

Linear Regression

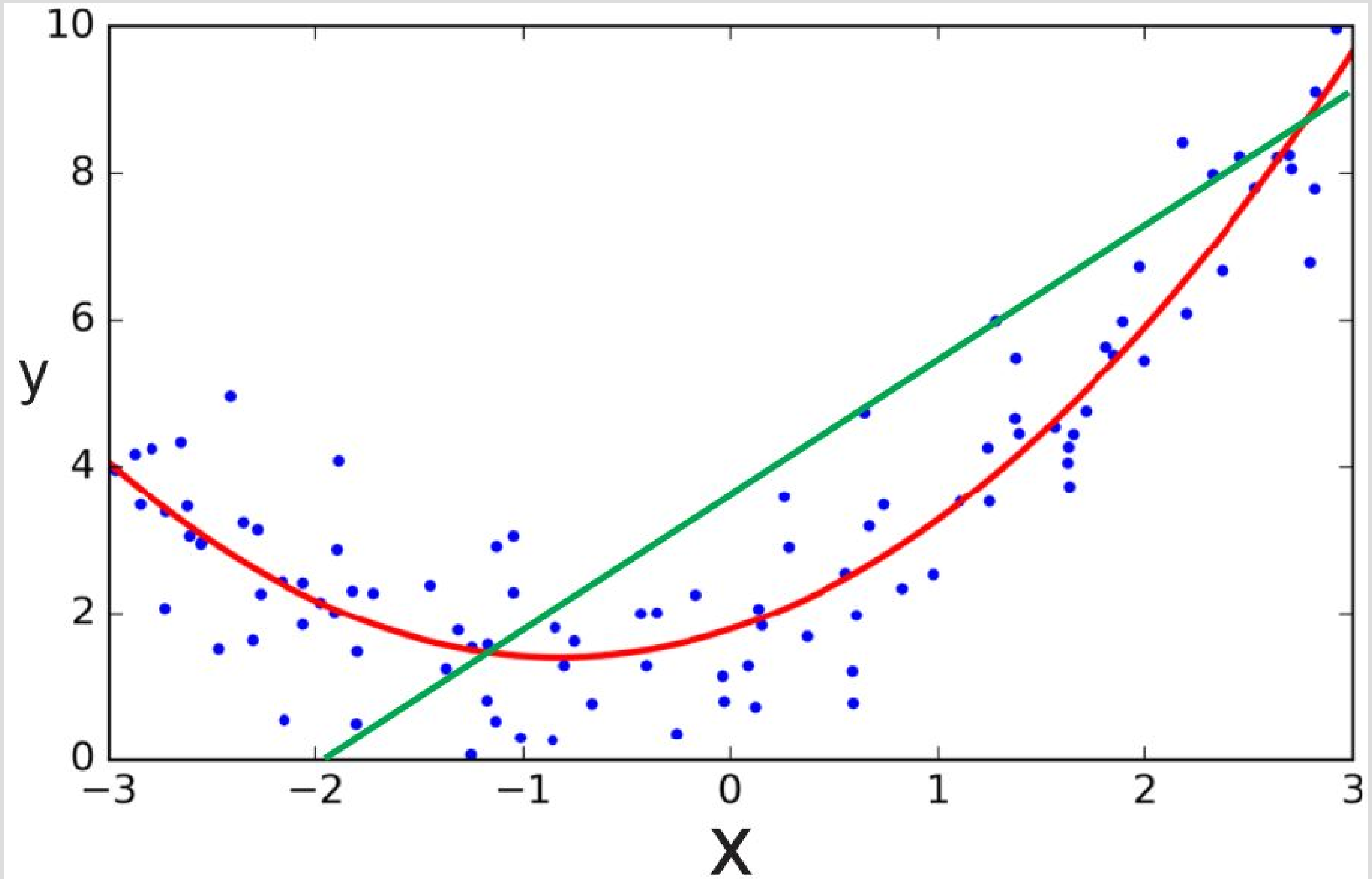
Idea: You have a bunch of data points, and you want to find the line “closest” to them





Linear Regression

Why linear and not some polynomial?



Linear Regression

Why linear and not some polynomial?

It is a lot harder to “overfit” with a linear fit, yet it still gets the major “trend” of data

Also hard to “visualize” data if high dimension

Another bonus is that it makes the calculations much easier (which is always nice...)

