Machine Learning

by Stanford University

Week3

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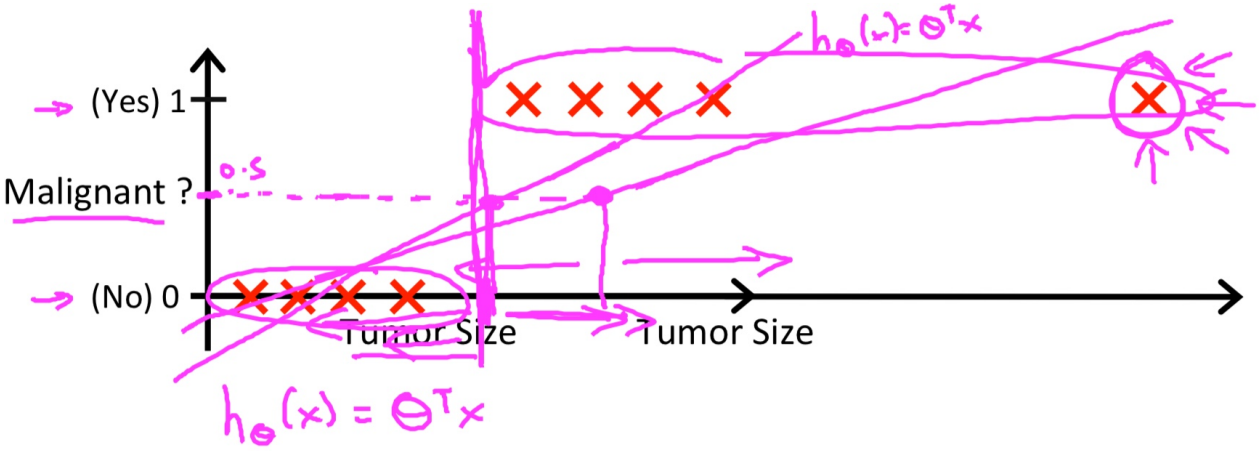
1 Logistic regresion

1.1 Classification and Representation

1.1.1 Classification

To attempt classification, one method is to use linear regression and map all predictions greater than 0.5 as a 1 and all less than 0.5 as a 0. However, this method doesn't work well because classification is not actually a linear function.

The classification problem is just like the regression problem, except that the values we now want to predict take on only a small number of discrete values. For now, we will focus on the **binary classification problem** in which y can take on only two values, 0 and 1. (Most of what we say here will also generalize to the multiple-class case.) For instance, if we are trying to build a spam classifier for email, then $x^{(i)}$ may be some features of a piece of email, and y may be 1 if it is a piece of spam mail, and 0 otherwise. Hence, y∈{0,1}. 0 is also called the negative class, and 1 the positive class, and they are sometimes also denoted by the symbols "-" and "+." Given $x^{(i)}$, the corresponding $y^{(i)}$ is also called the label for the training example.



→ Threshold classifier output $h_\theta(x)$ at 0.5:

→ If $h_\theta(x) \geq 0.5$, predict "y = 1"

If $h_\theta(x) < 0.5$, predict "y = 0"

Which of the following statements is true?

- If linear regression doesn't work on a classification task as in the previous example shown in the video, applying feature scaling may help.
- If the training set satisfies $0 \leq y^{(i)} \leq 1$ for every training example $(x^{(i)}, y^{(i)})$, then linear regression's prediction will also satisfy $0 \leq h_\theta(x) \leq 1$ for all values of x.
- If there is a feature x that perfectly predicts y, i.e. if $y = 1$ when $x \geq c$ and $y = 0$ whenever $x < c$ (for some constant c), then linear regression will obtain zero classification error.
- None of the above statements are true.

Correct

1.1.2 Hipothesis representation

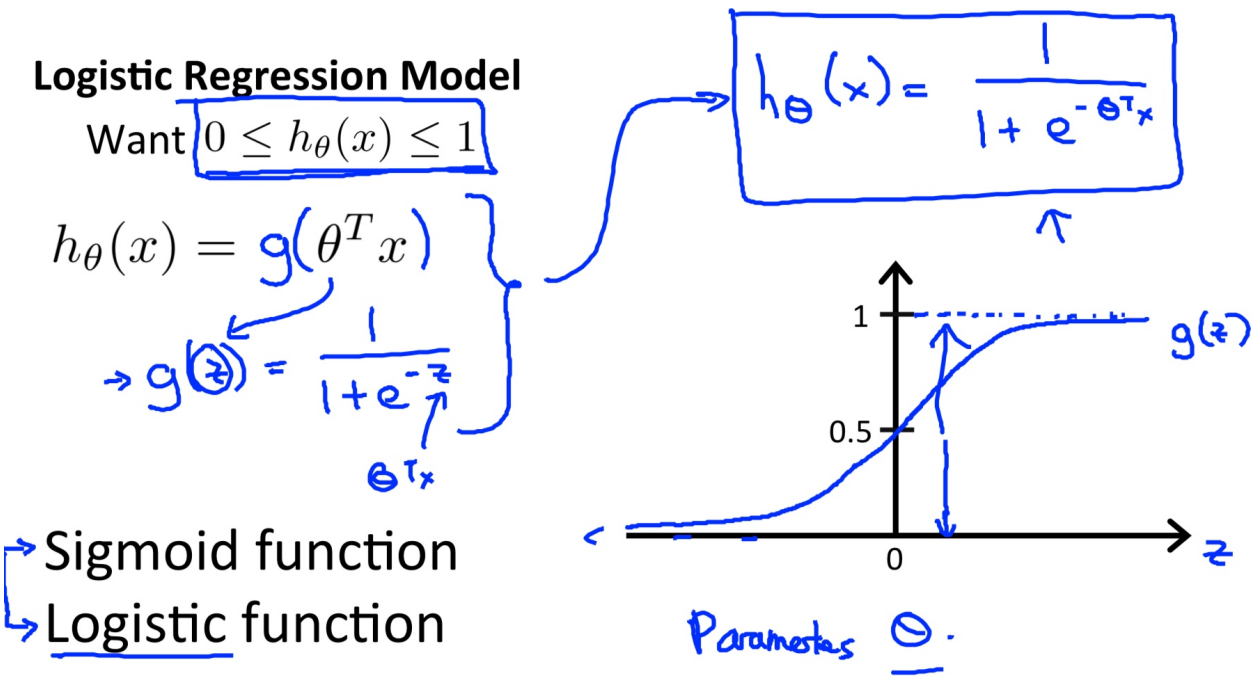
We could approach the classification problem ignoring the fact that y is discrete-valued, and use our old linear regression algorithm to try to predict y given x. However, it is easy to construct examples where this method performs very poorly. Intuitively, it also doesn't make sense for $h_\theta(x)$ to take values larger than 1 or smaller than 0 when we know that y ∈ {0, 1}. To fix this, let's change the form for our hypotheses $h_\theta(x)$ to satisfy $0 \leq h_\theta(x) \leq 1$. This is accomplished by plugging $\theta^T x$ into the Logistic Function.

Our new form uses the "Sigmoid Function," also called the "Logistic Function":

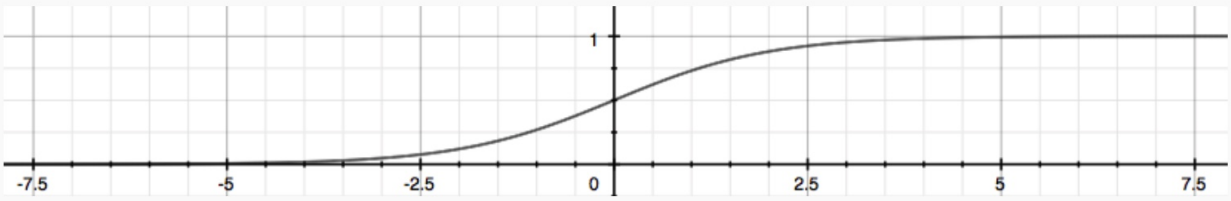
$$h_\theta(x) = g(\theta^T x)$$

$$z = \theta^T x$$

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



The following image shows us what the sigmoid function looks like:



The function g(z), shown here, maps any real number to the (0, 1) interval, making it useful for transforming an arbitrary-valued function into a function better suited for classification.

