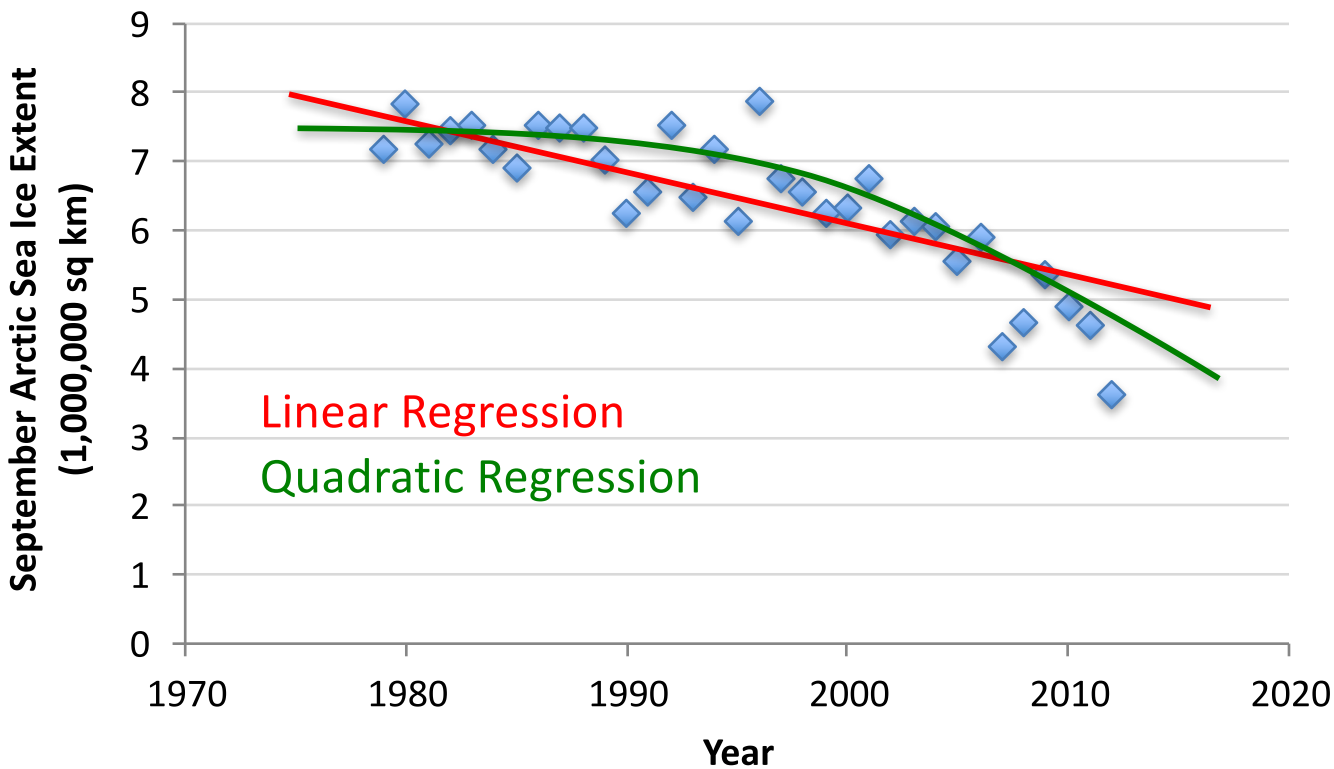
Linear Regression

These slides were assembled by Eric Eaton, with grateful acknowledgement of the many others who made their course materials freely available online. Feel free to reuse or adapt these slides for your own academic purposes, provided that you include proper attribution. Please send comments and corrections to Eric.

Regression

Given:

- Data $\boldsymbol{X} = \left\{ \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)} \right\}$ where $\boldsymbol{x}^{(i)} \in \mathbb{R}^d$
- Corresponding labels $\boldsymbol{y} = \left\{ y^{(1)}, \ldots, y^{(n)} \right\}$ where $y^{(i)} \in \mathbb{R}$



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

Prostate Cancer Dataset

- 97 samples, partitioned into 67 train / 30 test
- Eight predictors (features):
  - 6 continuous (4 log transforms), 1 binary, 1 ordinal
- Continuous outcome variable:
  - lpsa: log(prostate specific antigen level)

TABLE 3.2. *Linear model fit to the prostate cancer data. The Z score is the coefficient divided by its standard error (3.12). Roughly a Z score larger than two in absolute value is significantly nonzero at the $p = 0.05$ level.*

Term	Coefficient	Std. Error	Z Score
Intercept	2.46	0.09	27.60
lcavol	0.68	0.13	5.37
lweight	0.26	0.10	2.75
age	−0.14	0.10	−1.40
lbph	0.21	0.10	2.06
svi	0.31	0.12	2.47
lcp	−0.29	0.15	−1.87
gleason	−0.02	0.15	−0.15
pgg45	0.27	0.15	1.74

Based on slide by Jeff Howbert

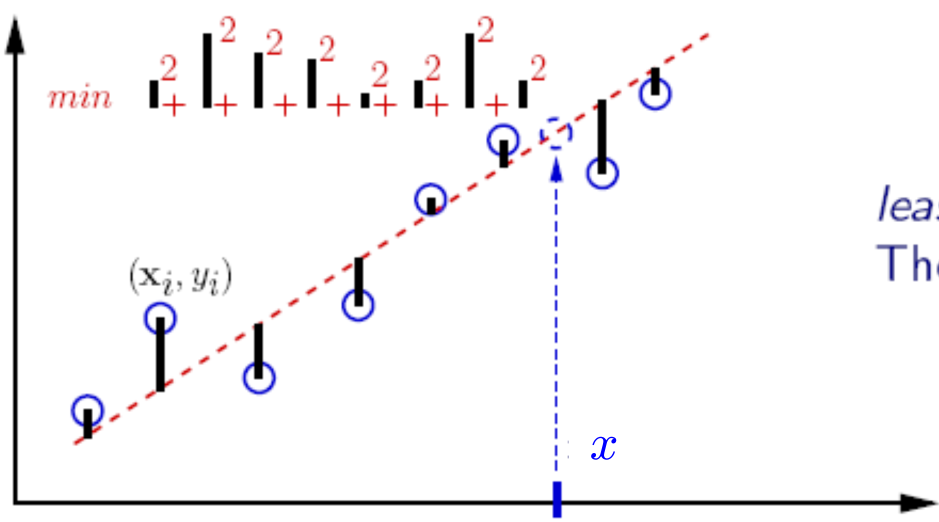
Linear Regression

- Hypothesis:

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \sum_{j=0}^{d} \theta_j x_j$$

Assume x_0 = 1

- Fit model by minimizing sum of squared errors



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

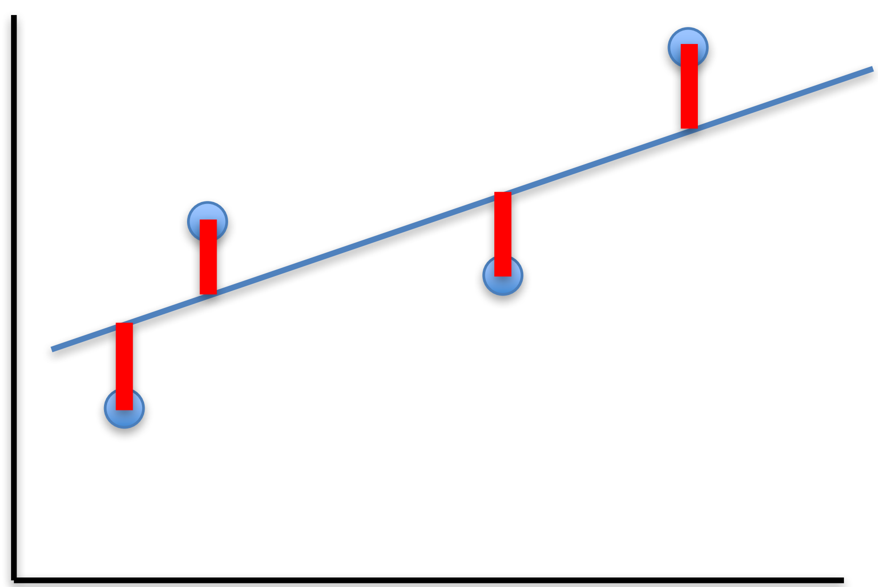
Figures are courtesy of Greg Shakhnarovich

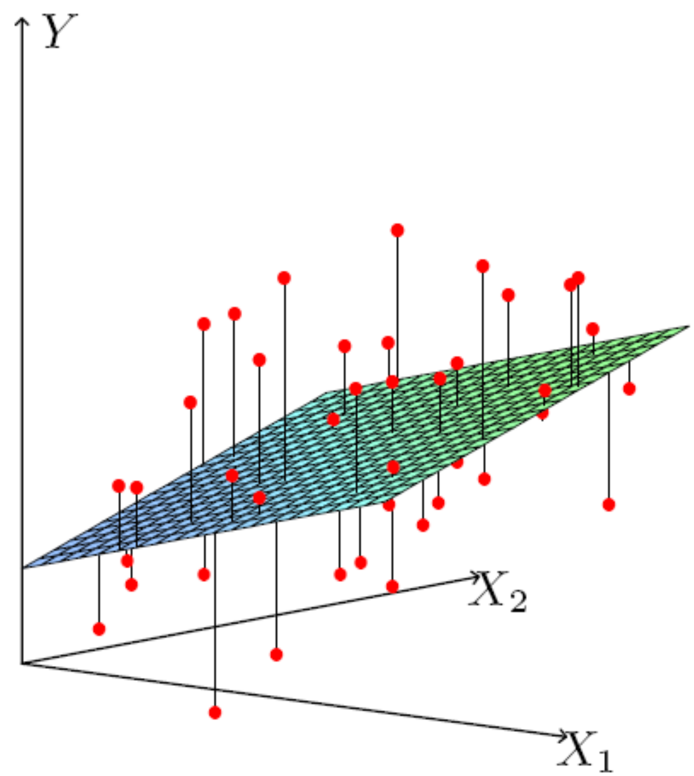
Least Squares Linear Regression

- Cost Function

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

- Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$





Intuition Behind Cost Function

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

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

Based on example
by Andrew Ng

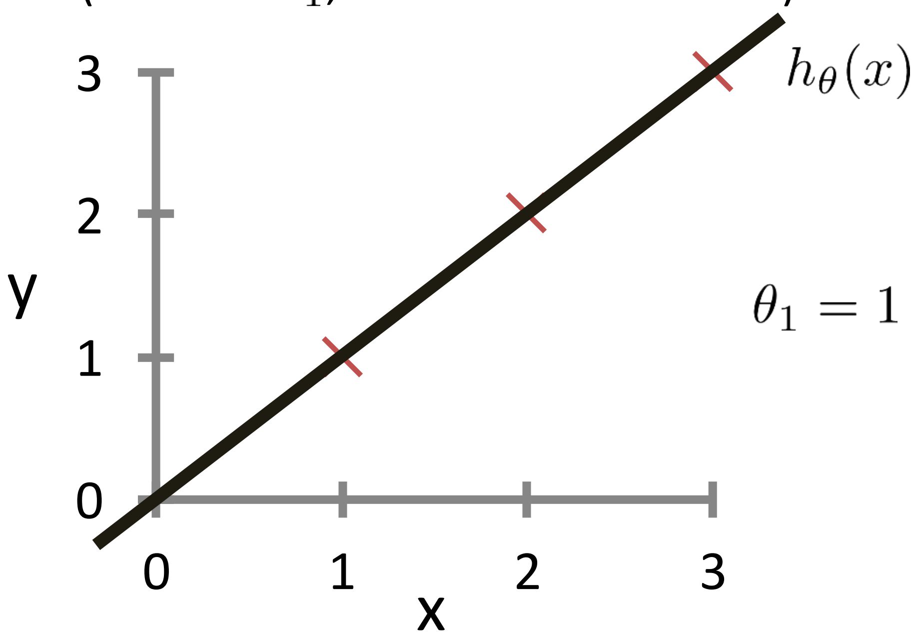
Intuition Behind Cost Function

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

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

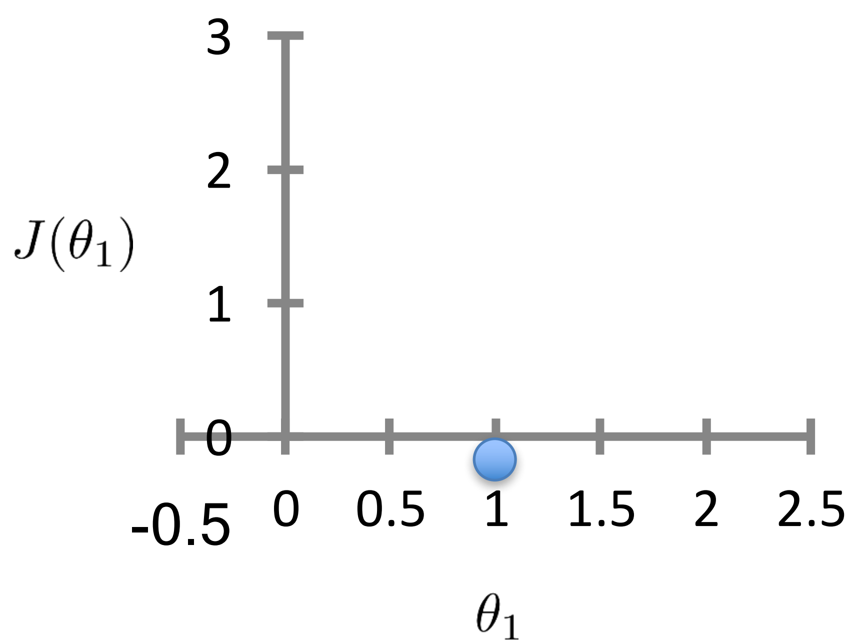
$h_\theta(x)$

(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

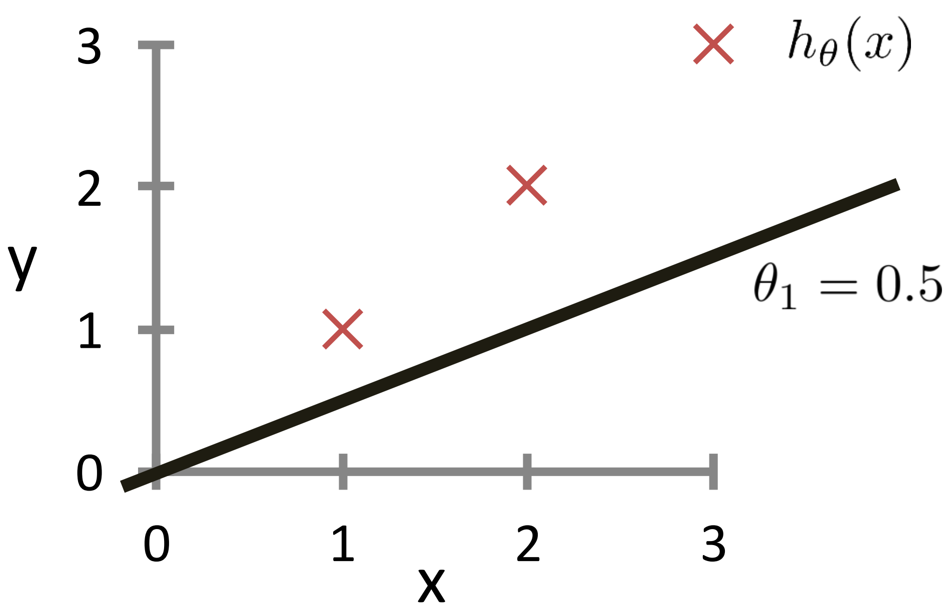
Intuition Behind Cost Function

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

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

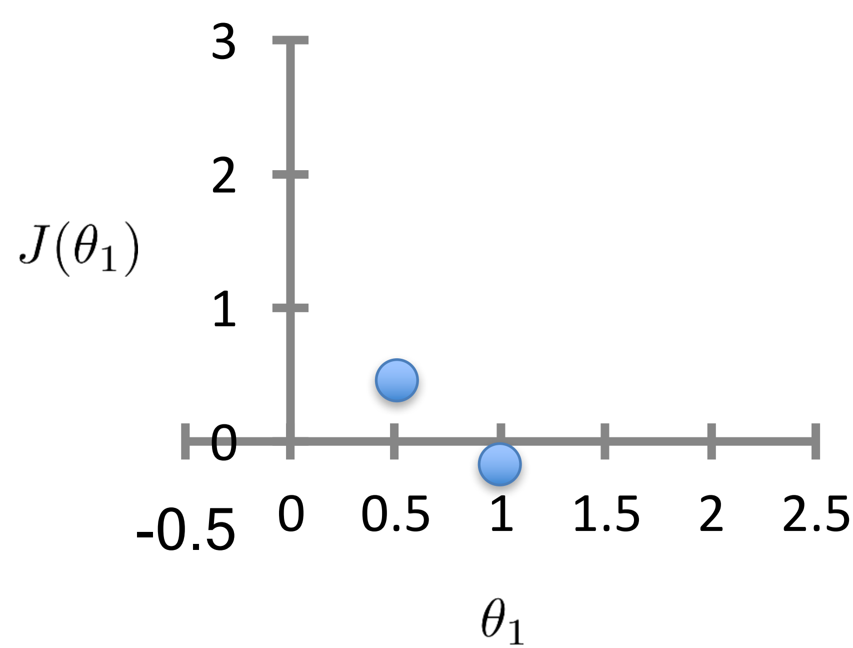
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



