Carnegie Mellon University
Language Technologies Institute

11-411/11-611 Natural Language Processing

Logistic Regression

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February 7, 2023

Language Technologies Institute

Learning Objectives

At the end of this lecture, students will be able to:

- Explain the difference between generative and discriminative classifiers
- Describe the basic requirements of an ML classifier and how these are satisfied by logistic regression classifiers
- Implement classification with logistic regression works (be able to calculate it)
- Explain why the sigmoid function is used in logistic regression
- Define GRADIENT in the context of logistic regression and explain how it is calculated
- Explain at a high level how gradient descent works
- Work through an example of training a logistic regression classifier using gradient descent
- Define and diagnose overfitting
- Implement L2 and L1 regularization as a solution to overfitting in logistic regression

The super villain Dendrobion plans to conquer the world in order to amass the world's largest collection of orchids

He needs to classify his collection by genus—**but how?**

An Example: Classifying Orchids

Cymbidium

Phalaenopsis

Features: terrestrial/epiphitic, stem shape (sympodial, monopodial, keikis), leaves (shape, pigments), roots (thickness, tuberous), flowers (dorsal sepal, other sepals, petals, labelum, pollinia)

Two Options for Classification

Build up a model of each class

Cymbidiums Semi-epiphetic, lithophytic, or terrestrial. Pseduobulb. Flowers in spikes. Bowl-shaped labellum. Glaborous seed capsule.

Phalaenopsis Epiphetic. Long, course roots. Short, leafy stems. Flowers in racemes or panicles. Spread sepals and petals. Petals much larger than sepals.

Find features that distinguish them

	Cymbs	Phals
pseudobulbs	T	F
spikes	T	F
panicles	F	T
petals much larger than sepals	F	T

Should Dendrobion Use Generative or Discriminative Classifiers?

1. **Generative**—builds a model of each of the categories, so it could **generate** instances of them
2. **Discriminative**—weights heavily the features that best discriminate between categories

Finding the Correct Class c from a Document d

Dendrobion can compare orchids to documents:

Naive Bayes

$$\hat{c} = \operatorname*{argmax}_{c \in C} P(d|c)P(c) \tag{1}$$

(compute the likelihood times the prior)

Logistic Regression

$$\hat{c} = \operatorname*{argmax}_{c \in C} P(c|d) \tag{2}$$

(compute the posterior directly)

What Goes into a (Discriminative) ML Classifier?

1. A feature representation
2. A classification function
3. An objective function
4. An algorithm for optimizing the objective function

What Goes into Logistic Regression?

GENERAL	IN LOGISTIC REGRESSION
feature representation	represent each observation $x^{(i)}$ as a **vector of features** $[x_1, x_2, \ldots x_n]$, as we did with orchids
classification function	**sigmoid function** (logistic function)
objective function	**cross-entropy loss**
optimization function	**gradient descent**

The Two Phases of Logistic Regression

train learn the weights w and b using stochastic gradient descent and cross-entropy loss.

test given a test example x, we compute $p(y|x)$ using the learned weights w and b and return the label ($y = 1$ or $y = 0$) that has higher probability.

Classification with Logistic Regression

Features in Logistic Regression

For feature x_i, weight w_i tells us how import x_i is

- 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 feature vector $x = [x_1, x_2, \ldots, x_n]$

weights one per feature $W = [w_1, w_2, \ldots, w_n]$ (which can also be called $\Theta = [\theta_1, \theta_2, \ldots, \theta_n]$

output a predicted class $\hat{y} \in \{0, 1\}$

How to Do Classification

For each feature x_i, weight w_i tells us the importance of x_i (and we also have the bias b)

We'll sum up all the weighted features and the bias

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

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

A Most Important Formula

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

If z is high, we say $y = 1$; if low, then $y = 0$

But We Want a Probabilistic Classifier

What does “sum is high” even mean?

Can’t our classifier be like Naive Bayes and give us a probability?

What we really want:

- $p(y = 1|x; \theta)$
- $p(y = 0|x; \theta)$

Where x is a vector of features and θ is a vector of weights/parameters.

The Problem: z Isn't a Probability!