$h_\theta(x)$ will give us the **probability** that our output is 1. For example, $h_\theta(x) = 0.7$ gives us a probability of 70% that our output is 1. Our probability that our prediction is 0 is just the complement of our probability that it is 1 (e.g. if probability that it is 1 is 70%, then the probability that it is 0 is 30%).

$$h_\theta(x) = P(y = 1|x; \theta) = 1 - P(y = 0|x; \theta)$$
$$P(y = 0|x; \theta) + P(y = 1|x; \theta) = 1$$

Interpretation of Hypothesis Output

$h_\theta(x)$

$h_\theta(x)$ = estimated probability that y = 1 on input x

Example: If $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$

$h_\theta(x) = 0.7$ $\quad$ $y=1$

Tell patient that 70% chance of tumor being malignant

$h_\theta(x) = P(y=1|x;\theta)$

"probability that y = 1, given x, parameterized by θ"

$y = 0$ or 1

$P(y = 0|x;\theta) + P(y = 1|x;\theta) = 1$

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

Suppose we want to predict, from data x about a tumor, whether it is malignant ($y = 1$) or benign ($y = 0$). Our logistic regression classifier outputs, for a specific tumor, $h_\theta(x) = P(y = 1|x; \theta) = 0.7$, so we estimate that there is a 70% chance of this tumor being malignant. What should be our estimate for $P(y = 0|x; \theta)$, the probability the tumor is benign?

- (•) $P(y = 0|x; \theta) = 0.3$

  Correct

- ( ) $P(y = 0|x; \theta) = 0.7$
- ( ) $P(y = 0|x; \theta) = 0.7^2$
- ( ) $P(y = 0|x; \theta) = 0.3 \times 0.7$

1.1.3 Decision boundary

In order to get our discrete 0 or 1 classification, we can translate the output of the hypothesis function as follows:

$$h_\theta(x) \geq 0.5 \rightarrow y = 1$$
$$h_\theta(x) < 0.5 \rightarrow y = 0$$

The way our logistic function g behaves is that when its input is greater than or equal to zero, its output is greater than or equal to 0.5:

$$g(z) \geq 0.5$$
$$when\ z \geq 0$$

Remember.

$$z = 0, e^0 = 1 \Rightarrow g(z) = 1/2$$
$$z \rightarrow \infty, e^{-\infty} \rightarrow 0 \Rightarrow g(z) = 1$$
$$z \rightarrow -\infty, e^{\infty} \rightarrow \infty \Rightarrow g(z) = 0$$

So if our input to g is $\theta^T X$, then that means:

$$h_\theta(x) = g(\theta^T x) \geq 0.5$$
$$when\ \theta^T x \geq 0$$

From these statements we can now say:

$$\theta^T x \geq 0 \Rightarrow y = 1$$
$$\theta^T x < 0 \Rightarrow y = 0$$

The **decision boundary** is the line that separates the area where y = 0 and where y = 1. It is created by our hypothesis function.

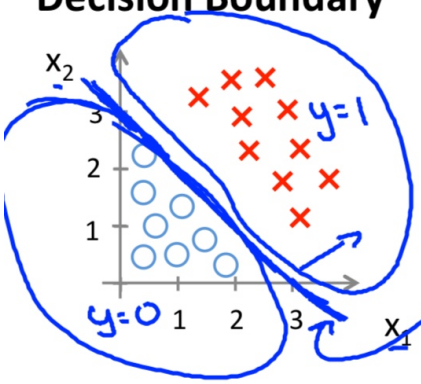
Example:

$$\theta = \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix}$$
$$y = 1\ if\ 5 + (-1)x_1 + 0x_2 \geq 0$$
$$5 - x_1 \geq 0$$
$$-x_1 \geq -5$$
$$x_1 \leq 5$$

In this case, our decision boundary is a straight vertical line placed on the graph where $x_1 = 5$, and everything to the left of that denotes y = 1, while everything to the right denotes y = 0.

Again, the input to the sigmoid function g(z) (e.g. $\theta^T X$) doesn't need to be linear, and could be a function that describes a circle (e.g. $z = \theta_0 + \theta_1 x_1^2 + \theta_2 x_2^2$) or any shape to fit our data.

Decision Boundary



$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$

$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$

$-3 \quad 1 \quad 1$

Decision boundary

Predict "$y = 1$" if $-3 + x_1 + x_2 \geq 0$

$\theta^T x$

$x_1 + x_2 \geq 3$

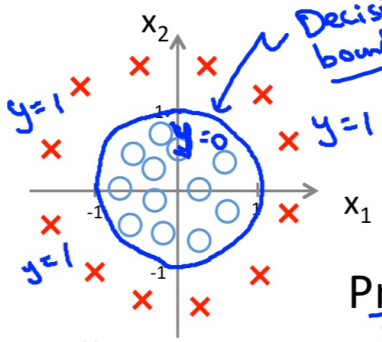
$x_1 + x_2 = 3$

$h_\theta(x) = 0.5$

$x_1 + x_2 < 3$

$y = 0$

Non-linear decision boundaries



$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$

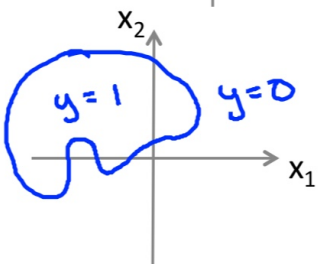
$-1 \quad 0 \quad 0 \quad 1 \quad 1$

$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$

Predict "$y = 1$" if $-1 + x_1^2 + x_2^2 \geq 0$

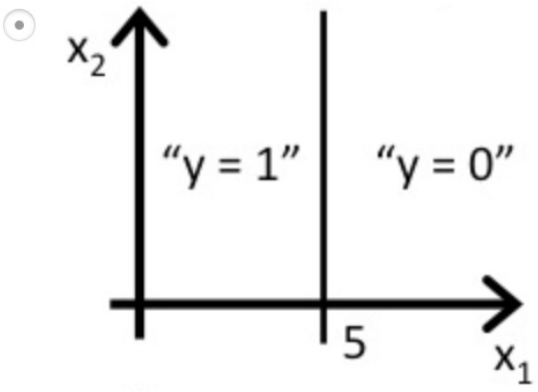
$x_1^2 + x_2^2 = 1$

$x_1^2 + x_2^2 \geq 1$



$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_1^2 x_2 + \theta_5 x_1^2 x_2^2 + \theta_6 x_1^3 x_2 + \dots)$

Consider logistic regression with two features x_1 and x_2. Suppose $\theta_0 = 5$, $\theta_1 = -1$, $\theta_2 = 0$, so that $h_\theta(x) = g(5 - x_1)$. Which of these shows the decision boundary of $h_\theta(x)$?



.

Correct

Predict Y = 0 if x_1 is greater than 5.

1.2 Logistic Regression Model

1.2.1 Cost Function

We cannot use the same cost function that we use for linear regression because the Logistic Function will cause the output to be wavy, causing many local optima. In other words, it will not be a convex function.

