



Machine Learning

CSCE 4205/5215

**Regression
Linear and Logistic**

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Goal of Linear Regression

Create a linear model that minimizes the sum of squares of the error

Independent variable- x axis (by convention)

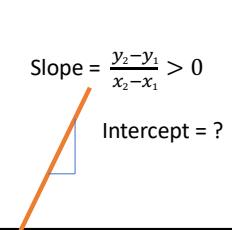
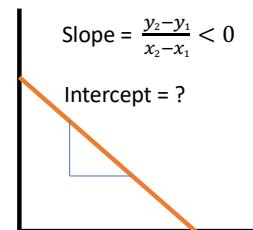
Dependent variable- y axis (by convention)

Predict one variable based on another variable, i.e.

y as a function of x

$$y = f(x)$$

e.g.: $y = a*x + b$ (a: slope, b: intercept)



Step 1: Calculate the best-fit line through the data

Is it $y = a + b*x$? It is a line

Step 2: Find the best fitting line that minimizes the SSE

Step 3: Make Predictions on unseen data to the simple linear regression model

Goal of Linear Regression

Succinctly, predicting numbers rather than labels, for example:

- Predicting the severity or strength, rather than presence or absence
 - e.g. how many **inches** of rain, rather than the presence or absence of rain
- Predicting the future for a quantity of interest
 - Resource allocation for future growth, stock valuation, etc
- Matching a data sample to a known quantity to help interpretation
 - e.g. predicting clinical scores on mobility based on obscure wearable device signals

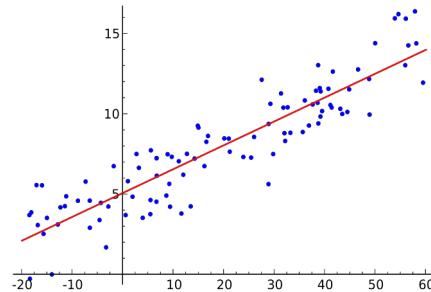
Linear regression

Finding the best a_k

$$y = a_1 x_1 + a_2 x_2 + a_3 x_3 \dots$$

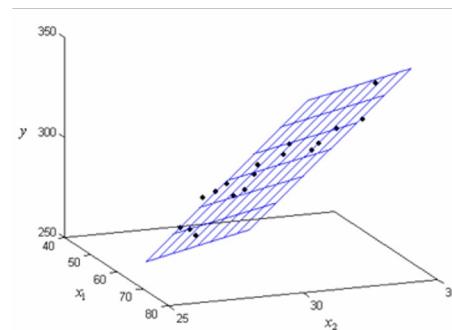
One of the simplest regression models, but also has a lot of subtle variations.

- Intercepts
- Extensible with complex features (e.g. polynomial with powers)
- Variations in error metrics
- How to handle overfitting (regularization)



Linear Model: $Y = mX + b$

Response Variable Covariate
Slope Intercept (bias)



Linear regression, more powerful than it may appear

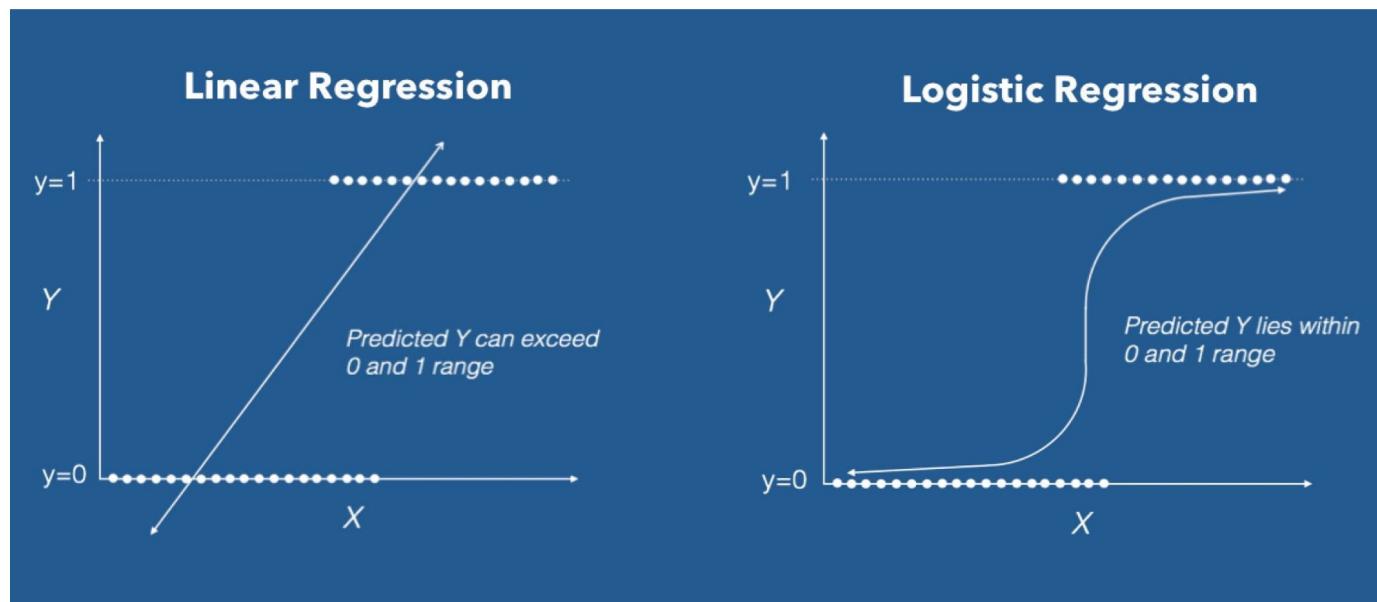
With more complex features, linear regression is arbitrarily powerful

- High frequency trader colleague used regularized linear regression a great deal, but with complex features

Linear regression can be used to provide a graded classification

- Binary classification is equivalent to a 0-1 regression with a threshold
- More on this when discussing logistic regression in upcoming slides
- And multiclass classification can be performed with a one-hot encoding scheme.