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

Based on example by Andrew Ng

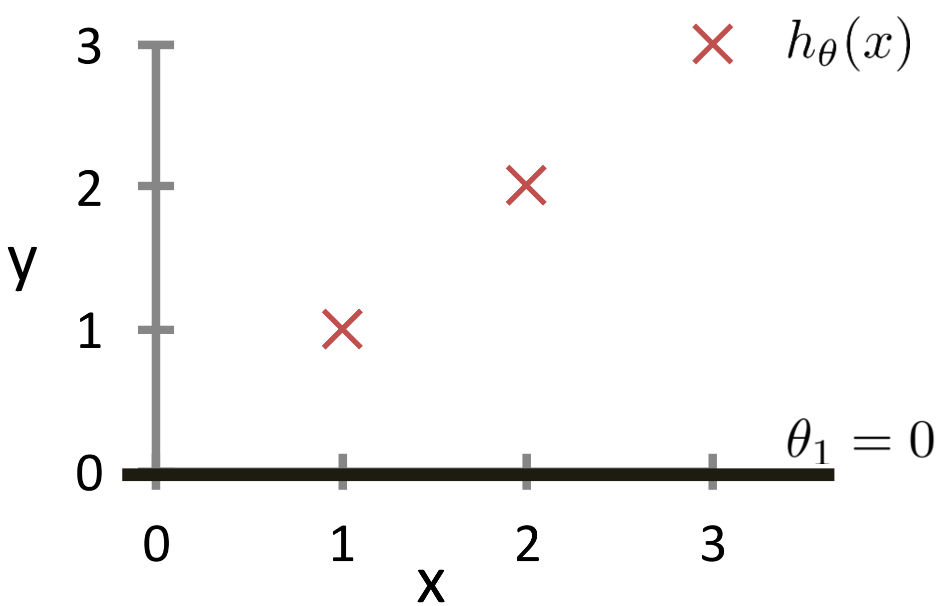
Intuition Behind Cost Function

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

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

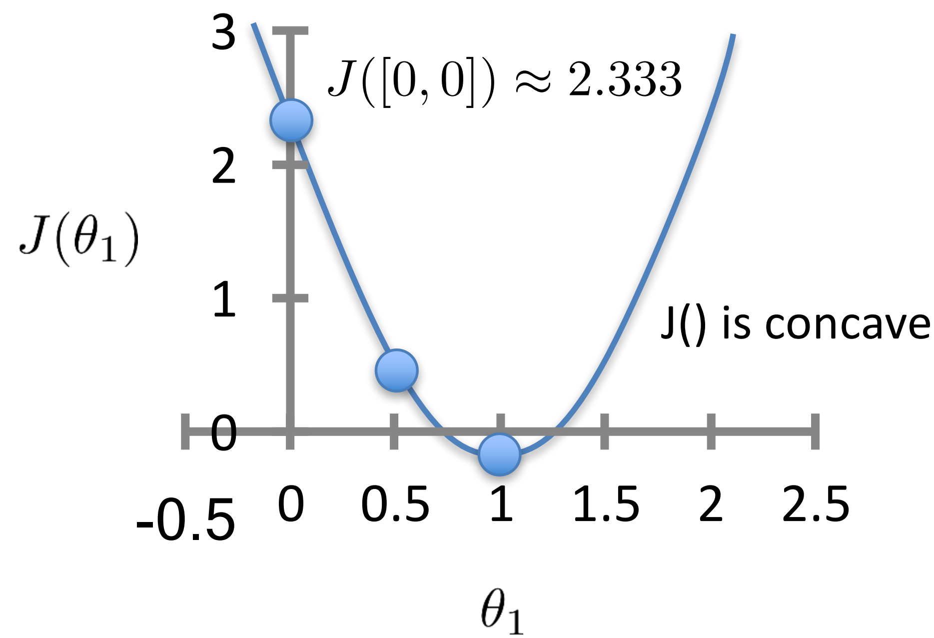
$h_\theta(x)$

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



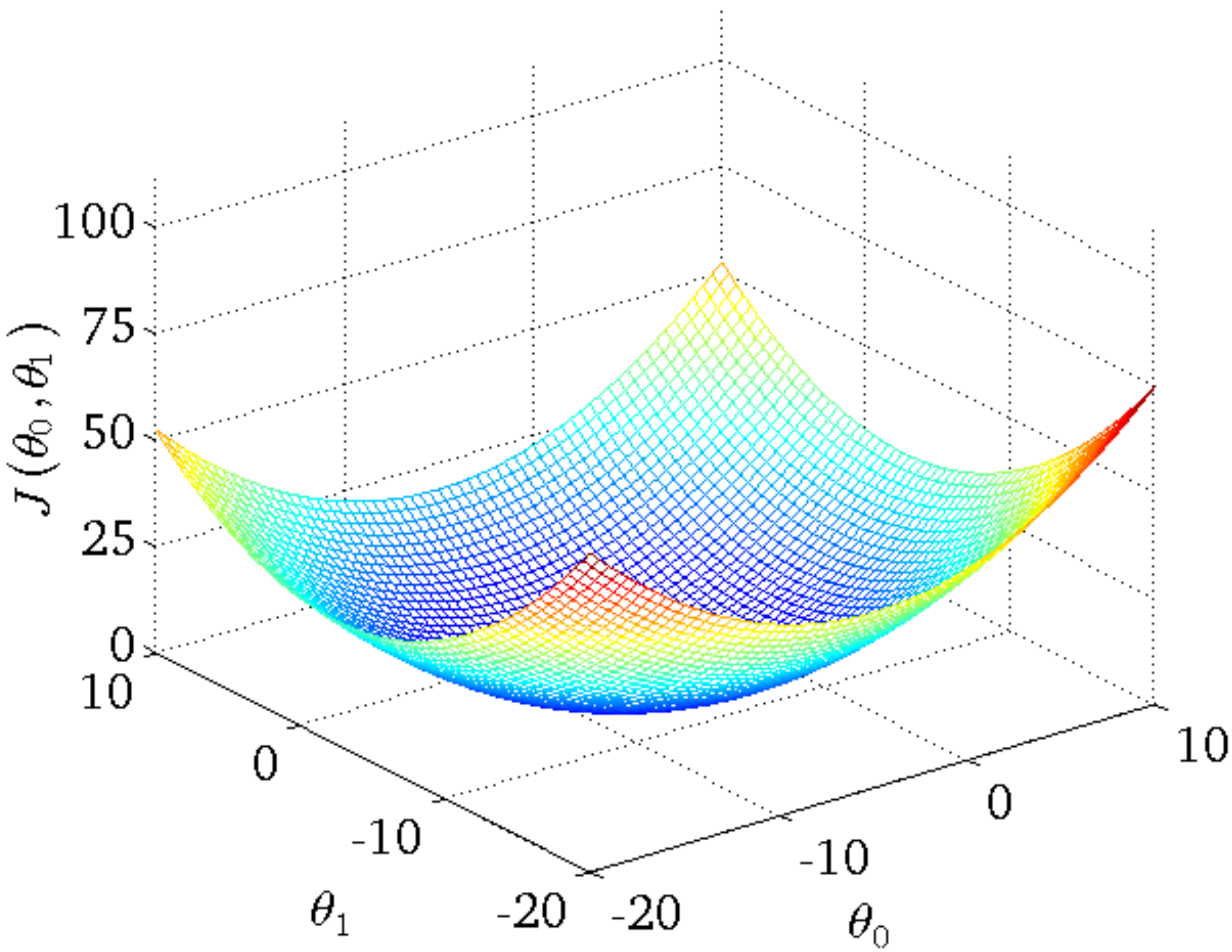
$J(\theta_1)$

(function of the parameter θ_1)



Based on example
by Andrew Ng

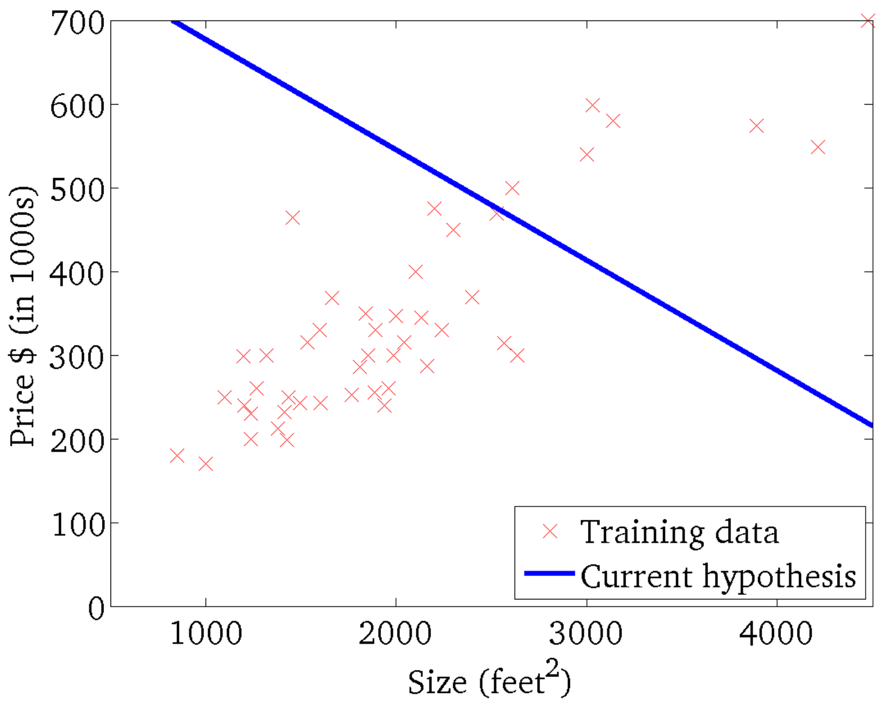
Intuition Behind Cost Function



Intuition Behind Cost Function

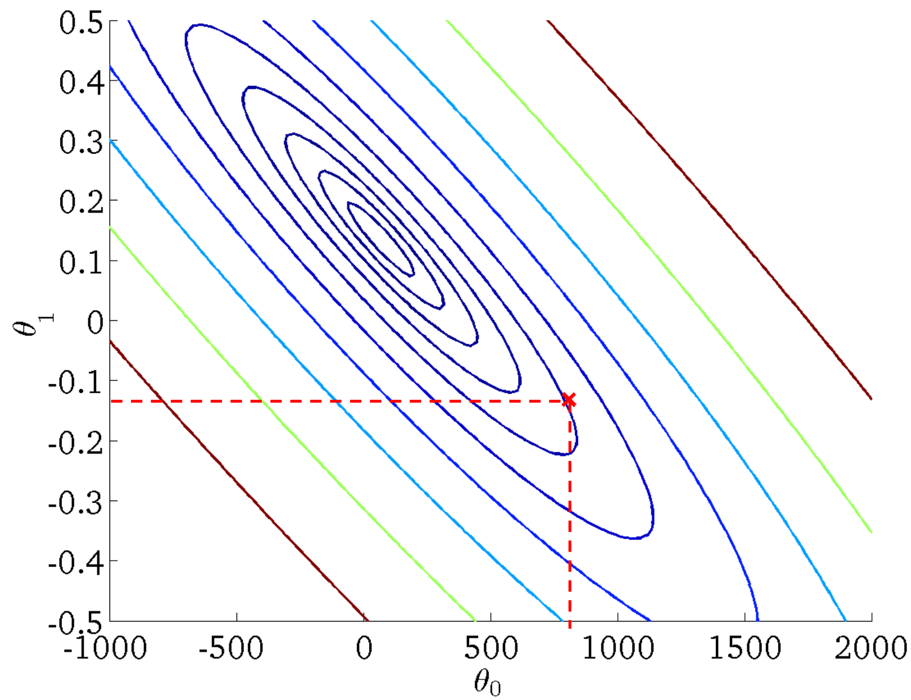
$$h_\theta(x)$$

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



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

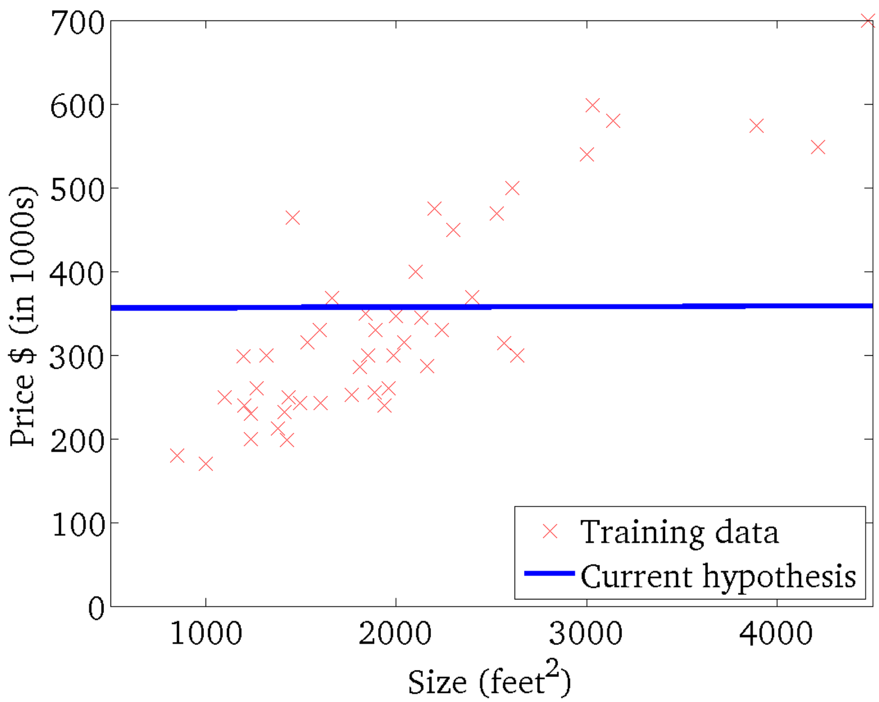
(function of the parameters θ_0, θ_1)



