

Linear Regression

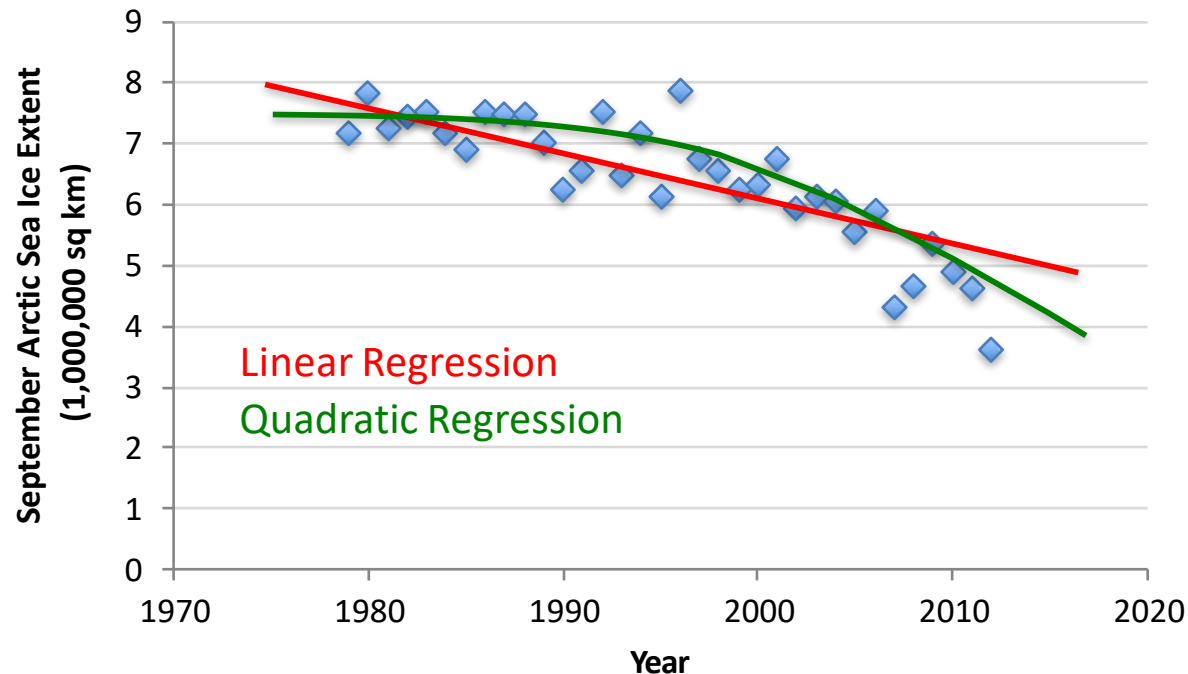
Machine Learning (AIM 5002-41)

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Regression

Given:

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



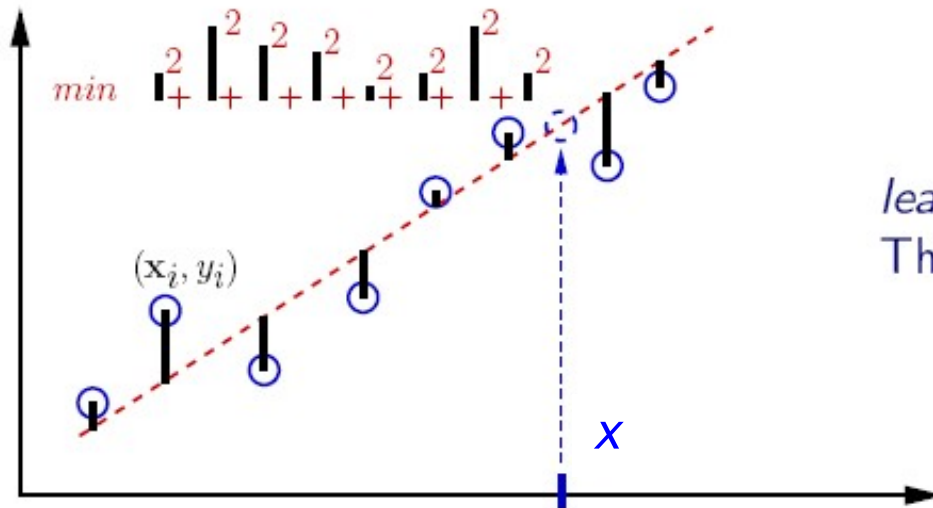
Linear Regression

- Hypothesis:

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

Assume $x_0 = 1$

- Fit model by minimizing sum of squared errors



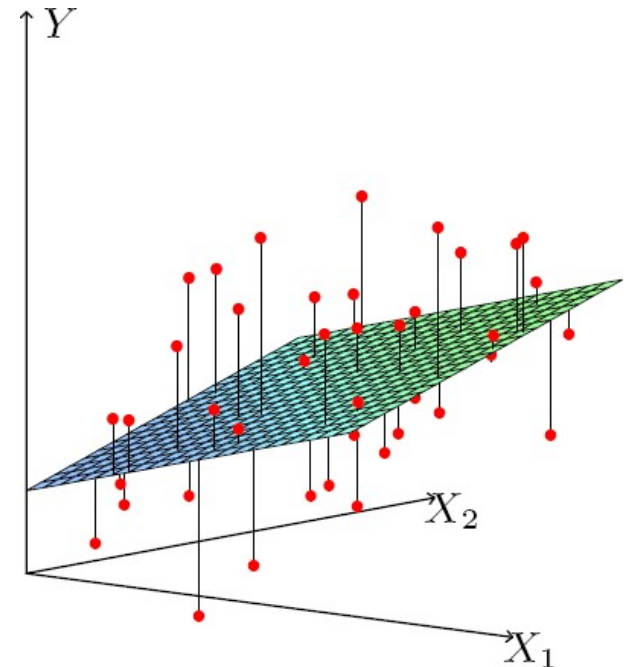
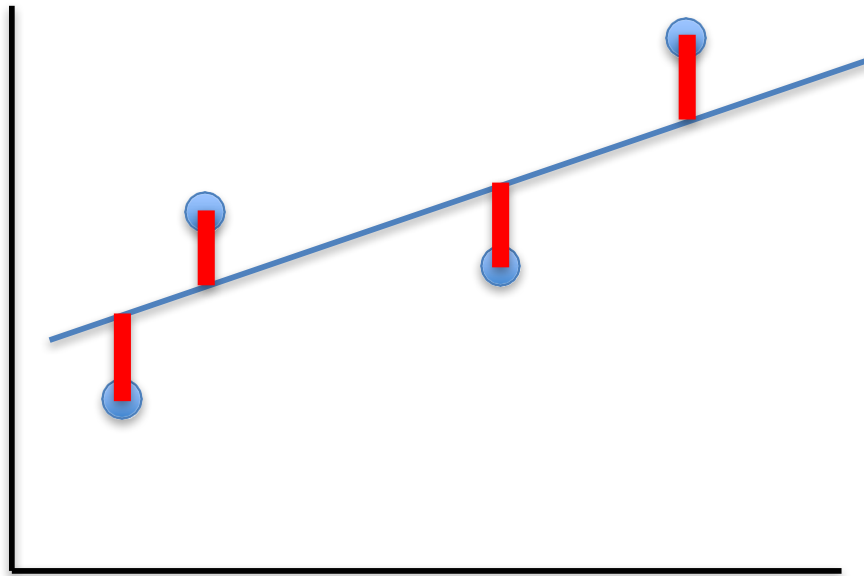
least squares (LSQ)
The fitted line is used as a predictor

Least Squares Linear Regression

- Cost Function

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

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



Intuition Behind Cost Function

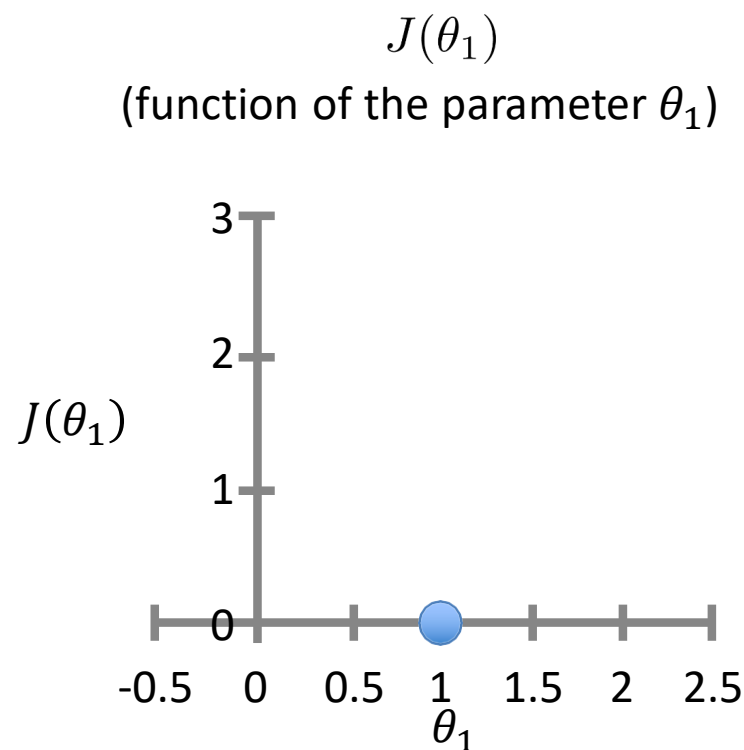
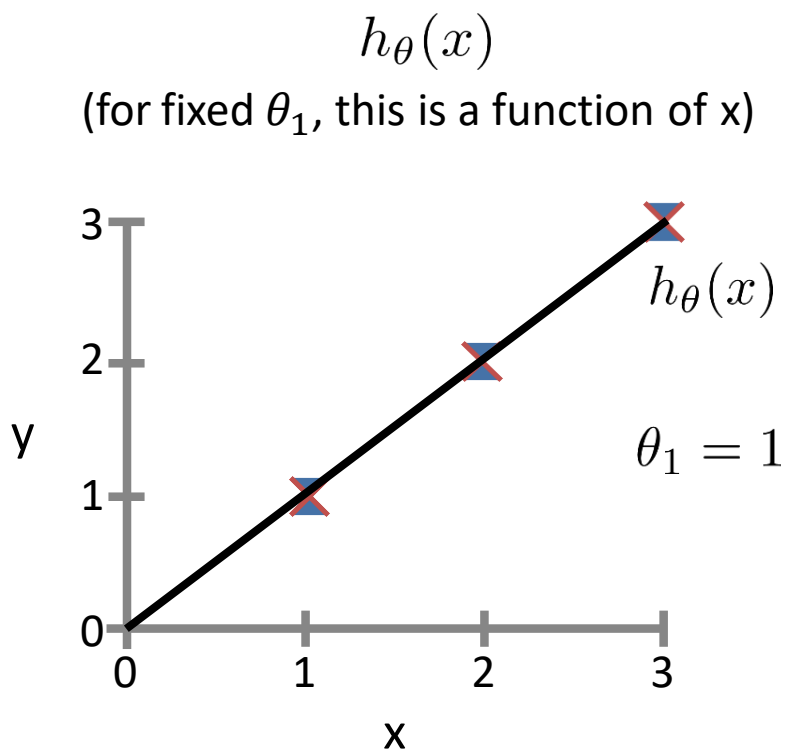
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For insight on $J()$, let's assume $y \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

