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Machine Learning
DSECL ZG565

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Lecture No. – 6 | Linear Regression

Date – 30/11/2019

Time – 11:00 AM – 1:00 PM

Session Content

- Regression (Andre Ng Notes)
- Bayesian linear regression (6.4 Tom Mitchell)
- Linear basis function models (3.1 Bishop)
- Bias-variance decomposition (3.2 Bishop)

Regression

So far, we've been interested in learning P(Y|X) where Y has discrete values (called 'classification')

What if Y is continuous? (called 'regression')

- predict weight from gender, height, age, …
- predict Google stock price today from Google, Yahoo, MSFT prices yesterday
- predict each pixel intensity in robot's current camera image, from previous image and previous action

Regression

Wish to learn f: X→ Y, where Y is real, given {<x^1,y^1>…<x^n,y^n>}

- Geometric Approach
  - Least squares function fitting given {<x^1,y^1>…<x^n,y^n>}

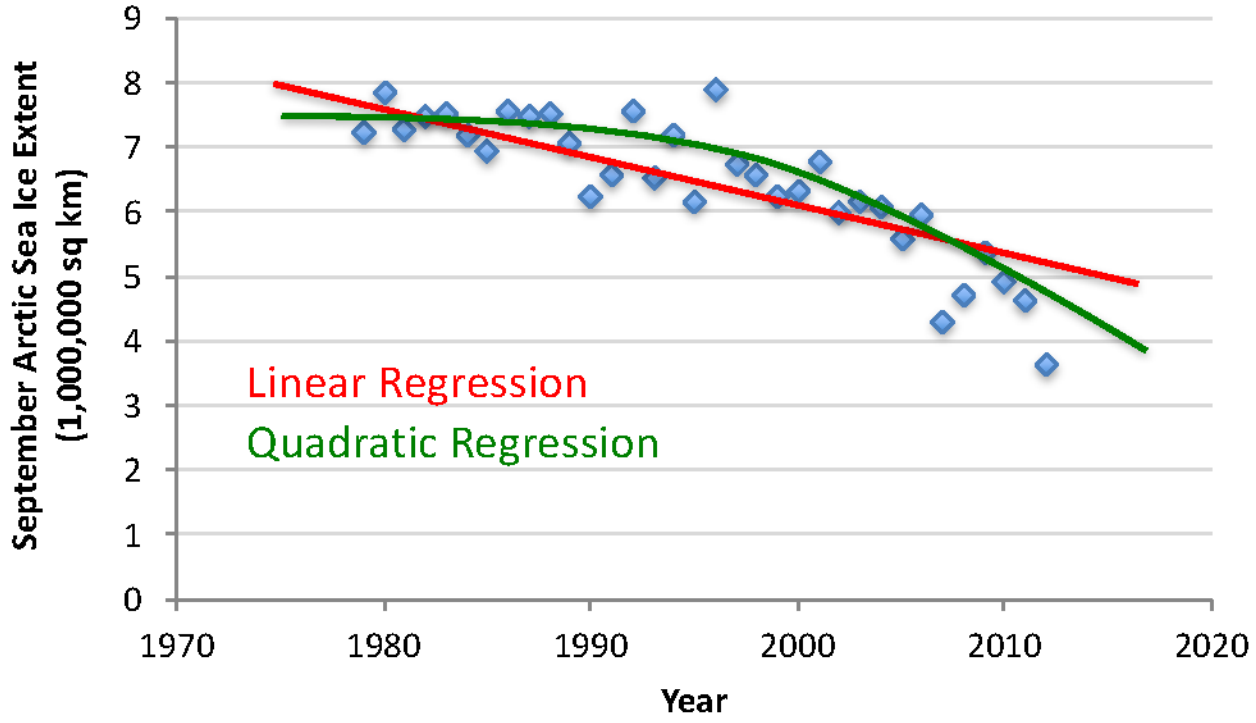
- Bayesian Approach
  - Choose some parameterized form for P(Y|X; θ)
    - (θ is the vector of parameters)

  - Derive learning algorithm as MCLE estimate for θ

Geometric Approach

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)

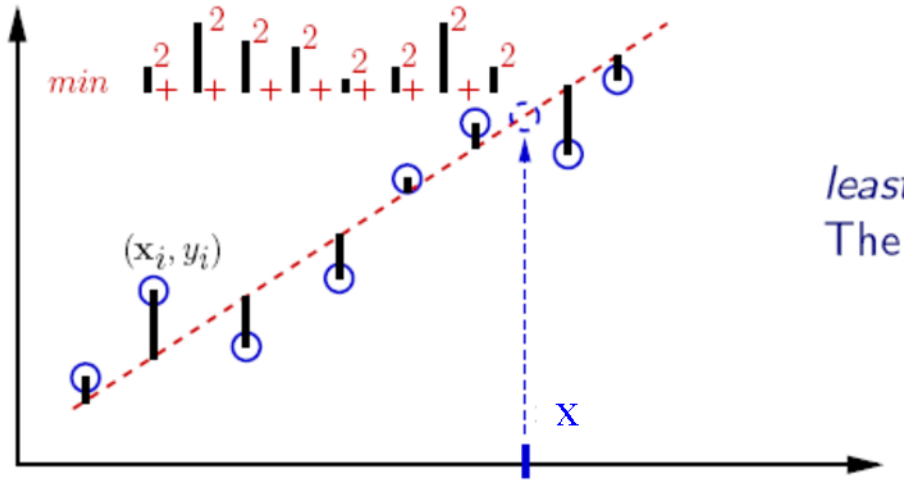
Linear Regression

- 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

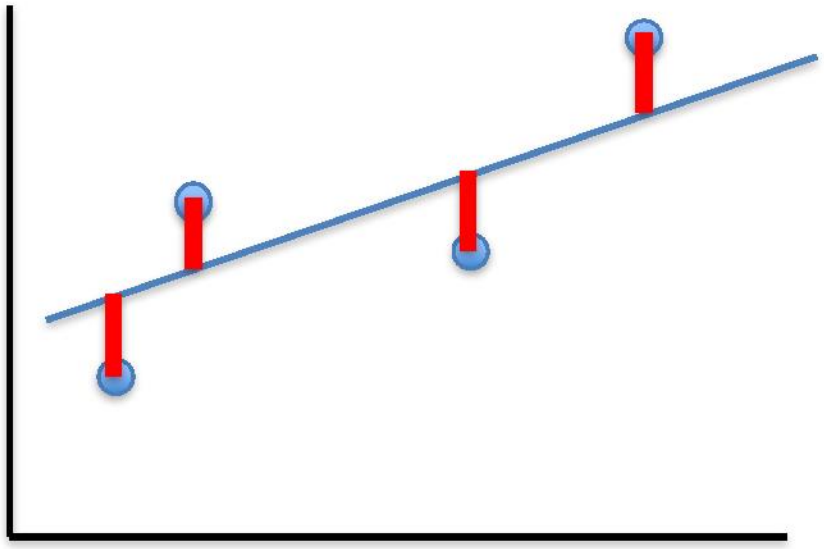
Figures are courtesy of Greg Shakhnarovich

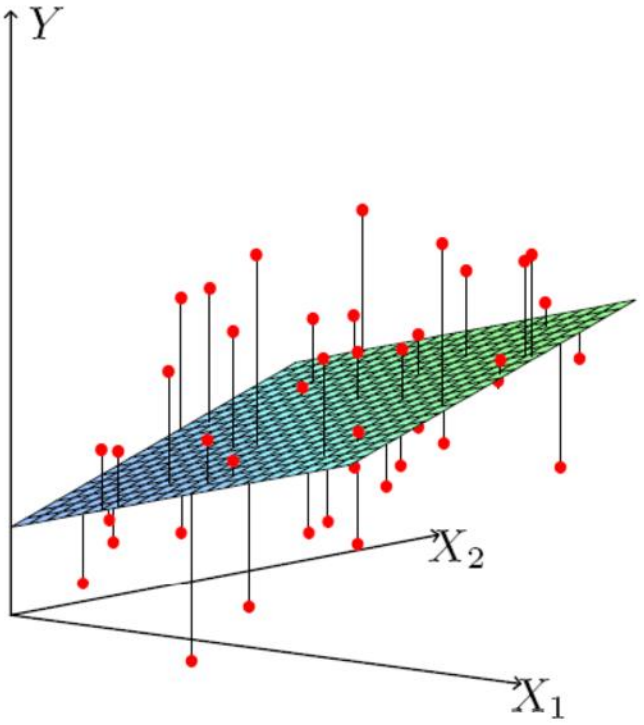
Least Squares Linear Regression

- 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

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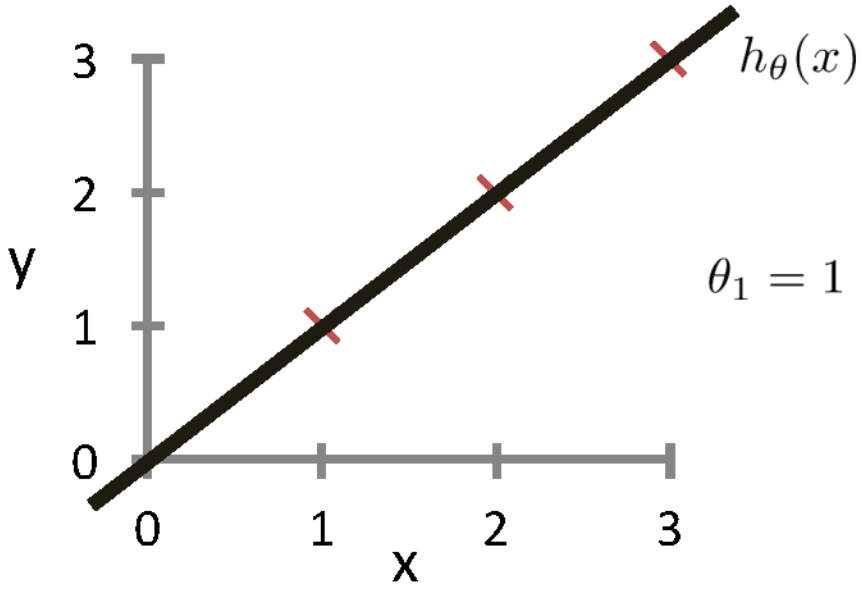
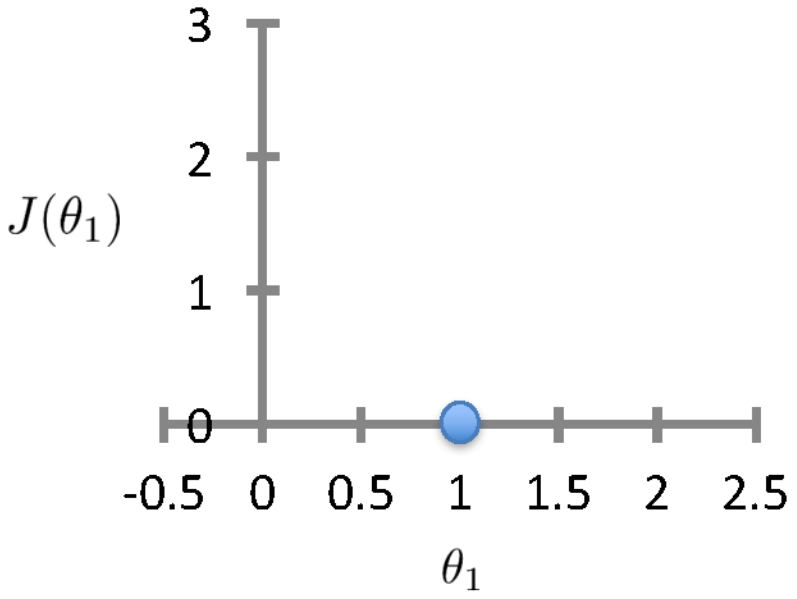
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



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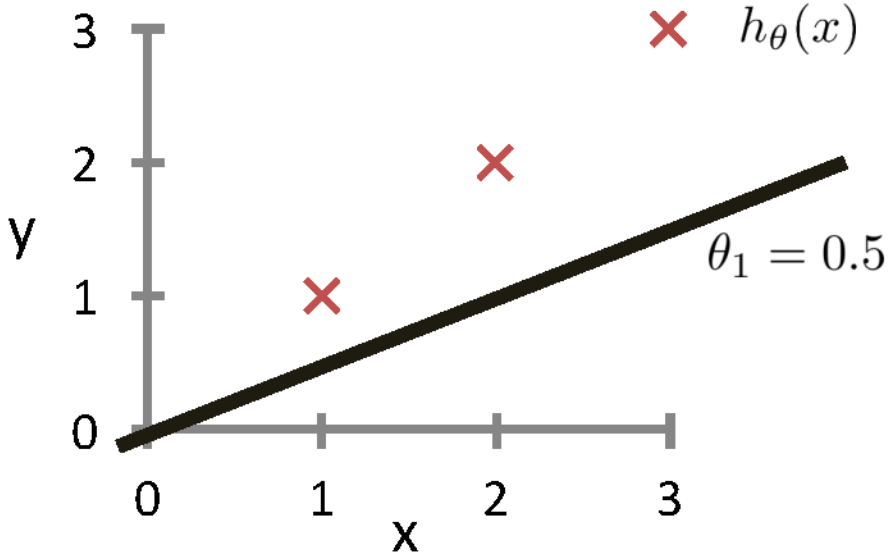

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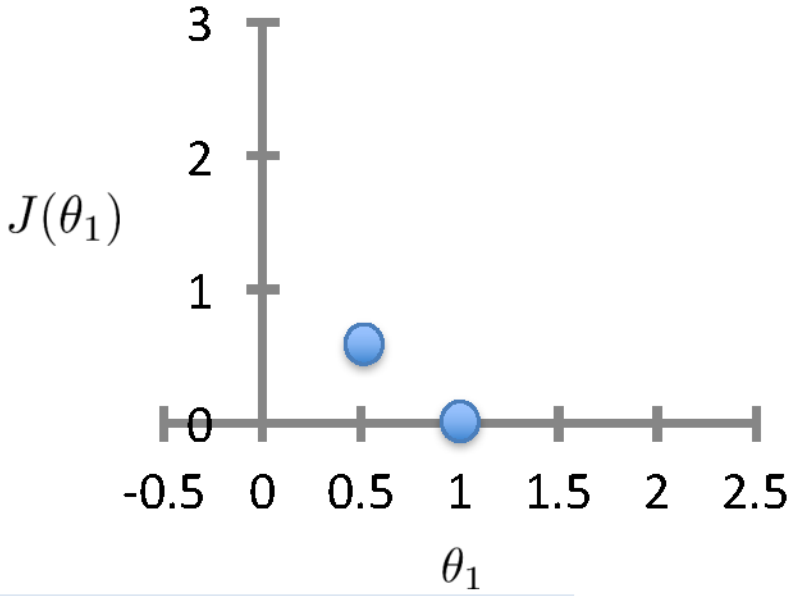

$$J([0, 0.5]) = \frac{1}{2 \times 3}\left[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2\right] \approx 0.58$$