Intuition Behind Cost Function

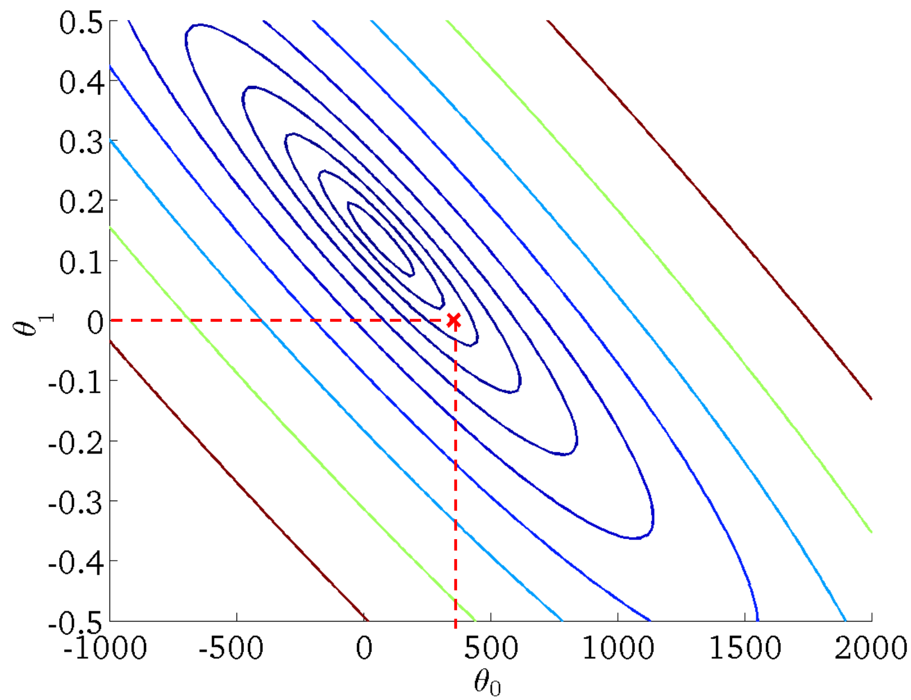
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

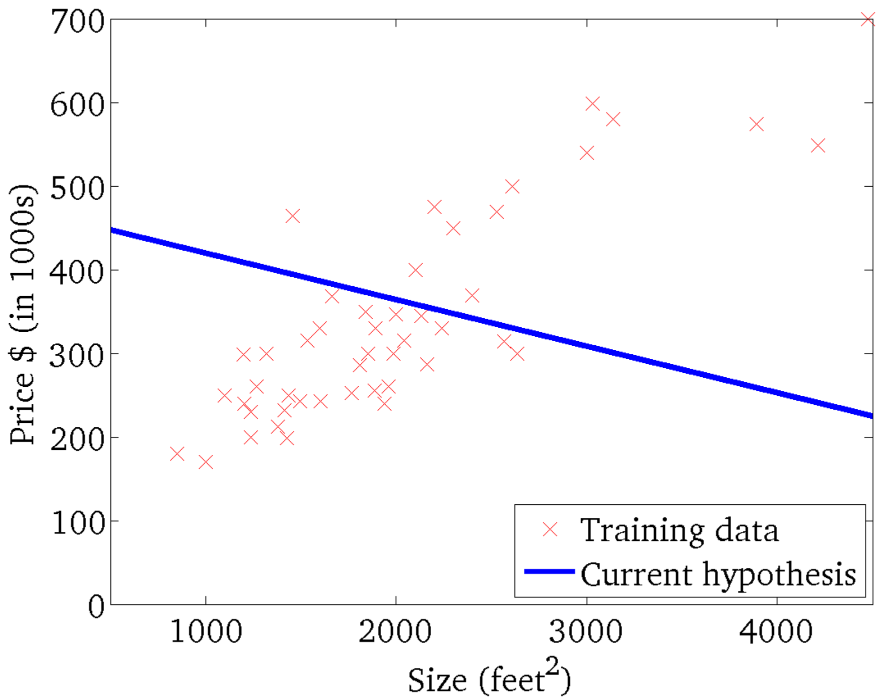
(function of the parameters θ_0, θ_1)



Intuition Behind Cost Function

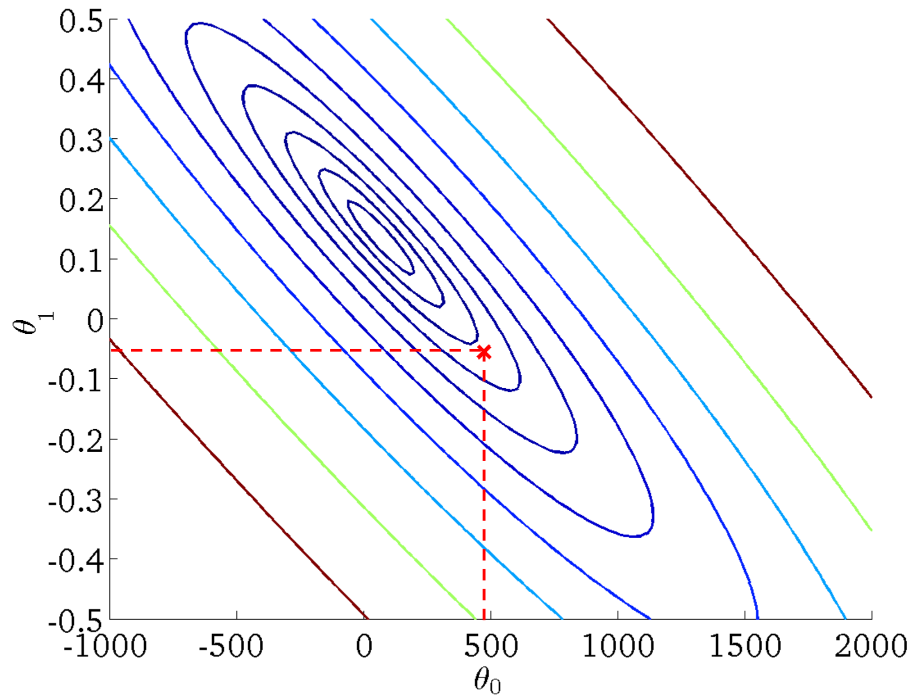
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

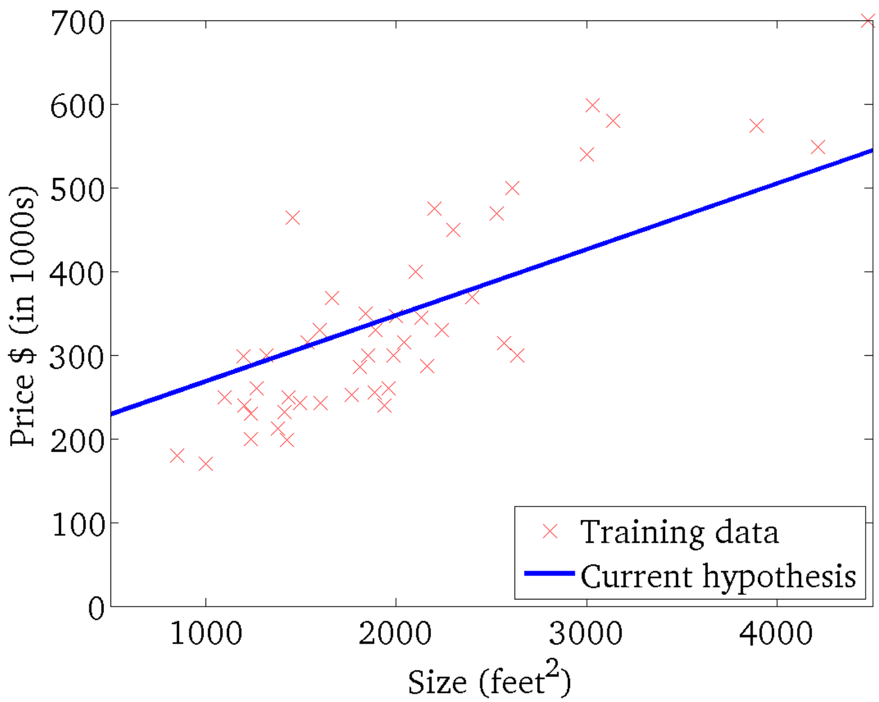
(function of the parameters θ_0, θ_1)



Intuition Behind Cost Function

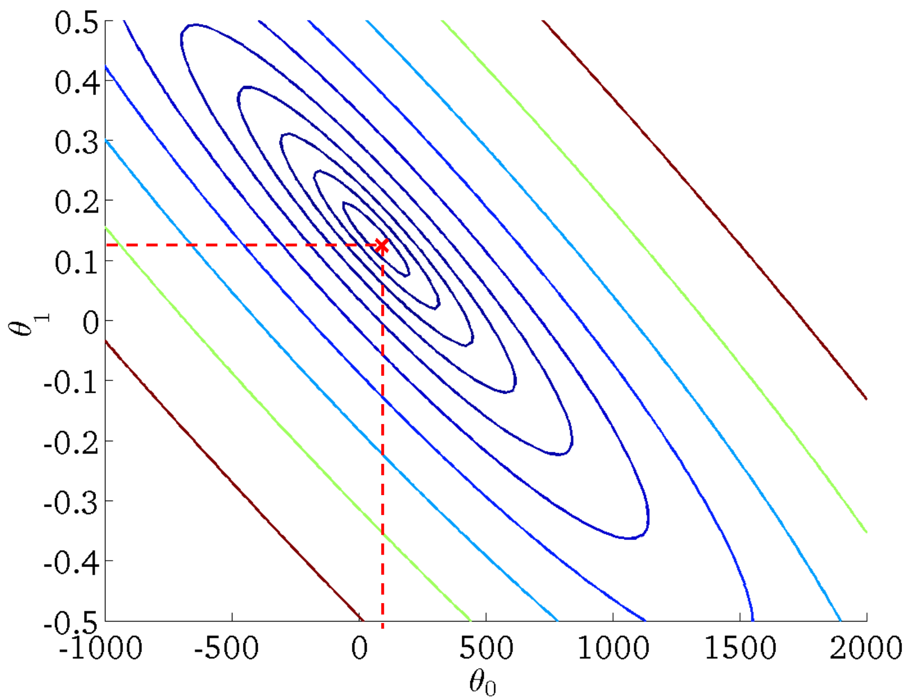
$h_\theta(x)$

(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 $\boldsymbol{\theta}$ to reduce $J(\boldsymbol{\theta})$

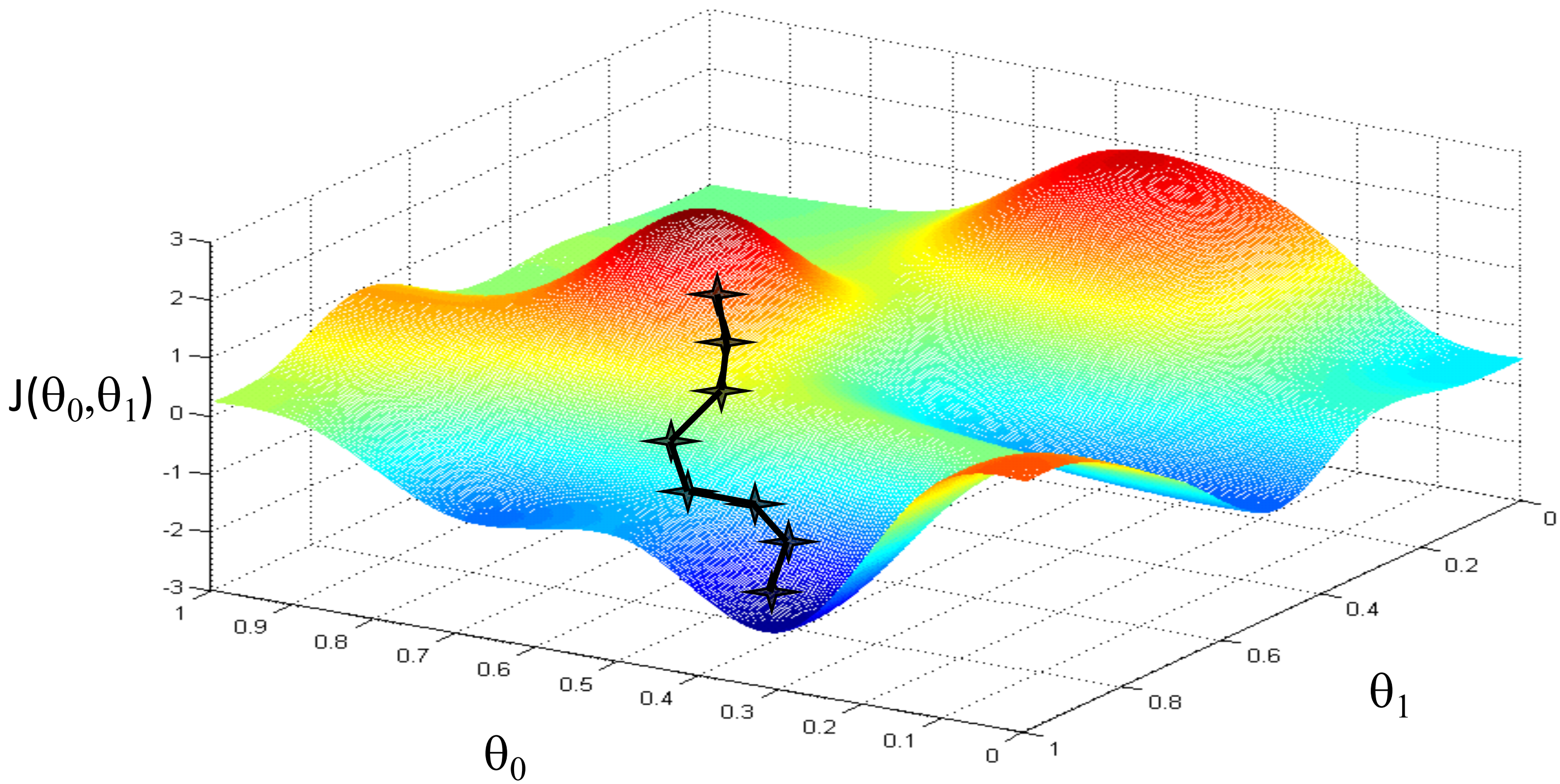


Figure by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for $\boldsymbol{\theta}$ to reduce $J(\boldsymbol{\theta})$