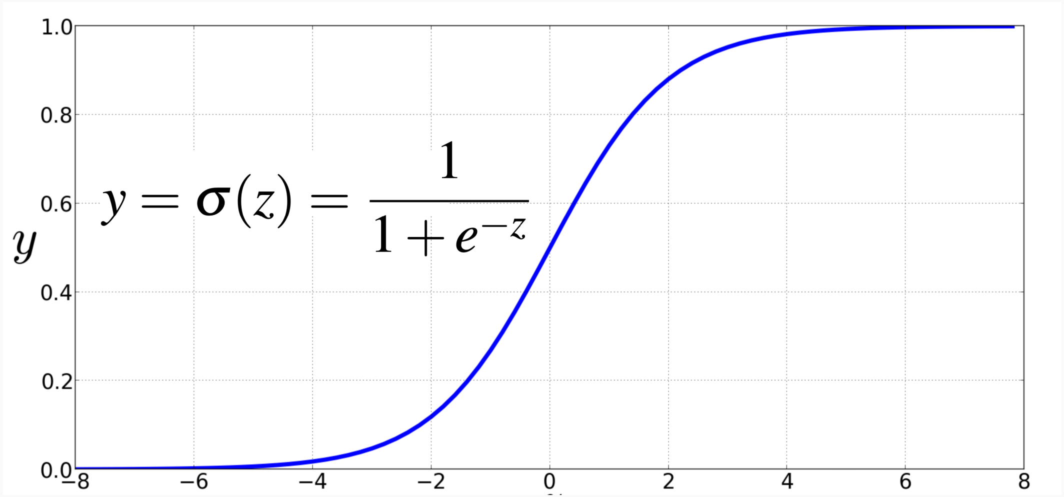
z is just a number:

$$z = w \cdot x + b \tag{3}$$

Solution: use a function of z that goes from 0 to 1, like the **logistic function** or **sigmoid function**:

$$\hat{y} = \sigma(z) = \frac{1}{1+e^{-z}} = \frac{1}{1+\exp(-z)} \tag{4}$$

The Sigmoid Function



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

Logistic Regression in Three Easy Steps

1. Compute $w \cdot x + b$
2. Pass it through the sigmoid function: $\sigma(w \cdot x + b)$
3. Treat the result as a probability

Making Probabilities with Sigmoids

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

Wait, what?

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

because

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

a very convenient property!

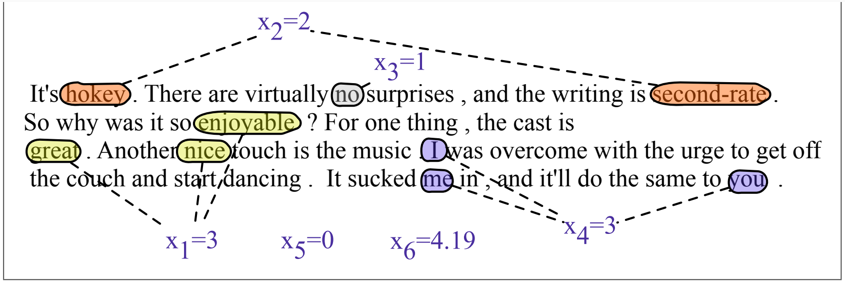
From Probability to Classification

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

0.5 here is called the **decision boundary**

Sentiment Classification: Movie Review

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 .



$x_2=2$
$x_3=1$
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 .
$x_4=3$
$x_1=3$
$x_5=0$
$x_6=4.19$

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)	$\ln(66) = 4.19$

Classifiying Sentiment for Input x

Var	Definition	Val
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
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x_6	log(word count of doc)	$\ln(66) = 4.19$

Suppose $w = [2.5, -0.5, -1.2, 0.5, 2.0, 0.7]$ **and** $b = 0.1$

Performing the Calculations

$$\begin{aligned}
p(+|x) = P(Y=1|x) &= \sigma(w \cdot x + b) \\
&= \sigma([2.5, -5.0, -1.2, 0.5.2.0, 0.7] \cdot [3, 2, 1, 3, 0, 4.19] + 0.1) \\
&= \sigma(0.833) \\
&= 0.70 \\
p(-|x) = P(Y=0|x) &= 1 - \sigma(w \cdot x + b) \\
&= 0.30
\end{aligned}$$

