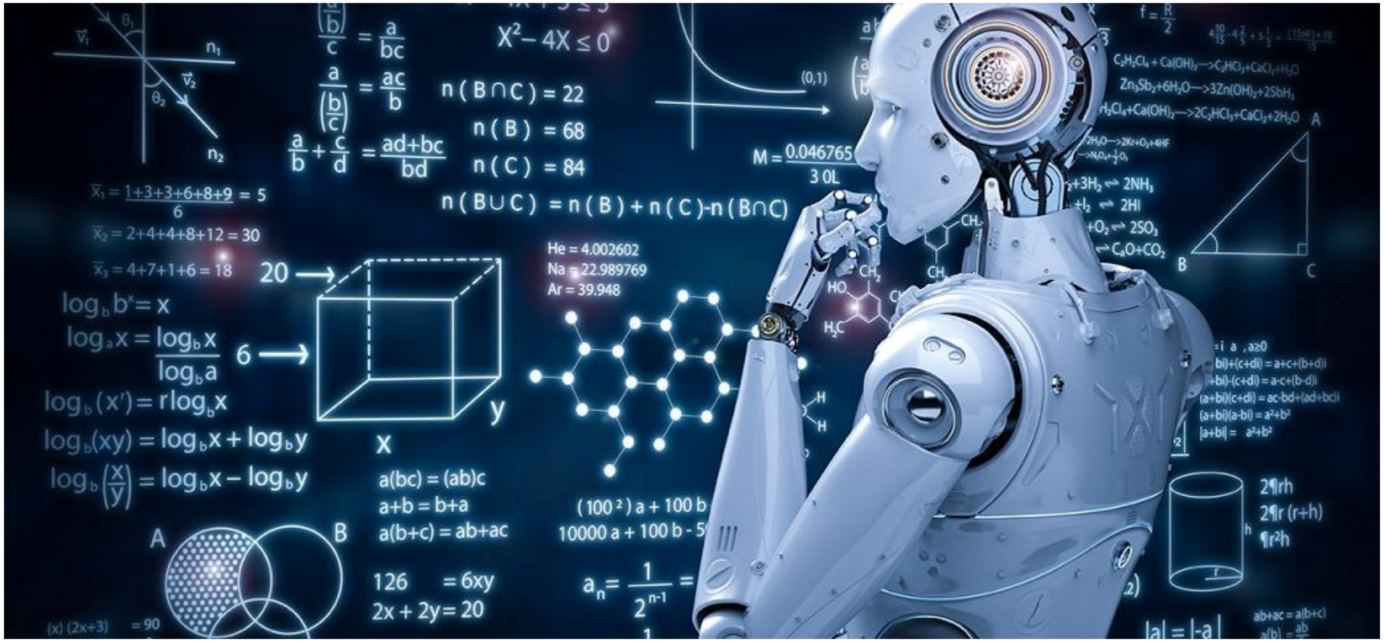


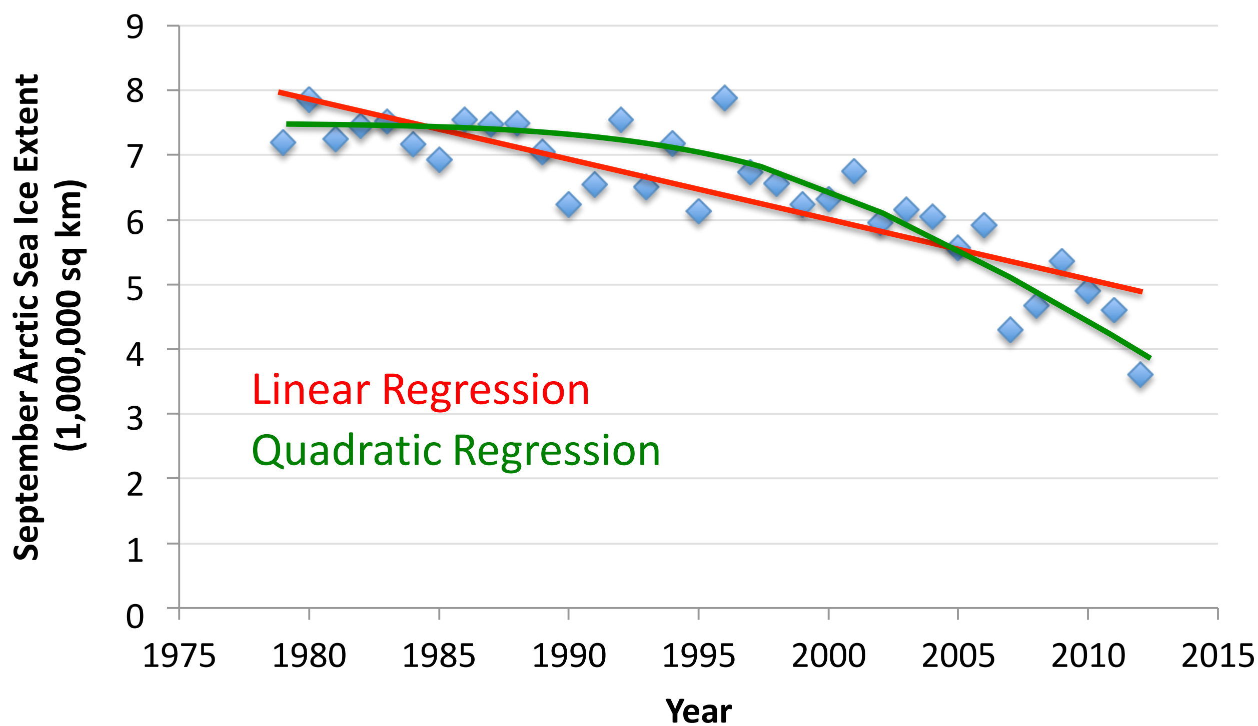
BBM406: Fundamentals of Machine Learning

Linear Regression, Cost Function, Gradient Descent

Regression

Given:

- Data $X = \{x^{(1)}, x^{(2)}, \cdots, x^{(n)}\}$, where $x^{(i)} \in R$
- Corresponding labels $y = \{y^{(1)}, y^{(2)}, \cdots, y^{(n)}\}$, where $y^{(i)} \in R$



Data from G. Witt. Journal of Statistics Education, Volume 21, Number 1 (2013)

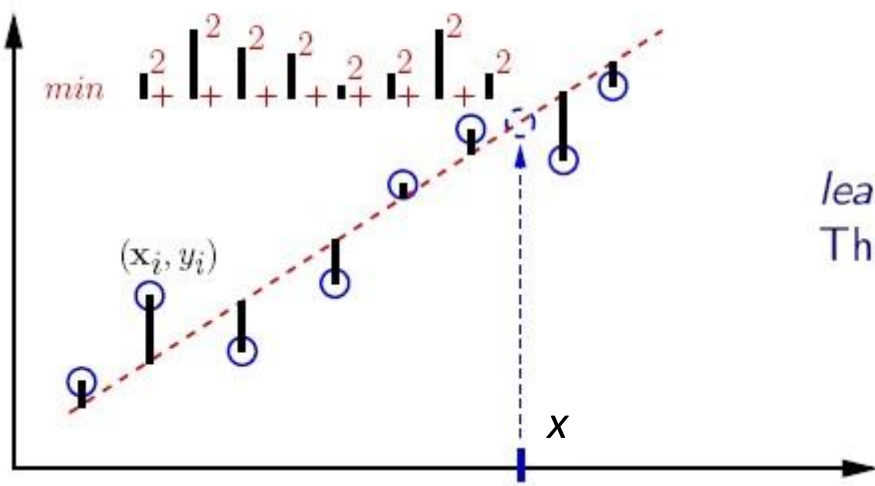
Linear Regression

- Hypothesis:

Assume $x_0 = 1$

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_d x_d = \sum_{j=0}^{d} \theta_j x_j = h_\theta(x)$$

- Fit model by minimizing sum of squared errors



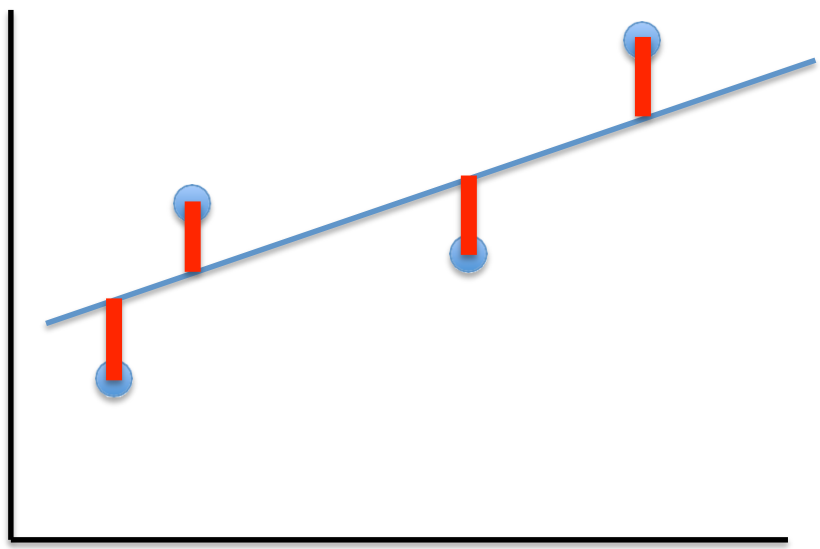
least squares (LSQ)
The fitted line is used as a predictor

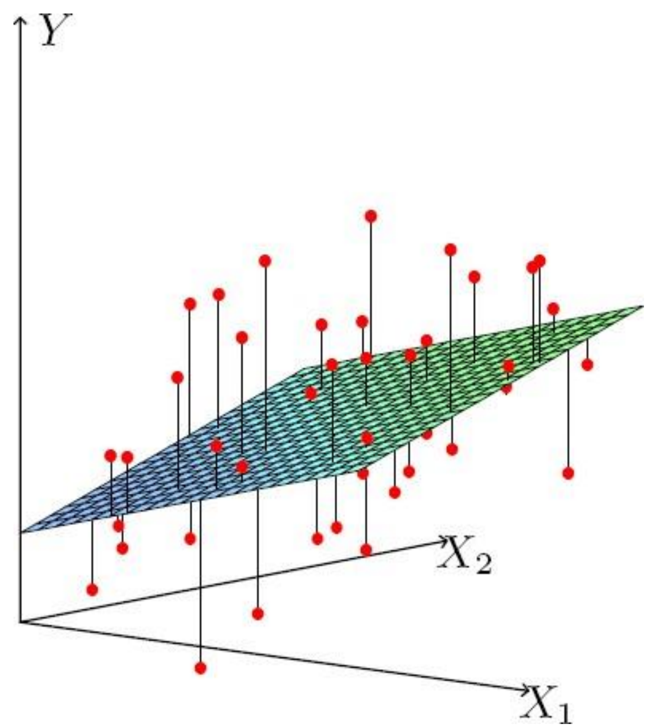
Least Squares Linear Regression

- Cost Function

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- Fit by solving





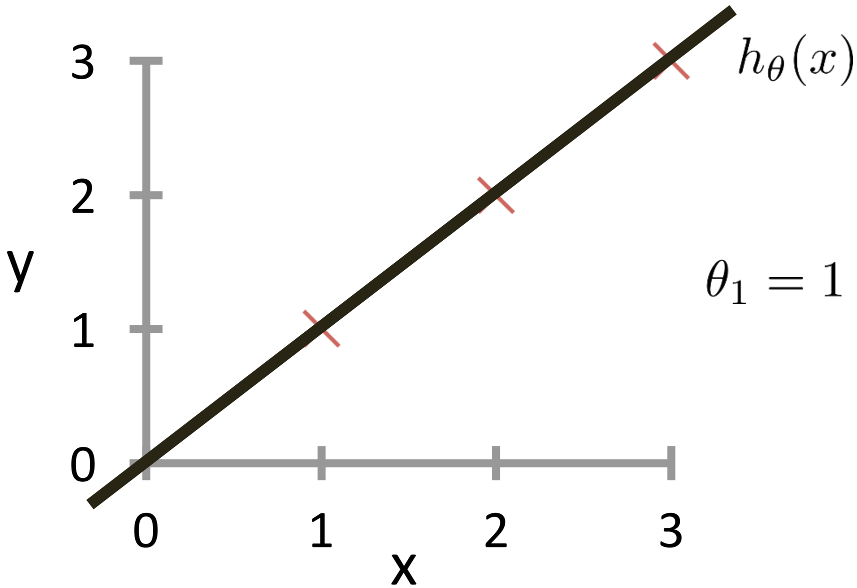
Intuition Behind Cost Function

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

For insight on $J()$, let's assume $x^{(i)} \in R$ and $\theta = [\theta_0, \theta_1]$

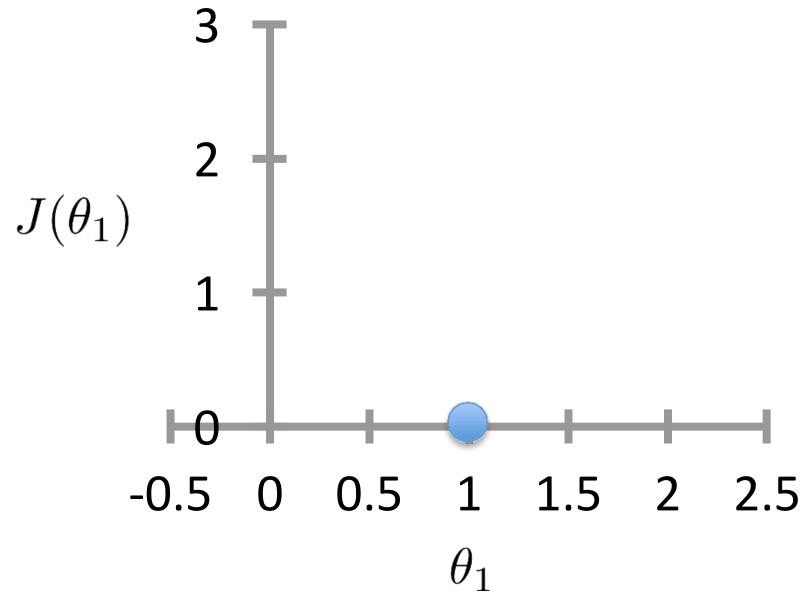
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



$$J([0,1]) = \frac{1}{2\times 3}\left[(1-1)^2 + (2-2)^2 + (3-3)^2\right] = 0$$

Based on example by Andrew Ng

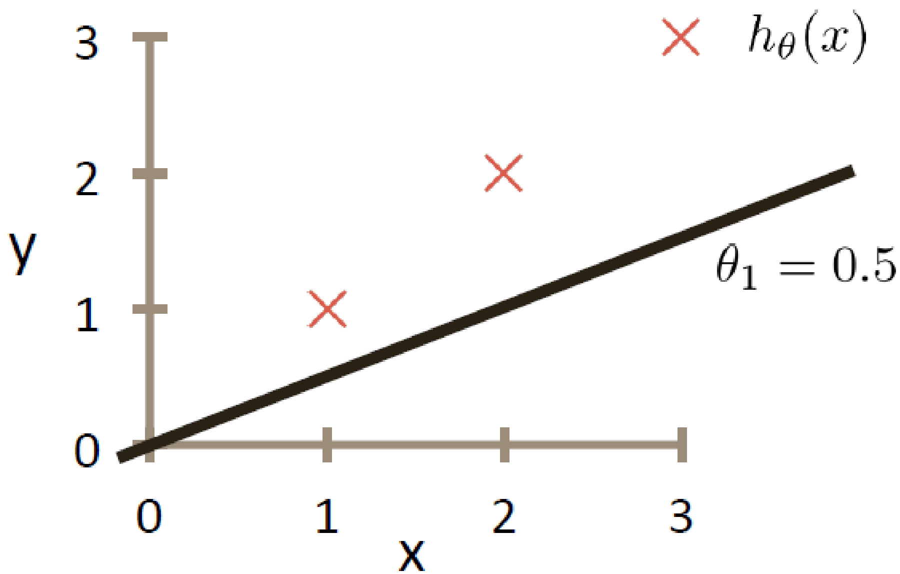
Intuition Behind Cost Function

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

For insight on $J()$, let's assume $x^{(i)} \in R$ and $\theta = [\theta_0, \theta_1]$

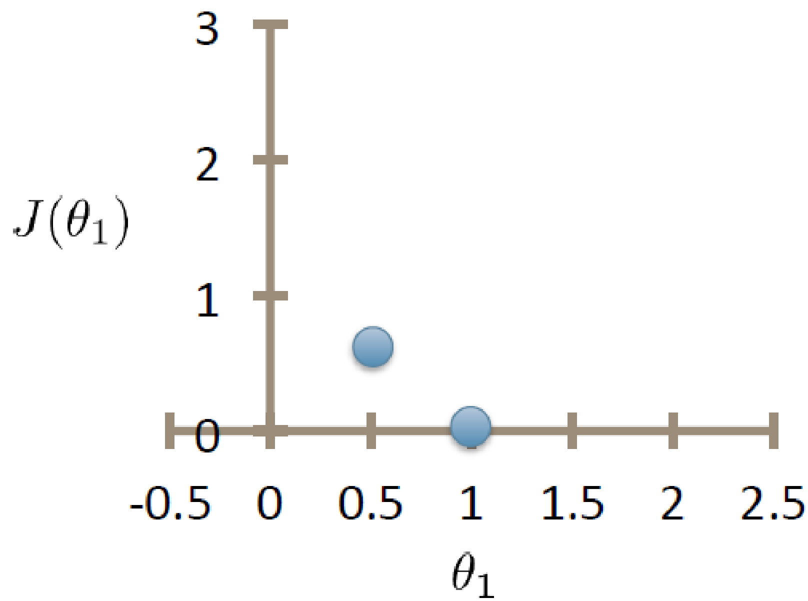
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



Based on example by Andrew Ng

$$J([0,0.5]) = \frac{1}{2\times 3}\left[(0.5-1)^2+(1-2)^2+(1.5-3)^2\right] \approx 0.58$$

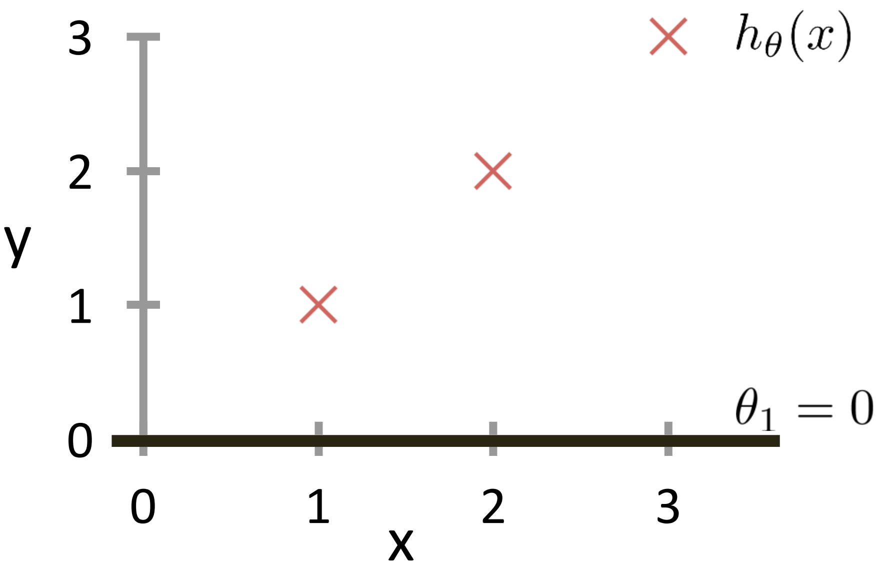
Intuition Behind Cost Function

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

For insight on $J()$, let's assume $x^{(i)} \in R$ and $\theta = [\theta_0, \theta_1]$

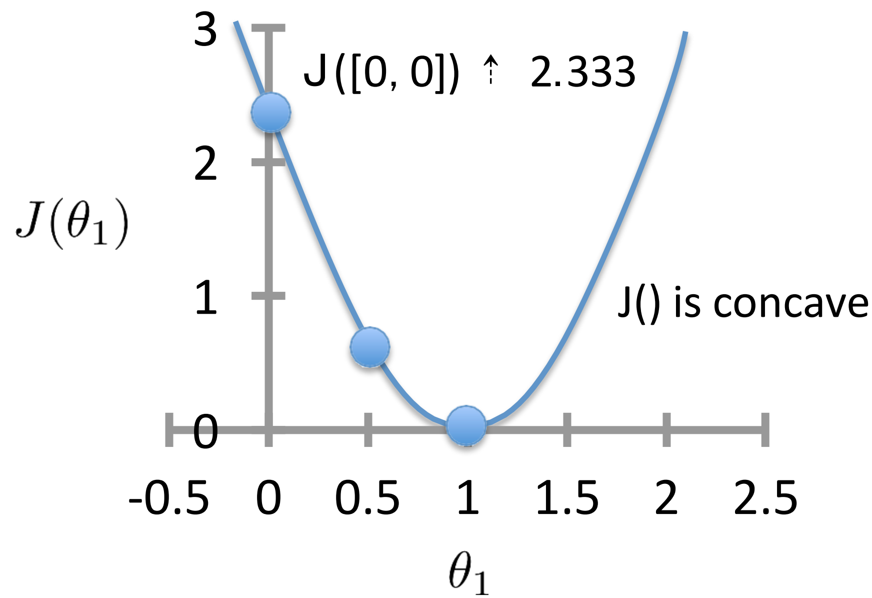
$h_\theta(x)$

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



$J(\theta_1)$

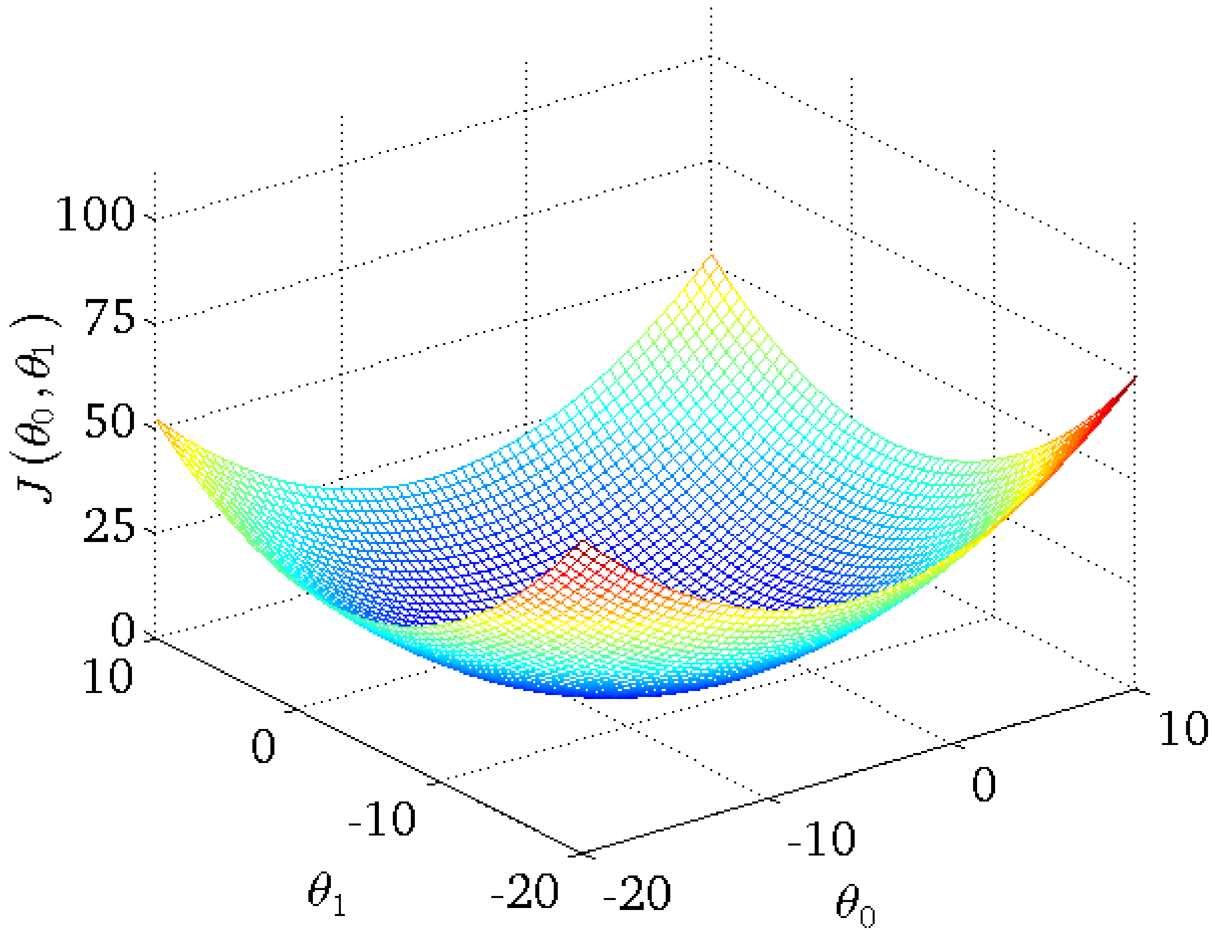
(function of the parameter θ_1)



Based on example
by Andrew Ng

$$J([0,0]) = \frac{1}{2\times 3}\left[(0-1)^2+(0-2)^2+(0-3)^2\right] \approx 2.33$$

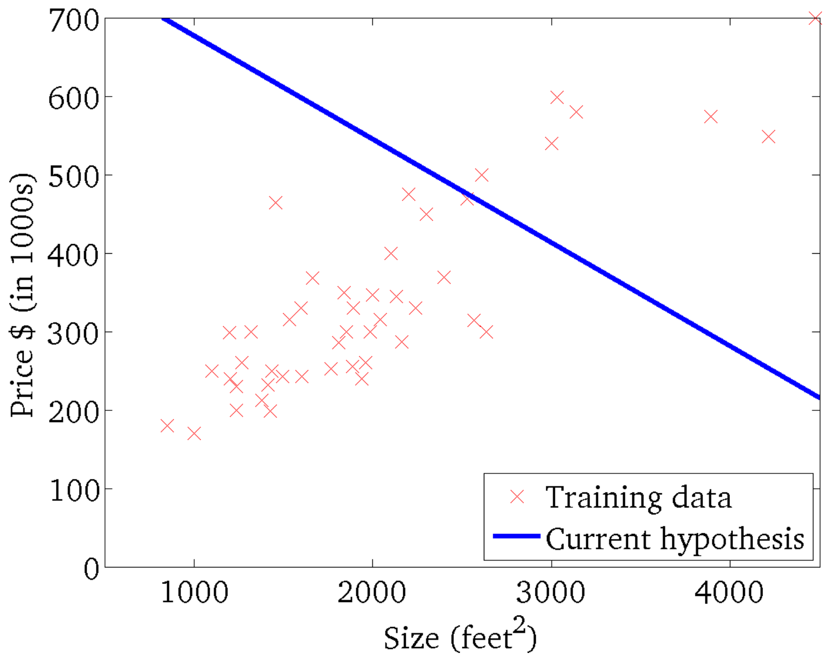
Intuition Behind Cost Function



Intuition Behind Cost Function

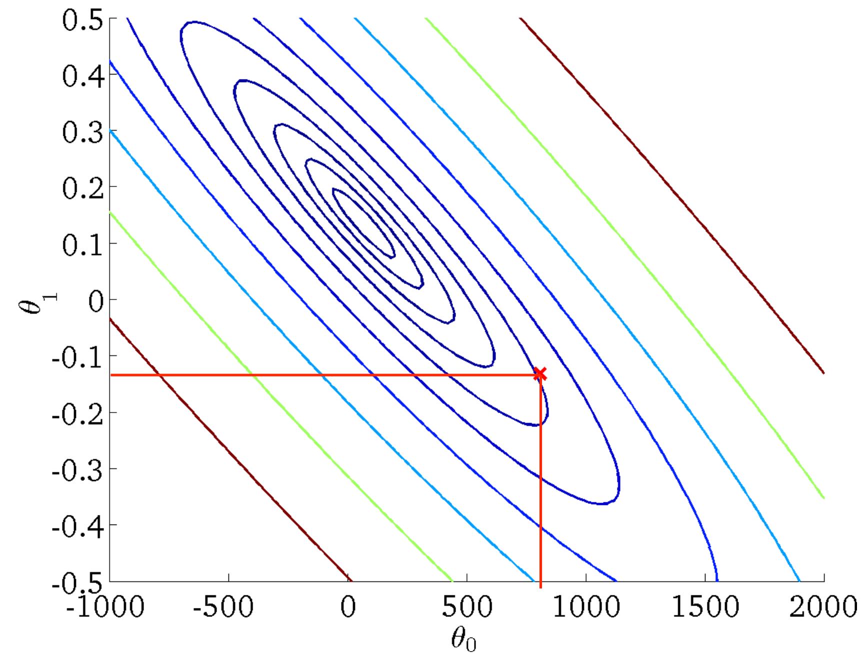
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

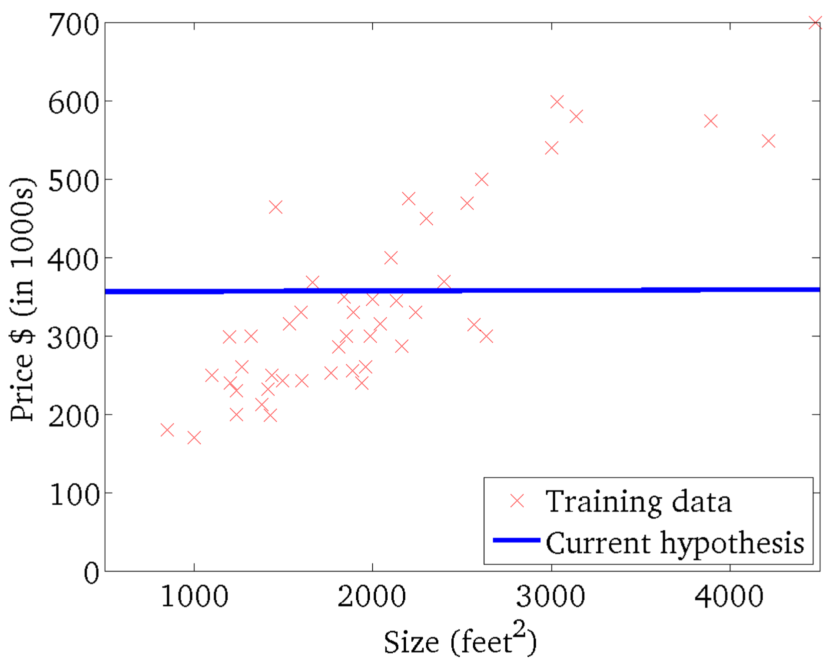
(function of the parameters θ_0, θ_1)



Intuition Behind Cost Function

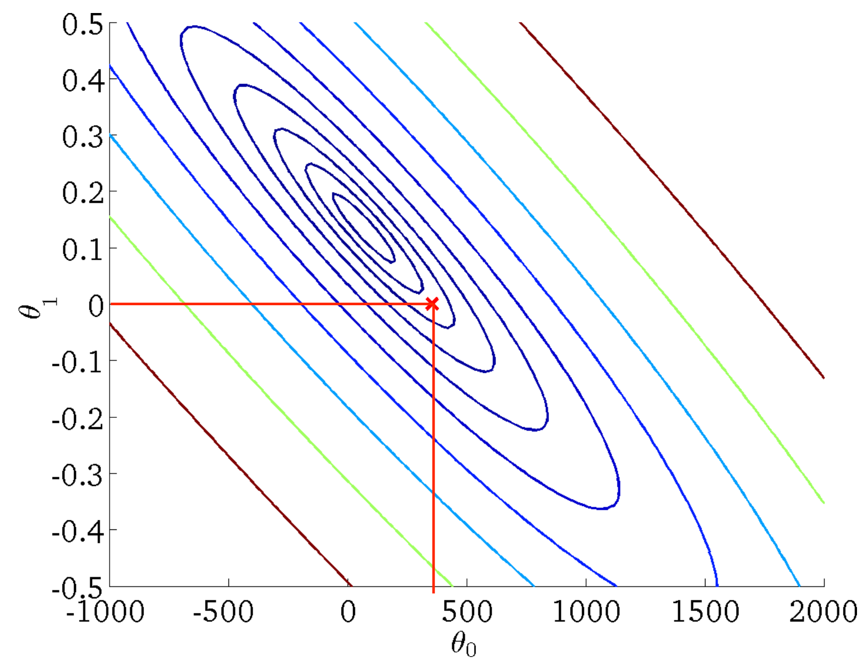
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

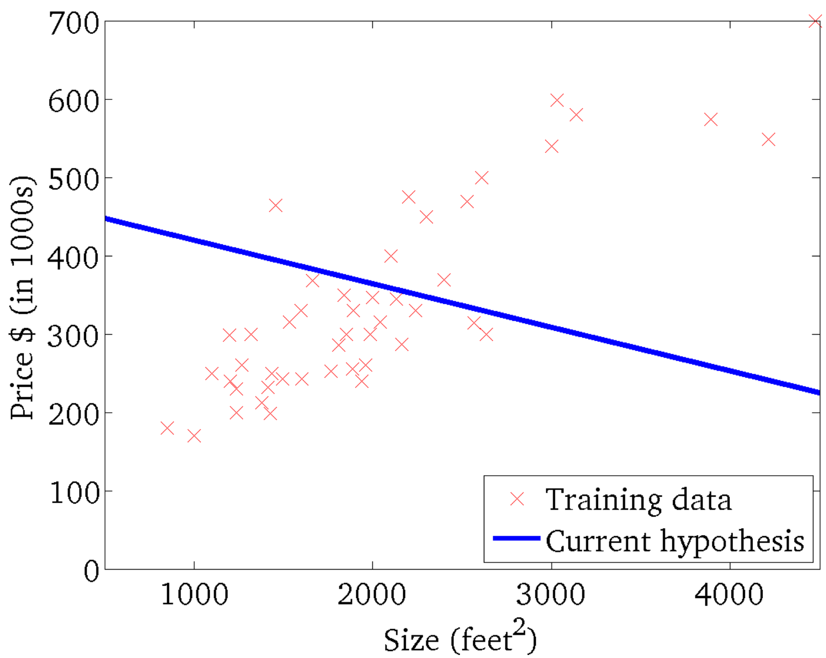
(function of the parameters θ_0, θ_1)



Intuition Behind Cost Function

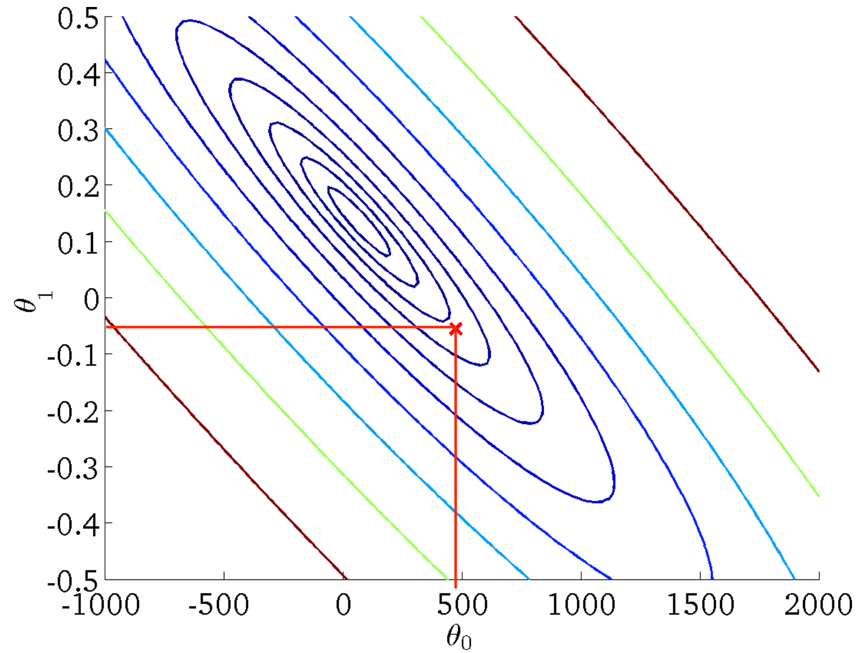
$$h_\theta(x)$$

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



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

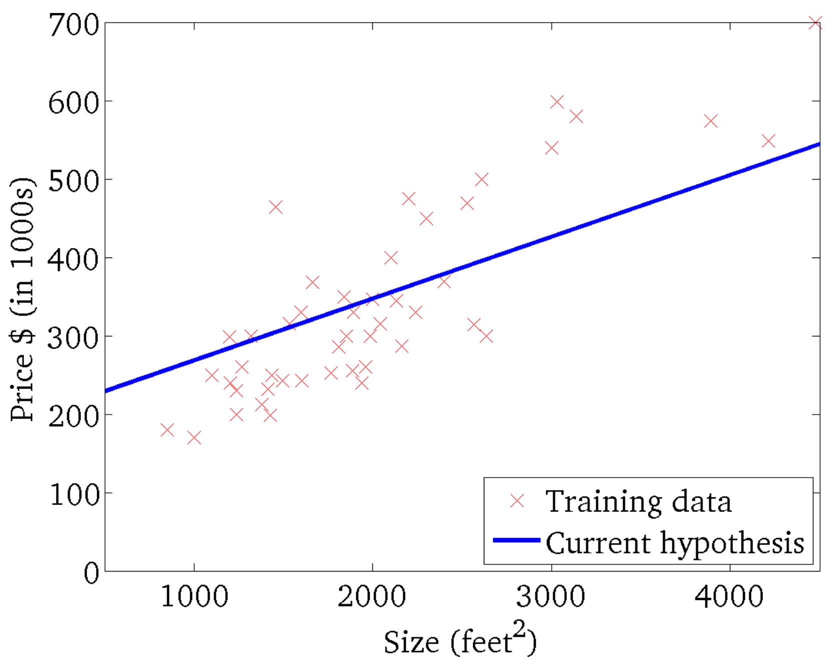
(function of the parameters θ_0, θ_1)



Intuition Behind Cost Function

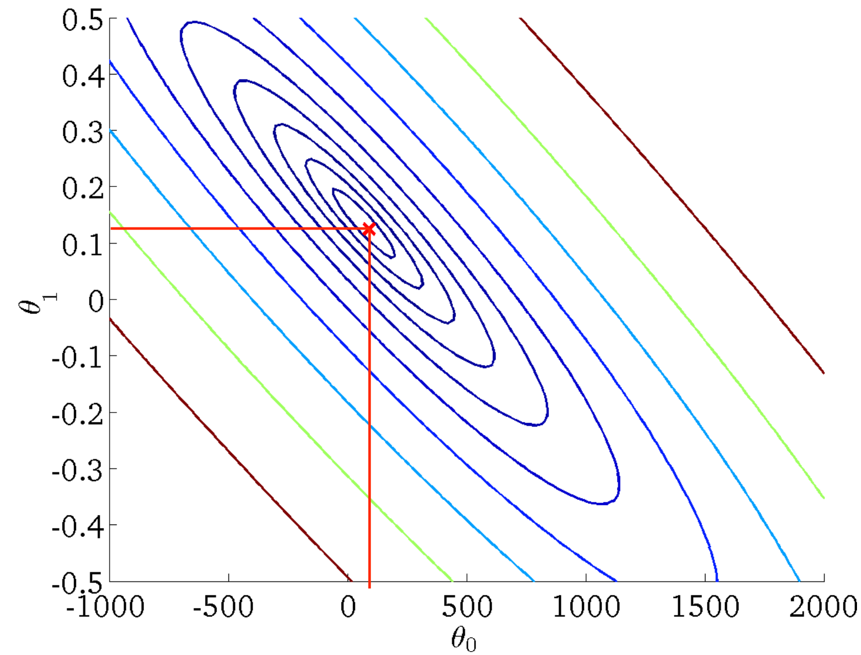
$$h_\theta(x)$$

(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)



Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for θ to reduce J(θ)

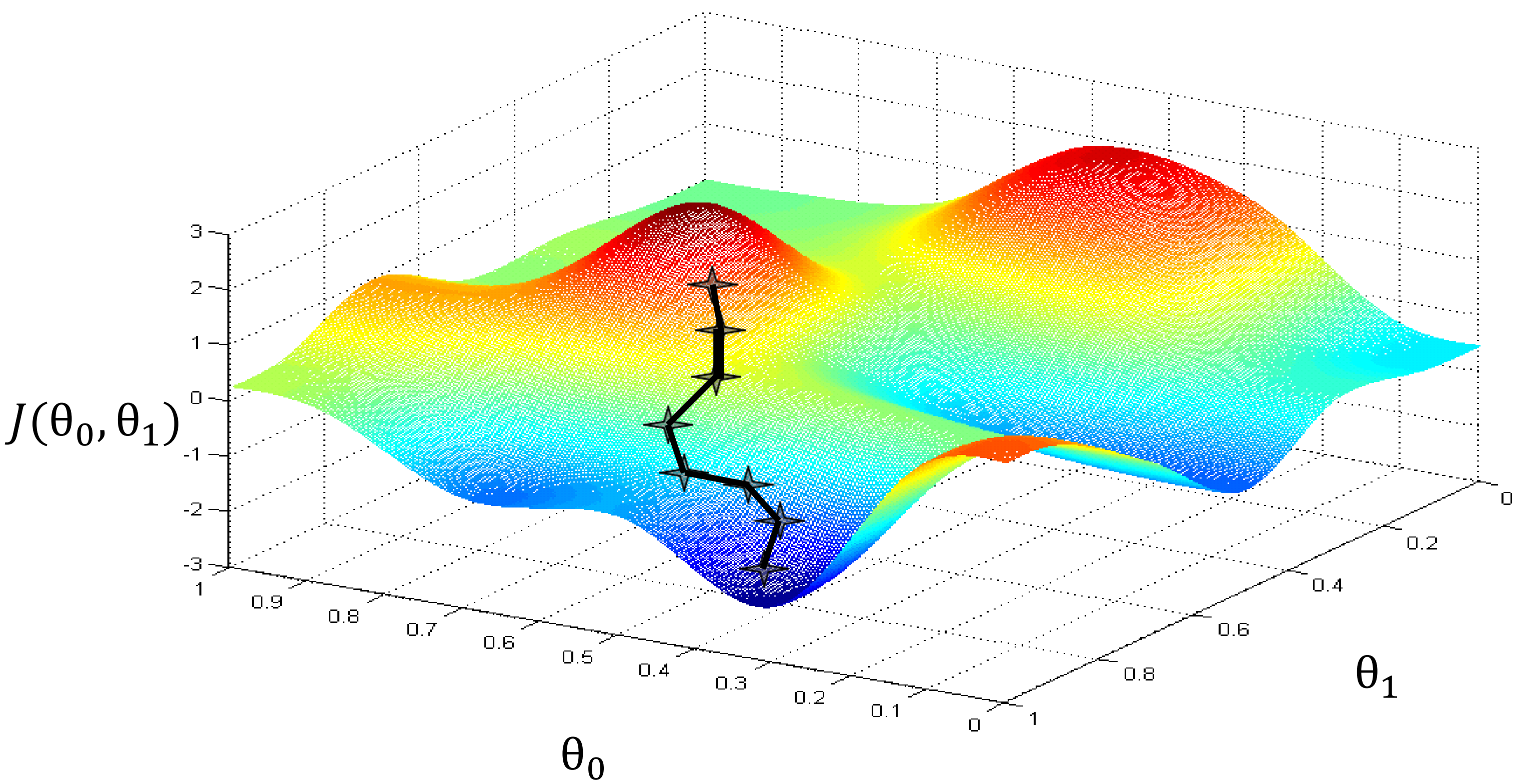


Figure by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for θ to reduce J (θ)

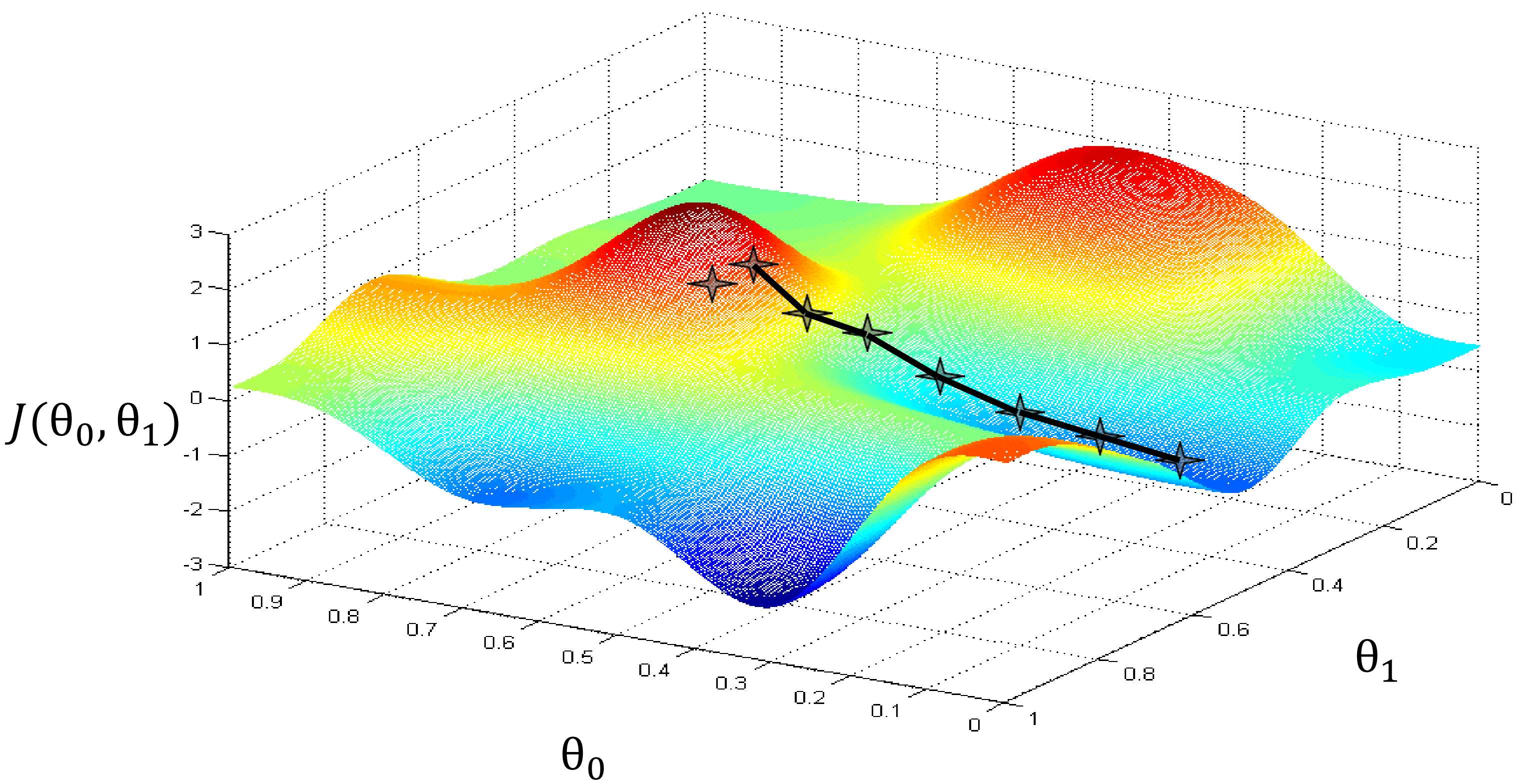
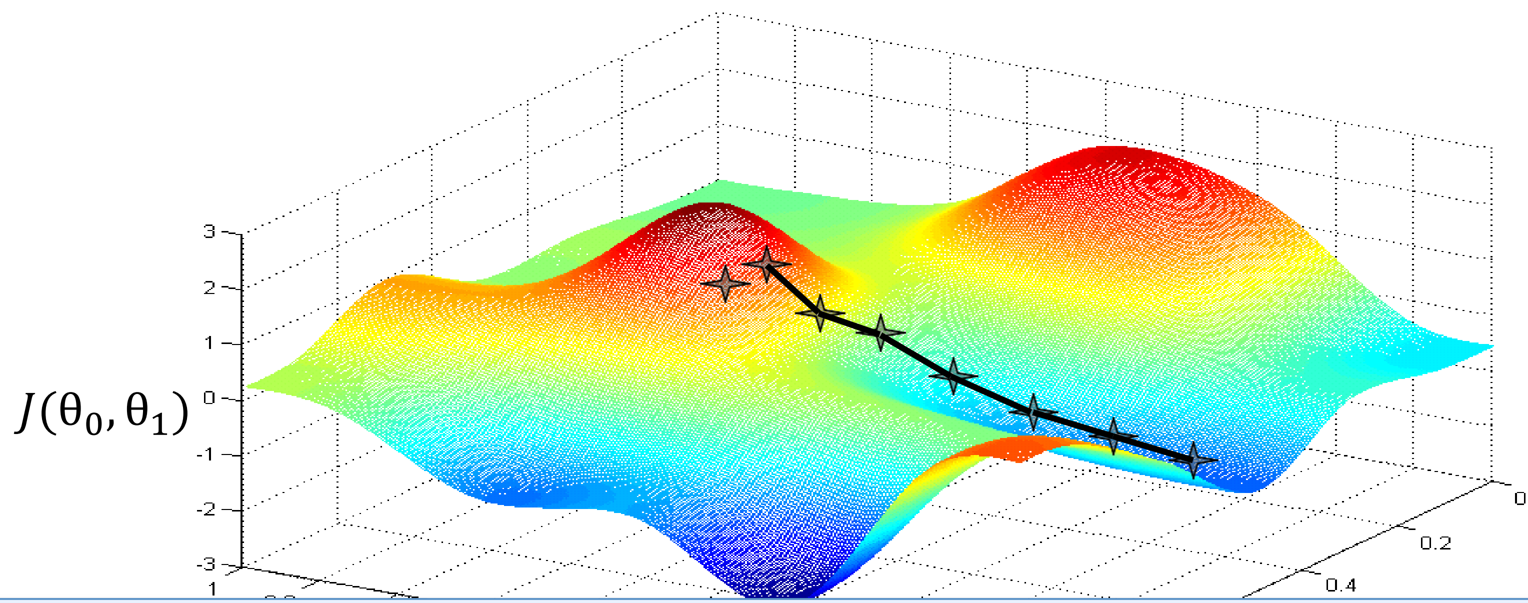


Figure by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for θ to reduce J(θ)



Since the least squares objective function is convex (concave), we don't need to worry about local minima

Figure by Andrew Ng

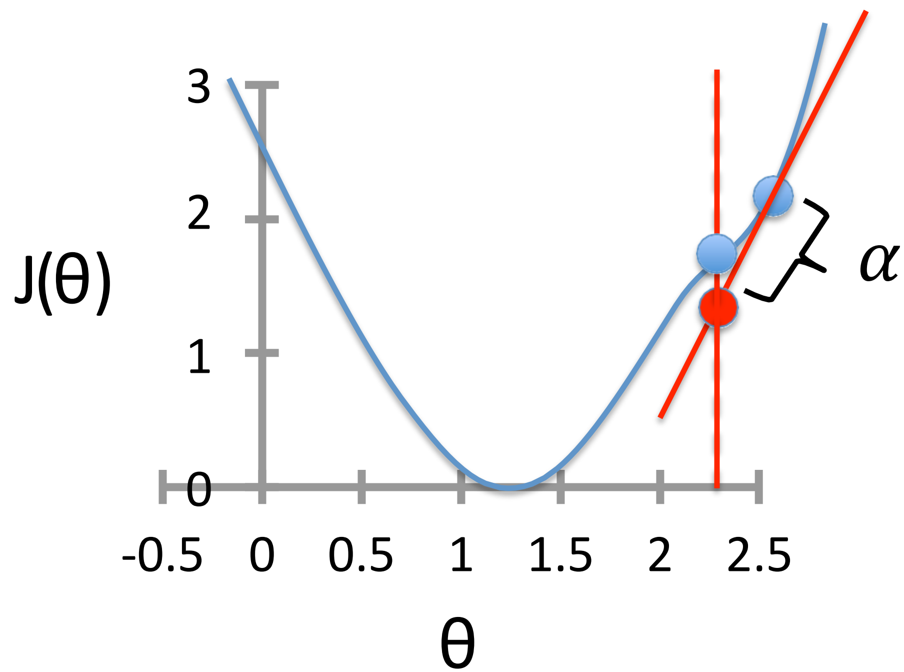
Gradient Descent

- Initialize θ
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



Gradient Descent

- Initialize θ
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

simultaneous update
for j = 0 ... d

$$J(\theta) = \frac{1}{2n} \sum_{i=1}^{n} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

For linear regression:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

Gradient Descent

- Initialize θ
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

simultaneous update
for j = 0 ... d

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_d x_d = \sum_{j=0}^{d} \theta_j x_j$$

For linear regression:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right)^2$$

$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(\sum_{j=0}^{d} \theta_j x_j^{(i)} - y^{(i)} \right)^2$$

Gradient Descent

- Initialize θ
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

simultaneous update
for j = 0 ... d

For linear regression:
$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(\sum_{j=0}^{d} \theta_j x_j^{(i)} - y^{(i)} \right)^2$$

$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=0}^{d} \theta_j x_j^{(i)} - y^{(i)} \right) \frac{\partial}{\partial \theta_j} \left(\sum_{j=0}^{d} \theta_j x_j^{(i)} - y^{(i)} \right)$$

$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=0}^{d} \theta_j x_j^{(i)} - y^{(i)} \right) x_j^{(i)}$$

Gradient Descent

- Initialize θ
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \propto \frac{1}{n}\sum_{i=1}^{n}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right) x_j^{(i)}$$

simultaneous update
for j = 0 ... d

- To achieve simultaneous update
  - At the start of each GD iteration, compute $h_\theta\left(x^{(i)}\right)$
  - Use this stored value in the update step loop

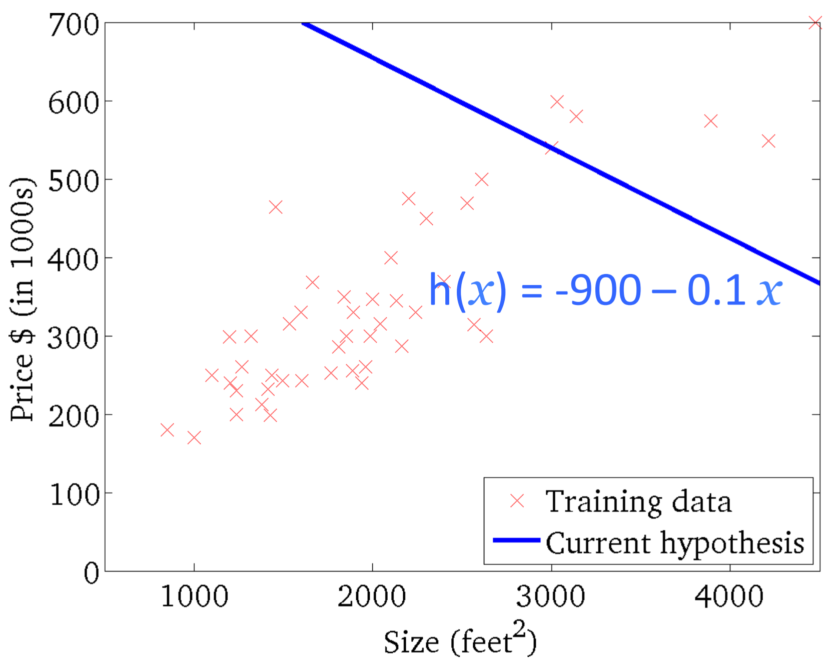
- Assume convergence when $\|\theta_{new} - \theta_{old}\|_2 < \epsilon$

L_2 norm : $\|v\|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \cdots + v_{|v|}^2}$

Gradient Descent

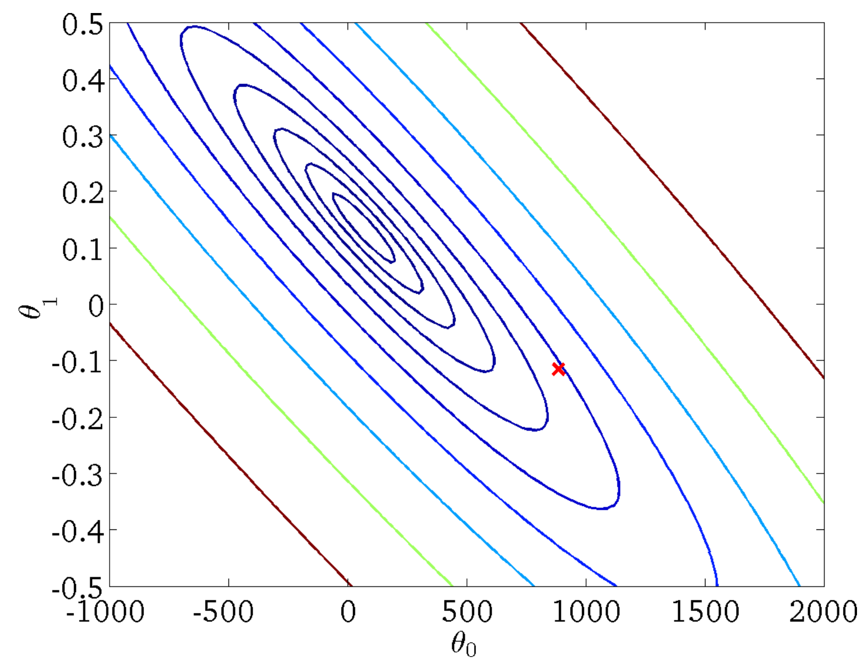
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

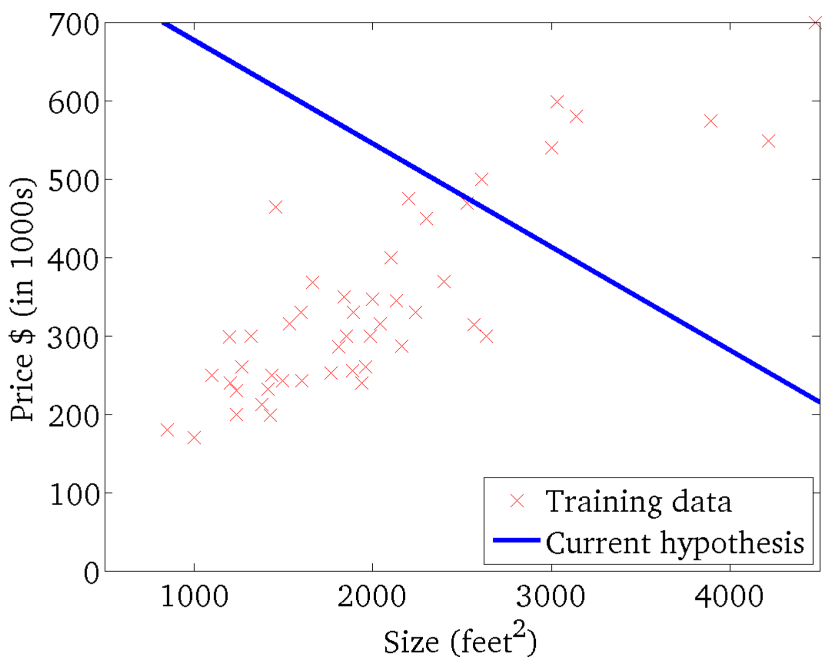
(function of the parameters θ_0, θ_1)



Gradient Descent

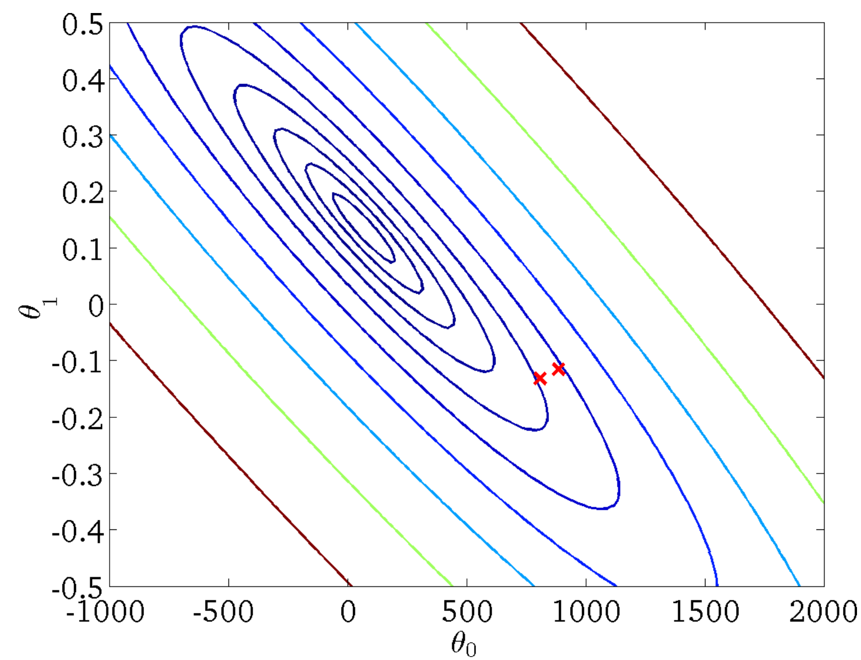
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

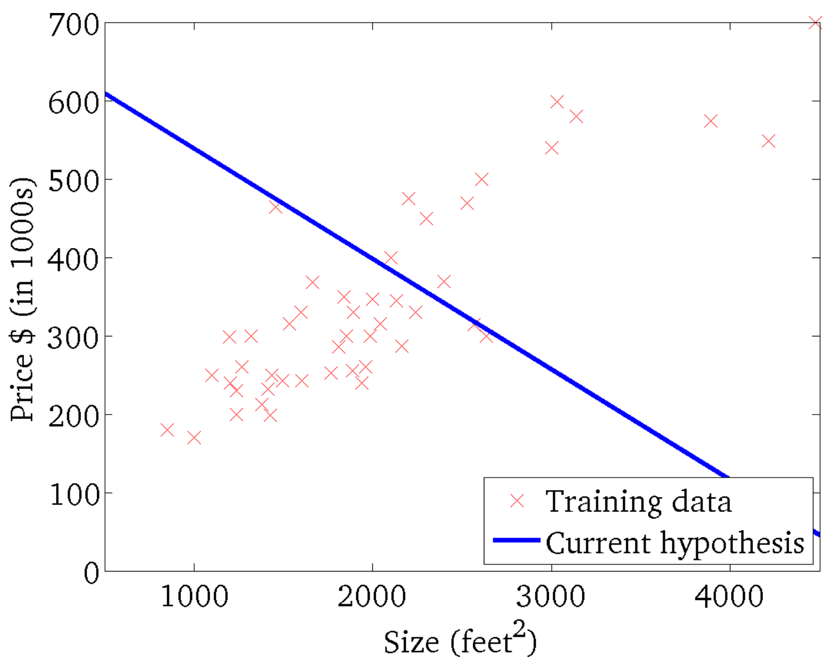
(function of the parameters θ_0, θ_1)



Gradient Descent

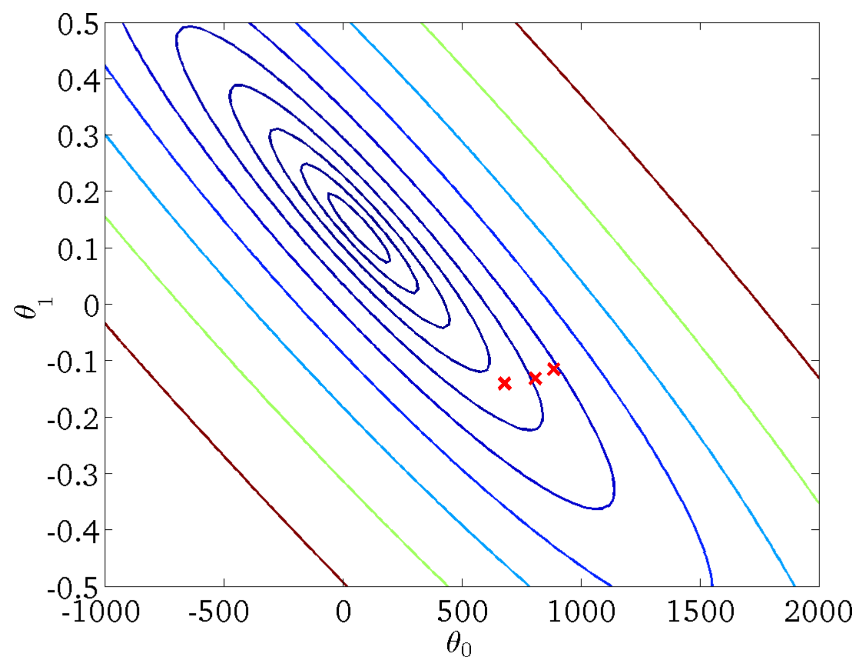
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

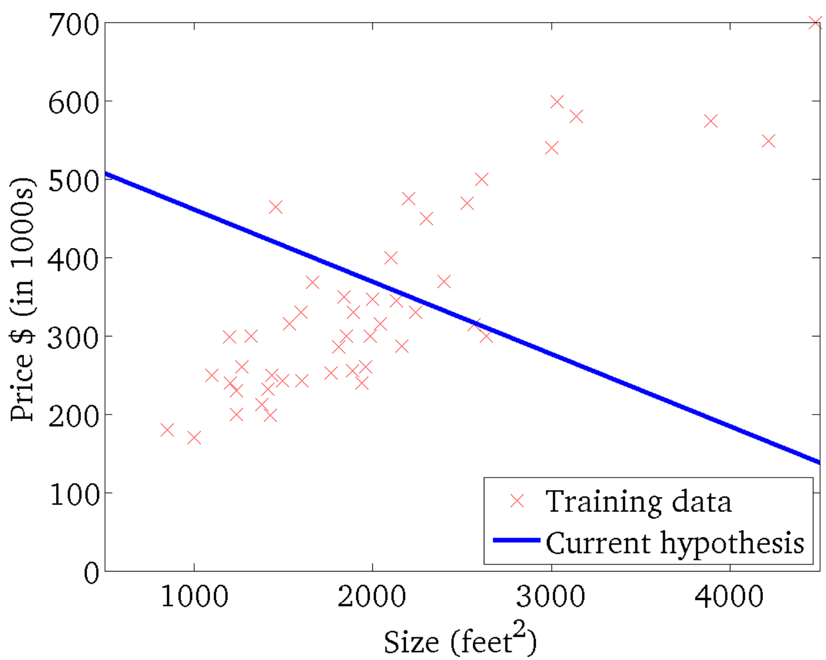
(function of the parameters θ_0, θ_1)



Gradient Descent

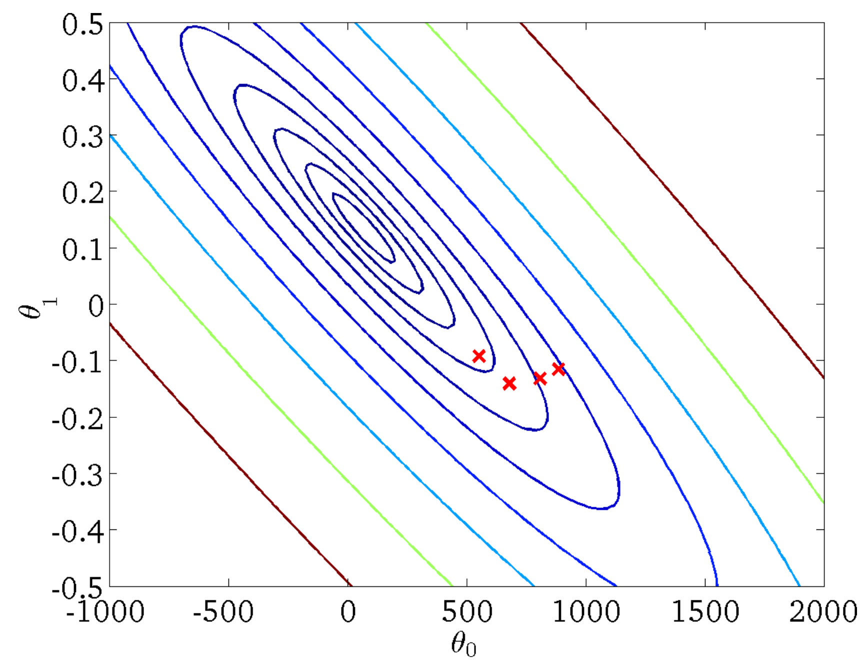
$$h_\theta(x)$$

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



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

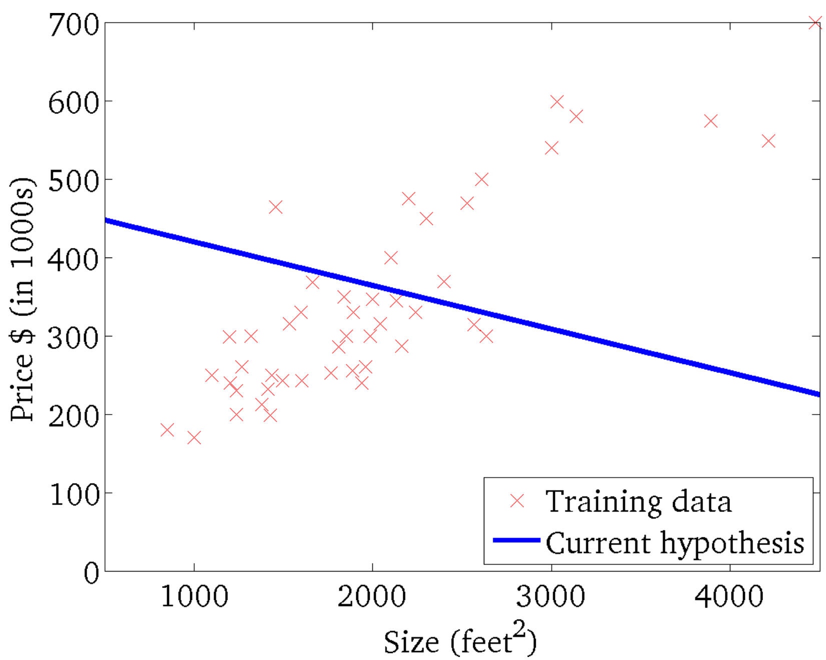
(function of the parameters θ_0, θ_1)



Gradient Descent

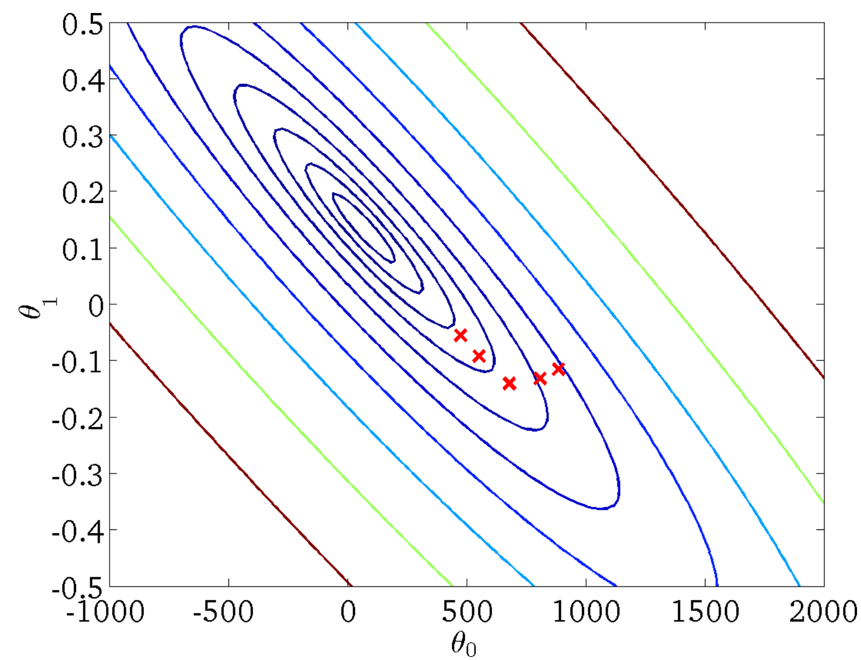
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

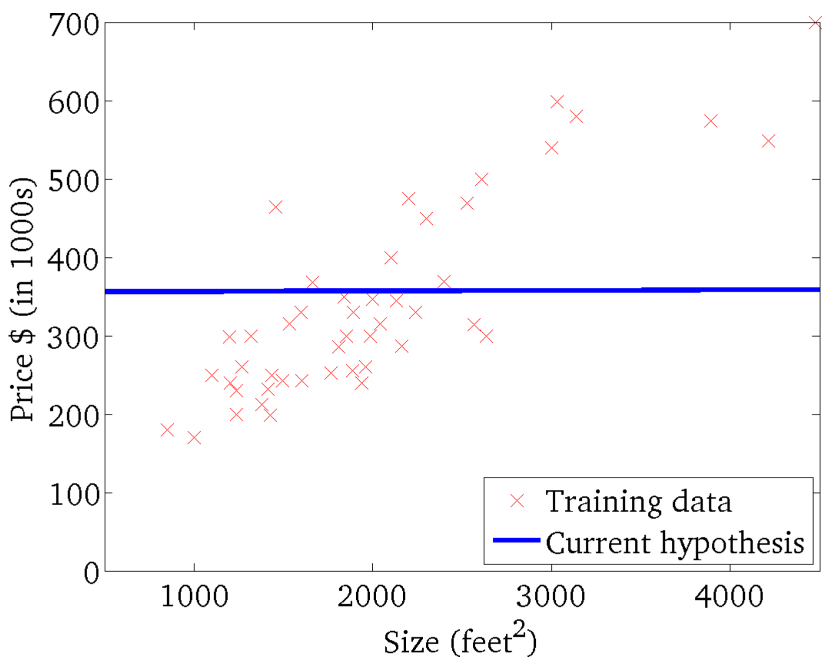
(function of the parameters θ_0, θ_1)



Gradient Descent

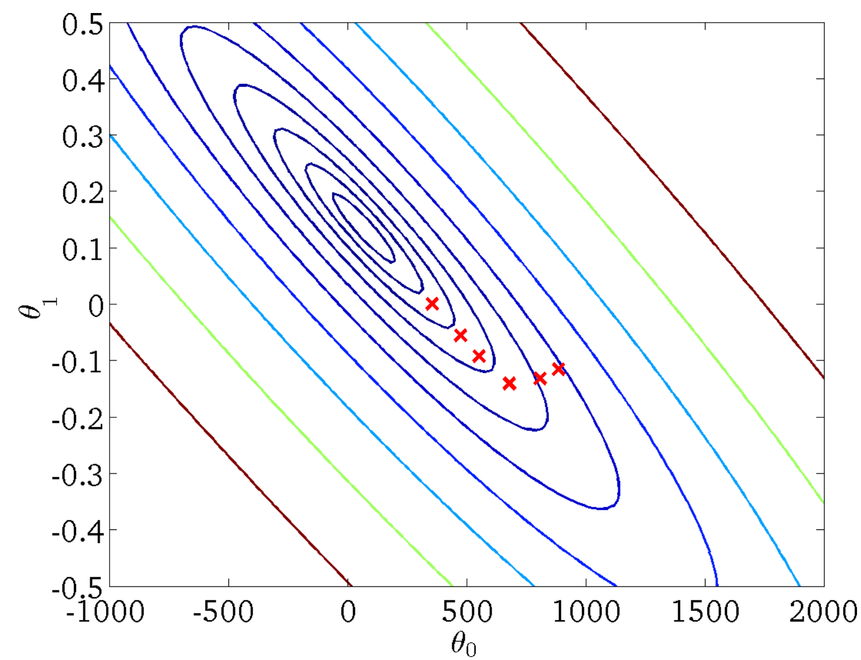
$h_\theta(x)$

(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)

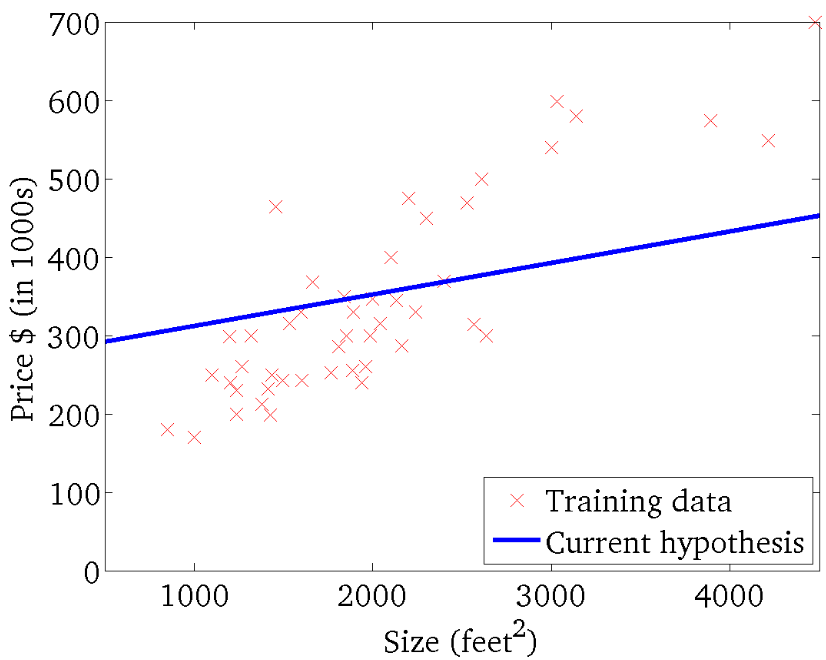


Slide by Andrew Ng

Gradient Descent

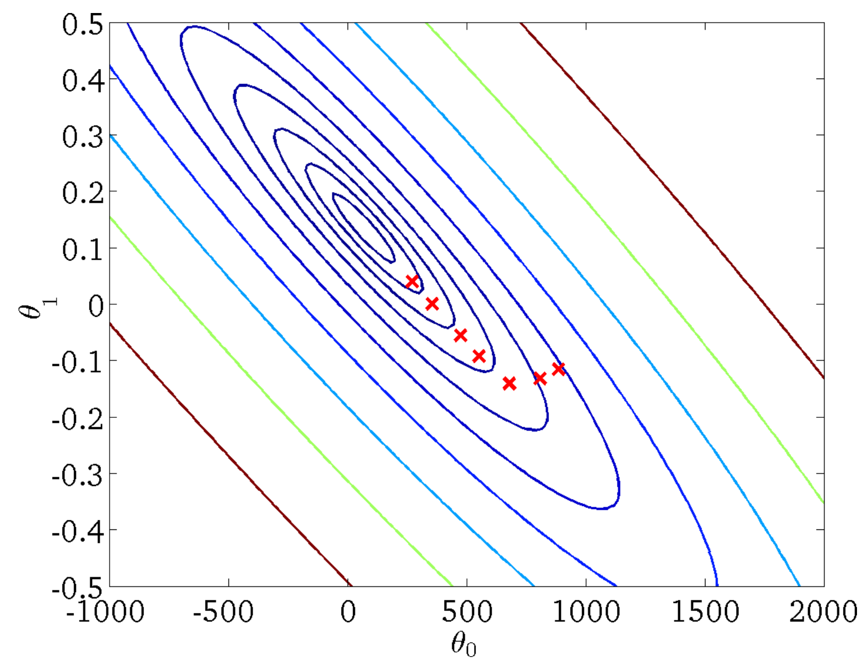
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

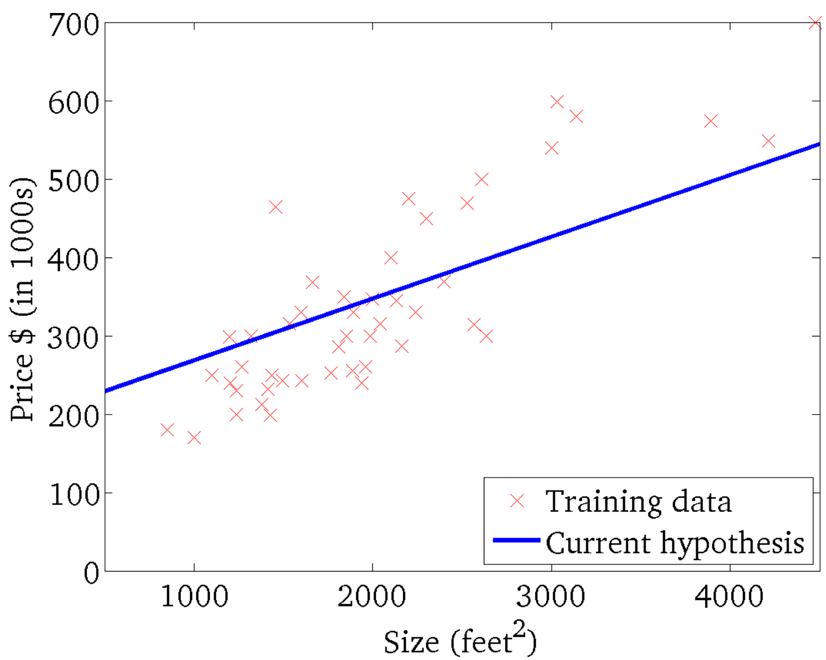
(function of the parameters θ_0, θ_1)



Gradient Descent

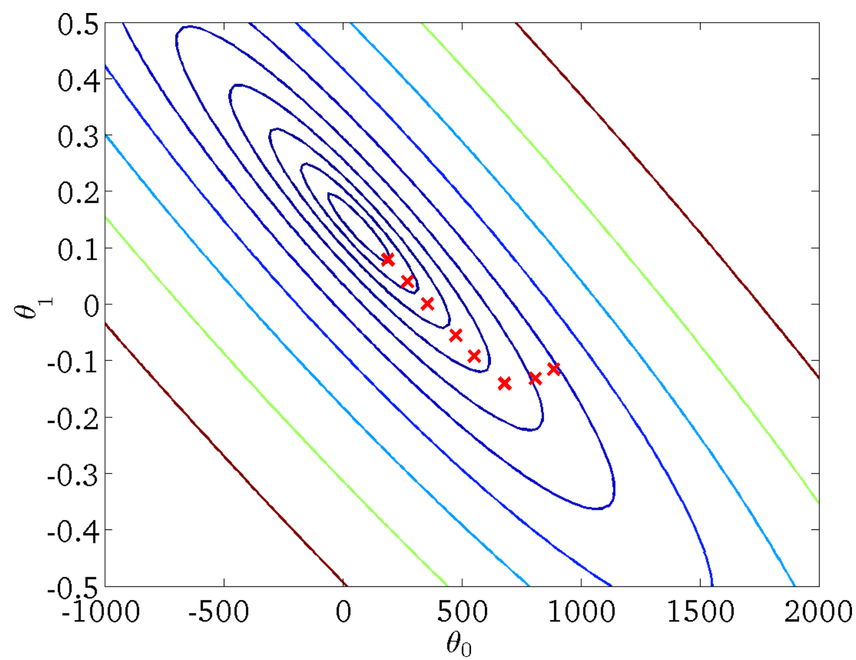
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

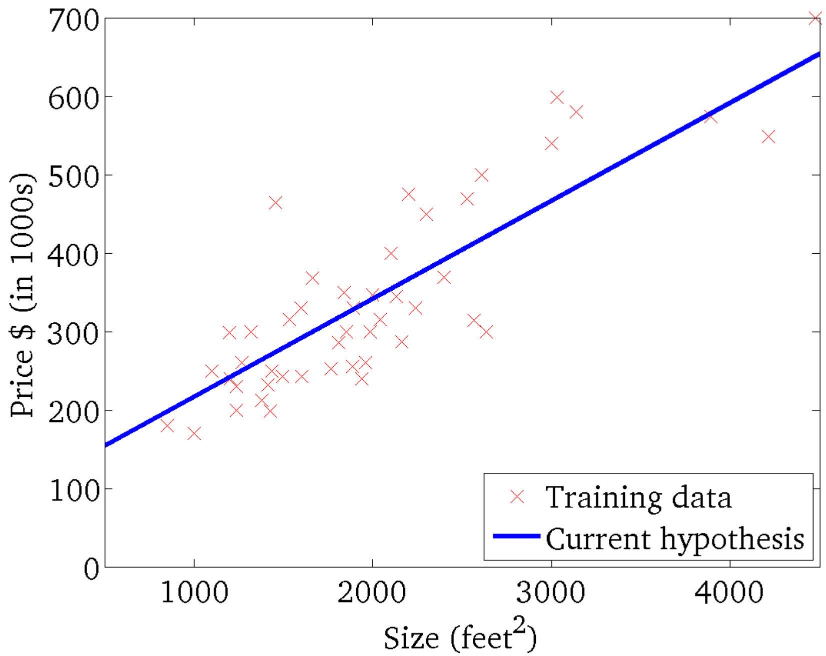
(function of the parameters θ_0, θ_1)



Gradient Descent

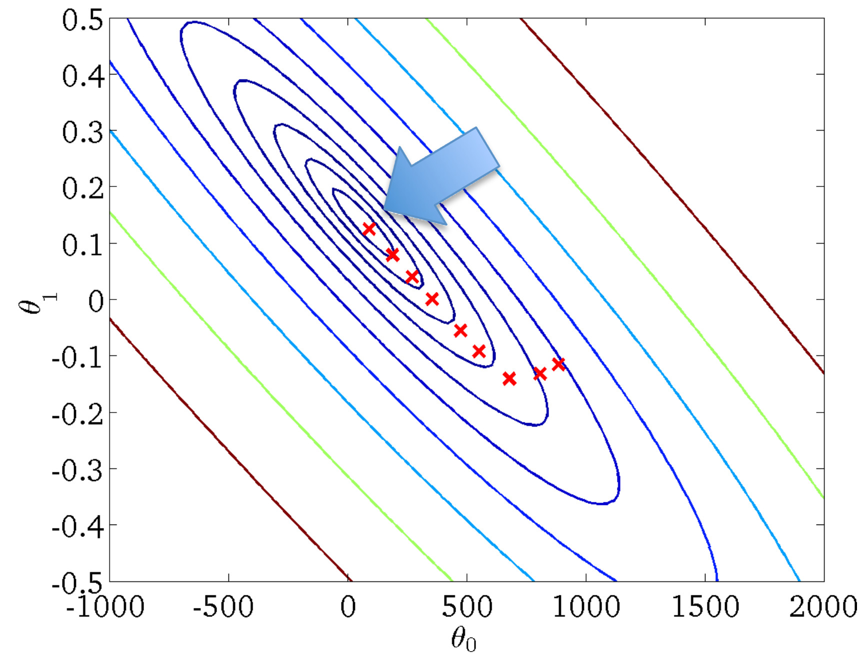
$$h_\theta(x)$$

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



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

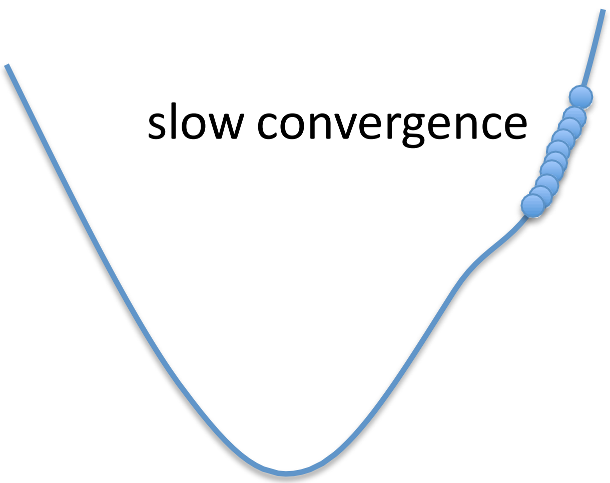
(function of the parameters θ_0, θ_1)



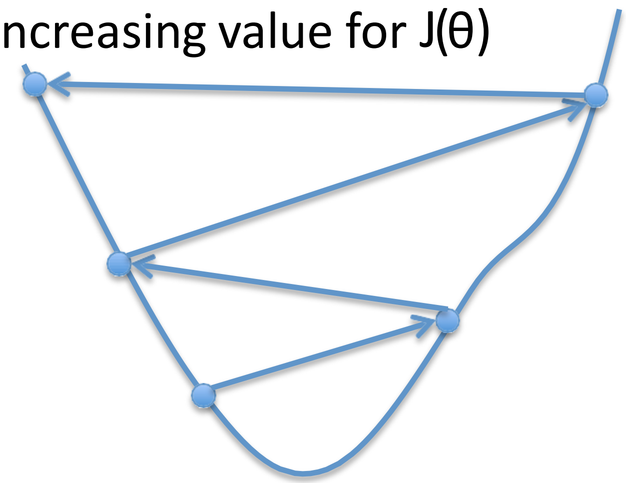
Slide by Andrew Ng

Choosing α

α too small



α too large



- May overshoot the minimum
- May fail to converge
- May even diverge

To see if gradient descent is working, print out $J(\theta)$ each iteration
- The value should decrease at each iteration
- If it doesn't, adjust α