

What do you call a bad dream about machine learning?

A logistic nightmare

CS 2731 Introduction to Natural Language Processing

Session 7: Logistic regression, part 2

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Course logistics

- [Project area and contribution form](#) is **due Thu 09-21, 11:59pm**
 - Please plan meeting with your groups to discuss project ideas
 - If you don't have any specific ideas, that's fine! We will help you come up with some.
 - No need to submit anything on Canvas. Just fill out the form
- Discussion forum post due **Mon 09-25, 12:00pm noon**
 - Discussion of bias in word embeddings. Additional reading of [Blodgett et al. 2020](#)
 - Michael will post prompt soon
 - No reading quiz
- Reading quizzes and discussion forums will be available until class, but considered late and will be given half credit if are submitted after 12 noon

Lecture overview: logistic regression part 2

- Learning the weights for features in logistic regression
- Cross-entropy loss function
- Stochastic gradient descent
- Batch and mini-batch training
- Regularization
- Training multinomial logistic regression

Logistic regression: learning 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:

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

from the true output:

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

We'll call this difference:

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

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:

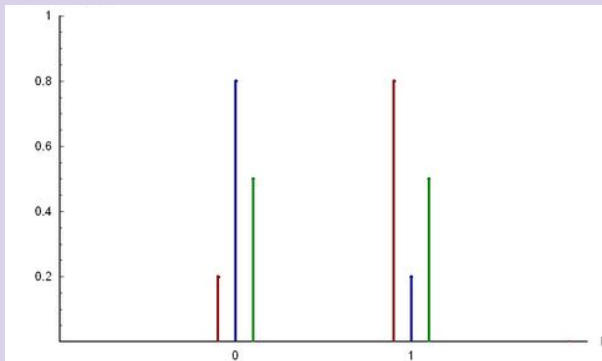
if $y=1$, this simplifies to \hat{y}

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



From the Bernoulli distribution, also expressed as:

$$p(y|x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$



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

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

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

Deriving cross-entropy loss for a single observation x

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

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

This happens to be the formula for **cross-entropy**, a measure of difference between distributions from information theory



Claude Shannon

Deriving cross-entropy loss for a single observation x

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

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

Plugging in the 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?

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

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 $y=0$.

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

What's the loss?

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

Let's see if this works for our sentiment example

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

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

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

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

Sure enough, loss was bigger when model was wrong!

Stochastic gradient descent

Our Goal: Minimize the Loss

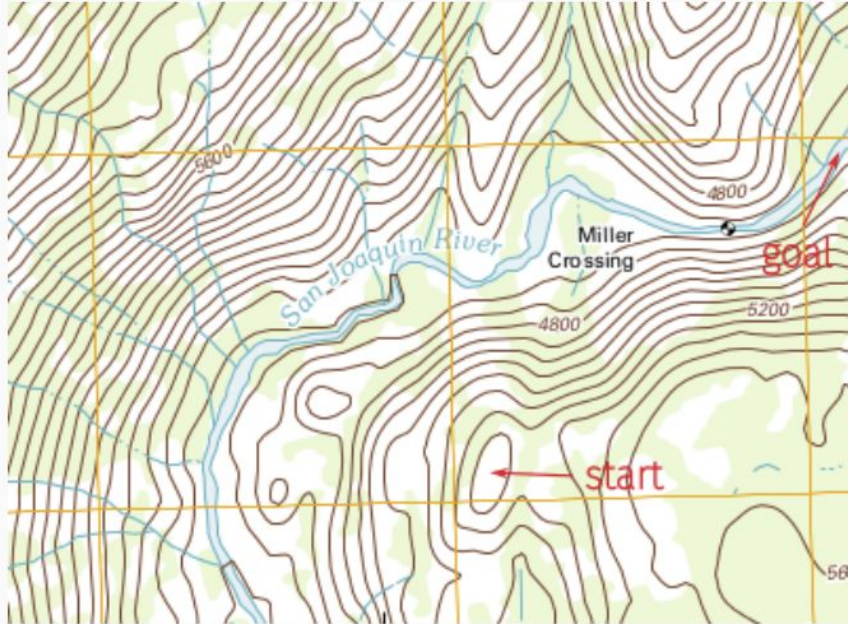
Let's make it explicit that the loss function is parameterized by weights $\theta = (w, b)$.