Performing the Calculations

$$\begin{aligned}
p(+|x) = P(Y=1|x) &= \sigma(w \cdot x + b) \\
&= \sigma([2.5, -5.0, -1.2, 0.5.2.0, 0.7] \cdot [3, 2, 1, 3, 0, 4.19] + 0.1) \\
&= \sigma(0.833) \\
&= \mathbf{0.70} \\
p(-|x) = P(Y=0|x) &= 1 - \sigma(w \cdot x + b) \\
&= \mathbf{0.30}
\end{aligned}$$

Learning to Classify with Logistic Regression

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, $\hat{y}$

The Loss Function

A loss function is a function that quantifies how much we are **“losing”**—how different our inferred outputs are from the gold, or ground truth, labels.

Cross-Entropy Loss:
For logistic regression, we can use Cross-Entropy Loss (L_{CE}). For discrete distributions, this has the following form:

$$L_{CE}(\hat{y}, y) = -\sum_{i=1}^{n} y_i \log(\hat{y}_i) \text{ for } n \text{ classes} \tag{5}$$

where y is ground truth and $\hat{y}$ is the probability assigned by the classifier.

Our Goal: Minimize the Loss

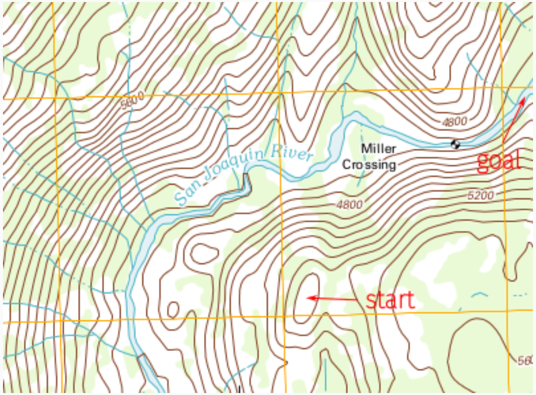
Let's make it explicit that the loss function is parameterized by weights $\theta = (w, b)$.

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

We want the weights that minimize the loss (L_{CE}), averaged over all examples:

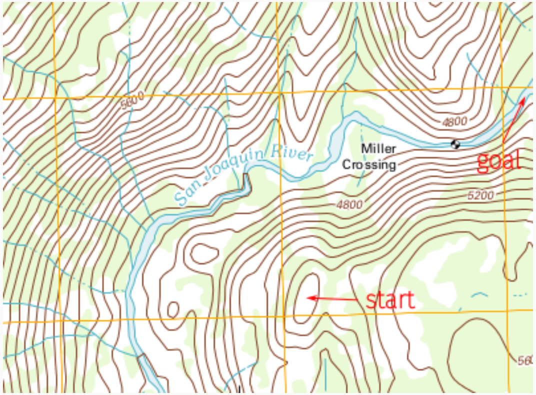
$$\hat{\theta} = \operatorname*{argmin}_{\theta} \frac{1}{m} \sum_{i=1}^{m} L_{CE}(f(x^{(i)}; \theta), y^{(i)}) \tag{6}$$

The Intuition of Gradient Descent



- You are on a hill
- It is your mission to reach the river at the bottom of the canyon (as quickly as possible)
- What is your strategy?

The Intuition of Gradient Descent



- You are on a hill
- It is your mission to reach the river at the bottom of the canyon (as quickly as possible)
- What is your strategy?
    1. Determine in which direction the steepest downhill slope lies
    2. Take a step in that direction
    3. Repeat until a step in any direction will take you up hill

