Logistic Regression

Background: Generative and Discriminative Classifiers

Edited from Dan Jurafsky’s book website: https://web.stanford.edu/~jurafsky/slp3/

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

Naive Bayes is a **generative** classifier

by contrast:

Logistic regression is a **discriminative** classifier

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

Generative vs. Discriminative

Classify a document (e.g., review) *d* into class *c* (e.g., positive/negative)

- **Generative** classifier assigns a class *c* to a document *d* by computing:

$$\hat{c} = \operatorname*{argmax}_{c \in C} \overbrace{P(d|c)}^{\text{likelihood}} \; \overbrace{P(c)}^{\text{prior}}$$

expresses how to *generate* the features of a document *if we knew it was of class c*

Generative vs. Discriminative

Discriminative classifier

- Directly computes *P(c|d)* instead of learning *P(d|c)* and *P(c)*
- For example, by assigning high weights to document features that can help it **discriminate** between possible classes

Finding the correct class c from a document d in Generative vs Discriminative Classifiers

Naive Bayes

$$\hat{c} = \underset{c \in C}{\operatorname{argmax}} \; \overbrace{P(d|c)}^{\text{likelihood}} \; \overbrace{P(c)}^{\text{prior}}$$

Logistic Regression

$$\hat{c} = \underset{c \in C}{\operatorname{argmax}} \; \overset{\text{posterior}}{P(c|d)}$$

Components of machine learning classifier

Training data: input/output pairs $(x^{(i)}, y^{(i)})$

Feature **representation** of input

- E.g., each $x^{(i)}$ is a vector of features $[x_1, x_2, \ldots, x_n]$

A **classification** function i.e., sigmoid, softmax, …

- E.g., how we compute an estimate $\hat{y}$ with $p(y|x)$

Objective function for learning e.g., to minimize error on training examples

Algorithm for optimizing the **objective function**

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

Logistic Regression

Background: Generative and Discriminative Classifiers

Logistic Regression

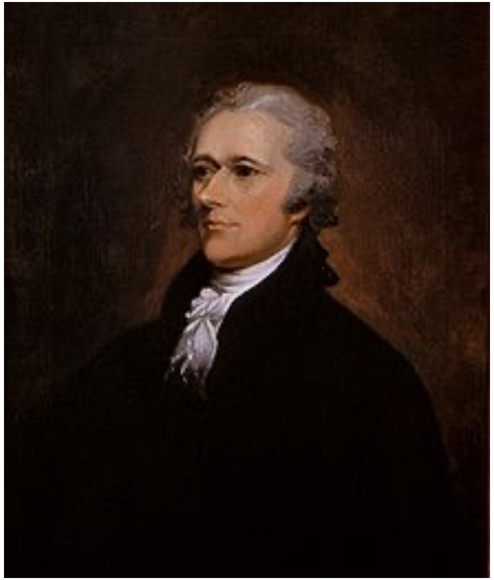
Classification in Logistic Regression

Classification Reminder

Positive/negative sentiment

Spam/not spam

Authorship attribution (Hamilton or Madison?)



Alexander Hamilton

Text Classification: definition

Input:

- a document x
- a fixed set of classes $C = \{c_1, c_2,\ldots, c_J\}$

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** $[x_1, x_2, \ldots, x_n]$
- We compute an output: a predicted class $\hat{y}^{(i)} \in \{0,1\}$

Weights and Bias

Logistic regression learns from the training set (1) a vector of weights **w** and (2) a bias/intercept term *b*

- Each **weight** w_i is associated with one of the input features x_i and represent how **important** that feature is to the classification **decision**
  - E.g., for a sentiment classification task, we would expect the word '*awesome*' to have a **high positive weight** with the **positive** class

Features in logistic regression

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

Logistic Regression for one observation x

Input observation: vector $x = [x_1, x_2, \ldots, x_n]$

Weights: one per feature: $W = [w_1, w_2, \ldots, w_n]$

- Sometimes we call the weights $\theta = [\theta_1, \theta_2, \ldots, \theta_n]$

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

- (Plus 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, just like Naive Bayes did

We want a model that can tell us:

$p(y=1|x; \theta)$

$p(y=0|x; \theta)$

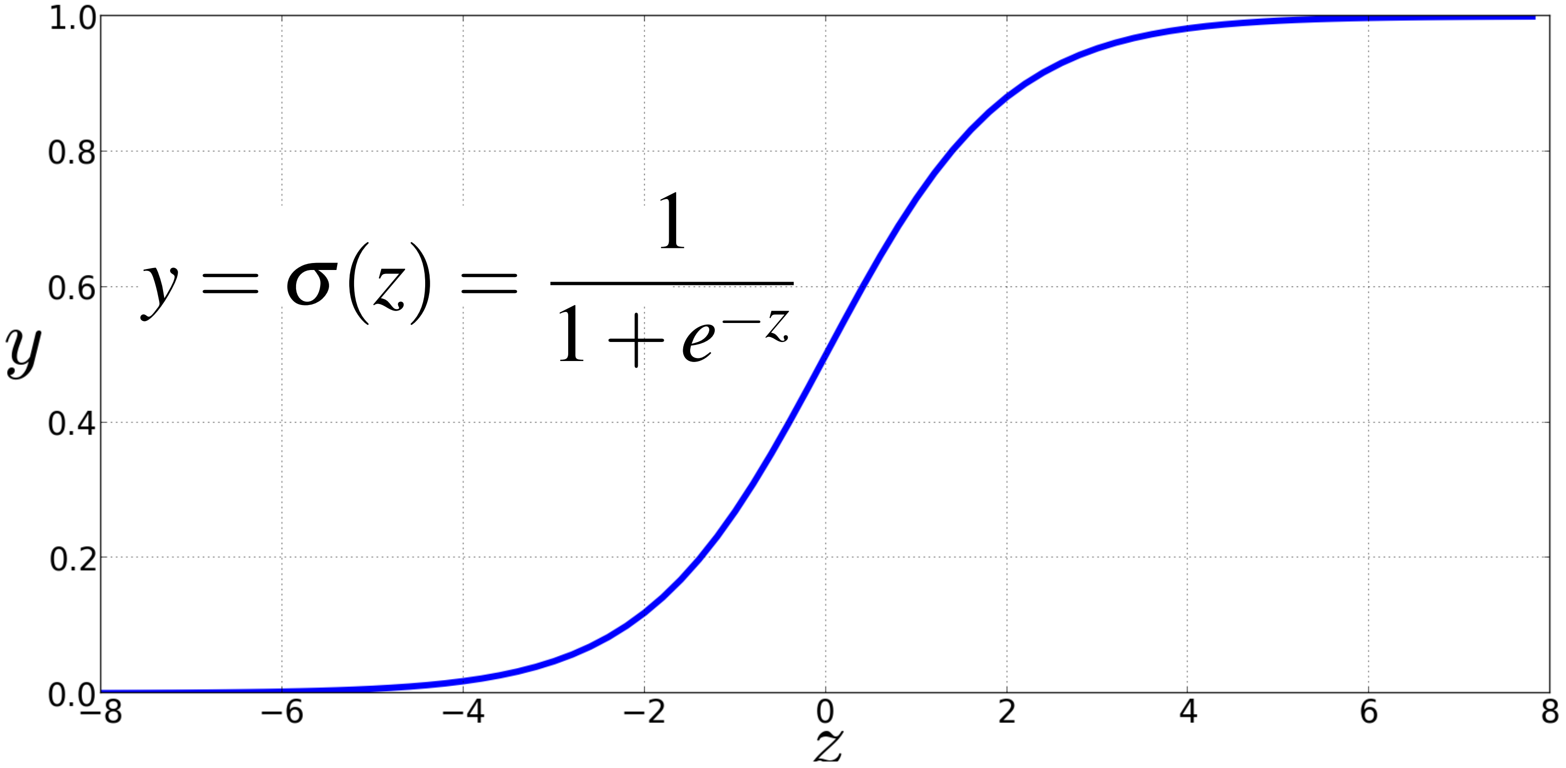
The problem: z isn't a probability, it's just a number!