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:

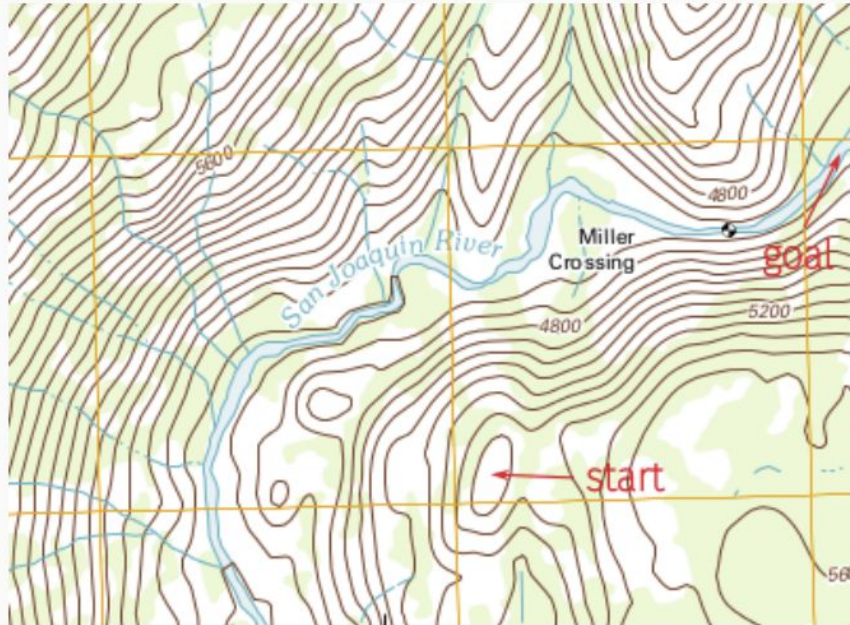
$$\hat{\theta} = \operatorname{argmin}_{\theta} \frac{1}{m} \sum_{i=1}^m L_{CE}(f(x^{(i)}; \theta), y^{(i)}) \quad (11)$$

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

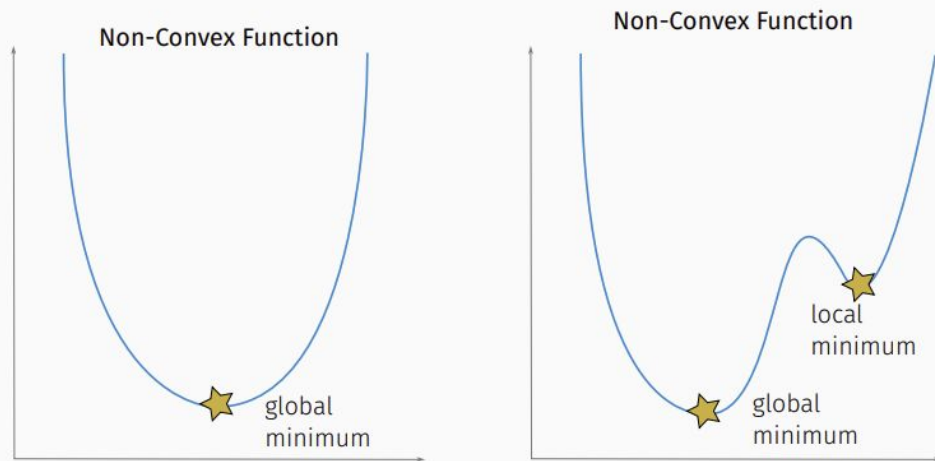


- You are on a hill
- It is your mission to reach the river at the bottom of the canyon (as quickly as possible)
- What is your strategy?
 1. Determine in which direction the steepest downhill slope lies
 2. Take a step in that direction
 3. Repeat until a step in any direction will take you up hill

