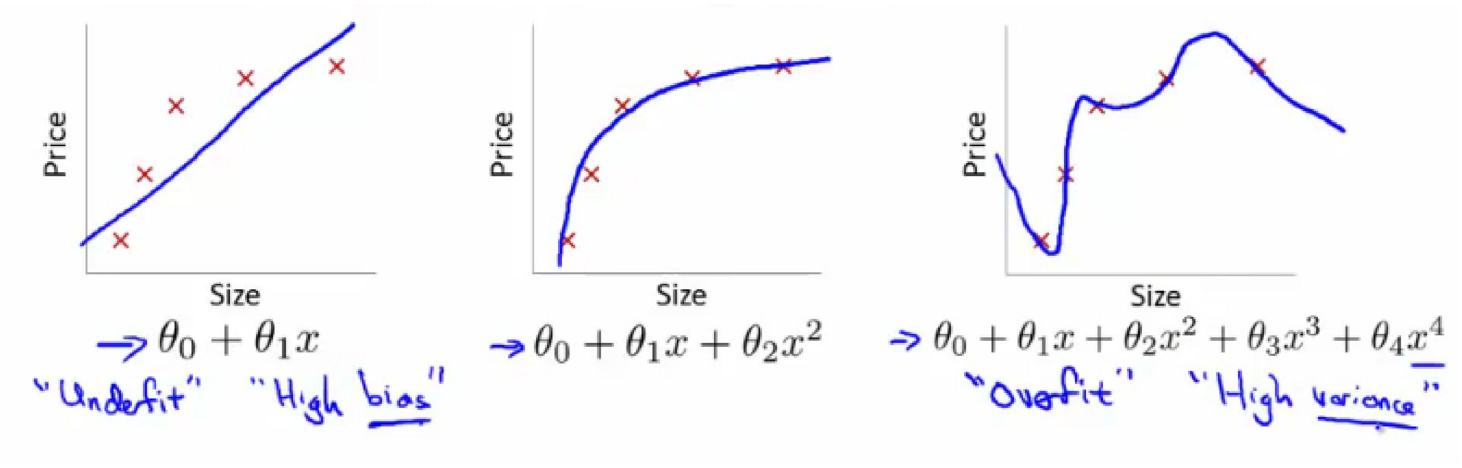
07: Regularization

The problem of overfitting

- So far we've seen a few algorithms - work well for many applications, but can suffer from the problem of overfitting
- What is overfitting?
- What is regularization and how does it help

Overfitting with linear regression

- Using our house pricing example again
    - Fit a linear function to the data - not a great model
        - This is **underfitting** - also known as **high bias**
        - Bias is a historic/technical one - if we're fitting a straight line to the data we have a strong preconception that there should be a linear fit
            - In this case, this is not correct, but a straight line can't help being straight!
    - Fit a quadratic function
        - Works well
    - Fit a 4th order polynomial
        - Now curve fit's through all five examples
            - Seems to do a good job fitting the training set
            - But, despite fitting the data we've provided very well, this is actually not such a good model
        - This is **overfitting** - also known as **high variance**
    - Algorithm has high variance
        - High variance - if fitting high order polynomial then the hypothesis can basically fit any data
        - Space of hypothesis is too large