Linear Regression: How To

To find this line, let's start with the simple case: only one variable

Then our line will look like (call them "h" just like our learning trees):

$$h_w(x) = y = w_0 + w_1 \cdot x$$

w is $\{w_0, w_1\}$ as parameters

Then we need to define what "fit to data" means (i.e. how do we calculate how "wrong" a line is, often called the "<u>loss</u>")

Linear Regression: How To

There are multiple options, but a common choice is the square difference, so “loss” is:

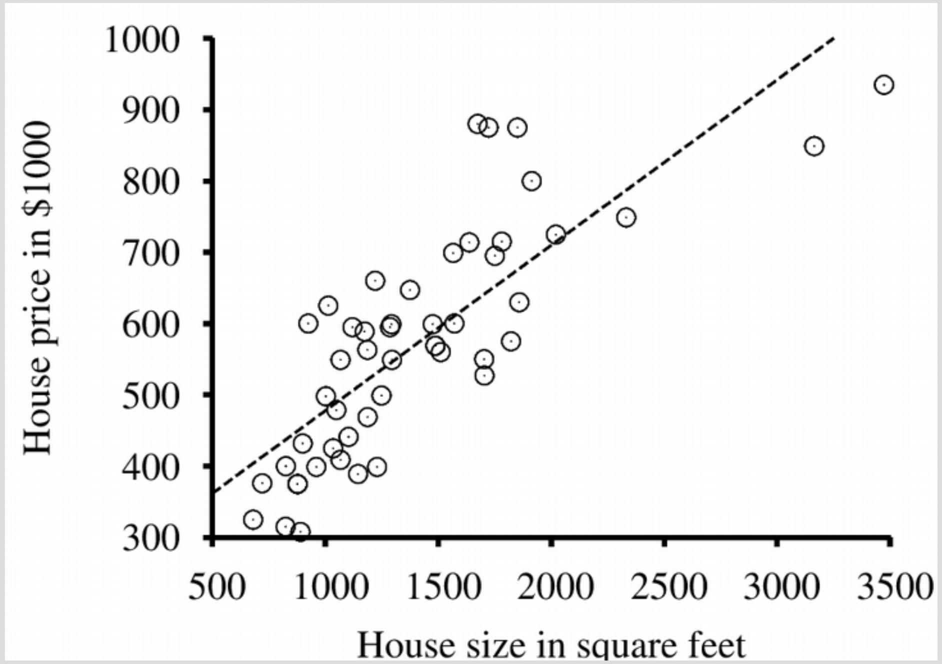
$$Loss(h_w) = \sum_{j=1}^{N} (\underbrace{y_j}_{y_j \text{ is actual y-coordinate}} - \underbrace{h_w(x_j)}_{h_w(x_j) \text{ is approximated (line) y-coordinate}})^2 = \sum_{j=1}^{N} (y_j - (w_0 + w_1 \cdot x_j))^2$$

... where N is the number of examples/points

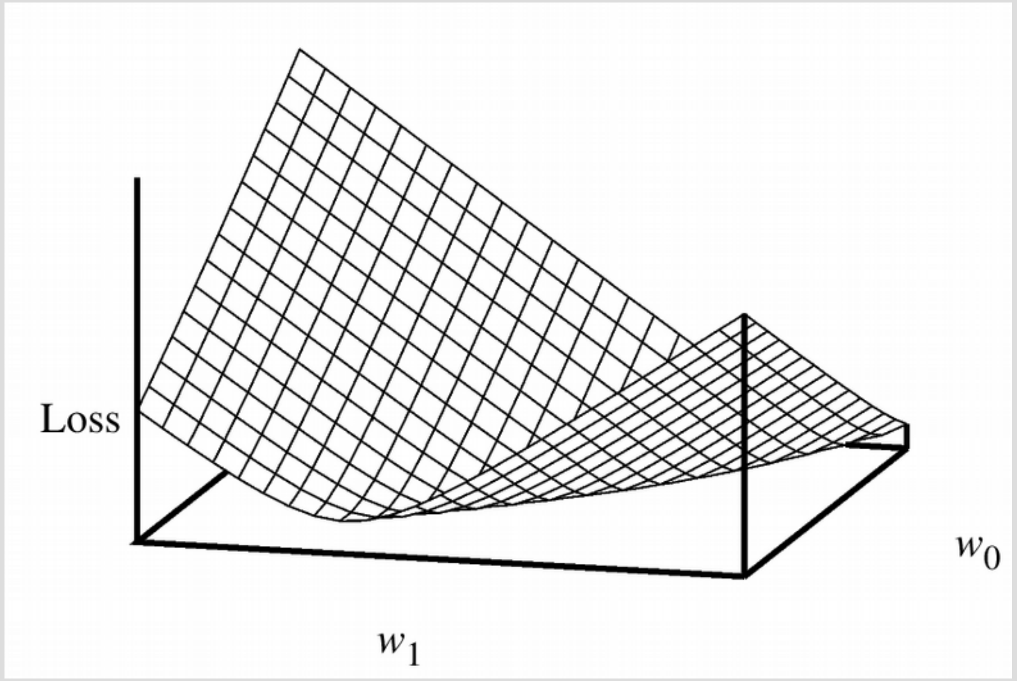
This makes sense as it penalizes “wrong” answers more the further they are away (two points off by 1 better than one off by 2)

Linear Regression: How To

You can plot this loss function (z-axis) with respect to the choice of w_0 and w_1