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

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

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

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

By the way:

$$P(y=0) = 1-\sigma(w\cdot x+b) = \sigma(-(w\cdot x+b))$$

$$= 1-\frac{1}{1+\exp(-(w\cdot x+b))}$$

$$= \frac{\exp(-(w\cdot x+b))}{1+\exp(-(w\cdot x+b))}$$

Because

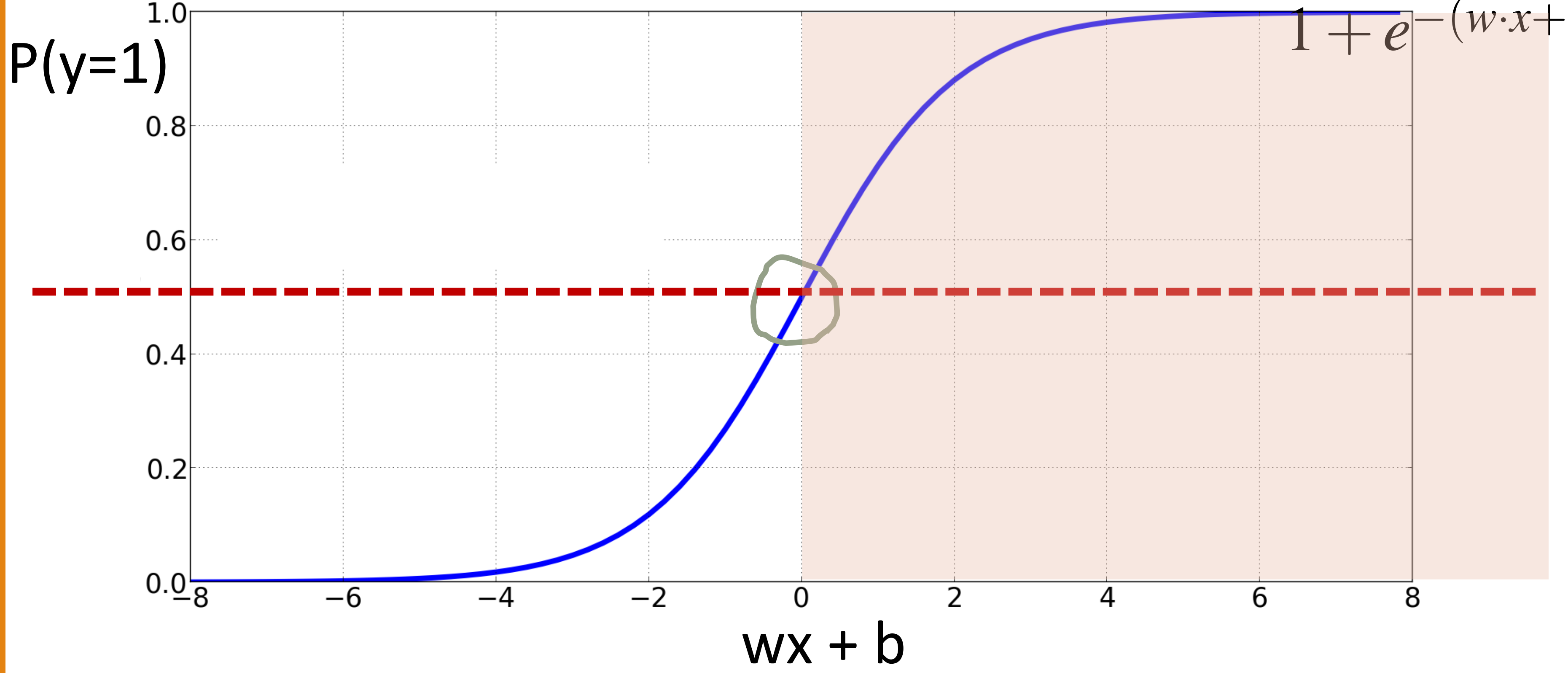
$$1-\sigma(x) = \sigma(-x)$$

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 $P(y=1) = \sigma(w \cdot x + b) = \frac{1}{1+e^{-(w \cdot x + b)}}$