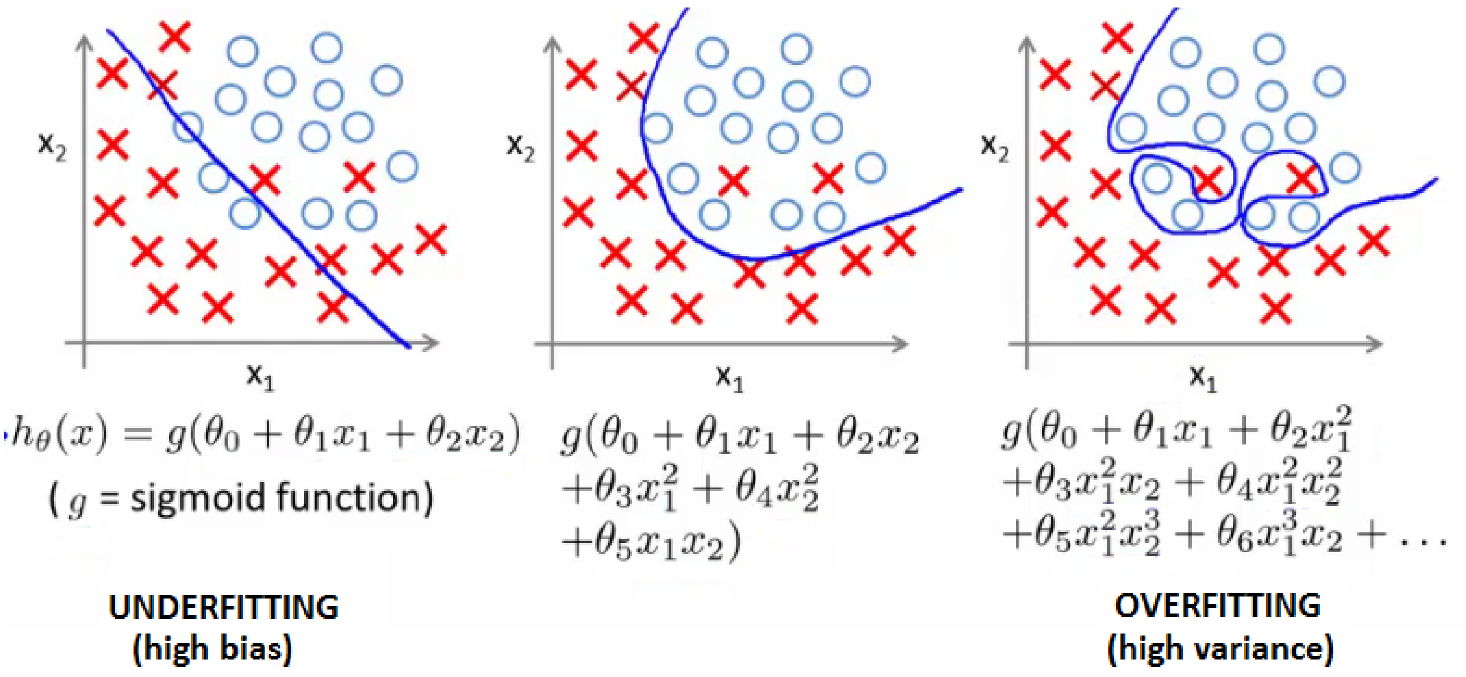


- To recap, if we have too many features then the learned hypothesis may give a cost function of exactly zero
    - But this tries too hard to fit the training set

    - Fails to provide a *general* solution - **unable to generalize** (apply to new examples)

Overfitting with logistic regression

- Same thing can happen to logistic regression
    - Sigmoidal function is an underfit
    - But a high order polynomial gives and overfitting (high variance hypothesis)



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

(g = sigmoid function)

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

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

UNDERFITTING (high bias)

OVERFITTING (high variance)

Addressing overfitting

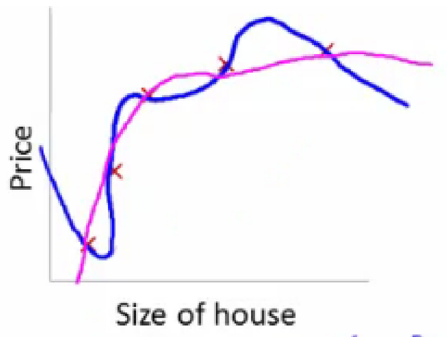
- Later we'll look at identifying when overfitting and underfitting is occurring
- Earlier we just plotted a higher order function - saw that it looks "too curvy"
    - Plotting hypothesis is one way to decide, but doesn't always work
    - Often have lots of a features - here it's not just a case of selecting a degree polynomial, but also harder to plot the data and visualize to decide what features to keep and which to drop
    - If you have lots of features and little data - overfitting can be a problem
- How do we deal with this?
    - 1) **Reduce number of features**
        - Manually select which features to keep
        - Model selection algorithms are discussed later (good for reducing number of features)
        - But, in reducing the number of features we lose some information
            - Ideally select those features which minimize data loss, but even so, some info is lost
    - 2) **Regularization**
        - Keep all features, but reduce magnitude of parameters θ
        - Works well when we have a lot of features, each of which contributes a bit to predicting y

