CS1138

Machine Learning

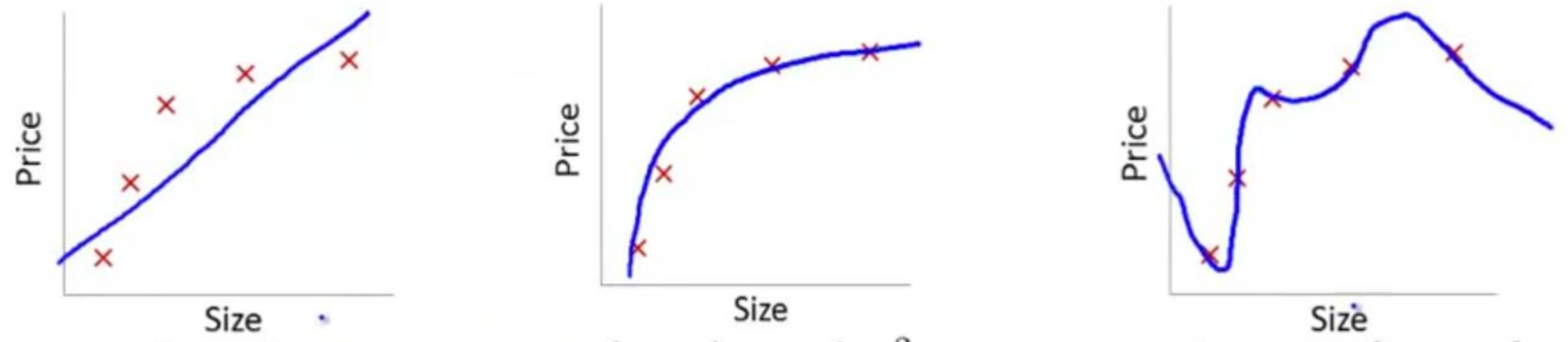
Lecture : Regularization: Problem of Overfitting

(Slide Credits: Andrew Ng)

Arpan Gupta

Problem of Overfitting

Example: Linear regression (housing prices)



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

Underfitting.
High Bias.

“Just right”

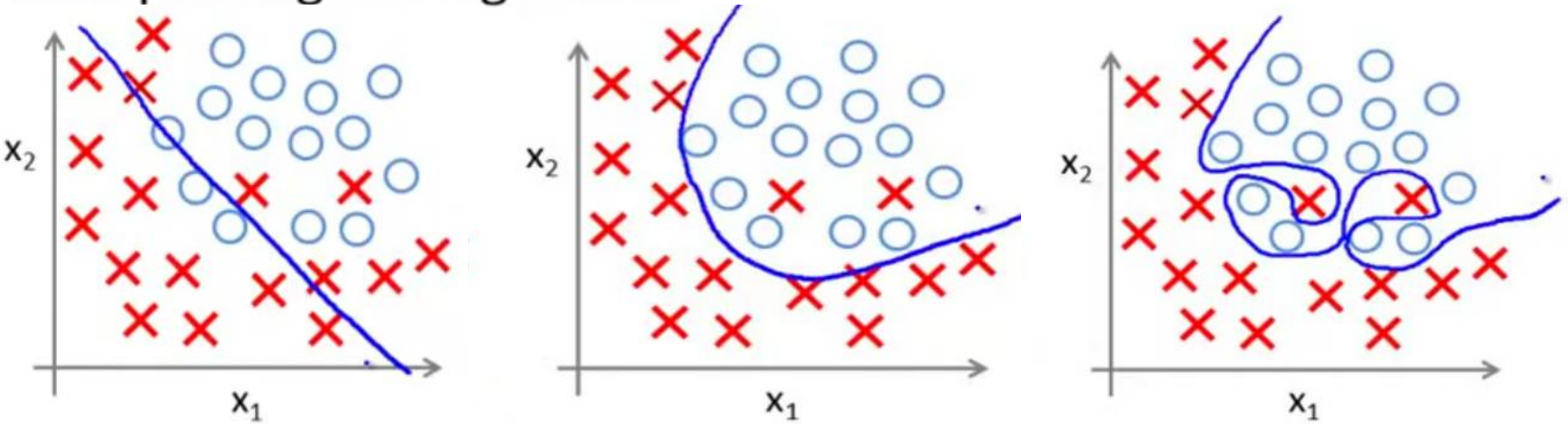
Overfitting.
High Variance

Problem of Overfitting

Overfitting: If we have too many features, the learned hypothesis may fit the training set very well ($J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$), but fail to generalize to new examples (predict prices on new examples).