Turning a probability into a classifier

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

$$\text{if } w \cdot x + b > 0$$

$$\text{if } w \cdot x + b \leq 0$$

Logistic Regression

Classification in Logistic Regression

Logistic Regression

Logistic Regression: a text example on sentiment classification

Example: sentiment classification

Input: Movie review text

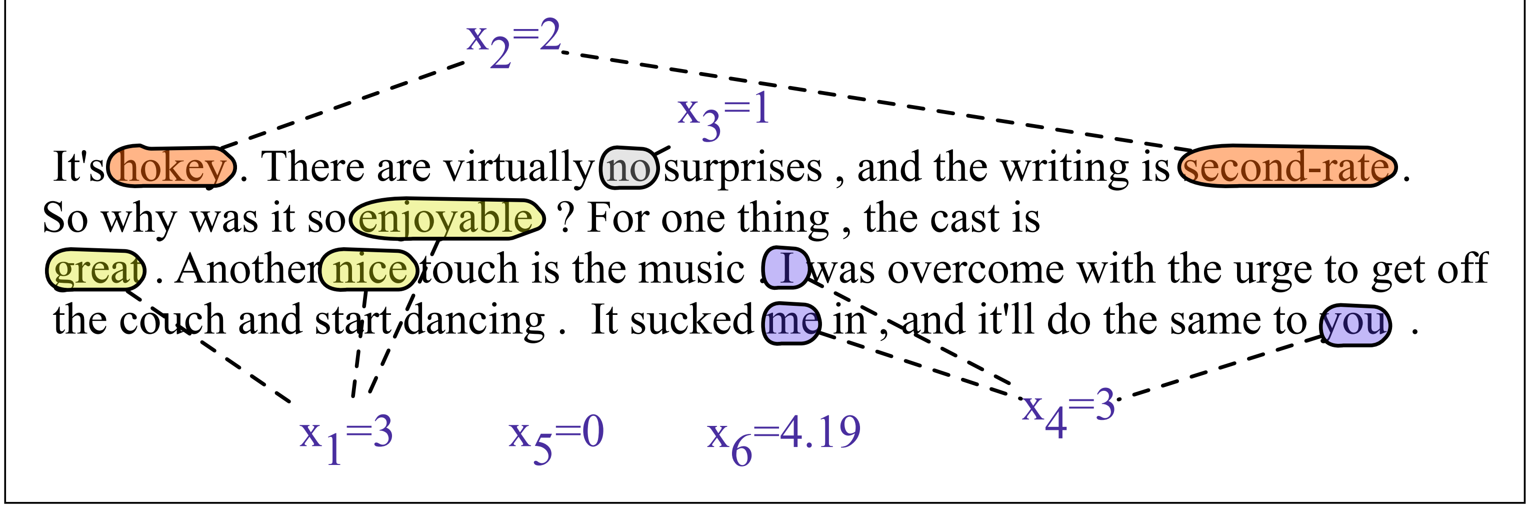
Output: +/-

Features:

Var	Definition
x_1	count(positive lexicon) $\in$ doc)
x_2	count(negative lexicon) $\in$ doc)
x_3	$\begin{cases} 1 & \text{if “no”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$
x_4	count(1st and 2nd pronouns $\in$ doc)
x_5	$\begin{cases} 1 & \text{if “!”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$
x_6	log(word count of doc)

Sentiment example: does y=1 or y=0?

It's hokey . There are virtually no surprises , and the writing is second-rate . So why was it so enjoyable ? For one thing , the cast is great . Another nice touch is the music . I was overcome with the urge to get off the couch and start dancing . It sucked me in , and it'll do the same to you .



Var	Definition	Value in Fig. 5.2
x_1	count(positive lexicon) $\in$ doc)	3
x_2	count(negative lexicon) $\in$ doc)	2
x_3	$\begin{cases} 1 & \text{if “no”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	1
x_4	count(1st and 2nd pronouns $\in$ doc)	3
x_5	$\begin{cases} 1 & \text{if “!”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	0
x_6	log(word count of doc)	$\ln(66) = 4.19$

Example: learned weights

Already learned the weights:

$$[2.5, -5.0, -1.2, 0.5, 2.0, 0.7]$$

w_1 w_2 w_3 w_4 w_5 w_6

Negative words are negatively associated with + label

Var	Definition
x_1	count(positive lexicon) $\in$ doc)
x_2	count(negative lexicon) $\in$ doc)
x_3	$\begin{cases} 1 & \text{if "no"} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$
x_4	count(1st and 2nd pronouns $\in$ doc)
x_5	$\begin{cases} 1 & \text{if "!"} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$
x_6	log(word count of doc)

Classifying sentiment for input x

Var	Definition	Val	5.2
x_1	count(positive lexicon) $\in$ doc)	3	
x_2	count(negative lexicon) $\in$ doc)	2	
x_3	$\begin{cases} 1 & \text{if “no”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	1	
x_4	count(1st and 2nd pronouns $\in$ doc)	3	
x_5	$\begin{cases} 1 & \text{if “!”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	0	
x_6	log(word count of doc)	$\ln(66) = 4.19$	

Suppose $w = [2.5, -5.0, -1.2, 0.5, 2.0, 0.7]$

$b = 0.1$

Classifying sentiment for input x

$$
\begin{aligned}
p(+|x) = P(Y=1|x) &= \sigma(w \cdot x + b) \\
&= \sigma([2.5, -5.0, -1.2, 0.5, 2.0, 0.7] \cdot [3, 2, 1, 3, 0, 4.19] + 0.1) \\
&= \sigma(.833) \\
&= 0.70
\end{aligned}
$$

$$
\begin{aligned}
p(-|x) = P(Y=0|x) &= 1 - \sigma(w \cdot x + b) \\
&= 0.30
\end{aligned}
$$

We can build features for logistic regression for any classification task: period disambiguation

End of sentence

This ends in a period.
The house at 465 Main St. is new.