Based on example by Andrew Ng

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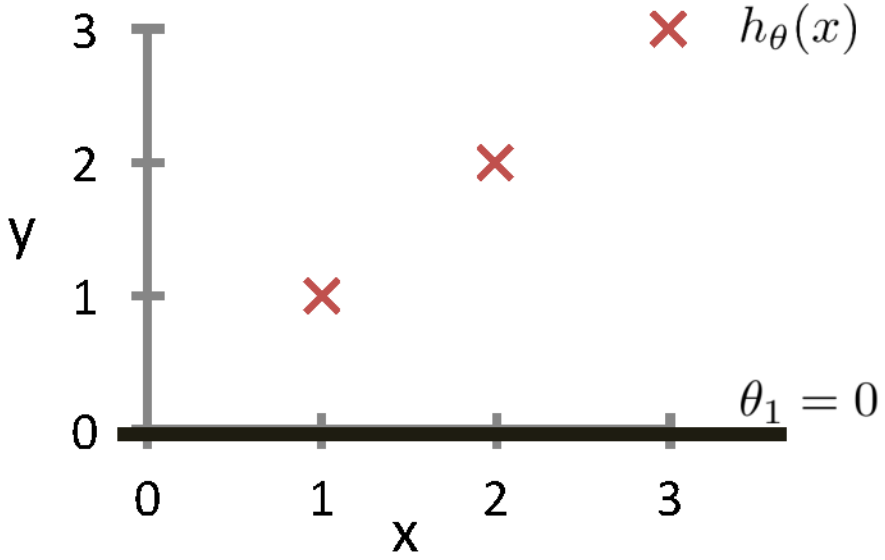

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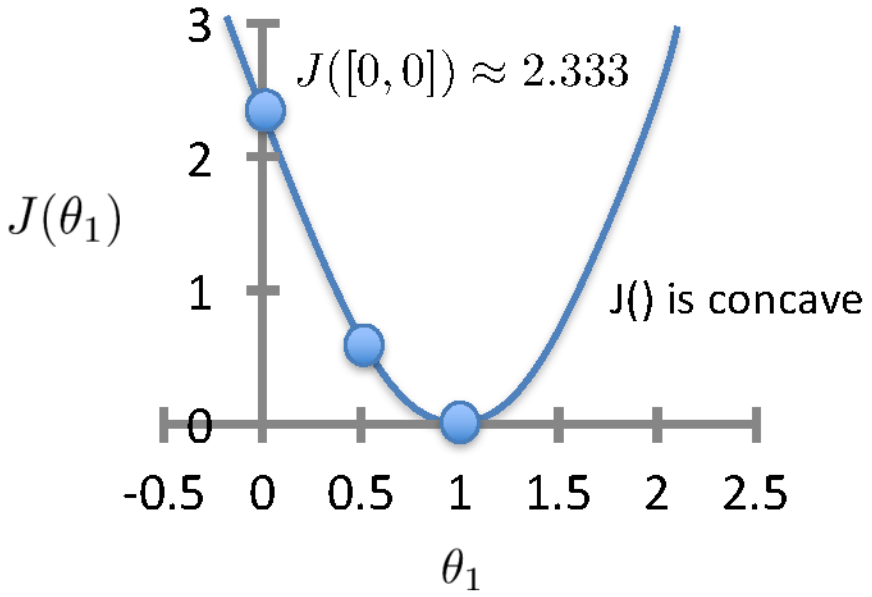

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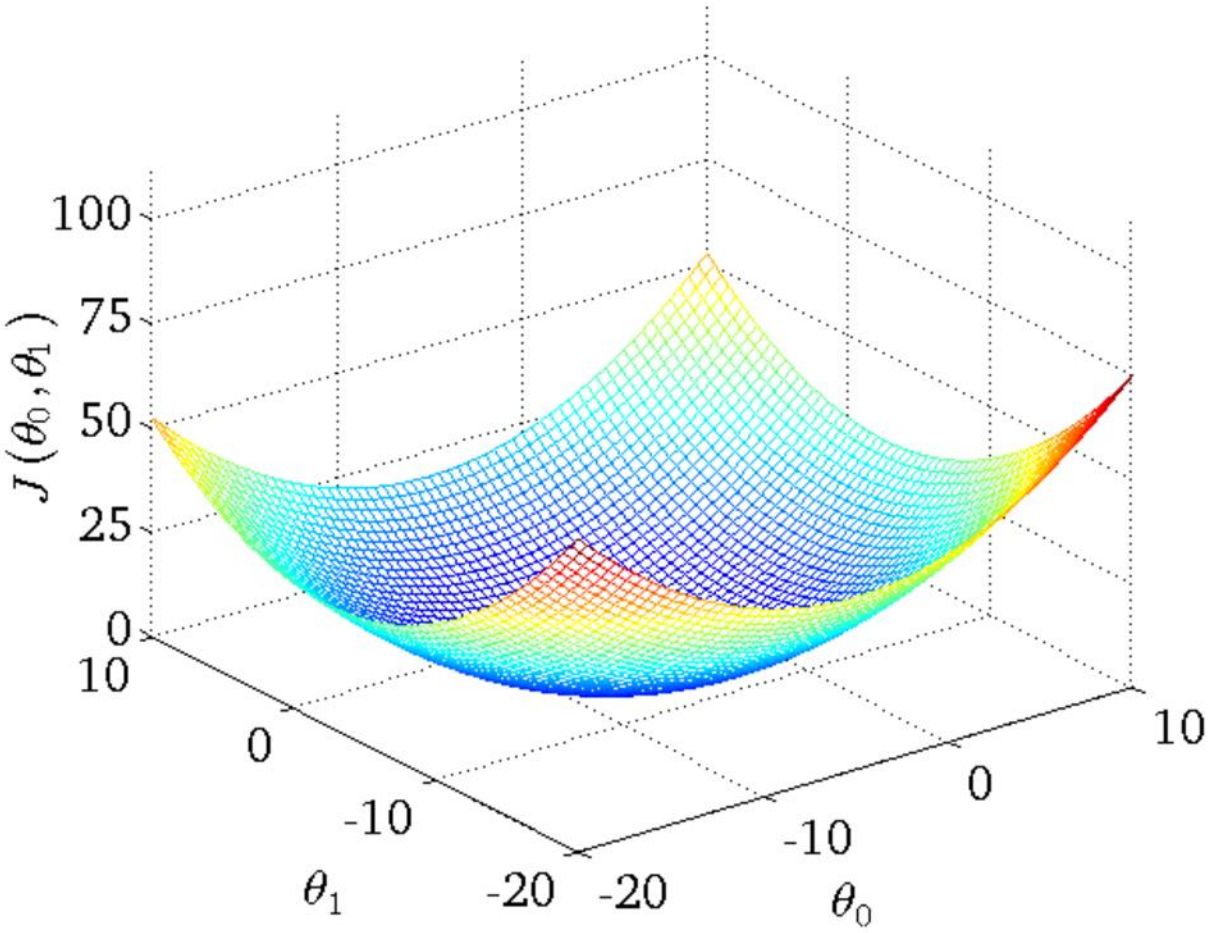

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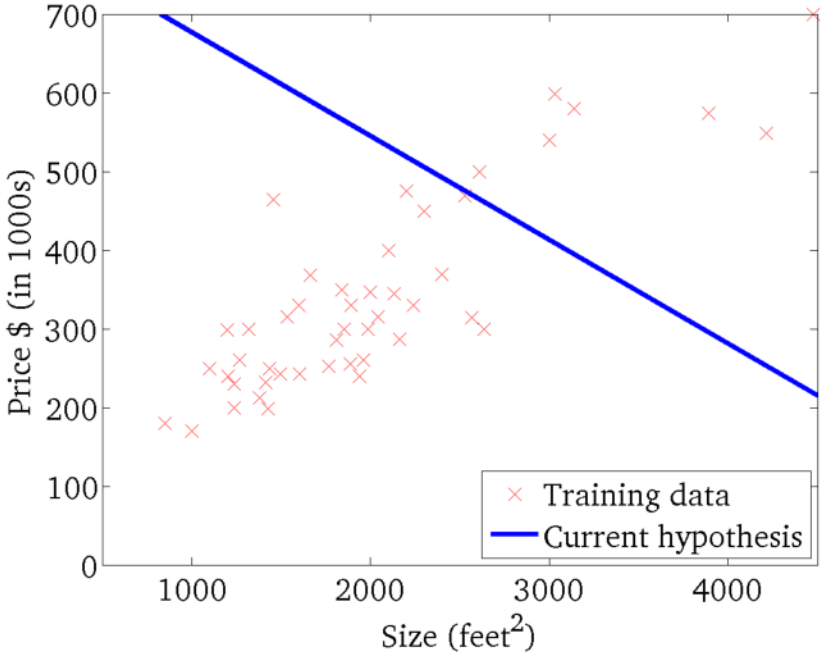
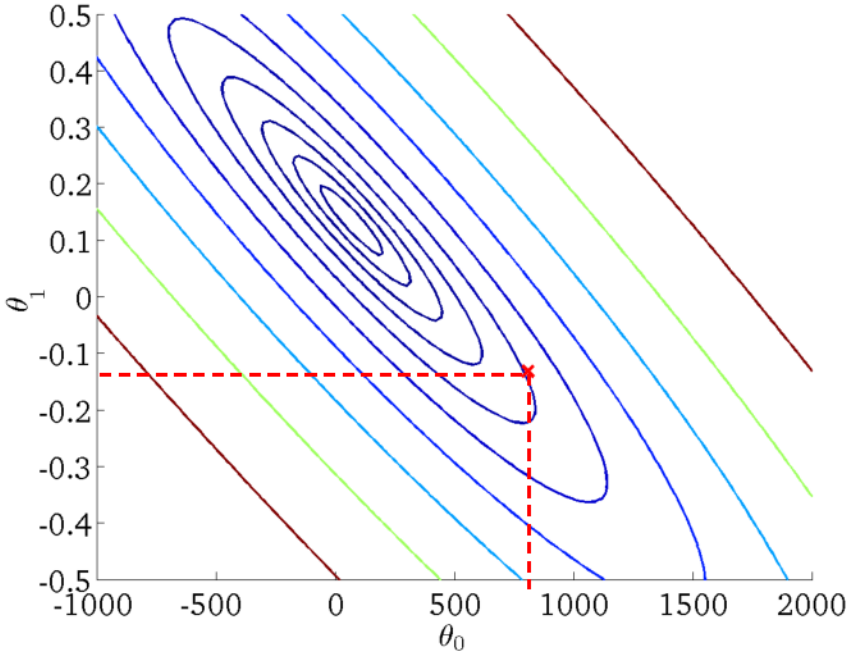


$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



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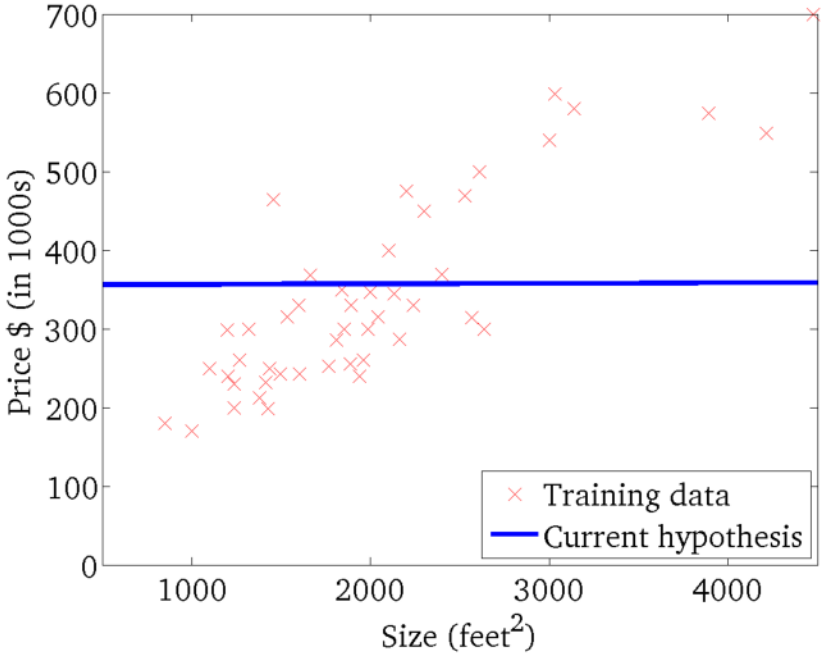

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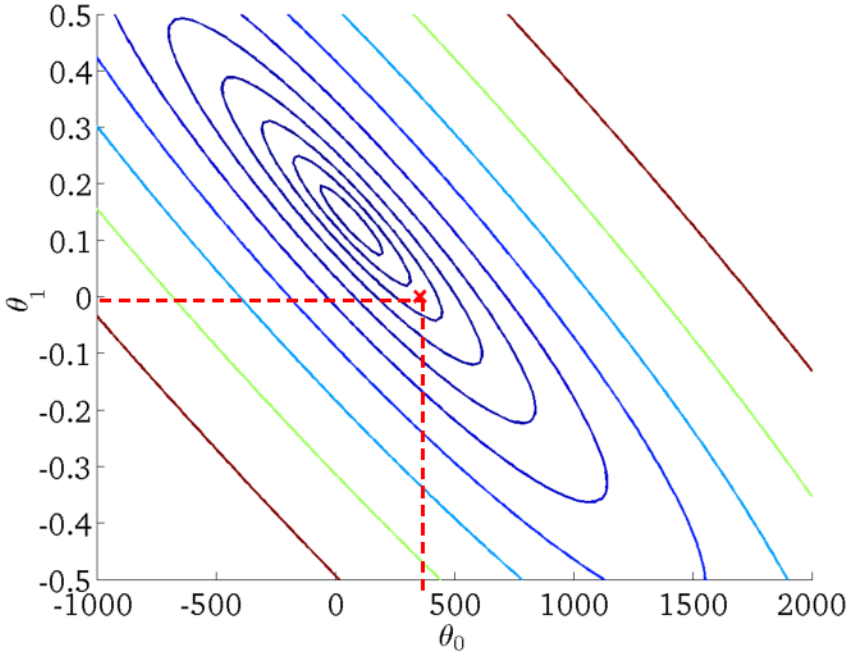