Regression



Loss

Linear Regression: How To

We want the regression line (w_0, w_1) to have the lowest loss possible

As the loss function looks convex (it is), the minimum is unique, so from calculus we want:

$$\frac{\partial}{\partial w_0} Loss(h_w) = 0 = \frac{\partial}{\partial w_0} \sum_{j=1}^{N} (y_j - (w_0 + w_1 \cdot x_j))^2$$

bottom is when both w_0 and w_1 derivatives zero

$$\frac{\partial}{\partial w_1} Loss(h_w) = 0 = \frac{\partial}{\partial w_1} \sum_{j=1}^{N} (y_j - (w_0 + w_1 \cdot x_j))^2$$

Linear Regression: How To

It is not too hard to do a bit of calculus to find the unique solution for w_0 and w_1:

$$w_1 = \frac{N\cdot(\sum_j x_j \cdot y_j) - (\sum_j x_j)\cdot(\sum_j y_j)}{N\cdot(\sum_j x_j^2) - (\sum_j x_j)^2}$$

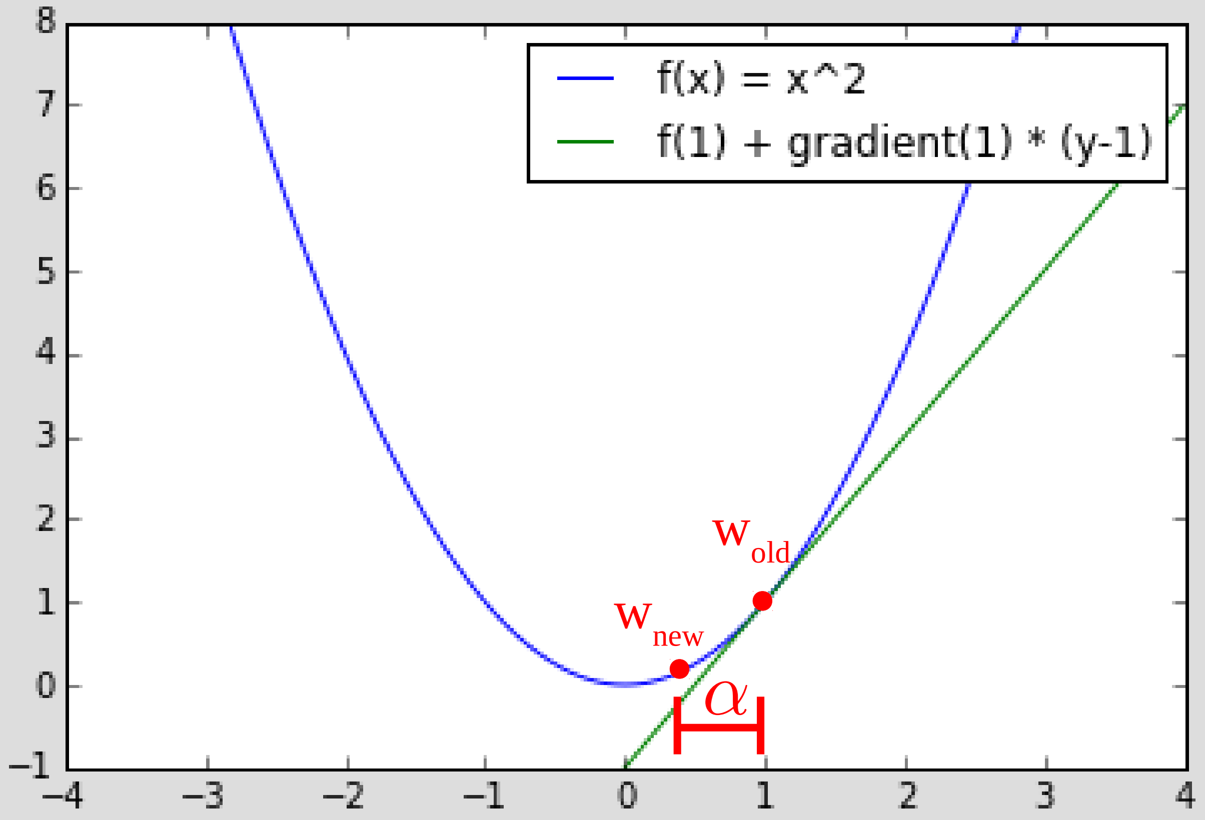
all sum from j=1 to N

$$w_0 = \frac{(\sum_j y_j) - w_1\cdot(\sum_j x_j)}{N}$$

Unfortunately, if you want to do polynomials, you might not have a closed form solution like this (i.e. no “easy” exact answer)

Linear Regression: Estimate

You can do a gradient descent (much like Newton’s method)(similar to “hill-climbing”)



Linear Regression: Estimate

Again, you need calculus to figure out what direction is "down hill", so to move the weights (w_0, w_1, ...) towards the bottom:

$$\underbrace{w_i}_{w_{new}} \leftarrow \underbrace{w_i}_{w_{old}} - \alpha \cdot \frac{\partial}{\partial w_i} Loss(h_{\underbrace{w_i}_{w_{old}}})$$