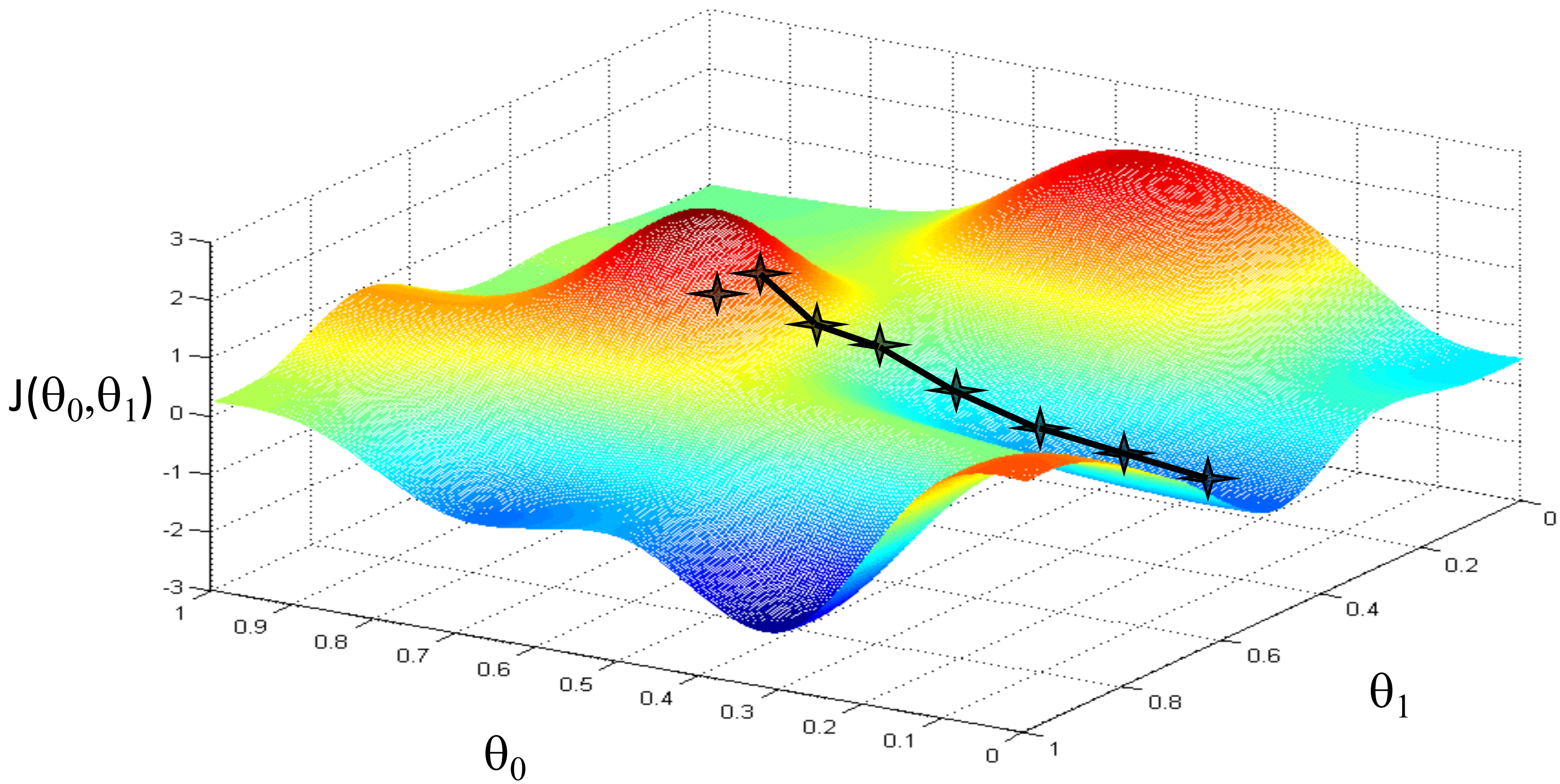
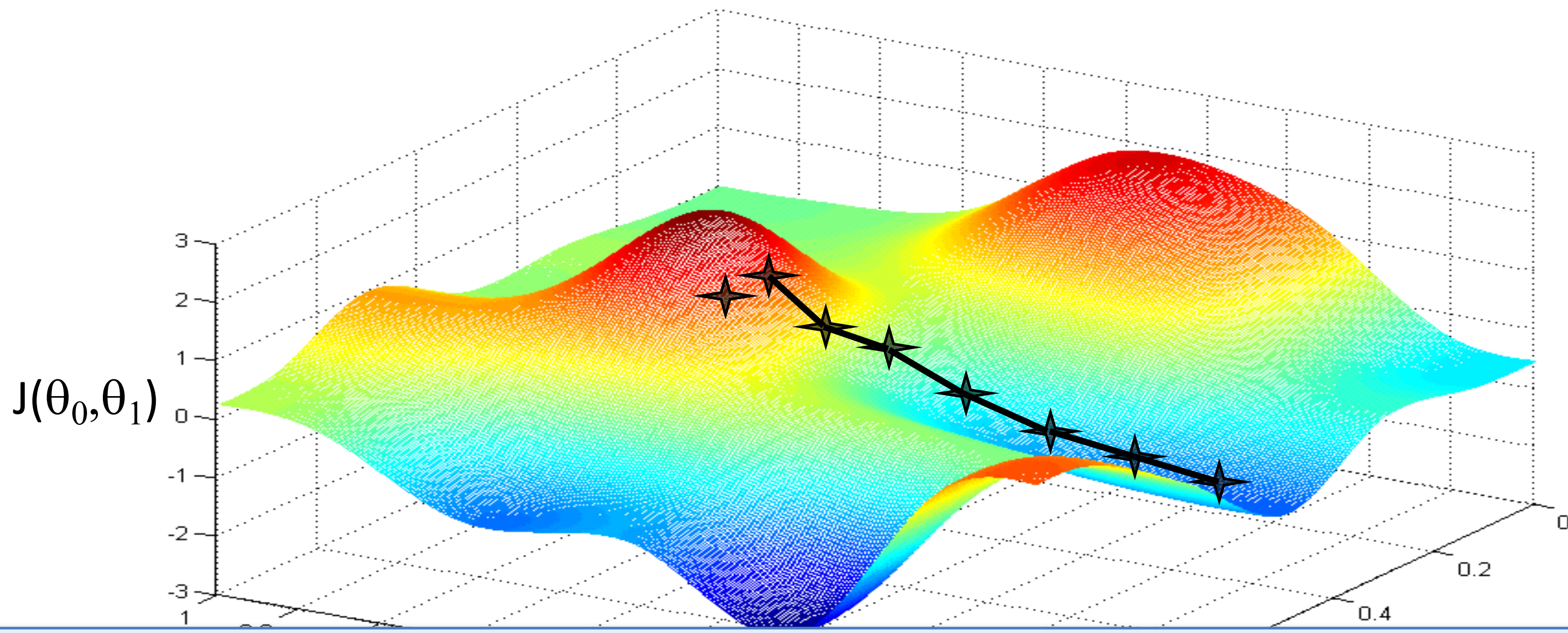


Figure by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for $\boldsymbol{\theta}$ to reduce $J(\boldsymbol{\theta})$



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

Figure by Andrew Ng

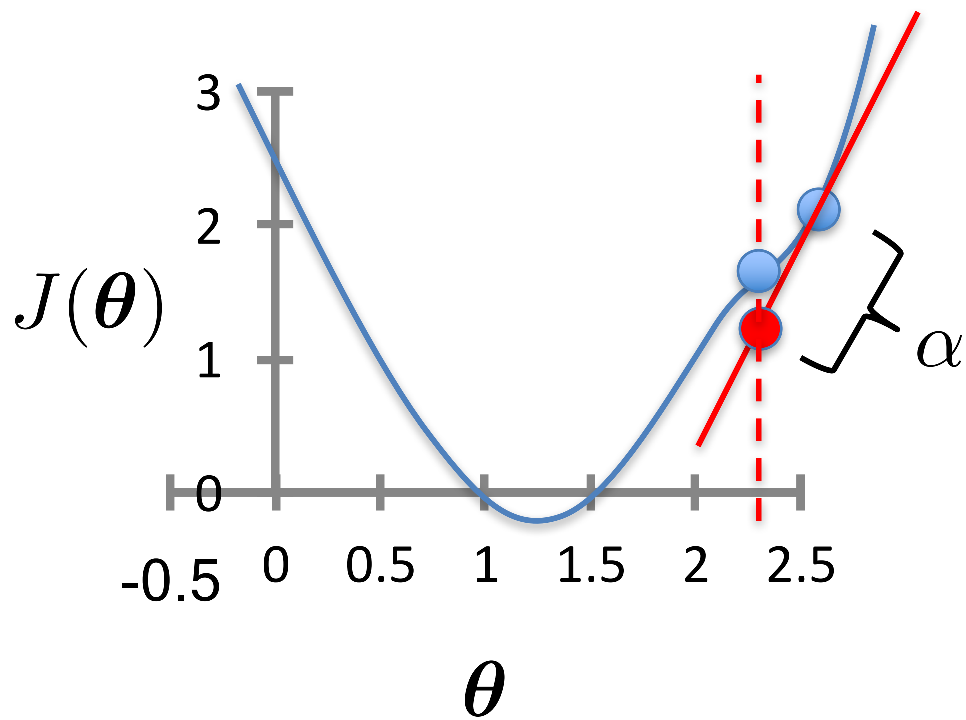
Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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

simultaneous update for j = 0 ... d

learning rate (small) e.g., α = 0.05



Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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

simultaneous update
for j = 0 ... d

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

Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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

simultaneous update
for j = 0 ... d

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

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

Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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

simultaneous update for j = 0 ... d

For Linear Regression:
$$\frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta}) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2$$
$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2$$
$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) \times \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)$$

Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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

simultaneous update for j = 0 ... d

For Linear Regression:
$$\frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta}) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2$$
$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2$$
$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) \times \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)$$
$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) x_j^{(i)}$$

Gradient Descent for Linear Regression

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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

simultaneous update for j = 0 ... d

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

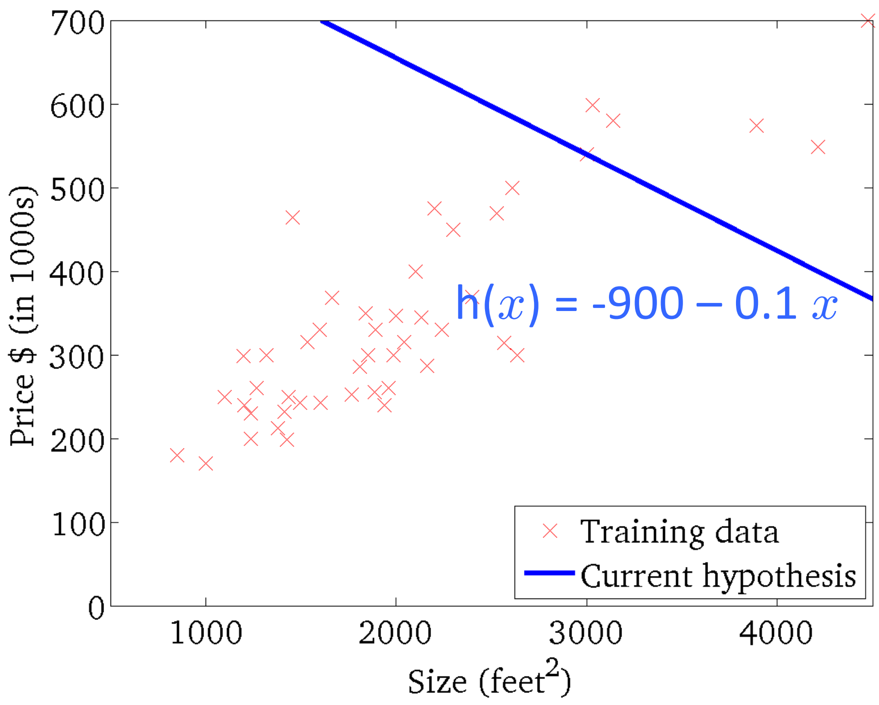
- Assume convergence when $\|\boldsymbol{\theta}_{new} - \boldsymbol{\theta}_{old}\|_2 < \epsilon$

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

Gradient Descent

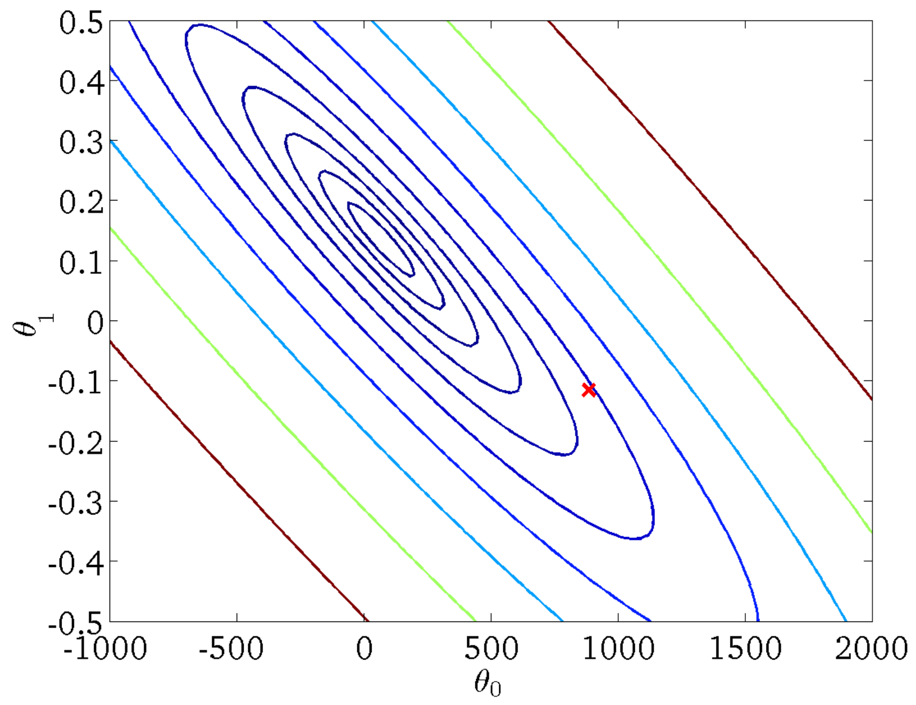
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

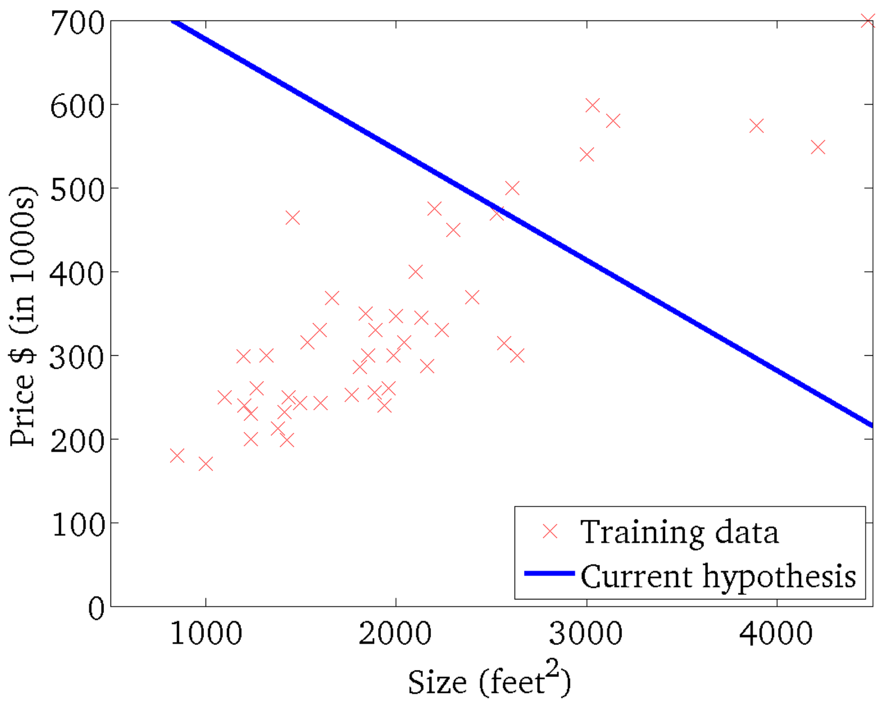
(function of the parameters θ_0, θ_1)