Compare Linear vs Logistic regression



Logistic Regression

- Important analytic tool in natural and social sciences
- Baseline supervised machine learning tool for classification
- Is also the foundation of neural networks

Generative and Discriminative Classifiers

Suppose we're distinguishing cat from dog images



imagenet



imagenet

Generative Classifier:

- Build a model of what's in a cat image
 - Knows about whiskers, ears, eyes
 - Assigns a probability to any image:
 - how cat-y is this image?



Also build a model for dog images

Now given a new image:

Run both models and see which one fits better

Discriminative Classifier

Just try to distinguish dogs from cats



Oh look, dogs have collars!
Let's ignore everything else

Finding the correct class c from a document d

- Logistic Regression

$$\hat{c} = \operatorname{argmax}_{c \in C} P(c|d) \quad \text{posterior}$$

Components of a probabilistic machine learning classifier

Given m input/output pairs $(x^{(i)}, y^{(i)})$:

1. A **feature representation** of the input. For each input observation $x^{(i)}$, a vector of features $[x_1, x_2, \dots, x_n]$. Feature j for input $x^{(i)}$ is x_j , more completely $x_j^{(i)}$, or sometimes $f_j(x)$.
2. A **classification function** that computes \hat{y} , the estimated class, via $p(y|x)$, like the **sigmoid** or **softmax** functions.
3. An objective function for learning, like **cross-entropy loss**.
4. An algorithm for optimizing the objective function: **stochastic gradient descent**.

The two phases of logistic regression

- **Training:** we learn weights w and b using **stochastic gradient descent** and **cross-entropy loss**.
- **Test:** Given a test example x we compute $p(y|x)$ using learned weights w and b , and return whichever label ($y = 1$ or $y = 0$) is higher probability

Classification Reminder

- Spam/not spam
- Fake/Real News
- Benign/Malignant
- Positive/negative sentiment
- Adm/No Adm

Text Classification: definition

- *Input:*
 - a document x
 - a fixed set of classes $C = \{c_1, c_2, \dots, c_J\}$
- *Output:* a predicted class $\hat{y} \in C$

Binary Classification in Logistic Regression

- Given a series of input/output pairs:
 - $(x^{(i)}, y^{(i)})$
- For each observation $x^{(i)}$
 - We represent $x^{(i)}$ by a **feature vector** $[x_1, x_2, \dots, x_n]$
 - We compute an output: a predicted class $\hat{y}^{(i)} \in \{0,1\}$

Features in logistic regression

- For feature x_i , weight w_i tells us how important is x_i
 - $x_i = \text{"review contains 'awesome'"}: w_i = +10$
 - $x_j = \text{"review contains 'abysmal'"}: w_j = -10$
 - $x_k = \text{"review contains 'mediocre'"}: w_k = -2$

Logistic Regression for one observation x

- Input observation: vector $x = [x_1, x_2, \dots, x_n]$
- Weights: one per feature: $W = [w_1, w_2, \dots, w_n]$
 - Sometimes we call the weights $\theta = [\theta_1, \theta_2, \dots, \theta_n]$
- Output: a predicted class $\hat{y} \in \{0, 1\}$

(multinomial logistic regression: $\hat{y} \in \{0, 1, 2, 3, 4\}$)

How to do classification

- For each feature x_i , weight w_i tells us importance of x_i
 - (Also we'll have a bias b)
- We'll sum up all the weighted features and the bias

$$z = \left(\sum_{i=1}^n w_i x_i \right) + b$$
$$z = w \cdot x + b$$

- If this sum is high, we say $y=1$; if low, then $y=0$

But we want a probabilistic classifier

- We need to formalize “sum is high”.
- We’d like a principled classifier that gives us a probability
- We want a model that can tell us:
 - $p(y=1|x; \theta)$
 - $p(y=0|x; \theta)$