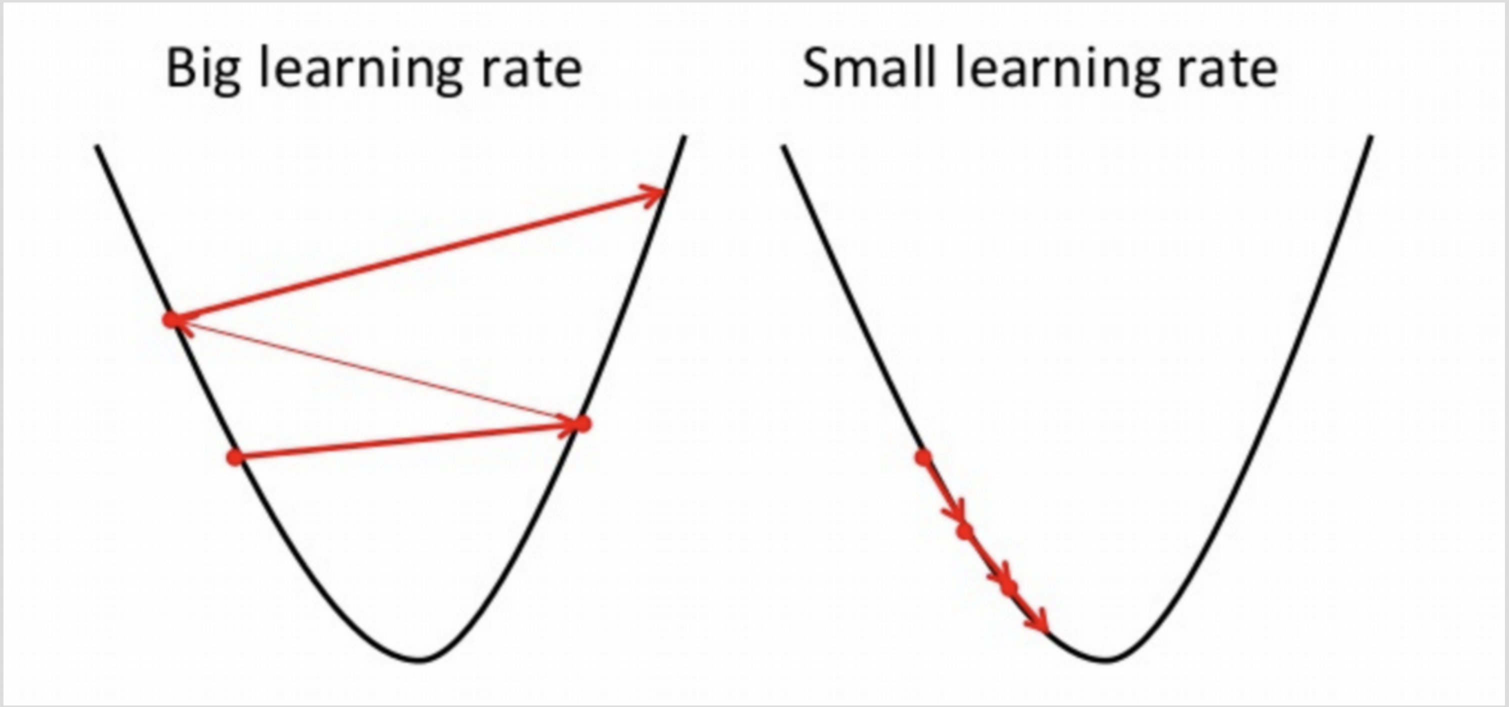
Loss function is what we minimizing (convex), so derivative of it

... where α is basically the "step size" (we will often use alpha in a similar fashion, but call it the "learning factor/rate")

Linear Regression: Estimate

The choice of α is somewhat arbitrary...

You don’t want it too big, but anything small is fine (even better if you shrink it over time)



Linear Regression: Estimate

You can extend this to more than just one variable (or attribute) in a similar fashion

If we have X as (for attributes a,b,c ...):

$$X = \begin{bmatrix} 1 & a_1 & b_1 & c_1 & \dots \\ 1 & a_2 & b_2 & c_2 & \dots \\ 1 & a_3 & b_3 & c_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

... and w as:

$$w^T = \begin{bmatrix} w_0 & w_1 & w_2 & w_3 & \dots \end{bmatrix}$$

Linear Regression: Estimate

Then if x_j is a single row of X:

$$(x_j)^T = [1 \quad a_j \quad b_j \quad c_j \quad \ldots]$$

Then our "line" is just the dot product:

$$w_0 + w_1 \cdot a_j + w_2 \cdot b_j + w_3 \cdot c_j + ... = w \cdot x_j = w^T x_j$$

Just like for the single variable case, we update our w's as: $w_i \leftarrow w_i - \alpha \cdot \frac{\partial}{\partial w_i} Loss(h_w)$

attribute for the corresponding weight in example, so if updating "w_2" then "b_j" as in line we do "$w_2 * b_j$"

... after math: $w_i \leftarrow w_i + \alpha \cdot \sum_{j=1}^{N} x_{j,i}(y_j - h_w(x_j))$

y_j is actual output for example/point number j

Linear Regression: Example

Let’s do an example...