Gradient Descent

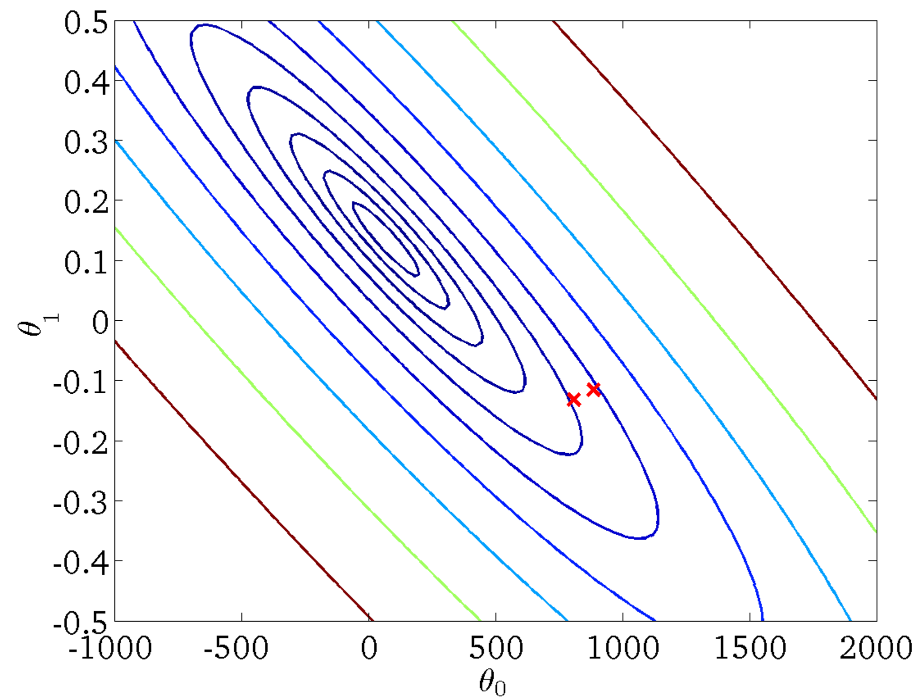
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

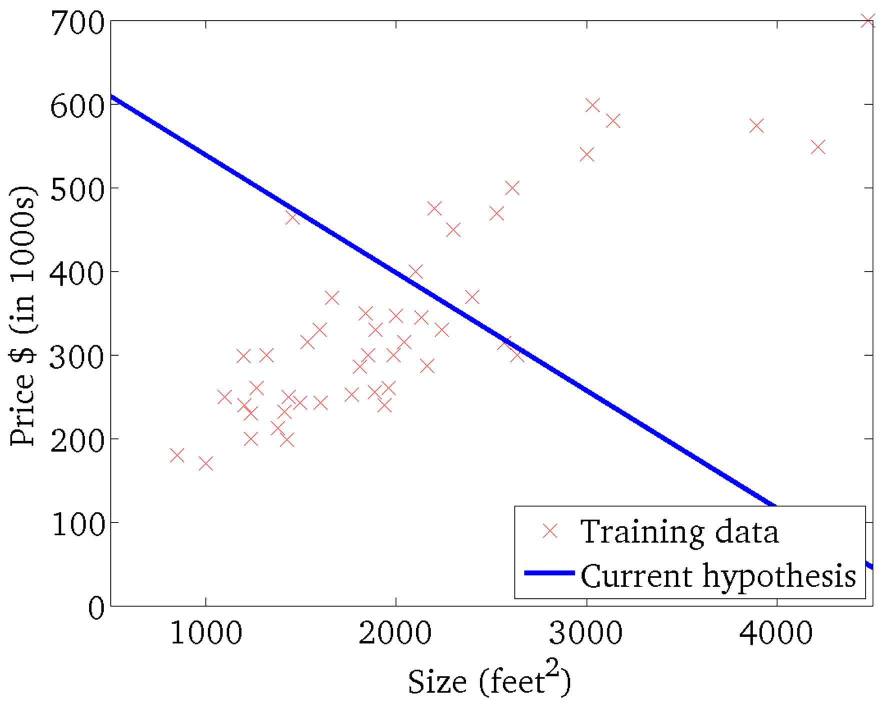
(function of the parameters θ_0, θ_1)



Gradient Descent

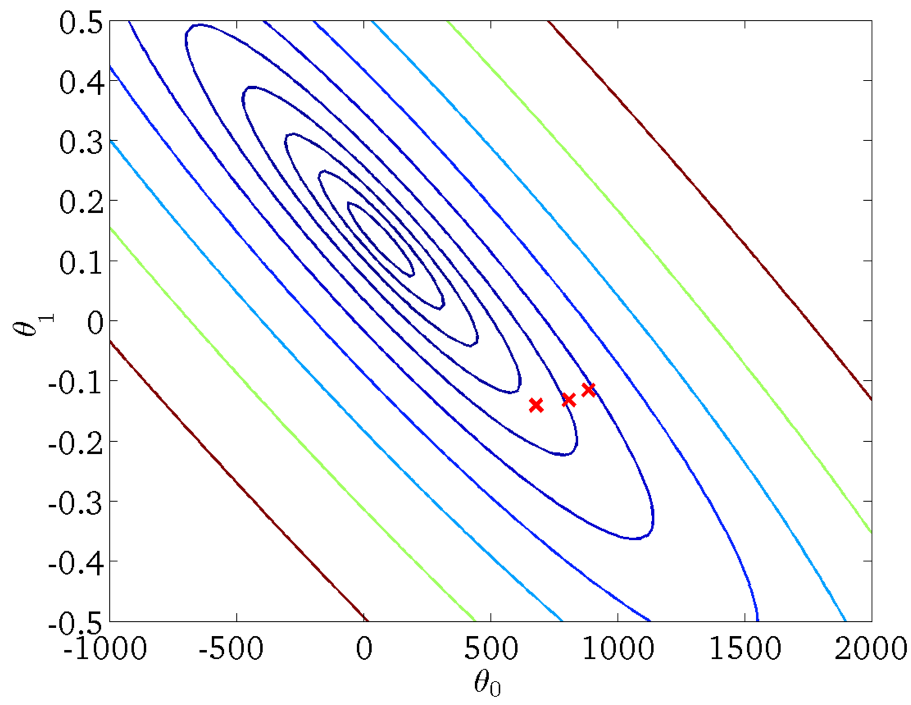
$$h_\theta(x)$$

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



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

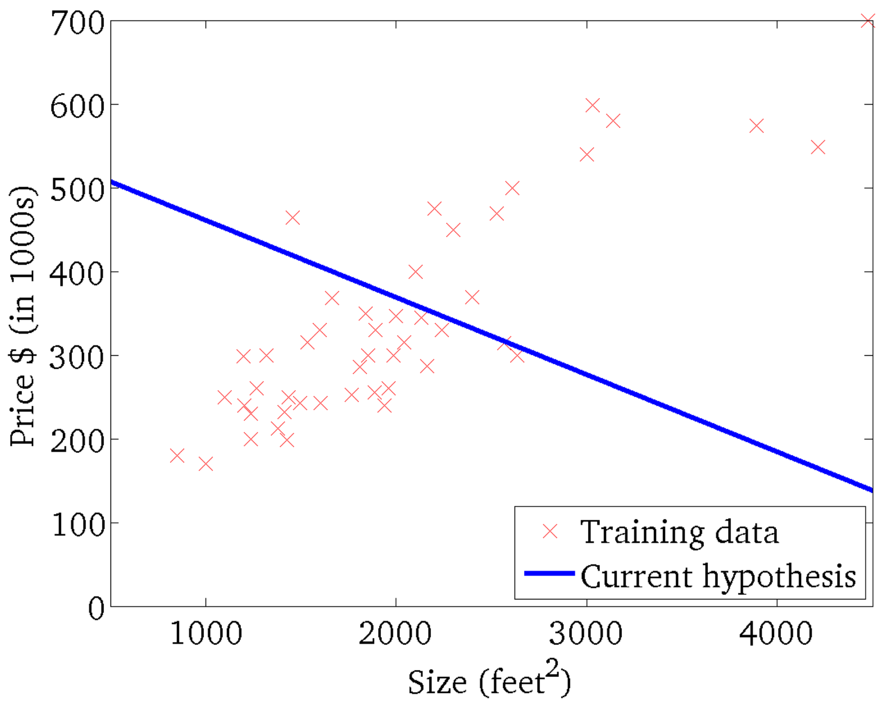
(function of the parameters θ_0, θ_1)



Gradient Descent

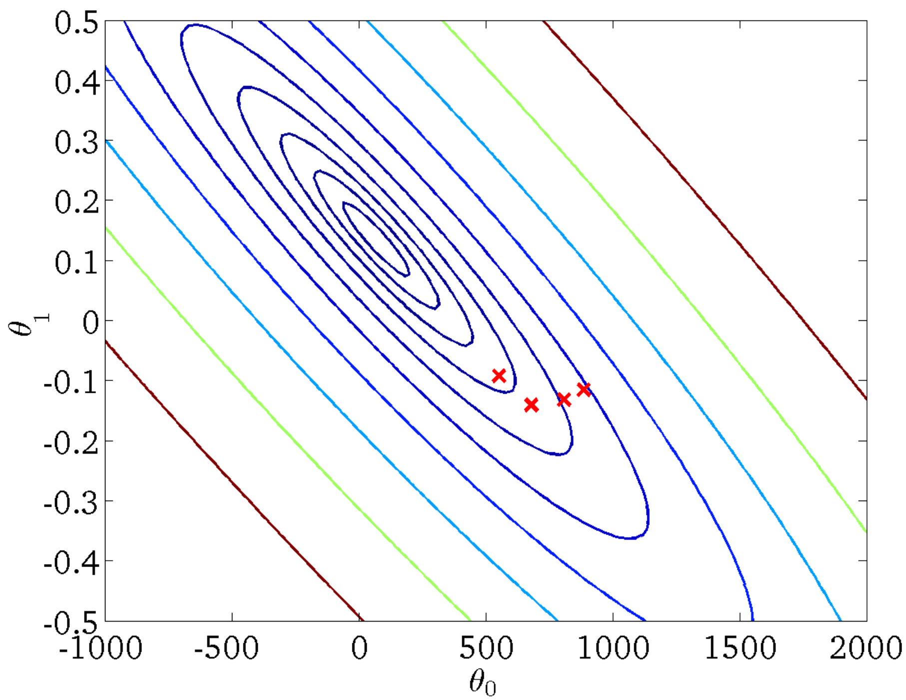
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

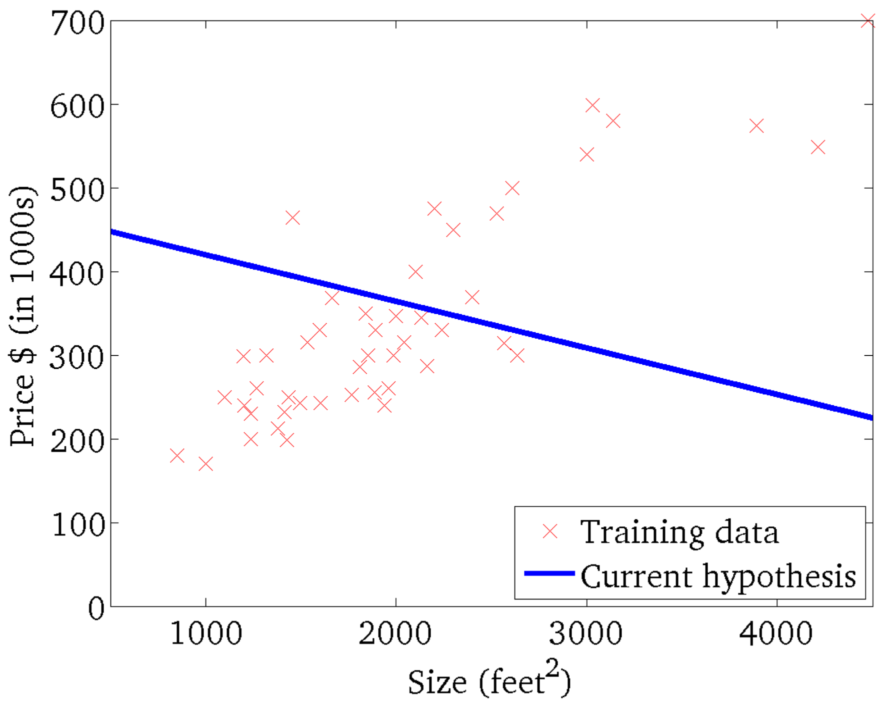
(function of the parameters θ_0, θ_1)



Gradient Descent

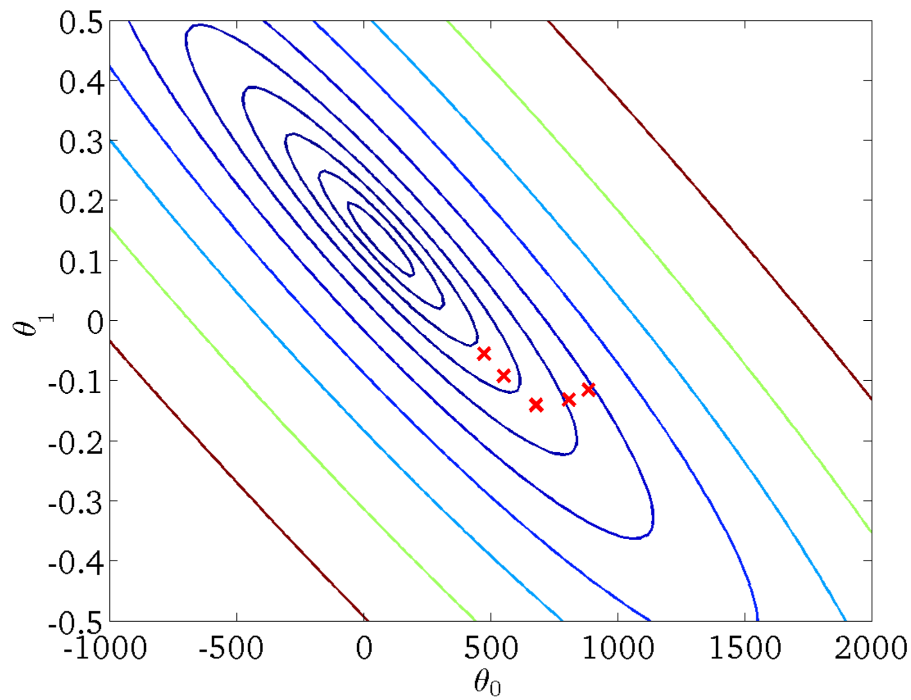
$h_\theta(x)$

(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)