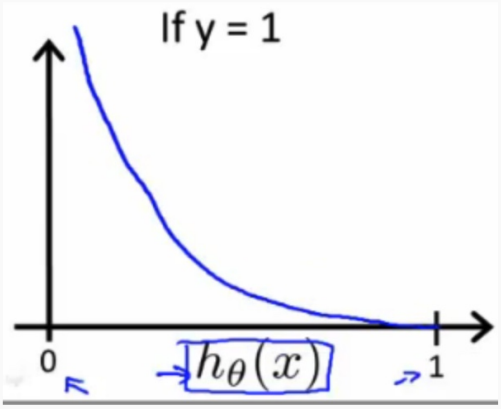
Instead, our cost function for logistic regression looks like:

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

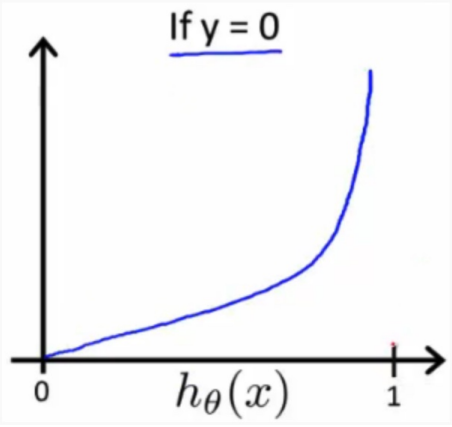
$$\text{Cost}(h_\theta(x), y) = -\log(h_\theta(x)) \qquad \text{if y} = 1$$

$$\text{Cost}(h_\theta(x), y) = -\log(1 - h_\theta(x)) \qquad \text{if y} = 0$$

When y = 1, we get the following plot for $J(\theta)$ vs $h_\theta(x)$:



Similarly, when y = 0, we get the following plot for $J(\theta)$ vs $h_\theta(x)$:



$$\text{Cost}(h_\theta(x), y) = 0 \text{ if } h_\theta(x) = y$$

$$\text{Cost}(h_\theta(x), y) \to \infty \text{ if } y = 0 \text{ and } h_\theta(x) \to 1$$

$$\text{Cost}(h_\theta(x), y) \to \infty \text{ if } y = 1 \text{ and } h_\theta(x) \to 0$$

If our correct answer 'y' is 0, then the cost function will be 0 if our hypothesis function also outputs 0. If our hypothesis approaches 1, then the cost function will approach infinity.

If our correct answer 'y' is 1, then the cost function will be 0 if our hypothesis function outputs 1. If our hypothesis approaches 0, then the cost function will approach infinity.

Note that writing the cost function in this way guarantees that J(θ) is convex for logistic regression.

Cost function

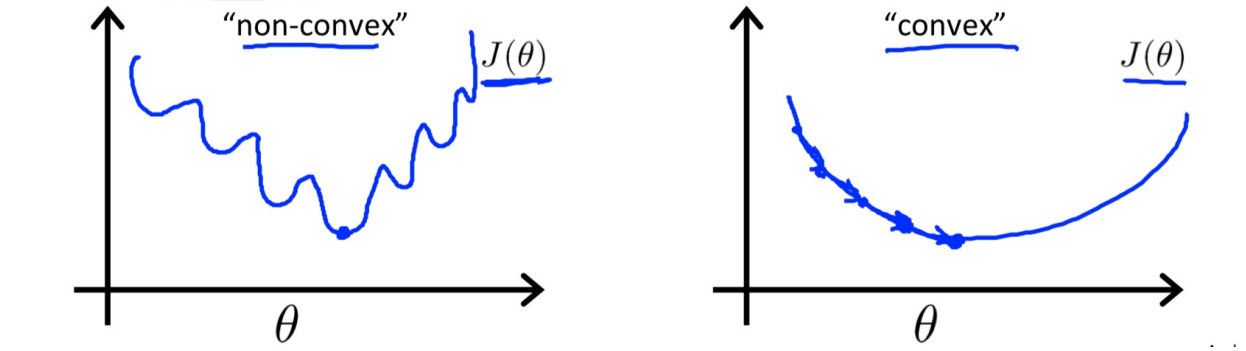
Linear regression: $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

Logistic

$\text{Cost}(h_\theta(x^{(i)}), y^{(i)}) = \frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

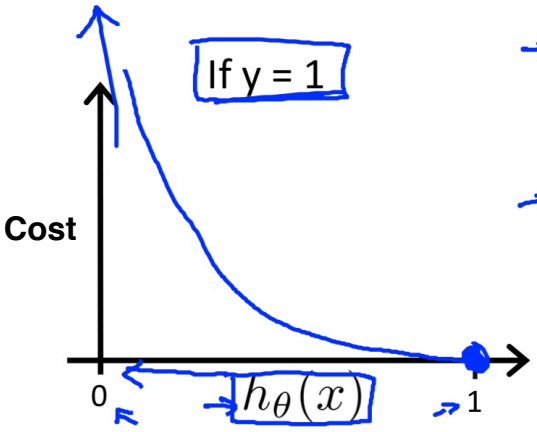
$\text{Cost}(h_\theta(x), y)$

$\frac{1}{1+e^{-\theta^T x}}$



Logistic regression cost function

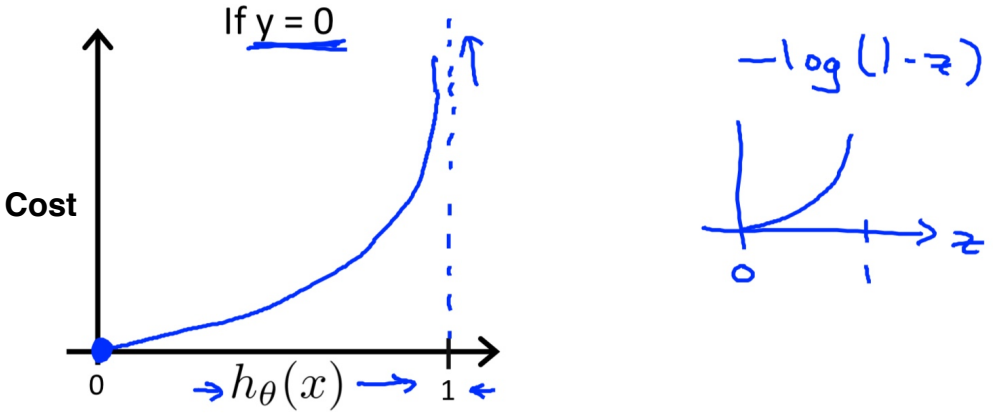
$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$



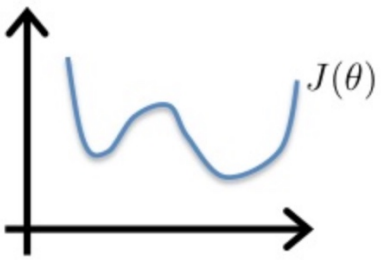
- Cost $= 0$ if $y = 1, h_\theta(x) = 1$
  But as $h_\theta(x) \to 0$
  $Cost \to \infty$
- Captures intuition that if $h_\theta(x) = 0$, (predict $P(y = 1|x;\theta) = 0$), but $y = 1$, we'll penalize learning algorithm by a very large cost.

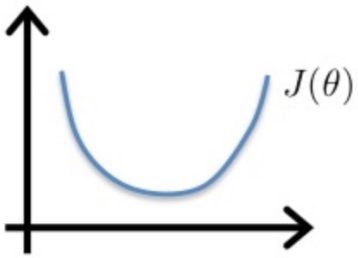
Logistic regression cost function

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$



Consider minimizing a cost function $J(\theta)$. Which one of these functions is convex?





Correct

In logistic regression, the cost function for our hypothesis outputting (predicting) $h_\theta(x)$ on a training example that has label $y \in \{0, 1\}$ is:

$$\text{cost}(h_\theta(x), y) = \begin{cases} -\log h_\theta(x) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Which of the following are true? Check all that apply.