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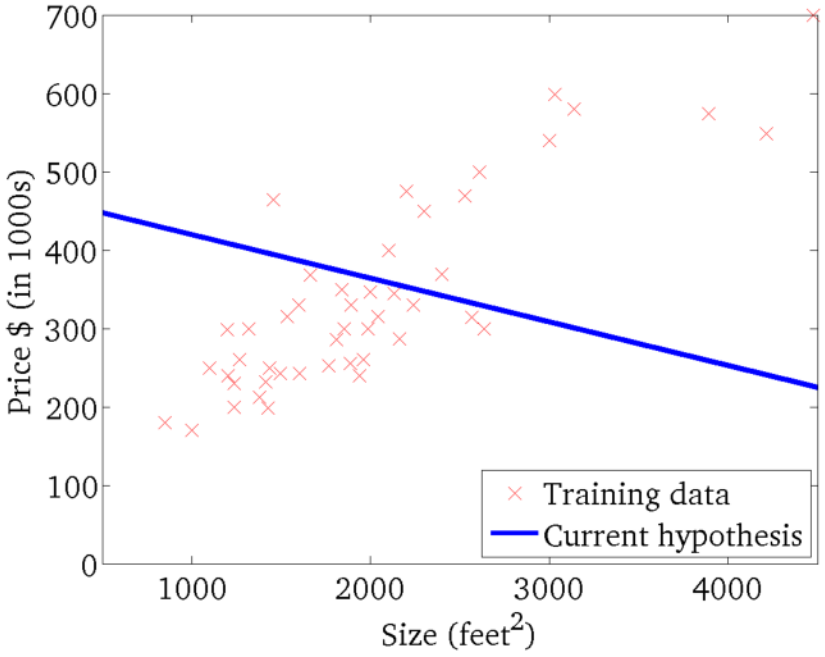

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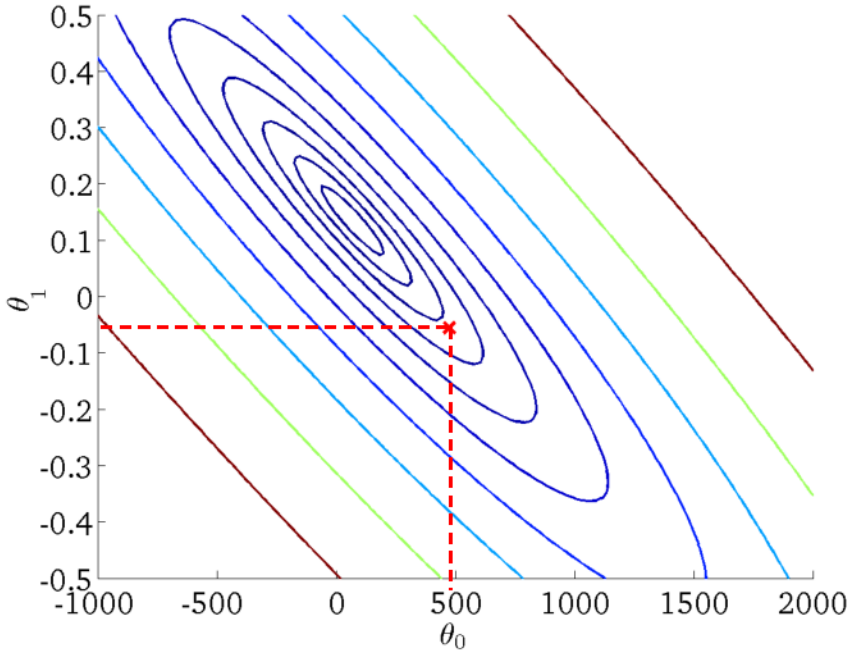

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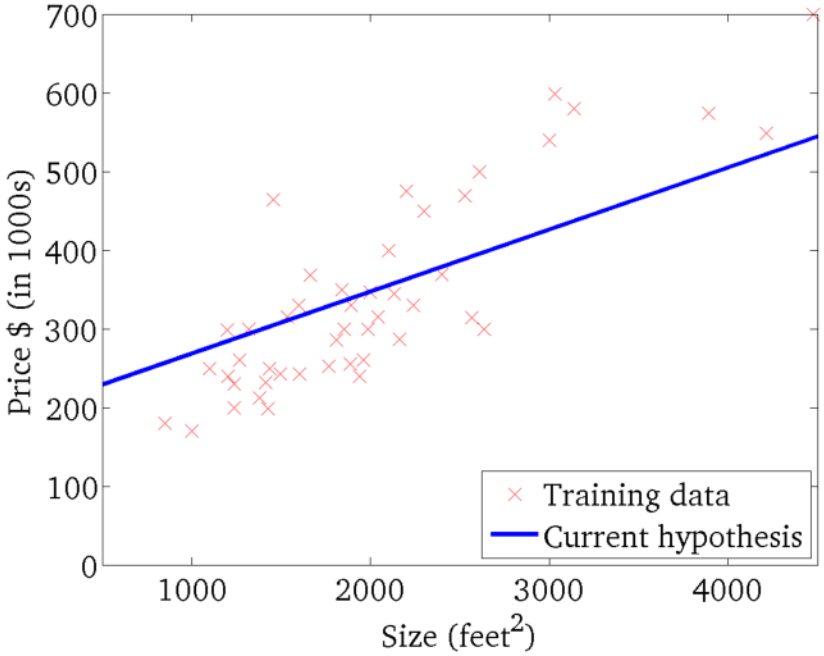

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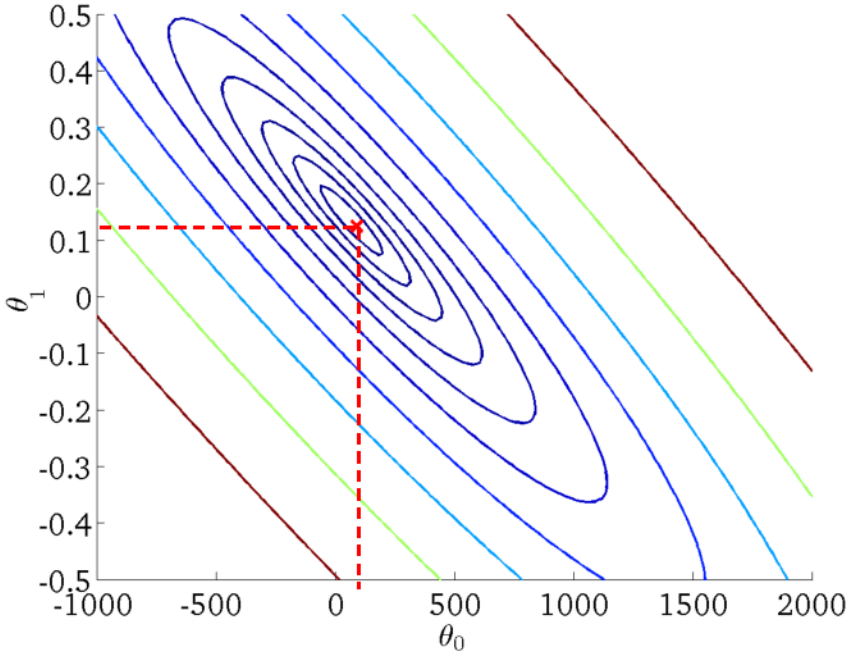

Basic Search Procedure

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

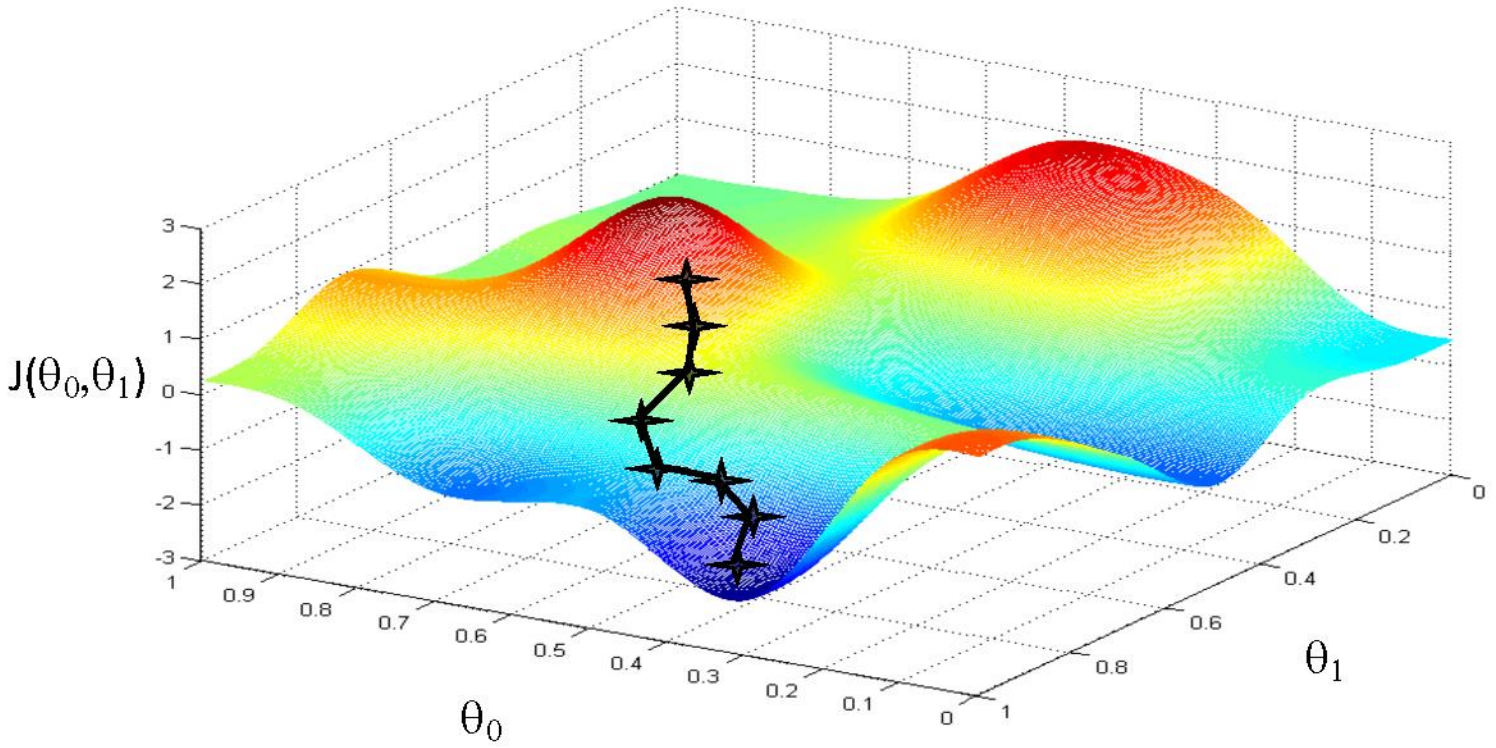

Figure by Andrew Ng

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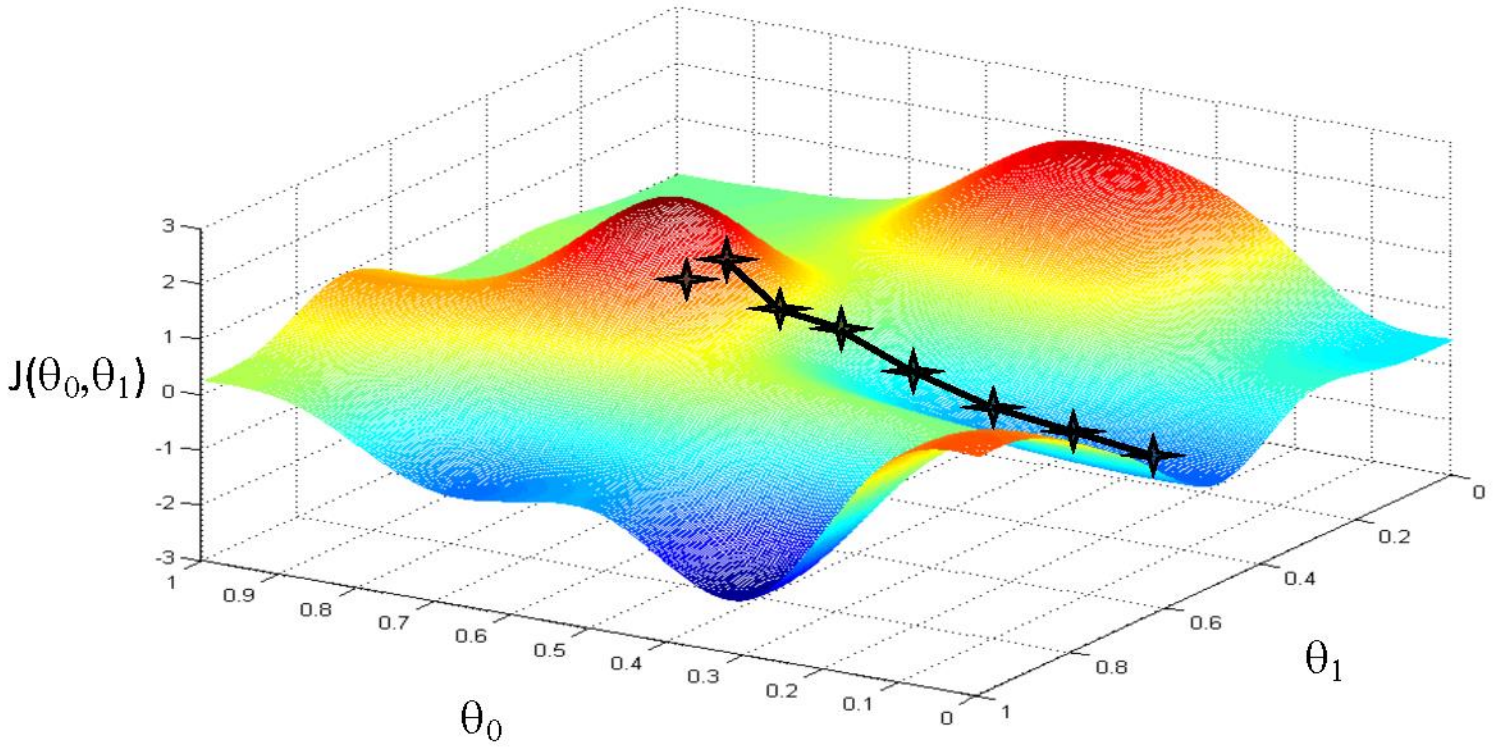