Assume we have the following data points:
(assume trying to calculate BMI or something)

Age:	Height:	Calories:
5	20	1500
22	50	2500
50	48	2000

We will try to fit (age + height) to estimate Cal

Linear Regression: Example

So we will need to come up with some equation to predict Calories in the form:
$w_0 + w_1$*age + w_2*height

Initially, we can pick whatever for the w's:
$w_0=550$, $w_1=-20$, $w_2=50$

From this we can calculate the loss:

$$Loss(h_w) = \sum_{j=1}^{N}(y_j - h_w(x_j))^2 = \sum_{j=1}^{N}(y_j - (w_0 + w_1 \cdot age + w_2 \cdot height))^2$$

Linear Regression: Example

$$Loss(h_w) = \sum_{j=1}^{N}(y_j - h_w(x_j))^2 = \sum_{j=1}^{N}(y_j - (w_0 + w_1 \cdot age + w_2 \cdot height))^2$$

From our data:

$$\begin{aligned} \text{Loss} = &(1500 - (550 + -20*5 + 50*20))^2 \\ &+(2500 - (550 + -20*22 + 50*50))^2 \\ &+(2000 - (550 + -20*50 + 50*48))^2 \end{aligned}$$

Loss = 17,100

... this is pretty big so, these w’s aren’t great

Let’s update w_2 to make it better!

Linear Regression: Estimate

$$w_i \leftarrow w_i + \alpha \cdot \sum_{j=1}^{N} x_{j,i}(y_j - h_w(x_j))$$

since w_2 is associated with height, we multiply by the height out front

Use update formula (with α=0.0001) for w_2:

w_2 = 50 + 0.0001 * [

20*(1500 – (550 + -20*5 + 50*20))

+50*(2500 – (550 + -20*22 + 50*50))

+48*(2000 – (550 + -20*50 + 50*48))]

w_2 = 49.79

(Note: α chosen small as Loss was large and we don't want w_2 to change by a large amount)

Linear Regression: Estimate

$$Loss(h_w) = \sum_{j=1}^{N} (y_j - h_w(x_j))^2 = \sum_{j=1}^{N} (y_j - (w_0 + w_1 \cdot age + w_2 \cdot height))^2$$

We can then re-calculate the loss with the new w_2=49.79:

Loss = $(1500 – (550 + -20*5 + 49.79*20))^2$
$+(2500 – (550 + -20*22 + 49.79*50))^2$
$+(2000 – (550 + -20*50 + 49.79*48))^2$

Loss = 16,447.5

... which is better than the old Loss = 17,100

Linear Regression: Exact

However, you can solve for linear regression exactly even with multiple inputs

Specifically, you can find optimal weights as:

$$w = (X^T X)^{-1} X^T y$$

This requires you to find a matrix inverse, which can be a bit ugly... but do-able

Thus we estimate our line as: $\overset{\text{matrix multiplication}}{Xw} \approx y$

Linear Regression: Exact

So for:

Age:	Height:	Calories:
5	20	1500
22	50	2500
50	48	2000

$$X = \begin{bmatrix} 1 & 5 & 20 \\ 1 & 22 & 50 \\ 1 & 50 & 48 \end{bmatrix}$$

... thus the “best fit” w’s are:

$$\begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \left(\begin{bmatrix} 1 & 1 & 1 \\ 5 & 22 & 50 \\ 20 & 50 & 48 \end{bmatrix} \begin{bmatrix} 1 & 5 & 20 \\ 1 & 22 & 50 \\ 1 & 50 & 48 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & 1 \\ 5 & 22 & 50 \\ 20 & 50 & 48 \end{bmatrix} \begin{bmatrix} 1500 \\ 2500 \\ 2000 \end{bmatrix}$$

Linear Regression: Overfitting

You actually still can overfit even with a linear approximation by using too many variables (can't overfit "trend")

Another option to minimize (rather than loss):

$$Cost(h_w) = Loss(h_w) + \lambda \cdot Complexity(h_w)$$

as before for line fit

... where we will treat λ as some constant

and: $Complexity(h_w) = L_p(w)$

... where $L_p(w)$ is similar to the p-norm

Side note: “Distance”

The p-norm is a generalized way of measuring distance (you already know some of these)