- [x] If $h_\theta(x) = y$, then $\text{cost}(h_\theta(x), y) = 0$ (for $y = 0$ and $y = 1$).

Correct

- [x] If $y = 0$, then $\text{cost}(h_\theta(x), y) \to \infty$ as $h_\theta(x) \to 1$.

Correct

- [ ] If $y = 0$, then $\text{cost}(h_\theta(x), y) \to \infty$ as $h_\theta(x) \to 0$.

Un-selected is correct

- [x] Regardless of whether $y = 0$ or $y = 1$, if $h_\theta(x) = 0.5$, then $\text{cost}(h_\theta(x), y) > 0$.

Correct

1.2.2 Simplified cost function

We can compress our cost function's two conditional cases into one case:

$$\text{Cost}(h_\theta(x), y) = -y \ \log(h_\theta(x)) - (1 - y) \log(1 - h_\theta(x))$$

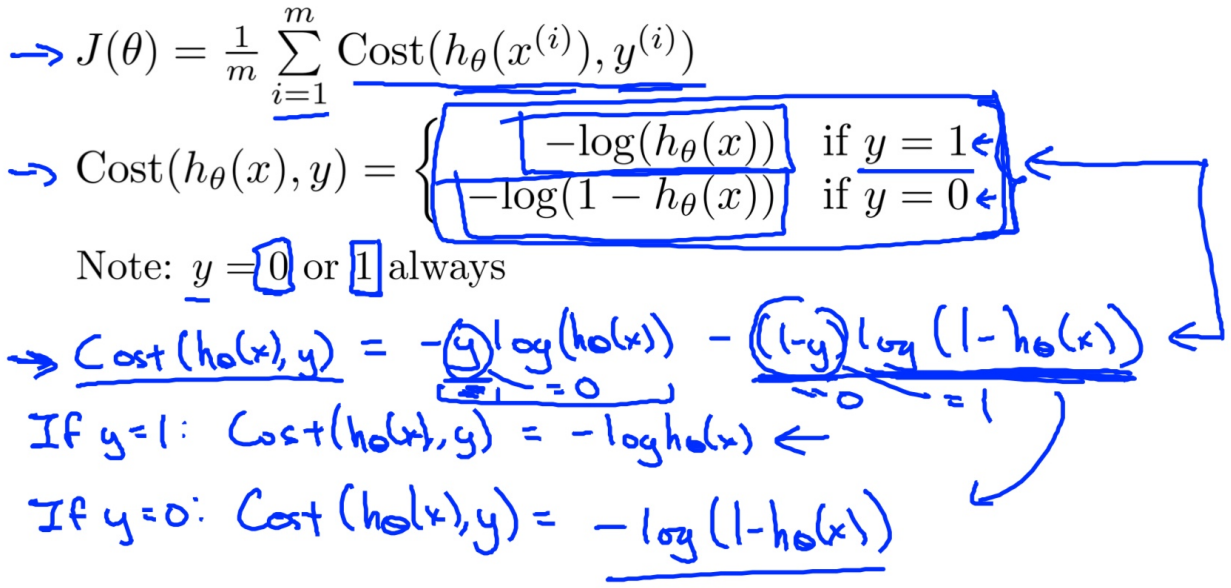
Notice that when y is equal to 1, then the second term $(1 - y) \log(1 - h_\theta(x))$ will be zero and will not affect the result. If y is equal to 0, then the first term $-y \log(h_\theta(x))$ will be zero and will not affect the result.

We can fully write out our entire cost function as follows:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} \log(h_\theta(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))]$$

A vectorized implementation is:

$$h = g(X\theta)$$
$$J(\theta) = \frac{1}{m} \cdot \left(-y^T \log(h) - (1 - y)^T \log(1 - h)\right)$$



$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$$
$$= -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

To fit parameters θ :

$$\min_\theta J(\theta)$$ Get θ

To make a prediction given new x:

Output $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$ $p(y=1 \mid x;\theta)$

1.2.3 Gradient descent

Remember that the general form of gradient descent is:

Repeat {

$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$

}

We can work out the derivative part using calculus to get:

Repeat {

$\theta_j := \theta_j - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$

}

Notice that this algorithm is identical to the one we used in linear regression. We still have to simultaneously update all values in theta.

A vectorized implementation is:

$\theta := \theta - \frac{\alpha}{m} X^T (g(X\theta) - \vec{y})$

Gradient Descent

$$J(\theta) = -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

Want $\min_\theta J(\theta)$:

Repeat $\{$

$$\theta_j := \theta_j - \alpha \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

(simultaneously update all θ_j)

$\}$

$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$ for $i = 0$ to n

$h_\theta(x) = \theta^T x$

$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$

Algorithm looks identical to linear regression!

Suppose you are running gradient descent to fit a logistic regression model with parameter $\theta \in \mathbb{R}^{n+1}$. Which of the following is a reasonable way to make sure the learning rate α is set properly and that gradient descent is running correctly?

- Plot $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$ as a function of the number of iterations (i.e. the horizontal axis is the iteration number) and make sure $J(\theta)$ is decreasing on every iteration.
- Plot $J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))]$ as a function of the number of iterations and make sure $J(\theta)$ is decreasing on every iteration.

  Correct

- Plot $J(\theta)$ as a function of θ and make sure it is decreasing on every iteration.
- Plot $J(\theta)$ as a function of θ and make sure it is convex.

One iteration of gradient descent simultaneously performs these updates:

$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_0^{(i)}$

$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)}$

$\vdots$

$\theta_n := \theta_n - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_n^{(i)}$

We would like a vectorized implementation of the form $\theta := \theta - \alpha\delta$ (for some vector $\delta \in \mathbb{R}^{n+1}$).

What should the vectorized implementation be?

- (•) $\theta := \theta - \alpha \frac{1}{m} \sum_{i=1}^{m} [(h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}]$

  Correct

- ( ) $\theta := \theta - \alpha \frac{1}{m} [\sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})] \cdot x^{(i)}$
- ( ) $\theta := \theta - \alpha \frac{1}{m} x^{(i)} [\sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})]$
- ( ) All of the above are correct implementations.

1.2.4 Advanced optimization

"Conjugate gradient", "BFGS", and "L-BFGS" are more sophisticated, faster ways to optimize θ that can be used instead of gradient descent. We suggest that you should not write these more sophisticated algorithms yourself (unless you are an expert in numerical computing) but use the libraries instead, as they're already tested and highly optimized. Octave provides them.

We first need to provide a function that evaluates the following two functions for a given input value θ:

$$J(\theta)$$
$$\frac{\partial}{\partial \theta_j} J(\theta)$$

Optimization algorithm

Given θ, we have code that can compute

- $J(\theta)$
- $\frac{\partial}{\partial \theta_j} J(\theta)$ (for $j = 0, 1, \ldots, n$)

Optimization algorithms:

- Gradient descent
- Conjugate gradient
- BFGS
- L-BFGS

Advantages:

- No need to manually pick α
- Often faster than gradient descent.