Not end

$$x_1 = \begin{cases} 1 & \text{if "}Case(w_i) = \text{Lower"} \\ 0 & \text{otherwise} \end{cases}$$

$$x_2 = \begin{cases} 1 & \text{if "}w_i \in \text{AcronymDict"} \\ 0 & \text{otherwise} \end{cases}$$

$$x_3 = \begin{cases} 1 & \text{if "}w_i = \text{St. \& }Case(w_{i-1}) = \text{Cap"} \\ 0 & \text{otherwise} \end{cases}$$

Feature Engineering

For logistic regression, some features that are combination features like x_3 have to be designed by hand

Recently, no need for feature engineering

- Representation learning: ways to learn features automatically in unsupervised manner
  - E.g., word2vec

Classification in (**binary**) logistic regression: summary

Given:

- a set of classes: (+ sentiment,- sentiment)
- a vector **x** of features `[x1, x2, …, xn]`
  - x1= count("awesome")
  - x2 = log(number of words in review)
- A vector **w** of weights `[w1, w2, …, wn]`
  - w_i for each feature f_i

$$P(y=1) = \sigma(w \cdot x + b) = \frac{1}{1+e^{-(w \cdot x + b)}}$$

Logistic Regression vs. Naïve Bayes

NB has strong conditional independence assumption between features

Logistic regression is more robust to correlated features

- E.g., if correlated features are x_1 and x_2, logistic regression simply assigns part of the weight to w_1 and part to w_2

However, NB is fast to train and works extremely well on some cases (e.g., when features are independent given the class)

Logistic Regression

Logistic Regression: a text example on sentiment classification

Learning: Cross-Entropy Loss

Parameter Learning

Given the data (x^i), the feature representation x^i=[x_1,x_2,…,x_n], and the classification function (sigmoid of the weighted sum of features $\sigma(w \cdot x + b)$)

How do we learn the weights?

Wait, 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:

$\hat{y}$ = σ(w·x+b)

from the true output:

y [= either 0 or 1]

We'll call this difference:

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

Parameter Learning

Learn **w** and b that make $\hat{y}$ as close as possible to the true *y*

- <u>**or**</u> learn **w** and b that **minimizes** the **distance** between $\hat{y}$ and *y*

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

How?

- By maximizing the probability of the true labels in the training data (x,y) i.e., maximizes P(y|x)

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

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

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

noting:

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

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

Cross entropy between the true distribution y and estimated distribution

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

Now flip sign to turn this into a loss: something to minimize

Cross-entropy loss (because 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 $\hat{y}$:

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

Let's see if this works for our sentiment example

We want loss to be:

- smaller if the model estimate is close to correct
- bigger if model is confused

Let's first suppose the true label of this is y=1 (positive)

It's hokey . There are virtually no surprises , and the writing is second-rate . So why was it so enjoyable ? For one thing , the cast is great . Another nice touch is the music . I was overcome with the urge to get off the couch and start dancing . It sucked me in , and it'll do the same to you .

Let's see if this works for our sentiment example

True value is y=1. How well is our model doing?

$$
\begin{aligned}
p(+|x) = P(Y=1|x) &= \sigma(w \cdot x + b) \\
&= \sigma([2.5, -5.0, -1.2, 0.5, 2.0, 0.7] \cdot [3, 2, 1, 3, 0, 4.19] + 0.1) \\
&= \sigma(.833) \\
&= 0.70 \qquad (5.6)
\end{aligned}
$$

Pretty well! What's the loss?

$$
\begin{aligned}
L_{\text{CE}}(\hat{y}, y) &= -[y \log \sigma(w \cdot x + b) + (1-y) \log (1 - \sigma(w \cdot x + b))] \\
&= -[\log \sigma(w \cdot x + b)] \\
&= -\log(.70) \\
&= .36
\end{aligned}
$$

Let's see if this works for our sentiment example

Suppose true value instead was y=0.

$$
\begin{aligned}
p(-|x) = P(Y=0|x) &= 1-\sigma(w\cdot x+b) \\
&= 0.30
\end{aligned}
$$

What's the loss?

$$
\begin{aligned}
L_{\mathrm{CE}}(\hat{y},y) &= -[y\log\sigma(w\cdot x+b)+(1-y)\log(1-\sigma(w\cdot x+b))] \\
&= -[\log(1-\sigma(w\cdot x+b))] \\
&= -\log(.30) \\
&= 1.2
\end{aligned}
$$

Let's see if this works for our sentiment example

The loss when model was right (if true y=1)

$$
\begin{aligned}
L_{\mathrm{CE}}(\hat{y},y) &= -[y\log\sigma(w\cdot x+b)+(1-y)\log(1-\sigma(w\cdot x+b))] \\
&= -[\log\sigma(w\cdot x+b)] \\
&= -\log(.70) \\
&= .36
\end{aligned}
$$

Is lower than the loss when model was wrong (if true y=0):

$$
\begin{aligned}
L_{\mathrm{CE}}(\hat{y},y) &= -[y\log\sigma(w\cdot x+b)+(1-y)\log(1-\sigma(w\cdot x+b))] \\
&= -[\log(1-\sigma(w\cdot x+b))] \\
&= -\log(.30) \\
&= 1.2
\end{aligned}
$$

Sure enough, loss was bigger when model was wrong!

Logistic Regression

Cross-Entropy Loss

Logistic Regression

Stochastic Gradient Descent

Our goal: minimize the loss

Let's make explicit that the loss function is parameterized by weights θ=(w,b)

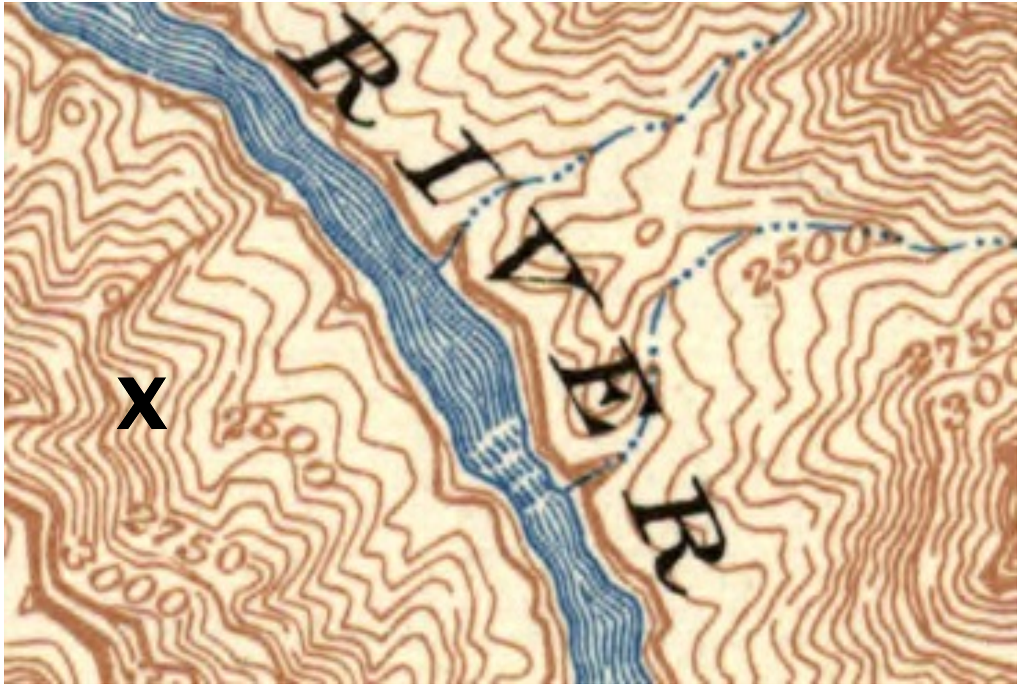
- And we'll represent $\hat{y}$ as $f(x; \theta)$ to make the dependence on θ more obvious