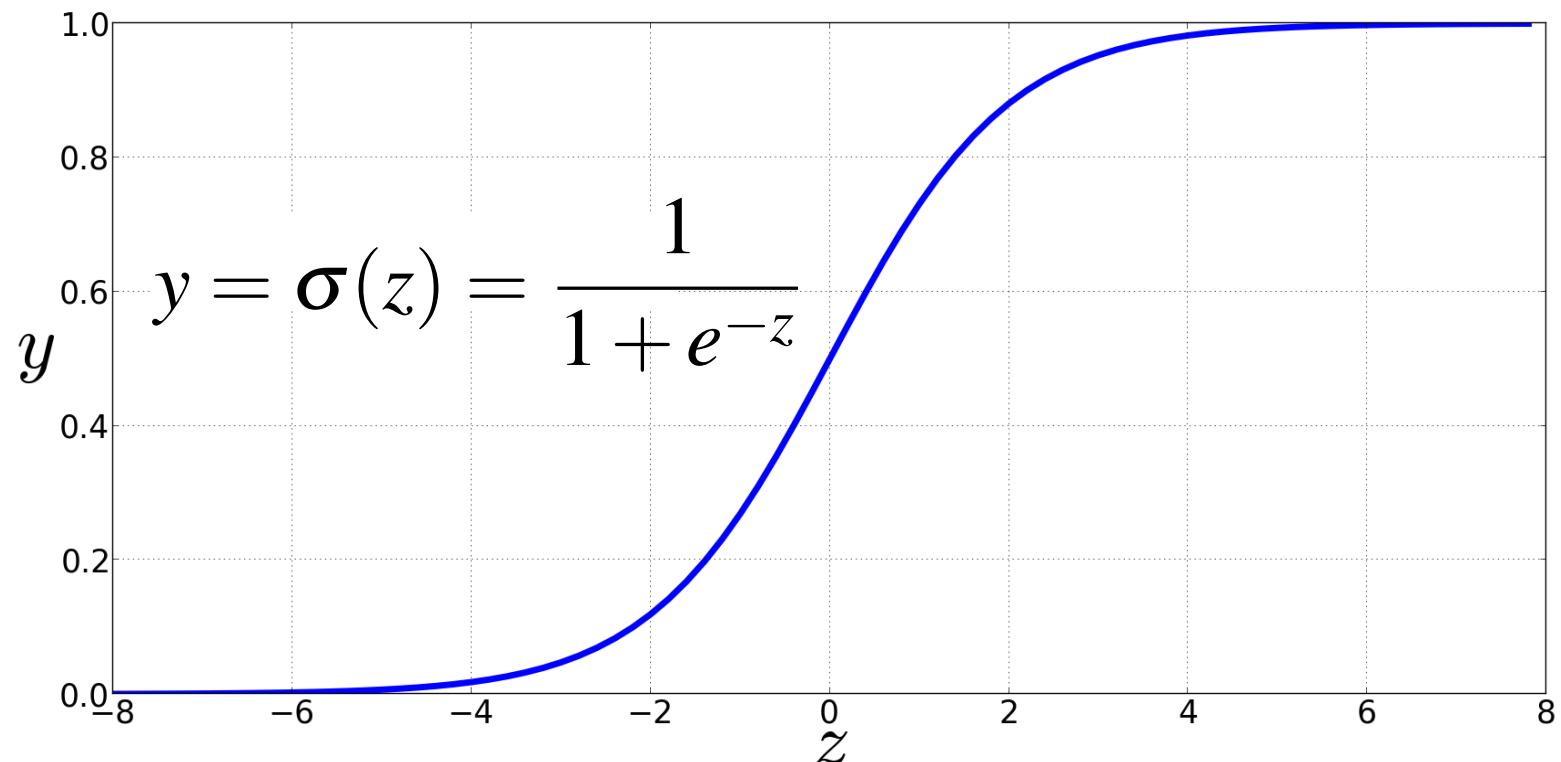
The problem: z isn't a probability, it's just a number!

$$z = w \cdot x + b$$

- Solution: use a function of z that goes from 0 to 1

$$y = \sigma(z) = \frac{1}{1 + e^{-z}} = \frac{1}{1 + \exp(-z)}$$

The very useful sigmoid or logistic function



Idea of logistic regression

- We'll compute $w \cdot x + b$
- And then we'll pass it through the sigmoid function:
$$\sigma(w \cdot x + b)$$
- And we'll just treat it as a probability

Making probabilities with sigmoids

$$\begin{aligned} P(y = 1) &= \sigma(w \cdot x + b) \\ &= \frac{1}{1 + \exp(-(w \cdot x + b))} \end{aligned}$$

$$\begin{aligned} P(y = 0) &= 1 - \sigma(w \cdot x + b) \\ &= 1 - \frac{1}{1 + \exp(-(w \cdot x + b))} \\ &= \frac{\exp(-(w \cdot x + b))}{1 + \exp(-(w \cdot x + b))} \end{aligned}$$

By the way:

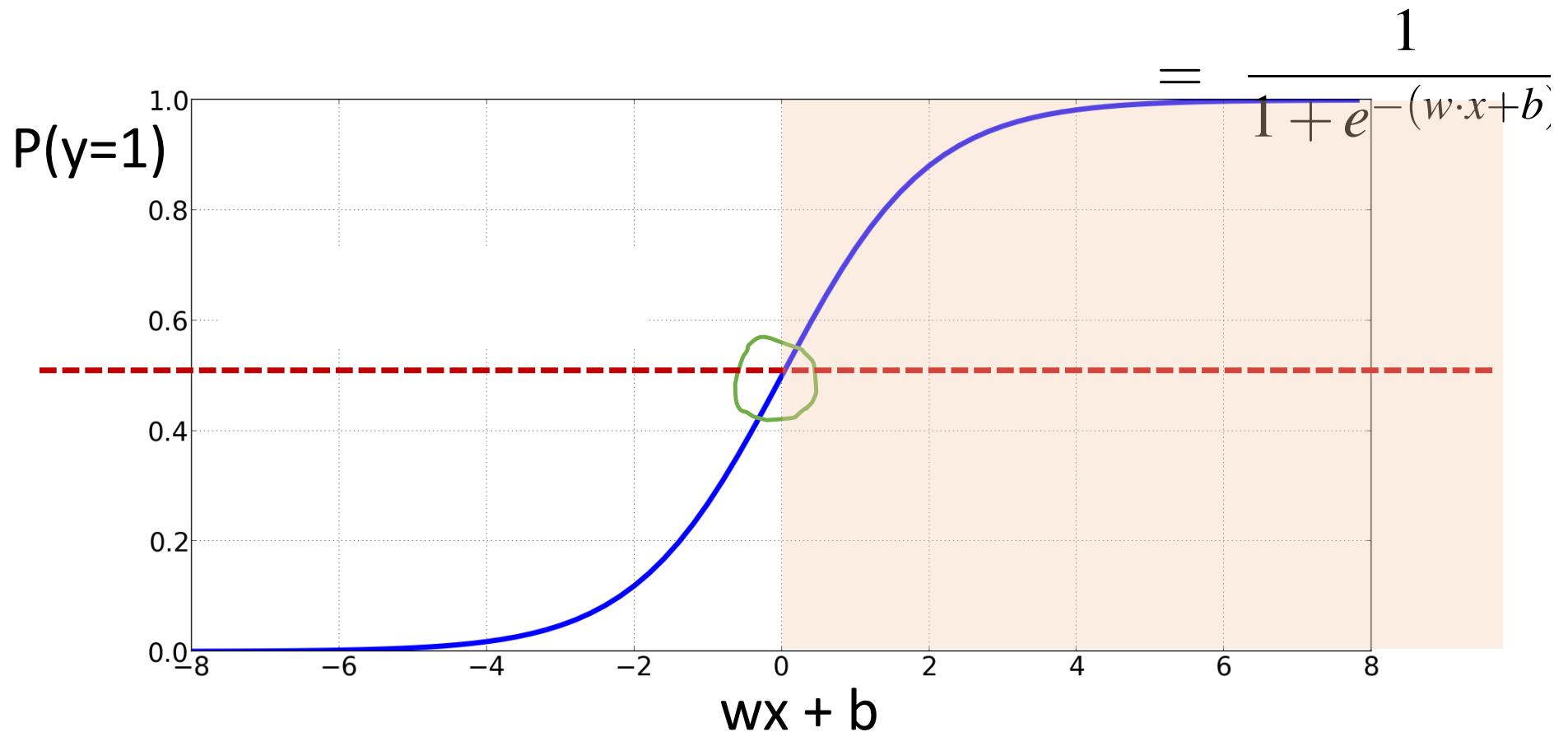
$$\begin{aligned} P(y = 0) &= 1 - \sigma(w \cdot x + b) &= \sigma(-(w \cdot x + b)) \\ &= 1 - \frac{1}{1 + \exp(-(w \cdot x + b))} && \text{Because} \\ &= \frac{\exp(-(w \cdot x + b))}{1 + \exp(-(w \cdot x + b))} &1 - \sigma(x) = \sigma(-x) \end{aligned}$$