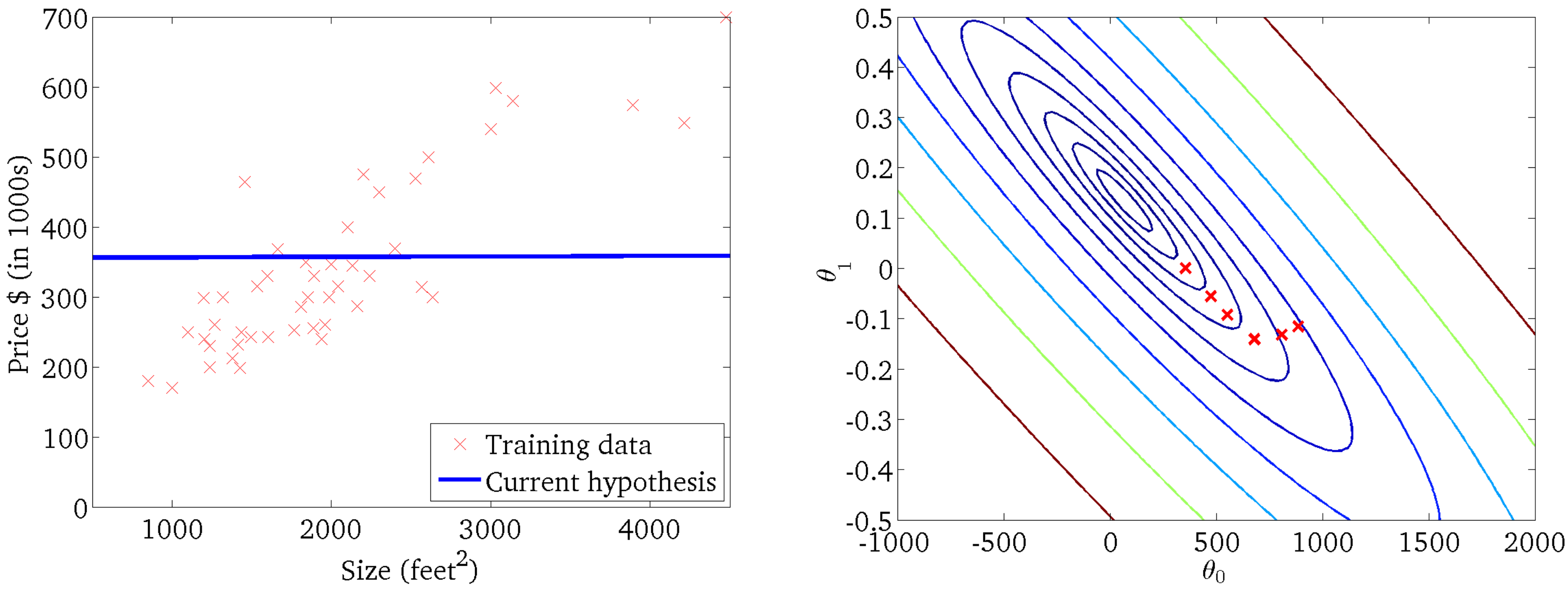
Gradient Descent

$$h_\theta(x)$$

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

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

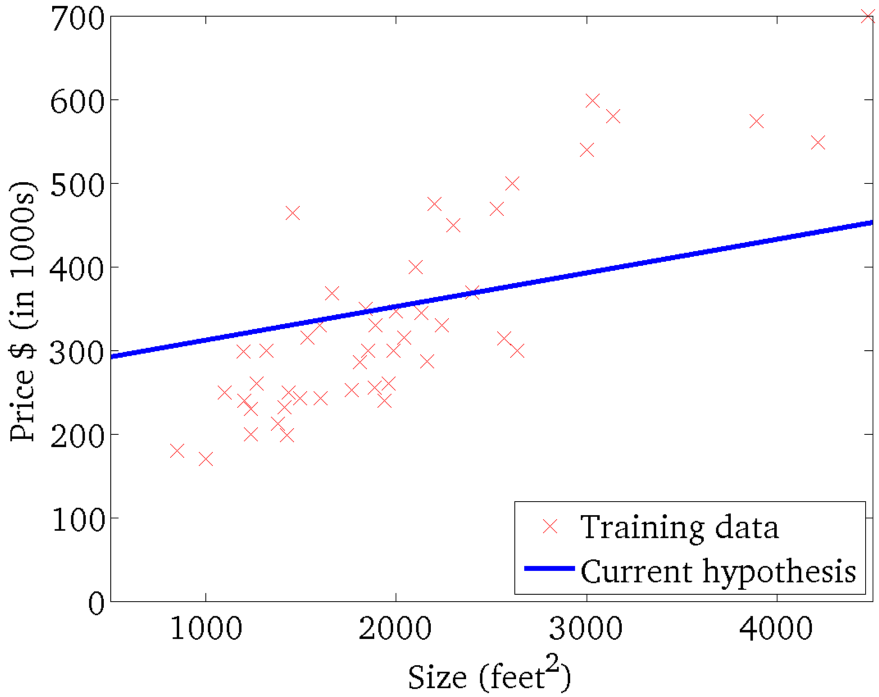
(function of the parameters θ_0, θ_1)



Gradient Descent

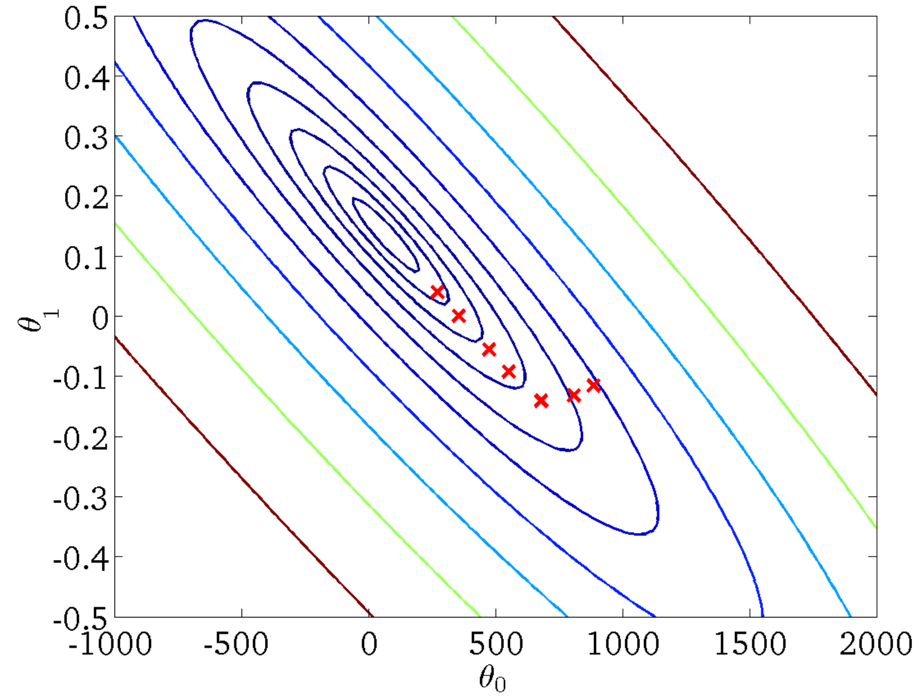
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

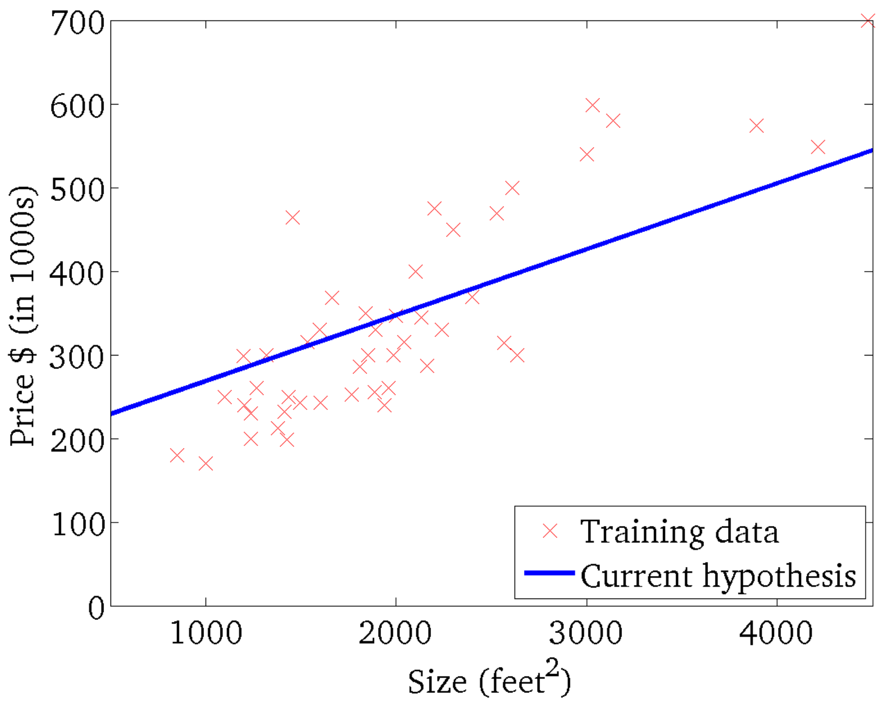
(function of the parameters θ_0, θ_1)



Gradient Descent

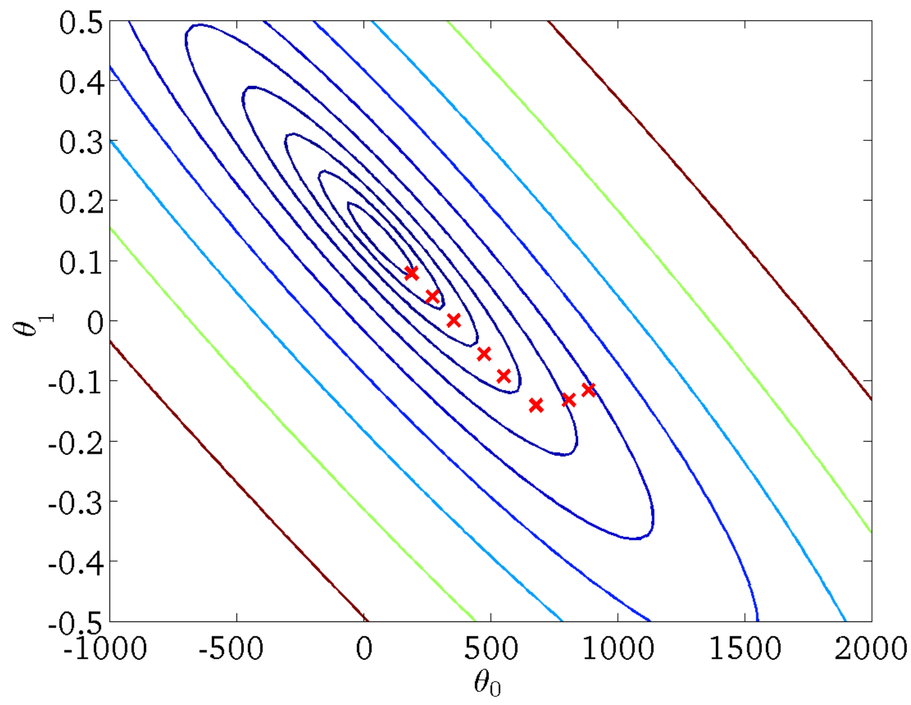
$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

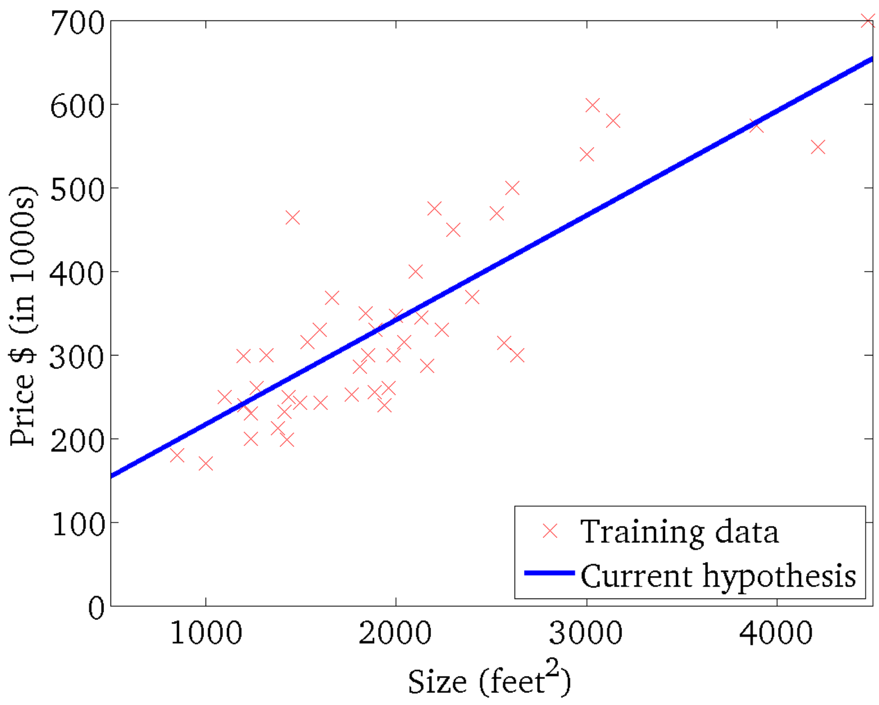
(function of the parameters θ_0, θ_1)



Gradient Descent

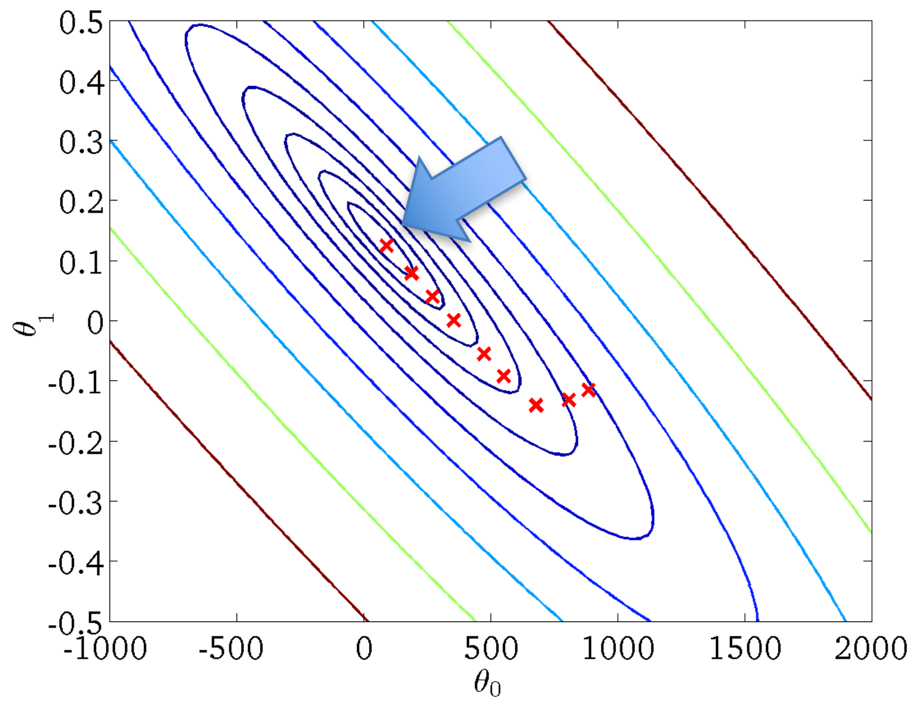
$h_\theta(x)$

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



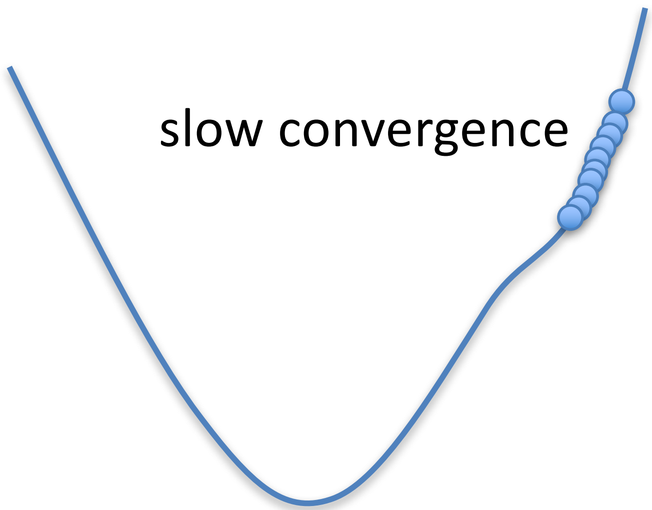
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