Figure by Andrew Ng

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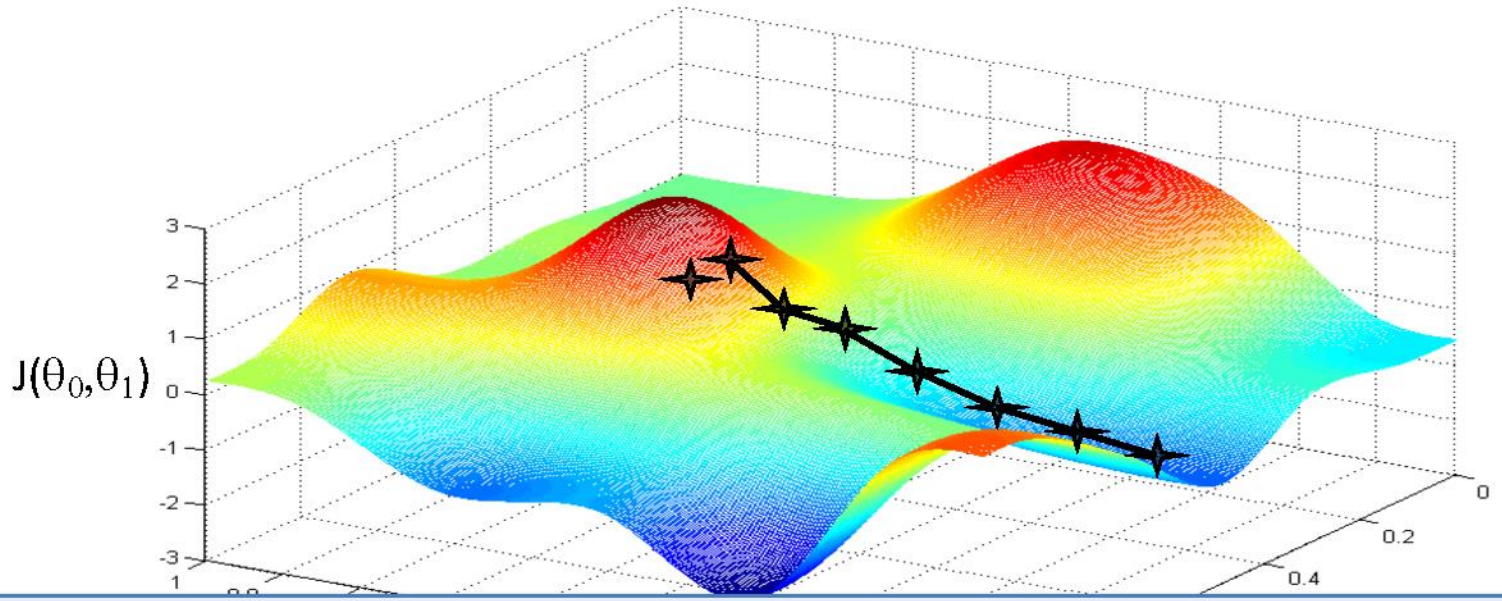


Since the least squares objective function is convex (concave), we don't need to worry about local minima

Figure by Andrew Ng

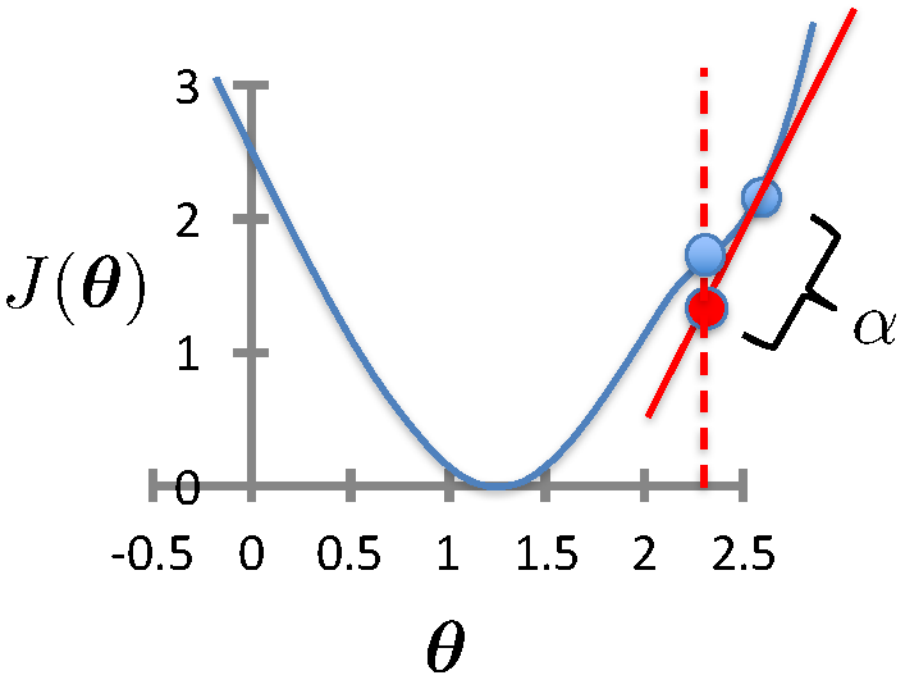
Gradient Descent

- 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



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

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

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simultaneous update
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For Linear Regression:

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta}) &= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2 \\
&= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) \times \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)
\end{aligned}$$

Gradient Descent

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&= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) x_j^{(i)}
\end{aligned}$$

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

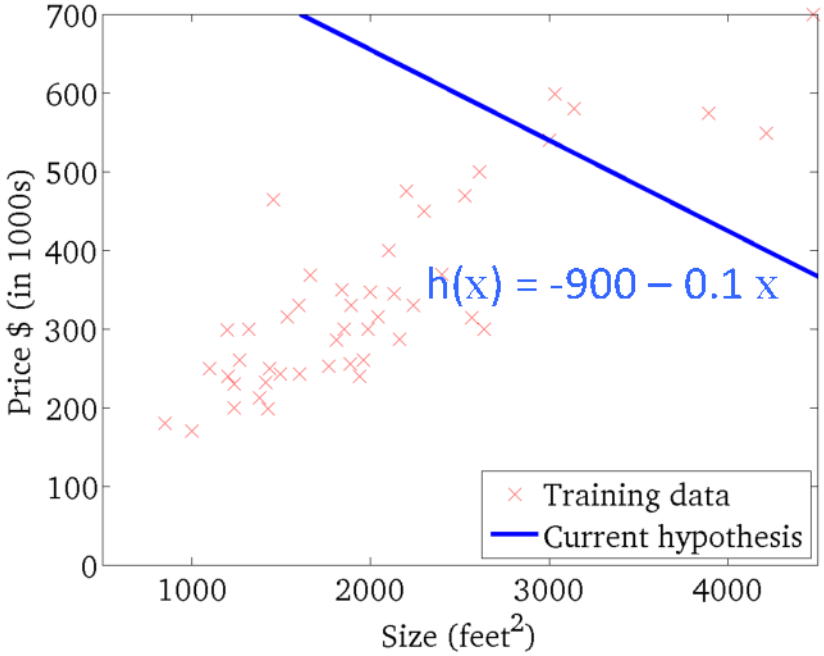
- Assume convergence when $\left\| \boldsymbol{\theta}_{new} - \boldsymbol{\theta}_{old} \right\|_2 < \epsilon$

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

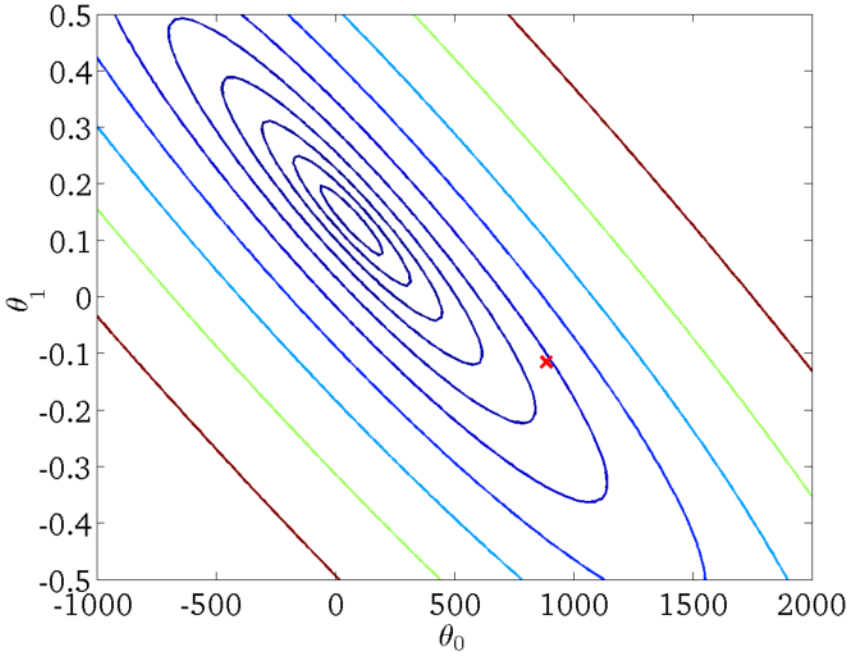
$h_\theta(x)$

(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)



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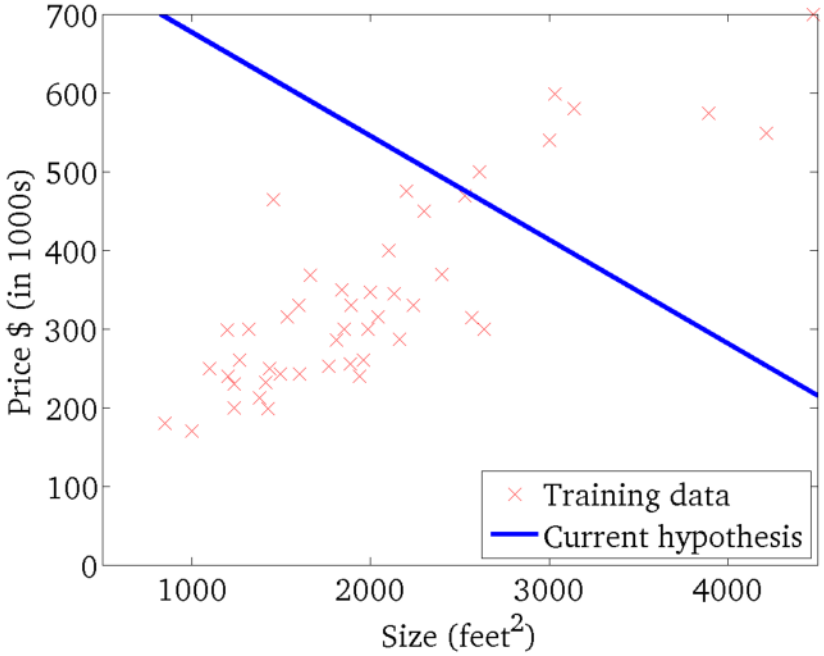

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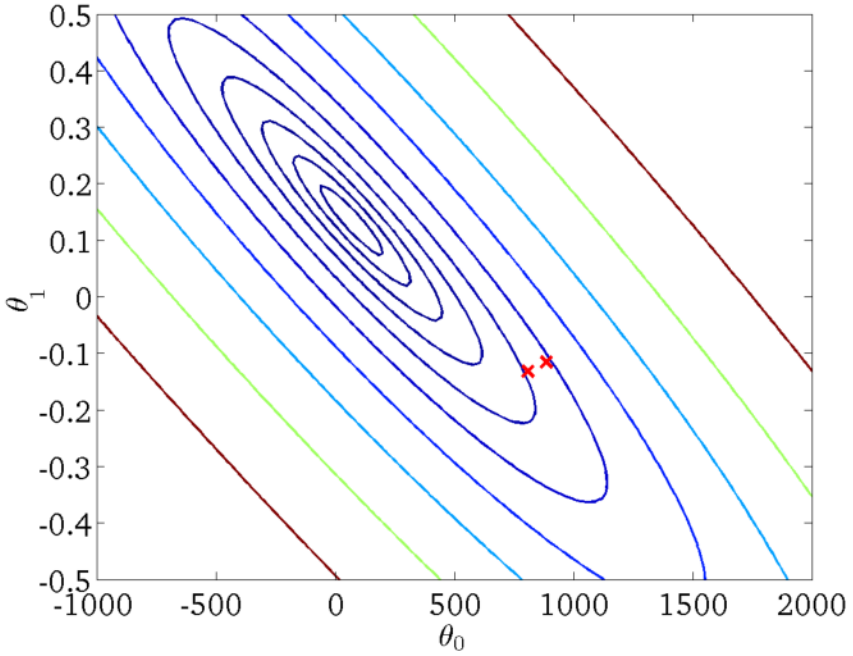

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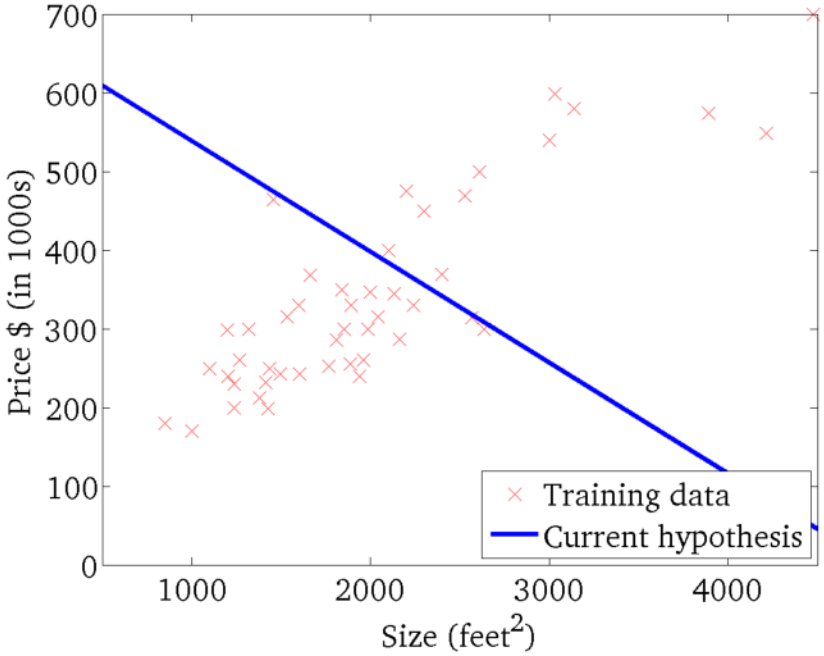