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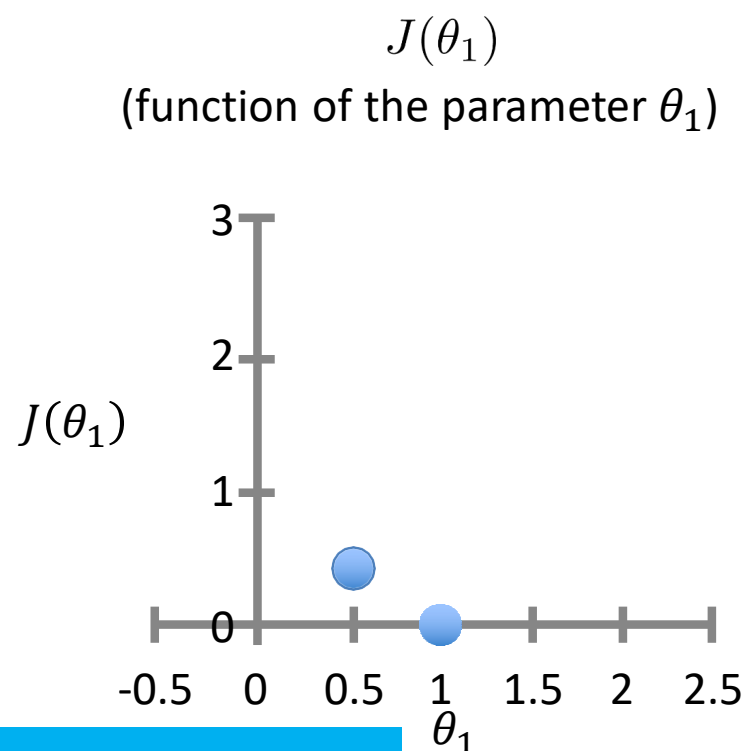
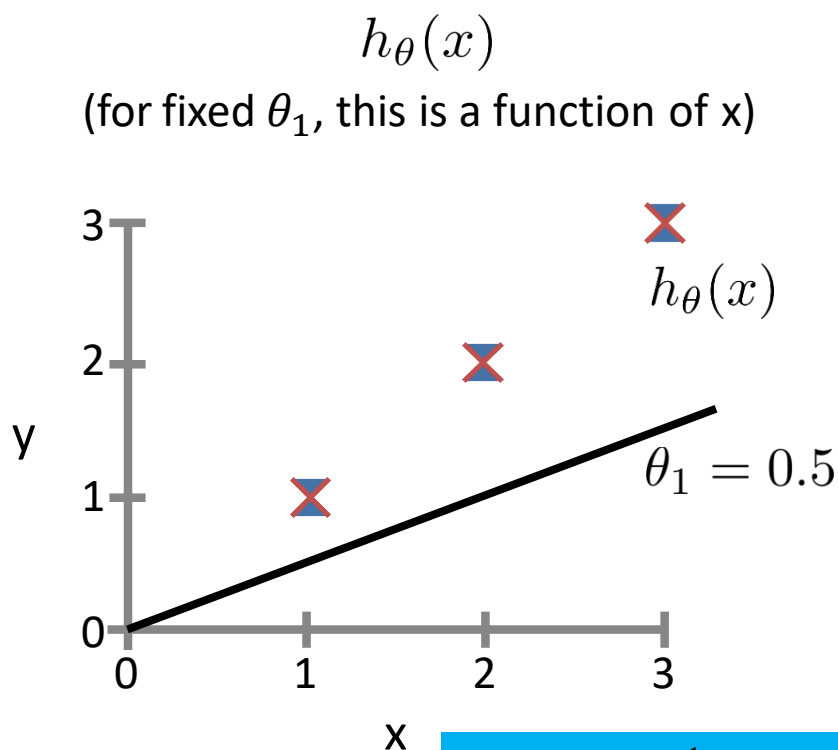