Turning a probability into a classifier

$$\hat{y} = \begin{cases} 1 & \text{if } P(y=1|x) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

0.5 here is called the **decision boundary**

The probabilistic classifier $P(y = 1) = \sigma(w \cdot x + b)$



Turning a probability into a classifier

$$\hat{y} = \begin{cases} 1 & \text{if } P(y=1|x) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

if $w \cdot x + b > 0$
if $w \cdot x + b \leq 0$

Logistic Regression Learning:

Where did the W's come from?

- Supervised classification:
 - We know the correct label y (either 0 or 1) for each x .
 - But what the system produces is an estimate, \hat{y}
 - We want to set w and b to minimize the **distance** between our estimate $\hat{y}^{(i)}$ and the true $y^{(i)}$.
 - We need a distance estimator: a **loss function** or a **cost function**
 - We need an optimization algorithm to update w and b to minimize the loss.

Learning components

- A loss function:
 - **cross-entropy loss**
- An optimization algorithm:
 - **stochastic gradient descent**

The distance between \hat{y} and y

- We want to know how far is the classifier output:

$$\hat{y} = \sigma(w \cdot x + b)$$

- from the true output:

$$y \quad [= \text{either 0 or 1}]$$

- We'll call this difference:

$$L(\hat{y}, y) = \text{how much } \hat{y} \text{ differs from the true } y$$

Intuition of negative log likelihood loss = cross-entropy loss

- A case of conditional maximum likelihood estimation
- We choose the parameters w, b that maximize
 - the log probability
 - of the true y labels in the training data
 - given the observations x

Deriving cross-entropy loss for a single observation x

- **Goal:** maximize probability of the correct label $p(y|x)$
- Since there are only 2 discrete outcomes (0 or 1) we can express the probability $p(y|x)$ from our classifier (the thing we want to maximize) as

noting:

$$p(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}$$

if $y=1$, this simplifies to \hat{y}

if $y=0$, this simplifies to $1 - \hat{y}$

Deriving cross-entropy loss for a single observation x

Goal: maximize probability of the correct label $p(y|x)$

Maximize:
$$p(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}$$

- Now take the log of both sides (mathematically handy)

Maximize:
$$\begin{aligned} \log p(y|x) &= \log [\hat{y}^y (1 - \hat{y})^{1-y}] \\ &= y \log \hat{y} + (1 - y) \log (1 - \hat{y}) \end{aligned}$$

- Whatever values maximize $\log p(y|x)$ will also maximize $p(y|x)$

Deriving cross-entropy loss for a single observation x

Goal: maximize probability of the correct label $p(y|x)$

Maximize:

$$\begin{aligned}\log p(y|x) &= \log [\hat{y}^y (1 - \hat{y})^{1-y}] \\ &= y \log \hat{y} + (1 - y) \log(1 - \hat{y})\end{aligned}$$

- Now flip sign to turn this into a loss: something to minimize
- **Cross-entropy loss** (because is formula for cross-entropy(y , \hat{y}))

Minimize: $L_{\text{CE}}(\hat{y}, y) = -\log p(y|x) = -[y \log \hat{y} + (1 - y) \log(1 - \hat{y})]$

- Or, plugging in definition of \hat{y} :

$$L_{\text{CE}}(\hat{y}, y) = -[y \log \sigma(w \cdot x + b) + (1 - y) \log(1 - \sigma(w \cdot x + b))]$$