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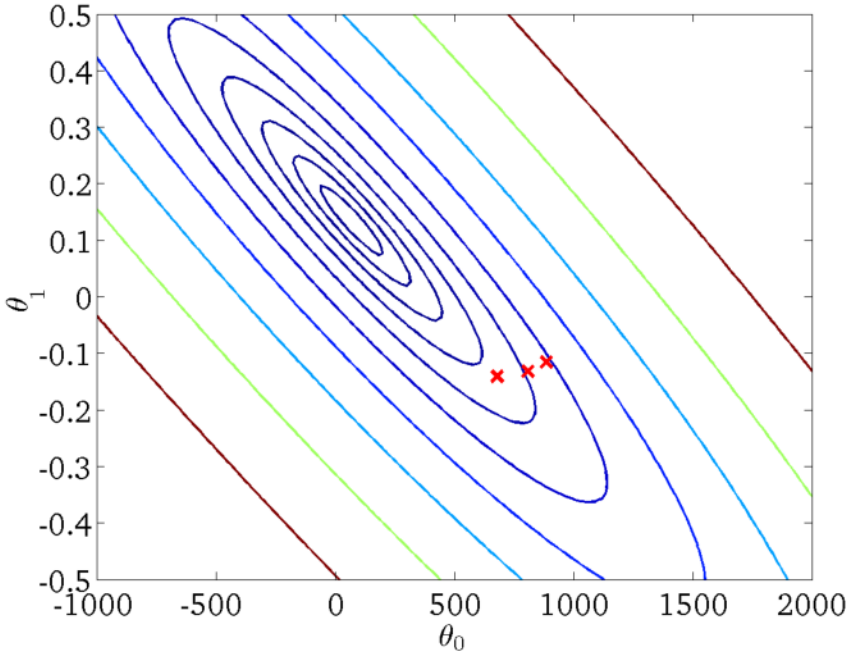

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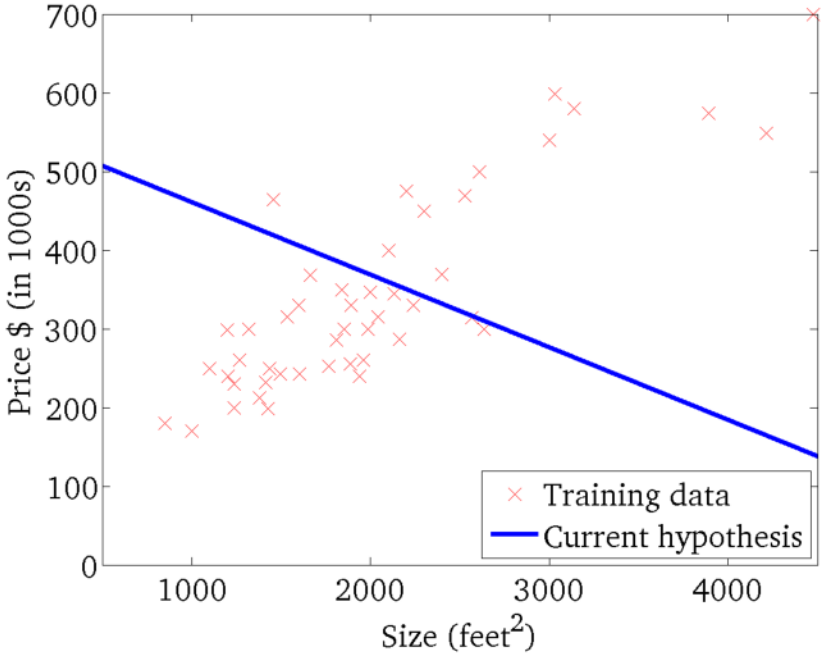

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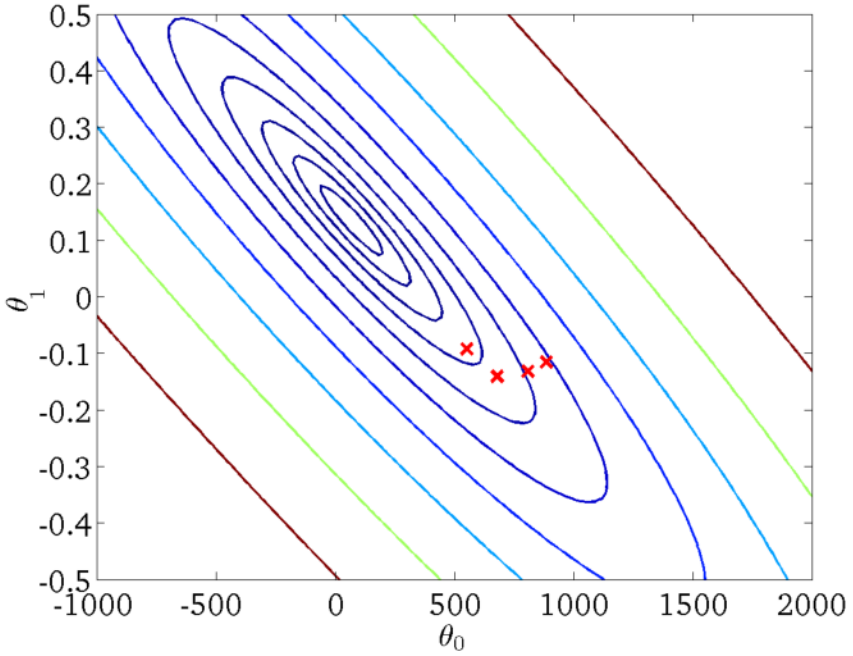

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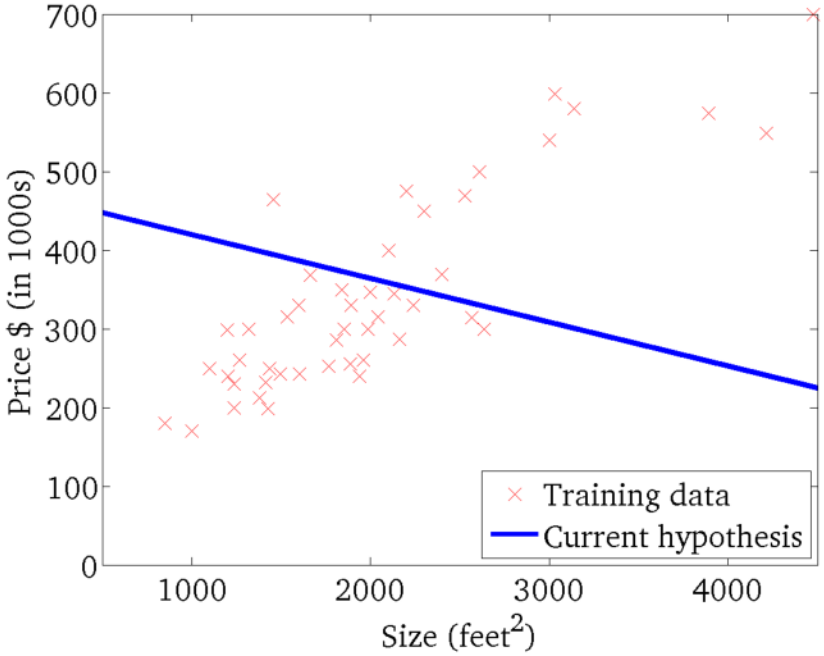
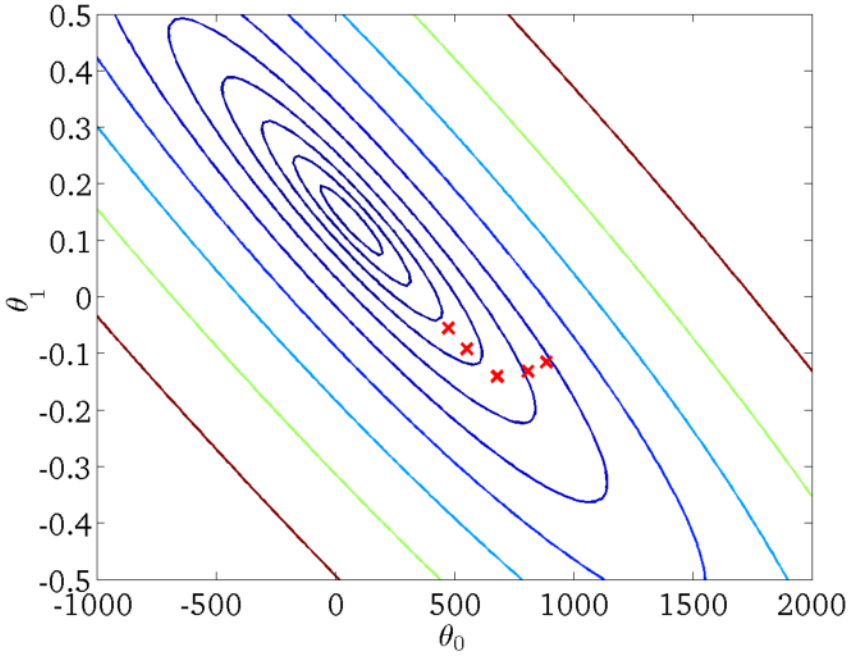


$J(\theta_0, \theta_1)$

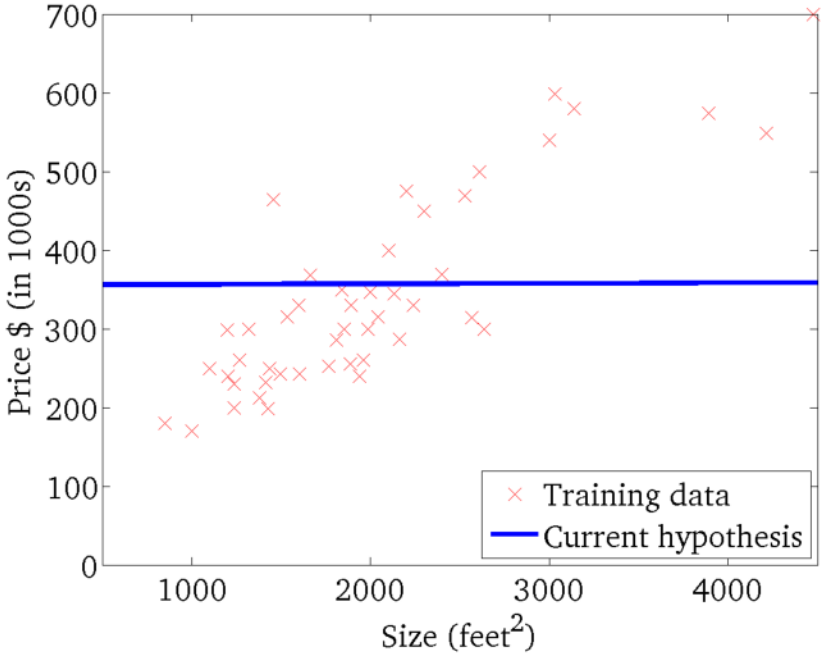
(function of the parameters θ_0, θ_1)



Gradient Descent

$h_\theta(x)$

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



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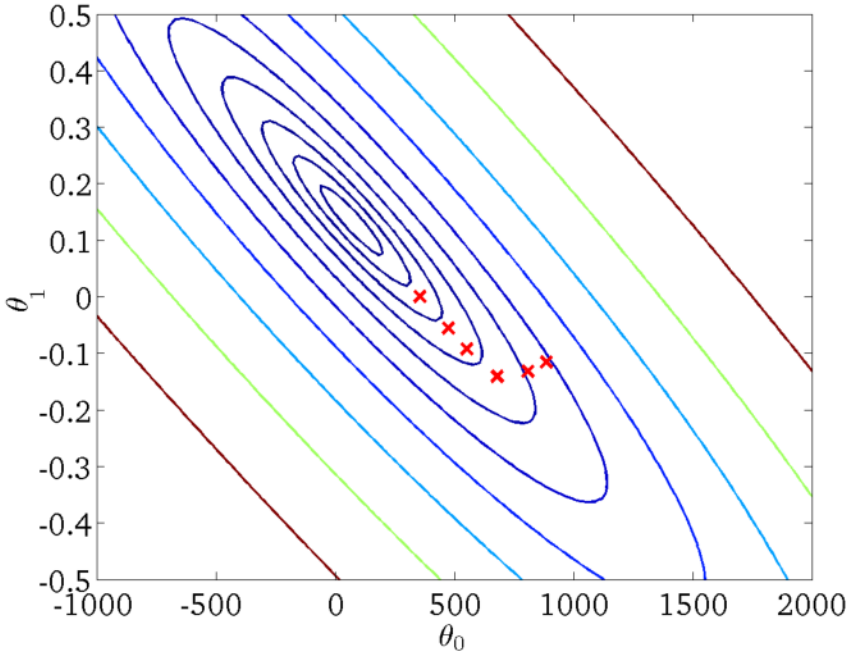

Gradient Descent

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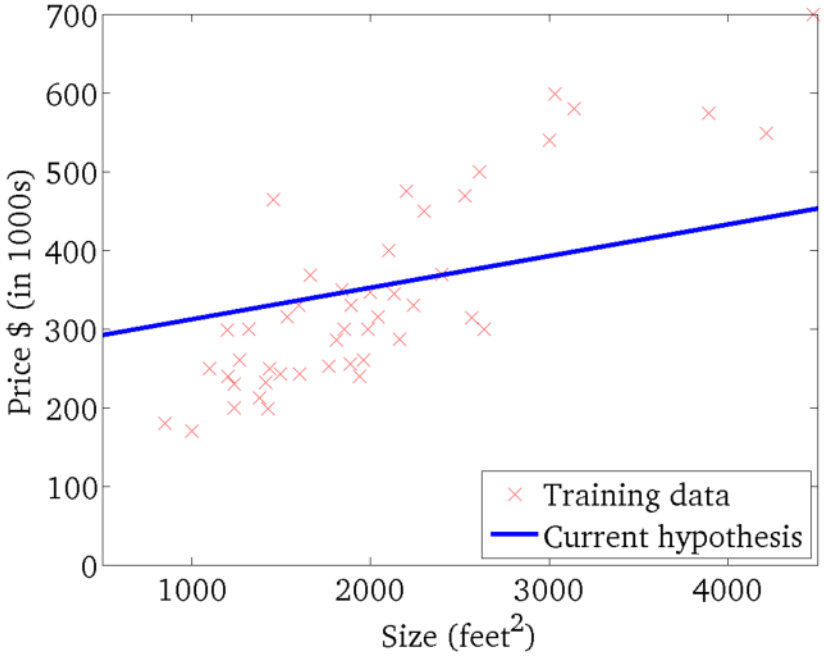
(for fixed θ_0, θ_1, this is a function of x)