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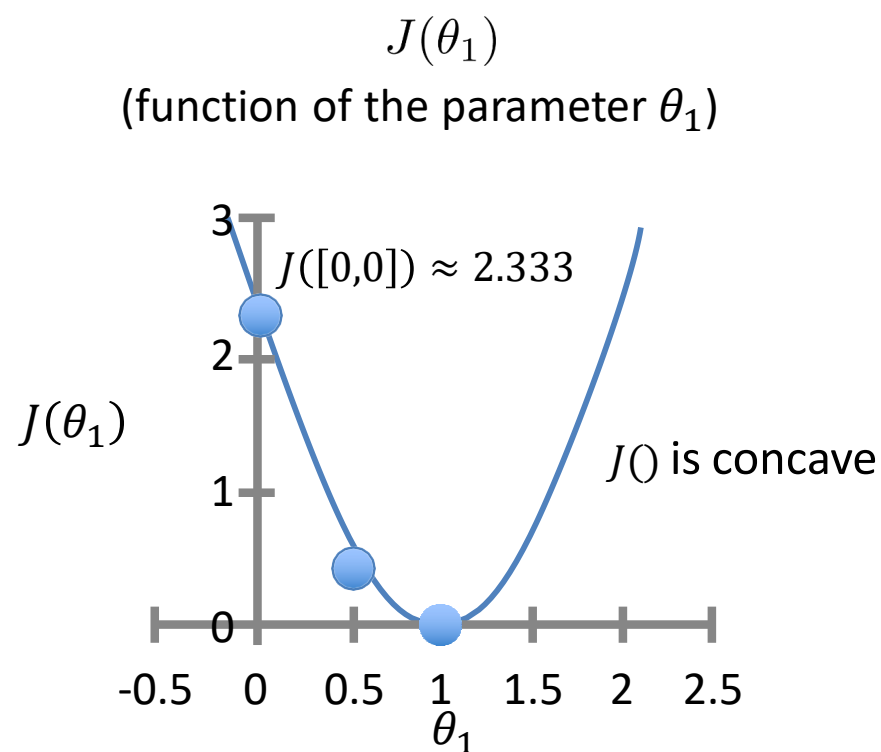
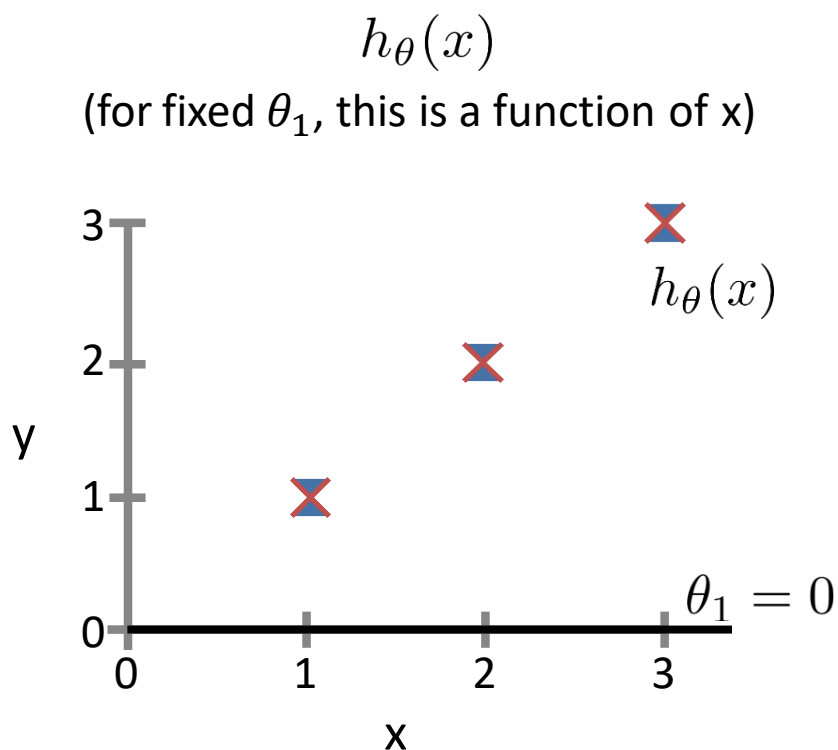