Our Goal: Minimize the Loss

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

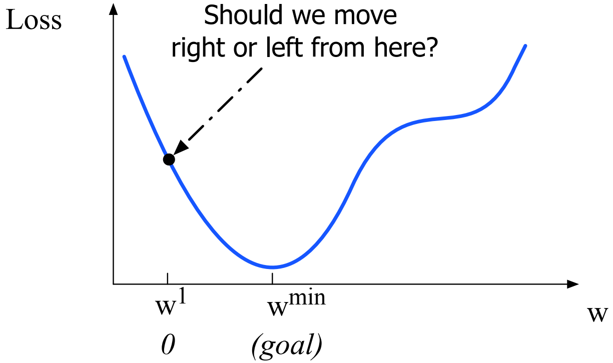
- Just one minimum
- Gradient descent is guaranteed to find the minimum, no matter where you start

(Loss for neural networks is non-convex; we'll talk more about that later)

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



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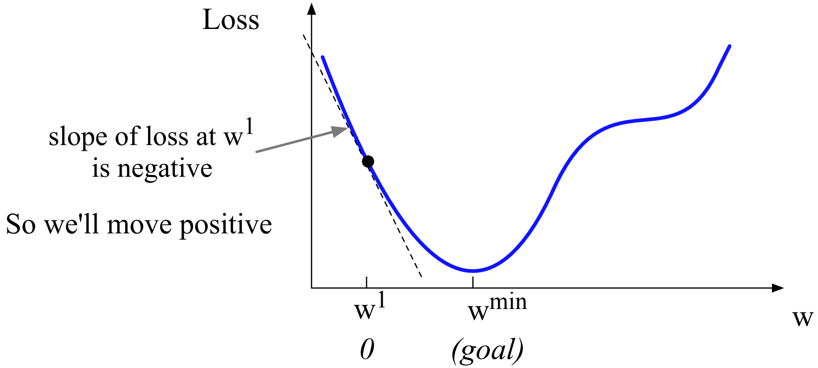

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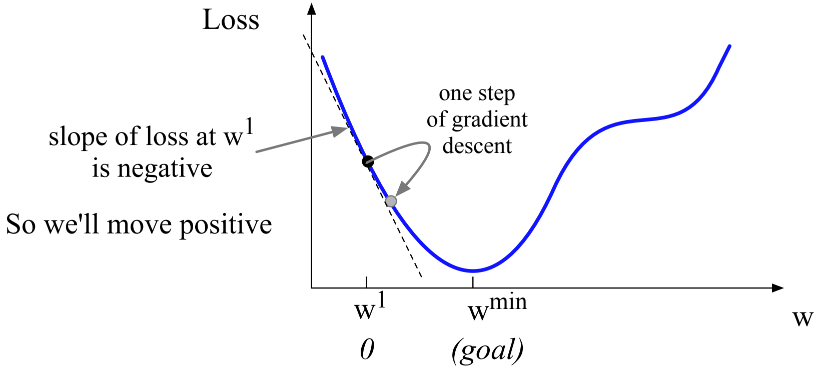

Loss
slope of loss at w^1 is negative
So we'll move positive
one step of gradient descent
w^1
w^{min}
w
0
(goal)

A Gradient is a Vector Pointing in the Direction of Greatest Increase

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 a Step?

- We move by the value of the gradient (in our example, the slope)

$$\frac{d}{dw} L_{CE}(f(x; w), y)$$

  weighted by the LEARNING RATE η
- The higher the learning rate, the faster w moves:

$$w_{t+1} = w_t - \eta \frac{d}{dw} L_{CE}(f(x; w), y) \tag{7}$$

How Do We Do Gradient Descent in N Dimensions?

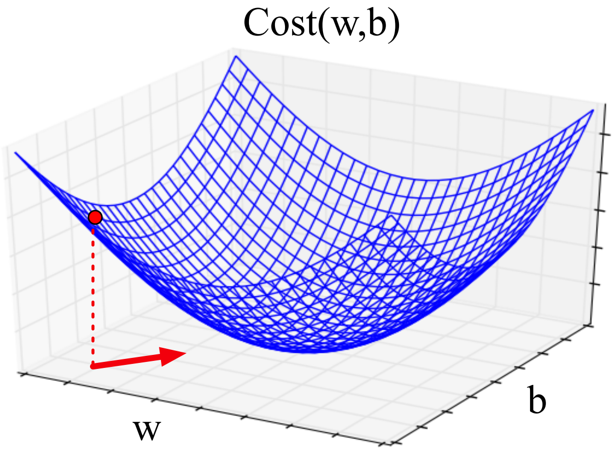
We want to know where in the N-dimensional space (of the N parameters that make up θ) we should move.

