

07: Regularization

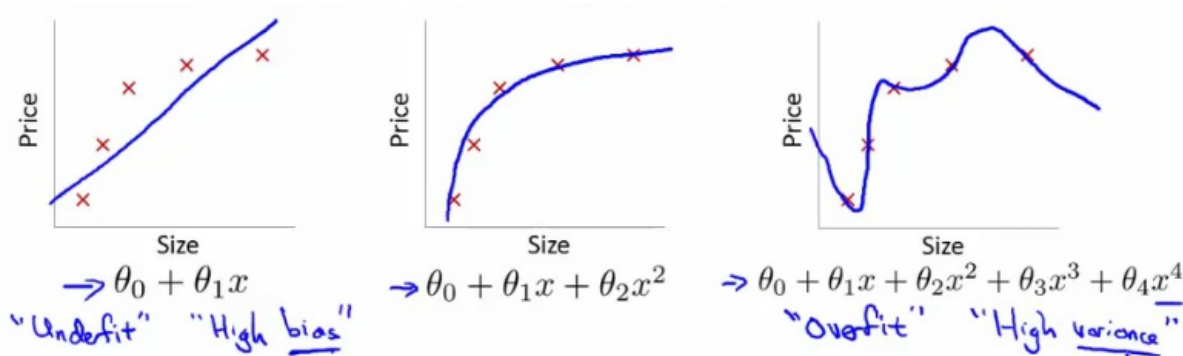
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The problem of overfitting

- 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

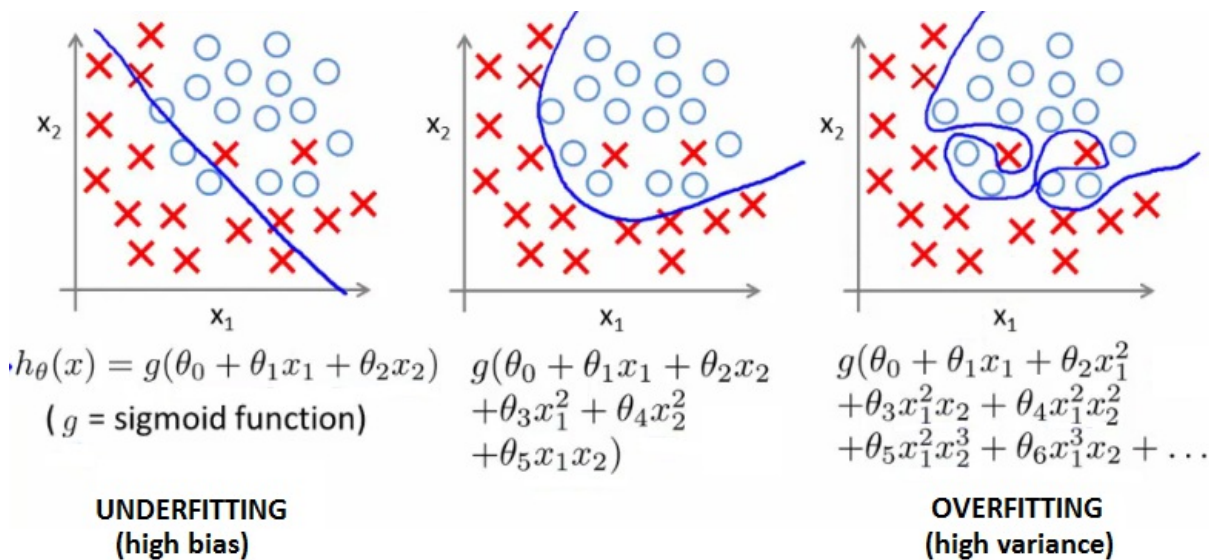
- Using our house pricing example again
 - Fit a linear function to the data - not a great model
 - This is **underfitting** - also known as **high bias**
 - Bias is a historic/technical one - if we're fitting a straight line to the data we have a strong preconception that there should be a linear fit
 - 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)



Addressing overfitting

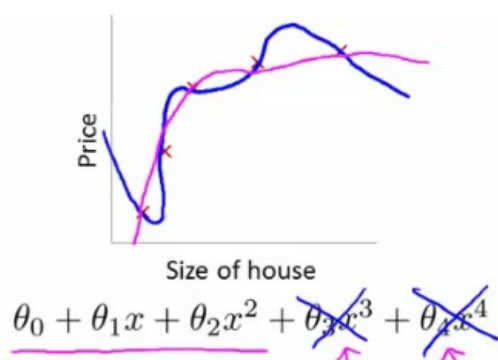
- Later we'll look at identifying when overfitting and underfitting is occurring
- Earlier we just plotted a higher order function - saw that it looks "too curvy"
 - Plotting hypothesis is one way to decide, but doesn't always work
 - Often have lots of features - here it's not just a case of selecting 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

Cost function optimization for regularization

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

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

- 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



- 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, \dots, 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

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

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

- 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 $j = 0, 1, 2, \dots, n$ simultaneously
 - Shown below

Repeat {

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

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

- 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 $J(\theta)$

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

(j = ~~red X~~, 1, 2, 3, ..., n)
 $\frac{\partial}{\partial \theta_j} J(\theta)$ regularized

- The update for θ_j
 - θ_j gets updated to
 - $\theta_j - \alpha * [\text{a big term which also depends on } \theta_j]$
- 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 $(1 - \text{a small number})$
 - 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 $J(\theta)$ using the normal equation
 - To use regularization we add a term $(+ \lambda [n+1 \times n+1])$ to the equation
 - $[n+1 \times n+1]$ is the $n+1$ identity matrix

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

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

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

$(j = 0, 1, 2, 3, \dots, n)$

- 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 $J(\theta)$
 - Need to include regularization term
- Gradient
 - Needs to be the partial derivative of $J(\theta)$ with respect to θ_i
 - Adding the appropriate term here is also necessary

```
function [jVal, gradient] = costFunction(theta)
```

```
jVal = [code to compute  $J(\theta)$ ];
```

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

```
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  $\frac{\partial}{\partial \theta_2} J(\theta)$ ];
```

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

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

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