Problem of Overfitting

Example: Logistic regression



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

(g = sigmoid function)

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

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

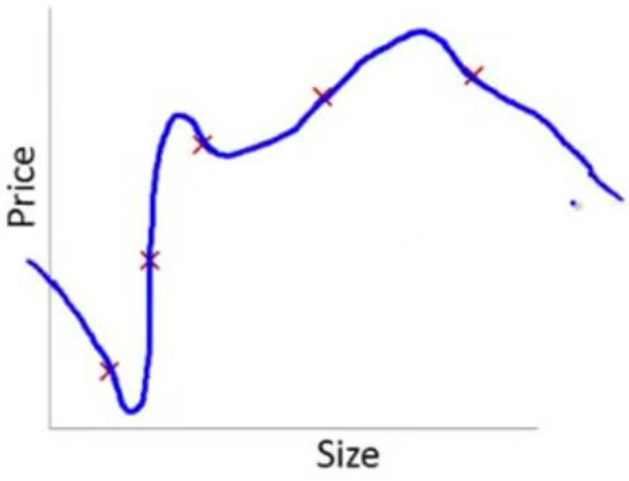
Underfitting.
High Bias.

Just right fit

Overfitting.
High Variance

Addressing Overfitting

- If overfitting is occurring, what to do to address it.
  - For 1D or 2D data, we can just plot and see which degree of polynomial best fits the data.
    - But it doesn’t always work.



Addressing Overfitting (Contd.)

- We may have a learning problem when there are a lot of features.
  - Becomes much harder to visualize for more features.
  - **If we have lot of features and very little data, then overfitting can occur.**

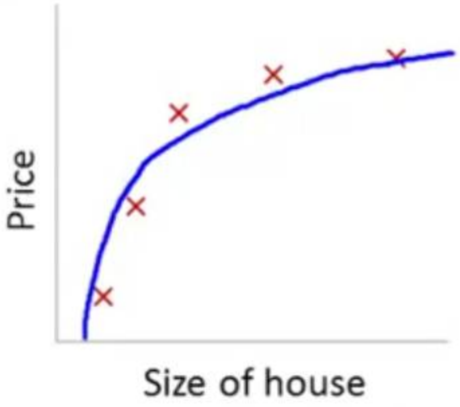
$x_1 =$ size of house
$x_2 =$ no. of bedrooms
$x_3 =$ no. of floors
$x_4 =$ age of house
$x_5 =$ average income in neighborhood
$x_6 =$ kitchen size
$\vdots$
x_{100}

Addressing Overfitting (contd.)

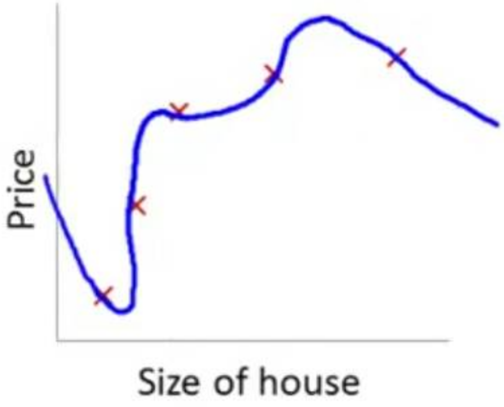
- Options:
  1) Reduce number of features
     a) Manually select which features to keep
     b) Use a model selection algorithm
  2) Regularization
     a) Keep all features, but reduce magnitude/values of parameters Θ_j.
     b) Works well when we have a lot of features, each of which contributes a bit to predicting **y**.

Regularization: Cost Function

Intuition



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



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

Suppose we penalize and make θ_3, θ_4 really small.

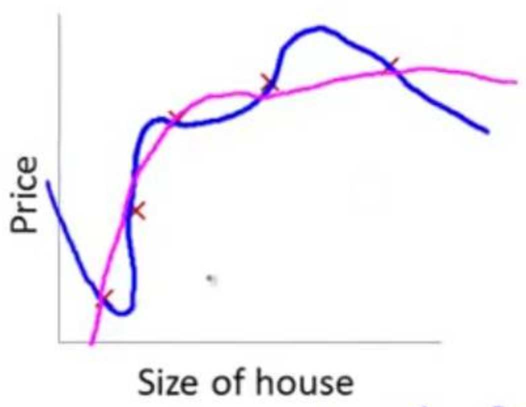
$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000\,\theta_3^2 + 1000\,\theta_4^2$$

Regularization: Cost Function

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

When we minimize this new function, then we have to make Θ_3 and Θ_4 very small.

We will end up with Θ_3 and Θ_4 close to 0. Similar to getting rid of the higher order terms in the hypothesis function.



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

Regularization

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

- "Simpler" hypothesis
- Less prone to overfitting

Housing:

- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

We may not know which parameters to shrink, so we select all of them.

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

Regularization

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

- The convention is to penalize Θ_1 to Θ_n and not penalize Θ_0 , i.e., summation j from 1 to n. But in practice, it does not make much difference.
- If we penalize Θ_0 (intercept -> 0) means that the hyperplane passes through the origin.
- The second term is the **regularization term** and **λ is the regularization parameter**.