$$J([0, 0.5]) = \frac{1}{2 \times 3} [(0.5 - 1)^2 + (1 - 2)^2 + (1.5 - 3)^2]$$

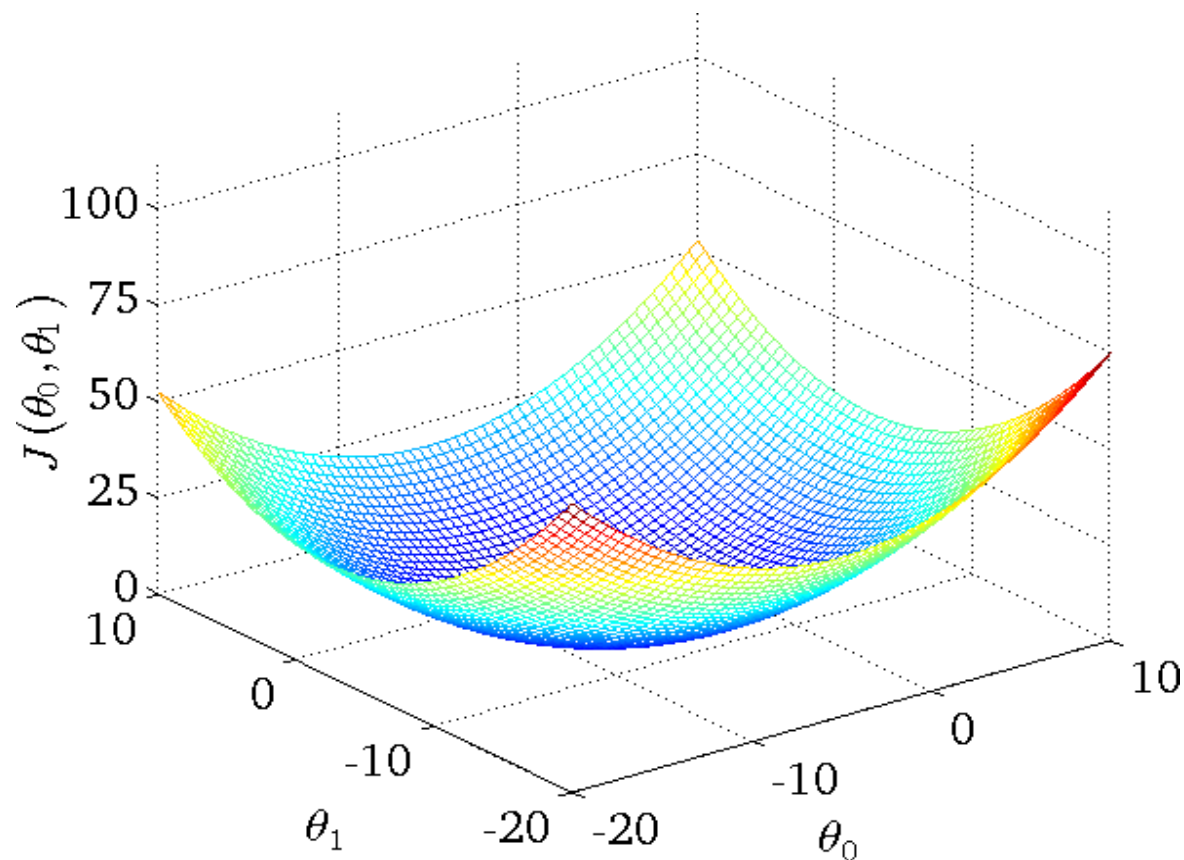
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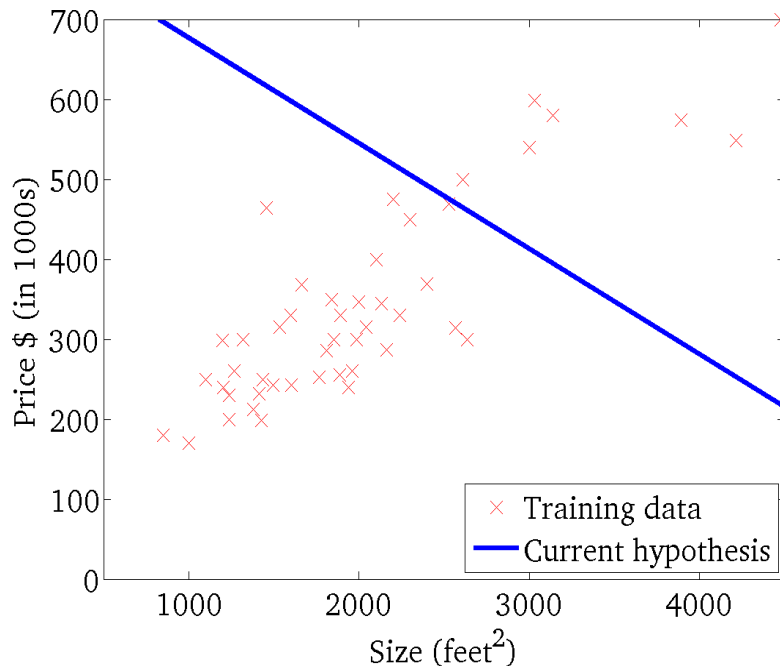
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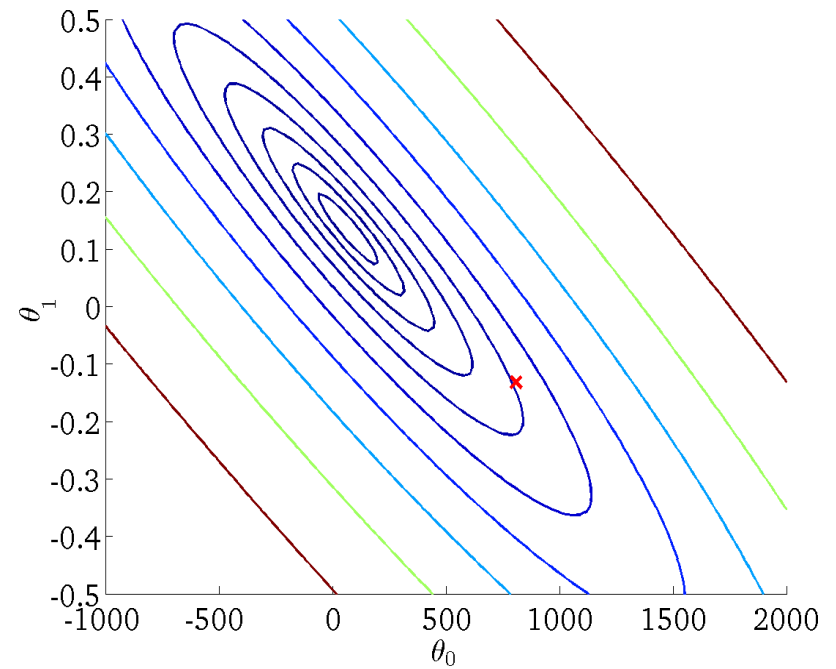
$$h_{\theta}(x)$$