We want the weights that minimize the loss, averaged over all examples:

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

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

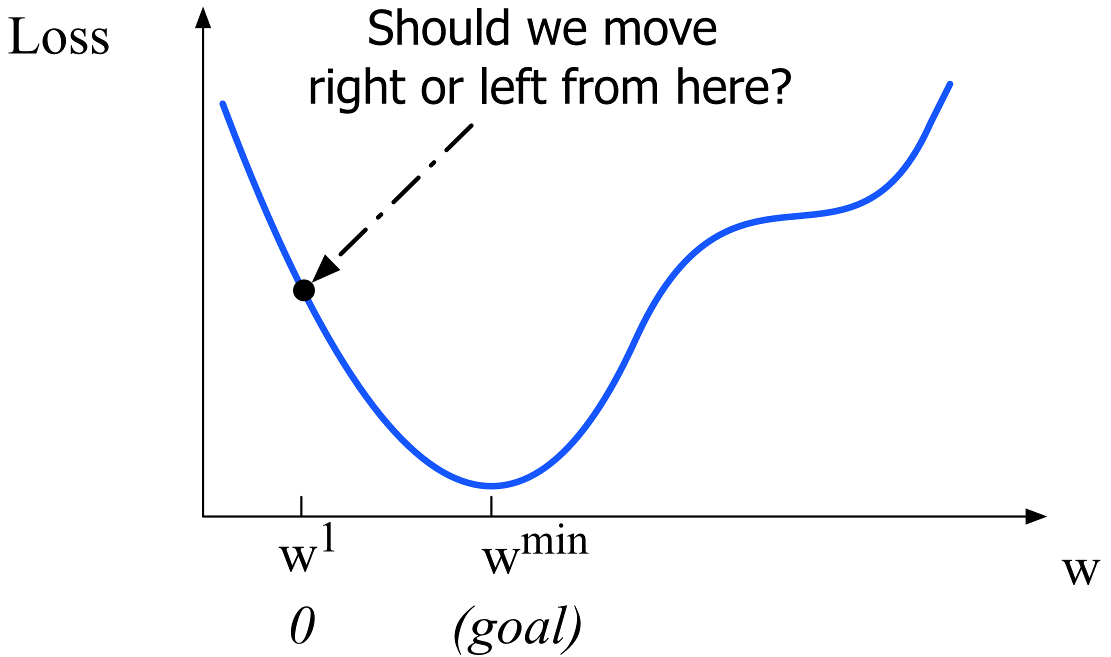
For logistic regression, loss function is **convex**

- 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?

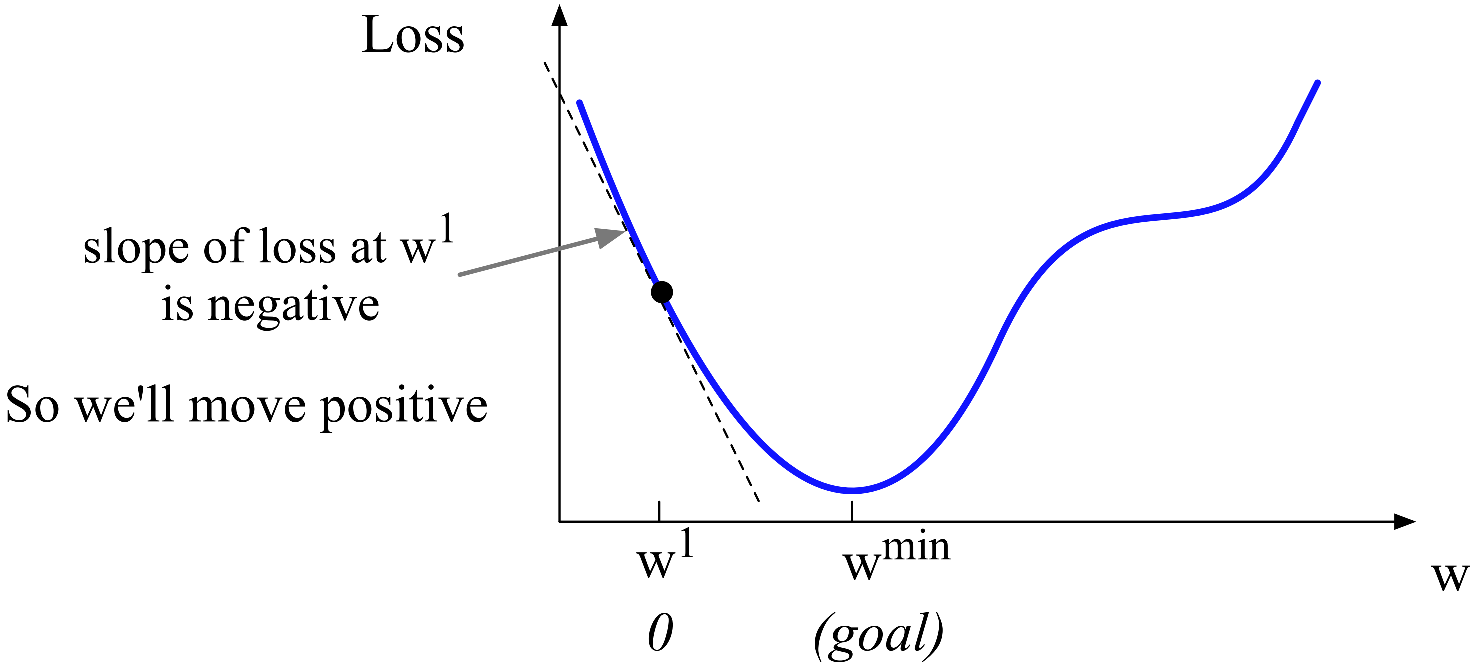
A: Move *w* in the reverse direction from the slope of the function