The definition is of a p-norm:

$$||x||_p = (|x_1|^p + |x_2|^p + ...)^{1/p}$$

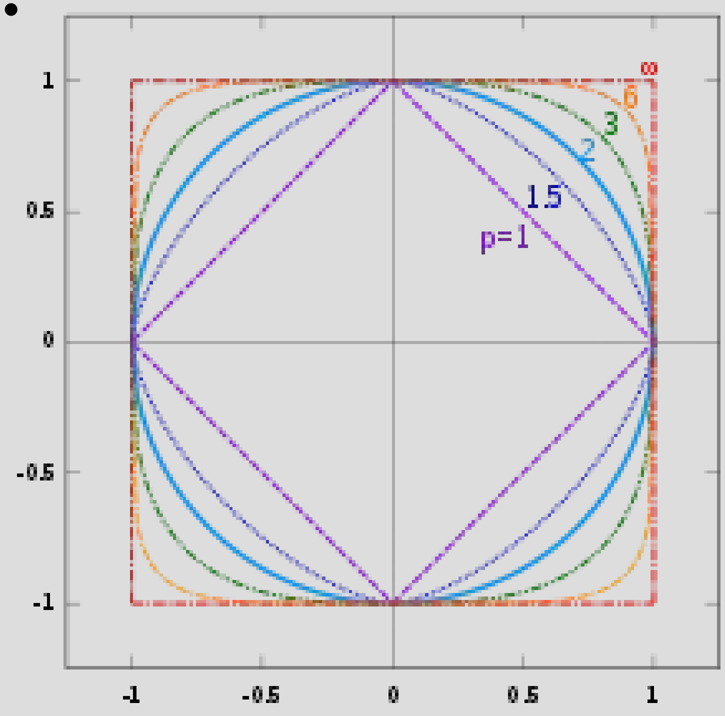
Specifically in 2 dimensions:

$$||(x, y)||_1 = |x| + |y|$$

(Manhattan distance)

$$||(x, y)||_2 = \sqrt{x^2 + y^2}$$

(Euclidean distance)



Linear Regression: Overfitting

We drop the exponent for L's, so in 2D:

$$||(x,y)||_2 = \sqrt{x^2 + y^2}$$

$$L_2(x,y) = x^2 + y^2$$

So we treat the weight vector's "distance" as the complexity (to minimize)

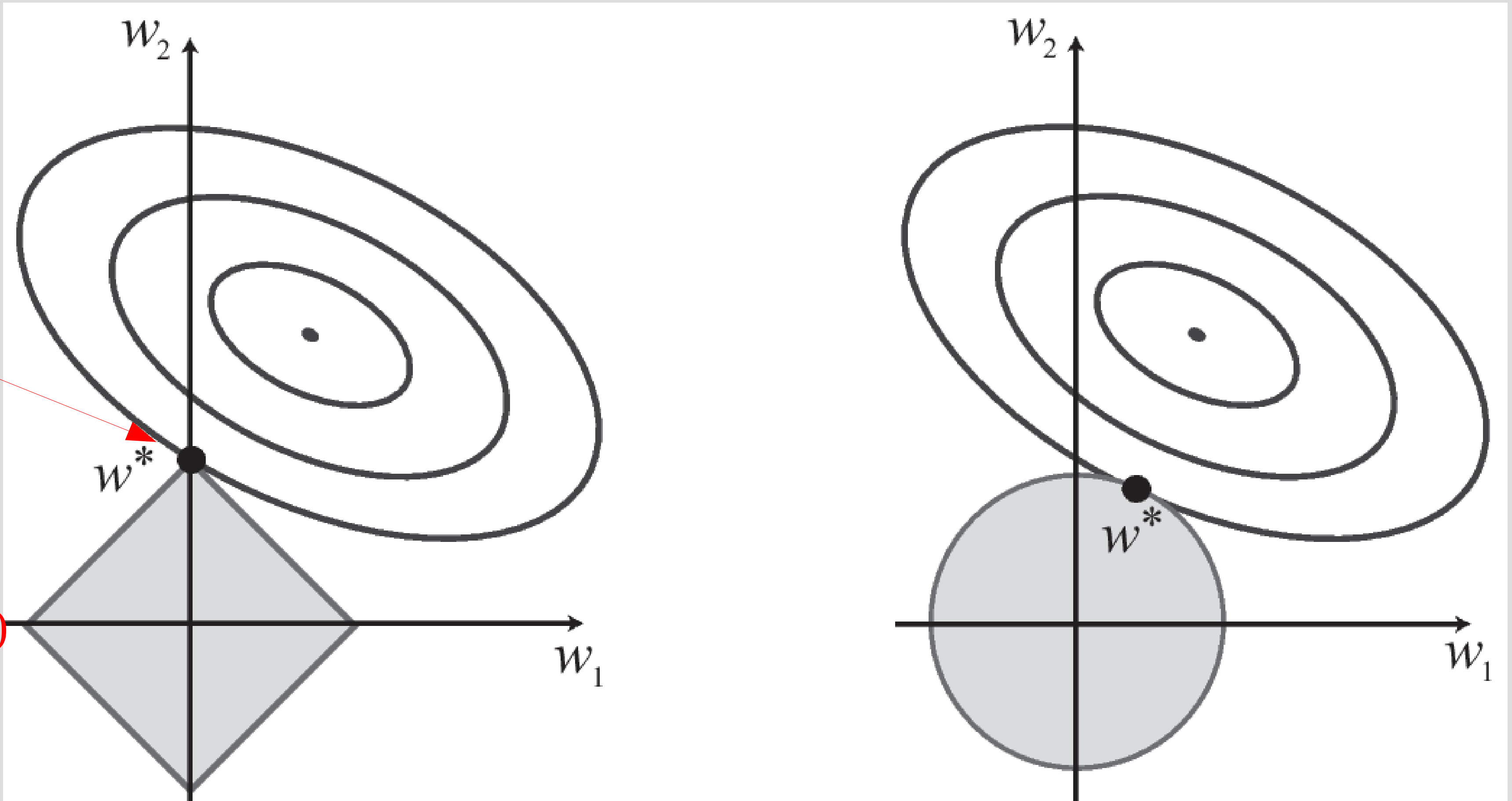
Here L_1 is often the best choice as it tends to have 0's on "irrelevant" attributes/varaibles