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



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

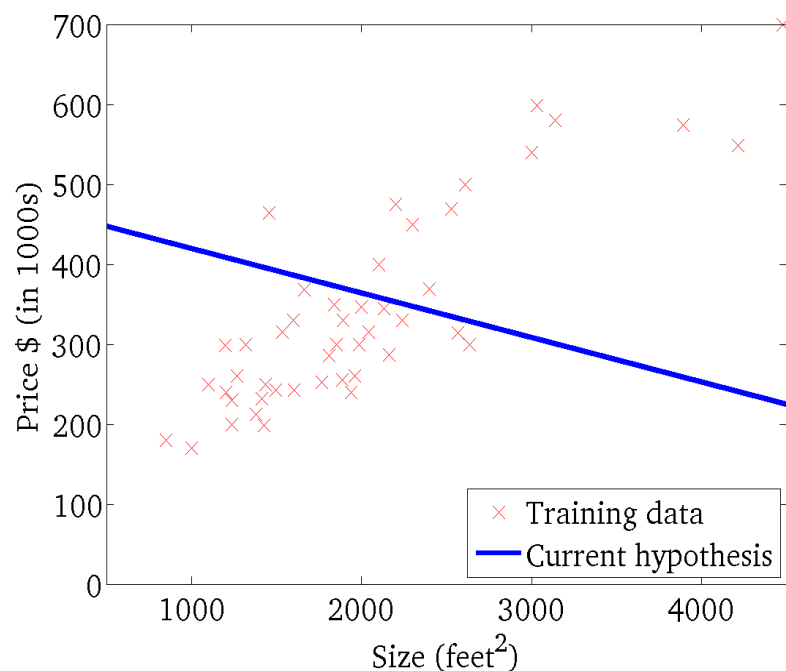
(function of the parameter(θ_0, θ_1))