Stochastic Gradient Descent

Our goal: minimize the loss

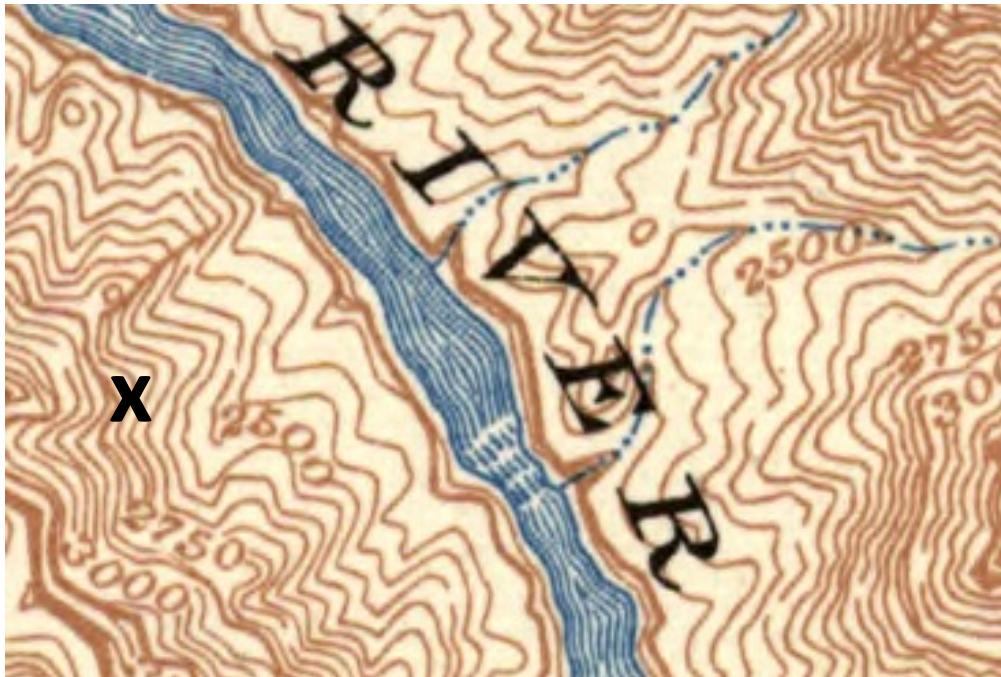
- Let's make explicit that the loss function is parameterized by weights $\theta=(w,b)$
- And we'll represent \hat{y} as $f(x; \theta)$ to make the dependence on θ more obvious
- We want the weights that minimize the loss, averaged over all examples:

•

$$\hat{\theta} = \operatorname{argmin}_{\theta} \frac{1}{m} \sum_{i=1}^m L_{\text{CE}}(f(x^{(i)}; \theta), y^{(i)})$$

Intuition of gradient descent

- How do I get to the bottom of this river canyon?



Look around me 360°
Find the direction of
steepest slope down
Go that way

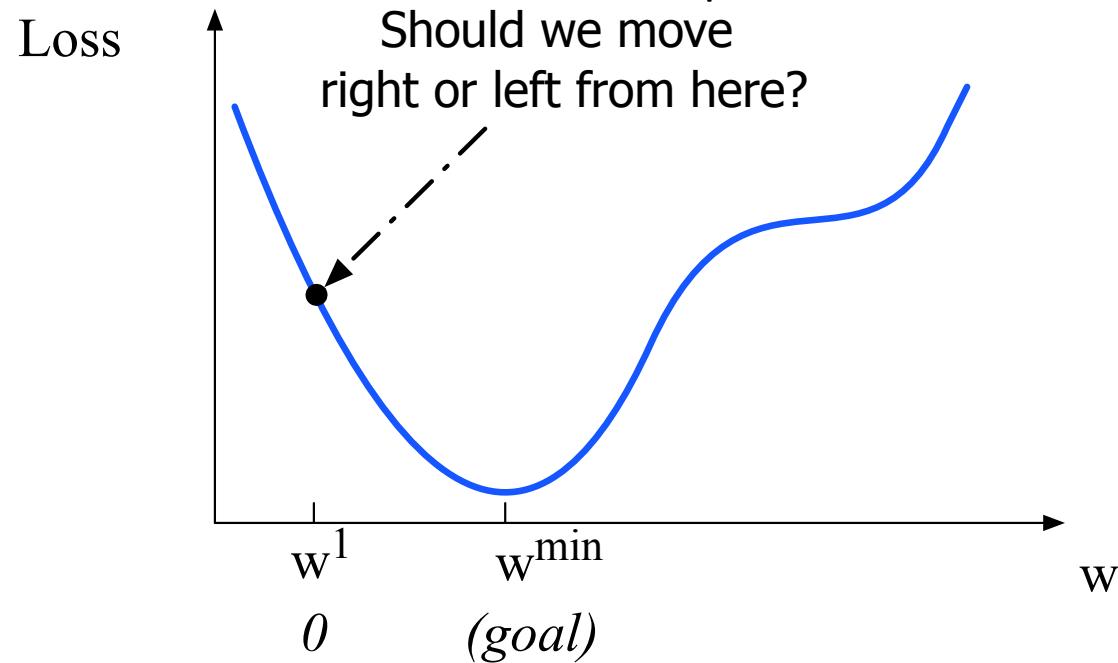
Our goal: minimize the loss

- For logistic regression, loss function is **convex**
 - A convex function has just one minimum
 - Gradient descent starting from any point is guaranteed to find the minimum
 - (Loss for neural networks is non-convex)

Let's first visualize for a single scalar w

Q: Given current w , should we make it bigger or smaller?