Our Goal: Minimize the Loss

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

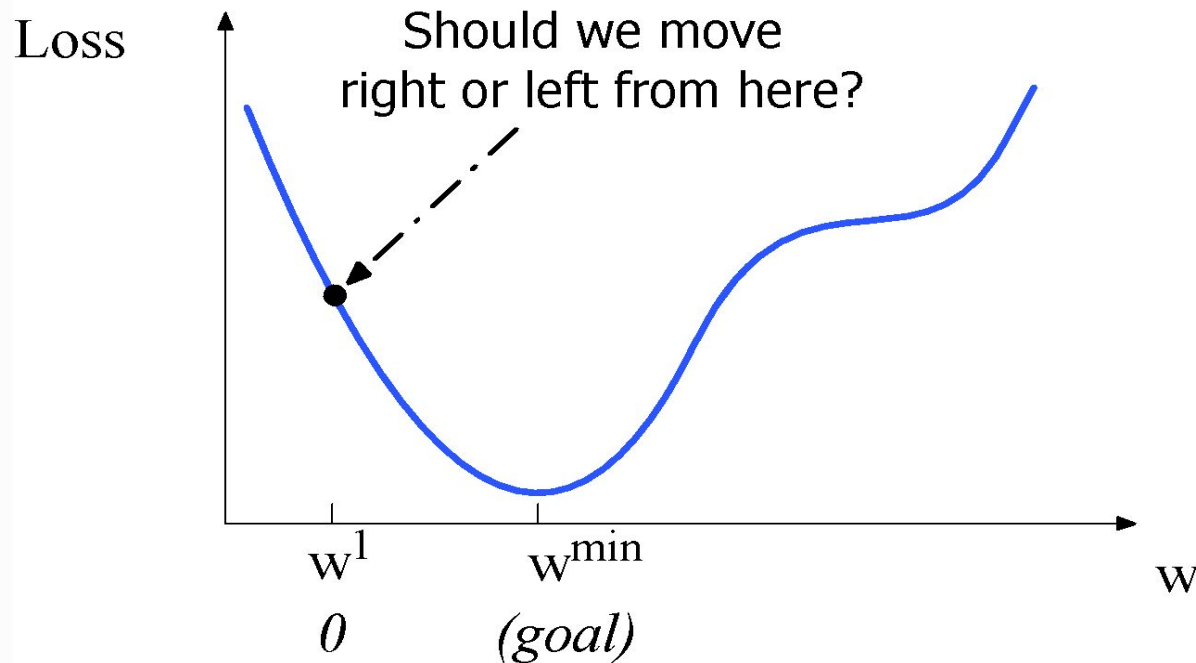
- Just one minimum
- Gradient descent is guaranteed to find the minimum, no matter where you start