Regularization

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

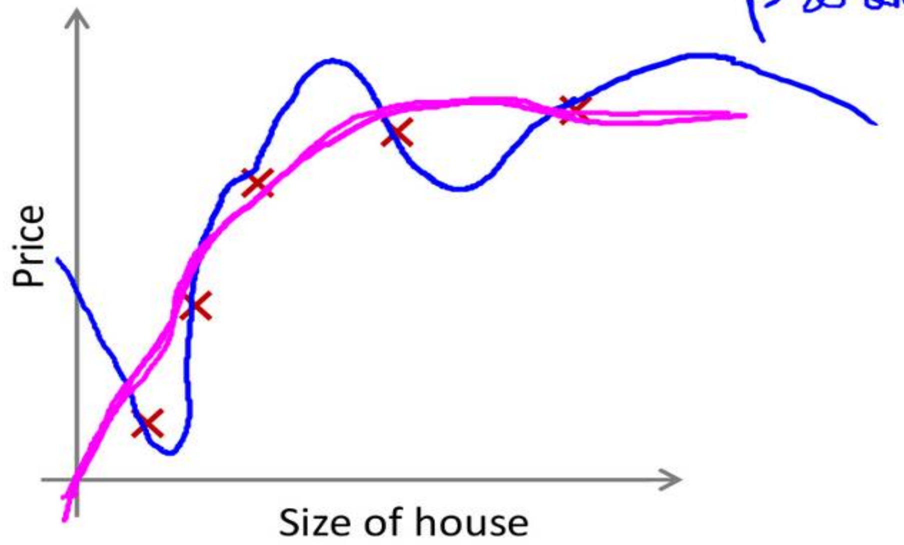
- This objective function ensures two goals, corresponding to the two summation terms.
  - **Fitting training set well:** The first term (squared error **$(h(x) - y)^2$**) tells that we want to fit the training set well.
  - **Keep the parameters small:** The second term (regularization term) tells that the chosen Θ values should be small.
- **λ** controls the tradeoff between the above two goals (fitting the training set well and keeping the parameters small), thereby, keeping the hypothesis relatively “simple” and avoid overfitting.

Regularization.

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

regularization parameter

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



Effect of λ

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 $\lambda = 10^{10}$)?

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

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

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

$\underline{h_\theta(x) = \theta_0}$

$h_\theta(x)$

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

Regularized Linear Regression

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

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

Gradient Descent for regularized linear regression

Repeat $\{$

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

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

$\}$

Gradient Descent for regularized linear regr

Repeat $\{$

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

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

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

$\}$

Gradient Descent for regularized linear regr

Repeat {

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

$$\frac{\partial}{\partial \theta_0} J(\theta)$$

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

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

}

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

Gradient Descent for regularized linear regr

Repeat {

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

$$\frac{\partial}{\partial \theta_0} J(\theta)$$

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

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

}

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

Gradient Descent for regularized linear regr

Repeat $\{$

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

$\frac{\partial}{\partial \theta_0} J(\theta)$

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

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

$\}$

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

$\rightarrow J(\theta)$

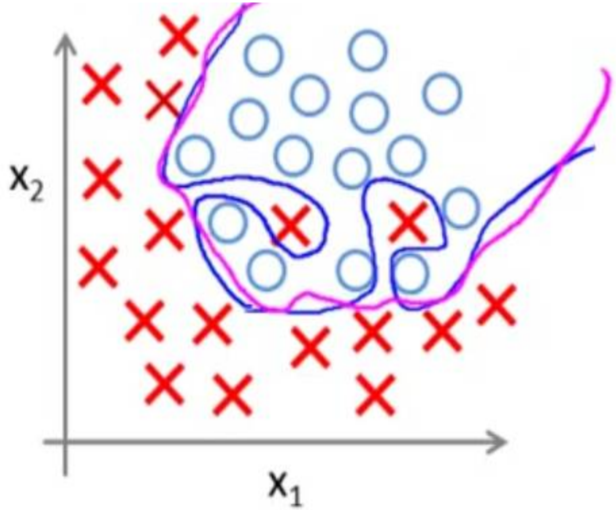
$1 - \alpha\frac{\lambda}{m} < 1$

0.99

$\theta_j \times 0.99$

$\boxed{\theta_j^2}$

Regularized Logistic Regression



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

Cost function:

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

$$+ \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2 \quad \Big| \quad \theta_1, \theta_2, \dots, \theta_n$$

Gradient Descent for regularized logistic regression

Repeat {

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

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

}

Gradient Descent for regularized logistic regression

Repeat {

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

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

$$(j = \cancel{0}, \underbrace{1, 2, 3, \ldots, n}_{\theta_1 \ldots \theta_n})$$

}

Similar to linear regression but hypothesis is different.

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

Gradient Descent for regularized logistic regression

Repeat {

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

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

$$(j = \cancel{0}, \underbrace{1, 2, 3, \ldots, n}_{\theta_1 \ldots \theta_n})$$

}

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

Ridge and Lasso

- Cost function where we take square of all parameters, is also known as **Ridge** regression.

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

- If we take the absolute values of parameters Θ, then it is called **Lasso** regression.

End of Lecture