<u>Cost function optimization for regularization</u>

- Penalize and make some of the θ parameters really small
  - e.g. here θ_3 and θ_4

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

- The addition in blue is a modification of our cost function to help penalize θ_3 and θ_4
  - So here we end up with θ_3 and θ_4 being close to zero (because the constants are massive)
  - So we're basically left with a quadratic function



$$\underline{\theta_0+\theta_1x+\theta_2x^2}+\cancel{\theta_3x^3}+\cancel{\theta_4x^4}$$

- In this example, we penalized two of the parameter values
  - More generally, regularization is as follows

- Regularization
  - Small values for parameters corresponds to a simpler hypothesis (you effectively get rid of some of the terms)
  - A simpler hypothesis is less prone to overfitting
- Another example
  - Have 100 features $x_1, x_2, \ldots, x_{100}$
  - Unlike the polynomial example, we don't know what are the high order terms
    - How do we pick the ones to pick to shrink?
  - With regularization, take cost function and modify it to shrink all the parameters
    - Add a term at the end
      - This regularization term shrinks every parameter
      - By convention you don't penalize θ_0 - minimization is from θ_1 onwards

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

$$\theta_1, \theta_2, \theta_3, \ldots, \theta_{100}$$

- In practice, if you include θ_0 has little impact
- λ is the **regularization parameter**

    - Controls a trade off between our two goals
        - 1) Want to fit the training set well
        - 2) Want to keep parameters small
- With our example, using the **regularized objective** (i.e. the cost function with the regularization term) you get a much smoother curve which fits the data and gives a much better hypothesis
    - If **λ** is very large we end up penalizing ALL the parameters (θ_1, θ_2 etc.) so all the parameters end up being close to zero
        - If this happens, it's like we got rid of all the terms in the hypothesis
            - This results here is then underfitting
        - So this hypothesis is too biased because of the absence of any parameters (effectively)
- So, **λ** should be chosen carefully - not too big...
    - We look at some automatic ways to select **λ** later in the course

Regularized linear regression

- Previously, we looked at two algorithms for linear regression
    - Gradient descent
    - Normal equation
- Our linear regression with regularization is shown below

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

$$\min_\theta J(\theta)$$

- Previously, gradient descent would repeatedly update the parameters θ_j, where j = 0,1,2...n simultaneously
    - Shown below

Repeat {

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

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

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

- We've got the θ_0 update here shown explicitly
    - This is because for regularization we don't penalize θ_0 so treat it slightly differently
- How do we regularize these two rules?
    - Take the term and add $\lambda/m * \theta_j$

        - Sum for every θ (i.e. j = 0 to n)
    - This gives regularization for gradient descent
- We can show using calculus that the equation given below is the partial derivative of the regularized J(θ)

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

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

$$\underline{\frac{\partial}{\partial \theta_j} \underline{J(\theta)}} \quad \text{regularized}$$

- The update for θ_j
    - θ_j gets updated to
        - $\theta_j - \alpha$ * [a big term which also depends on θ_j]
- So if you group the θ_j terms together

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

- The term

$$(1 - \alpha\frac{\lambda}{m})$$

    - Is going to be a number less than 1 usually
    - Usually learning rate is small and m is large
        - So this typically evaluates to (1 - a small number)
        - So the term is often around 0.99 to 0.95
- This in effect means θ_j gets multiplied by 0.99
    - Means the squared norm of θ_j a little smaller
    - The second term is exactly the same as the original gradient descent

Regularization with the normal equation

- Normal equation is the other linear regression model
    - Minimize the J(θ) using the normal equation
    - To use regularization we add a term (+ λ [n+1 x n+1]) to the equation
        - [n+1 x n+1] is the n+1 identity matrix

$$\Theta = \left(X^T X + \lambda \underbrace{\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}}_{(n+1)\times(n+1)} \right)^{-1} X^T y$$

e.g. if n = 2 $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Regularization for logistic regression

- We saw earlier that logistic regression can be prone to overfitting with lots of features
- Logistic regression cost function is as follows;