Let's first visualize for a single scalar w

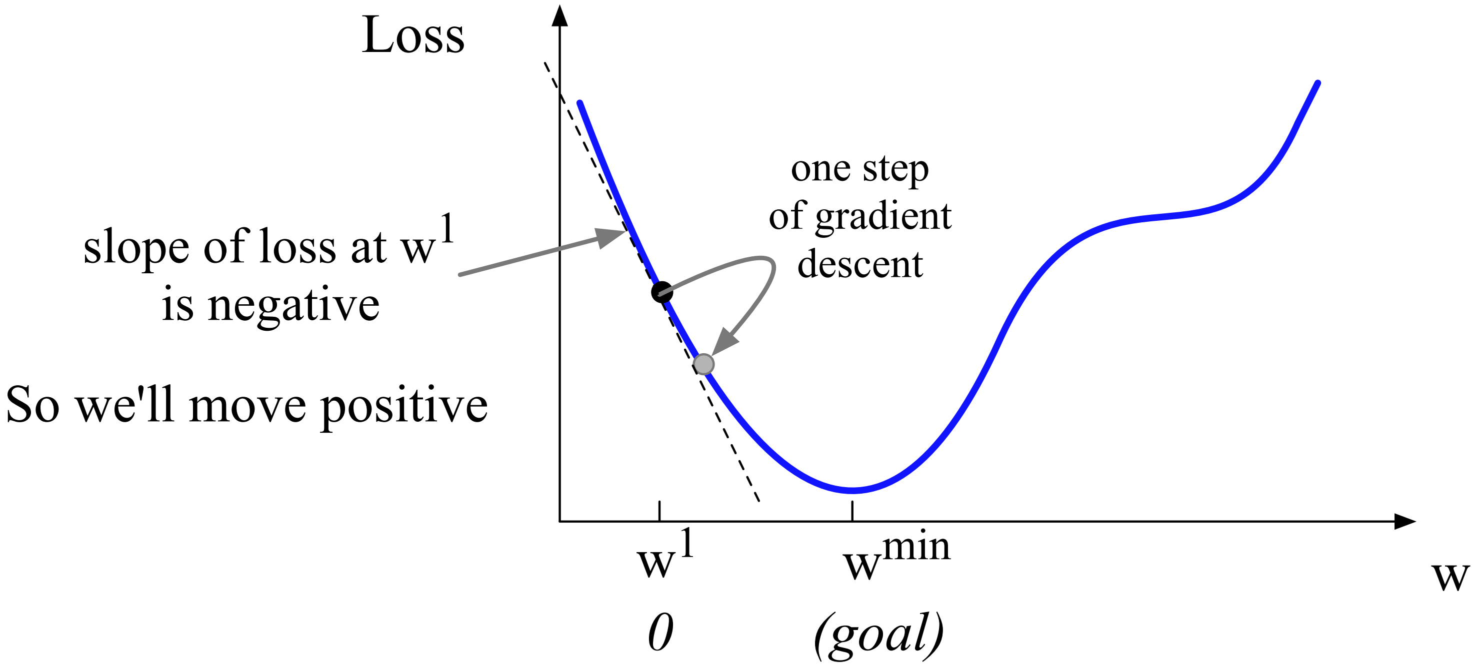
Q: Given current w, should we make it bigger or smaller?

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



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

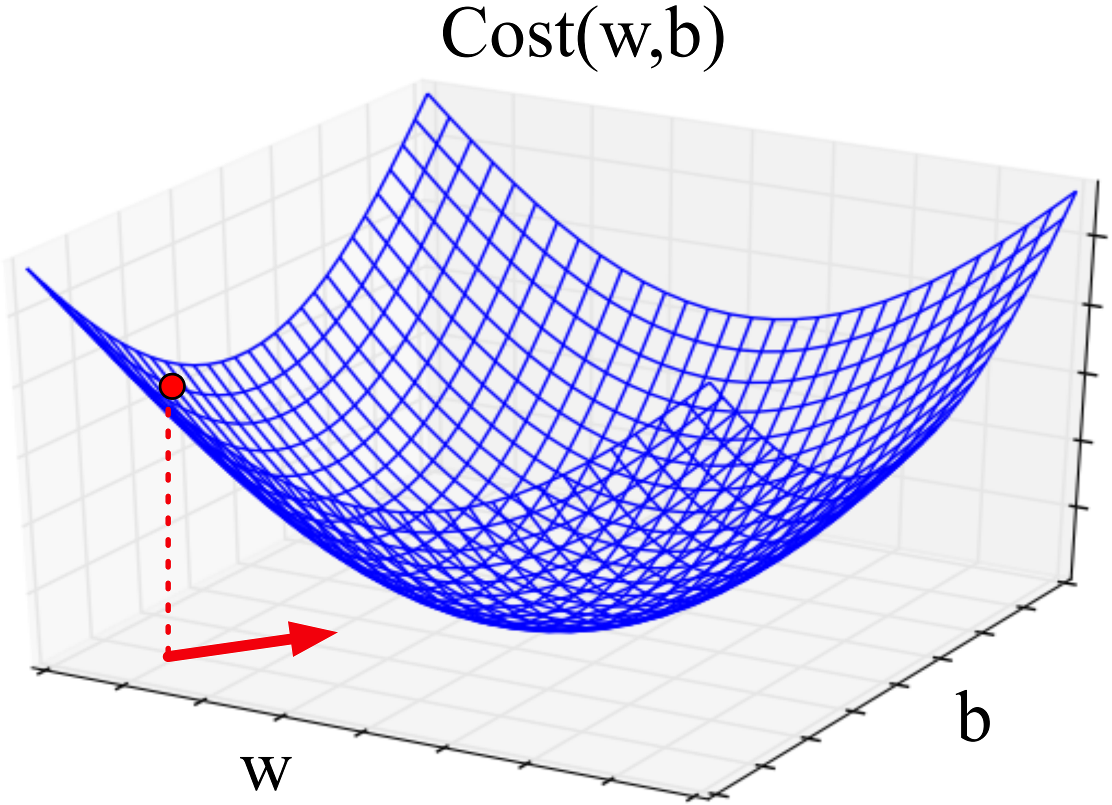
We want to know where in the N-dimensional space (of the *N* parameters that make up θ) we should move.