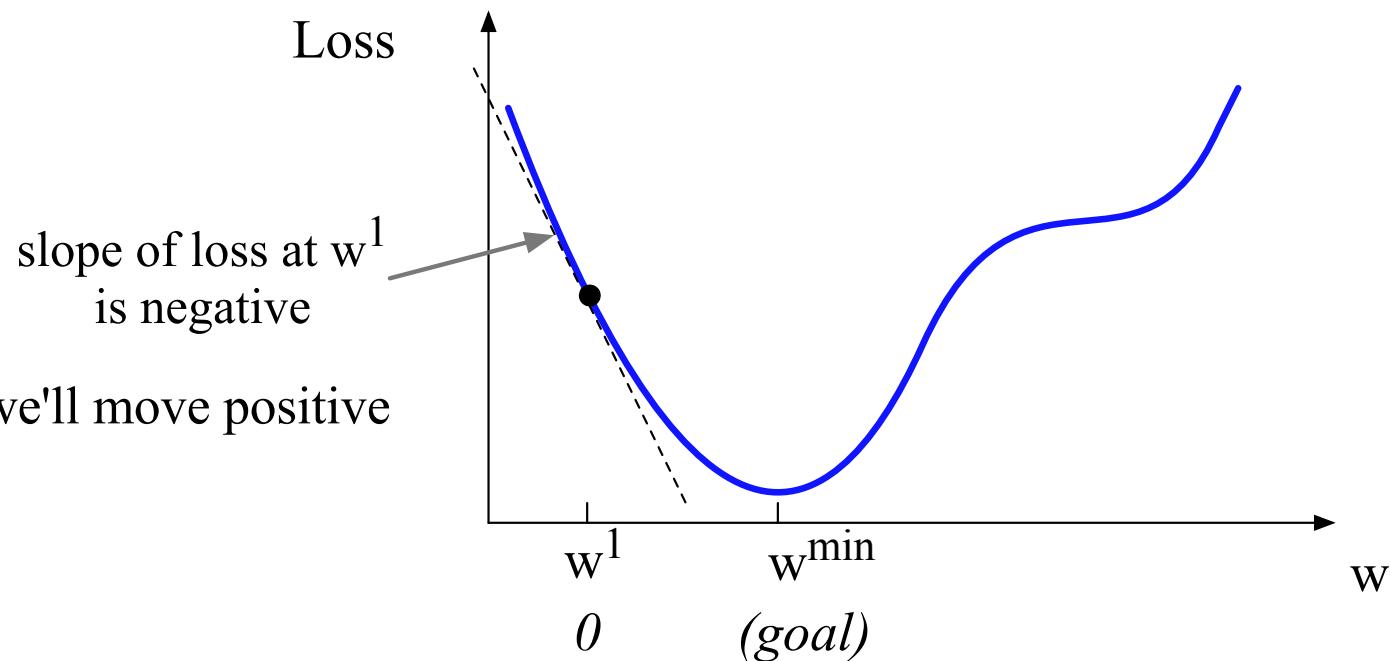
A: Move w in the reverse direction from the slope of the function



Let's first visualize for a single scalar w

Q: Given current w , should we make it bigger or smaller?

A: Move w in the reverse direction from the slope of the function

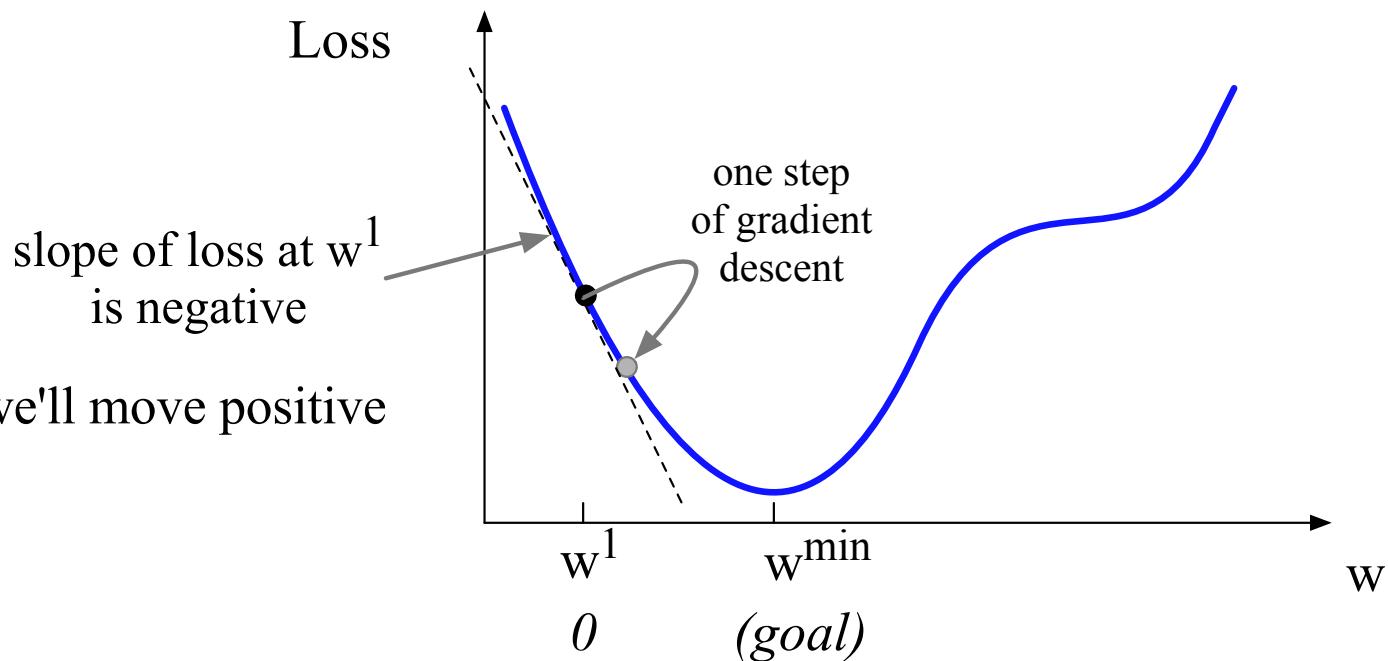


So we'll move positive

Let's first visualize for a single scalar w

Q: Given current w , should we make it bigger or smaller?

A: Move w in the reverse direction from the slope of the function



Gradients

- The **gradient** of a function of many variables is a vector pointing in the direction of the greatest increase in a function.
- **Gradient Descent:** Find the gradient of the loss function at the current point and move in the **opposite** direction.

