Regularization

GA DAT5

Agenda

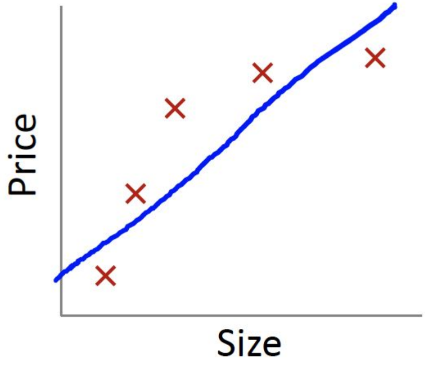
The Problem Of Overfitting

Cost Function

Regularized Regressions

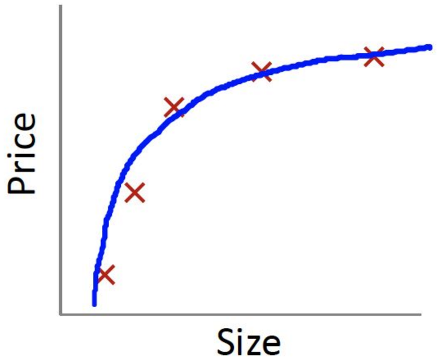
The Problem of Overfitting

Example: Linear regression (housing prices)



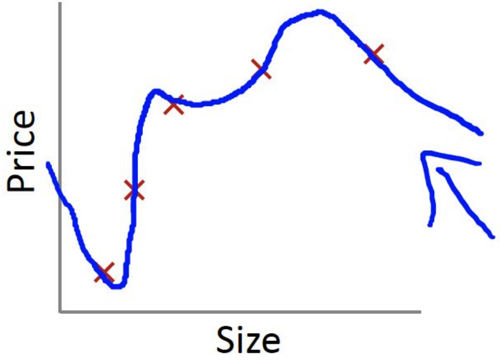
→ $\theta_0 + \theta_1 x$

"Underfit" "High bias"



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

"Just right"



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

"Overfit" "High variance"

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

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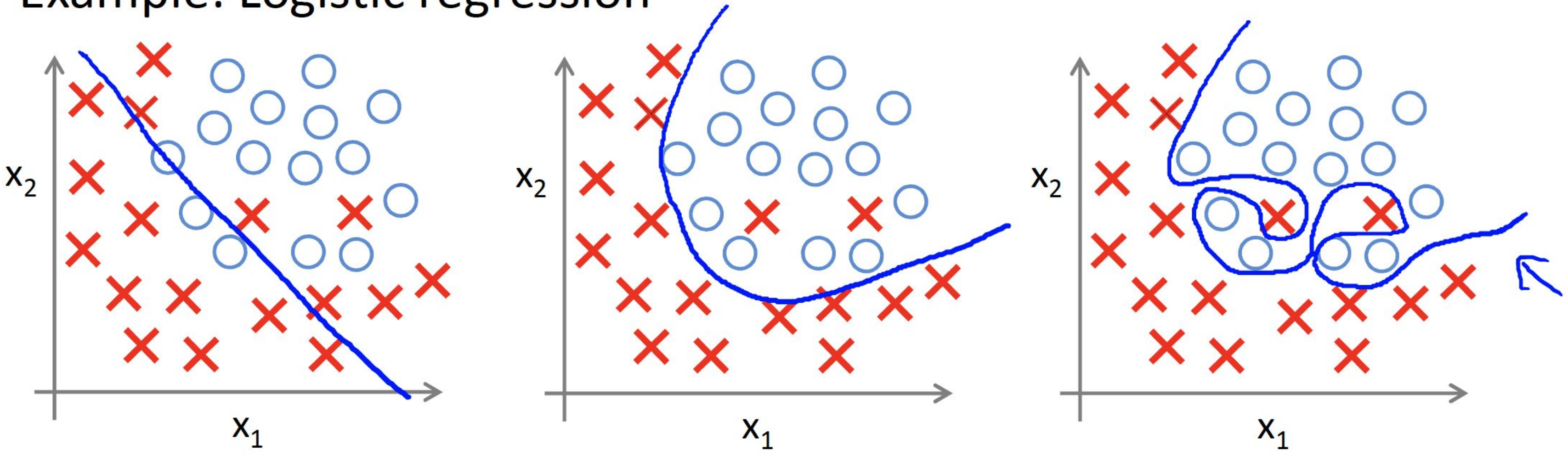
Example: Logistic regression