Disadvantages:

- More complex

1.3 Multiclass classification

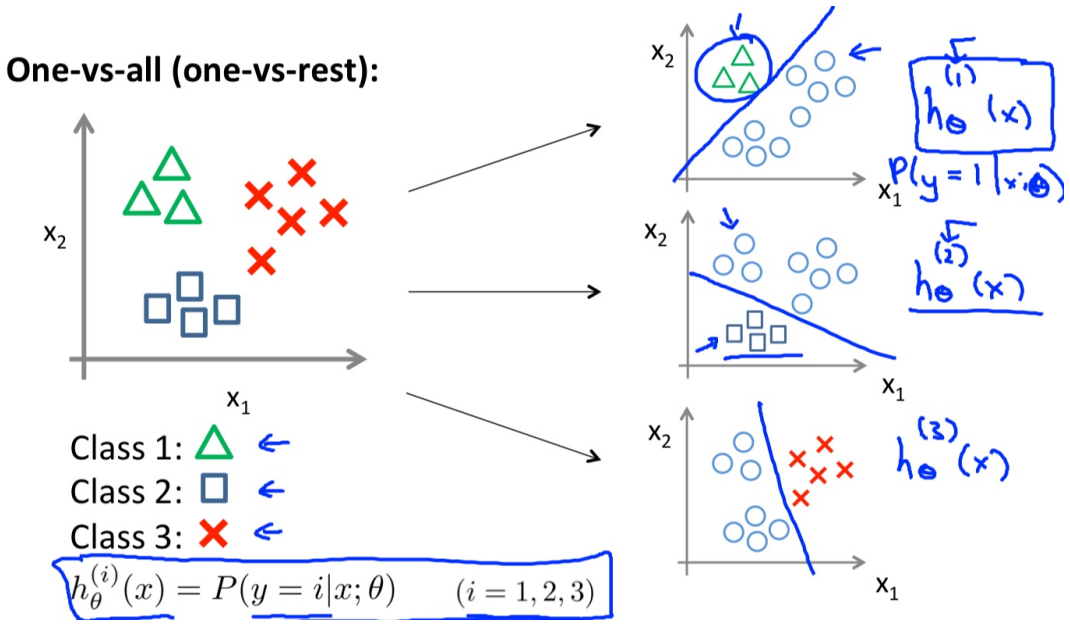
1.3.1 One-vs-all

Now we will approach the classification of data when we have more than two categories. Instead of y = {0,1} we will expand our definition so that y = {0,1...n}.

Since y = {0,1...n}, we divide our problem into n+1 (+1 because the index starts at 0) binary classification problems; in each one, we predict the probability that 'y' is a member of one of our classes.

$$
\begin{aligned}
&y \in \{0, 1 \dots n\} \\
&h_\theta^{(0)}(x) = P(y = 0 | x; \theta) \\
&h_\theta^{(1)}(x) = P(y = 1 | x; \theta) \\
&\cdots \\
&h_\theta^{(n)}(x) = P(y = n | x; \theta) \\
&\text{prediction} = \max_i (h_\theta^{(i)}(x))
\end{aligned}
$$

We are basically choosing one class and then lumping all the others into a single second class. We do this repeatedly, applying binary logistic regression to each case, and then use the hypothesis that returned the highest value as our prediction.



To summarize:

Train a logistic regression classifier $h_\theta(x)$ for each class to predict the probability that y = i .

To make a prediction on a new x, pick the class that maximizes $h_\theta(x)$

Suppose you have a multi-class classification problem with k classes (so $y \in \{1, 2, \ldots, k\}$). Using the 1-vs.-all method, how many different logistic regression classifiers will you end up training?

- $k - 1$
- k

  Correct

- $k + 1$
- Approximately $\log_2(k)$

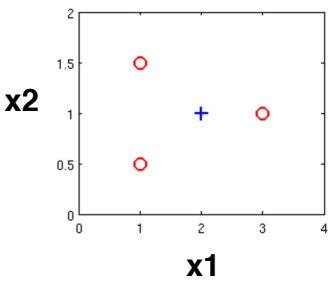
1.4 Test

1. Suppose that you have trained a logistic regression classifier, and it outputs on a new example x a prediction $h_\theta(x)$ = 0.2. This means (check all that apply):

- [x] Our estimate for $P(y = 1|x; \theta)$ is 0.2.
- [ ] Our estimate for $P(y = 0|x; \theta)$ is 0.2.
- [ ] Our estimate for $P(y = 1|x; \theta)$ is 0.8.
- [x] Our estimate for $P(y = 0|x; \theta)$ is 0.8.

2. Suppose you have the following training set, and fit a logistic regression classifier $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$.

x_1	x_2	y
1	0.5	0
1	1.5	0
2	1	1
3	1	0



Which of the following are true? Check all that apply.

- [x] $J(\theta)$ will be a convex function, so gradient descent should converge to the global minimum.
- [x] Adding polynomial features (e.g., instead using $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_1 x_2 + \theta_5 x_2^2)$) could increase how well we can fit the training data.
- [ ] The positive and negative examples cannot be separated using a straight line. So, gradient descent will fail to converge.
- [ ] Because the positive and negative examples cannot be separated using a straight line, linear regression will perform as well as logistic regression on this data.

3. For logistic regression, the gradient is given by $\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$. Which of these is a correct gradient descent update for logistic regression with a learning rate of α? Check all that apply.

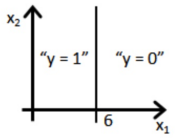
- [x] $\theta := \theta - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}$.
- [ ] $\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(\theta^T x - y^{(i)}\right) x_j^{(i)}$ (simultaneously update for all j).
- [ ] $\theta := \theta - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(\theta^T x - y^{(i)}\right) x^{(i)}$.
- [x] $\theta := \theta - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(\frac{1}{1+e^{-\theta^T x^{(i)}}} - y^{(i)}\right) x^{(i)}$.

4. Which of the following statements are true? Check all that apply.

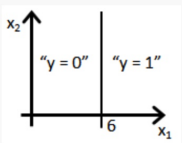
- [x] Since we train one classifier when there are two classes, we train two classifiers when there are three classes (and we do one-vs-all classification).
- [ ] For logistic regression, sometimes gradient descent will converge to a local minimum (and fail to find the global minimum). This is the reason we prefer more advanced optimization algorithms such as fminunc (conjugate gradient/BFGS/L-BFGS/etc).
- [ ] The one-vs-all technique allows you to use logistic regression for problems in which each $y^{(i)}$ comes from a fixed, discrete set of values.
- [x] The cost function $J(\theta)$ for logistic regression trained with $m \geq 1$ examples is always greater than or equal to zero.

5. Suppose you train a logistic classifier $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$. Suppose $\theta_0 = -6, \theta_1 = 1, \theta_2 = 0$. Which of the following figures represents the decision boundary found by your classifier?

- [ ] Figure:



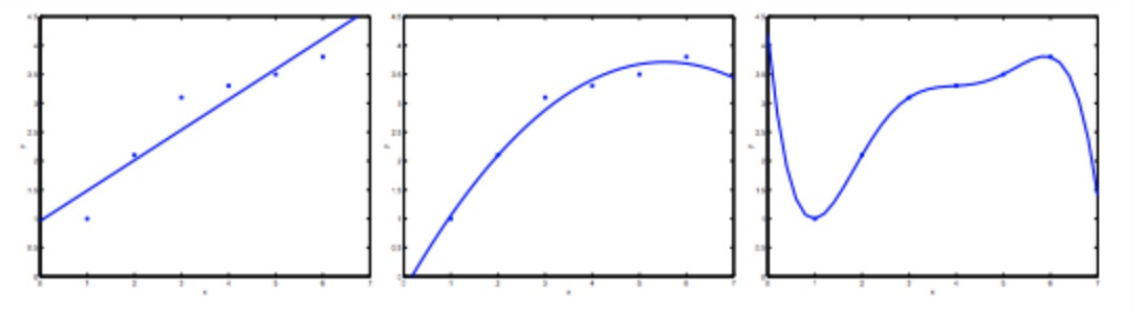
- [x] Figure:



2 Solving the problem of overfitting

2.1 The problem of overfitting

Consider the problem of predicting y from x ∈ R. The leftmost figure below shows the result of fitting a $y = \theta_0 + \theta_1 x$ to a dataset. We see that the data doesn't really lie on straight line, and so the fit is not very good.