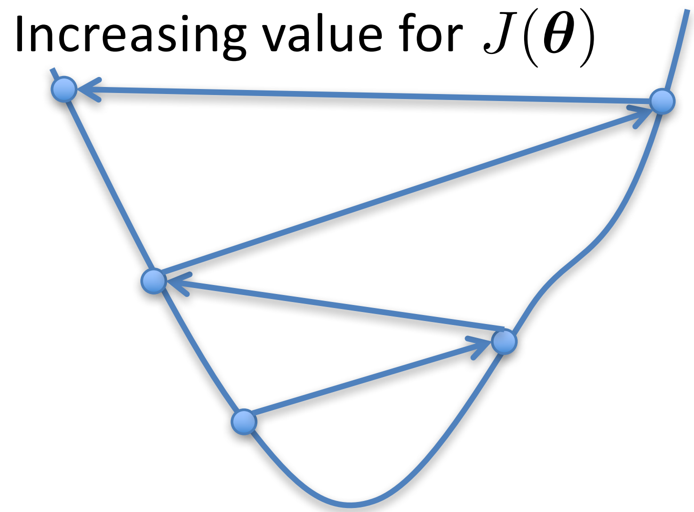


Choosing α

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 $J(\boldsymbol{\theta})$ each iteration

- The value should decrease at each iteration
- If it doesn't, adjust α

Extending Linear Regression to More Complex Models

- The inputs **X** for linear regression can be:
  - Original quantitative inputs
  - Transformation of quantitative inputs
    - e.g. log, exp, square root, square, etc.
  - Polynomial transformation
    - example: $y = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 + \beta_3 \cdot x^3$
  - Basis expansions
  - Dummy coding of categorical inputs
  - Interactions between variables
    - example: $x_3 = x_1 \cdot x_2$

This allows use of linear regression techniques to fit non-linear datasets.

Linear Basis Function Models

- Generally,

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j \underbrace{\phi_j(\boldsymbol{x})}_{\text{basis function}}$$

- Typically, $\phi_0(\boldsymbol{x}) = 1$ so that θ_0 acts as a bias
- In the simplest case, we use linear basis functions :

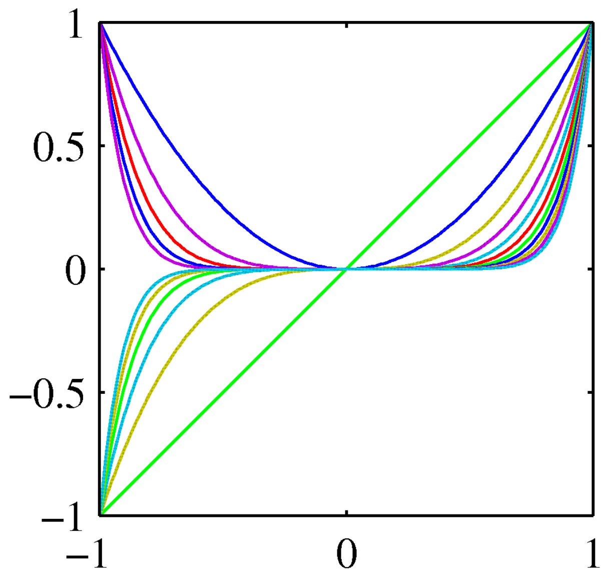
$$\phi_j(\boldsymbol{x}) = x_j$$

Linear Basis Function Models

- Polynomial basis functions:

$$\phi_j(x) = x^j$$

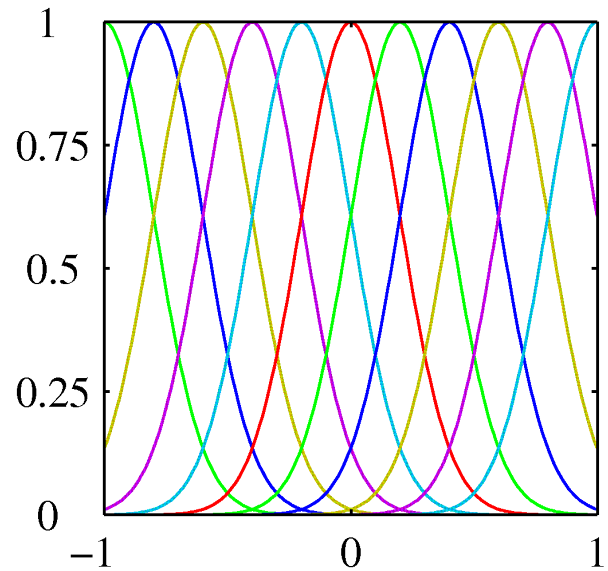
  - These are global; a small change in x affects all basis functions



- Gaussian basis functions:

$$\phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$

  - These are local; a small change in x only affect nearby basis functions. μ_j and s control location and scale (width).



Linear Basis Function Models

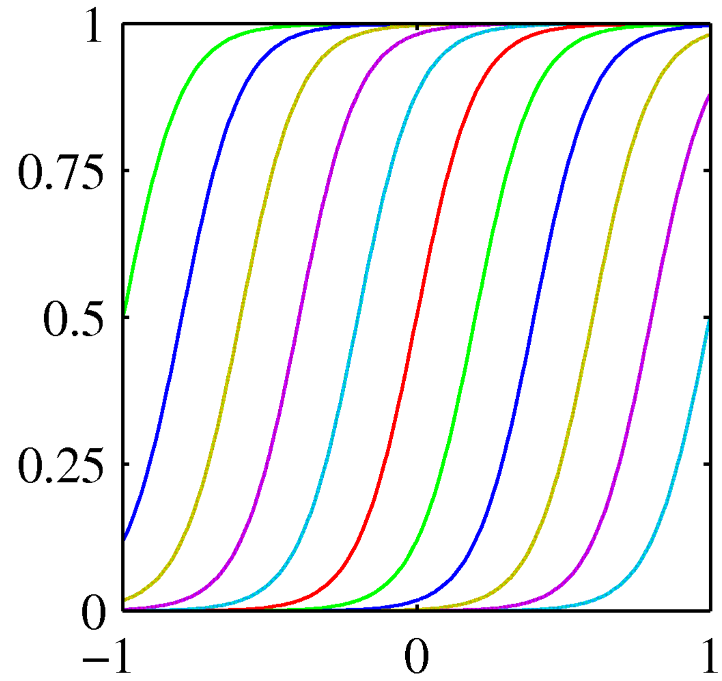
- Sigmoidal basis functions:

$$\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

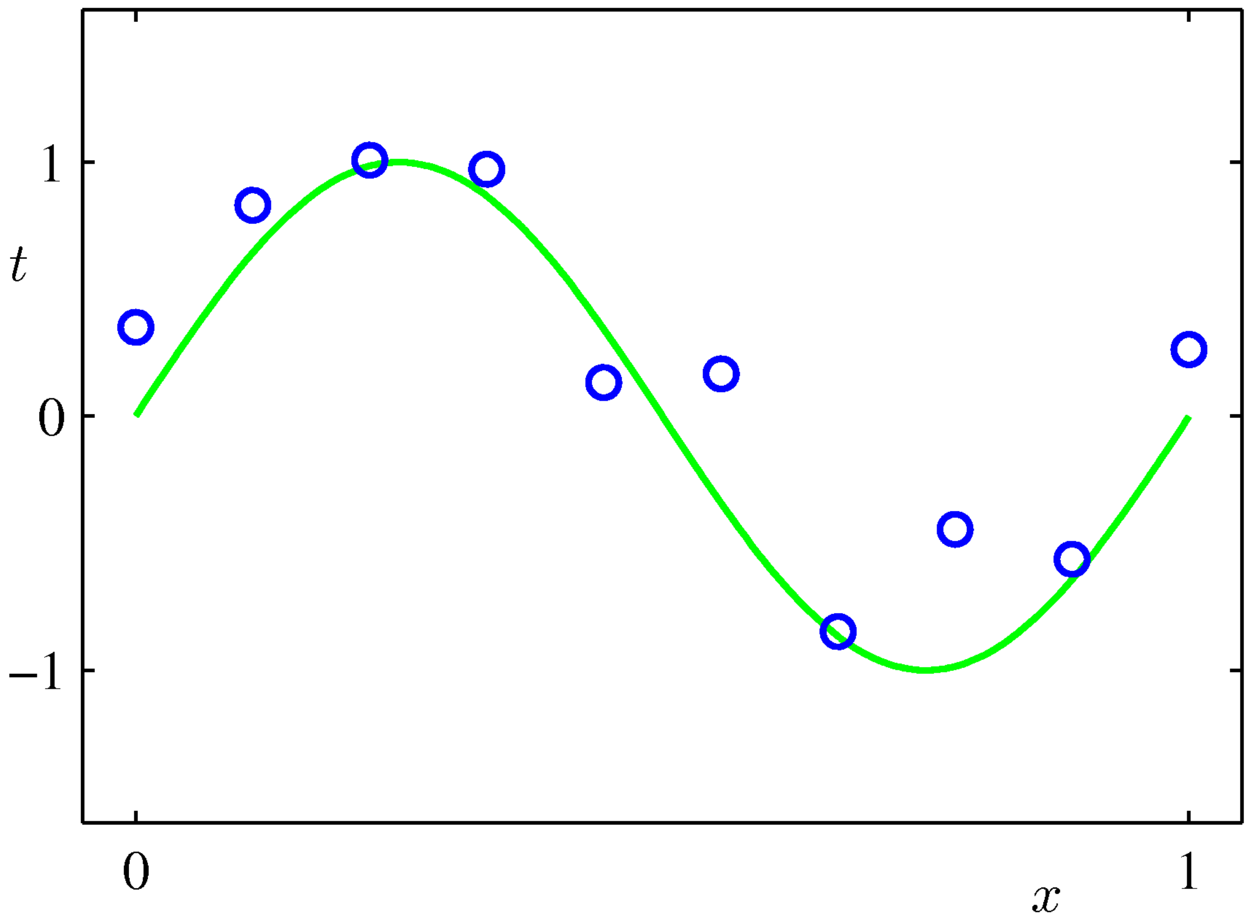
where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

  - These are also local; a small change in x only affects nearby basis functions. μ_j and s control location and scale (slope).



Example of Fitting a Polynomial Curve with a Linear Model



$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_p x^p = \sum_{j=0}^{p} \theta_j x^j$$

Linear Basis Function Models

- Basic Linear Model: $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$
- Generalized Linear Model: $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j \phi_j(\boldsymbol{x})$
- Once we have replaced the data by the outputs of the basis functions, fitting the generalized model is exactly the same problem as fitting the basic model
  - Unless we use the kernel trick – more on that when we cover support vector machines
  - Therefore, there is no point in cluttering the math with basis functions

Based on slide by Geoff Hinton

Linear Algebra Concepts

- *Vector* in $\mathbb{R}^d$ is an ordered set of d real numbers
  - e.g., v = [1,6,3,4] is in $\mathbb{R}^4$
  - "[1,6,3,4]" is a column vector: $\begin{pmatrix} 1 \\ 6 \\ 3 \\ 4 \end{pmatrix}$
  - as opposed to a row vector: $\begin{pmatrix} 1 & 6 & 3 & 4 \end{pmatrix}$

- An m-by-n *matrix* is an object with m rows and n columns, where each entry is a real number:

$$\begin{pmatrix} 1 & 2 & 8 \\ 4 & 78 & 6 \\ 9 & 3 & 2 \end{pmatrix}$$

Linear Algebra Concepts

- Transpose: reflect vector/matrix on line: ╲

$$\begin{pmatrix} a \\ b \end{pmatrix}^T = \begin{pmatrix} a & b \end{pmatrix} \qquad \begin{pmatrix} a & b \\ c & d \end{pmatrix}^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

  - Note: $(\boldsymbol{A}\boldsymbol{x})^T = \boldsymbol{x}^T\boldsymbol{A}^T$ (We'll define multiplication soon…)

- Vector norms:
  - L_p norm of $\boldsymbol{v} = (\boldsymbol{v}_1, \ldots, v_k)$ is $\left(\sum_i |v_i|^p\right)^{\frac{1}{p}}$
  - Common norms: L_1, L_2
  - $L_{infinity} = \max_i |v_i|$
- Length of a vector v is $L_2(v)$

Linear Algebra Concepts

- Vector dot product: $$u \bullet v = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \bullet \begin{pmatrix} v_1 & v_2 \end{pmatrix} = u_1 v_1 + u_2 v_2$$
  - Note: dot product of $\boldsymbol{u}$ with itself = length($\boldsymbol{u}$)^2 = $\|\boldsymbol{u}\|_2^2$
- Matrix product:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$AB = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}$$

Linear Algebra Concepts

- Vector products:
  - Dot product: $$u \bullet v = u^T v = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = u_1 v_1 + u_2 v_2$$
  - Outer product:

$$uv^T = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \begin{pmatrix} v_1 & v_2 \end{pmatrix} = \begin{pmatrix} u_1 v_1 & u_1 v_2 \\ u_2 v_1 & u_2 v_2 \end{pmatrix}$$

Vectorization

- Benefits of vectorization
  - More compact equations
  - Faster code (using optimized matrix libraries)
- Consider our model:

$$h(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$$

- Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \qquad \boldsymbol{x}^\intercal = \begin{bmatrix} 1 & x_1 & \ldots & x_d \end{bmatrix}$$

- Can write the model in vectorized form as $h(\boldsymbol{x}) = \boldsymbol{\theta}^\intercal \boldsymbol{x}$

Vectorization

- Consider our model for n instances:

$$h\left(\boldsymbol{x}^{(i)}\right) = \sum_{j=0}^{d} \theta_j x_j^{(i)}$$

- Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \qquad \boldsymbol{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(i)} & \dots & x_d^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_d^{(n)} \end{bmatrix}$$

$\mathbb{R}^{(d+1)\times 1}$ $\qquad$ $\mathbb{R}^{n\times(d+1)}$

- Can write the model in vectorized form as $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{X}\boldsymbol{\theta}$

Vectorization

- For the linear regression cost function:

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

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

$$= \frac{1}{2n} \underbrace{(\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y})^{\intercal}}_{\mathbb{R}^{1 \times n}} \underbrace{(\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y})}_{\mathbb{R}^{n \times 1}}$$

$\boldsymbol{X} \in \mathbb{R}^{n \times (d+1)}$

$\boldsymbol{\theta} \in \mathbb{R}^{(d+1) \times 1}$

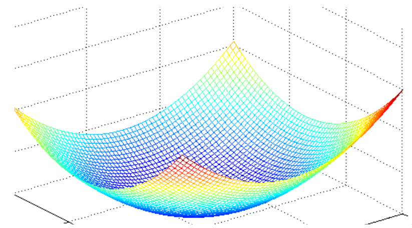
$\boldsymbol{X}\boldsymbol{\theta},\ \boldsymbol{y} \in \mathbb{R}^{n \times 1}$