... why are 0's good? Why does it happen?

Linear Regression: Overfitting

This is because the L_1 (Manhattan distance) has a sharper "angle" than a circle (L_2)

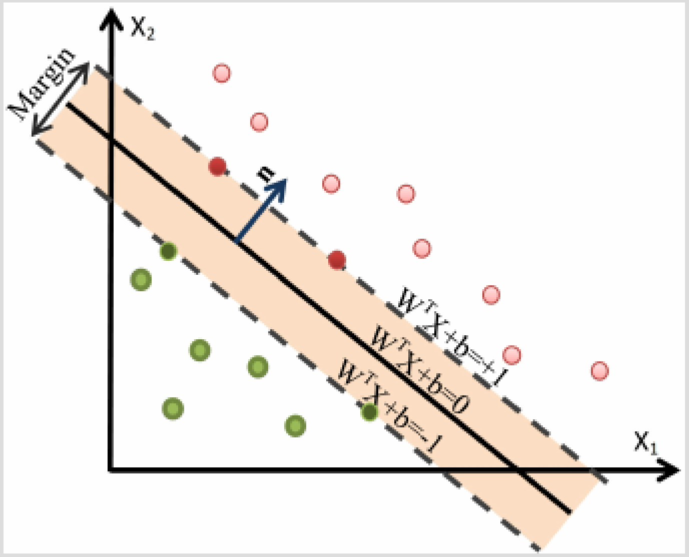
has w_1 = 0, as on y-axis ... so w_1 seems irrelevant (less overfit)



Linear Classification

A similar problem is instead of finding the "closest" line, we want to find a line that separates the data points (assume T/F for data)

This is more similar to what we were doing with decision trees, except we will use lines rather than trees



Linear Classification

This is actually a bit harder than linear regression as you can wiggle the line, yet the classification stays the same

This means, most places the derivative are zero, so we cannot do simple gradient descent

To classify we check if:

$h_w(x) = w \cdot x > y$ same as before: line defined by weights

... if yes, then guess True... otherwise guess F

Linear Classification

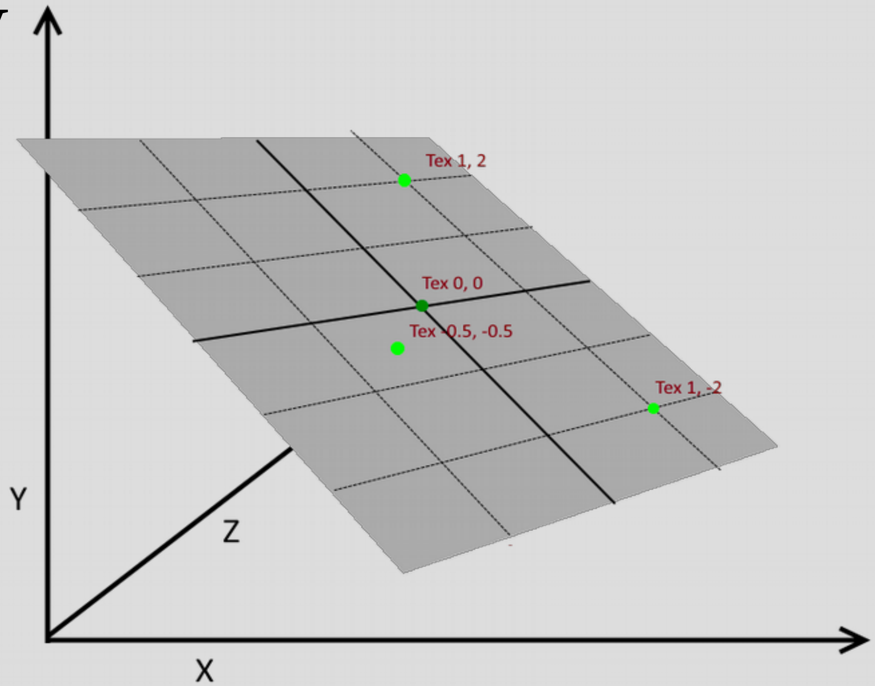
For example, in three dimensions:

$$w_1 \cdot x + w_2 \cdot y + w_3 \cdot z > c$$

y is not “output” atm

$c = -w_0$

This is simply one side of a plane in 3D, so this is trying to classify all possible points using a single plane...