Instead, if we had added an extra feature x^2 , and fit $y = \theta_0 + \theta_1 x + \theta_2 x^2$, then we obtain a slightly better fit to the data (See middle figure). Naively, it might seem that the more features we add, the better. However, there is also a danger in adding too many features: The rightmost figure is the result of fitting a 5^{th} order polynomial $y = \sum_{j=0}^{5} \theta_j x^j$. We see that even though the fitted curve passes through the data perfectly, we would not expect this to be a very good predictor of, say, housing prices (y) for different living areas (x). Without formally defining what these terms mean, we'll say the figure on the left shows an instance of **underfitting**—in which the data clearly shows structure not captured by the model—and the figure on the right is an example of **overfitting**.

Underfitting, or high bias, is when the form of our hypothesis function h maps poorly to the trend of the data. It is usually caused by a function that is too simple or uses too few features. At the other extreme, overfitting, or high variance, is caused by a hypothesis function that fits the available data but does not generalize well to predict new data. It is usually caused by a complicated function that creates a lot of unnecessary curves and angles unrelated to the data.

This terminology is applied to both linear and logistic regression. There are two main options to address the issue of overfitting:

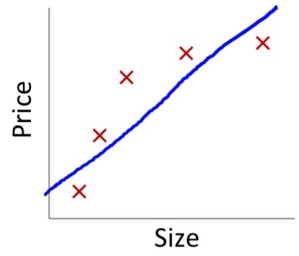
1) Reduce the number of features:

- Manually select which features to keep.
- Use a model selection algorithm (studied later in the course).

2) Regularization

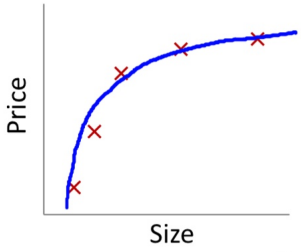
- Keep all the features, but reduce the magnitude of parameters θ_j.
- Regularization works well when we have a lot of slightly useful features.

Example: Linear regression (housing prices)



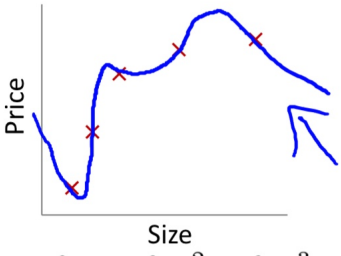
$\rightarrow \theta_0 + \theta_1 x$

"Underfit" "High bias"



$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2$

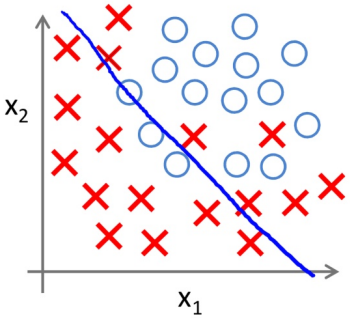
"Just right"



$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

"Overfit" "High variance"

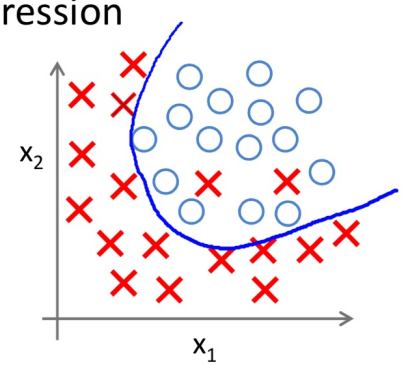
Example: Logistic regression



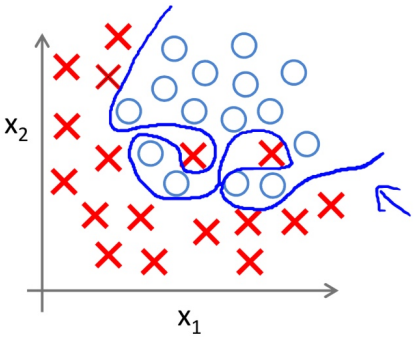
$\rightarrow h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$

(g = sigmoid function)

"Underfit"



$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$



$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$

"Overfit"

2.2 Cost function

If we have overfitting from our hypothesis function, we can reduce the weight that some of the terms in our function carry by increasing their cost.

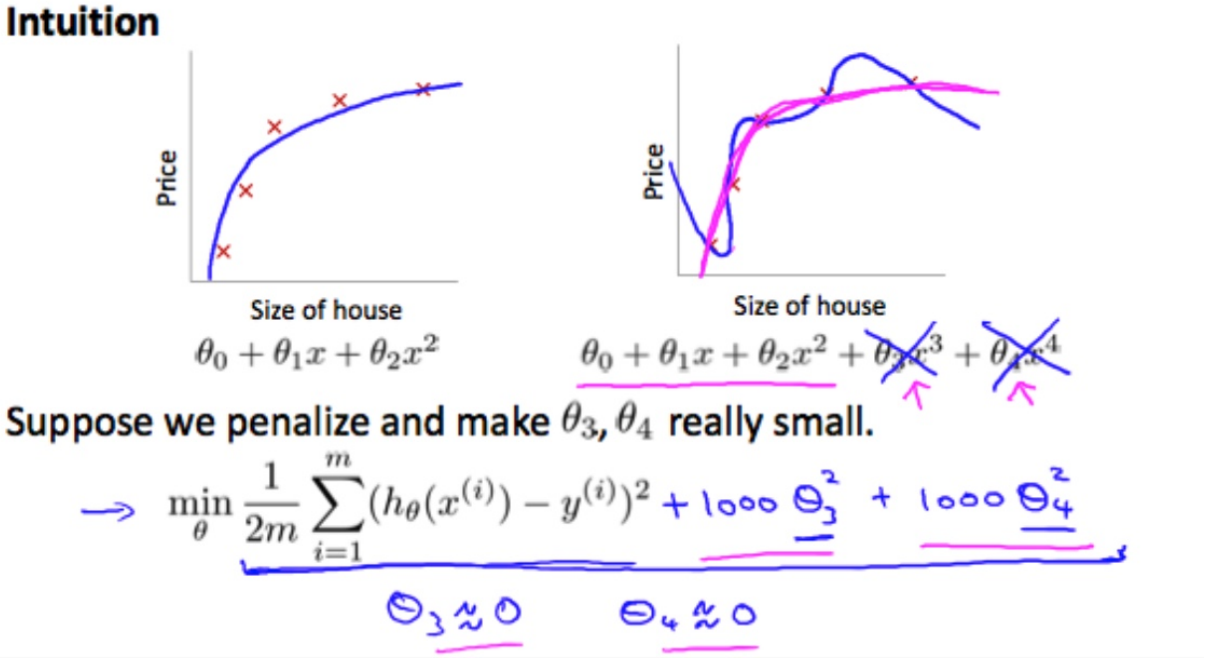
Say we wanted to make the following function more quadratic:

$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

We'll want to eliminate the influence of $\theta_3 x^3$ and $\theta_4 x^4$. Without actually getting rid of these features or changing the form of our hypothesis, we can instead modify our **cost function**:

$min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2$

We've added two extra terms at the end to inflate the cost of θ_3 and θ_4. Now, in order for the cost function to get close to zero, we will have to reduce the values of θ_3 and θ_4 to near zero. This will in turn greatly reduce the values of $\theta_3 x^3$ and $\theta_4 x^4$ in our hypothesis function. As a result, we see that the new hypothesis (depicted by the pink curve) looks like a quadratic function but fits the data better due to the extra small terms $\theta_3 x^3$ and $\theta_4 x^4$.