How much do we move in that direction ?

- The value of the gradient (slope in our example) $\frac{d}{dw} L(f(x; w), y)$ weighted by a **learning rate** η
- Higher learning rate means move w faster

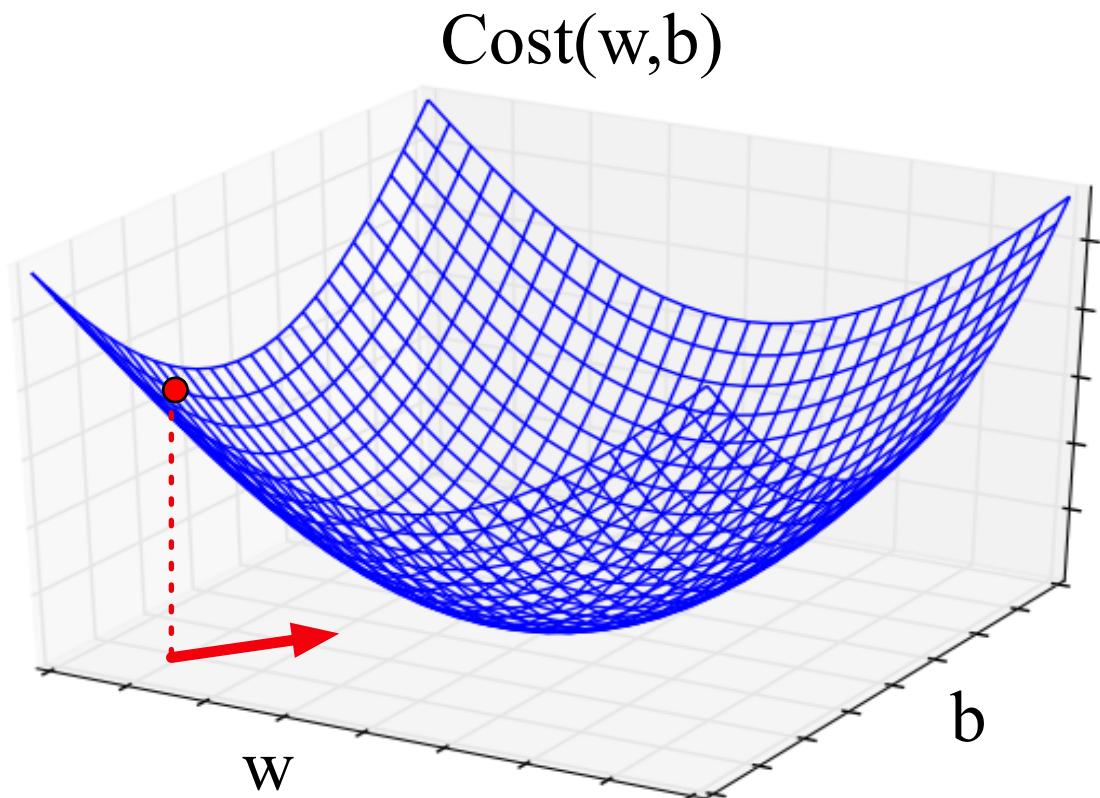
$$w^{t+1} = w^t - \eta \frac{d}{dw} L(f(x; w), y)$$

Now let's consider N dimensions

- We want to know where in the N -dimensional space (of the N parameters that make up θ) we should move.
- The gradient is just such a vector; it expresses the directional components of the sharpest slope along each of the N dimensions.

Imagine 2 dimensions, w and b

- Visualizing the gradient vector at the red point
- It has two dimensions shown in the x-y plane



Real gradients

- Are much longer; lots and lots of weights
- For each dimension w_i , the gradient component i tells us the slope with respect to that variable.
 - “How much would a small change in w_i influence the total loss function L ? ”
 - We express the slope as a partial derivative ∂ of the loss ∂w_i ,
- The gradient is then defined as a vector of these partials.

The gradient

We'll represent \hat{y} as $f(x; \theta)$ to make the dependence on θ more obvious:

$$\nabla_{\theta} L(f(x; \theta), y) = \begin{bmatrix} \frac{\partial}{\partial w_1} L(f(x; \theta), y) \\ \frac{\partial}{\partial w_2} L(f(x; \theta), y) \\ \vdots \\ \frac{\partial}{\partial w_n} L(f(x; \theta), y) \end{bmatrix}$$

The final equation for updating θ based on the gradient is thus

$$\theta_{t+1} = \theta_t - \eta \nabla L(f(x; \theta), y)$$

What are these partial derivatives for logistic regression?

The loss function

$$L_{\text{CE}}(\hat{y}, y) = -[y \log \sigma(w \cdot x + b) + (1 - y) \log (1 - \sigma(w \cdot x + b))]$$

$$\frac{\partial L_{\text{CE}}(\hat{y}, y)}{\partial w_j} = [\sigma(w \cdot x + b) - y]x_j$$

function STOCHASTIC GRADIENT DESCENT($L()$, $f()$, x , y) **returns** θ

where: L is the loss function

f is a function parameterized by θ

x is the set of training inputs $x^{(1)}$, $x^{(2)}$, ..., $x^{(m)}$

y is the set of training outputs (labels) $y^{(1)}$, $y^{(2)}$, ..., $y^{(m)}$

$\theta \leftarrow 0$

repeat til done

For each training tuple $(x^{(i)}, y^{(i)})$ (in random order)

1. Optional (for reporting): # How are we doing on this tuple?

 Compute $\hat{y}^{(i)} = f(x^{(i)}; \theta)$ # What is our estimated output \hat{y} ?

 Compute the loss $L(\hat{y}^{(i)}, y^{(i)})$ # How far off is $\hat{y}^{(i)}$ from the true output $y^{(i)}$?