Let's first visualize for a single scalar w

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

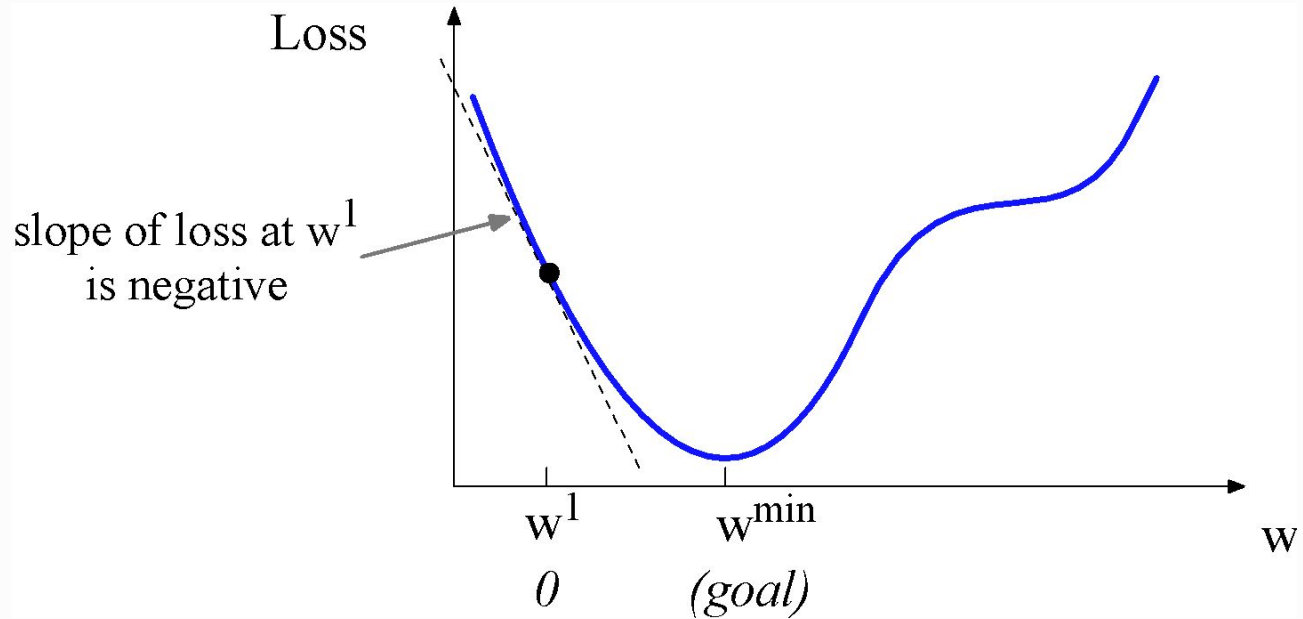
A: Move w in the reverse direction from the slope of the function



Let's first visualize for a single scalar w

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

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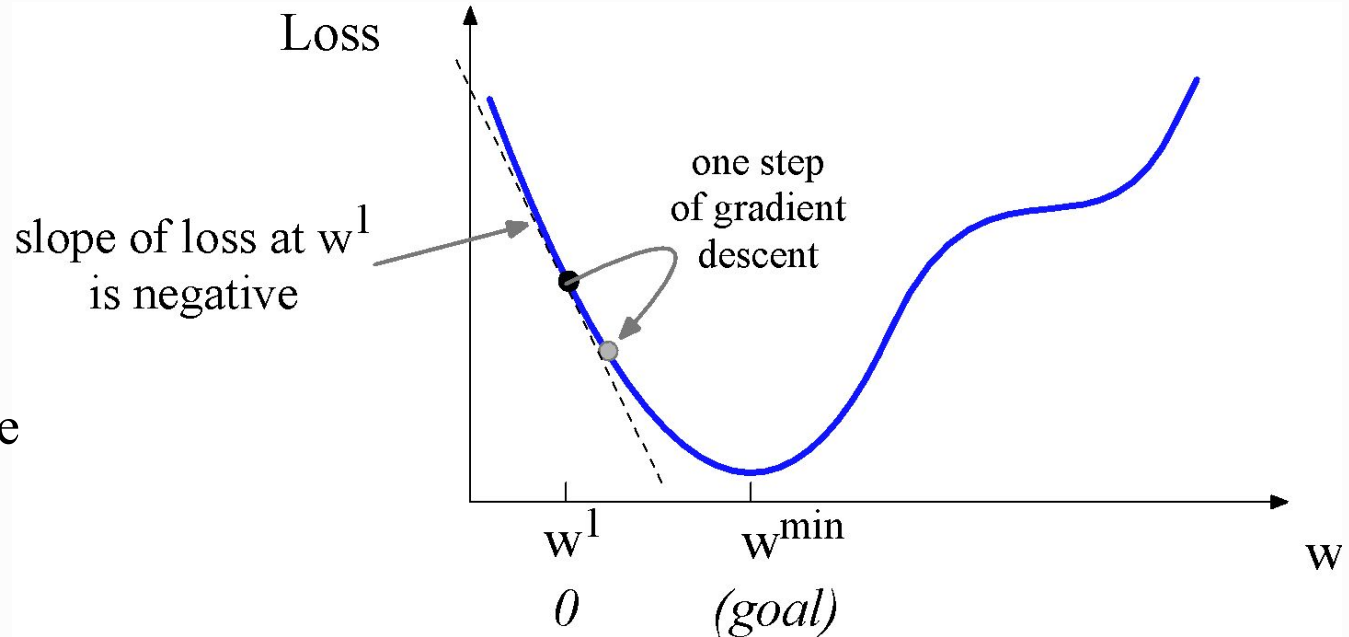


