

Regression and Gradient Descent

Source: Intro. to Machine Learning
By Andrew Ng, Stanford, Coursera

Training set of housing prices (Portland, OR)	Size in feet² (x)	Price (\$) in 1000's (y)
	2104	460
	1416	232
	1534	315
	852	178

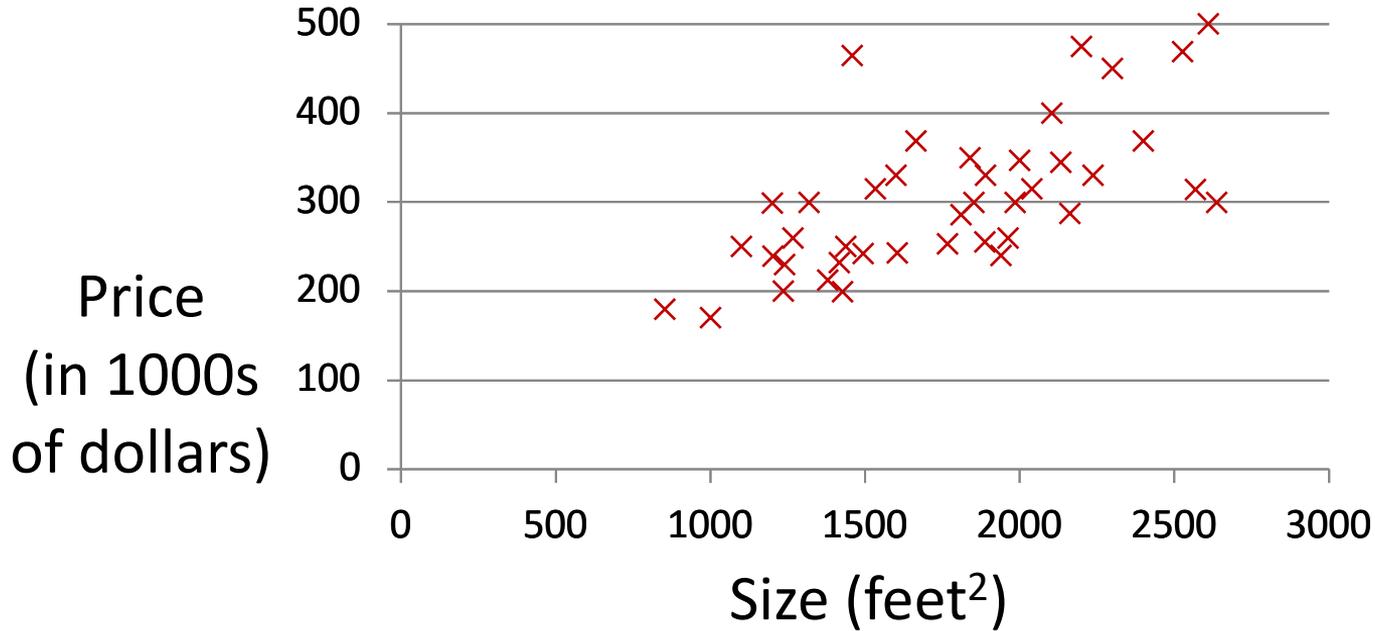
Notation:

m = Number of training examples

x's = "input" variable / features

y's = "output" variable / "target" variable

Housing Prices (Portland, OR)



Regression Problem

Predict real-valued output

Training Set	Size in feet ² (x)	Price (\$) in 1000's (y)
	2104	460
	1416	232
	1534	315
	852	178

Hypothesis: $h_{\theta}(x) = \theta_0 + \theta_1 x$

θ_i 's: Parameters

How to choose θ_i 's ?

Hypothesis:

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

Parameters:

$$\theta_0, \theta_1$$

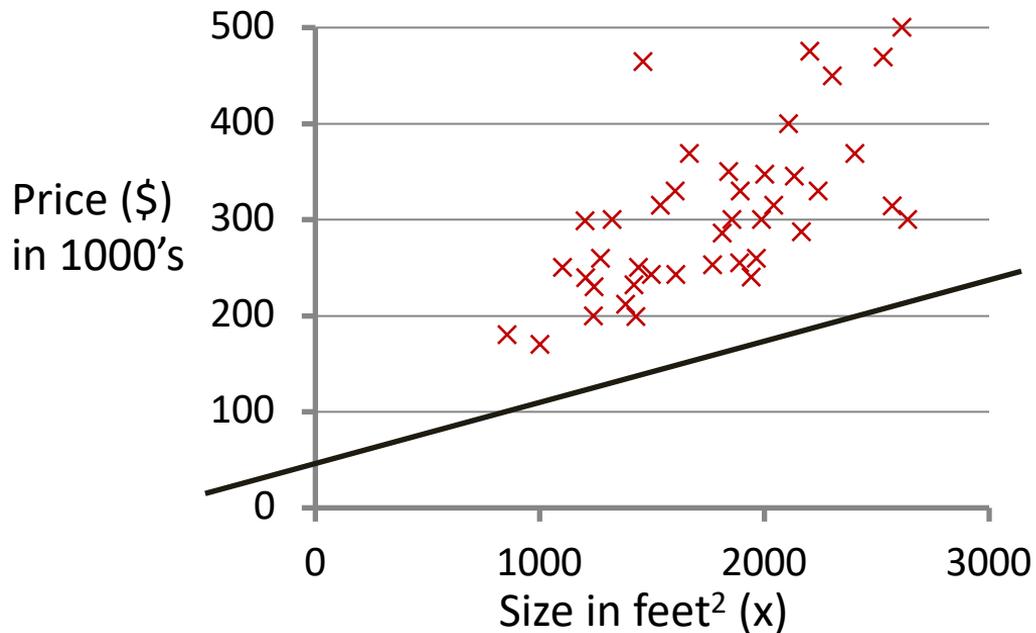
Cost Function (aka Loss Function):

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

Goal: minimize $J(\theta_0, \theta_1)$
 θ_0, θ_1

$$h_{\theta}(x)$$

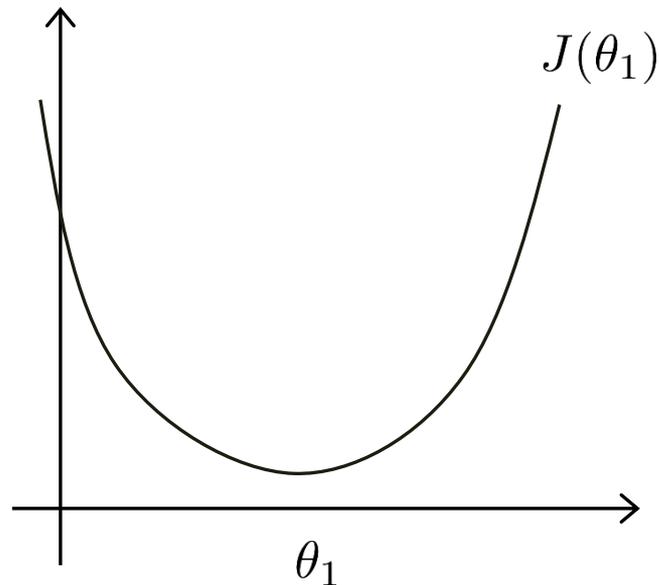
(for fixed θ_0, θ_1 , this is a function of x)

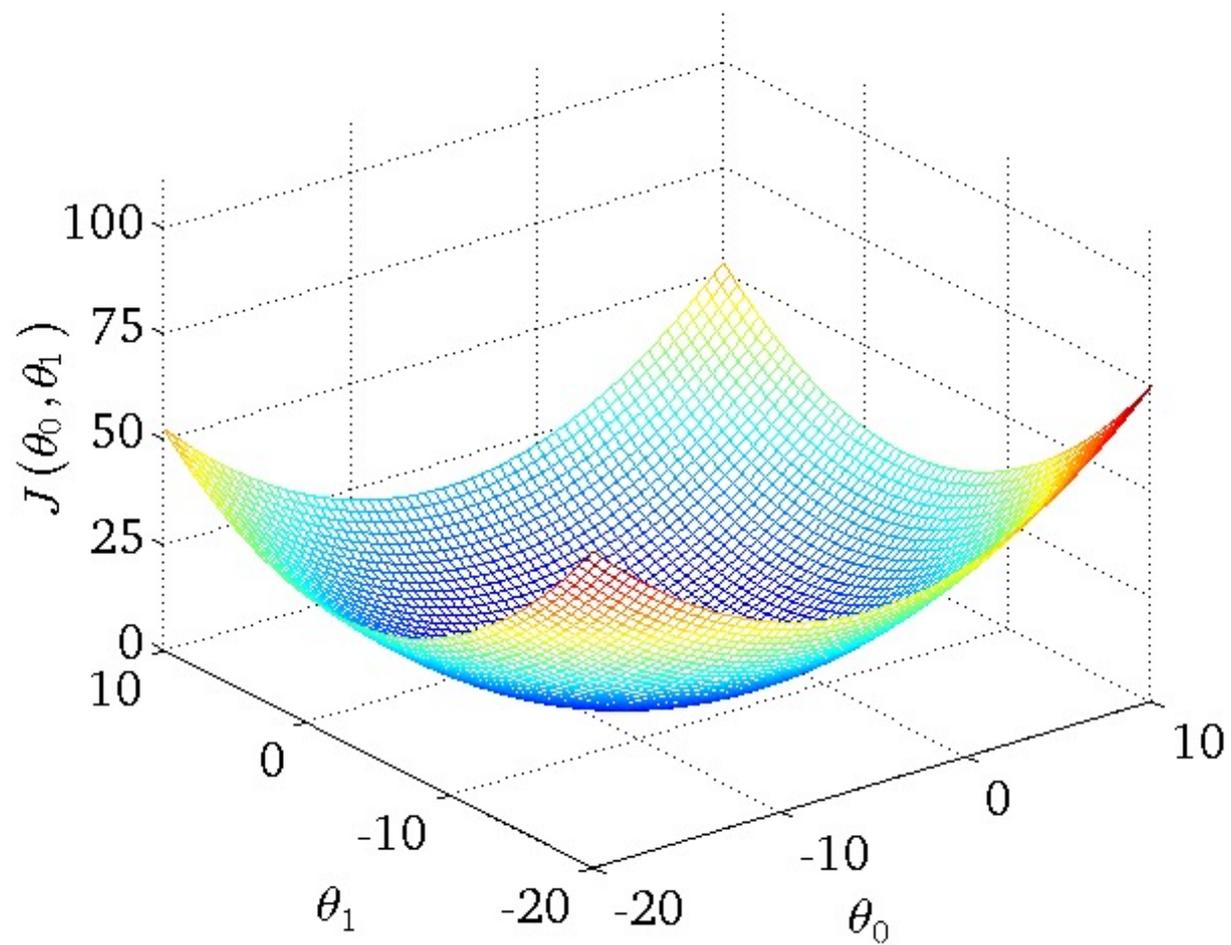


$$h_{\theta}(x) = 50 + 0.06x$$

$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)





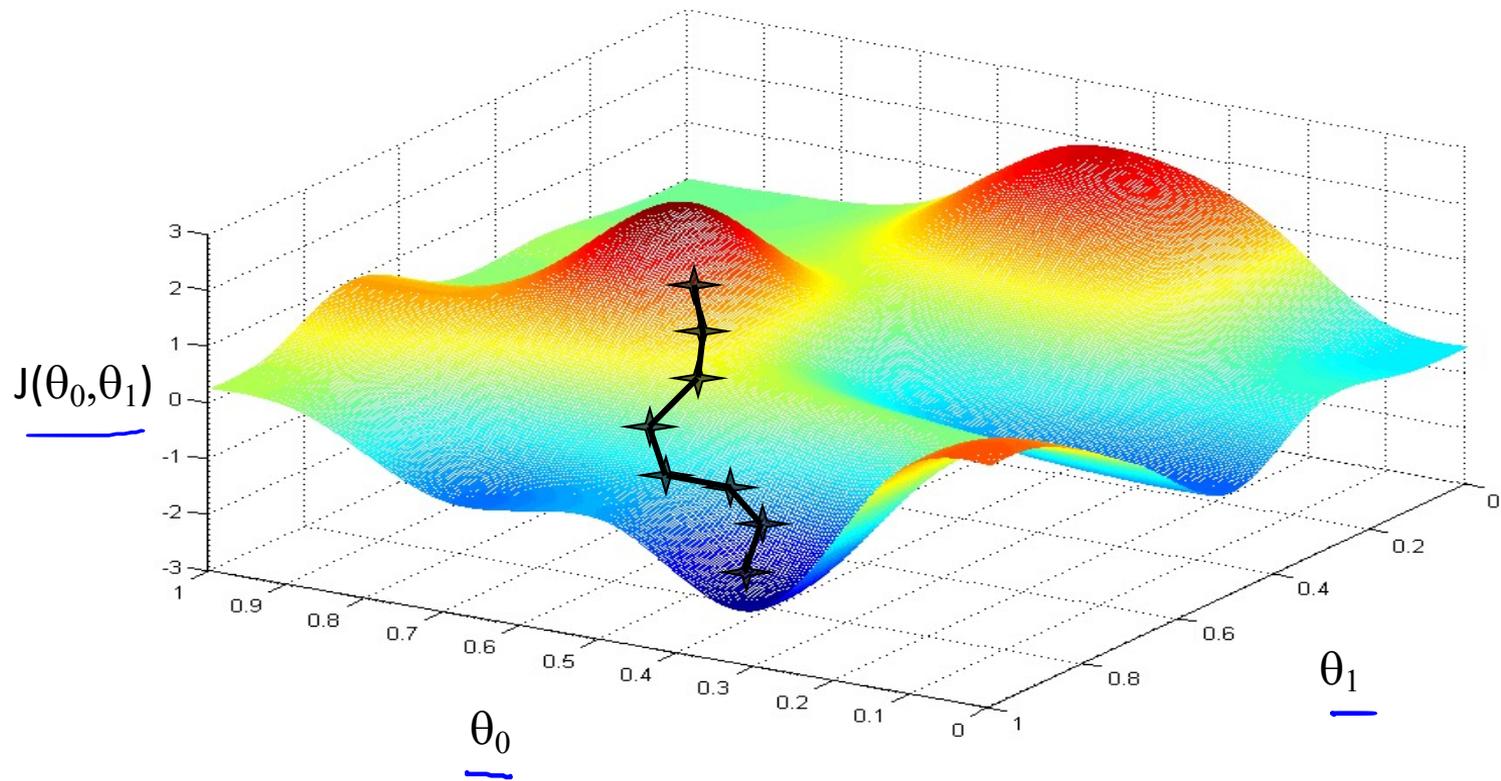
Gradient descent

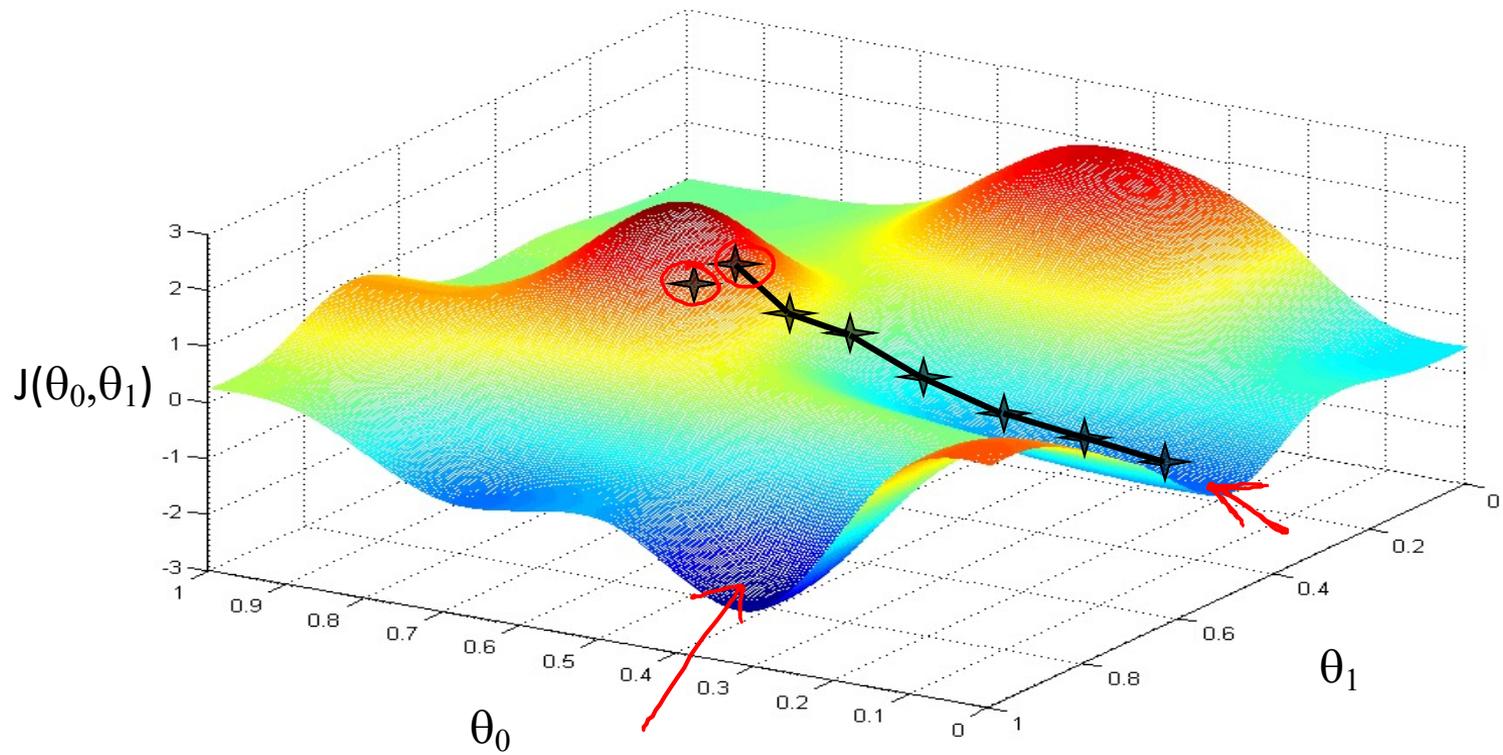
Have some function $J(\theta_0, \theta_1)$

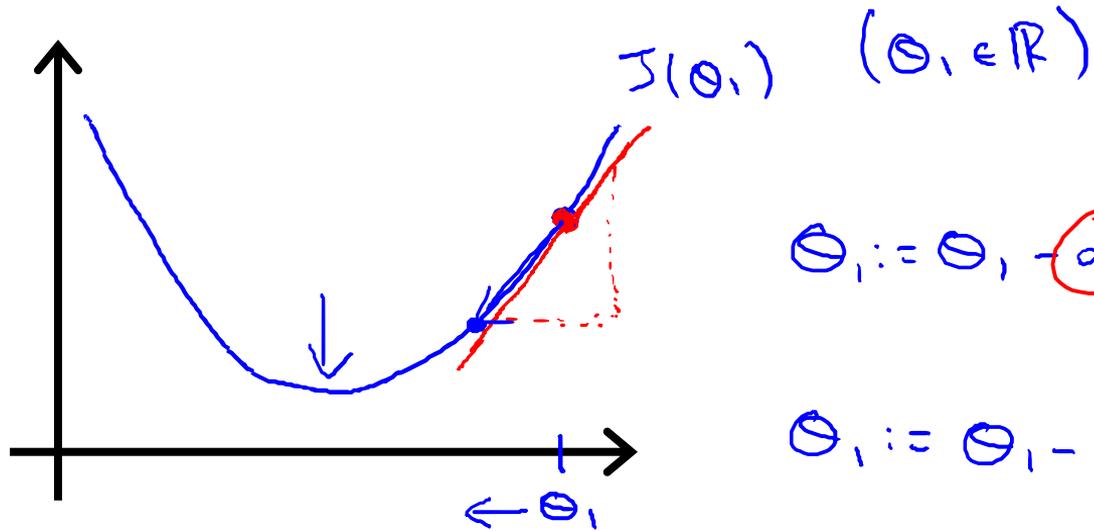
Want $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$

Outline:

- Start with some θ_0, θ_1
- Keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$
until we hopefully end up at a minimum





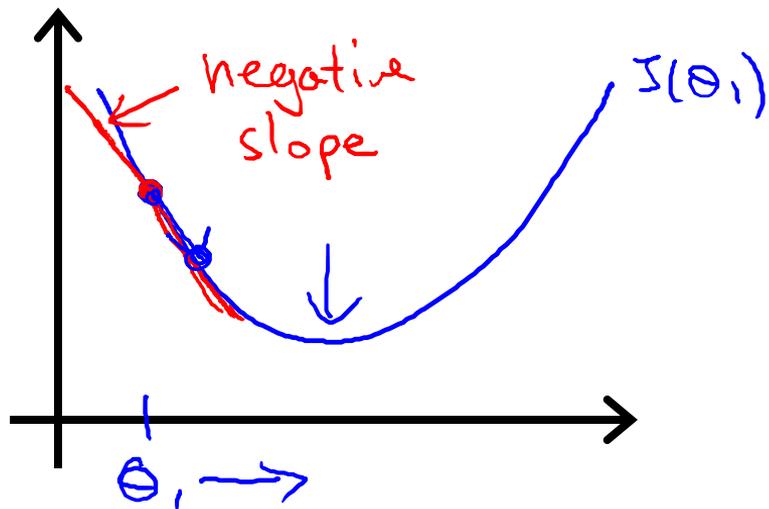


$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

$\frac{\partial}{\partial \theta_1} J(\theta_1) \leftarrow$

≥ 0

$$\theta_1 := \theta_1 - \alpha \cdot (\text{positive number})$$



$$\frac{\partial}{\partial \theta_1} J(\theta_1)$$

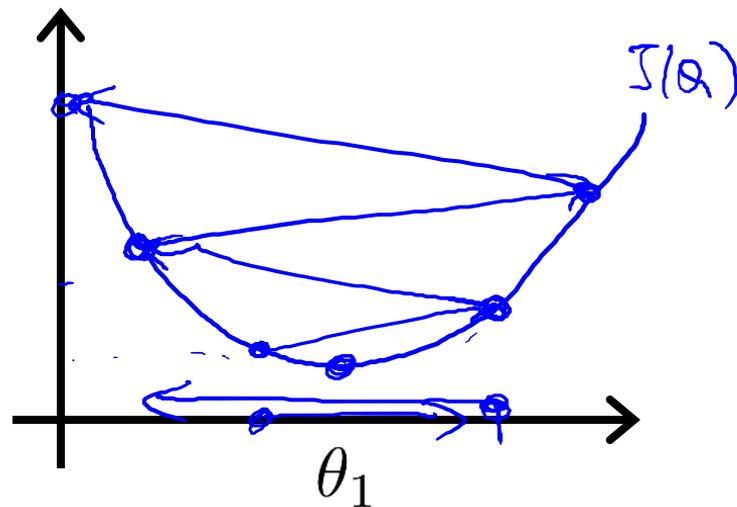
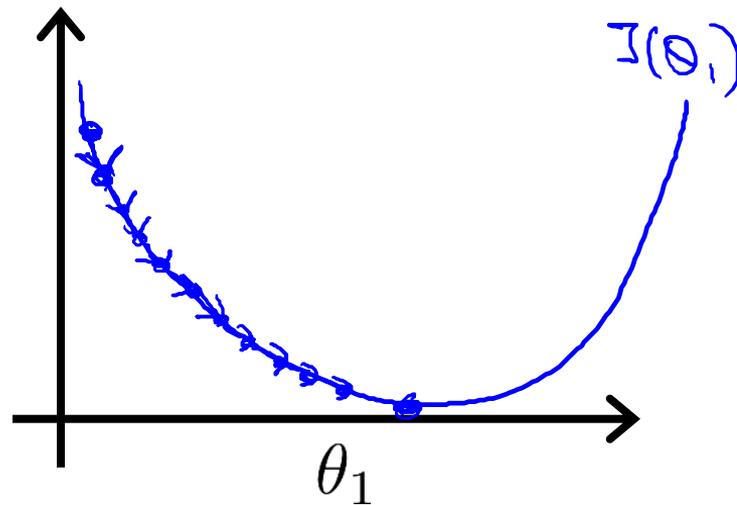
≤ 0

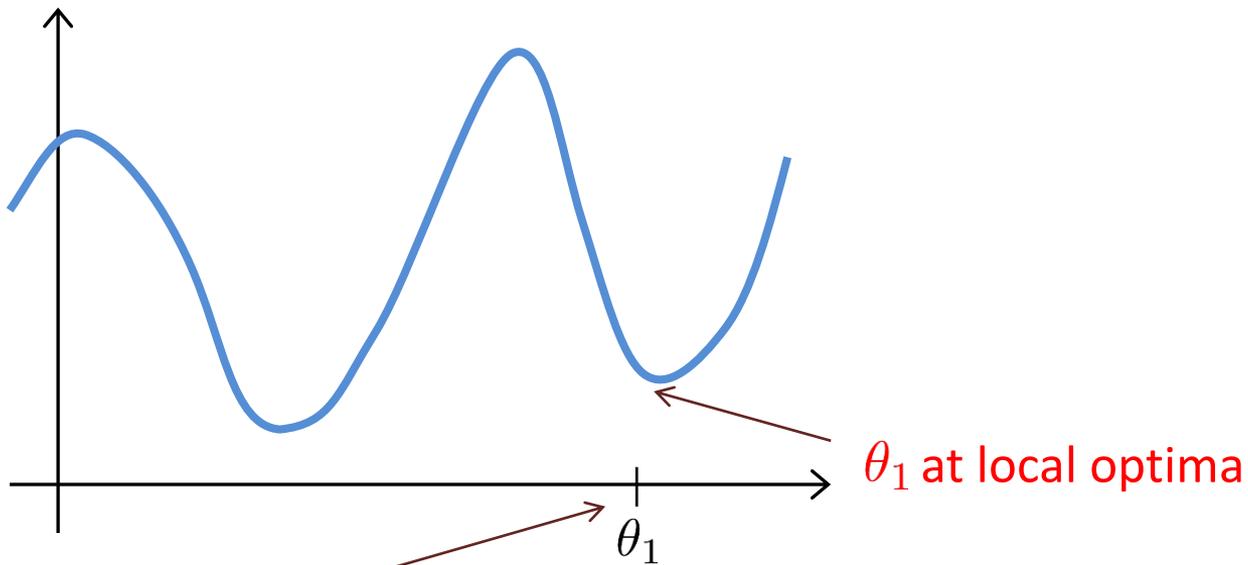
$$\theta_1 := \theta_1 - \alpha (\text{negative number})$$

$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If α is too small, gradient descent can be slow.

If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.





Current value of θ_1

$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

Gradient descent algorithm

repeat until convergence {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad (\text{simultaneously update } j = 0 \text{ and } j = 1)$$

}

Gradient descent algorithm

repeat until convergence {
 $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ (for $j = 0$ and $j = 1$)
}

Correct: Simultaneous update

$$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_0 := \text{temp0}$$

$$\theta_1 := \text{temp1}$$

Incorrect:

$$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$\theta_0 := \text{temp0}$$

$$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_1 := \text{temp1}$$

Gradient descent algorithm

repeat until convergence {
 $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$
 (for $j = 1$ and $j = 0$)
}

Linear Regression Model

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$\begin{aligned}\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) &= \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^m (\underbrace{h_{\theta}(x^{(i)}) - y^{(i)}}_{\text{green line}})^2 \\ &= \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^m (\underbrace{\theta_0 + \theta_1 x^{(i)} - y^{(i)}}_{\text{red line}})^2\end{aligned}$$

$$j = 0 : \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})$$

$$j = 1 : \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

Gradient descent algorithm

repeat until convergence {

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

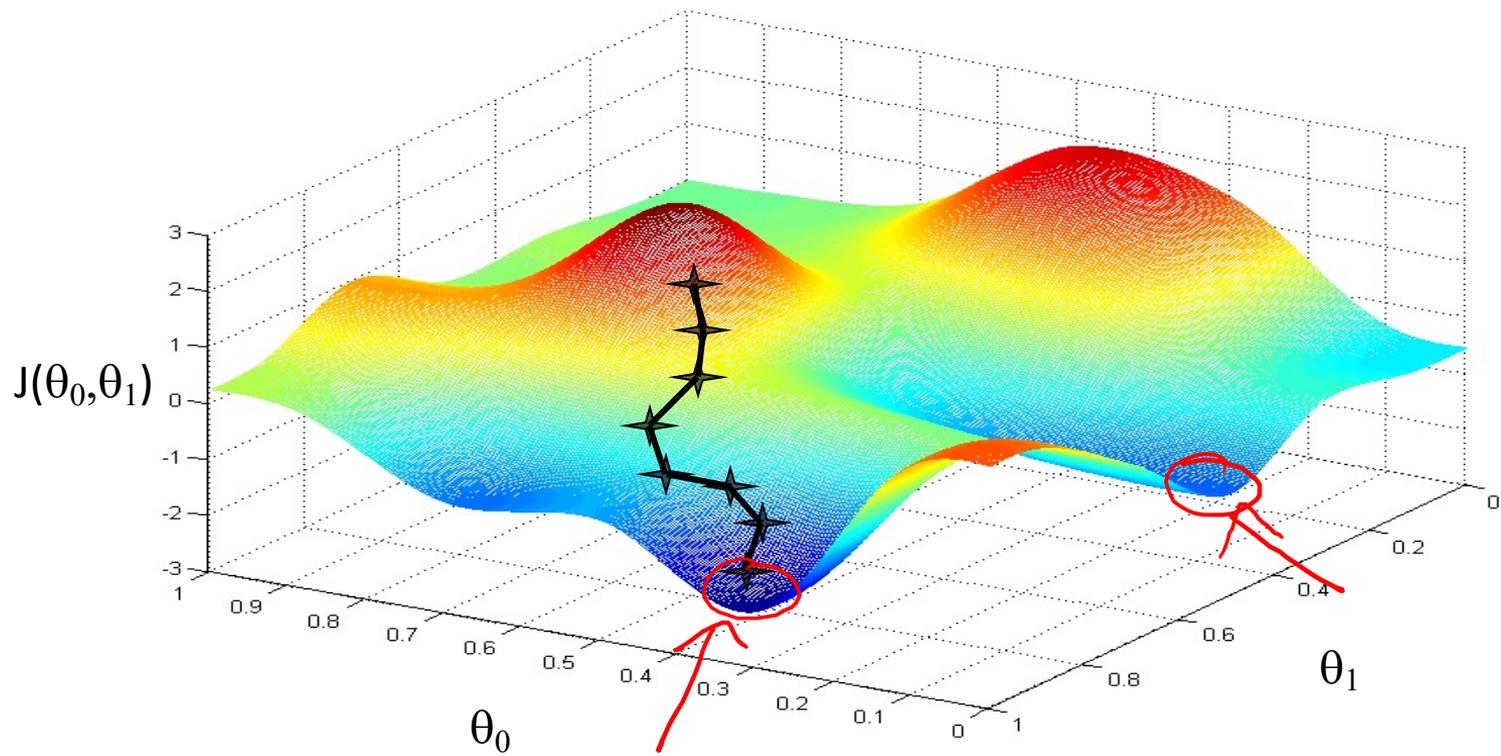
$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

}

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

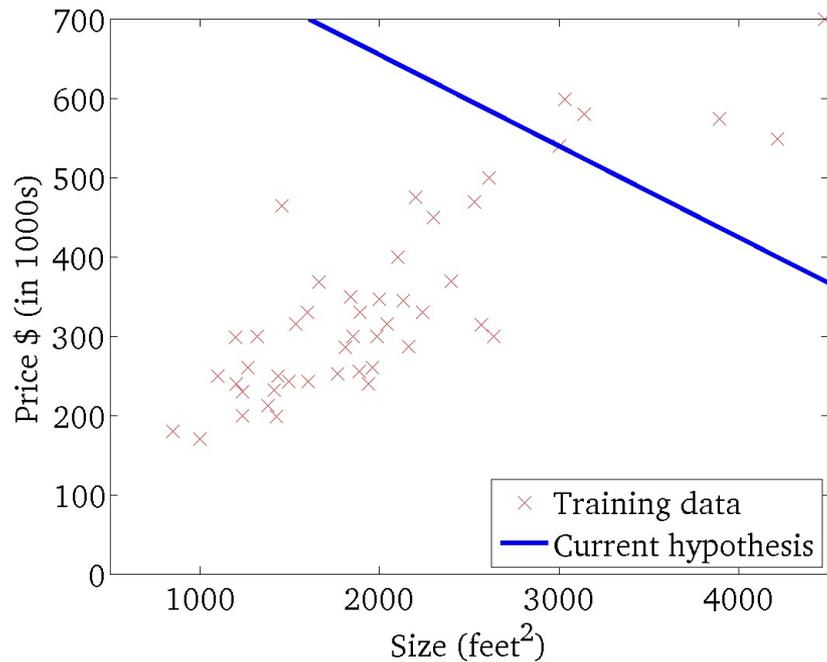
update
 θ_0 and θ_1
simultaneously

$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$



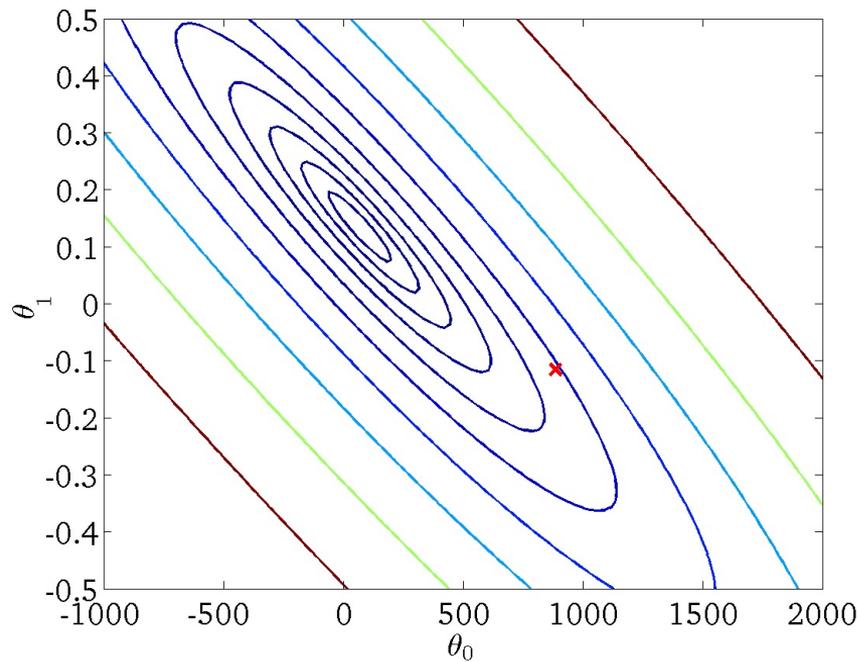
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



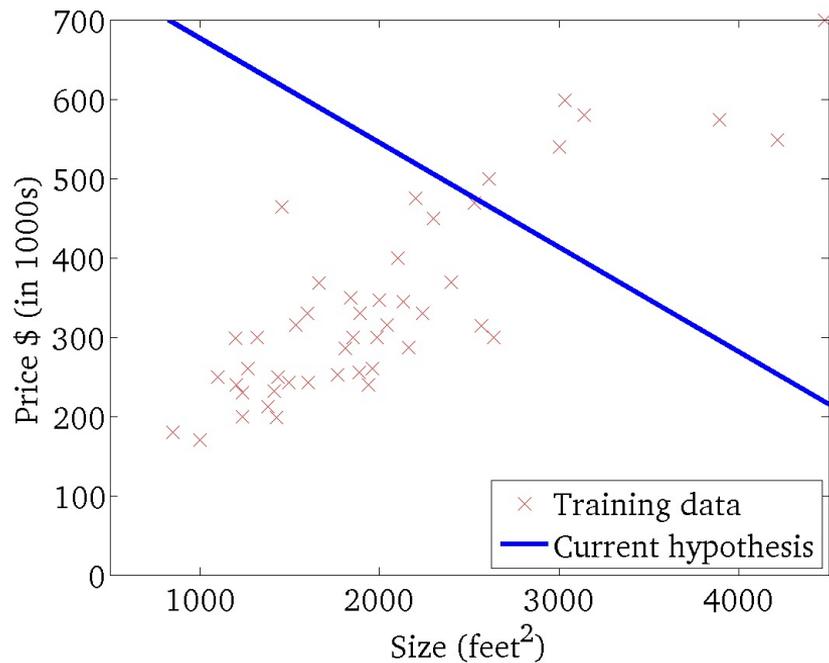
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



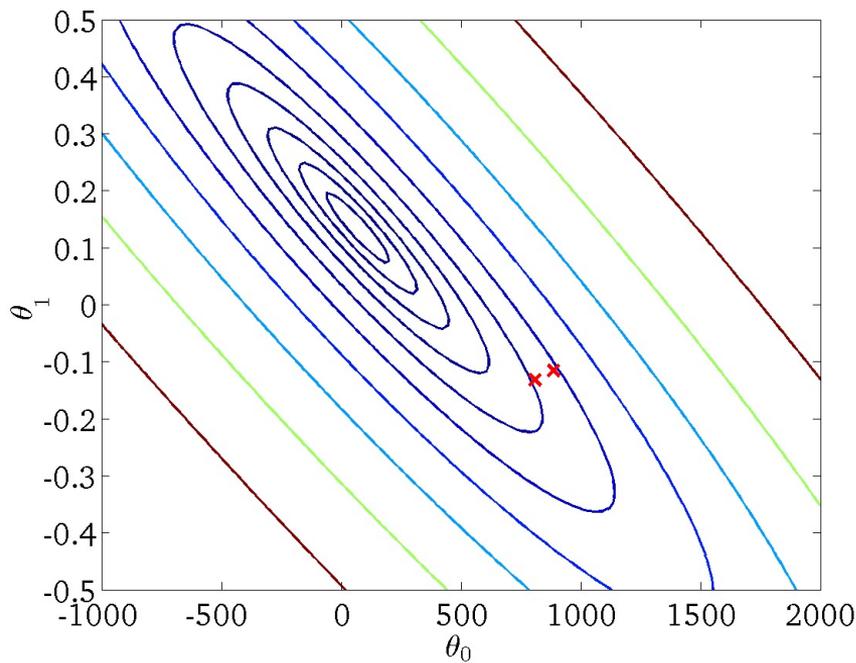
$$h_{\theta}(x)$$

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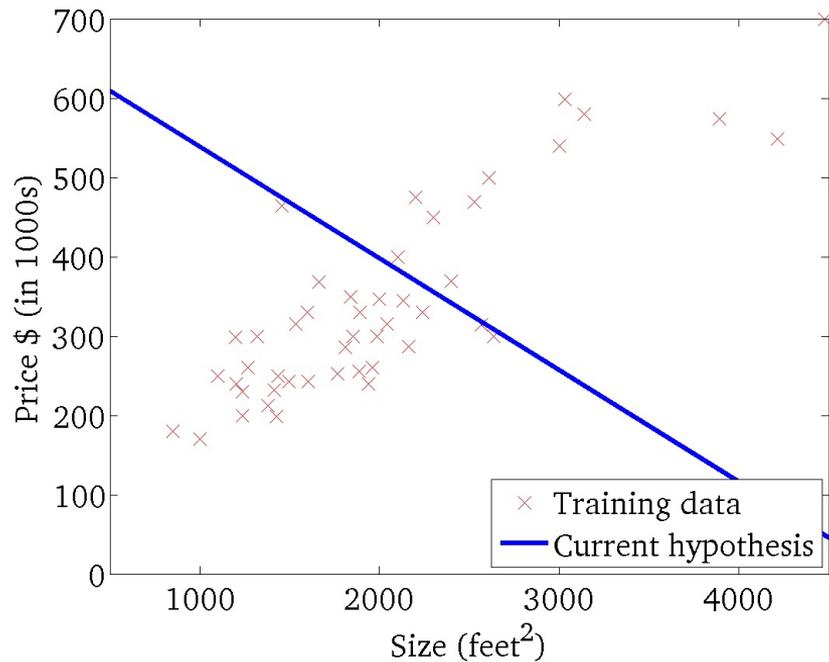
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



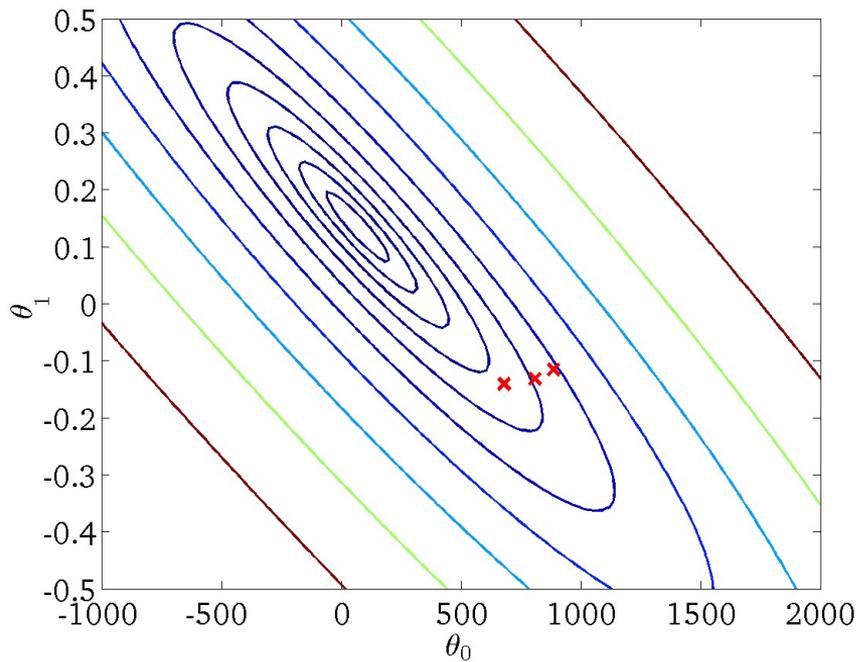
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



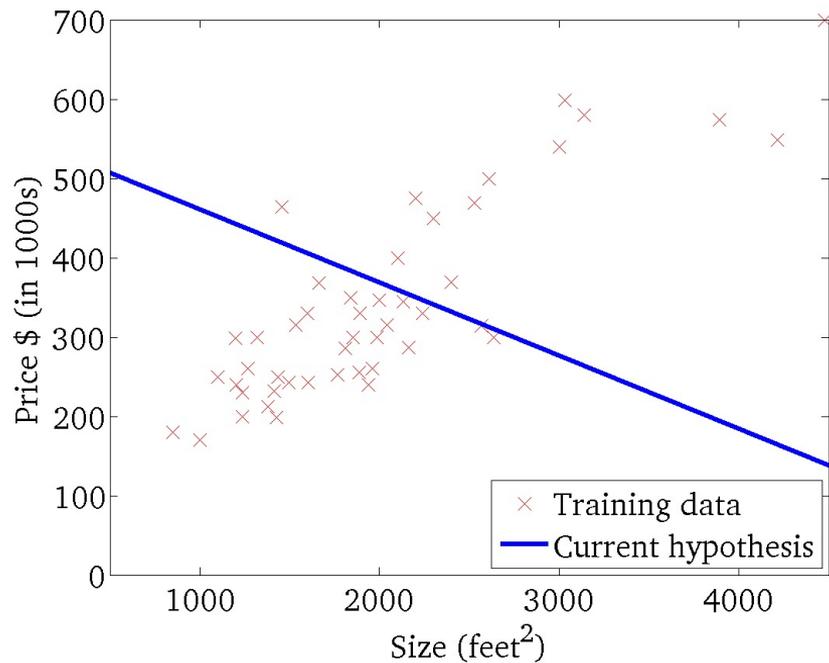
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



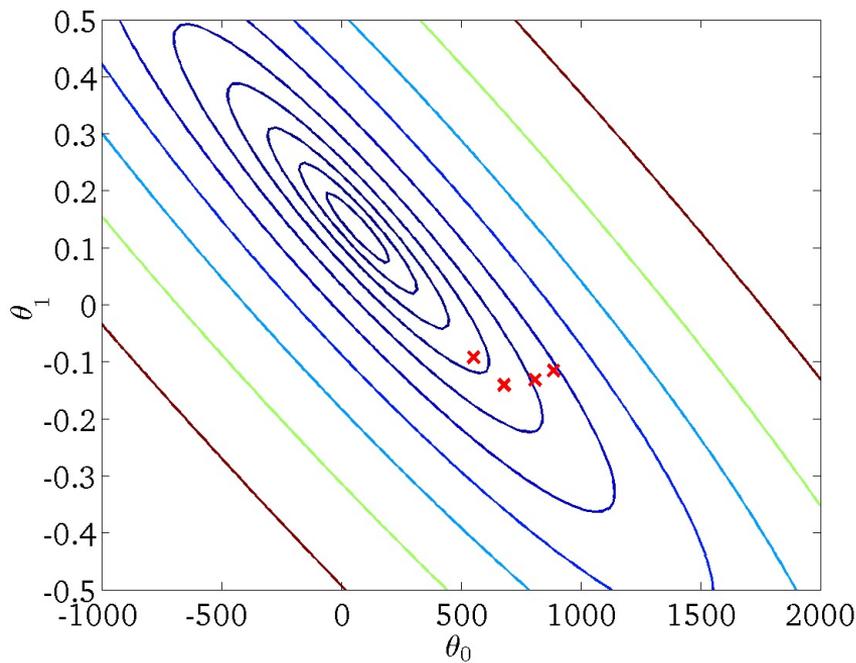
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



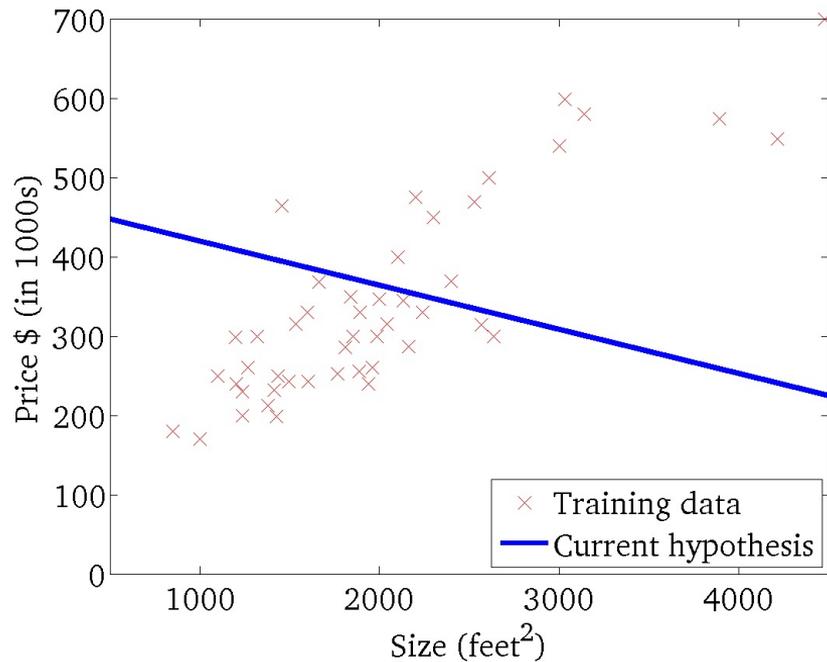
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



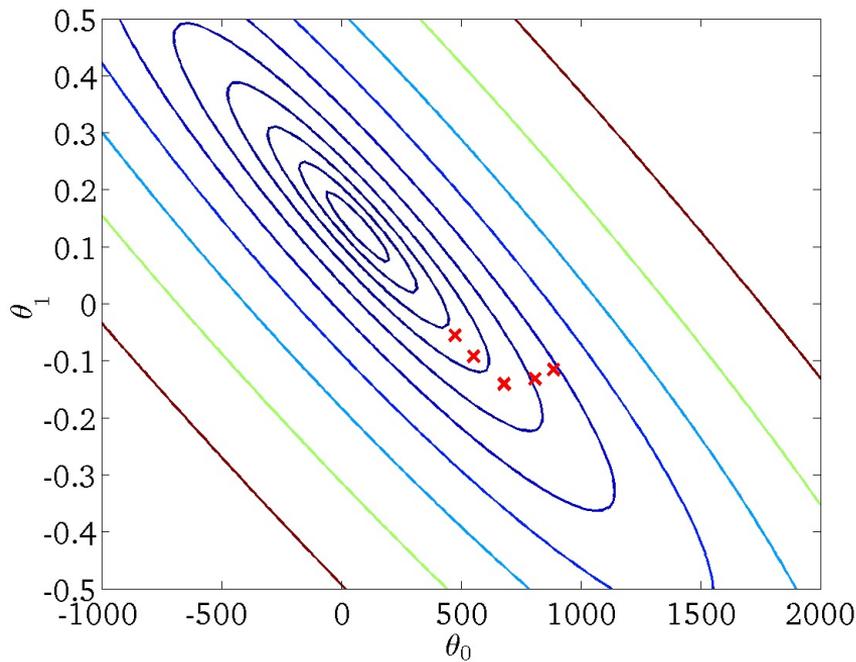
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



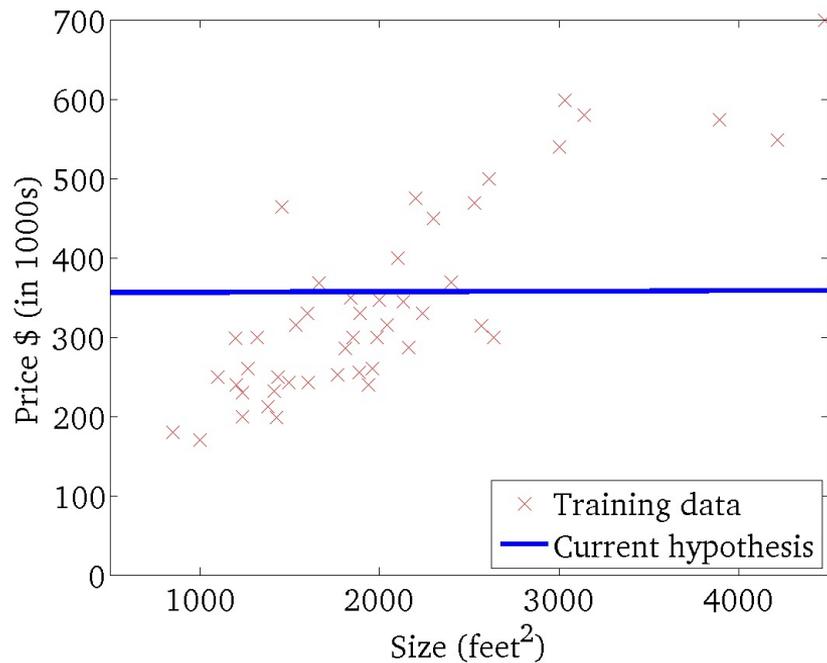
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



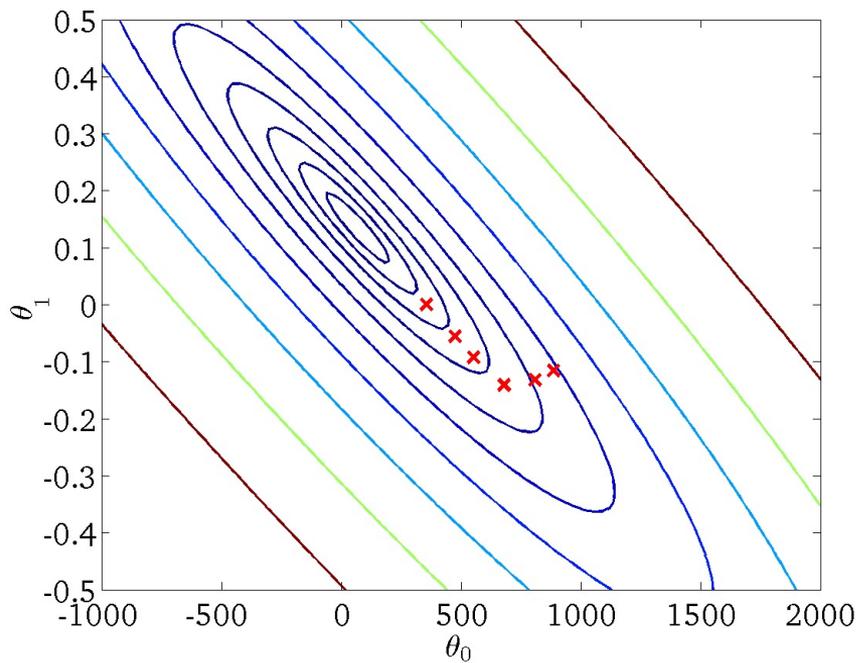
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



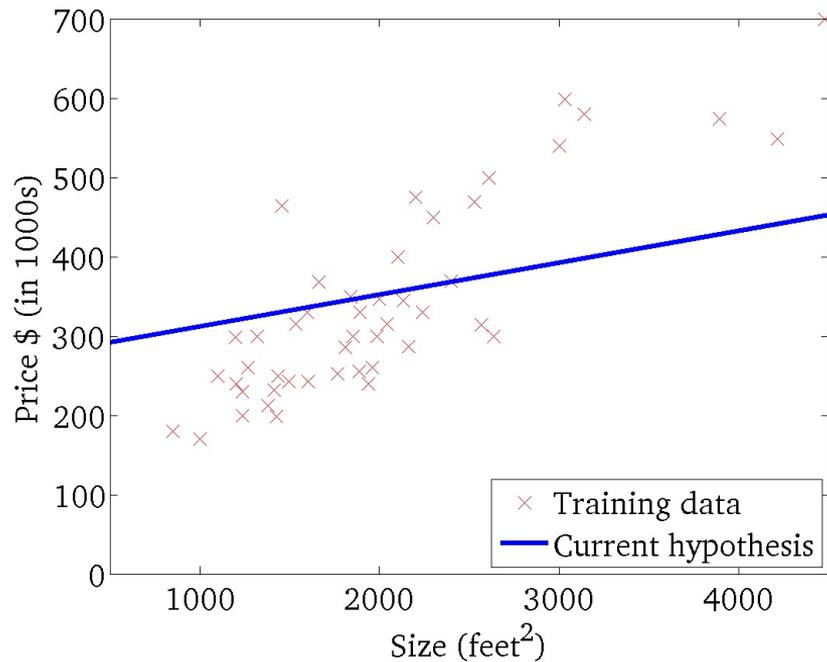
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



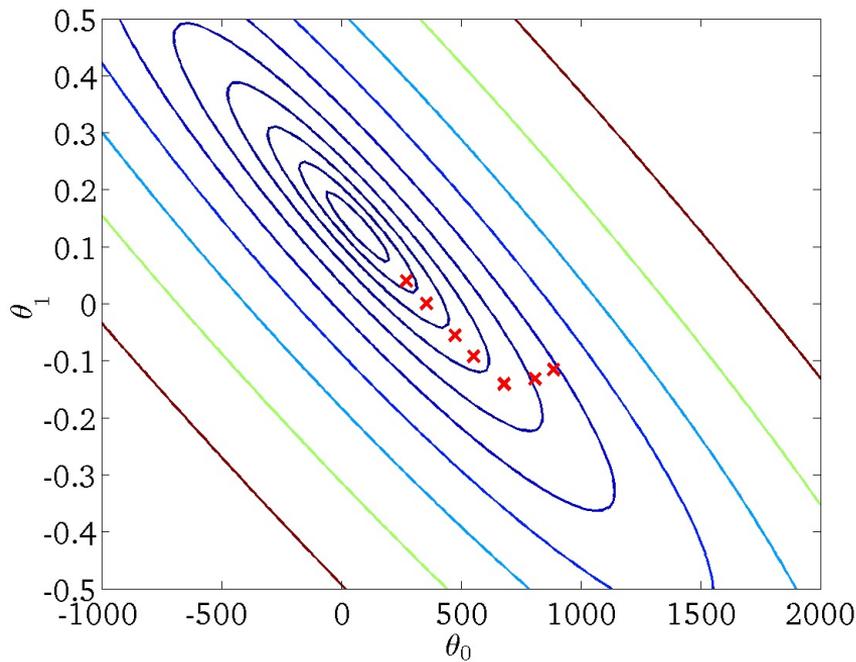
$$h_{\theta}(x)$$

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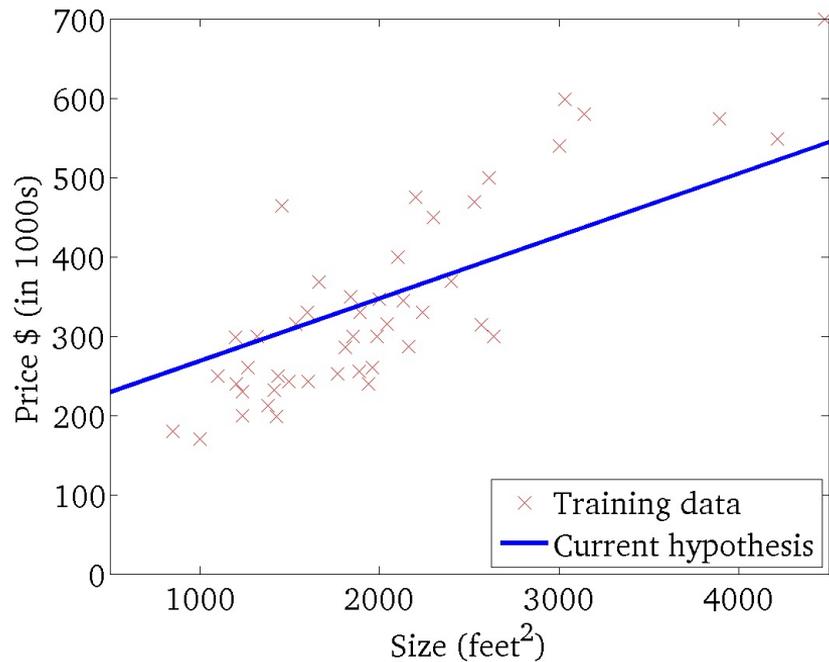
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



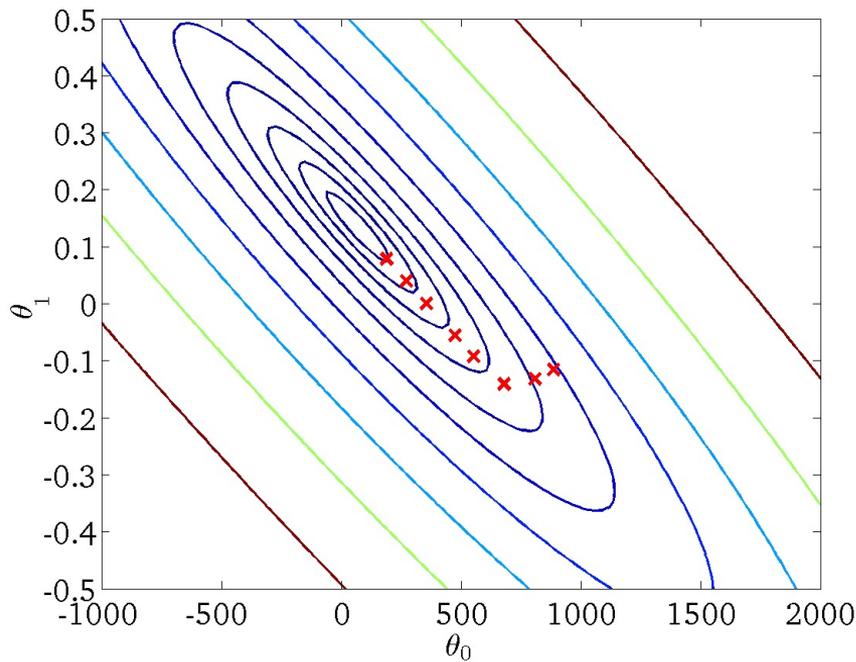
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



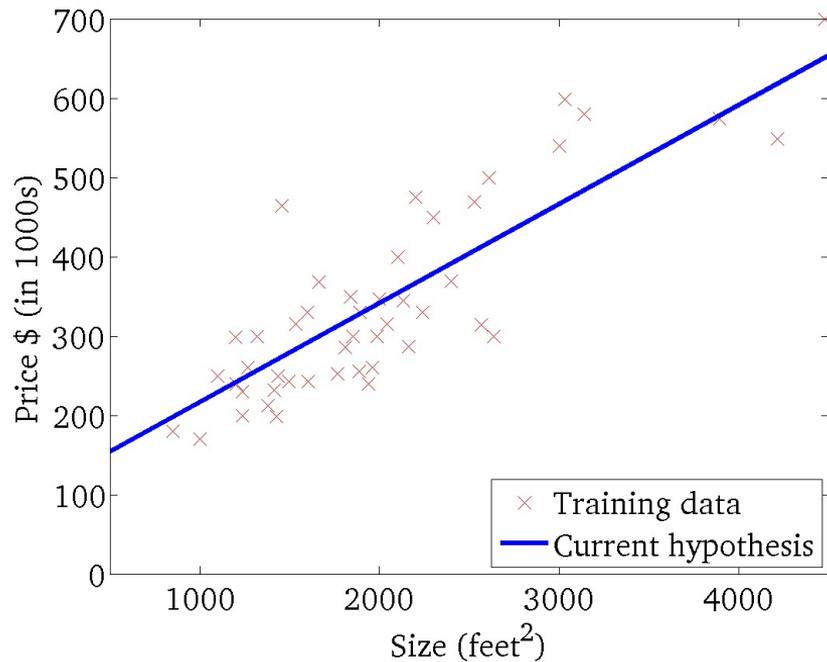
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



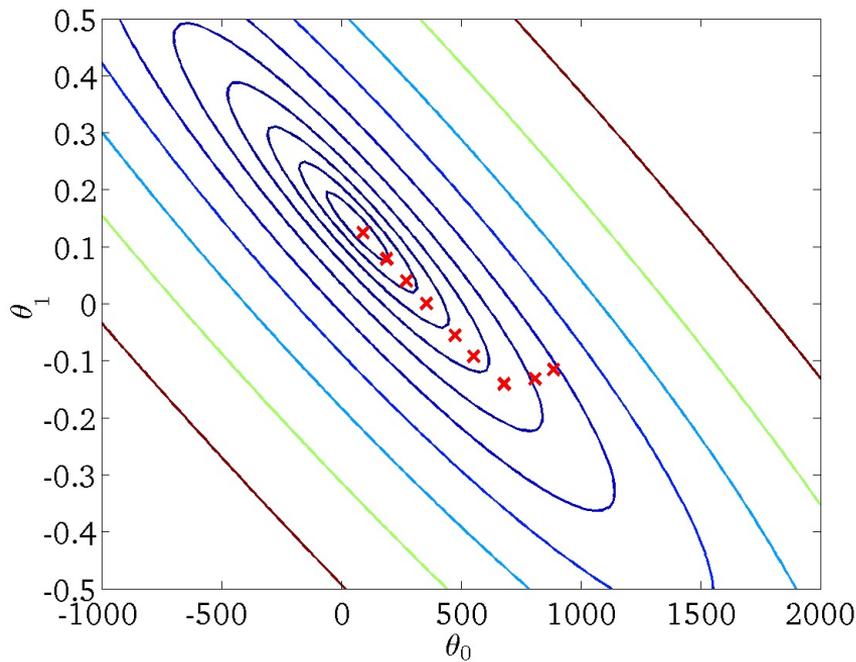
$$h_{\theta}(x)$$

(for fixed θ_0, θ_1 , this is a function of x)



$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



Linear regression with gradient descent

$$h_{\theta}(x) = \sum_{j=0}^n \theta_j x_j$$

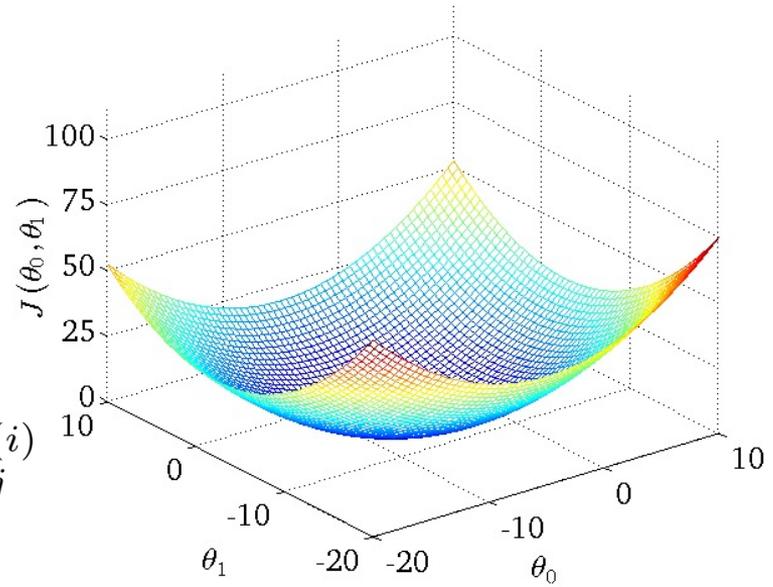
$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

Repeat {

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

(for every $j = 0, \dots, n$)

}



Linear regression with Batch Gradient Descent

$$h_{\theta}(x) = \sum_{j=0}^n \theta_j x_j$$

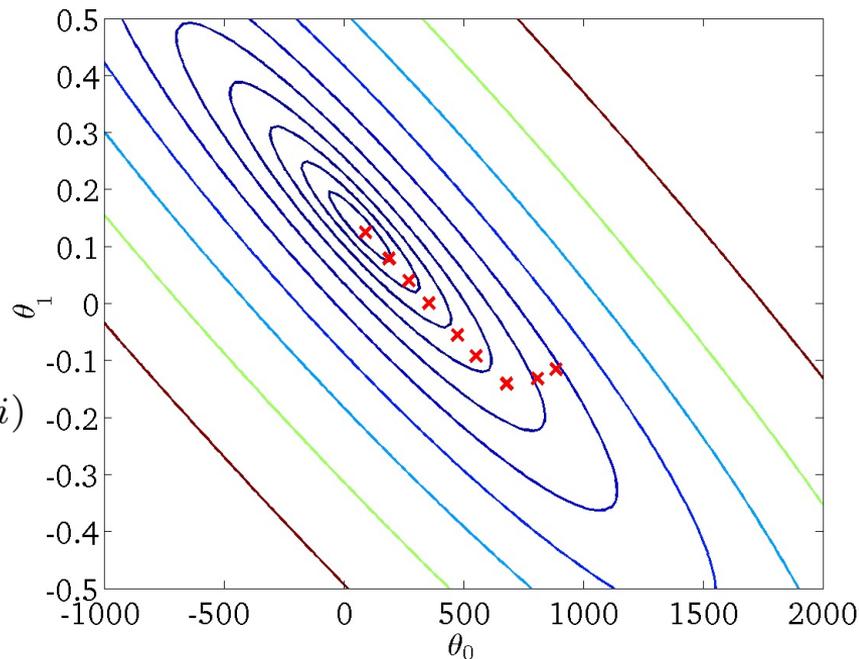
$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

Repeat {

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

(for every $j = 0, \dots, n$)

}



Stochastic gradient descent

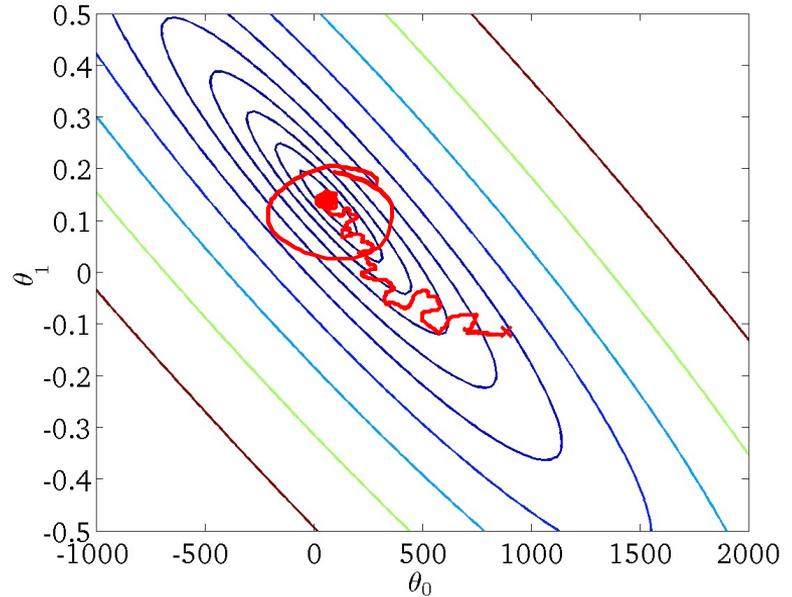
1. Randomly shuffle dataset.

2. Repeat {

$$\text{for } i := 1, \dots, m \quad \left\{ \begin{array}{l} \theta_j := \theta_j - \alpha (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} \\ \quad \text{(for } j = 0, \dots, n) \end{array} \right.$$

}

}



Learning rate α is typically held constant. Can slowly decrease α over time if we want θ to converge. (E.g. $\alpha = \frac{\text{const1}}{\text{iterationNumber} + \text{const2}}$) $\alpha \rightarrow 0$

Mini-Batch Gradient Descent

Say $b = 10, m = 1000$.

Repeat {

for $i = 1, 11, 21, 31, \dots, 991$ {

$$\theta_j := \theta_j - \alpha \frac{1}{10} \sum_{k=i}^{i+9} (h_{\theta}(x^{(k)}) - y^{(k)}) x_j^{(k)}$$

(for every $j = 0, \dots, n$)

}

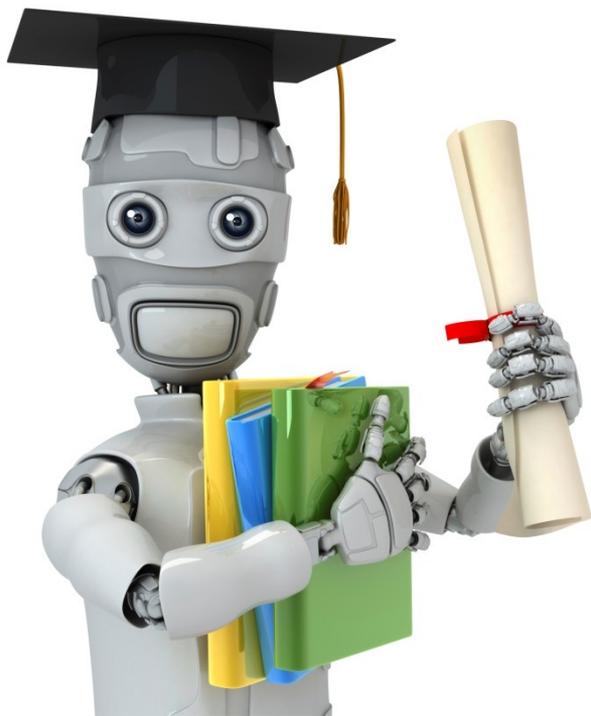
}

Mini-batch gradient descent

Batch gradient descent: Use all m examples in each iteration

Stochastic gradient descent: Use 1 example in each iteration

Mini-batch gradient descent: Use b examples in each iteration

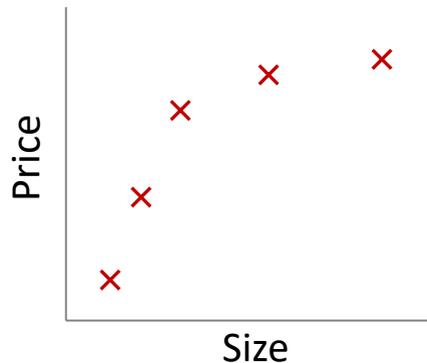


Machine Learning

Advice for applying
machine learning

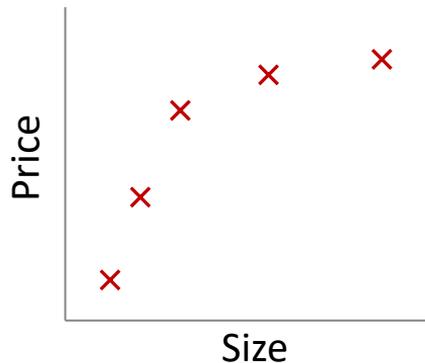
Diagnosing bias vs.
variance

Bias/variance



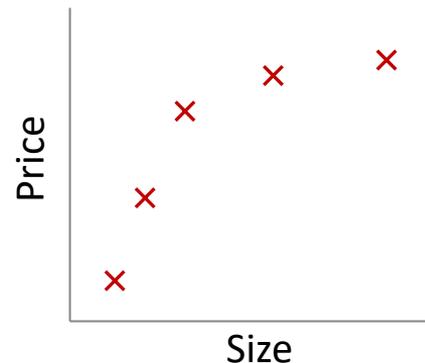
$$\theta_0 + \theta_1 x$$

High bias
(underfit)



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

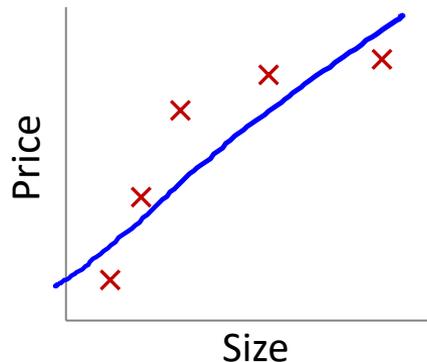
“Just right”



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

High variance
(overfit)

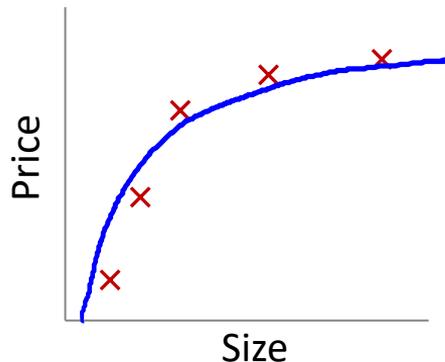
Bias/variance



$$\theta_0 + \theta_1 x$$

High bias
(underfit)

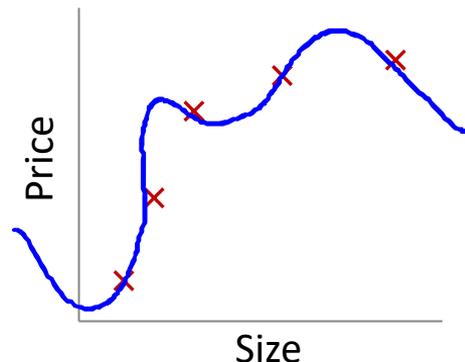
$$d=1$$



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

“Just right”

$$d=2$$



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

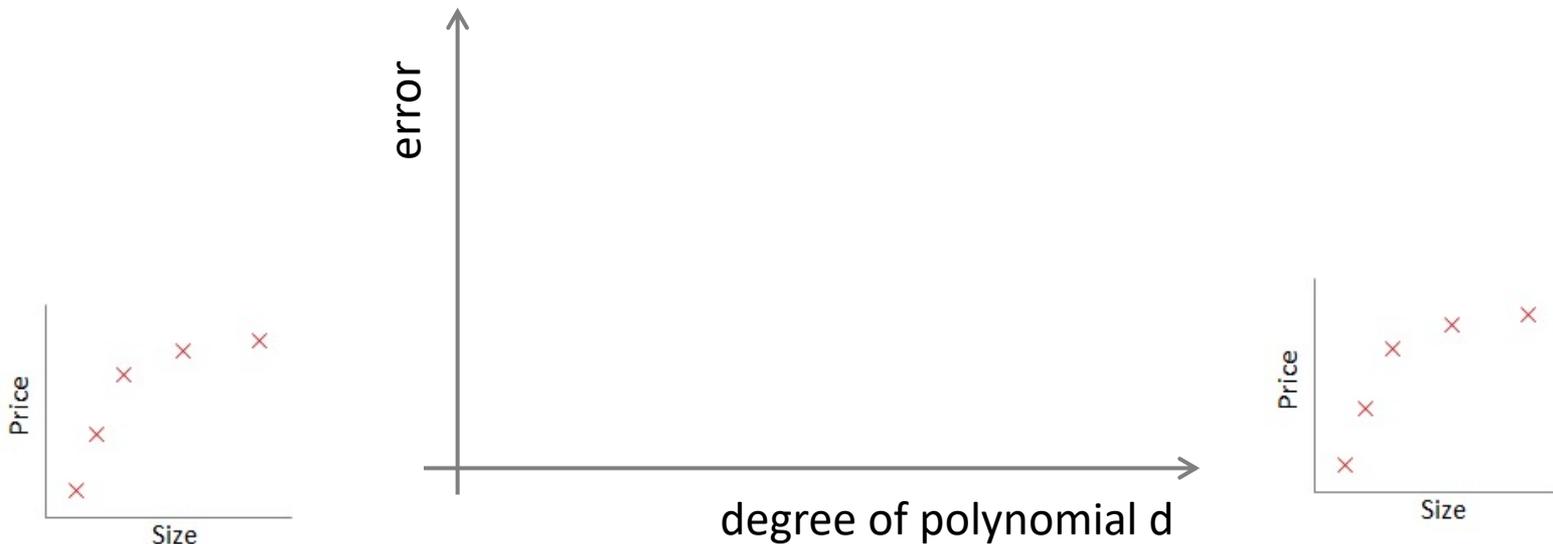
High variance
(overfit)

$$d=4$$

Bias/variance

Training error: $J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$

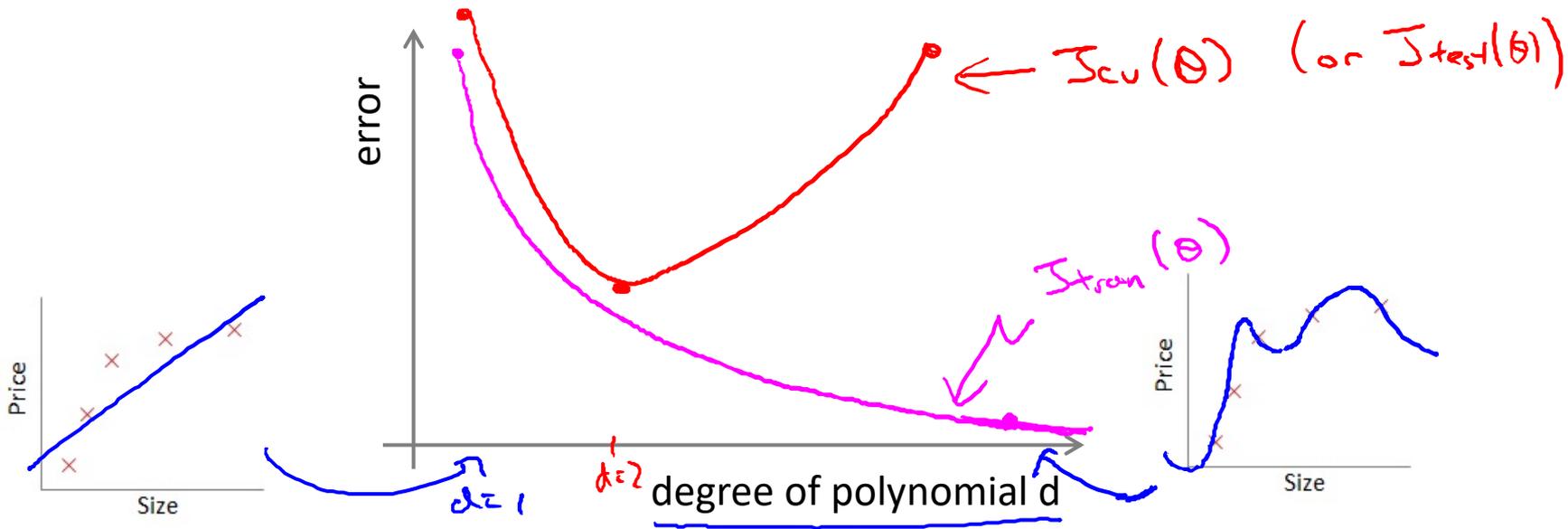
Cross validation error: $J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$



Bias/variance

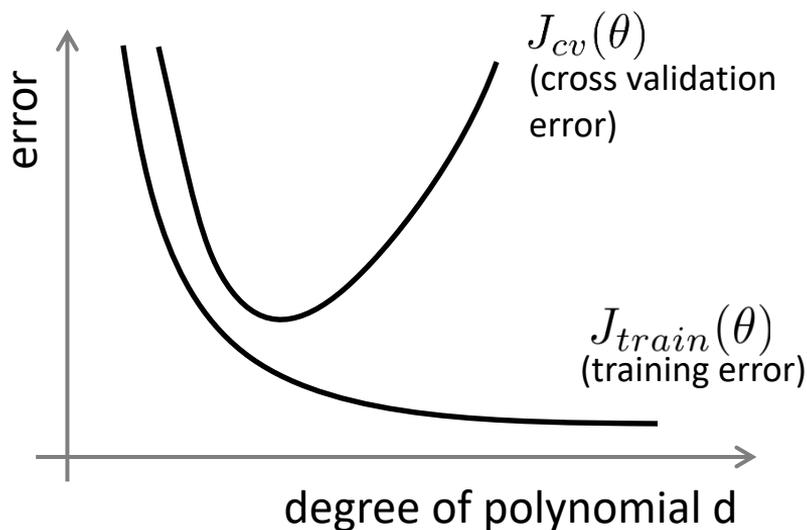
Training error: $J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$

Cross validation error: $J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$ (or $J_{test}(\theta)$)



Diagnosing bias vs. variance

Suppose your learning algorithm is performing less well than you were hoping. ($J_{cv}(\theta)$ or $J_{test}(\theta)$ is high.) Is it a bias problem or a variance problem?

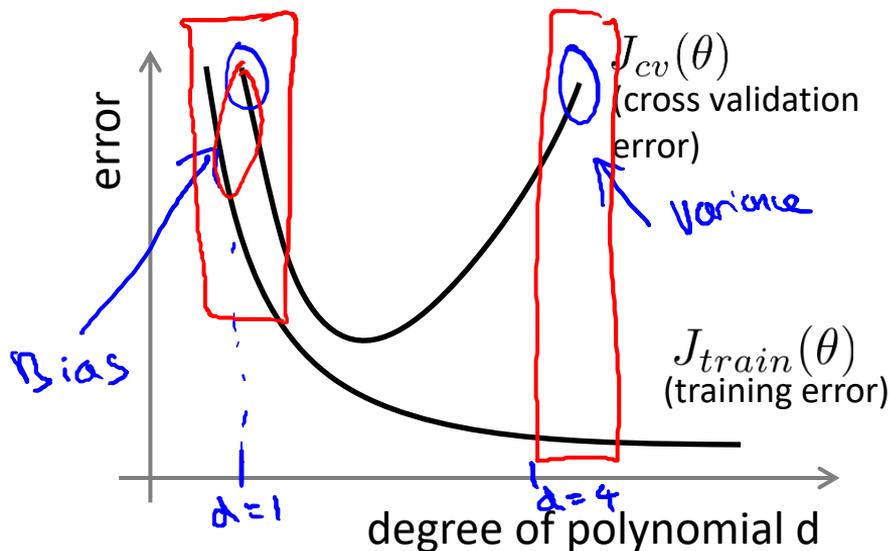


Bias (underfit):

Variance (overfit):

Diagnosing bias vs. variance

Suppose your learning algorithm is performing less well than you were hoping. ($J_{cv}(\theta)$ or $J_{test}(\theta)$ is high.) Is it a bias problem or a variance problem?



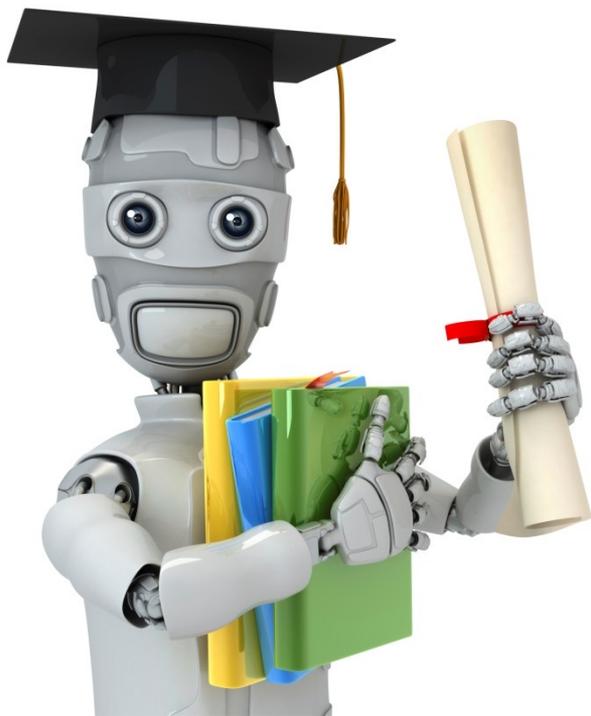
Bias (underfit):

$\rightarrow J_{train}(\theta)$ will be high
 $J_{cv}(\theta) \approx J_{train}(\theta)$

Variance (overfit):

$\rightarrow J_{train}(\theta)$ will be low
 $J_{cv}(\theta) \gg J_{train}(\theta)$

\Rightarrow



Machine Learning

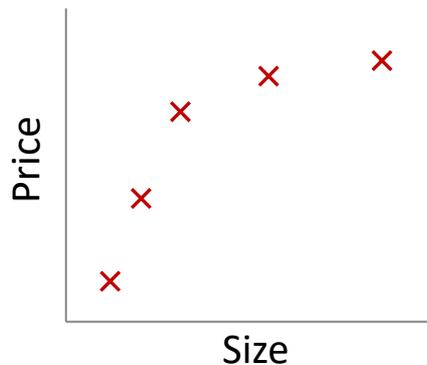
Advice for applying
machine learning

Regularization and
bias/variance

Linear regression with regularization

Model: $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

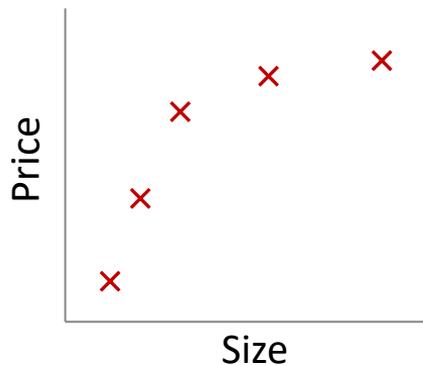


Large λ

High bias (underfit)

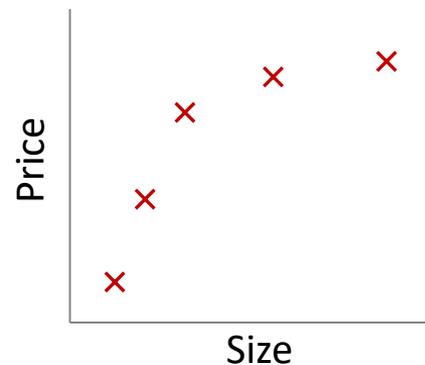
$\lambda = 10000$. $\theta_1 \approx 0, \theta_2 \approx 0, \dots$

$h_{\theta}(x) \approx \theta_0$



Intermediate λ

“Just right”



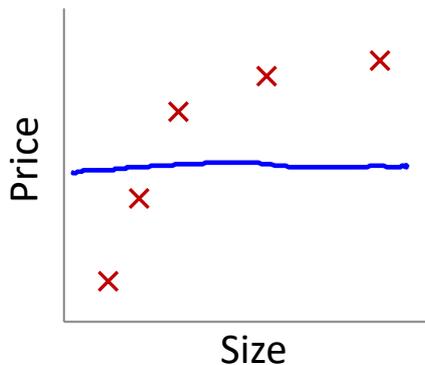
Small λ

High variance (overfit)

Linear regression with regularization

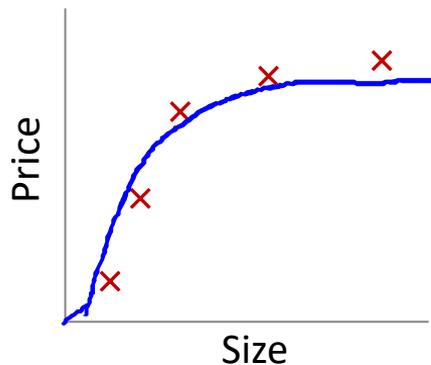
Model: $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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



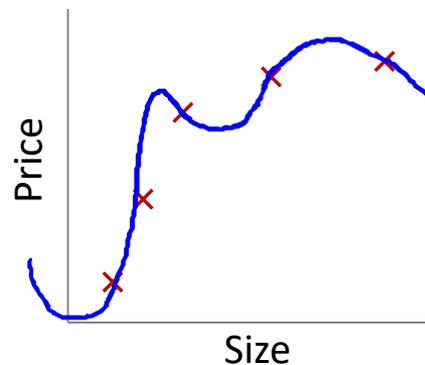
Large λ ←

↪ High bias (underfit)



Intermediate λ ←

“Just right”



↪ Small λ

High variance (overfit)

↪ $\lambda = 0$

↪ $\lambda = 10000$. $\theta_1 \approx 0, \theta_2 \approx 0, \dots$
 $h_{\theta}(x) \approx \theta_0$

Choosing the regularization parameter λ

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

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

$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

$$J_{test}(\theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_{\theta}(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

Choosing the regularization parameter λ

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4 \quad \leftarrow$$

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

$$\rightarrow J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 \quad J(\theta)$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

$$J_{test}(\theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_{\theta}(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

J_{train}
 J_{cv}
 J_{test}

Choosing the regularization parameter λ

Model: $h_{\theta}(x) = \theta_0 + \theta_1x + \theta_2x^2 + \theta_3x^3 + \theta_4x^4$

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

$$\lambda = 0$$

$$\lambda = 0.01$$

$$\lambda = 0.02$$

$$\lambda = 0.04$$

$$\lambda = 0.08$$

⋮

$$\lambda = 10$$

Pick (say) $\theta^{(5)}$. Test error:

Choosing the regularization parameter λ

Model: $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

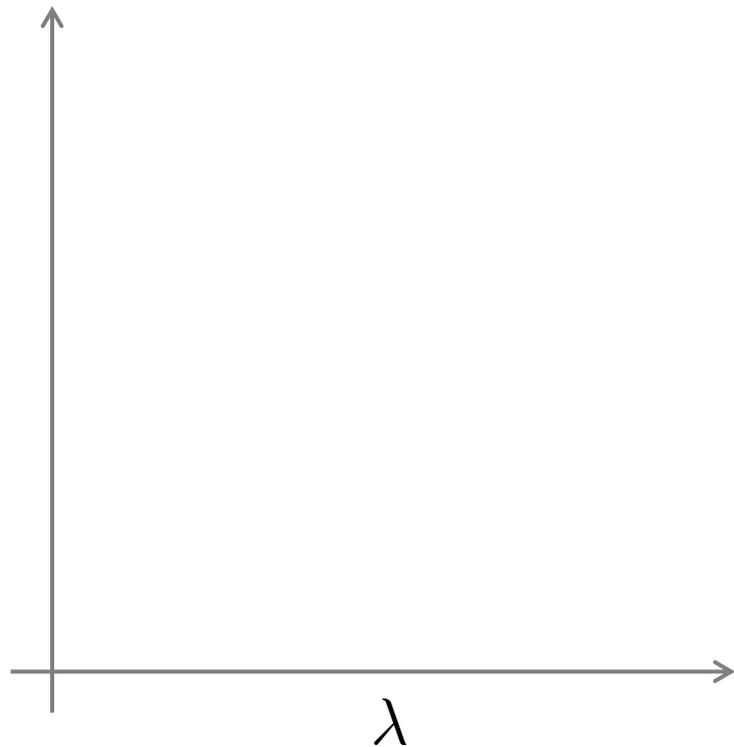
1. Try $\lambda = 0$ \leftarrow $\rightarrow \min_{\theta} J(\theta) \rightarrow \theta^{(1)} \rightarrow J_{cv}(\theta^{(1)})$
 2. Try $\lambda = 0.01$ $\rightarrow \min_{\theta} J(\theta) \rightarrow \theta^{(2)} \rightarrow J_{cv}(\theta^{(2)})$
 3. Try $\lambda = 0.02$ $\rightarrow \theta^{(3)} \rightarrow J_{cv}(\theta^{(3)})$
 4. Try $\lambda = 0.04$
 5. Try $\lambda = 0.08$ $\rightarrow \theta^{(5)} \rightarrow J_{cv}(\theta^{(5)})$
 - \vdots
 12. Try $\lambda = 10$ $\rightarrow \theta^{(12)} \rightarrow J_{cv}(\theta^{(12)})$
 \uparrow 10.24
- Pick (say) $\theta^{(5)}$. Test error: $J_{test}(\theta^{(5)})$

Bias/variance as a function of the regularization parameter λ

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

$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

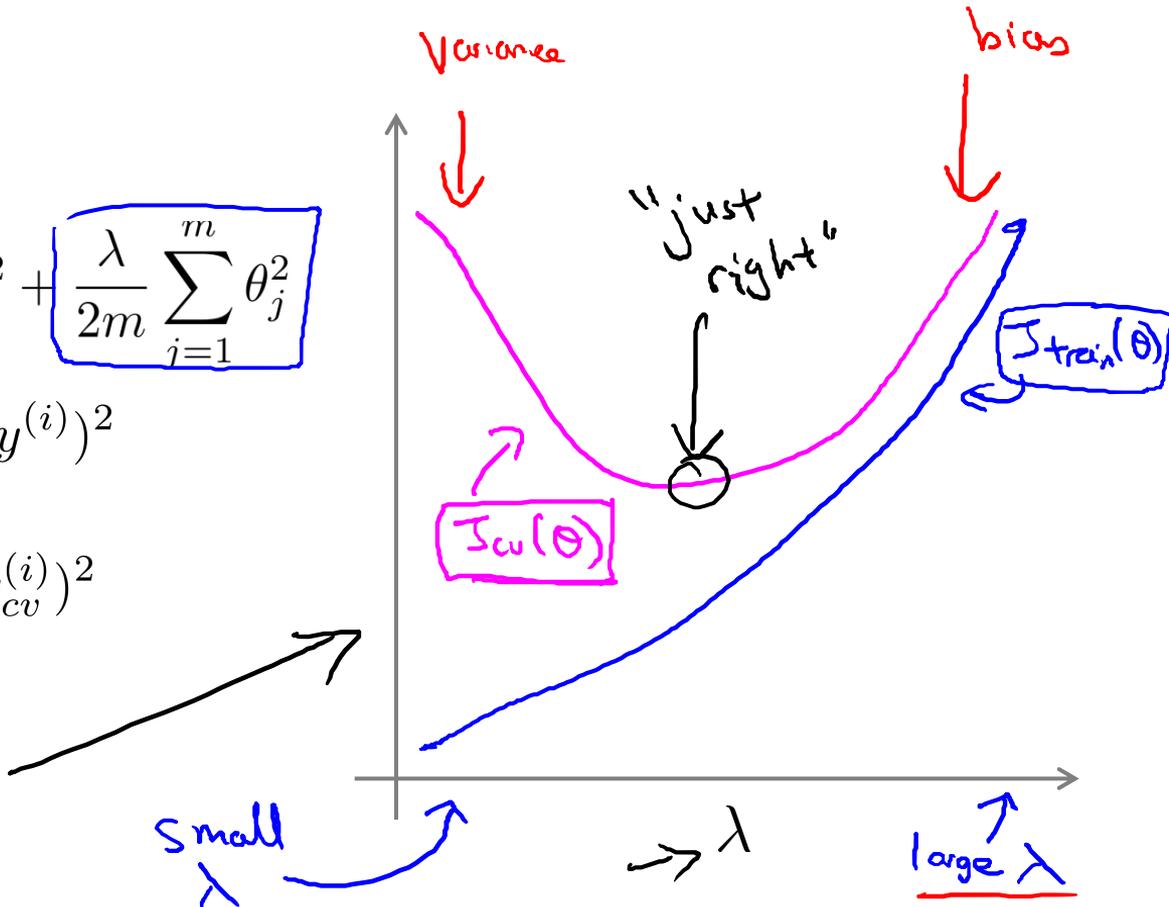


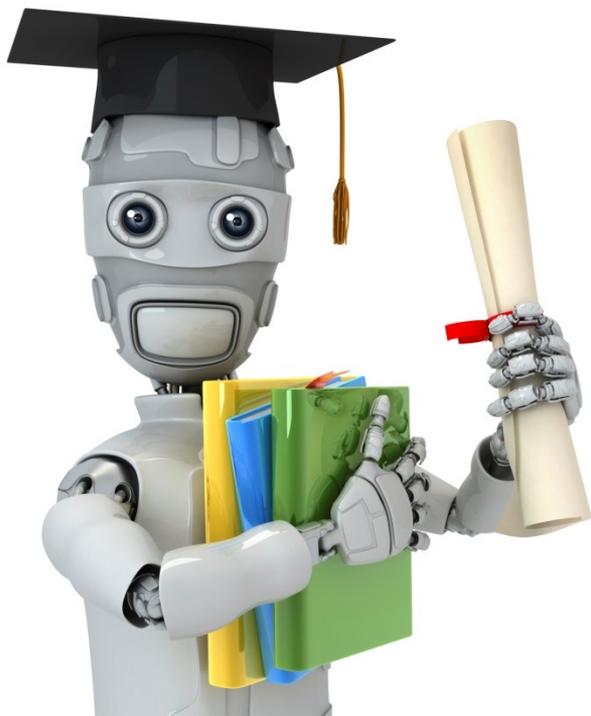
Bias/variance as a function of the regularization parameter λ

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

$$\rightarrow \underline{J_{train}(\theta)} = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$\rightarrow \underline{J_{cv}(\theta)} = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$





Machine Learning

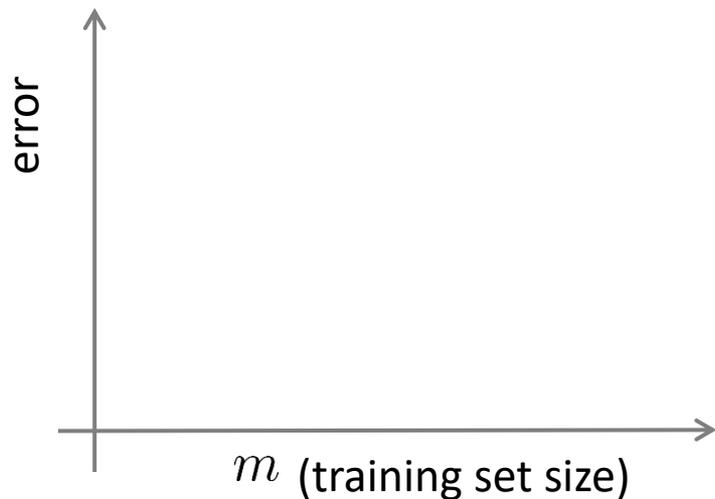
Advice for applying machine learning

Learning curves

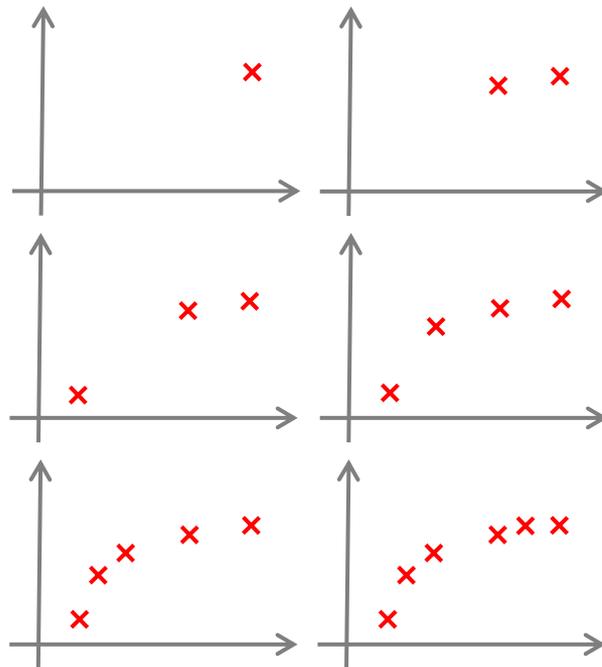
Learning curves

$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

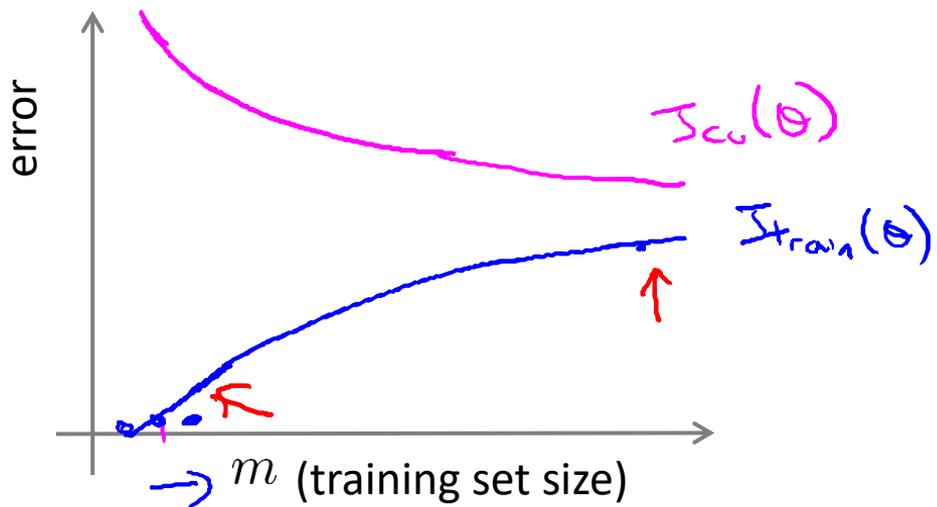
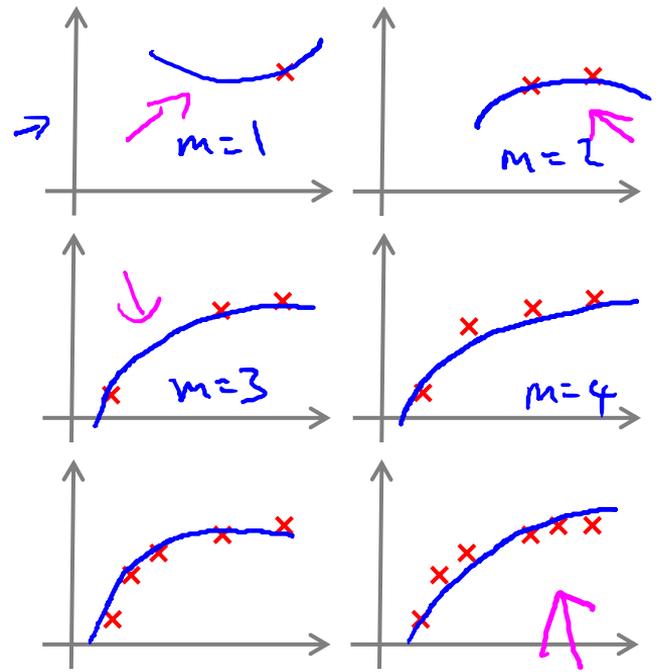


Learning curves

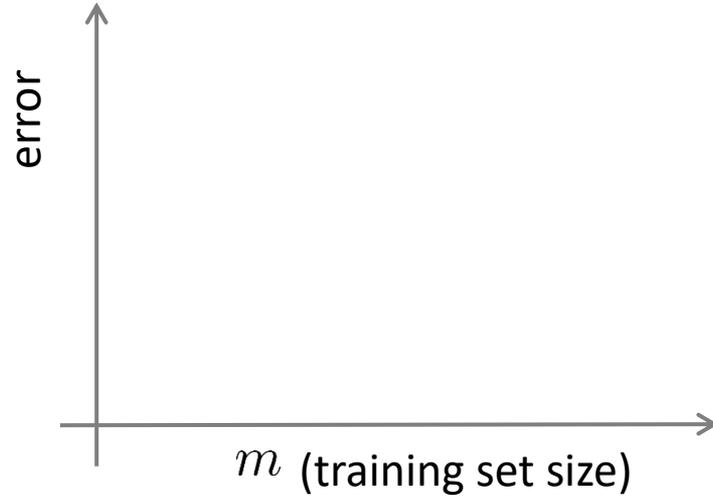
$$\rightarrow \underline{J_{train}(\theta)} = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 \leftarrow$$

$$\rightarrow J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

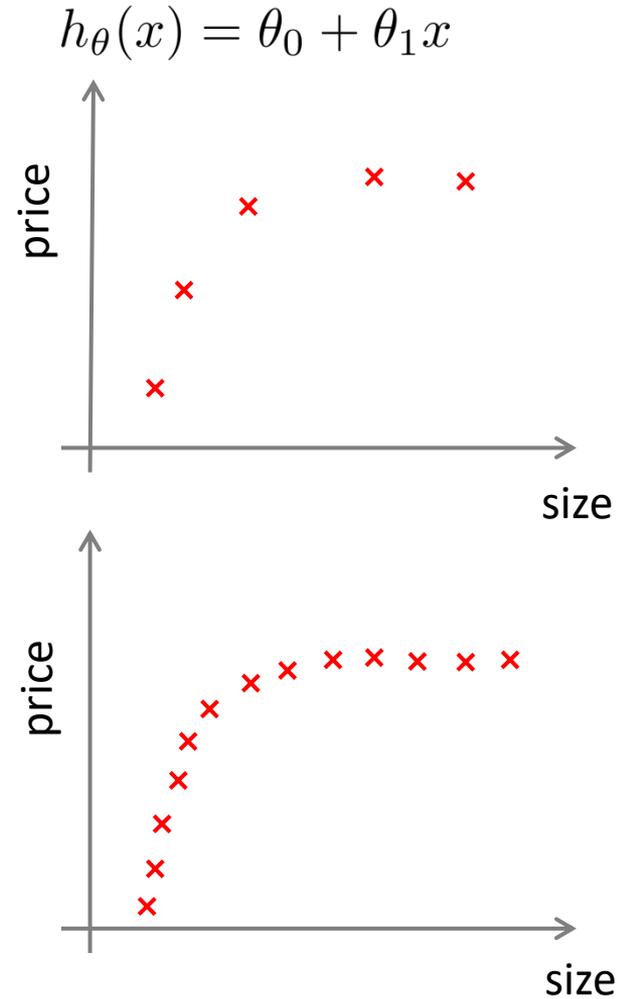
$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$



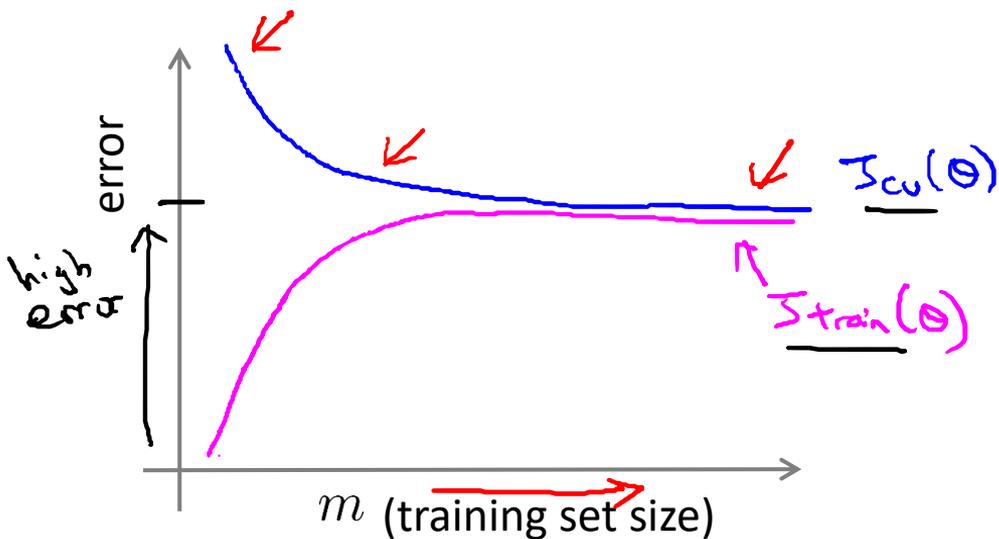
High bias



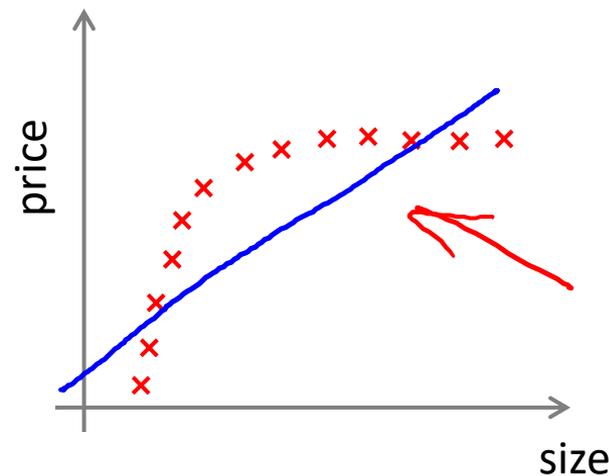
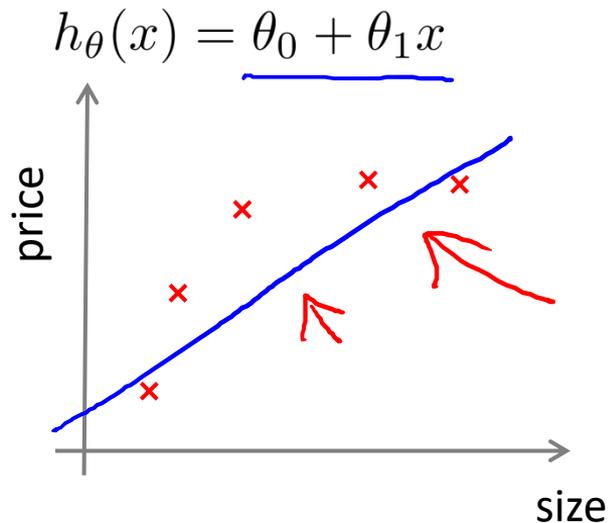
If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.



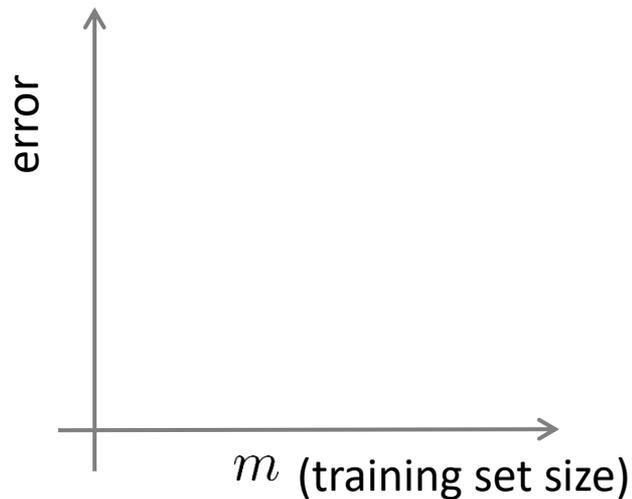
High bias



If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.



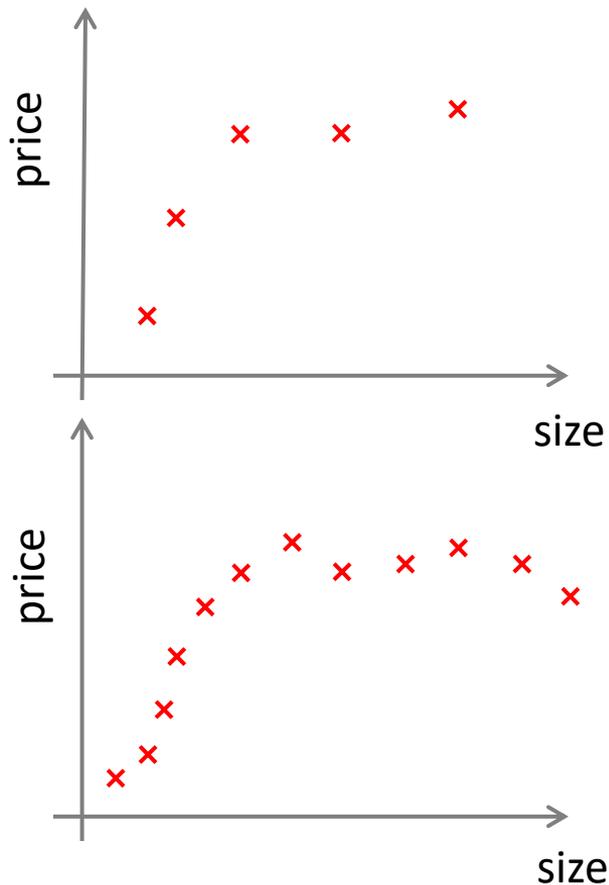
High variance



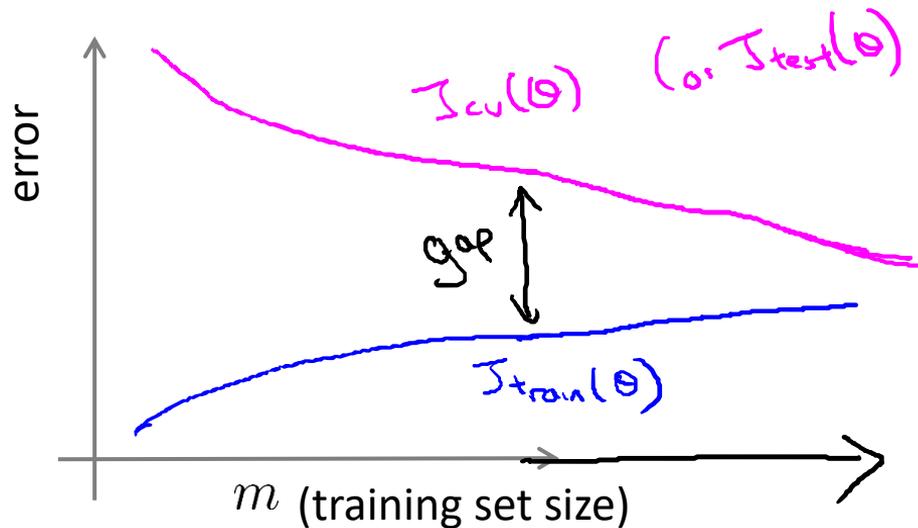
If a learning algorithm is suffering from high variance, getting more training data is likely to help.

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \dots + \theta_{100} x^{100}$$

(and small λ)



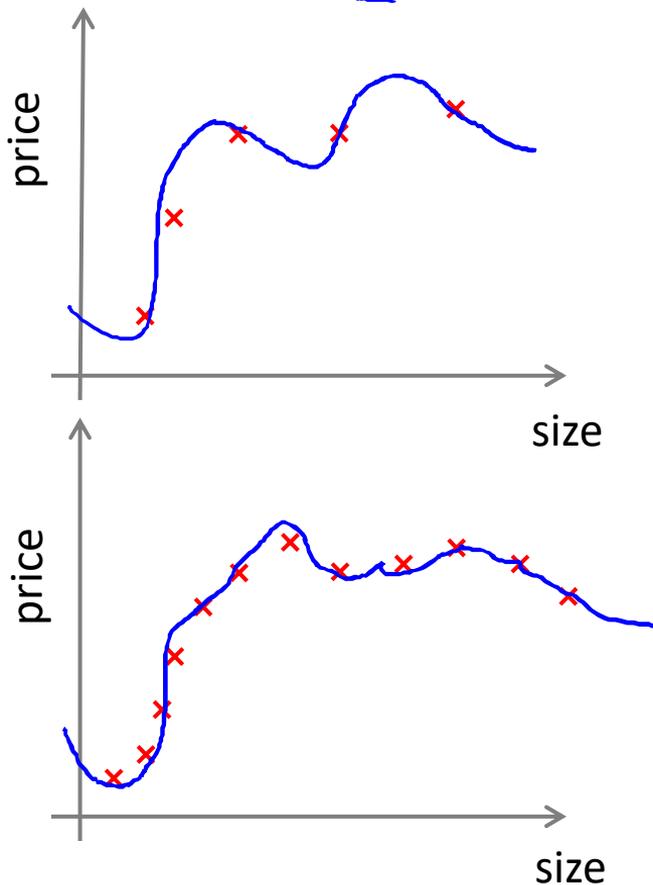
High variance

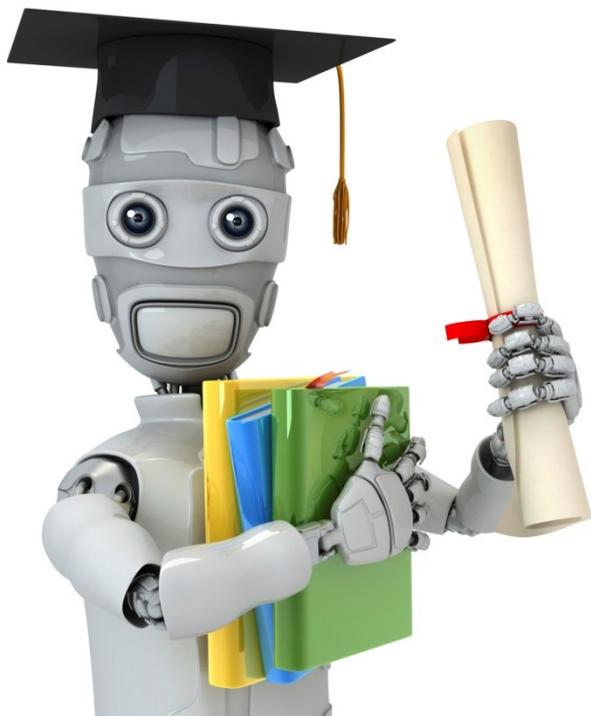


If a learning algorithm is suffering from high variance, getting more training data is likely to help. ←

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \dots + \theta_{100} x^{100}$$

(and small λ)





Machine Learning

Advice for applying
machine learning

Deciding what to
try next (revisited)

Debugging a learning algorithm:

Suppose you have implemented regularized linear regression to predict housing prices. However, when you test your hypothesis in a new set of houses, you find that it makes unacceptably large errors in its prediction. What should you try next?

- Get more training examples
- Try smaller sets of features
- Try getting additional features
- Try adding polynomial features ($x_1^2, x_2^2, x_1x_2, \text{etc}$)
- Try decreasing λ
- Try increasing λ

Debugging a learning algorithm:

Suppose you have implemented regularized linear regression to predict housing prices. However, when you test your hypothesis in a new set of houses, you find that it makes unacceptably large errors in its prediction. What should you try next?

- Get more training examples → fixes high variance
- Try smaller sets of features → fixes high variance
- Try getting additional features → fixes high bias
- Try adding polynomial features ($x_1^2, x_2^2, x_1x_2, \text{etc}$) → fixes high bias.
- Try decreasing λ → fixes high bias
- Try increasing λ → fixes high variance