2. $g \leftarrow \nabla_{\theta} L(f(x^{(i)}; \theta), y^{(i)})$ # How should we move θ to maximize loss?

3. $\theta \leftarrow \theta - \eta g$ # Go the other way instead

return θ

Hyperparameters

- The learning rate η is a **hyperparameter**
 - too high: the learner will take big steps and overshoot
 - too low: the learner will take too long
- Hyperparameters:
 - Briefly, a special kind of parameter for an ML model
 - Instead of being learned by algorithm from supervision (like regular parameters), they are chosen by algorithm designer.

Regularization

Overfitting

- A model that perfectly match the training data has a problem.
- It will also **overfit** to the data, modeling noise
 - A random word that perfectly predicts y (it happens to only occur in one class) will get a very high weight.
 - Failing to generalize to a test set without this word.
- A good model should be able to **generalize**

Overfitting

+

- This movie drew me in, and it'll do the same to you.

Useful or harmless features

X1 = "this"

X2 = "movie"

X3 = "hated"

X4 = "drew me in"

-

I can't tell you how much I hated this movie. It sucked.

features that just "memorize" training set and might cause problems

X5 = "the same to you"

X7 = "tell you how much"

Overfitting

- Model on tiny data will just memorize the data
 - 100% accuracy on the training set
- But it will be surprised by the novel 4-grams in the test data
 - Low accuracy on test set
- Models that are too powerful can **overfit** the data
 - Fitting the details of the training data so exactly that the model doesn't generalize well to the test set
 - How to avoid overfitting?
 - Regularization in logistic regression
 - Dropout in neural networks

Regularization

- A solution for overfitting
- Add a regularization term $R(\theta)$ to the loss function (for now written as maximizing logprob rather than minimizing loss)

$$\hat{\theta} = \operatorname{argmax}_{\theta} \sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) - \alpha R(\theta)$$

- Idea: choose an $R(\theta)$ that penalizes large weights
 - fitting the data well with lots of big weights not as good as fitting the data a little less well, with small weights

L2 Regularization (= ridge regression)

- The sum of the squares of the weights
- The name is because this is the (square of the) **L2 norm** $\|\theta\|_2$, = **Euclidean distance** of θ to the origin.

$$R(\theta) = \|\theta\|_2^2 = \sum_{j=1}^n \theta_j^2$$

- L2 regularized objective function:

$$\hat{\theta} = \operatorname{argmax}_{\theta} \left[\sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) \right] - \alpha \sum_{j=1}^n \theta_j^2$$

L1 Regularization (= lasso regression)

- The sum of the (absolute value of the) weights
- Named after the **L1 norm** $\|W\|_1$, = sum of the absolute values of the weights, = **Manhattan distance**

$$R(\theta) = \|\theta\|_1 = \sum_{i=1}^n |\theta_i|$$

- L1 regularized objective function:

$$\hat{\theta} = \operatorname{argmax}_{\theta} \left[\sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) \right] - \alpha \sum_{j=1}^n |\theta_j|$$

Multinomial Logistic Regression

Multinomial Logistic Regression

- Often we need more than 2 classes
 - Positive/negative/neutral
 - Real Numbers
 - Mnist images
- If >2 classes we use **multinomial logistic regression**
 - = Softmax regression
 - = Multinomial logit
 - = (defunct names : Maximum entropy modeling or MaxEnt
- So "logistic regression" will just mean binary (2 output classes)

Multinomial Logistic Regression

- The probability of everything must still sum to 1

$$P(\text{positive} \mid \text{doc}) + P(\text{negative} \mid \text{doc}) + P(\text{neutral} \mid \text{doc}) = 1$$

- Need a generalization of the sigmoid called the **softmax**
 - Takes a vector $z = [z_1, z_2, \dots, z_k]$ of k arbitrary values
 - Outputs a probability distribution
 - each value in the range $[0,1]$
 - all the values summing to 1

The softmax function

Turns a vector $z = [z_1, z_2, \dots, z_k]$ of k arbitrary values into probabilities

$$\text{softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^k \exp(z_j)} \quad 1 \leq i \leq k$$

The denominator $\sum_{i=1}^k e^{z_i}$ is used to normalize all the values into probabilities.

$$\text{softmax}(z) = \left[\frac{\exp(z_1)}{\sum_{i=1}^k \exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^k \exp(z_i)}, \dots, \frac{\exp(z_k)}{\sum_{i=1}^k \exp(z_i)} \right]$$

The softmax function

- Turns a vector $z = [z_1, z_2, \dots, z_k]$ of k arbitrary values into probabilities

$$z = [0.6, 1.1, -1.5, 1.2, 3.2, -1.1]$$

$$\text{softmax}(z) = \left[\frac{\exp(z_1)}{\sum_{i=1}^k \exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^k \exp(z_i)}, \dots, \frac{\exp(z_k)}{\sum_{i=1}^k \exp(z_i)} \right]$$

$$[0.055, 0.090, 0.0067, 0.10, 0.74, 0.010]$$

Softmax in multinomial logistic regression

$$p(y = c|x) = \frac{\exp(w_c \cdot x + b_c)}{\sum_{j=1}^k \exp(w_j \cdot x + b_j)}$$

Input is still the dot product between weight vector w and input vector x
But now we'll need separate weight vectors for each of the K classes.

Features in binary versus multinomial logistic regression

- Binary: positive weight $\rightarrow y=1$ neg weight $\rightarrow y=0$

$$x_5 = \begin{cases} 1 & \text{if “!”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases} \quad w_5 = 3.0$$

- Multinomial: separate weights for each class:

Feature	Definition	$w_{5,+}$	$w_{5,-}$	$w_{5,0}$
$f_5(x)$	$\begin{cases} 1 & \text{if “!”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	3.5	3.1	-5.3