Intuition Behind Cost Function

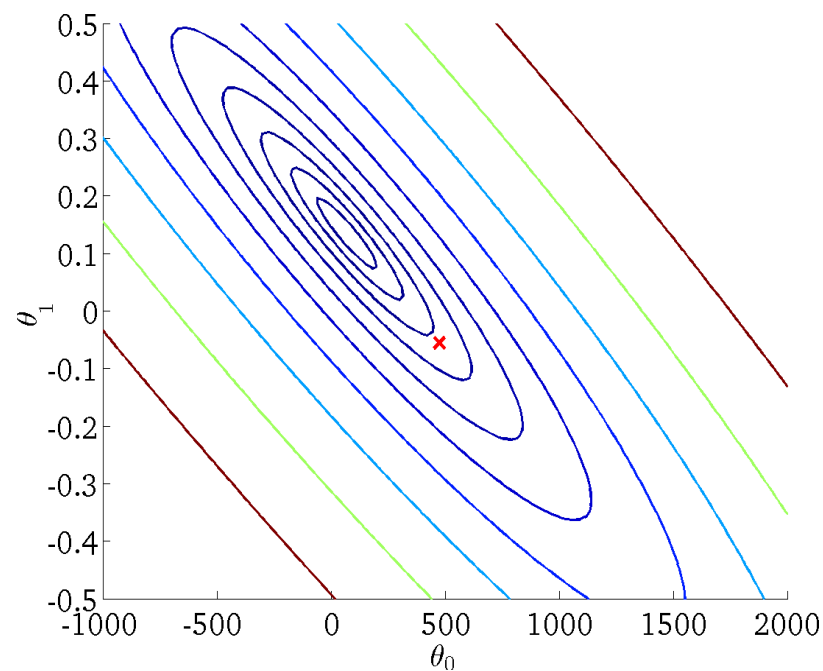
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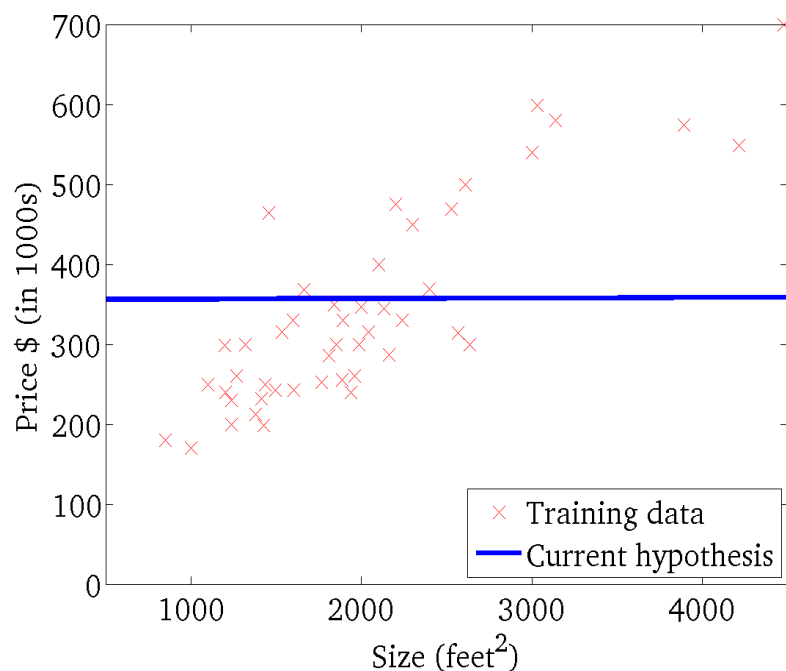
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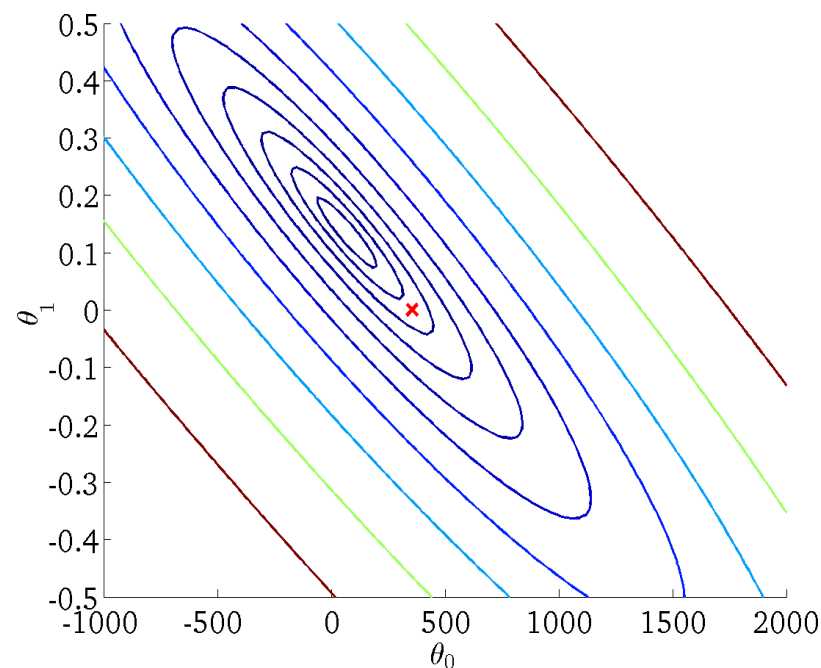