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



Find the error!

But Real Gradients Have More than Two Dimensions

- They are much longer
- They have lots of weights
- For each dimension w_i, the gradient component i tells us the slope w.r.t. that variable
    - "How much would a small change in w_i influence the total loss function L?"
    - The slope is expressed as the partial derivative ∂ of the loss ∂w_i
- We can then define the gradient as **a vector of these partials**

Computing the Gradient

Let's represent $\hat{y}$ as $f(x;\theta)$ to make things clearer:

$$\nabla_{\theta} L(f(x;\theta), y) = \begin{bmatrix} \frac{\partial}{\partial w_1} L(f(x;\theta), y) \\ \frac{\partial}{\partial w_2} L(f(x;\theta), y) \\ \vdots \\ \frac{\partial}{\partial w_n} L(f(x;\theta), y) \end{bmatrix} \tag{8}$$

What is the final equation for updating θ based on the gradient?

$$\theta_{t+1} = \theta_t - \eta \nabla L(f(x;\theta), y) \tag{9}$$

(For us, L is the cross-entropy loss L_{CE}).

So What Are These Partial Derivatives for Logistic Regression?

The textbook lays out the derivation in §5.8, but here's the basic idea:

Here is the loss function (for binary classification):

$$L_{CE}(\hat{y}, y) = -[y \log \sigma(w \cdot x + b) + (1 - y) \log(1 - \sigma(w \cdot x + b))] \tag{10}$$

The derivative of this function is:

$$\frac{\partial L_{CE}(\hat{y}, y)}{\partial w_j} = [\sigma(w \cdot x + b) - y]x_j \tag{11}$$

which looks very manageable!

```
function STOCHASTIC GRADIENT DESCENT($L()$, $f()$, $x$, $y$) returns $\theta$
    # where: L is the loss function
    #        f is a function parameterized by $\theta$
    #        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 $\theta$ to maximize loss?
    3. $\theta \leftarrow \theta - \eta\ g$                # Go the other way instead
return $\theta$
```

A Sidenote: Hyperparameters

The learning rate (our η) is a **hyperparameter**, a term you will keep hearing

- **Set it too high?** The learner will catapult itself across the minimum and may not converge
- **Set it too low?** The learner will take a long time to get to the minimum, and may not converge in our lifetime

But what are hyperparameters again?

- Hyperparameters are parameters in a machine learning model that are not learned empirically
- They have to be set by the human who is designing the algorithm

A Worked Example from Jurafsky and Martin

Time permitting, let’s work through an example of gradient descent borrowed directly from the textbook authors.

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:

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

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Example of gradient descent

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Example of gradient descent

$w_1 = w_2 = b = 0;$
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Update step for update θ is:

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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

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

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

$\eta = 0.1;$

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

Example of gradient descent

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

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

$\eta = 0.1;$

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

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-batching

- In stochastic gradient descent, the algorithm chooses one random example at each iteration
- The result? Sometimes movements are choppy and abrupt
- In practice, instead, we usually compute the gradient over **batches** of training instances
- Entire dataset: BATCH TRAINING
- m examples (e.g., 512 or 1024): MINI-BATCH TRAINING

Regularization

Don’t Fight Yesterday’s War

In fact a 4-gram model trained on small data can and will memorize the data, achieving perfect accuracy on the training set. Sounds great, right?

But what happens when it encounters 4-grams that were not in the training set? It will get low accuracy on the test set. The combination of a too-powerful model and small data can be disastrous.

This is called overfitting

OVERFITTING is when the model fits the details of the training set **so exactly** that it cannot generalize to a test set. How to avoid overfitting?

- REGULARIZATION (logistic regression)
- DROPOUT (neural networks)

Regularization

A solution for overfitting

Add a regularization term *R*(θ) to the loss function
(for now written as maximizing logprob 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*(θ) 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:

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

Questions?