Let:

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

Closed Form Solution

- Instead of using GD, solve for optimal $\boldsymbol{\theta}$ analytically
  - Notice that the solution is when $\frac{\partial}{\partial \boldsymbol{\theta}} J(\boldsymbol{\theta}) = 0$



- Derivation:

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{2n} (\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y})^\intercal (\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y})$$

$$\propto \boldsymbol{\theta}^\intercal \boldsymbol{X}^\intercal \boldsymbol{X} \boldsymbol{\theta} - \boxed{\boldsymbol{y}^\intercal \boldsymbol{X} \boldsymbol{\theta}} - \boxed{\boldsymbol{\theta}^\intercal \boldsymbol{X}^\intercal \boldsymbol{y}} + \boldsymbol{y}^\intercal \boldsymbol{y}$$

1 x 1

$$\propto \boldsymbol{\theta}^\intercal \boldsymbol{X}^\intercal \boldsymbol{X} \boldsymbol{\theta} - 2\boldsymbol{\theta}^\intercal \boldsymbol{X}^\intercal \boldsymbol{y} + \boldsymbol{y}^\intercal \boldsymbol{y}$$

Take derivative and set equal to 0, then solve for $\boldsymbol{\theta}$:

$$\frac{\partial}{\partial \boldsymbol{\theta}} \left(\boldsymbol{\theta}^\intercal \boldsymbol{X}^\intercal \boldsymbol{X} \boldsymbol{\theta} - 2\boldsymbol{\theta}^\intercal \boldsymbol{X}^\intercal \boldsymbol{y} + \cancel{\boldsymbol{y}^\intercal \boldsymbol{y}}\right) = 0$$

$$(\boldsymbol{X}^\intercal \boldsymbol{X})\boldsymbol{\theta} - \boldsymbol{X}^\intercal \boldsymbol{y} = 0$$

$$(\boldsymbol{X}^\intercal \boldsymbol{X})\boldsymbol{\theta} = \boldsymbol{X}^\intercal \boldsymbol{y}$$

Closed Form Solution: $\boldsymbol{\theta} = (\boldsymbol{X}^\intercal \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal \boldsymbol{y}$

Closed Form Solution

- Can obtain $\boldsymbol{\theta}$ by simply plugging $\boldsymbol{X}$ and $\boldsymbol{y}$ into

$$\boldsymbol{\theta} = (\boldsymbol{X}^\intercal \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal \boldsymbol{y}$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(i)} & \dots & x_d^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_d^{(n)} \end{bmatrix} \qquad \boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

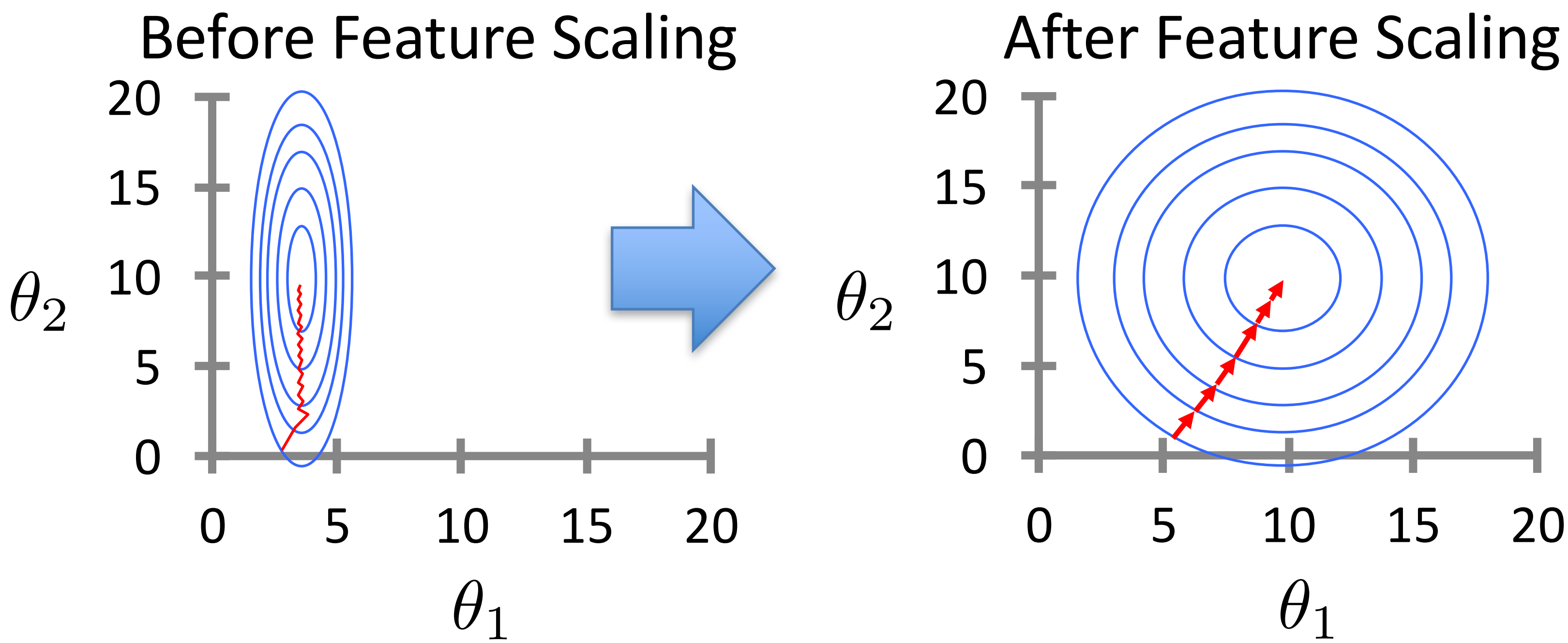
- If $\boldsymbol{X}^\intercal \boldsymbol{X}$ is not invertible (i.e., singular), may need to:
  - Use pseudo-inverse instead of the inverse
    - In python, `numpy.linalg.pinv(a)`
  - Remove redundant (not linearly independent) features
  - Remove extra features to ensure that $d \leq n$

Gradient Descent vs Closed Form

Gradient Descent	Closed Form Solution
• Requires multiple iterations • Need to choose α • Works well when n is large • Can support incremental learning	• Non-iterative • No need for α • Slow if n is large – Computing $(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$ is roughly $O(n^3)$

Improving Learning: Feature Scaling

- **Idea:** Ensure that feature have similar scales



- Makes gradient descent converge *much* faster

Feature Standardization

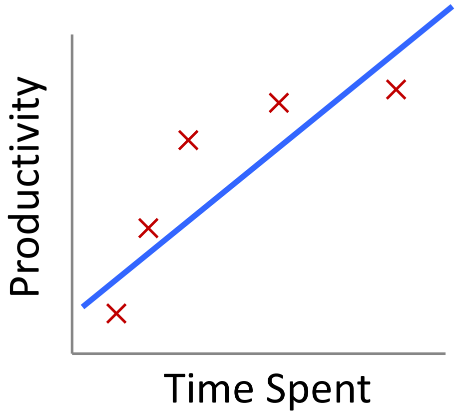
- Rescales features to have zero mean and unit variance
  - Let μ_j be the mean of feature j: $\mu_j = \frac{1}{n} \sum_{i=1}^{n} x_j^{(i)}$
  - Replace each value with:

$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}$$

for j = 1...d
(not x_0!)

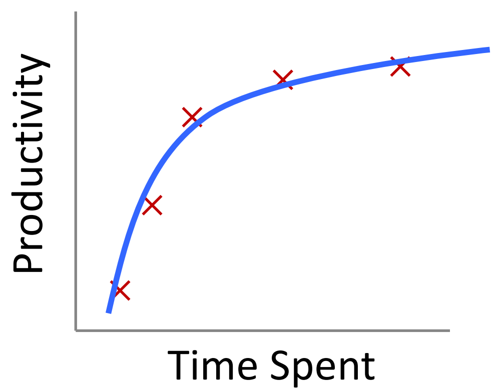
    - s_j is the standard deviation of feature j
    - Could also use the range of feature j ($\max_j - \min_j$) for s_j
- Must apply the same transformation to instances for both training and prediction
- Outliers can cause problems

Quality of Fit



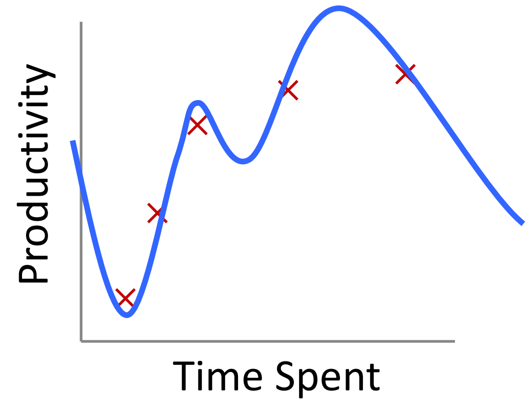
$\theta_0 + \theta_1 x$

Underfitting
(high bias)



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

Correct fit



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

Overfitting
(high variance)

Overfitting:

- The learned hypothesis may fit the training set very well ($J(\boldsymbol{\theta}) \approx 0$)
- ...but fails to generalize to new examples

Regularization

- A method for automatically controlling the complexity of the learned hypothesis
- **Idea**: penalize for large values of θ_j
  - Can incorporate into the cost function
  - Works well when we have a lot of features, each that contributes a bit to predicting the label
- Can also address overfitting by eliminating features (either manually or via model selection)

Regularization

- Linear regression objective function

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

model fit to data — regularization

  - λ is the regularization parameter ($\lambda \geq 0$)
  - No regularization on θ_0!

Understanding Regularization

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

- Note that $\sum_{j=1}^{d}\theta_j^2 = \|\boldsymbol{\theta}_{1:d}\|_2^2$
  - This is the magnitude of the feature coefficient vector!

- We can also think of this as:

$$\sum_{j=1}^{d}(\theta_j - 0)^2 = \|\boldsymbol{\theta}_{1:d} - \vec{\mathbf{0}}\|_2^2$$

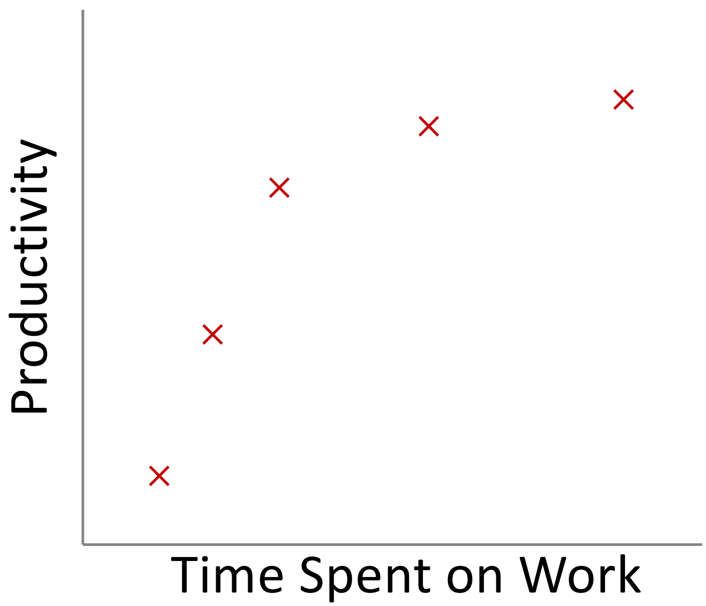
  - L_2 regularization pulls coefficients toward 0

Understanding Regularization

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

- What happens as $\lambda \to \infty$?

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

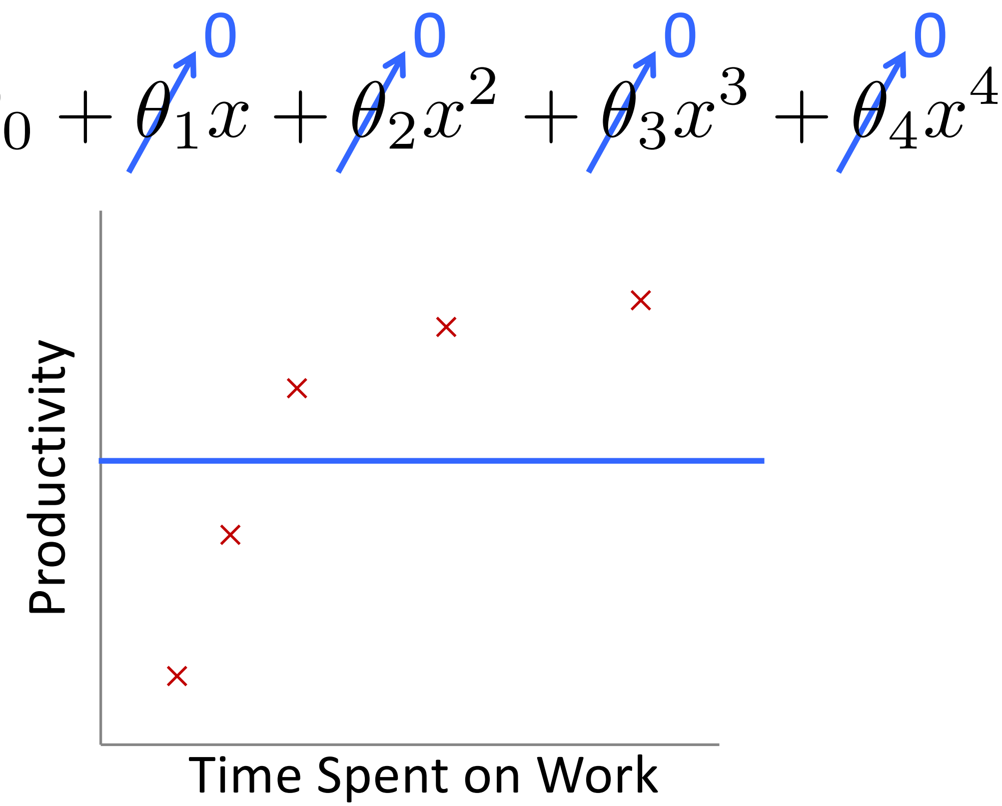


Understanding Regularization

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

- What happens as $\lambda \rightarrow \infty$?

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



Regularized Linear Regression

- Cost Function

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

- Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Gradient update:

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

$$\theta_0 \leftarrow \theta_0 - \alpha\frac{1}{n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)$$

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

$$\theta_j \leftarrow \theta_j - \alpha\frac{1}{n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)x_j^{(i)} \underbrace{- \alpha\lambda\theta_j}_{\text{regularization}}$$

Regularized Linear Regression

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

$$\theta_0 \leftarrow \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)$$

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

- We can rewrite the gradient step as:

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

Regularized Linear Regression

- To incorporate regularization into the closed form solution:

$$\boldsymbol{\theta} = \left(\boldsymbol{X}^\intercal \boldsymbol{X} \qquad\qquad\qquad\qquad \right)^{-1} \boldsymbol{X}^\intercal \boldsymbol{y}$$

Regularized Linear Regression

- To incorporate regularization into the closed form solution:

$$\boldsymbol{\theta} = \left(\boldsymbol{X}^\intercal \boldsymbol{X} + \lambda \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \right)^{-1} \boldsymbol{X}^\intercal \boldsymbol{y}$$

- Can derive this the same way, by solving $\frac{\partial}{\partial \boldsymbol{\theta}} J(\boldsymbol{\theta}) = 0$
- Can prove that for $\lambda > 0$, inverse exists in the equation above