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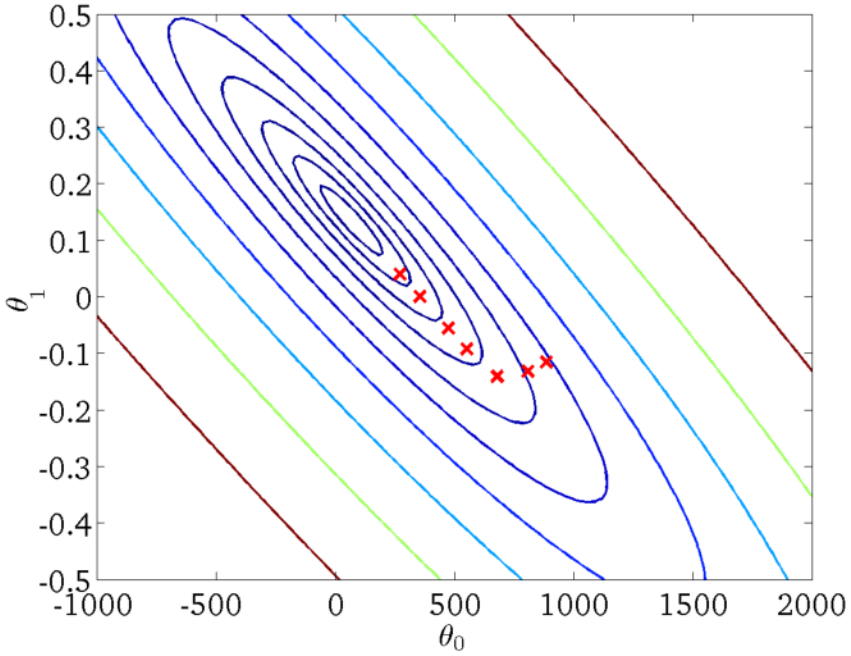
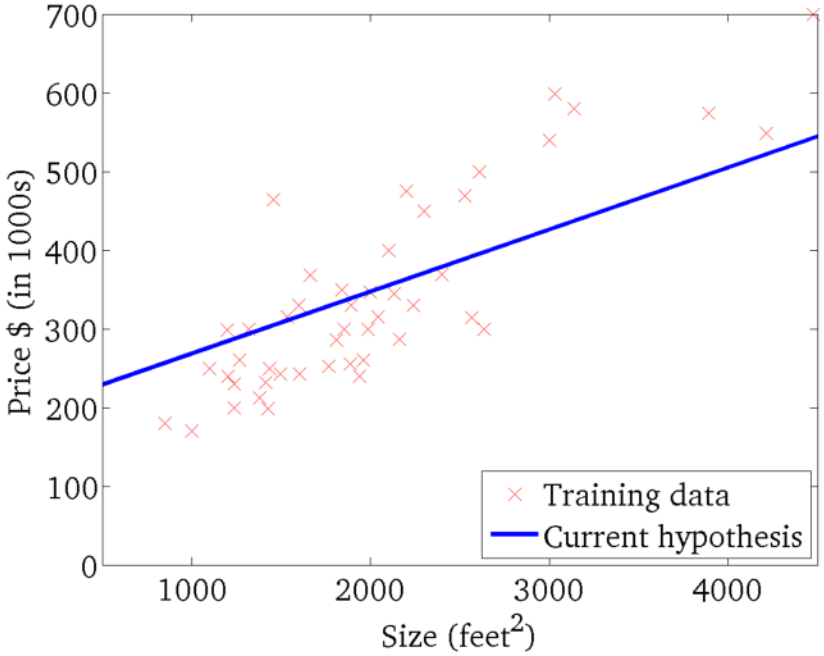


Gradient Descent

$h_\theta(x)$

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



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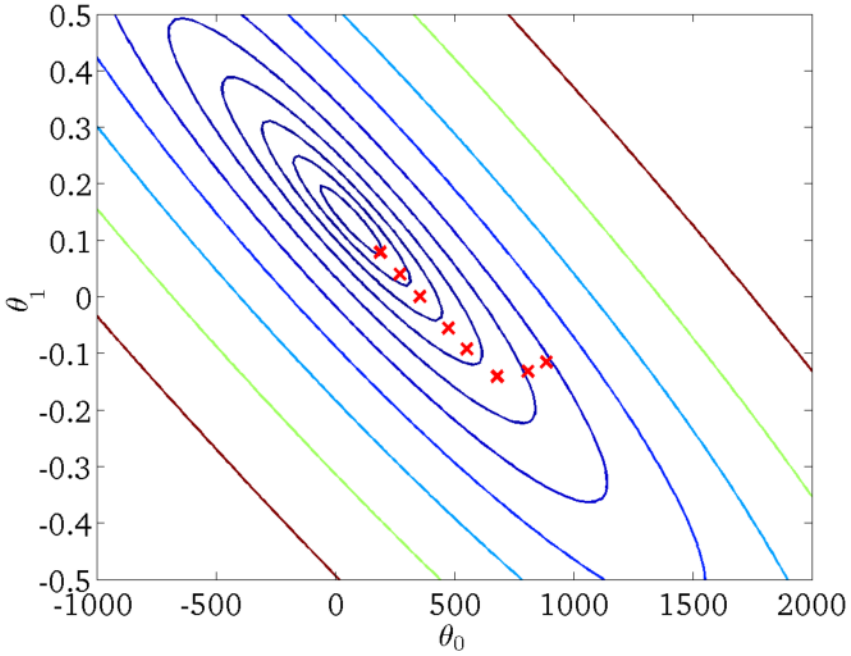
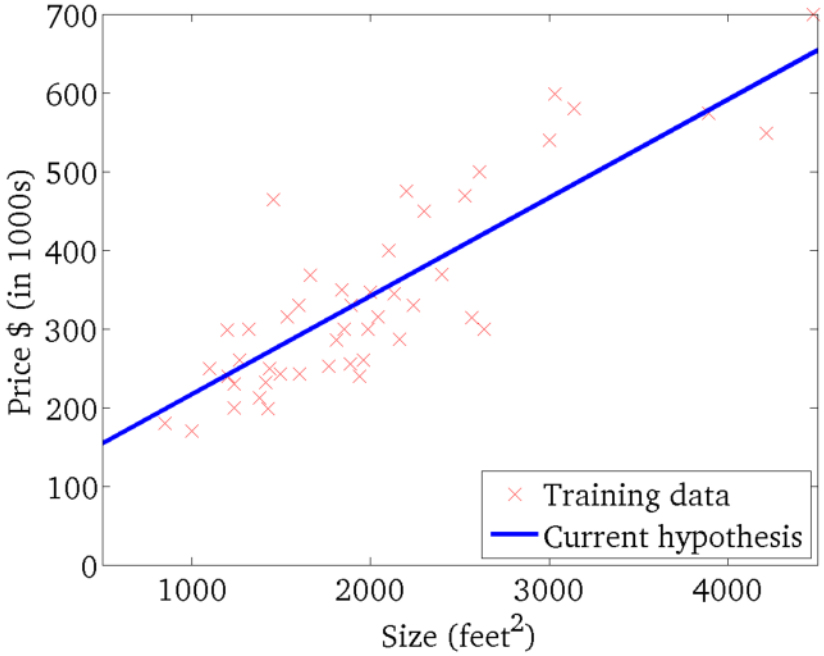


Gradient Descent

$h_\theta(x)$

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



$J(\theta_0, \theta_1)$

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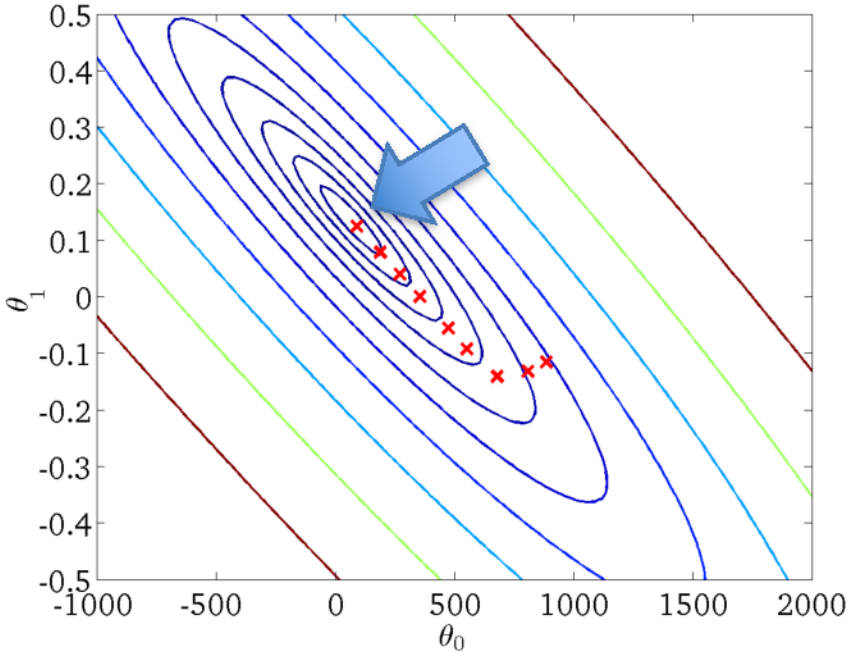
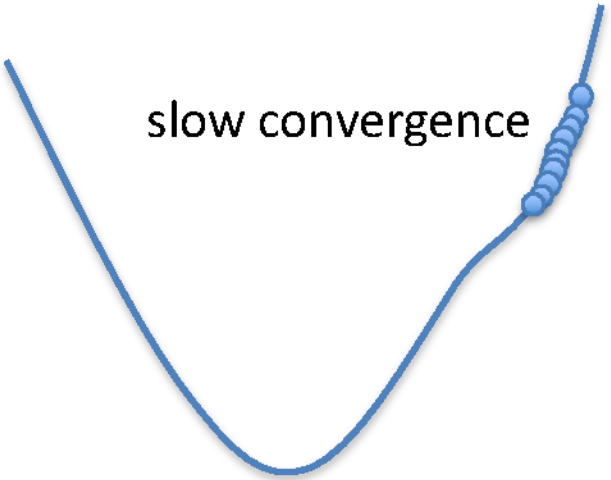
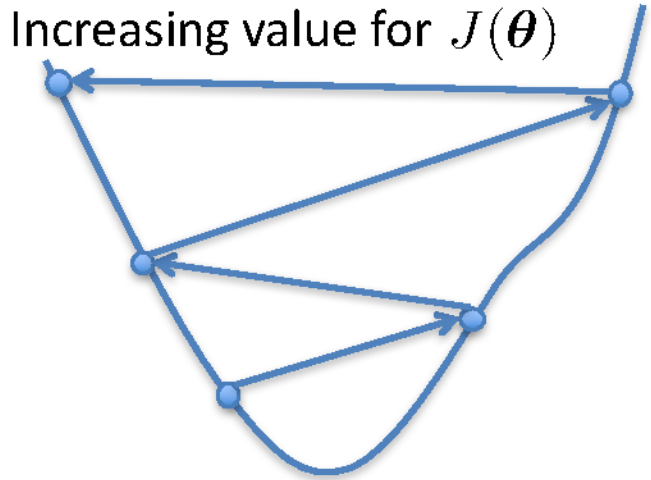


Choosing α

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

Learning Model Parameters – Closed Form Solution (using vectorization)

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

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

- 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

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

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

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

Vectorization

- For the linear regression cost function:

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

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

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

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

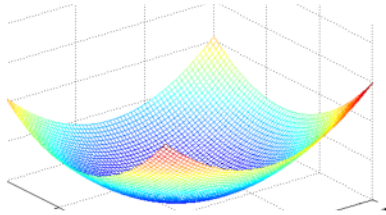
$\mathbb{R}^{(d+1)\times 1}$

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:

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

1 x 1

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

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

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

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

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

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

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 $\mathrm{d} \leq \mathrm{n}$

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 $(X^T X)^{-1}$ is roughly $O(n^3)$

Bayesian linear regression

Bayesian analysis

- Bayesian analysis will show that
  - under certain assumptions any learning algorithm that minimizes the squared error between the output hypothesis predictions and the training data will output a maximum likelihood hypothesis

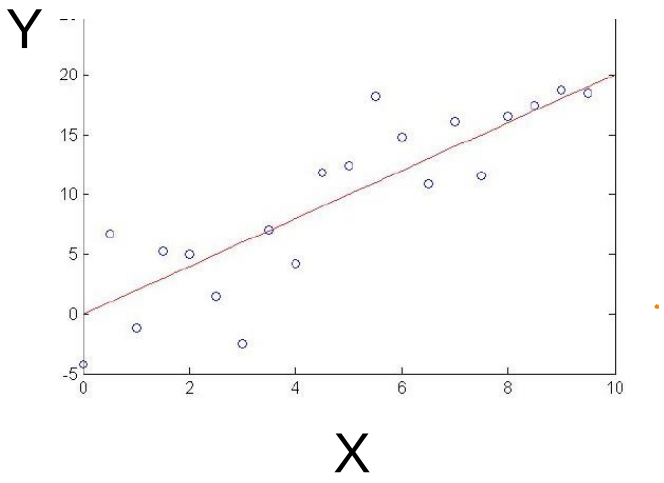
Maximum likelihood and least-squared error hypotheses

- A set of m training examples is provided, where the target value of each example is corrupted by random noise drawn according to a Normal probability distribution.
- Each training example is a pair of the form

(x_i, d_i) where $d_i = f(x_i) + e_i$. Here $f(x_i)$ is the noise-free value of the target function and e_i is a random variable representing the noise.