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

- To modify it we have to add an extra term

$$+ \frac{\lambda}{2m} \sum_{j=1}^{n} \Theta_j^2$$

- This has the effect of penalizing the parameters θ_1, θ_2 up to θ_n
  - Means, like with linear regression, we can get what appears to be a better fitting lower order hypothesis
- How do we implement this?
  - Original logistic regression with gradient descent function was as follows

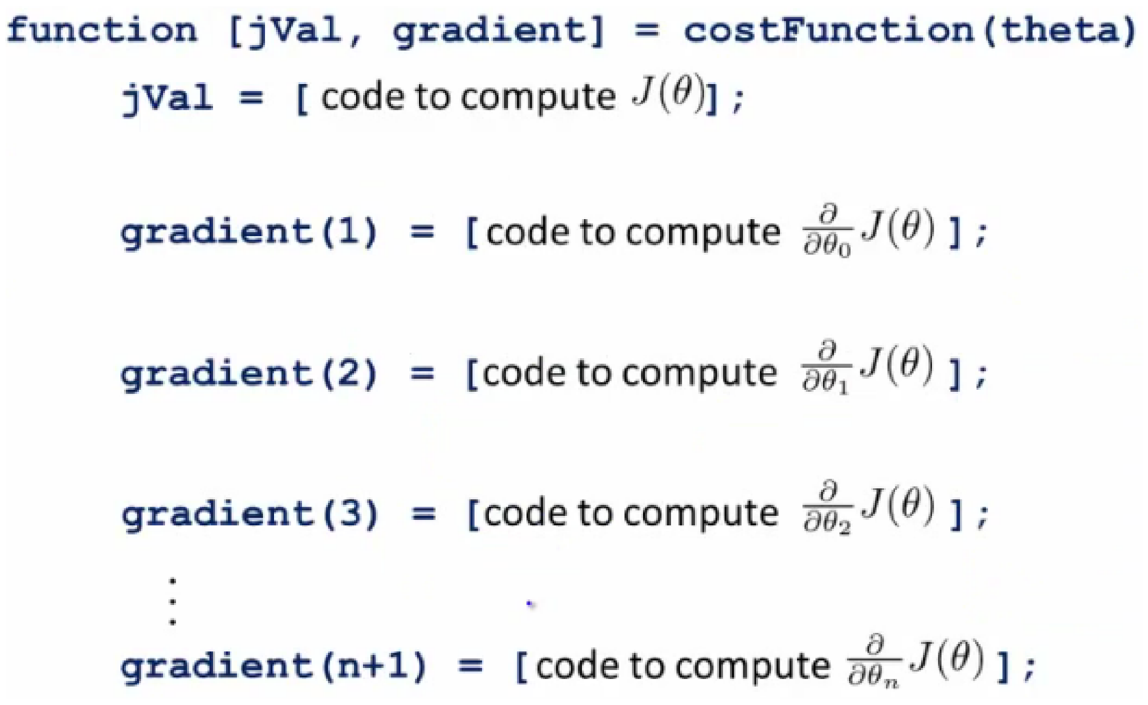
$$\theta_j := \theta_j - \alpha \quad \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$
$$(j = 0, 1, 2, 3, \ldots, n)$$

- Again, to modify the algorithm we simply need to modify the update rule for θ_1, onwards
  - Looks cosmetically the same as linear regression, except obviously the hypothesis is very different

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

Advanced optimization of regularized linear regression

- As before, define a costFunction which takes a θ parameter and gives jVal and gradient back