We could also regularize all of our theta parameters in a single summation as:

$$min_\theta \frac{1}{2m} \sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2$$

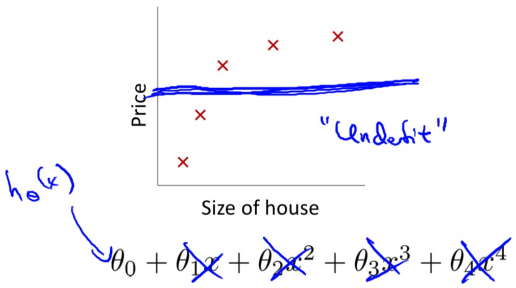
The λ, or lambda, is the **regularization parameter**. It determines how much the costs of our theta parameters are inflated.

Using the above cost function with the extra summation, we can smooth the output of our hypothesis function to reduce overfitting. If lambda is chosen to be too large, it may smooth out the function too much and cause underfitting. Hence, what would happen if $\lambda = 0$ or is too small ?

In regularized linear regression, we choose θ to minimize

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2\right]$$

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?



$\theta_1, \theta_2, \theta_3, \theta_4$

$\theta_1 \approx 0$, $\theta_2 \approx 0$

$\theta_3 \approx 0$, $\theta_4 \approx 0$

$h_\theta(x) = \theta_0$

In regularized linear regression, we choose θ to minimize:

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2\right]$$

What if λ is set to an extremely large value (perhaps too large for our problem, say $\lambda = 10^{10}$)?

- Algorithm works fine; setting λ to be very large can't hurt it.
- Algorithm fails to eliminate overfitting.
- (•) Algorithm results in underfitting (fails to fit even the training set).

Correct

- Gradient descent will fail to converge.

2.3 Regularized linear regression

Gradient Descent

We will modify our gradient descent function to separate out θ_0 from the rest of the parameters because we do not want to penalize θ_0.

Repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

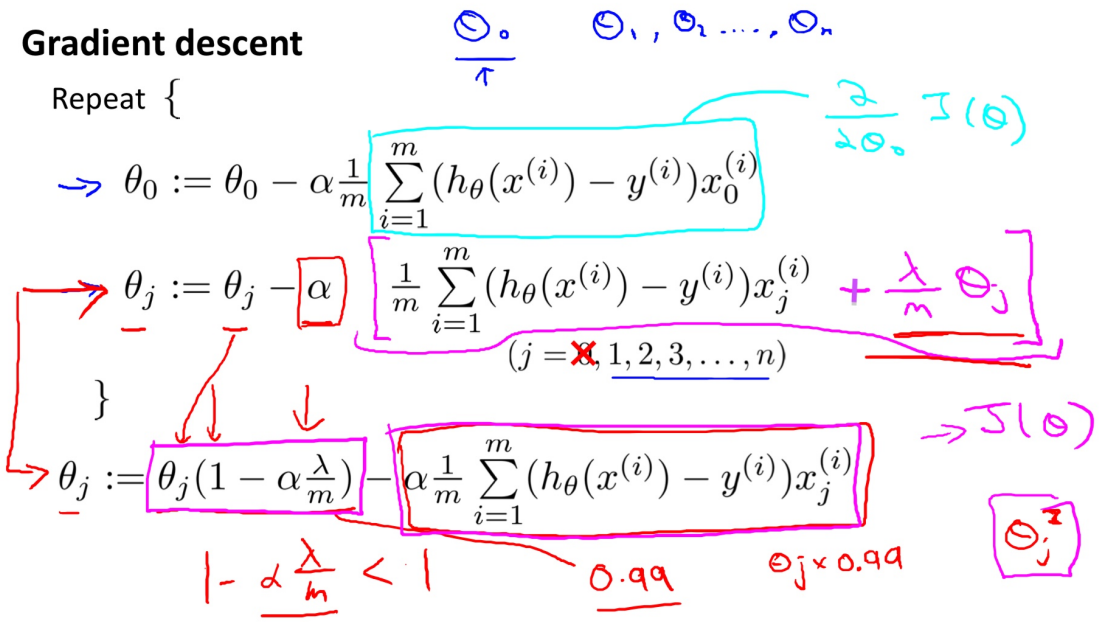
$$\theta_j := \theta_j - \alpha \left[\left(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right] \qquad j \in \{1, 2 ... n\}$$

}

The term $\frac{\lambda}{m}\theta_j$ performs our regularization. With some manipulation our update rule can also be represented as:

$$\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

The first term in the above equation, $1 - \alpha\frac{\lambda}{m}$ will always be less than 1. Intuitively you can see it as reducing the value of θ_j by some amount on every update. Notice that the second term is now exactly the same as it was before.



Normal Equation

Now let's approach regularization using the alternate method of the non-iterative normal equation.

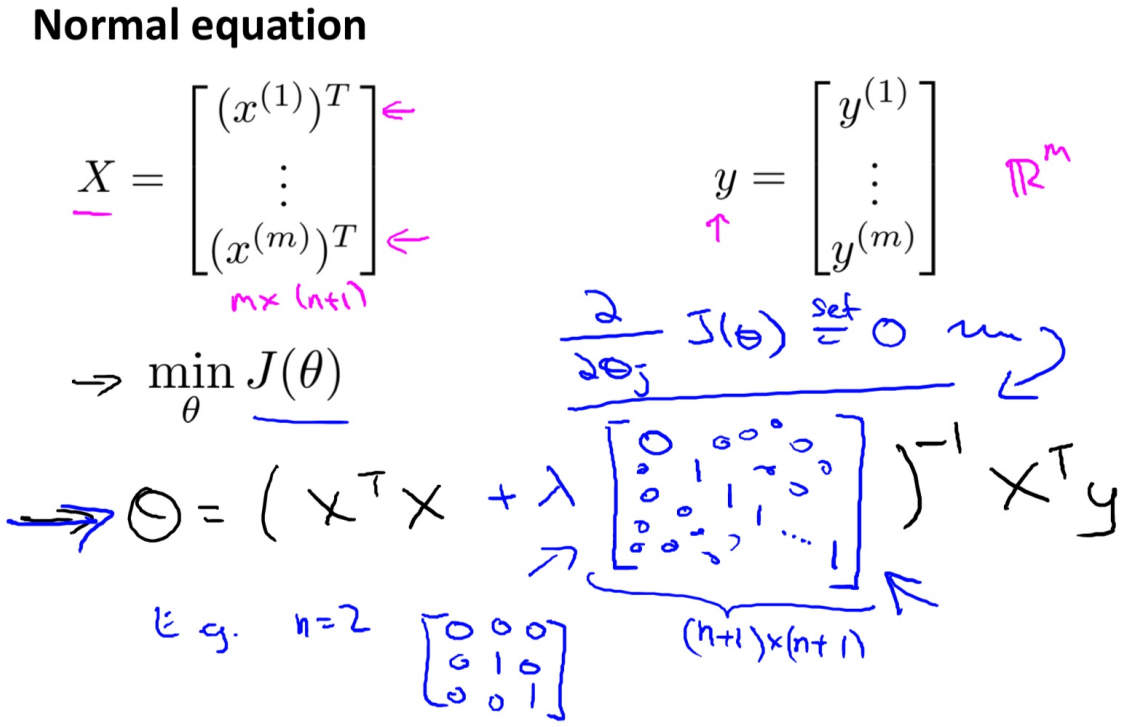
To add in regularization, the equation is the same as our original, except that we add another term inside the parentheses:

$$\theta = \left(X^T X + \lambda \cdot L\right)^{-1} X^T y$$

$$\text{where } L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$

L is a matrix with 0 at the top left and 1's down the diagonal, with 0's everywhere else. It should have dimension (n+1)×(n+1). Intuitively, this is the identity matrix (though we are not including x_0), multiplied with a single real number λ.

Recall that if m < n, then $X^T X$ is non-invertible. However, when we add the term λ·L, then $X^T X$ + λ·L becomes invertible.