  - values of the e_i are drawn independently and that they are distributed according to a Normal distribution with zero mean

Choose parameterized form for P(Y|X; θ)



Assume Y is some deterministic f(X), plus random noise

$$y = f(x) + \epsilon \qquad \text{where} \quad \epsilon \sim N(0, \sigma)$$

Therefore Y is a random variable that follows the distribution

$$p(y|x) = N(f(x), \sigma)$$

and the expected value of y for any given x is f(x)

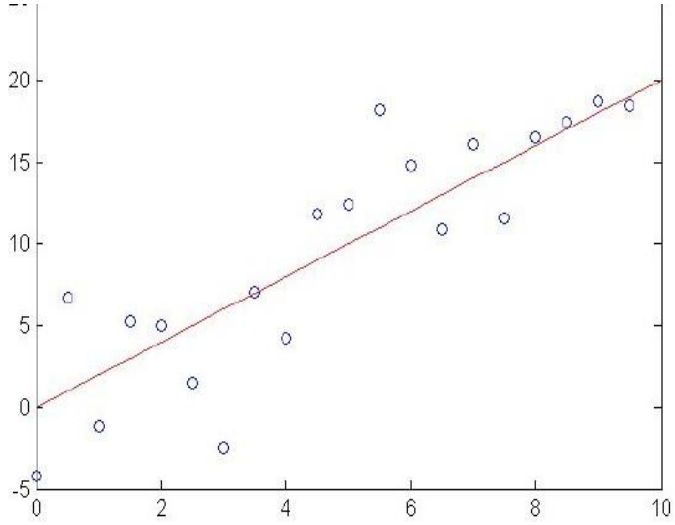
Consider Linear Regression

$$p(y|x) = N(f(x), \sigma)$$

E.g., assume f(x) is linear function of x

$$p(y|x) = N(w_0 + w_1 x, \sigma)$$

$$E[y|x] = w_0 + w_1 x$$



Notation: to make our parameters explicit, let's write

$$W =< w_0, w_1 >$$

$$p(y|x; W) = N(w_0 + w_1 x, \sigma)$$

Training Linear Regression : Maximum Conditional Likelihood Estimate (MCLE)

$$p(y|x;W) = N(w_0 + w_1 x, \sigma)$$

How can we learn W from the training data?

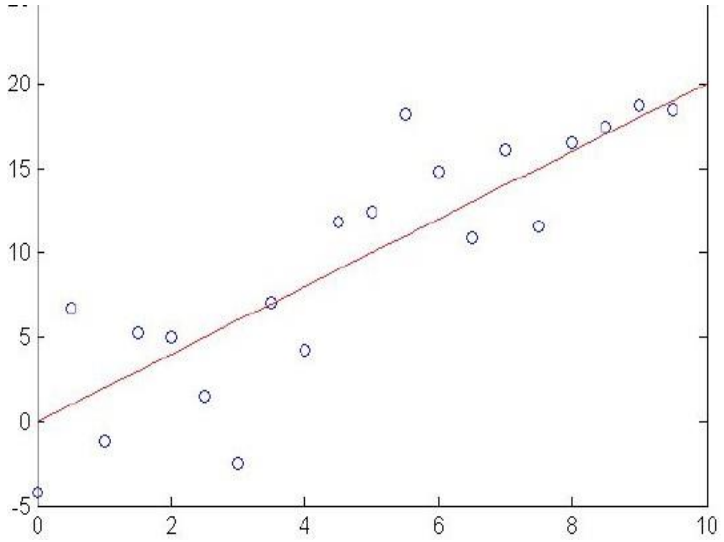
Learn Maximum Conditional Likelihood Estimate!

$$W_{MCLE} = \arg\max_W \prod_l p(y^l|x^l, W)$$

$$W_{MCLE} = \arg\max_W \sum_l \ln p(y^l|x^l, W)$$

where

$$p(y|x;W) = \frac{1}{\sqrt{2\pi\sigma^2}} \; e^{-\frac{1}{2}(\frac{y-f(x;W)}{\sigma})^2}$$



Training Linear Regression: MCLE

Learn Maximum Conditional Likelihood Estimate

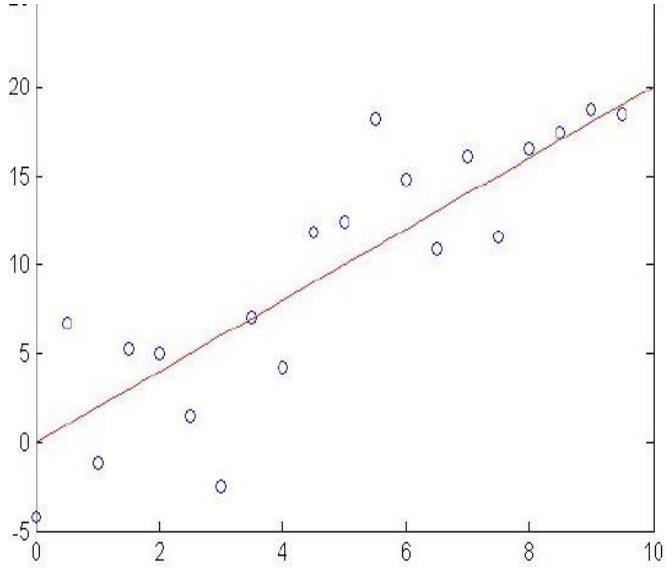
$$W_{MCLE} = \arg\max_W \sum_l \ln p(y^l|x^l, W)$$

where

$$p(y|x; W) = \frac{1}{\sqrt{2\pi\sigma^2}} \; e^{-\frac{1}{2}(\frac{y-f(x;W)}{\sigma})^2}$$

so:

$$W_{MCLE} = \arg\min_W \sum_l (y - f(x; W))^2$$



Training Linear Regression: MCLE, MLE

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

The first term in this expression is a constant independent of h, and can therefore be discarded, yielding

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} -\frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

Maximizing this negative quantity is equivalent to minimizing the corresponding positive quantity.

$$h_{ML} = \underset{h \in H}{\operatorname{argmin}} \sum_{i=1}^{m} \frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

Finally, we can again discard constants that are independent of h.

$$h_{ML} = \underset{h \in H}{\operatorname{argmin}} \sum_{i=1}^{m} (d_i - h(x_i))^2 \qquad (6.6)$$

Training Linear Regression

Maximum Conditional Likelihood Estimate is equivalent to minimizing the squared error loss

$$W_{MCLE} = \arg\min_{W} \sum_{l} (y - f(x; W))^2$$

Can we derive gradient descent rule for training?

$$\frac{\partial \sum_l (y - f(x; W))^2}{\partial w_i} = \sum_l 2(y - f(x; W)) \frac{\partial (y - f(x; W))}{\partial w_i}$$

$$= \sum_l -2(y - f(x; W)) \frac{\partial f(x; W)}{\partial w_i}$$

Regression – What you should know

Under general assumption

$$p(y|x;W) = N(f(x;W),\sigma)$$

- We can use gradient descent as a general learning algorithm
  - as long as our objective function is differentiable wrt W
  - though we might learn local optima

- Almost nothing we said here required that f(x) be linear in x

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

Linear Basis Function

- Simplest linear model for regression is one that involves a linear combination of the input variables

$$y(x,w)=w_0 +w_1x_1 +...+w_Dx_D$$

- Extend the class of models by considering linear combinations of fixed nonlinear functions of the input variables, of the form

$$y(x,w)=w_0 + \sum_{j=1}^{M-1} w_j\varphi_j(x)$$

  - where $\varphi_j(x)$ are known as basis functions.
  - By denoting the maximum value of the index j by M −1, the total number of parameters in this model will be M.

Linear Basis Function

- Convenient to define an additional dummy 'basis function' $\phi_0(x)=1$. So,

$$y(x,w) = \sum_{j=1}^{M-1} w_j \varphi_j(x) = \mathbf{w}^T \boldsymbol{\phi}_j(\mathbf{x})$$

where $\mathbf{w} = (w_0,\ldots,w_{M-1})^T$ and $\boldsymbol{\phi} = (\phi_0, \phi_1, \ldots\ldots \phi_n)$

- If the original variables comprise the vector x, then the features can be expressed in terms of the basis functions $\{\phi j(x)\}$

Linear Basis Function Models

- Generally,

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j \phi_j(\boldsymbol{x})$$

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 :

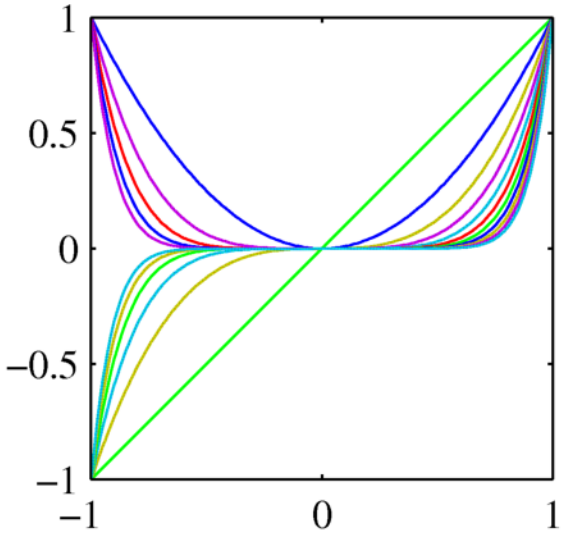
$$\phi_j(\boldsymbol{x}) = x_j$$

Linear Basis Function Models

- Polynomial basis functions:

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

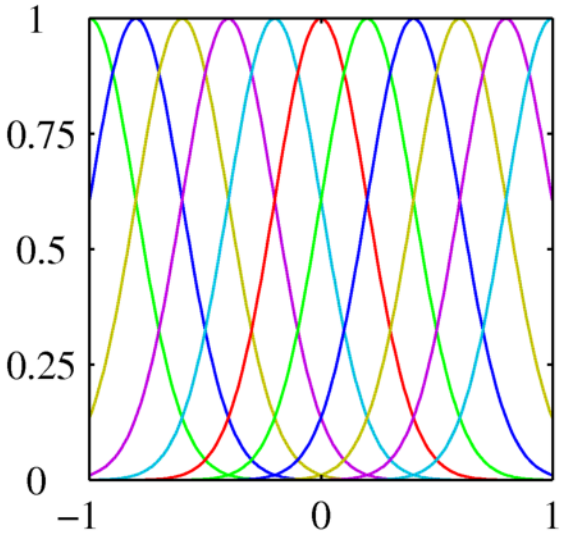
  - These are global; a small change in x affects all basis functions



- 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

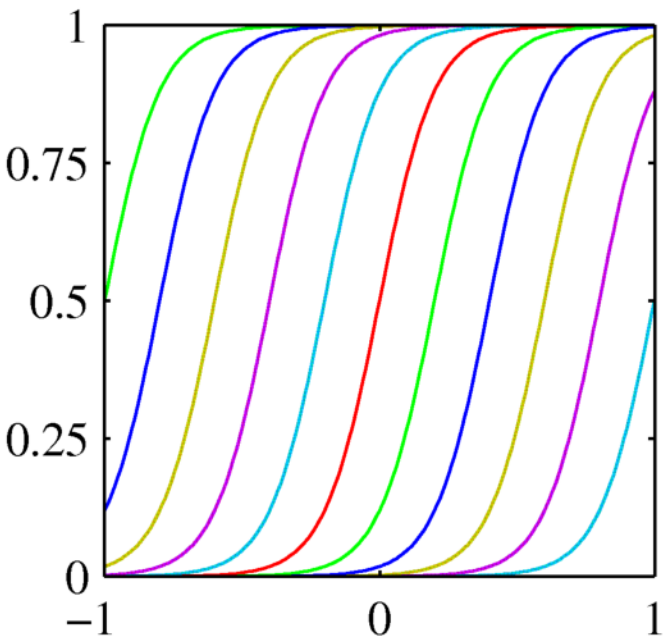
- Sigmoidal basis functions:

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

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).

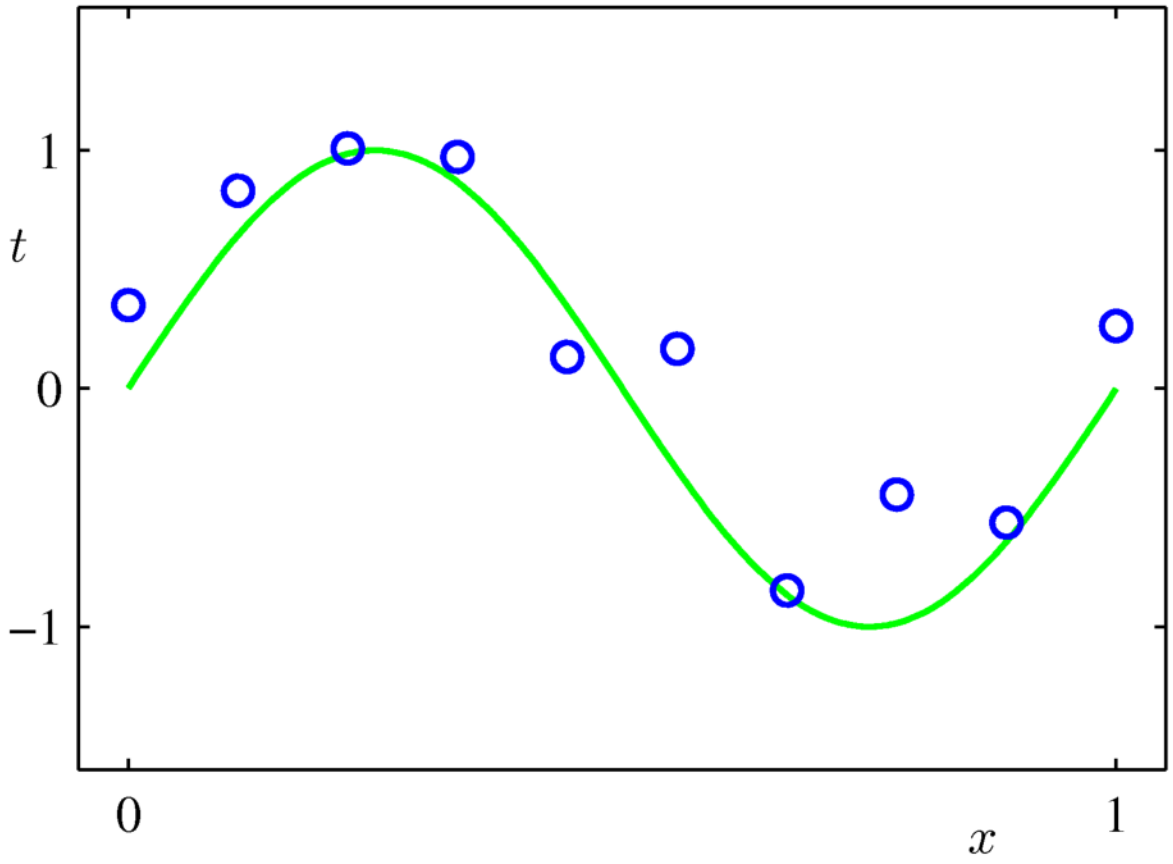


Linear Basis Function Models

- 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

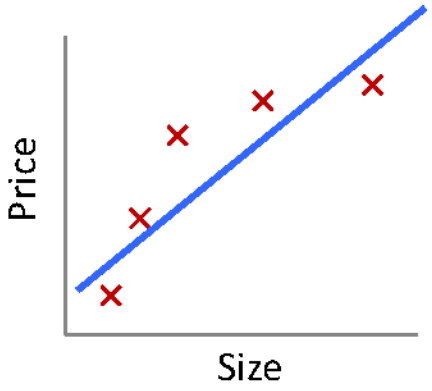
Example of Fitting a Polynomial Curve with a Linear Model