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

(g = sigmoid function)

"Underfit"

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

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

"Overfit"

Addressing overfitting:

$x_1 =$ size of house

$x_2 =$ no. of bedrooms

$x_3 =$ no. of floors

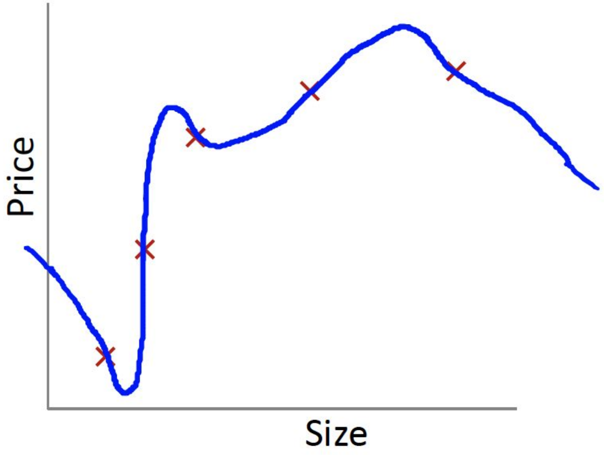
$x_4 =$ age of house

$x_5 =$ average income in neighborhood

$x_6 =$ kitchen size

$\vdots$

x_{100}



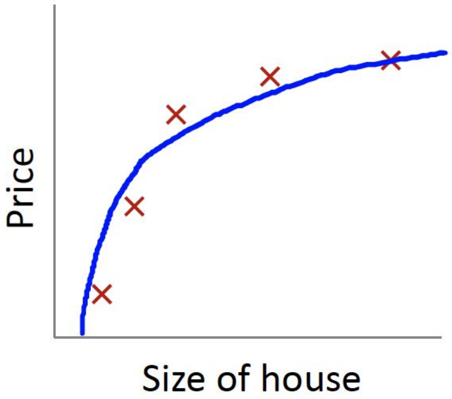
Addressing overfitting:

Options:

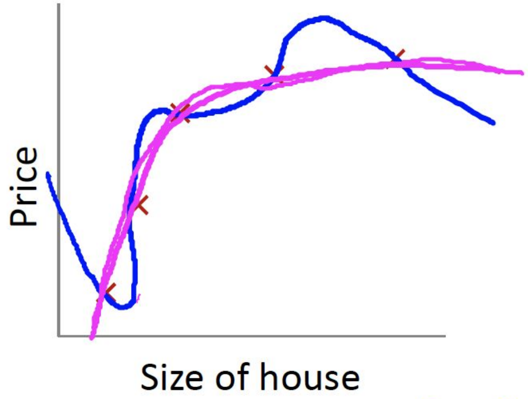
1. Reduce number of features.
   - → Manually select which features to keep.
   - → Model selection algorithm (later in course).
2. Regularization.
   - → Keep all the features, but reduce magnitude/values of parameters $\underline{\theta_j}$.
   - Works well when we have a lot of features, each of which contributes a bit to predicting y.

Cost Function

Intuition



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



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

Suppose we penalize and make θ_3, θ_4 really small.

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

$$\underline{\theta_3 \approx 0} \qquad \underline{\theta_4 \approx 0}$$

Regularization.

Small values for parameters $\boxed{\theta_0, \theta_1, \ldots, \theta_n}$

- "Simpler" hypothesis
- Less prone to overfitting

$\boxed{\theta_3, \theta_4} \approx 0$

Housing:

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

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

$\cancel{\theta_0}$ $\theta_1, \theta_2, \theta_3, \ldots, \theta_{100}$ $\cancel{\theta_0}$

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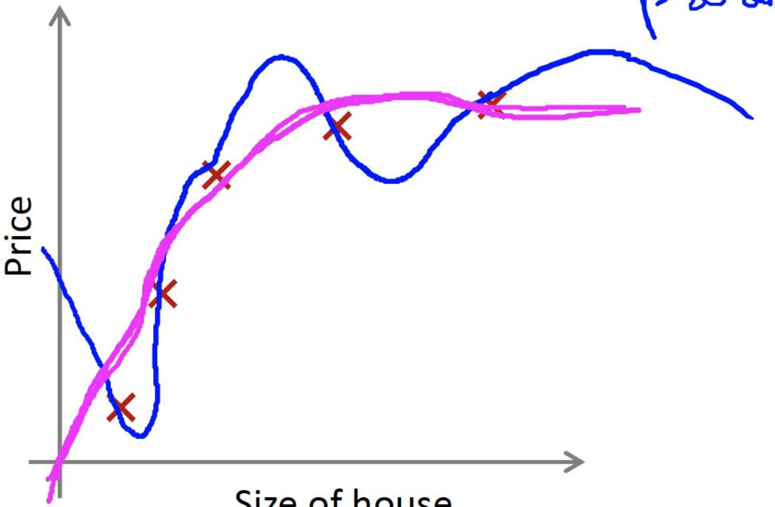
Regularization.

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

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



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

- Algorithm works fine; setting λ to be very large can't hurt it
- Algortihm fails to eliminate overfitting.
- Algorithm results in underfitting. (Fails to fit even training data well).
- Gradient descent will fail to converge.

In regularized linear regression, we choose θ to minimize

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

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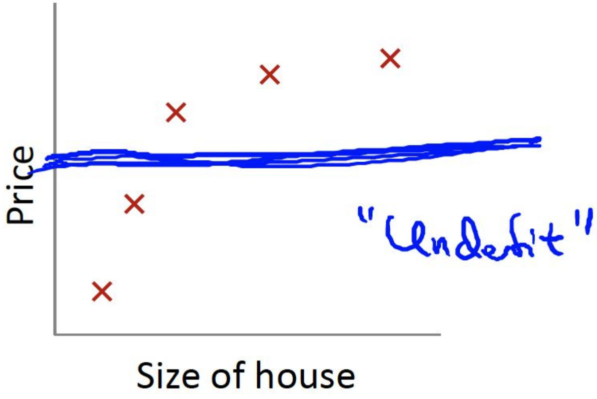

$h_\theta(x)$

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

$\underline{\theta_1}, \underline{\theta_2}, \underline{\theta_3}, \underline{\theta_4}$

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

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

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

Regularized Regressions

Regularized linear regression

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

$$\min_{\underset{\uparrow}{\theta}} \underline{J(\theta)}$$

Gradient descent

$\underline{\theta_0}$ ↑ $\theta_1, \theta_2, \dots, \theta_n$

Repeat {

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

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

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

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

}

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

$\rightarrow J(\theta)$

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

$\underline{0.99}$

$\theta_j \times 0.99$

$\boxed{\theta_j}$

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Normal equation

$$X = \underbrace{\begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix}}_{m \times (n+1)} \qquad y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \mathbb{R}^m$$

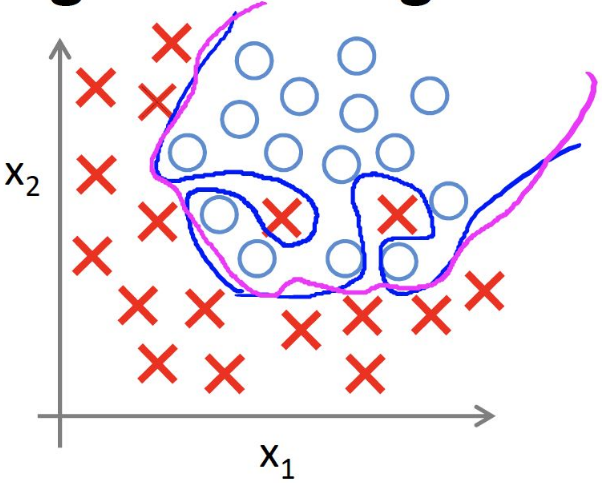
$$\min_{\theta} J(\theta)$$

$$\frac{\partial}{\partial \theta_j} J(\theta) \overset{\text{set}}{=} 0$$

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

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

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:

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

$$\boxed{\theta_1, \theta_2, \dots, \theta_n}$$

Gradient descent

Repeat $\{$

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

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

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

$\}$

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

Q??