So we'll move positive

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

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So we'll move positive

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)

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

weighted by the LEARNING RATE η

- The higher the learning rate, the faster \mathbf{w} changes:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{d}{d\mathbf{w}} L_{CE}(f(\mathbf{x}; \mathbf{w}), y) \quad (12)$$

How Do We Do Gradient Descent in N Dimensions?

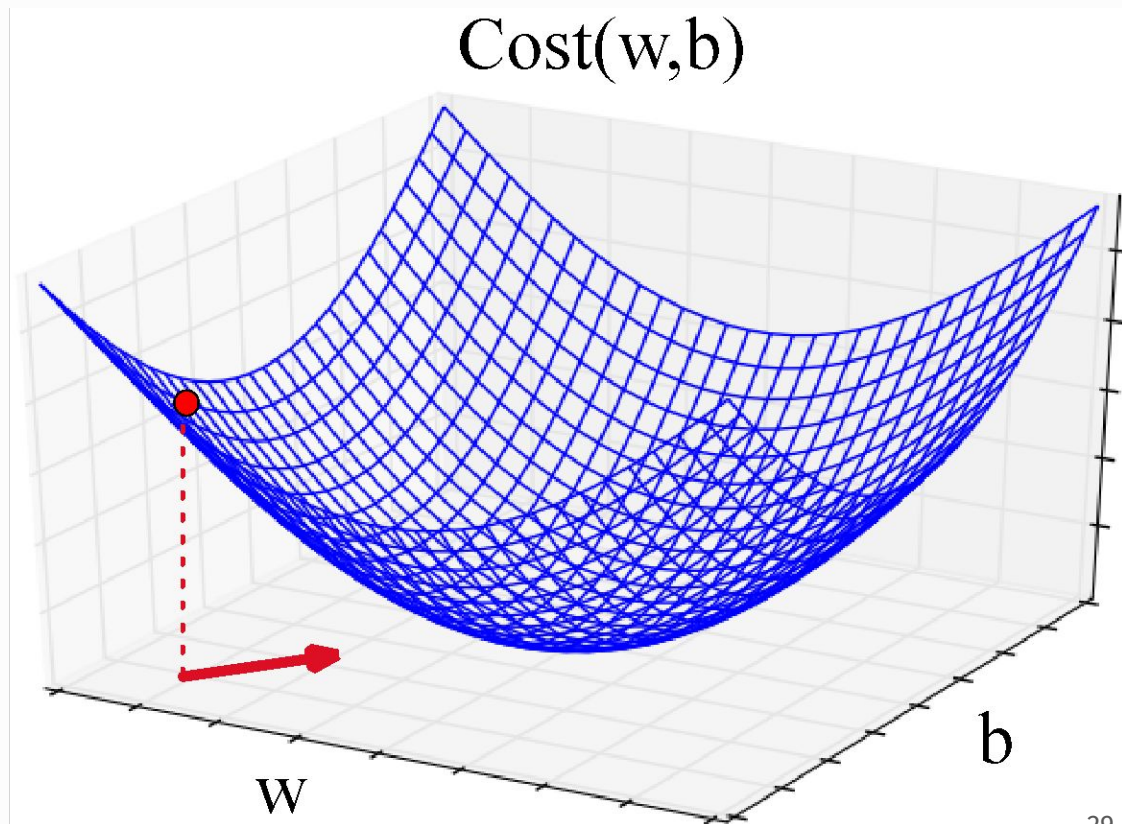
We want to know where in the N -dimensional space (of the N parameters that make up θ) we should move.