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

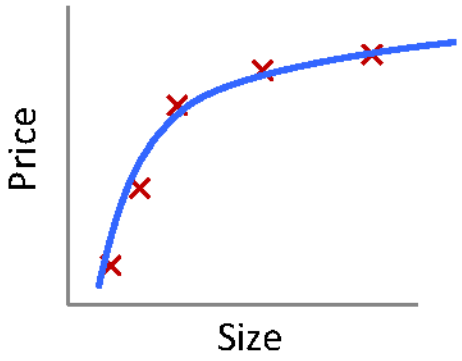
Bias-Variance Decomposition

Quality of Fit



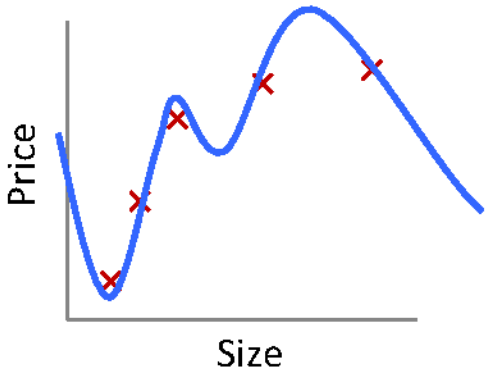
$\theta_0 + \theta_1 x$

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

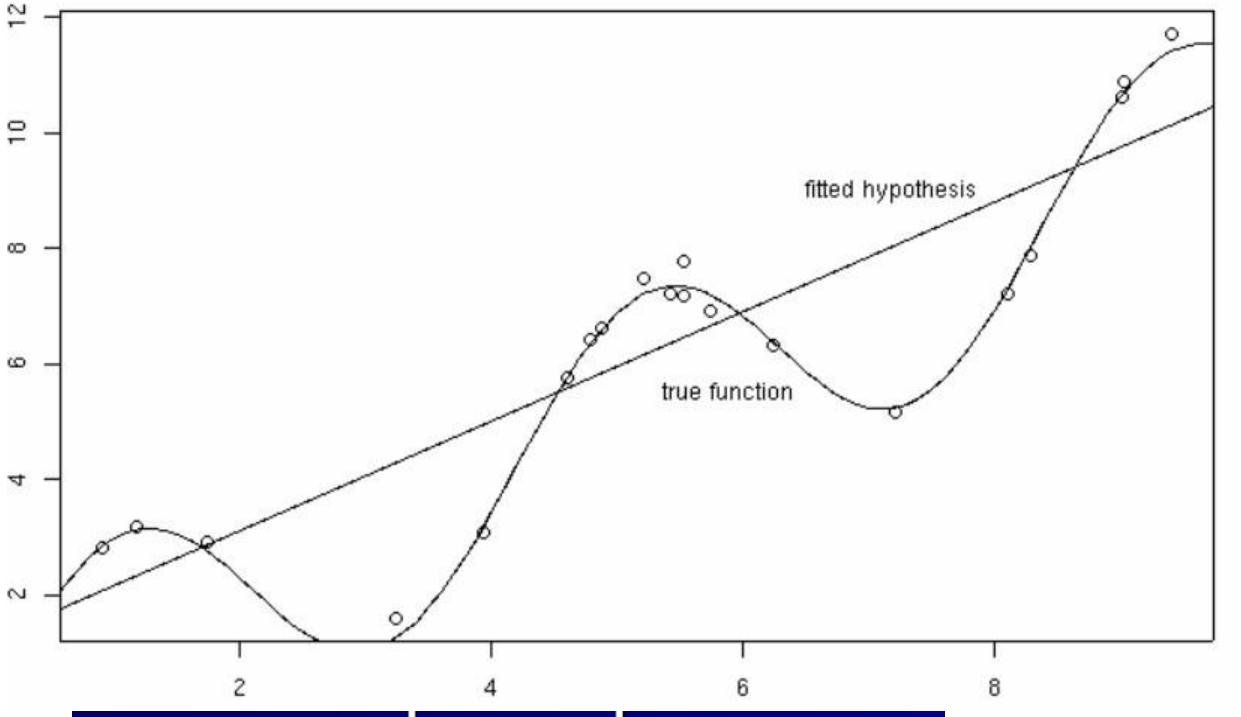
Bias-Variance Tradeoff

- **Bias:** difference between
  what you expect to learn and **truth**
  - Measures how well you expect to represent true solution
  - Decreases with more complex model

- **Variance:** difference between
  what you expect to learn and
  what you learn from a particular dataset
  - Measures how sensitive learner is to specific dataset
  - Increases with more complex model

Example

Tom Dietterich, Oregon St



$y = x + 2 \sin(1.5x) + N(0,0.2)$

True Function :
$y=f(x)$

Bias – Variance decomposition of error

$$E_{D,\varepsilon}\left\{\left(f(x)+\varepsilon-h_D(x)\right)^2\right\}$$

dataset and noise

true function

noise

learned from D

Fix test case *x*, then do this experiment:

1. Draw size *n* sample D=$(x_1,y_1),\ldots.(x_n,y_n)$
2. Train linear regressor h_D *using* D
3. Draw one test example $(x, f(x)+\varepsilon)$
4. Measure squared error of h_D on that example *x*
5. What's the expected error?

Bias – Variance decomposition of error

Notation - to simplify this

$$f \equiv f(x) + \varepsilon \qquad \hat{y} = \hat{y}_D \equiv h_D(x)$$

$$E_{D,\varepsilon}\left\{\left(f(x)+\varepsilon-h_D(x)\right)^2\right\}$$

dataset and noise

true function

noise

learned from D

$$h \equiv E_D\{h_D(x)\}$$

long-term expectation of learner's prediction on this *x* averaged over many data sets *D*

Bias – Variance decomposition of error

$$h = E_D\{\hat{y}_D\}$$

$$E_{D,\varepsilon}\left\{(f-\hat{y})^2\right\}$$

$$= E\left\{\left([f-h]+[h-\hat{y}]\right)^2\right\}$$

$$= E\left\{[f-h]^2+[h-\hat{y}]^2+2[f-h][h-\hat{y}]\right\}$$

$$= E\left\{[f-h]^2+[h-\hat{y}]^2+2[fh-f\hat{y}-h^2+h\hat{y}]\right\}$$

$$= E[(f-h)^2]+E[(h-\hat{y})^2]+2\left(E[fh]-E[f\hat{y}]-E[h^2]+E[h\hat{y}]\right)$$

$$\hat{y} = \hat{y}_D \equiv h_D(x)$$

$$f \equiv f(x)+\varepsilon$$

Bias – Variance decomposition of error

$$h = E_D\{\hat{y}_D\}$$

$$E_{D,\varepsilon}\left\{(f-\hat{y})^2\right\}$$

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$$= E[(f-h)^2]+E[(h-\hat{y})^2]+2\left(E[fh]-E[f\hat{y}]-E[h^2]+E[h\hat{y}]\right)$$

$$\hat{y} = \hat{y}_D \equiv h_D(x)$$

$$f \equiv f(x)+\varepsilon$$

Bias – Variance decomposition of error

$h = E_D\{\hat{y}_D\}$ $\quad \hat{y} = \hat{y}_D$ $\quad f \equiv f(x) + \varepsilon$

$$
\begin{aligned}
& 2(E[fh] - E[f\hat{y}] - E[h^2] + E[h\hat{y}]) \\
&= E[f]E[h] - E[f]E[\hat{y}] - E[h]E[h] + E[h]E[\hat{y}] \\
&= E[f]E[E[\hat{y}]] - E[f]E[\hat{y}] - E[h]E[E[\hat{y}]] + E[h]E[\hat{y}] \\
&= E[f]E[\hat{y}] - E[f]E[\hat{y}] - E[h]E[\hat{y}] + E[h]E[\hat{y}] \\
&= 0
\end{aligned}
$$

Bias – Variance decomposition of error

$$E_{D,\varepsilon}\left\{(f-\hat{y})^2\right\}$$
$$= E\left\{\left([f-h]+[h-\hat{y}]\right)\right\}^2$$
$$= E\left\{[f-h]^2+[h-\hat{y}]^2+2[f-h][h-\hat{y}]\right\}$$
$$= E[(f-h)^2]+E[(h-\hat{y})^2]$$

$$h \equiv E_D\{h_D(x)\}$$
$$\hat{y} = \hat{y}_D \equiv h_D(x)$$
$$f \equiv f(x) + \varepsilon$$

BIAS^2

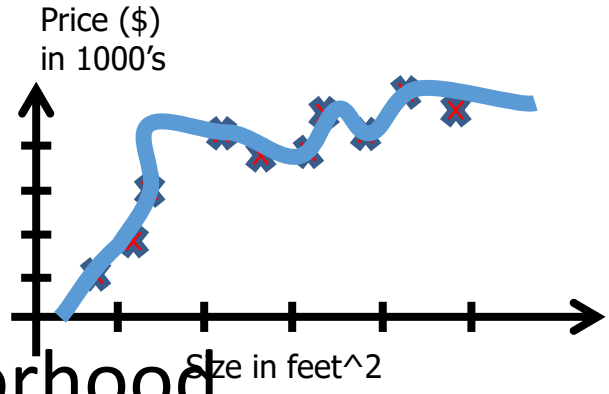
Squared difference between best possible prediction for x, f(x), and our "long-term" expectation for what the learner will do if we averaged over many datasets D, $E_D[h_D(x)]$

VARIANCE

Squared difference btwn our long-term expectation for the learners performance, $E_D[h_D(x)]$, and what we expect in a representative run on a dataset D (hat y)

Addressing overfitting

- $x_1 =$ size of house
- $x_2 =$ no. of bedrooms
- $x_3 =$ no. of floors
- $x_4 =$ age of house
- $x_5 =$ average income in neighborhood
- $x_6 =$ kitchen size
- $\vdots$
- x_{100}



Slide credit: Andrew Ng

Addressing overfitting

- **1. Reduce number of features.**
  - Manually select which features to keep.
  - Model selection algorithm

- **2. Regularization.**
  - Keep all the features, but reduce magnitude/values of parameters θ_j.
  - Works well when we have a lot of features, each of which contributes a bit to predicting y.

Slide credit: Andrew Ng

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

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

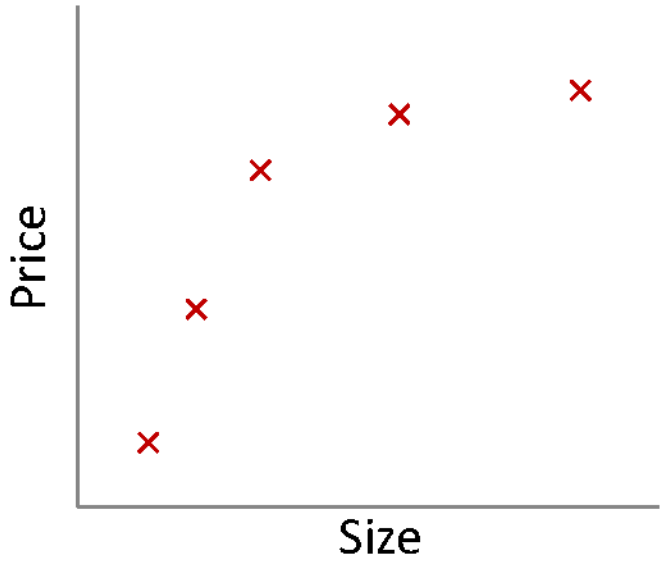
model fit to data — regularization

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

Understanding Regularization

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

- What happens if we set λ to be huge (e.g., 10^{10})?



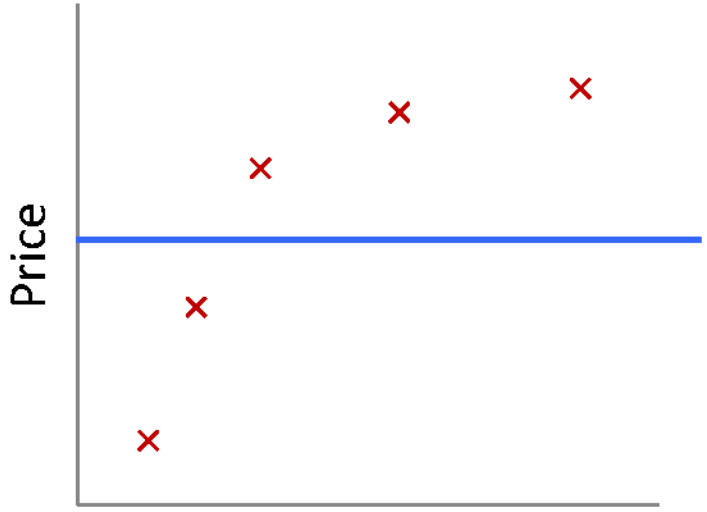
$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Based on example by Andrew Ng

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 if we set λ to be huge (e.g., 10^{10})?



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

0 0 0 0

Based on example by Andrew Ng

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:

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

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

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

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

regularization

Regularized Linear Regression

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

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

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

- We can rewrite the gradient step as:

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

Funny but simple explanation about bias and variance

- https://www.youtube.com/watch?v=EuBBz3bI-aA

In our next session

innovate achieve lead

We will cover:

Tom Mitchell - Chapter 3

- Decision Tree
- Handling overfitting
- Continuous values
- Missing Values
- Random Forest