Linear Classification

Despite gradient descent not working, we can still “update” weights until convergence as:

$$w_i \leftarrow w_i + \alpha \cdot (y - h_w(x)) \cdot x_i$$

Start weight randomly, then update weight for every example with above equation

... what does this equation look like?

Linear Classification

Despite gradient descent not working, we can still "update" weights until convergence as:

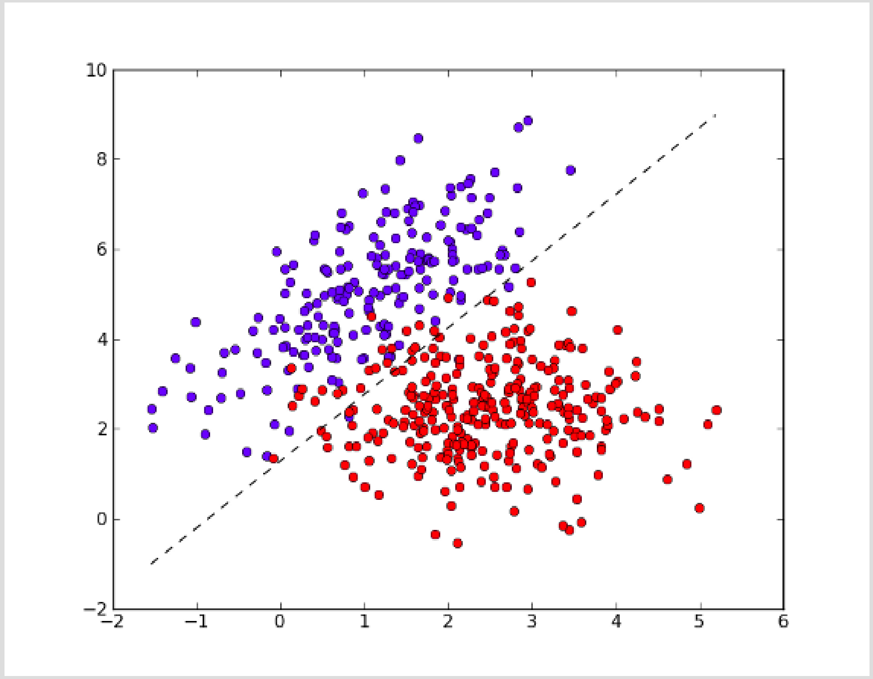
$$w_i \leftarrow w_i + \alpha \cdot (y - h_w(x)) \cdot x_i$$

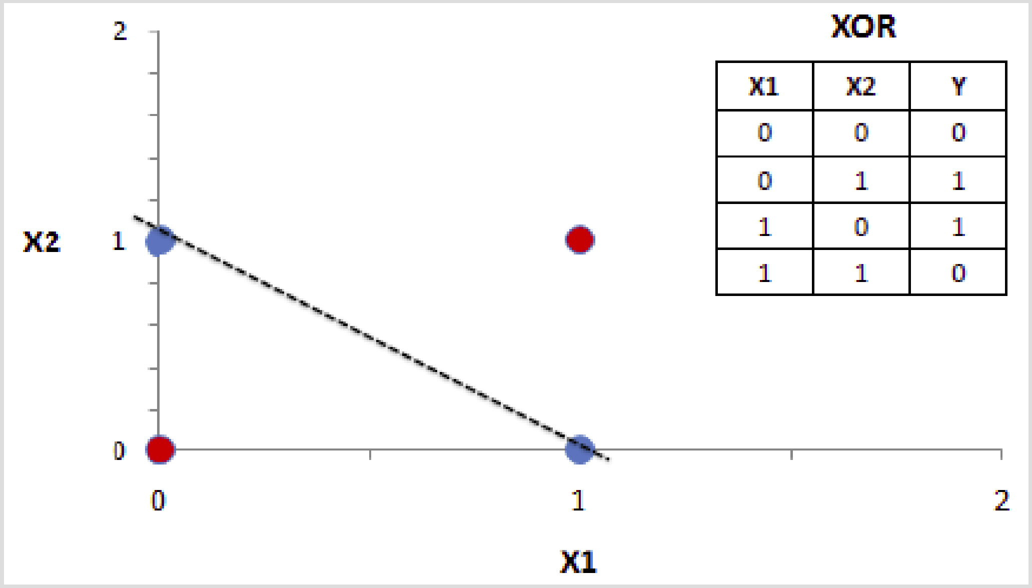
Start weight randomly, then update weight for every example with above equation

... what does this equation look like?
Just the gradient descent (but I thought you said we couldn't since derivative messed up!)

Linear Classification

If we had only 2 inputs, it would be everything above a line in 2D, but consider XOR on right





X1	X2	Y
0	0	0
0	1	1
1	0	1
1	1	0

There is no way a single line can classify XOR ... what should we do?

Linear Classification

If one line isn't enough... use more!
Our next topic will do just this...