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



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 $f(\mathbf{x}; \theta)$ to make things clearer:

$$\nabla_{\theta} L(f(\mathbf{x}; \theta), y) = \begin{bmatrix} \frac{\partial}{\partial w_0} L(f(\mathbf{x}; \theta), y) \\ \frac{\partial}{\partial w_1} L(f(\mathbf{x}; \theta), y) \\ \frac{\partial}{\partial w_2} L(f(\mathbf{x}; \theta), y) \\ \vdots \\ \frac{\partial}{\partial w_n} L(f(\mathbf{x}; \theta), y) \end{bmatrix}$$

Note that, since we are representing the bias b as w_0 , θ is more-or-less equivalent to \mathbf{w} .

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

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

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

So What Are These Partial Derivatives Used in Logistic Regression?

The textbook lays out the derivation in §5.10 but here's the basic idea:

Here is the cross-entropy loss function (for binary classification):

$$L_{CE}(\hat{y}, y) = -[y \log \sigma(w \cdot x + b) + (1 - y) \log(1 - \sigma(w \cdot x + b))] \quad (15)$$

The derivative of this function is:

$$\frac{\partial L_{CE}(\hat{y}, y)}{\partial w_j} = [\sigma(w \cdot x + b) - y]x_j \quad (16)$$

which is very manageable!

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 $x^{(1)}, x^{(2)}, \dots, x^{(m)}$

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

$\theta \leftarrow 0$

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

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

Working through an example

One step of gradient descent

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

Two features:

$$x_1 = 3 \quad (\text{count of positive lexicon words})$$

$$x_2 = 2 \quad (\text{count of negative lexicon words})$$

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

Update step for update θ is:

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

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

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:

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

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Example of gradient descent

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Example of gradient descent

Update step for update θ is:

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

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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:

$$\theta_{t+1} = \theta_t - \eta \frac{d}{d\theta} L(f(x; \theta), y) \quad \eta = 0.1;$$

$$\theta^1 =$$

Example of gradient descent

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

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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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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Note that enough negative examples would eventually make w_2 negative

Batch and mini-batch training

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

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**

Regularization Is One Solution to Overfitting

Add a regularization term $R(\theta)$ to the loss function (which we will write, for now, as maximizing log probability rather than minimizing loss):

$$\hat{\theta} = \operatorname{argmax}_{\theta} \sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) - \alpha R(\theta) \quad (29)$$

The insight: we choose, for $R(\theta)$, a function that **penalizes large weights** because fitting the data well with **big weights** is not as good as fitting the data a bit less well with **small weights**.

In L2 Regularization, One Regularizes by the Sum of the Squares of the Weights

We can define $R(\theta)$ as the (square of the) **L2 norm**, that is, the Euclidean distance from θ to the origin.

$$R(\theta) = \|\theta\|_2^2 = \sum_{j=1}^n \theta_j^2 \quad (30)$$

If we L2 regularize the objective function, we get:

$$\hat{\theta} = \operatorname{argmax}_{\theta} \left[\sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) \right] - \alpha \sum_{j=1}^n \theta_j^2 \quad (31)$$

The larger the weights are, the farther the vector will be from the origin, and thus the more will be deducted from the log probability.

L1 Regularization Regularizes by the Sum of the Absolute Value of the Weights

L1 Regularization (or the lasso regression) is named after the **L1 norm** $\|W\|_1$:

- The sum of the absolute value of the weights
- The MANHATTAN DISTANCE

$$R(\theta) = \|\theta\|_1 = \sum_{i=1}^n |\theta_i| \quad (32)$$

When added (or rather, subtracted) from an objective function, it looks like this:

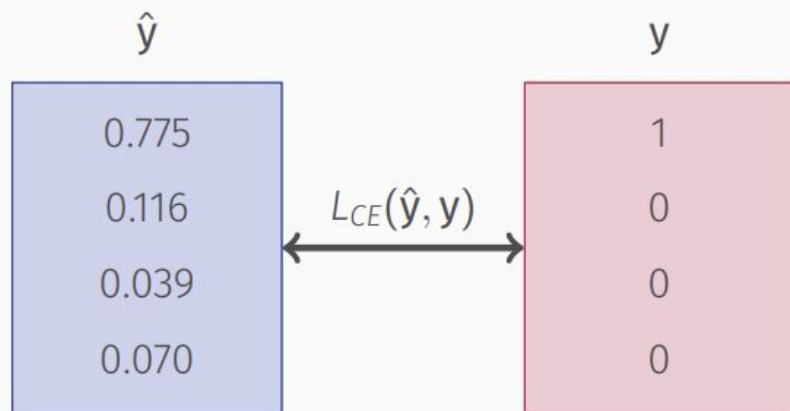
$$\hat{\theta} = \operatorname{argmax}_{\theta} \left[\sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) \right] - \alpha \sum_{j=1}^n |\theta_j| \quad (33)$$

While the function is different, the insight is similar to that for the L2 norm.

Training multinomial logistic regression

Categorical Cross-Entropy Loss for Multinomial Logistic Regression

Compare \mathbf{y} , a ONE-HOT VECTOR (one one, all other elements zero) and



How “distant” is $\hat{\mathbf{y}}$ from \mathbf{y} ? One measure is categorical cross-entropy loss:

$$\begin{aligned}L_{CE} &= -\sum_{i=1} T_i \log S_i \\&= -[1 \log_2 0.775 + 0 \log_2 0.126 + \\&\quad 0 \log_2 0.039 + 0 \log_2 0.070] \\&= -\log_2 0.775 \\&= 0.3677\end{aligned}$$

The elements of $\hat{\mathbf{y}}$ that correspond to 0-elements in \mathbf{y} are effectively ignored.

Generalizing Your Losses: The Negative Log Likelihood Loss

Reminder: the loss function for binary logistic regression (LR with two classes) is

$$L_{CE}(\hat{y}, y) = -\log p(y | x) = -[y \log \hat{y} + (1 - y) \log(1 - \hat{y})] \quad (23)$$

Note that we have two terms—one for when $y = 1$ and one for when $y = 0$ —corresponding to the two classes. What if we have K classes?

$$L_{CE}(\hat{y}, y) = -\sum_{k=1}^K y_k \log \hat{y}_k \quad (24)$$

$$= -\log \hat{y}_c \quad (\text{where } c \text{ is the correct class}) \quad (25)$$

$$= -\log \hat{p}(y_c = 1 | \mathbf{x}) \quad (\text{where } c \text{ is the correct class}) \quad (26)$$

$$= -\log \frac{\exp(\mathbf{w}_c \cdot \mathbf{x} + b_c)}{\sum_{j=1}^K \exp(\mathbf{w}_j \cdot \mathbf{x} + b_j)} \quad (c \text{ is the correct class}) \quad (27)$$

How did we get from (24) to (25)? **There is only one correct class.**

What We Actually Need to Compute Gradient Descent is the Gradient of the Loss

Consider one piece of the gradient—the derivative with respect to one weight.

- For each class k the weight of the i th element of \mathbf{x} (the input features) is $\mathbf{w}_{k,i}$.
- What is the partial derivative of $L_{CE}(\hat{\mathbf{y}}, \mathbf{y})$ wrt $\mathbf{w}_{k,i}$?
- It turns out, after some math, that the difference between the true value for the class k (either 1 or 0) and the probability that the class outputs class k (weighted by the value of the input \mathbf{x}_i corresponding to the i th element of the weight vector for class k).

$$\frac{\partial L_{CE}}{\partial \mathbf{w}_{k,i}} = -(\mathbf{y}_k - \hat{\mathbf{y}}_k)\mathbf{x}_i \quad (28)$$

- The rest of the procedure for training multinomial LR is the same as for binary LR.

Questions?

Homework 1 due Sun, Sep 17