Suppose you are doing gradient descent on a training set of $m > 0$ examples, using a fairly small learning rate $\alpha > 0$ and some regularization parameter $\lambda > 0$. Consider the update rule:

$$\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}.$$

Which of the following statements about the term $(1 - \alpha\frac{\lambda}{m})$ must be true?

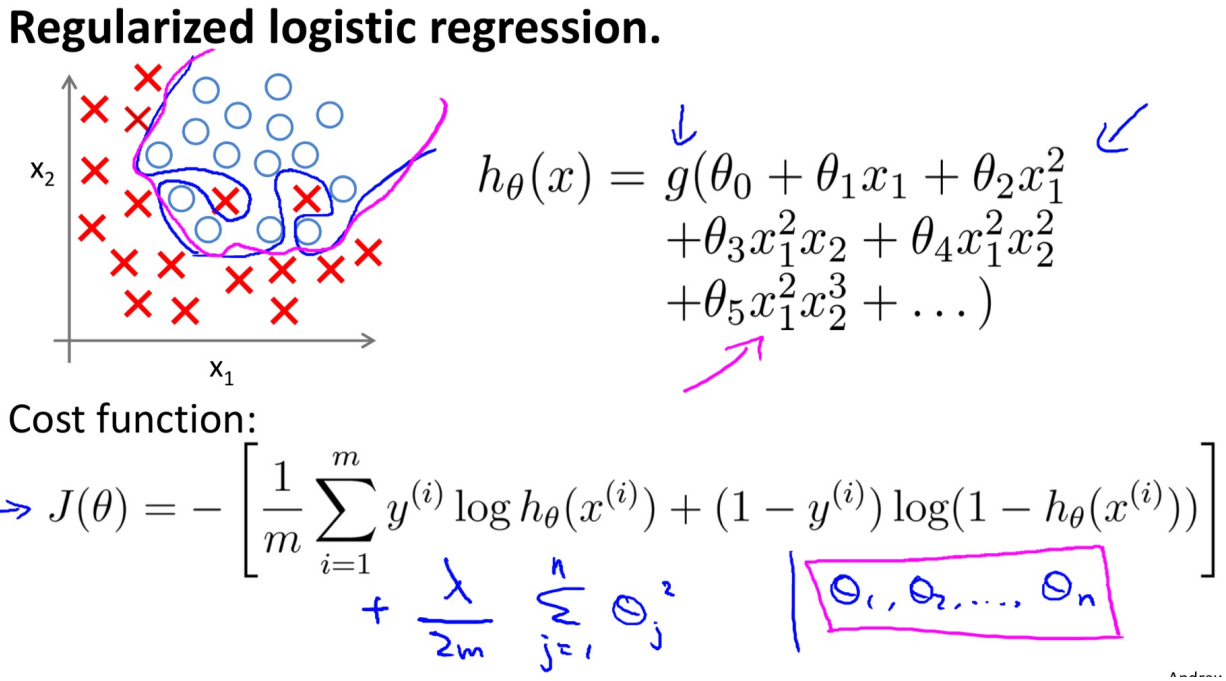
- $1 - \alpha\frac{\lambda}{m} > 1$
- $1 - \alpha\frac{\lambda}{m} = 1$
- $1 - \alpha\frac{\lambda}{m} < 1$

Correct

- None of the above.

2.4 Regularized logistic regression

We can regularize logistic regression in a similar way that we regularize linear regression. As a result, we can avoid overfitting. The following image shows how the regularized function, displayed by the pink line, is less likely to overfit than the non-regularized function represented by the blue line:



Cost Function

Recall that our cost function for logistic regression was:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\ \log(h_\theta(x^{(i)})) + (1-y^{(i)})\ \log(1-h_\theta(x^{(i)}))]$$

We can regularize this equation by adding a term to the end:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\ \log(h_\theta(x^{(i)})) + (1-y^{(i)})\ \log(1-h_\theta(x^{(i)}))] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

The second sum, $\sum_{j=1}^{n}\theta_j^2$ **means to explicitly exclude** the bias term, θ_0. I.e. the θ vector is indexed from 0 to n (holding n+1 values, θ_0 through θ_n), and this sum explicitly skips θ_0, by running from 1 to n, skipping 0. Thus, when computing the equation, we should continuously update the two following equations:

Gradient descent

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

$(j = \cancel{0}, 1, 2, 3, \ldots, n)$

$\theta_1 \ldots \theta_n$

$\}$

$\frac{\partial}{\partial \theta_j} J(\theta)$

$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$

Advanced optimization

fminunc (@ costFunction, θ = [θ_0 theta(1); θ_1 theta(2); θ_n theta(n+1)])

```
function [jVal, gradient] = costFunction(theta)
    jVal = [code to compute J(θ)];
        J(θ) = [ -(1/m) Σ_{i=1}^{m} y^(i) log(h_θ(x^(i))) + (1 - y^(i)) log 1 - h_θ(x^(i)) ] + (λ/2m) Σ_{j=1}^{n} θ_j^2
    gradient(1) = [code to compute ∂/∂θ_0 J(θ)];
        (1/m) Σ_{i=1}^{m} (h_θ(x^(i)) - y^(i)) x_0^(i)
    gradient(2) = [code to compute ∂/∂θ_1 J(θ)];
        (1/m) Σ_{i=1}^{m} (h_θ(x^(i)) - y^(i)) x_1^(i) - (λ/m) θ_1
    gradient(3) = [code to compute ∂/∂θ_2 J(θ)];
        (1/m) Σ_{i=1}^{m} (h_θ(x^(i)) - y^(i)) x_2^(i) - (λ/m) θ_2
    ⋮
    gradient(n+1) = [code to compute ∂/∂θ_n J(θ)];
```

J(θ)

2.5 Test

1. You are training a classification model with logistic regression. Which of the following statements are true? Check all that apply.

- [ ] Introducing regularization to the model always results in equal or better performance on the training set.
- [ ] Adding a new feature to the model always results in equal or better performance on examples not in the training set.
- [ ] Introducing regularization to the model always results in equal or better performance on examples not in the training set.
- [ ] Adding many new features to the model makes it more likely to overfit the training set.

2. Suppose you ran logistic regression twice, once with $\lambda = 0$, and once with $\lambda = 1$. One of the times, you got parameters $\theta = \begin{bmatrix} 23.4 \\ 37.9 \end{bmatrix}$, and the other time you got $\theta = \begin{bmatrix} 1.03 \\ 0.28 \end{bmatrix}$. However, you forgot which value of λ corresponds to which value of θ. Which one do you think corresponds to $\lambda = 1$?

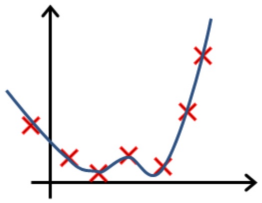
- ( ) $\theta = \begin{bmatrix} 23.4 \\ 37.9 \end{bmatrix}$
- (•) $\theta = \begin{bmatrix} 1.03 \\ 0.28 \end{bmatrix}$

3. Which of the following statements about regularization are true? Check all that apply.

- [ ] Because logistic regression outputs values $0 \leq h_\theta(x) \leq 1$, its range of output values can only be "shrunk" slightly by regularization anyway, so regularization is generally not helpful for it.
- [ ] Because regularization causes $J(\theta)$ to no longer be convex, gradient descent may not always converge to the global minimum (when $\lambda > 0$, and when using an appropriate learning rate α).
- [ ] Using a very large value of λ cannot hurt the performance of your hypothesis; the only reason we do not set λ to be too large is to avoid numerical problems.
- [x] Using too large a value of λ can cause your hypothesis to underfit the data.

4. In which one of the following figures do you think the hypothesis has overfit the training set?

(•) Figure:



5. In which one of the following figures do you think the hypothesis has underfit the training set?

(•) Figure: