UCK358E – INTR. TO ARTIFICIAL INTELLIGENCE

SPRING ‘23

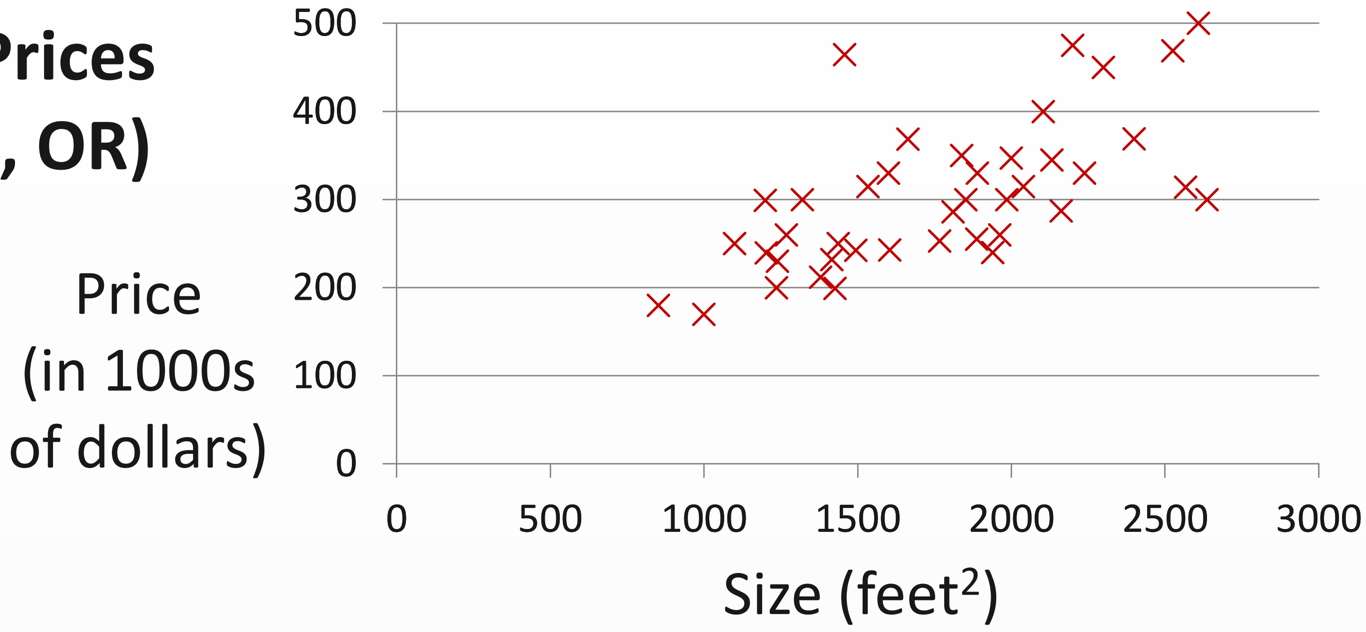
LECTURE 3

LINEAR AND POLYNOMIAL REGRESSION

Instructor: Asst. Prof. Barış Başpınar

Model Representation

Housing Prices (Portland, OR)



<u>Supervised Learning</u>

Given the “right answer” for each example in the data.

<u>Regression Problem</u>

Predict real-valued output

Model Representation

Training set of housing prices (Portland, OR)

Size in feet² (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
…	…

m = 50

Notation:

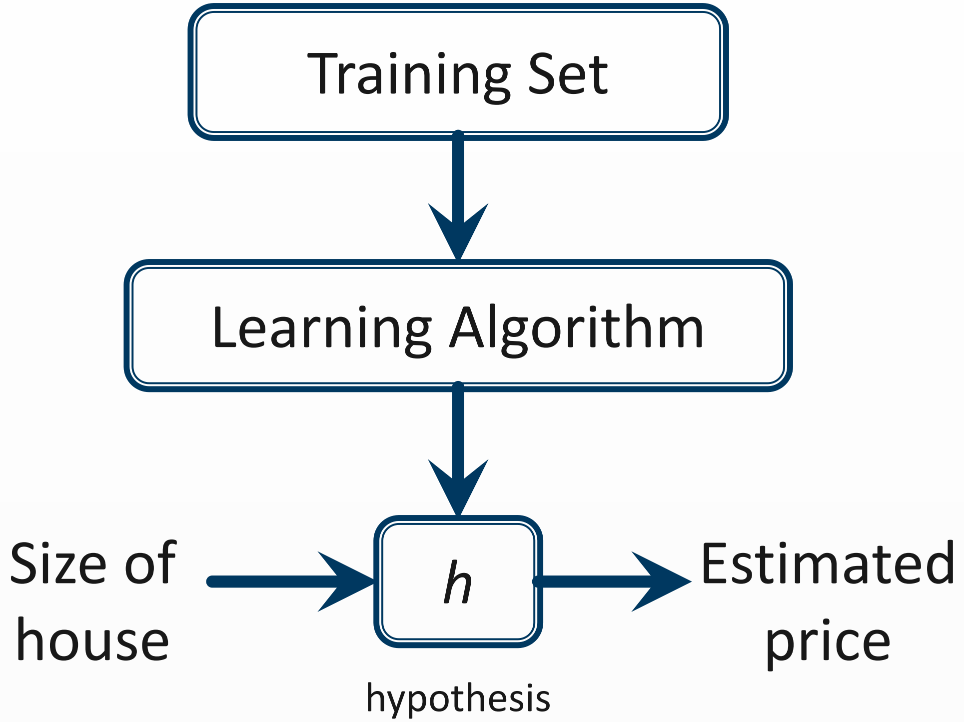
m = Number of training examples
x's = "input" variable / features
y's = "output" variable / "target" variable

$\left(x^{(1)}, y^{(1)}\right) = (2104, 460)$

$\left(x^{(2)}, y^{(2)}\right) = (1416, 232)$

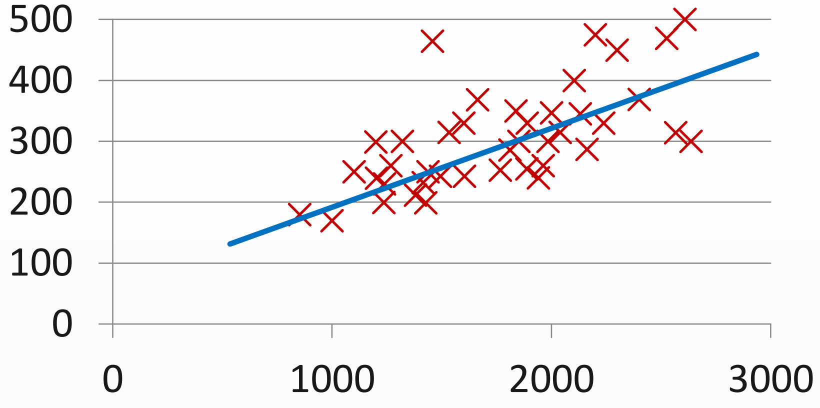
$\left(x^{(i)}, y^{(i)}\right) \rightarrow i^{th}$ training example

Model Representation: linear regression



How do we represent *h* ?

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



Linear regression with one variable.
Univariate linear regression.

Cost Function

Training Set

Size in feet² (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
…	…

m = 50

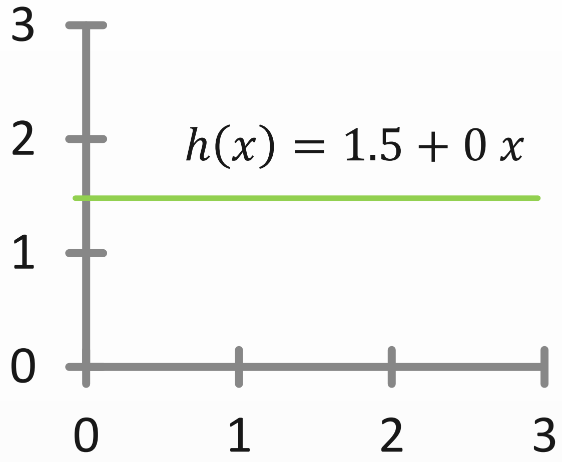
Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x$

θ_i's: Parameters

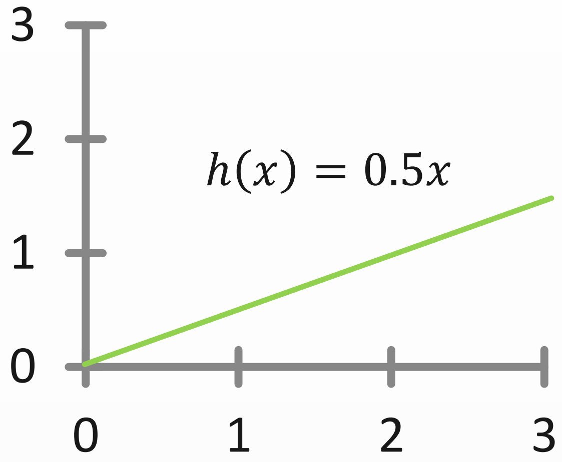
How to choose θ_i's ?

Cost Function

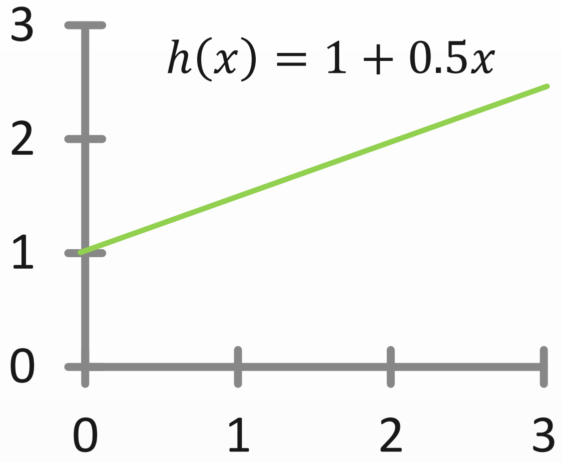
$$h_\theta(x) = \theta_0 + \theta_1 x$$



$\theta_0 = 1.5$
$\theta_1 = 0$

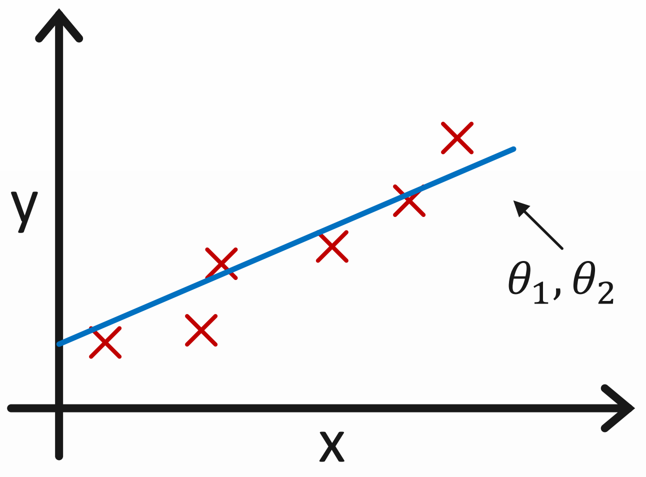


$\theta_0 = 0$
$\theta_1 = 0.5$



$\theta_0 = 1$
$\theta_1 = 0.5$

Cost Function



Number of training examples

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \overbrace{\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2}^{\text{Squared error function}}$$

Cost function

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

$$\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$$

Idea: Choose θ_0, θ_1 so that $h_\theta(x)$ is close to y for our training examples (x, y)

Cost Function Intuition

Hypothesis:

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

Parameters:

$$\theta_0, \theta_1$$

Cost Function:

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

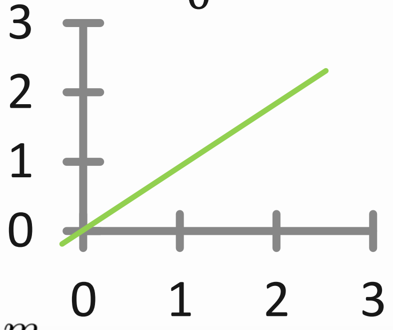
Goal: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

Simplified

$$h_\theta(x) = \theta_1 x$$

$\theta_0 = 0$

θ_1



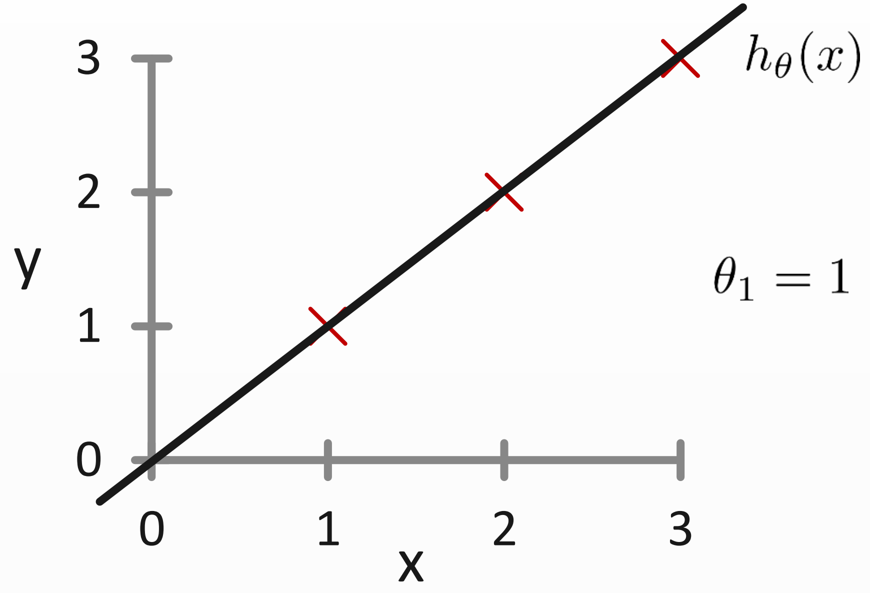
$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$\underset{\theta_1}{\text{minimize}}\ J(\theta_1)$

Cost Function Intuition

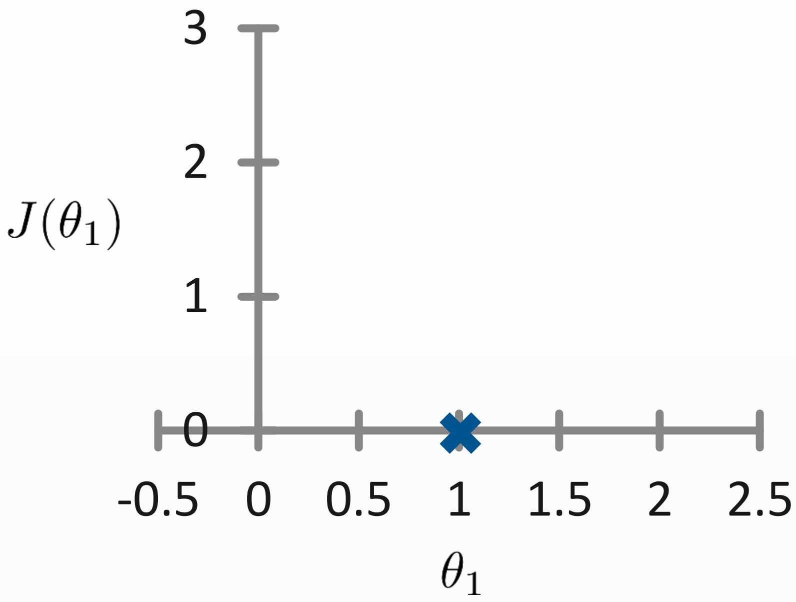
$$h_\theta(x)$$

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



$$J(\theta_1)$$

(function of the parameter θ_1)



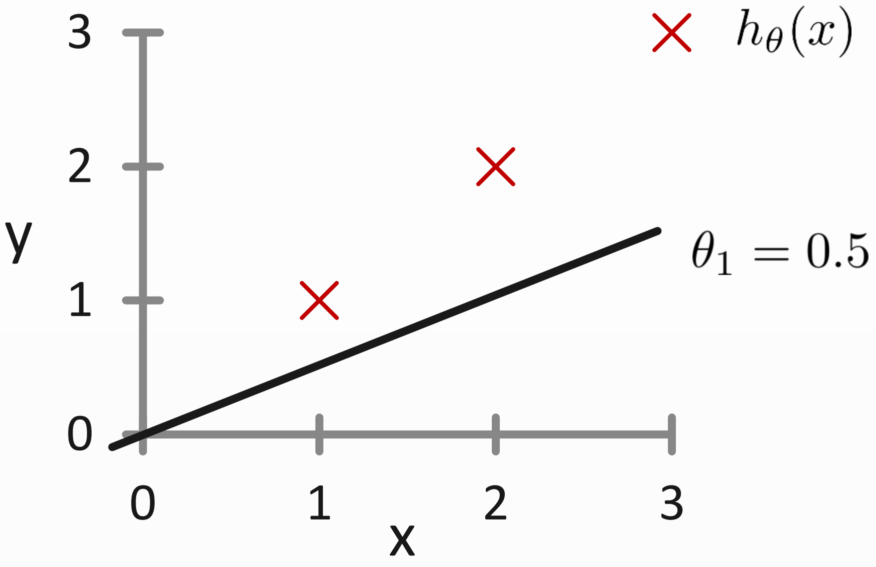
$$J(\theta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

$$= \frac{1}{2m}\sum_{i=1}^{m}\left(\theta_1 x^{(i)} - y^{(i)}\right)^2 \longrightarrow J(1) = \frac{1}{2m}(0+0+0)^2 = 0$$

Cost Function Intuition

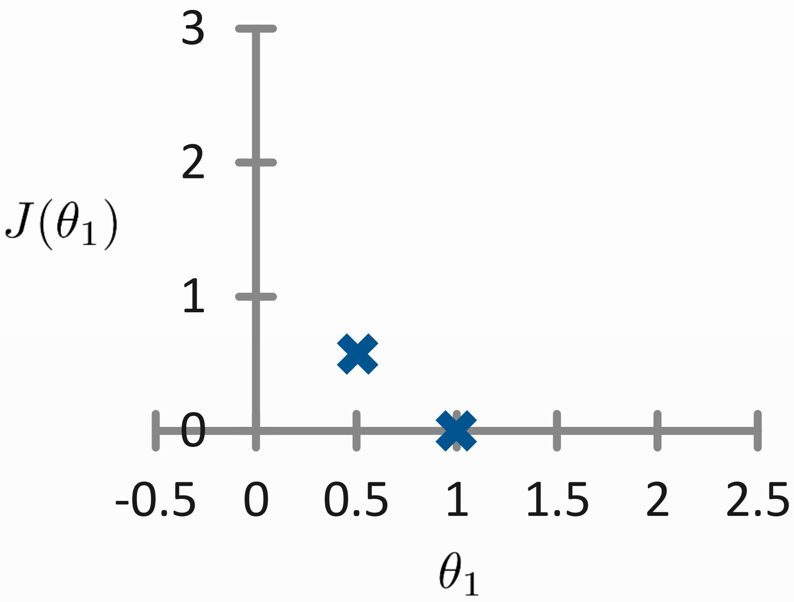
$$h_\theta(x)$$

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



$$J(\theta_1)$$

(function of the parameter θ_1)

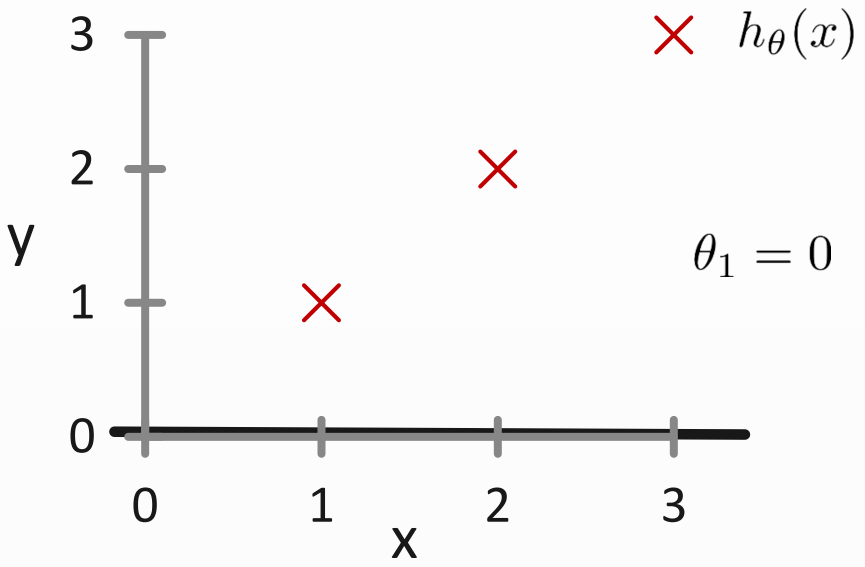


$$J(0.5) = \frac{1}{2 \times 3}[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2] = \frac{3.5}{6} = 0.58$$

Cost Function Intuition

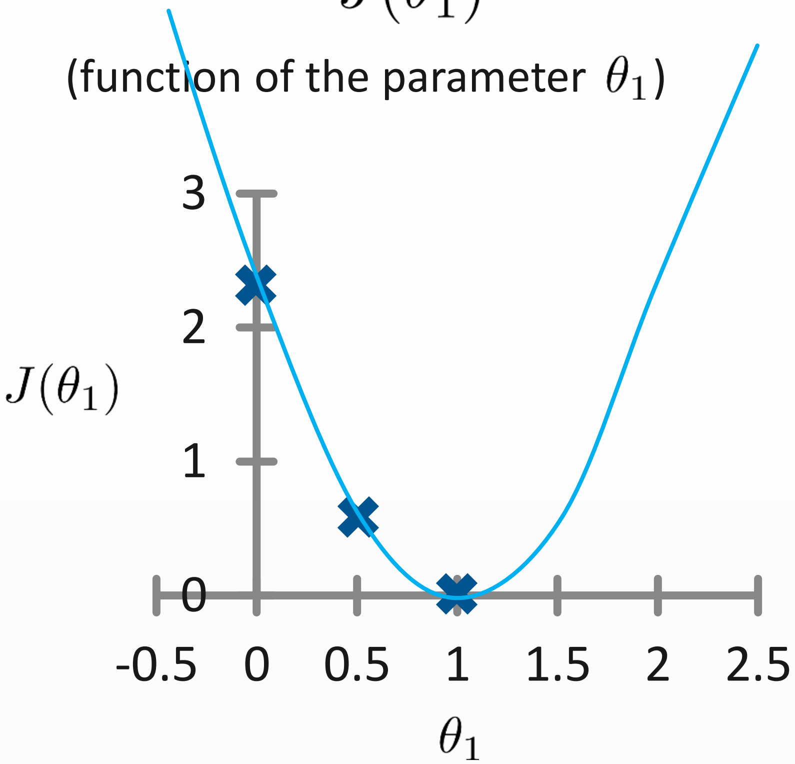
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



$\min_{\theta_1} J(\theta_1)$

$$J(0) = \frac{1}{2 \times 3}[(0-1)^2 + (0-2)^2 + (0-3)^2] = \frac{14}{6} = 2.33$$

Cost Function Intuition

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

Parameters: θ_0, θ_1

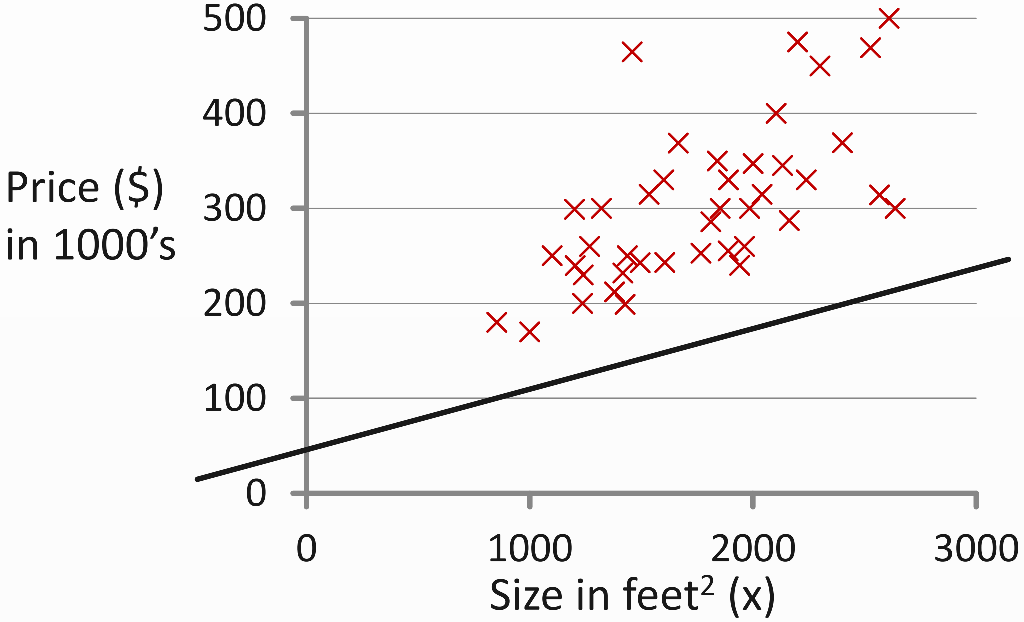
Cost Function: $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$

Goal: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

Cost Function Intuition

$$h_\theta(x)$$

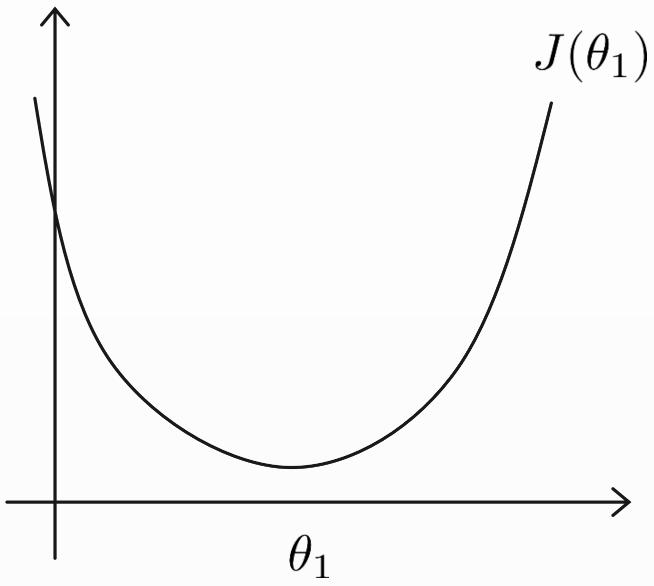
(for fixed θ_0, θ_1, this is a function of x)



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

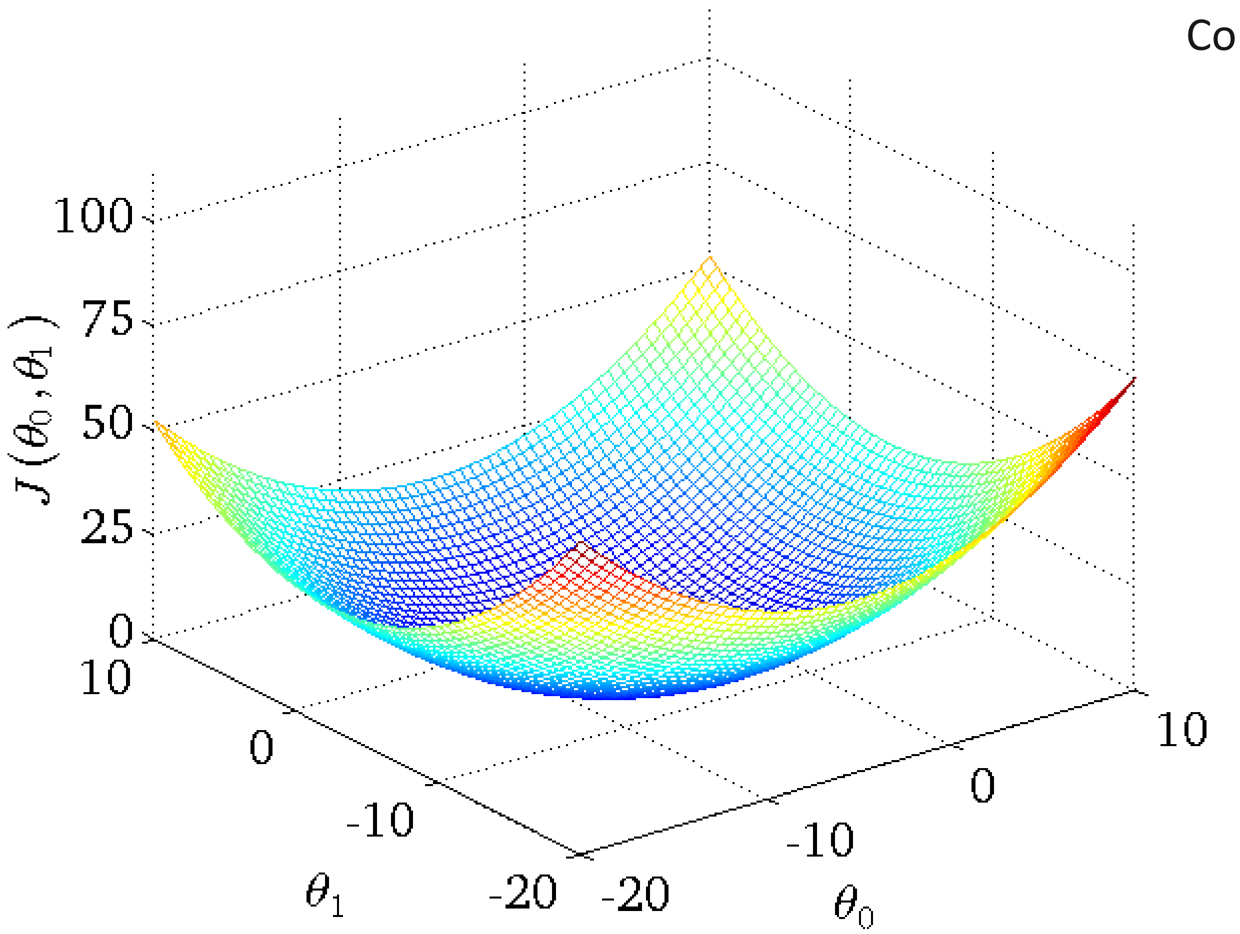
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



$\boxed{\theta_0, \theta_1}$

Cost Function Intuition



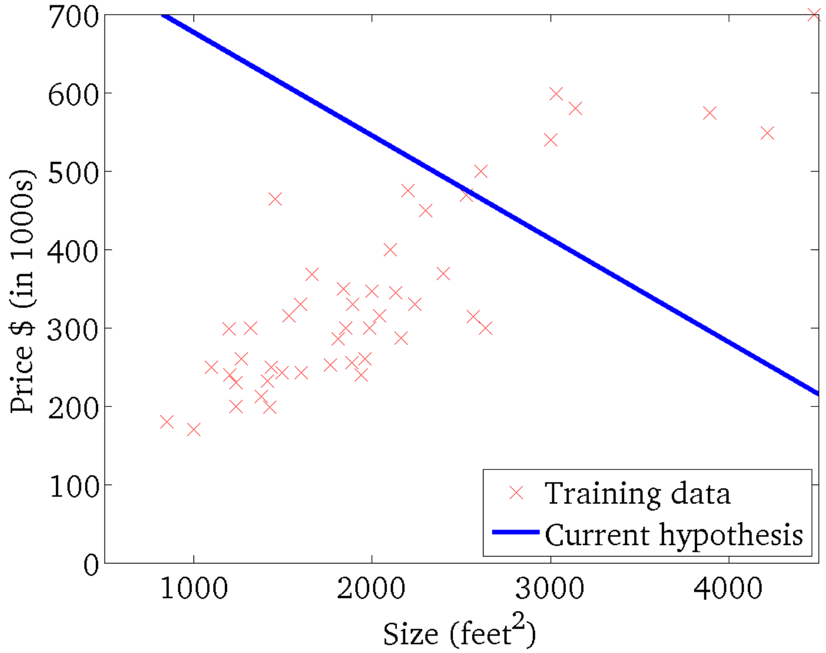
Contour plots

$J(\theta_0, \theta_1)$

Cost Function Intuition

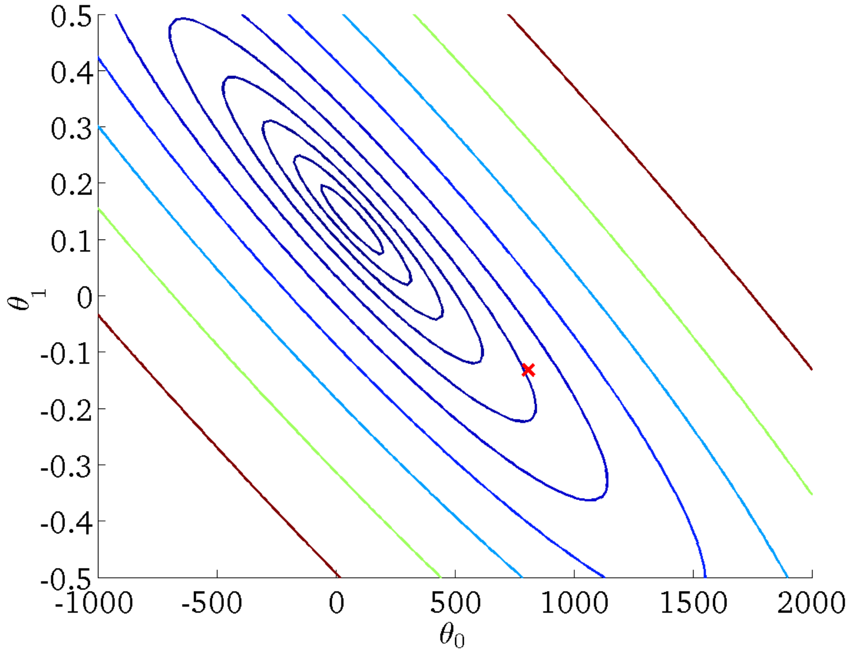
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

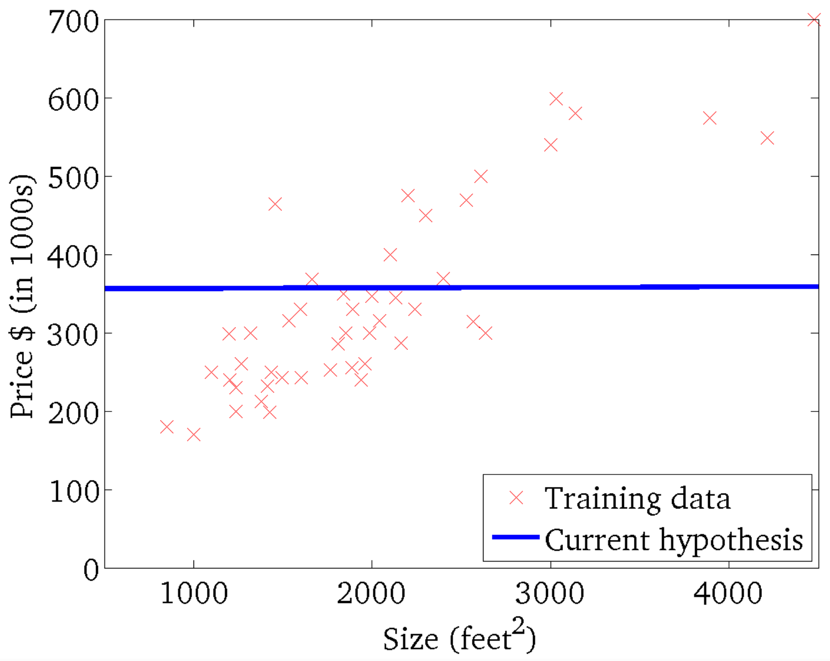
(function of the parameters θ_0, θ_1)



Cost Function Intuition

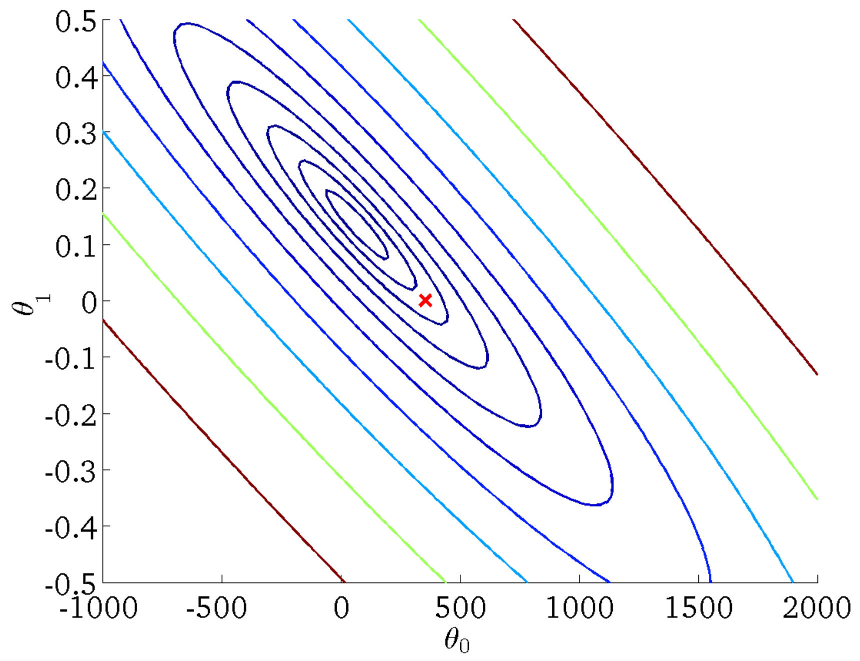
$$h_\theta(x)$$

(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

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

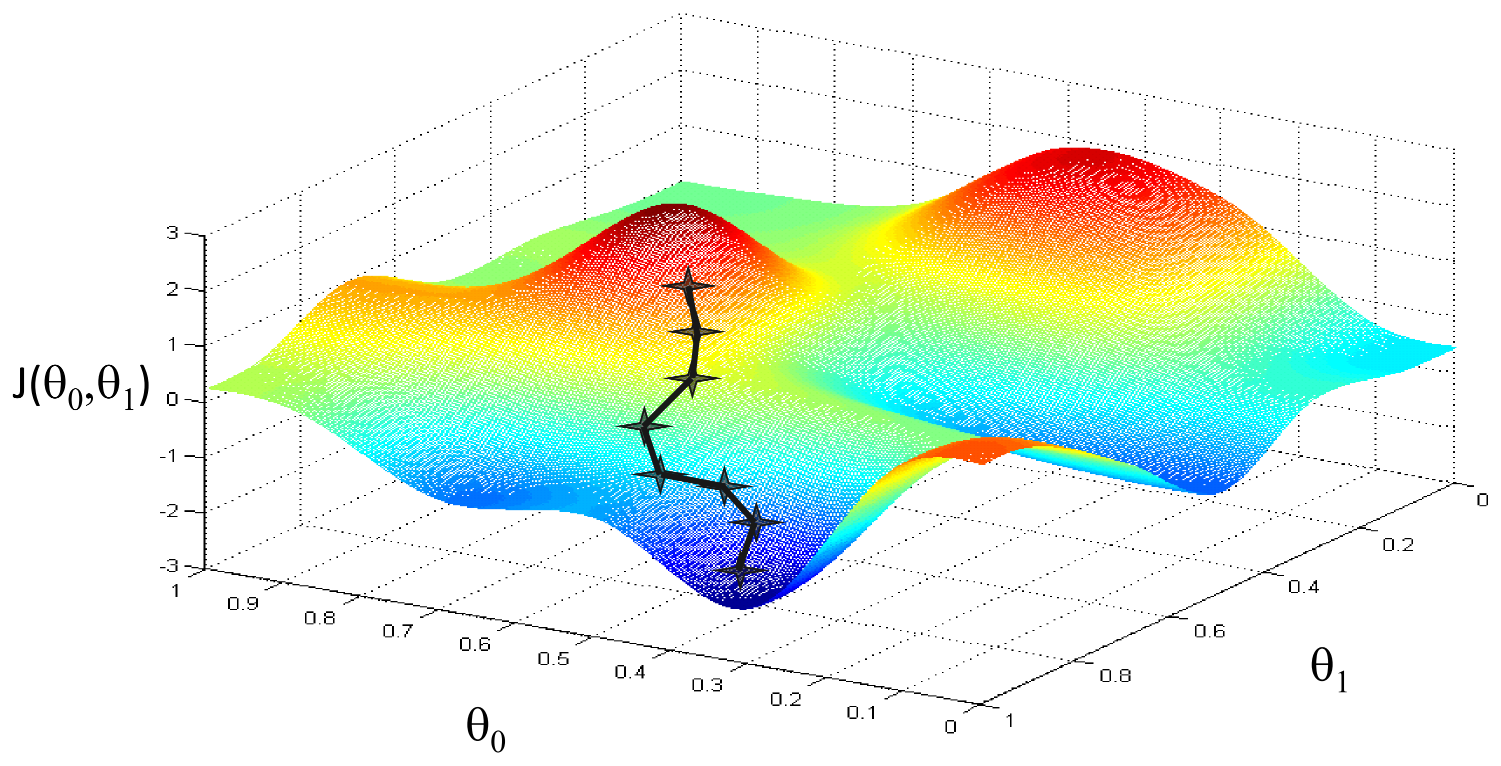
Want $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$

Outline:

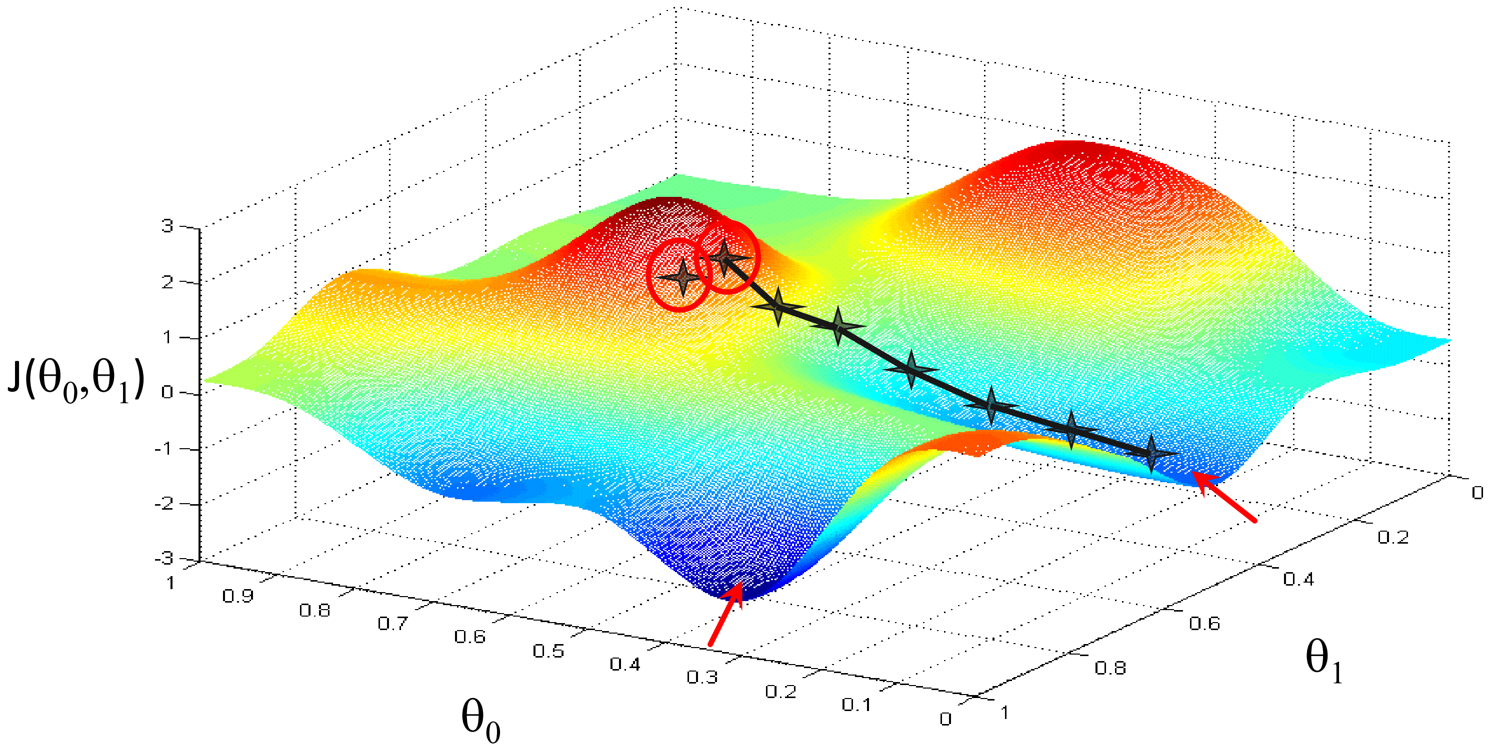
- Start with some θ_0, θ_1
- Keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$

  until we hopefully end up at a minimum

Gradient Descent



Gradient Descent



Gradient Descent Algorithm

$$
\begin{aligned}
&\text{repeat until convergence } \{ \\
&\quad \theta_j := \theta_j - \underbrace{\alpha}_{\text{learning rate}} \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \qquad (\text{for } j = 0 \text{ and } j = 1) \\
&\}
\end{aligned}
$$

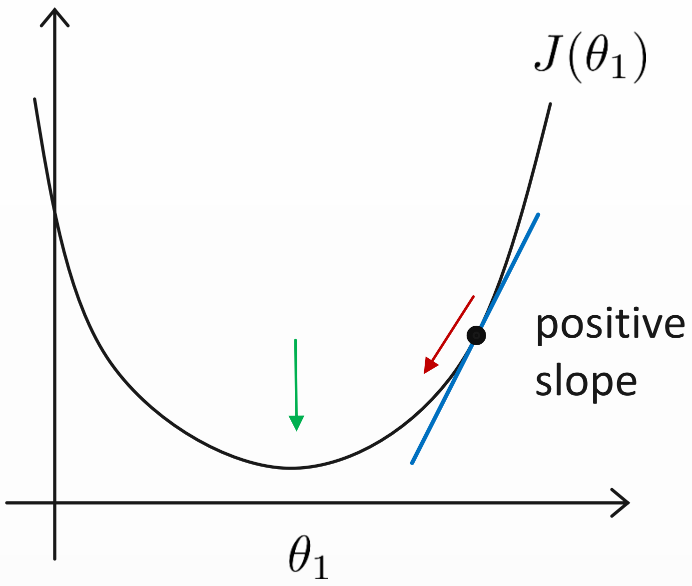
Correct: Simultaneous update

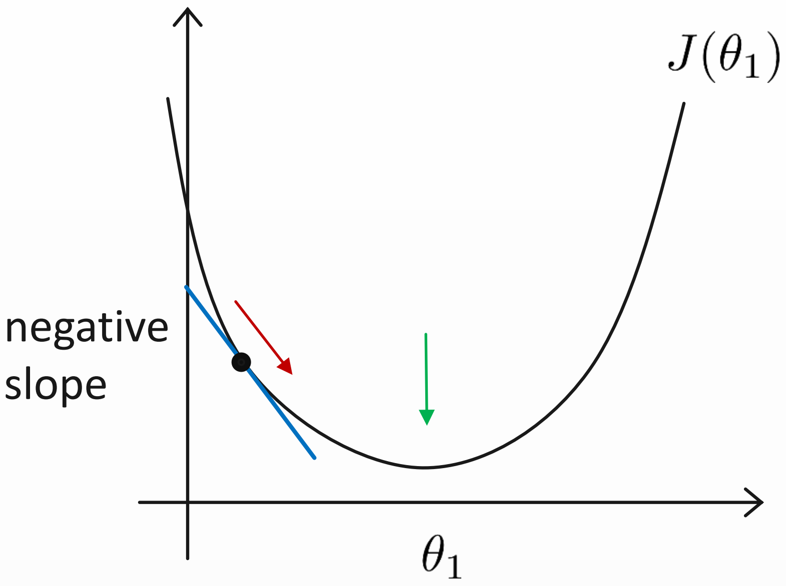
$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$
$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$
$\theta_0 := \text{temp0}$
$\theta_1 := \text{temp1}$

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 Intuition





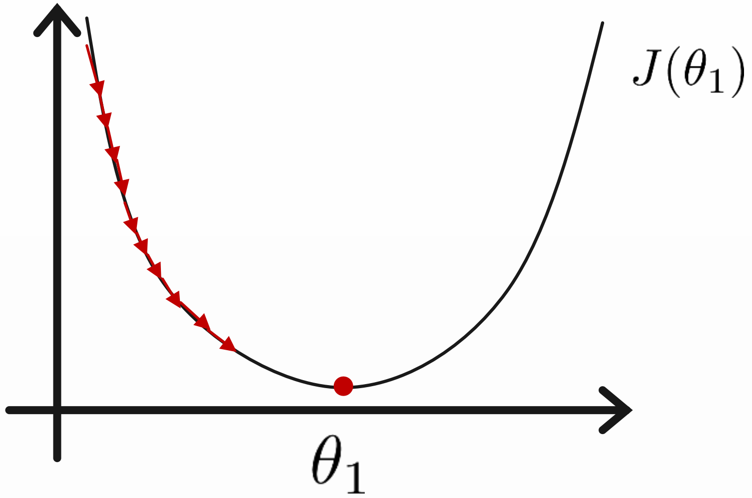
$$\theta_1 := \theta_1 - \alpha \underbrace{\boxed{\frac{\partial}{\partial \theta_1} J(\theta_1)}}_{\geq 0}$$

$$\theta_1 := \theta_1 - \alpha \underbrace{\boxed{\frac{\partial}{\partial \theta_1} J(\theta_1)}}_{\leq 0}$$

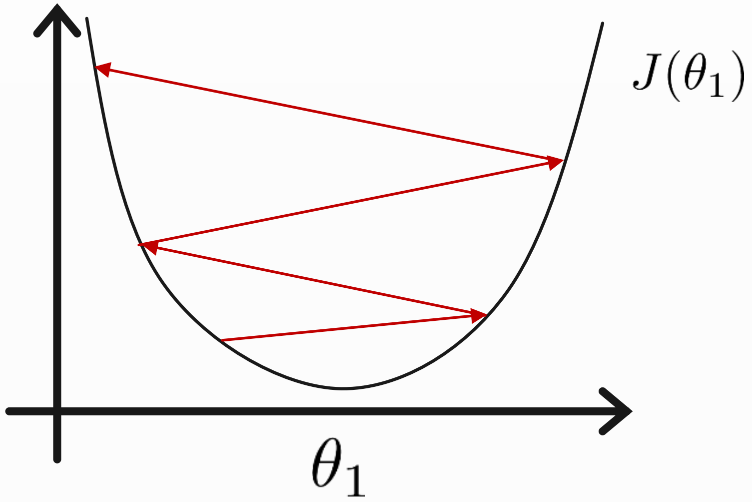
Gradient Descent Intuition

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

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

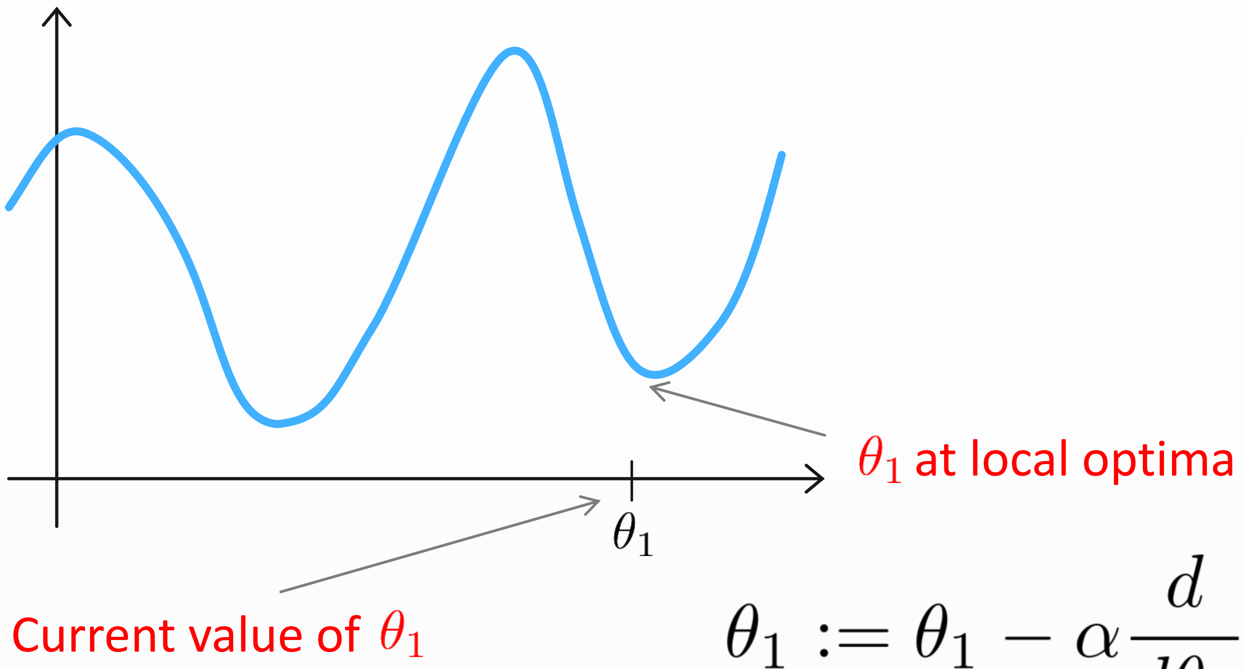


If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.



Gradient Descent Intuition

- Gradient descent can converge to a local minimum, even with the learning rate α fixed



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

- As we approach a local minimum, gradient descent will automatically take smaller steps

Gradient Descent for Linear Regression

Gradient descent algorithm

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

Linear Regression Model

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

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

Gradient Descent for Linear Regression

In order to implement this algorithm, we need to calculate the partial derivatives:

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

$$\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) = \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right)^2$$

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

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

Gradient Descent for Linear Regression

repeat until convergence {

$$\theta_0 := \theta_0 - \alpha \overbrace{\boxed{\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)}}^{\frac{\partial}{\partial\theta_0}J(\theta_0,\theta_1)}$$

$$\theta_1 := \theta_1 - \alpha \underbrace{\boxed{\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)\cdot x^{(i)}}}_{\frac{\partial}{\partial\theta_1}J(\theta_0,\theta_1)}$$

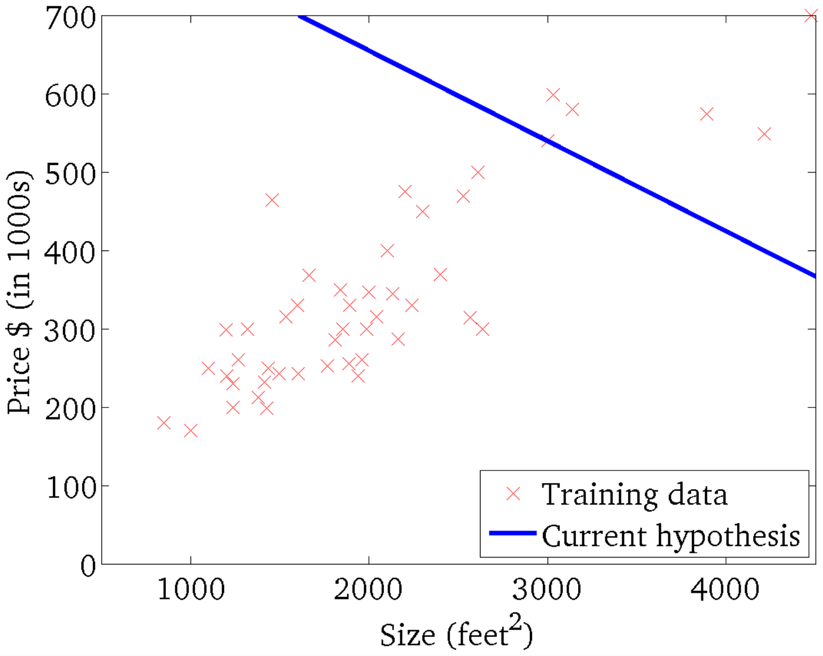
}

update θ_0 and θ_1 simultaneously

Gradient Descent for Linear Regression

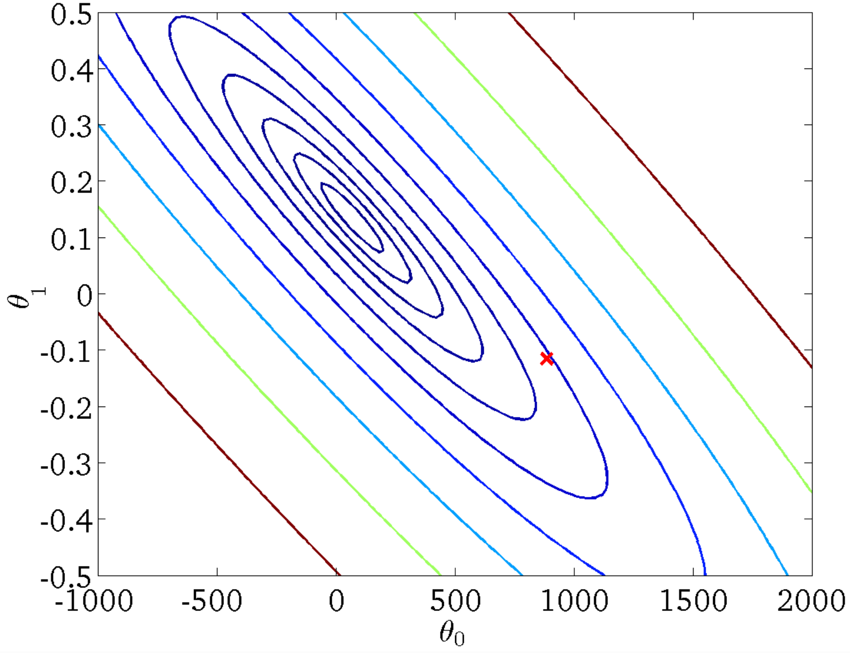
$$h_\theta(x)$$

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



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

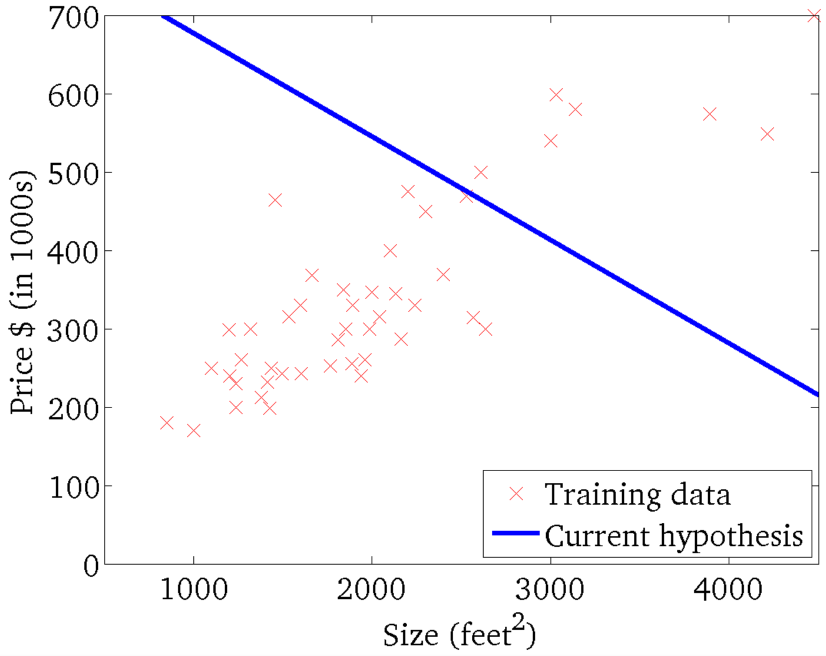
(function of the parameters θ_0, θ_1)



Gradient Descent for Linear Regression

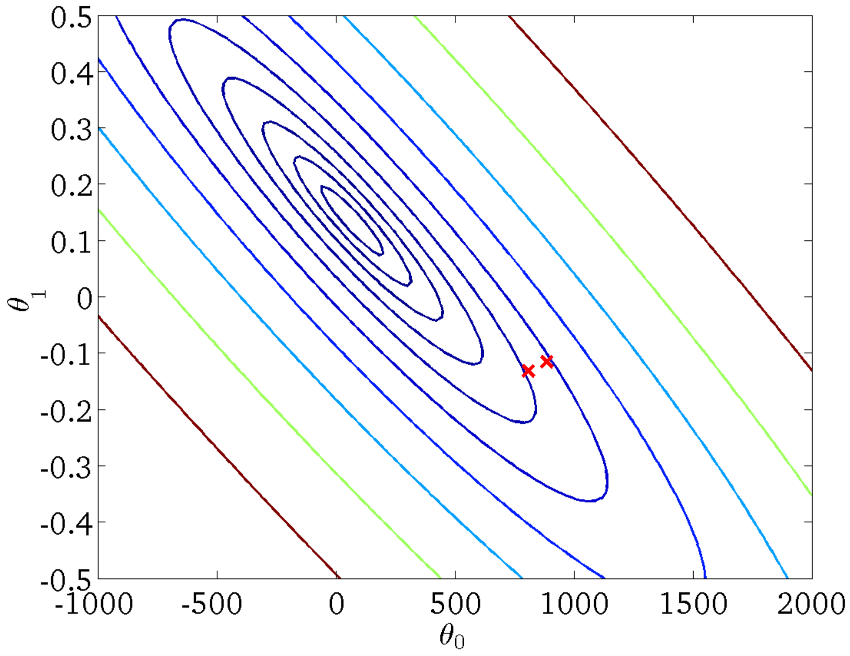
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

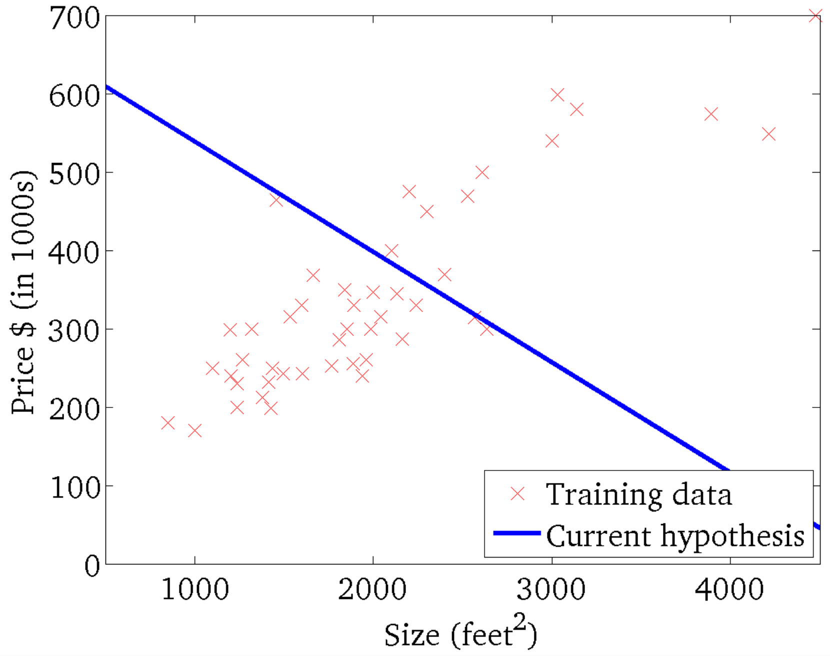
(function of the parameters θ_0, θ_1)



Gradient Descent for Linear Regression

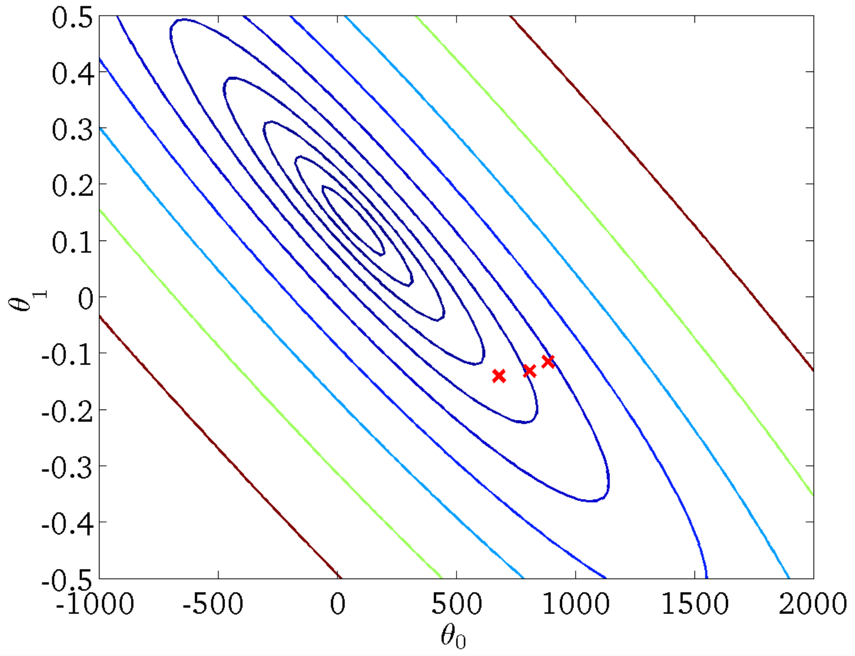
$$h_\theta(x)$$

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



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

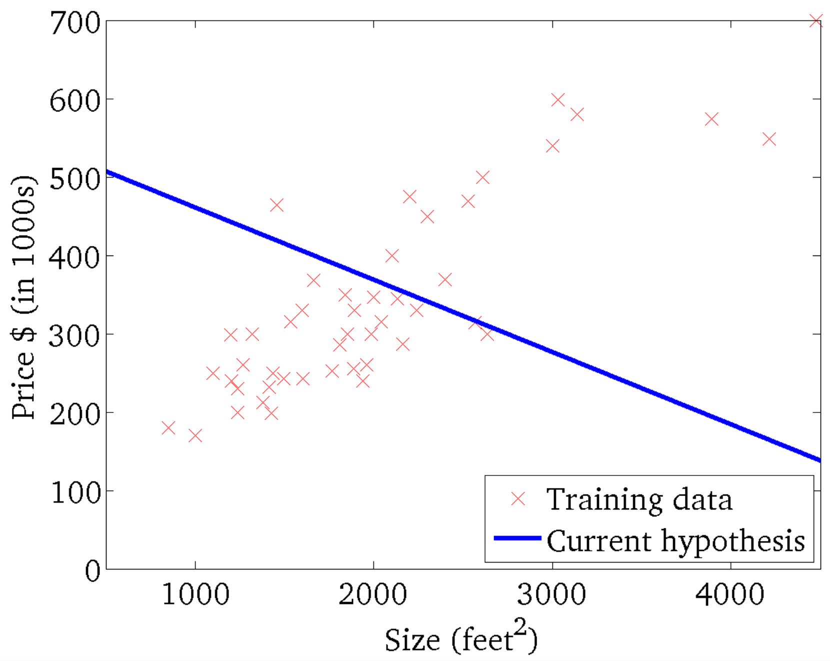
(function of the parameters θ_0, θ_1)



Gradient Descent for Linear Regression

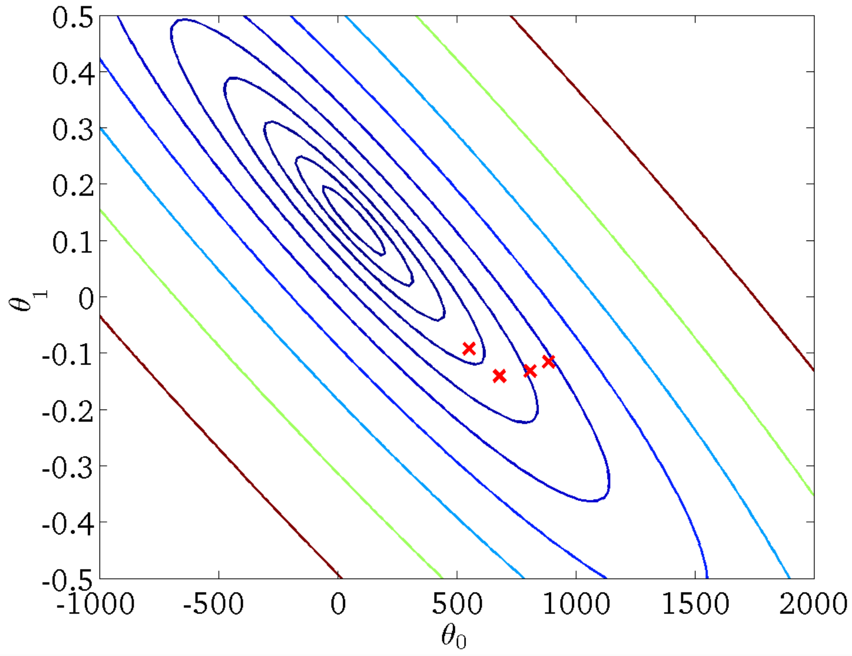
$$h_\theta(x)$$

(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)



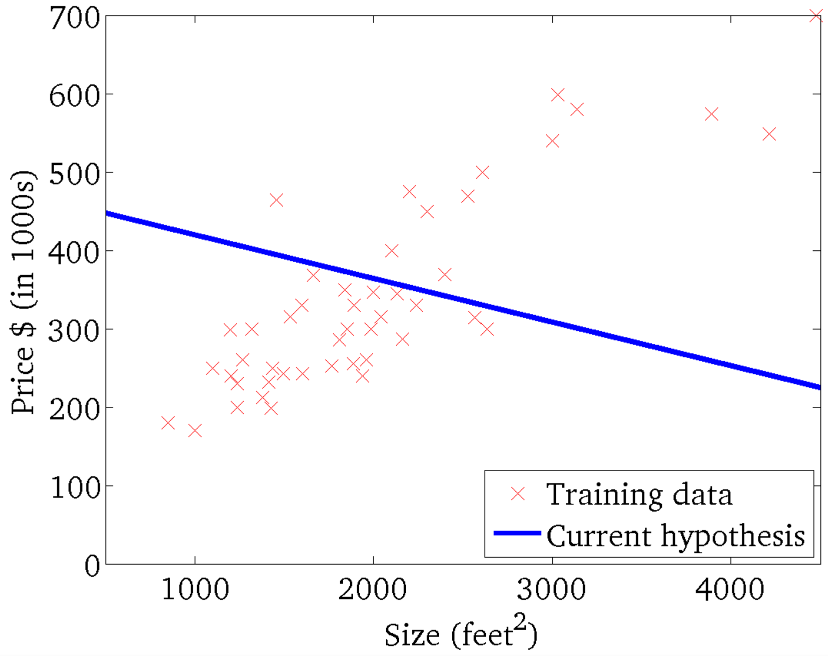
Gradient Descent for Linear Regression

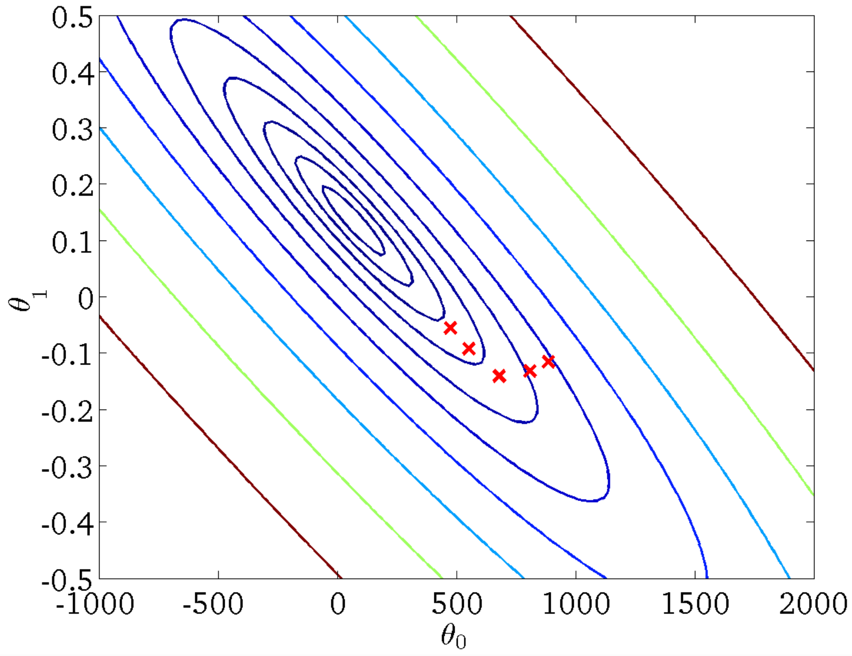
$$h_\theta(x)$$

(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)

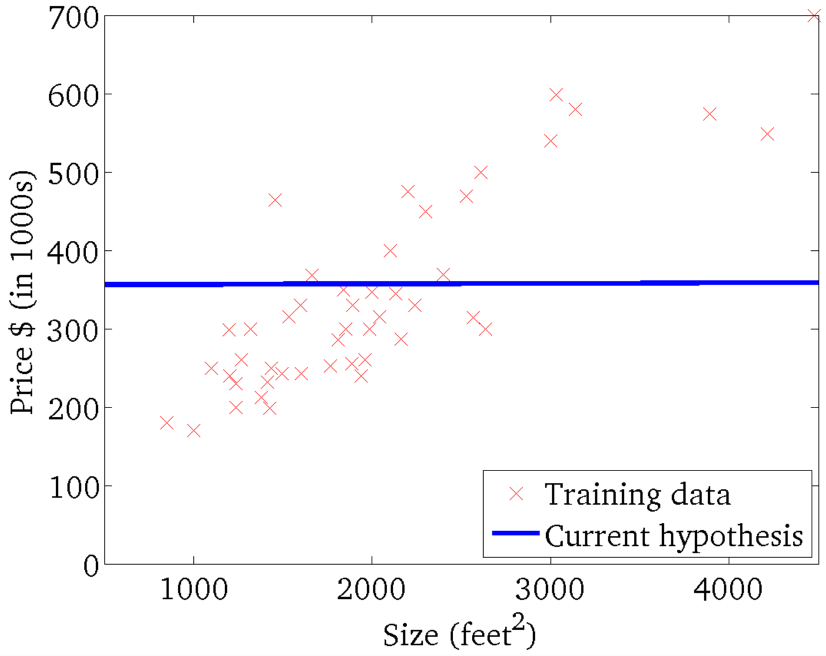




Gradient Descent for Linear Regression

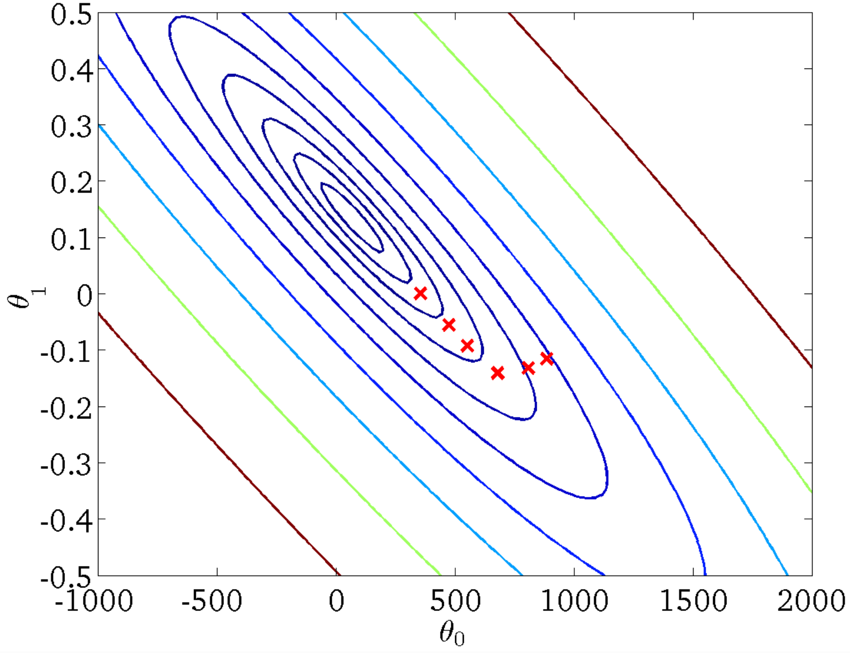
$$h_\theta(x)$$

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



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

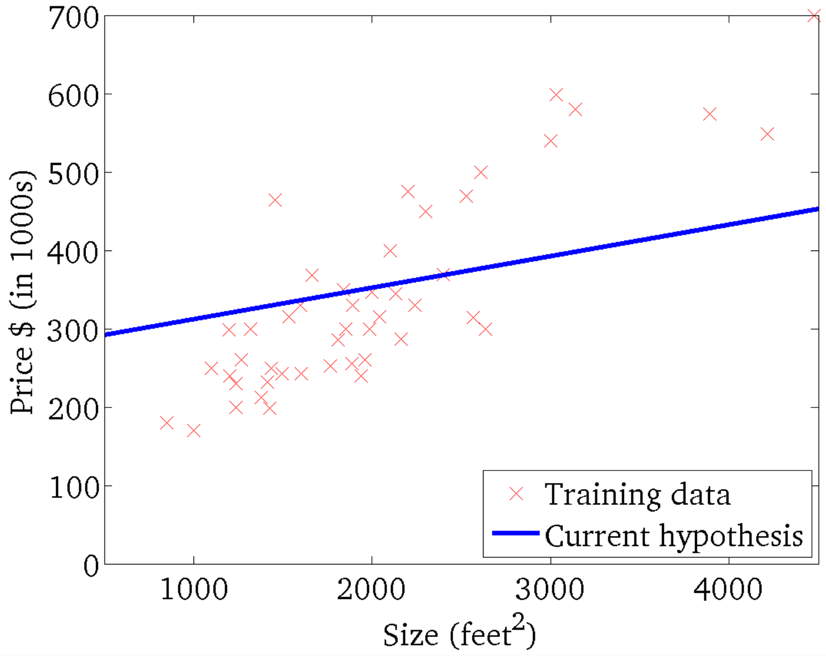
(function of the parameters θ_0, θ_1)



Gradient Descent for Linear Regression

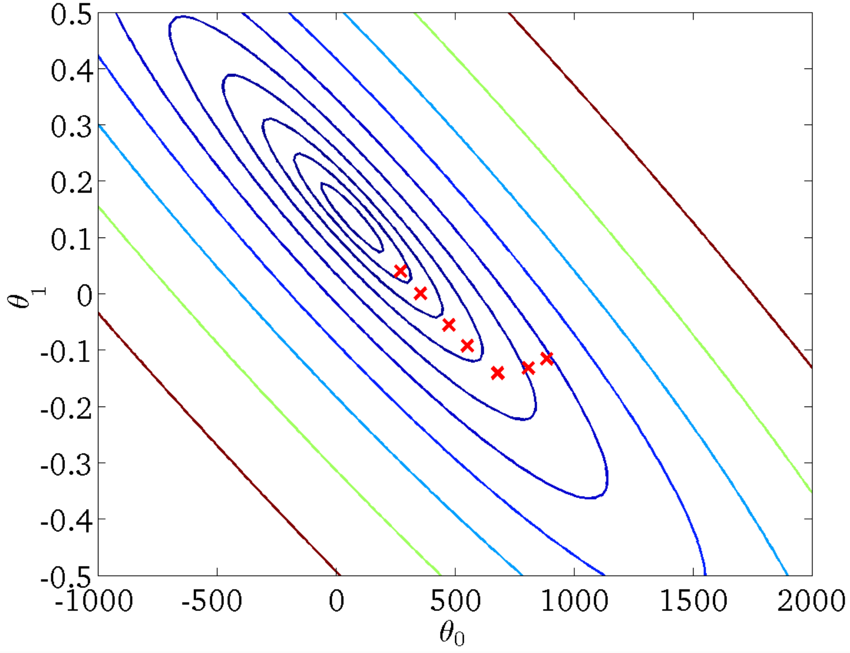
$$h_\theta(x)$$

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



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

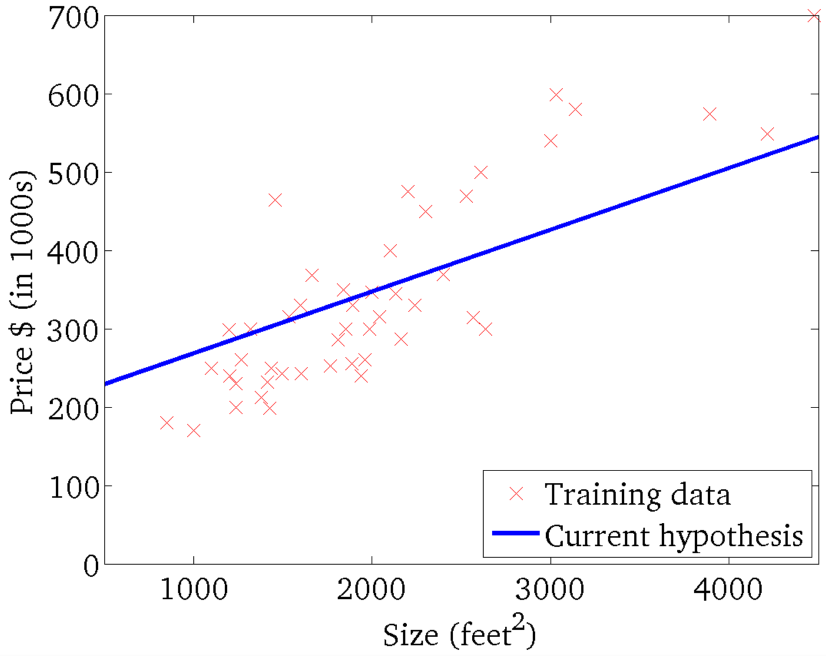
(function of the parameters θ_0, θ_1)



Gradient Descent for Linear Regression

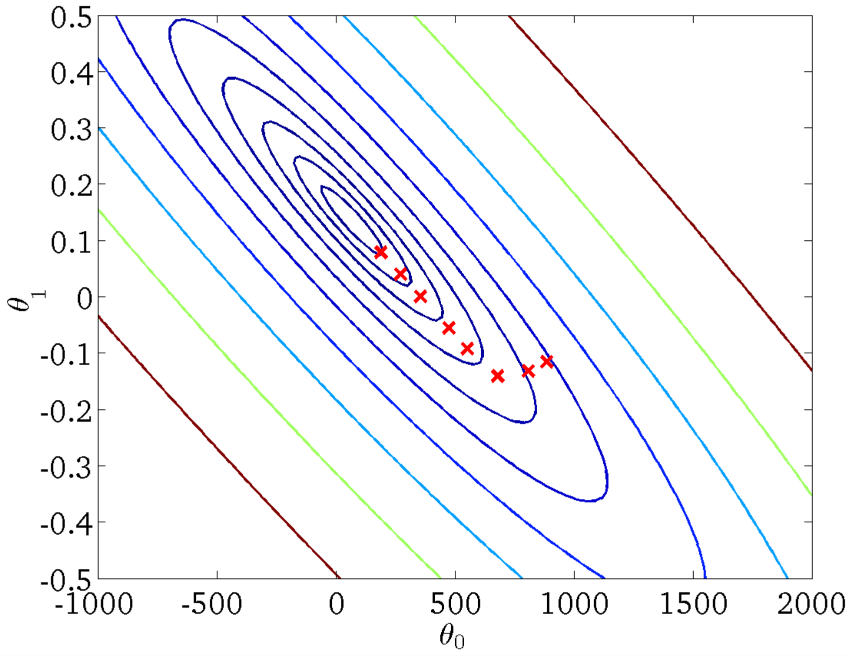
$$h_\theta(x)$$

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



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

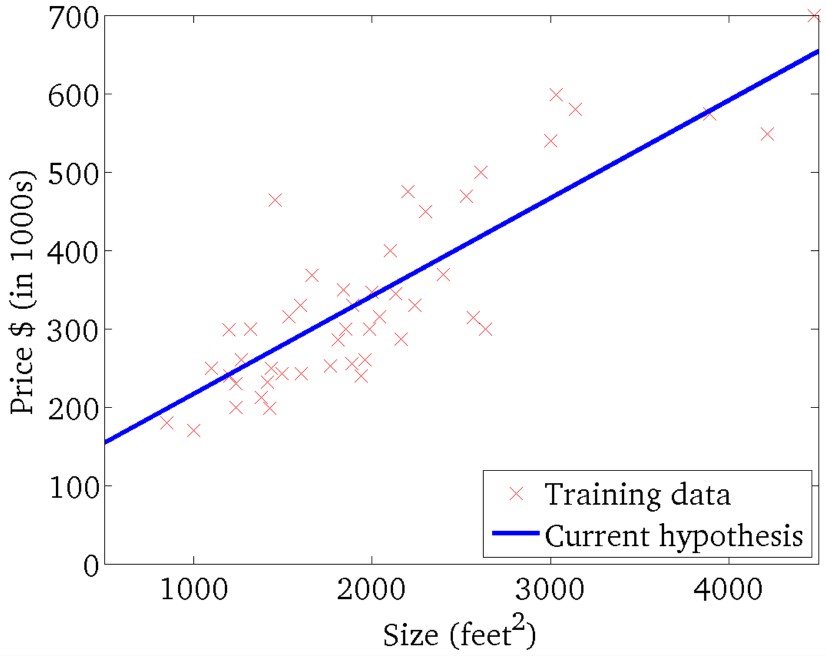
(function of the parameters θ_0, θ_1)



Gradient Descent for Linear Regression

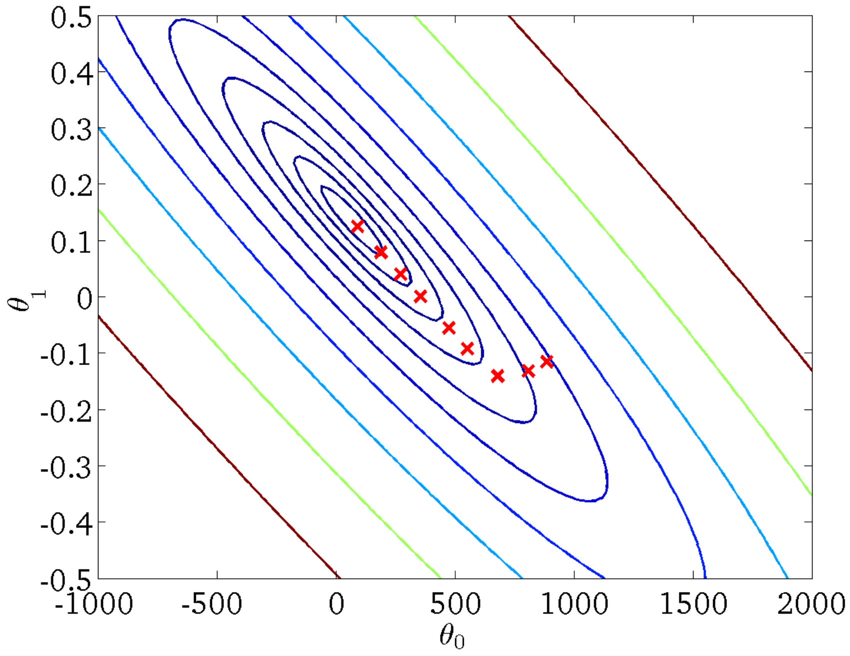
$$h_\theta(x)$$

(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)



Multiple Features (Variables)

Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

Notation:

n = number of features

$x^{(i)}$ = input (features) of i^{th} training example.

$x_j^{(i)}$ = value of feature j in i^{th} training example.

$$x^{(2)} = \begin{bmatrix} 1416 \\ 3 \\ 2 \\ 40 \end{bmatrix}$$

$$x_3^{(2)} = 2$$

Multiple Features (Variables)

Hypothesis:

Previously: $h_\theta(x) = \theta_0 + \theta_1 x$

Now: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$

For convenience of notation, define $x_0 = 1$

$$h_\theta(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

Multivariate linear regression

Gradient Descent with Multiple Variables

Gradient Descent

Previously (n=1):

Repeat $\{$

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

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

(simultaneously update θ_0, θ_1)

$\}$

New algorithm $(n \geq 1)$:

Repeat $\{$

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

(simultaneously update θ_j for $j = 0, \ldots, n$)

$\}$

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

$x_0^{(i)} = 1$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

$$\theta_2 := \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_2^{(i)}$$

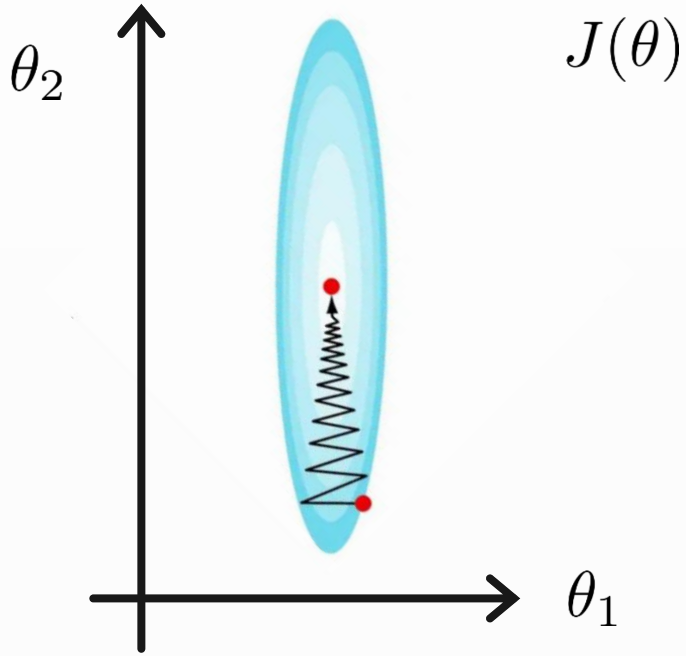
$\ldots$

Gradient Descent: Feature Scaling

Idea: Make sure features are on a similar scale

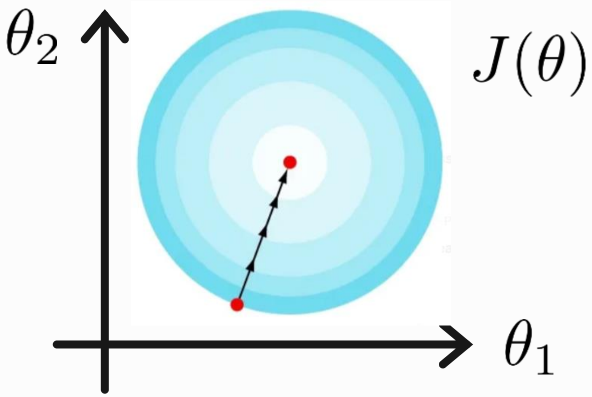
E.g. x_1 = size (0-2000 feet^2)

x_2 = number of bedrooms (1-5)



$$x_1 = \frac{\text{size (feet}^2\text{)}}{2000}$$

$$x_2 = \frac{\text{number of bedrooms}}{5}$$



Gradient Descent: Feature Scaling – Mean Normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (Do not apply to $x_0 = 1$).

E.g. $x_1 = \frac{size - 1000}{2000}$

$$x_2 = \frac{\#bedrooms - 2}{5}$$

$$-0.5 \leq x_1 \leq 0.5, -0.5 \leq x_2 \leq 0.5$$

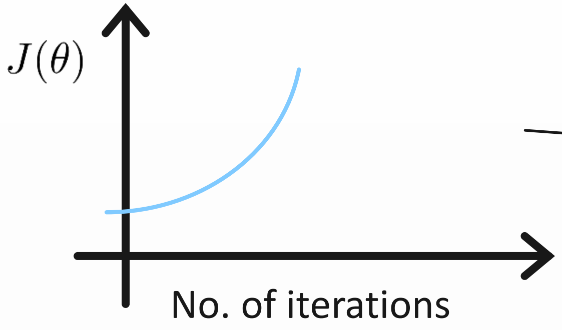
$$x_1 \leftarrow \frac{x_1 - \mu_1}{s_1} \qquad x_2 \leftarrow \frac{x_2 - \mu_2}{s_2}$$

μ_i: average value of x_i in training set

s_i: range (max-min) or standard deviation

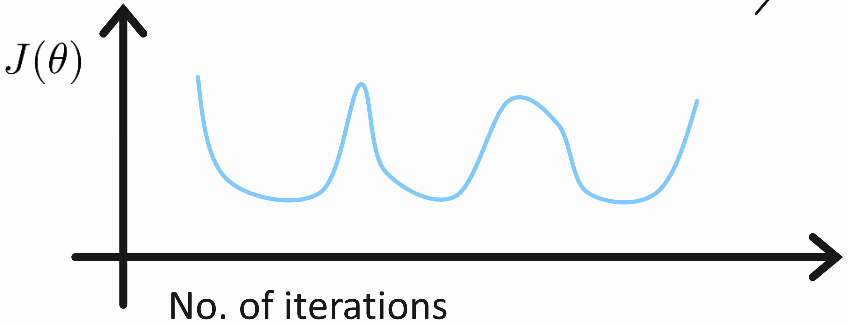
Gradient Descent: Learning Rate

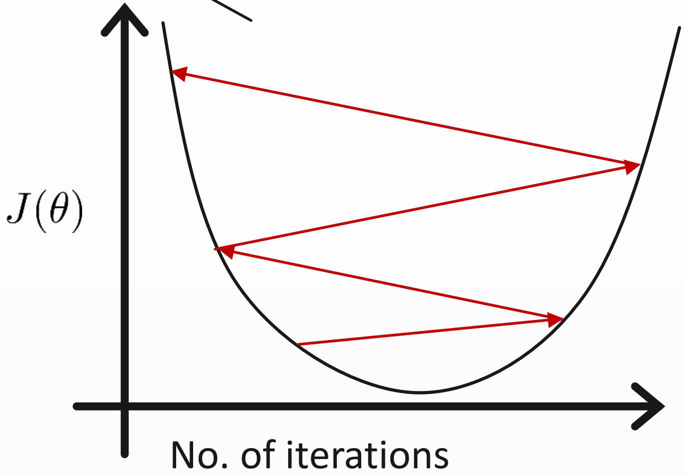
Making sure gradient descent is working correctly.



Gradient descent not working.

Use smaller α.





- For sufficiently small α, $J(\theta)$ should decrease on every iteration.
- But if α is too small, gradient descent can be slow to converge.

Gradient Descent: Learning Rate

- If α is too small: slow convergence.
- If α is too large: $J(\theta)$ may not decrease on every iteration; may not converge.

To choose α, try

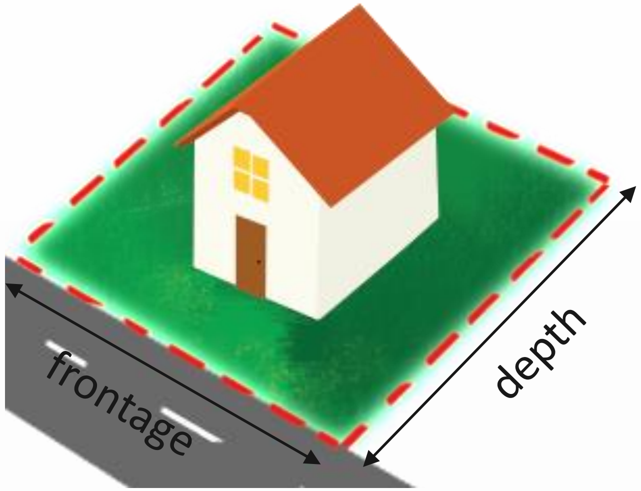
$$\ldots, 0.001, 0.003, 0.01, 0.03, 0.1, \ldots$$

$\xrightarrow{}$
3x

Features and Polynomial Regression

Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times frontage + \theta_2 \times depth$$



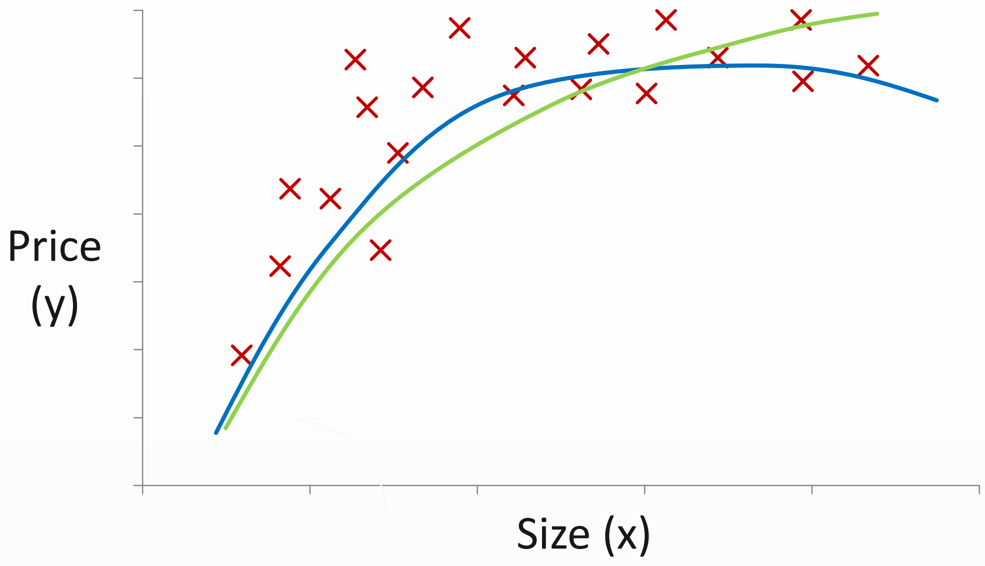
Area:

x = frontage * depth

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

Features and Polynomial Regression

Choice of features



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

$$h_\theta(x) = \theta_0 + \theta_1(size) + \theta_2\sqrt{(size)}$$

Normal Equation

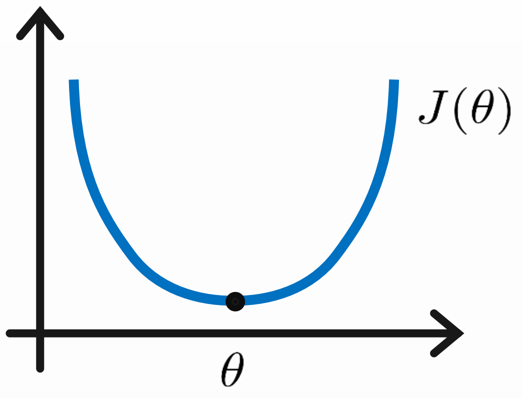
Normal equation: Method to solve for analytically.

Intuition: If 1D $(\theta \in \mathbb{R})$

$$J(\theta) = a\theta^2 + b\theta + c$$

$$\frac{\partial}{\partial\theta} J(\theta) = 0$$

Solve for θ



$\theta \in \mathbb{R}^{n+1}$ $\quad J(\theta_0, \theta_1, \ldots, \theta_m) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$

$$\frac{\partial}{\partial\theta_j} J(\theta) = \cdots = 0 \qquad \text{(for every } j\text{)}$$

Solve for $\theta_0, \theta_1, \ldots, \theta_n$

Normal Equation

Examples: $m = 5$.

x_0	Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
1	2104	5	1	45	460
1	1416	3	2	40	232
1	1534	3	2	30	315
1	852	2	1	36	178
1					

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \\ 1 & 3000 & 4 & 1 & 38 \end{bmatrix} \qquad y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \\ 540 \end{bmatrix}$$

$$\Theta = (X^T X)^{-1} X^T y$$

Gradient Descent vs Normal Equation

m training examples, n features.

Gradient Descent

- Need to choose α.
- Needs many iterations.
- Works well even when n is large.

Normal Equation

- No need to choose α.
- Don't need to iterate.
- Need to compute $(X^T X)^{-1}$
- Slow if n is very large.

References

- A. Ng. Machine Learning, Lecture Notes.
- I. Goodfellow, Y. Bengio and A. Courville, “Deep Learning”, 2016.