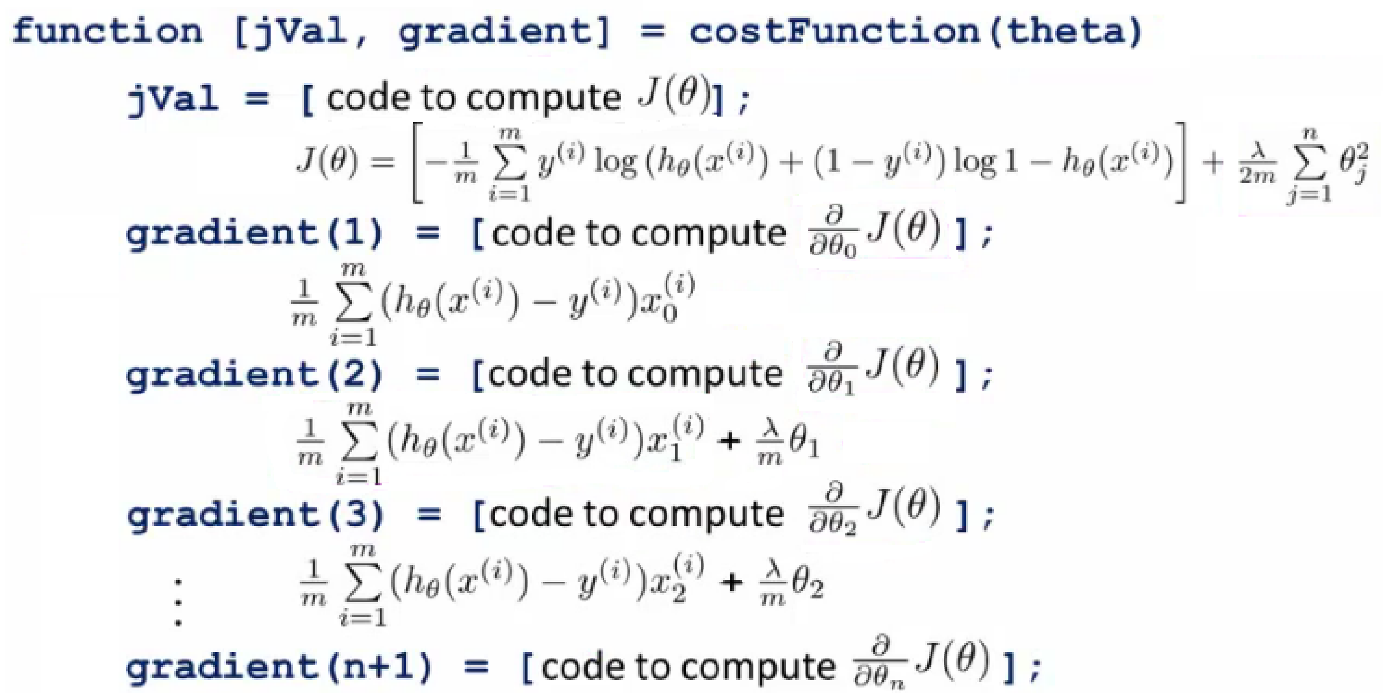
```
function [jVal, gradient] = costFunction(theta)
      jVal = [ code to compute $J(\theta)$] ;

      gradient(1) = [code to compute $\frac{\partial}{\partial\theta_0}J(\theta)$ ] ;

      gradient(2) = [code to compute $\frac{\partial}{\partial\theta_1}J(\theta)$ ] ;

      gradient(3) = [code to compute $\frac{\partial}{\partial\theta_2}J(\theta)$ ] ;
        ⋮
      gradient(n+1) = [code to compute $\frac{\partial}{\partial\theta_n}J(\theta)$ ] ;
```

- use **`fminunc`**
  - Pass it an **`@costfunction`** argument
  - Minimizes in an optimized manner using the cost function
- **`jVal`**
  - Need code to compute J(θ)
    - Need to include regularization term
- Gradient
  - Needs to be the partial derivative of J(θ) with respect to θ_i
  - Adding the appropriate term here is also necessary



```
function [jVal, gradient] = costFunction(theta)
      jVal = [ code to compute $J(\theta)$] ;
```

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

```
      gradient(1) = [code to compute $\frac{\partial}{\partial\theta_0}J(\theta)$ ] ;
```

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

```
      gradient(2) = [code to compute $\frac{\partial}{\partial\theta_1}J(\theta)$ ] ;
```

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

```
      gradient(3) = [code to compute $\frac{\partial}{\partial\theta_2}J(\theta)$ ] ;
```

$$\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_2^{(i)} + \frac{\lambda}{m}\theta_2$$

```
        ⋮
      gradient(n+1) = [code to compute $\frac{\partial}{\partial\theta_n}J(\theta)$ ] ;
```

- Ensure summation doesn't extend to to the lambda term!
    - It doesn't, but, you know, don't be daft!