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

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

The elegant derivative of this function (see textbook 5.8 for derivation)

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

difference between
estimated label and true label

Gradient Descent for Logistic Regression

$$w^{t+1} = w^t \underbrace{- \eta[\underbrace{\sigma(w \cdot x + b) -}_{<=0} y]}_{>=0} x_j$$

1

positively correlated with y=1

$w^{t+1} >= w^t$

If seeing more y=1example with high counts of x_j,
weight w^{t+1} will shift more and more towards a positive value

Gradient Descent for Logistic Regression

$$w^{t+1} = w^t - \eta\Big[\underbrace{\underbrace{\sigma(w \cdot x + b)}_{>=0} - \underbrace{y}_{0}}_{<=0}\Big]x_j$$

Negatively correlated with y=1

$w^{t+1} <= w^t$

If seeing more y=0 example with high counts of x_j,
weight w^{t+1} will shift more and more towards a negative value

Gradient Descent for Logistic Regression

Batch loss = average loss over training examples

$$Cost(w,b) = -\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log \sigma(w \cdot x^{(i)} + b) + (1 - y^{(i)}) \log\left(1 - \sigma(w \cdot x^{(i)} + b)\right)$$

Batch gradient

$$\frac{\partial Cost(w,b)}{\partial w_j} = \frac{1}{m}\sum_{i=1}^{m}\left[\sigma(w \cdot x^{(i)} + b) - y^{(i)}\right] x_j^{(i)}$$

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 $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$
    #   y is the set of training outputs (labels) $y^{(1)}, y^{(2)}, \ldots, y^{(m)}$

$\theta \leftarrow 0$

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.

Learning rate

Common practice:

- Begin at a higher value and slowly decrease as you iterate
- Begin at some value and reset value + decrease if the loss increases (you've skipped the minimum! so you should reset and take smaller steps) or increase if the loss decreases (you're still some distance away from the minimum, so move faster!) (**Bold Driver**)

Adapt learning rate in each iteration

Logistic Regression

Stochastic Gradient Descent

Logistic Regression

Stochastic Gradient Descent: An example and more details

Working through an example

One step of gradient descent

A mini-sentiment example, where the true y=1 (positive)

Two features:

$x_1 = 3$ (count of positive lexicon words)

$x_2 = 2$ (count of negative lexicon words)

Assume 3 parameters (2 weights and 1 bias) in Θ^0 are zero:

$w_1 = w_2 = b = 0$

$\eta = 0.1$

Example of gradient descent

$w_1 = w_2 = b = 0;$
$x_1 = 3; \quad x_2 = 2$

Update step for update θ is:

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

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

Gradient vector has 3 dimensions:

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix}$$

Example of gradient descent

$w_1 = w_2 = b = 0;$
$x_1 = 3; \quad x_2 = 2$

Update step for update θ is:

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

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

Gradient vector has 3 dimensions:

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} \quad \end{bmatrix}$$

Example of gradient descent

$w_1 = w_2 = b = 0;$

$x_1 = 3; \quad x_2 = 2$

Update step for update θ is:

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

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

Gradient vector has 3 dimensions:

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w \cdot x + b) - y)x_1 \\ (\sigma(w \cdot x + b) - y)x_2 \\ \sigma(w \cdot x + b) - y \end{bmatrix}$$

Example of gradient descent

$w_1 = w_2 = b = 0;$
$x_1 = 3; \quad x_2 = 2$

Update step for update θ is:

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

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

Gradient vector has 3 dimensions:

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w \cdot x + b) - y)x_1 \\ (\sigma(w \cdot x + b) - y)x_2 \\ \sigma(w \cdot x + b) - y \end{bmatrix} = \begin{bmatrix} (\sigma(0) - 1)x_1 \\ (\sigma(0) - 1)x_2 \\ \sigma(0) - 1 \end{bmatrix} =$$

Example of gradient descent

$w_1 = w_2 = b = 0;$
$x_1 = 3; \quad x_2 = 2$

Update step for update θ is:

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

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

Gradient vector has 3 dimensions:

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\text{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\text{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\text{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w \cdot x + b) - y)x_1 \\ (\sigma(w \cdot x + b) - y)x_2 \\ \sigma(w \cdot x + b) - y \end{bmatrix} = \begin{bmatrix} (\sigma(0) - 1)x_1 \\ (\sigma(0) - 1)x_2 \\ \sigma(0) - 1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

Example of gradient descent

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\text{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\text{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\text{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w\cdot x+b)-y)x_1 \\ (\sigma(w\cdot x+b)-y)x_2 \\ \sigma(w\cdot x+b)-y \end{bmatrix} = \begin{bmatrix} (\sigma(0)-1)x_1 \\ (\sigma(0)-1)x_2 \\ \sigma(0)-1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

Now that we have a gradient, we compute the new parameter vector θ^1 by moving θ^0 in the opposite direction from the gradient:

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

$\eta = 0.1;$

$$\theta^1 =$$

Example of gradient descent

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w\cdot x+b)-y)x_1 \\ (\sigma(w\cdot x+b)-y)x_2 \\ \sigma(w\cdot x+b)-y \end{bmatrix} = \begin{bmatrix} (\sigma(0)-1)x_1 \\ (\sigma(0)-1)x_2 \\ \sigma(0)-1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

Now that we have a gradient, we compute the new parameter vector θ^1 by moving θ^0 in the opposite direction from the gradient:

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

$\eta = 0.1$;

$$\theta^1 = \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix} - \eta \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

Example of gradient descent

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w \cdot x + b) - y)x_1 \\ (\sigma(w \cdot x + b) - y)x_2 \\ \sigma(w \cdot x + b) - y \end{bmatrix} = \begin{bmatrix} (\sigma(0) - 1)x_1 \\ (\sigma(0) - 1)x_2 \\ \sigma(0) - 1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

Now that we have a gradient, we compute the new parameter vector θ^1 by moving θ^0 in the opposite direction from the gradient:

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

$\eta = 0.1;$

$$\theta^1 = \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix} - \eta \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix} = \begin{bmatrix} .15 \\ .1 \\ .05 \end{bmatrix}$$

Example of gradient descent

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w \cdot x + b) - y)x_1 \\ (\sigma(w \cdot x + b) - y)x_2 \\ \sigma(w \cdot x + b) - y \end{bmatrix} = \begin{bmatrix} (\sigma(0) - 1)x_1 \\ (\sigma(0) - 1)x_2 \\ \sigma(0) - 1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

Now that we have a gradient, we compute the new parameter vector θ^1 by moving θ^0 in the opposite direction from the gradient:

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

$\eta = 0.1$;

$$\theta^1 = \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix} - \eta \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix} = \begin{bmatrix} .15 \\ .1 \\ .05 \end{bmatrix}$$

Note that enough negative examples would eventually make w_2 negative

Mini-batch training

Stochastic gradient descent chooses a single random example at a time.

That can result in choppy movements

More common to compute gradient over batches of training instances.

Batch training: entire dataset

Mini-batch training: *m* examples (512, or 1024)

Logistic Regression

Stochastic Gradient Descent: An example and more details

Logistic Regression

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.

-

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

Useful or harmless features

X1 = "this"
X2 = "movie
X3 = "hated"
X4 = "drew me in"

4gram features that just "memorize" training set and might cause problems

X5 = "the same to you"
X7 = "tell you how much"

Overfitting

4-gram 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 log prob rather than minimizing loss)

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

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:

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

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:

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

Regularization

Constraints on **the prior** of how the weights should look

- L1 regularization → Laplace prior on weights
- L2 regularization → Gaussian prior on weights with mean = 0
  - i.e., the "weights" prefer to have the value 0

$$\hat{w} = \underbrace{\underbrace{\underset{w}{\operatorname{argmax}} \prod_{i=1}^{M} P(y^{(i)}|x^{(i)})}_{\text{likelihood}} \times \prod_{j=1}^{n} \underbrace{\frac{1}{\sqrt{2\pi\sigma_j^2}} \exp\left(-\frac{(w_j - \mu_j)^2}{2\sigma_j^2}\right)}_{\text{prior}}}_{\text{posterior}}$$

MAP est.

Detour: Maximum A Posteriori Estimation

$$\theta_{MLE} = \arg\max_{\theta} P(X|\theta)$$ likelihood

$$\theta_{MAP} = \arg\max_{\theta} P(X|\theta)P(\theta)$$ prior

posterior $$P(\theta|X) = \frac{P(X|\theta)P(\theta)}{P(X)}$$ Bayes Rule

$$\propto P(X|\theta)P(\theta)$$

MLE is a special case of MAP where the prior is a constant

Regularization and MAP

$$\hat{w} \;=\; \underset{w}{\operatorname{argmax}} \prod_{i=1}^{M} P(y^{(i)}|x^{(i)}) \times \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi\sigma_j^2}} \exp\left(-\frac{(w_j-\mu_j)^2}{2\sigma_j^2}\right)$$

likelihood weighted by prior (**MAP**)

in log space, with $\mu = 0$, and assuming $2\sigma^2 = 1$

$$\hat{w} \;=\; \underset{w}{\operatorname{argmax}} \sum_{i=1}^{m} \log P(y^{(i)}|x^{(i)}) - \alpha \sum_{j=1}^{n} w_j^2$$

regularized objective

Logistic Regression

Regularization

Logistic Regression

Multinomial Logistic Regression

Multinomial Logistic Regression

Often we need more than 2 classes

- Positive/negative/neutral
- Parts of speech (noun, verb, adjective, adverb, preposition, etc.)
- Classify emergency SMSs into different actionable classes

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(positive|doc) + P(negative|doc) + P(neutral|doc) = 1

Need a generalization of the sigmoid called the **softmax**

- Takes a vector *z* = [*z*1, *z*2, ..., *zk*] 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 $z = [z_1, z_2, \ldots , z_k]$ of k arbitrary values into probabilities

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

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

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

The **softmax** function

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

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

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

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

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 → y=1 neg weight → y=0

$$x_5 = \begin{cases} 1 & \text{if "!"} \in \text{doc} \\ 0 & \text{otherwise} \end{cases} \qquad w_5 = 0.1$$

Multinominal: 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

Multinomial Logistic Regression

Logistic regression loss: (with 2 classes, y=0 or y=1)

$$L_{CE}(\hat{y},y) = -\log p(y|x) \;=\; -\log\left[\hat{y}^{y}\,(1-\hat{y})^{1-y}\right] \;=\; -\left[y\log\hat{y} + (1-y)\log(1-\hat{y})\right]$$

Now that we have K classes, the loss function is :

$$\begin{aligned} L_{CE}(\hat{y},y) &= -\sum_{k=1}^{K} 1\{y=k\}\log p(y=k|x) \\ &= -\sum_{k=1}^{K} 1\{y=k\}\log \frac{e^{w_k\cdot x+b_k}}{\sum_{j=1}^{K} e^{w_j\cdot x+b_j}} \end{aligned}$$

Multinomial Logistic Regression

Gradient of the update:

$$\frac{\partial L_{CE}}{\partial w_k} = -(1\{y=k\} - p(y=k|x))x_f$$

$$= -\left(1\{y=k\} - \frac{e^{w_k \cdot x + b_k}}{\sum_{j=1}^{K} e^{w_j \cdot x + b_j}}\right)x_f$$

logistic regression

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

true label

1/0

predicted label

p(y=k|x)/p(y=1|x)

Logistic Regression

Multinomial Logistic Regression