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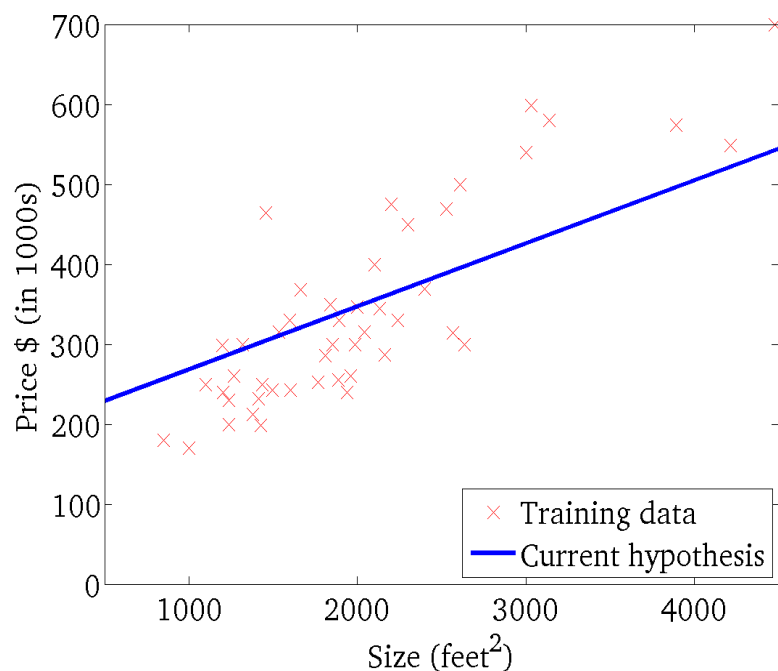
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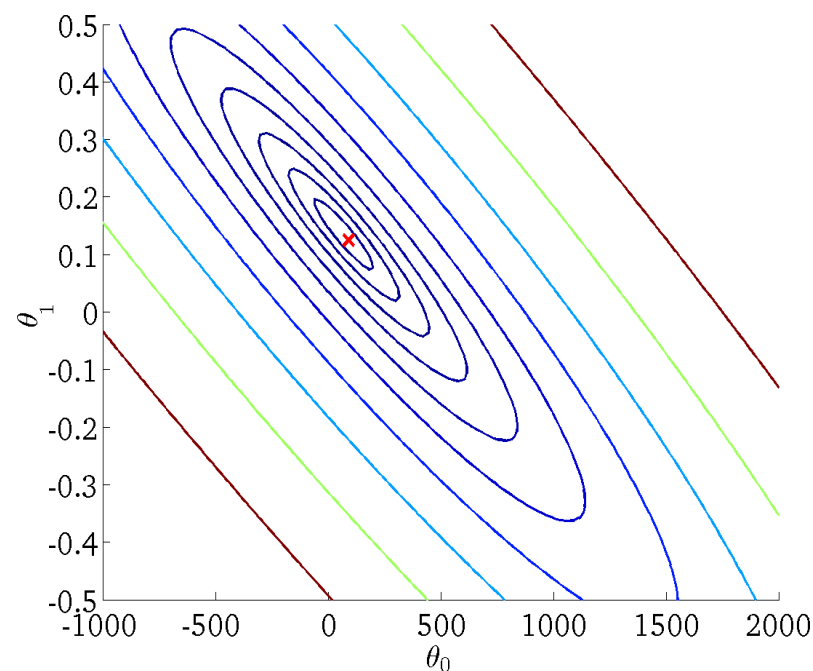
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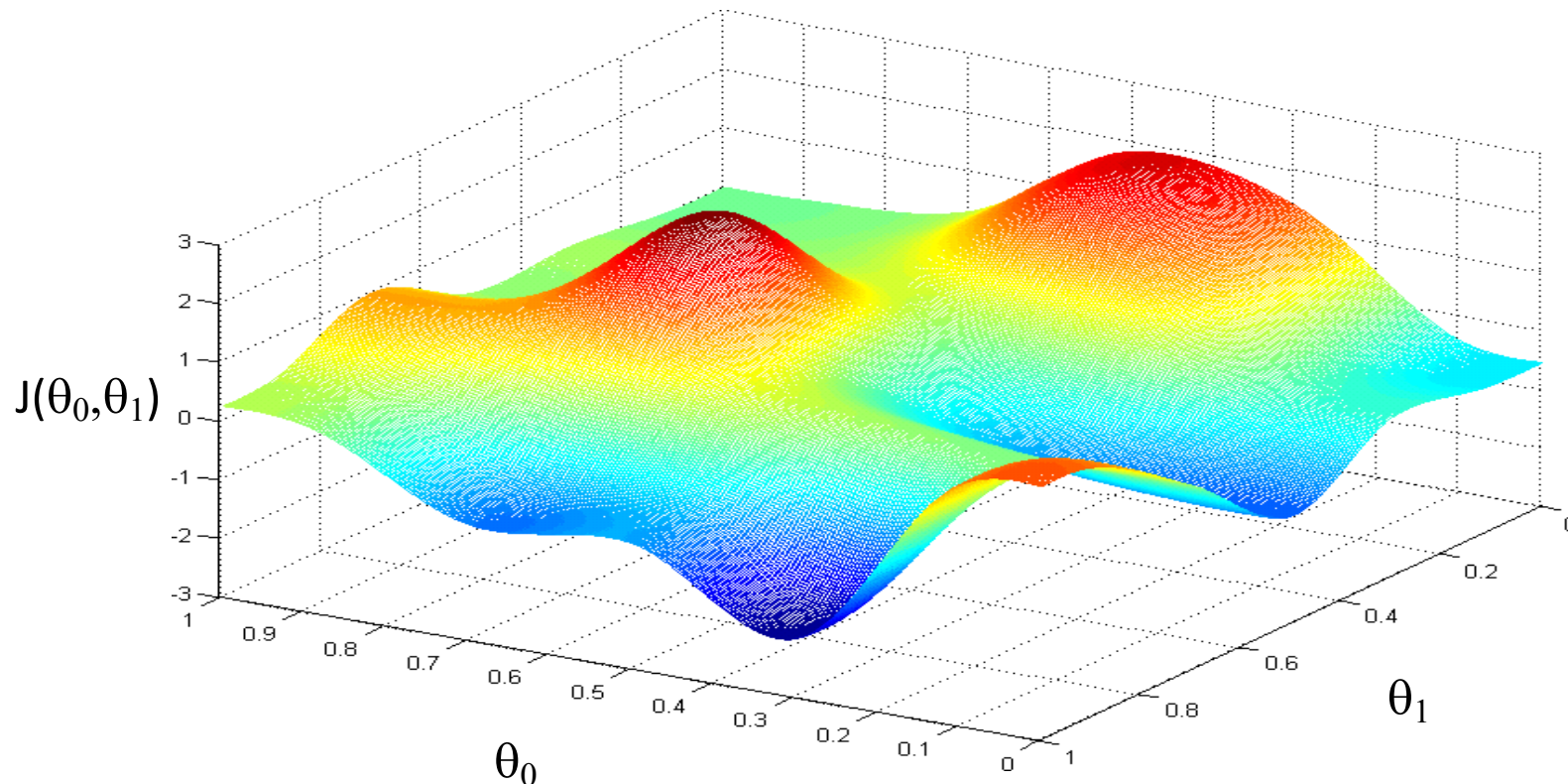
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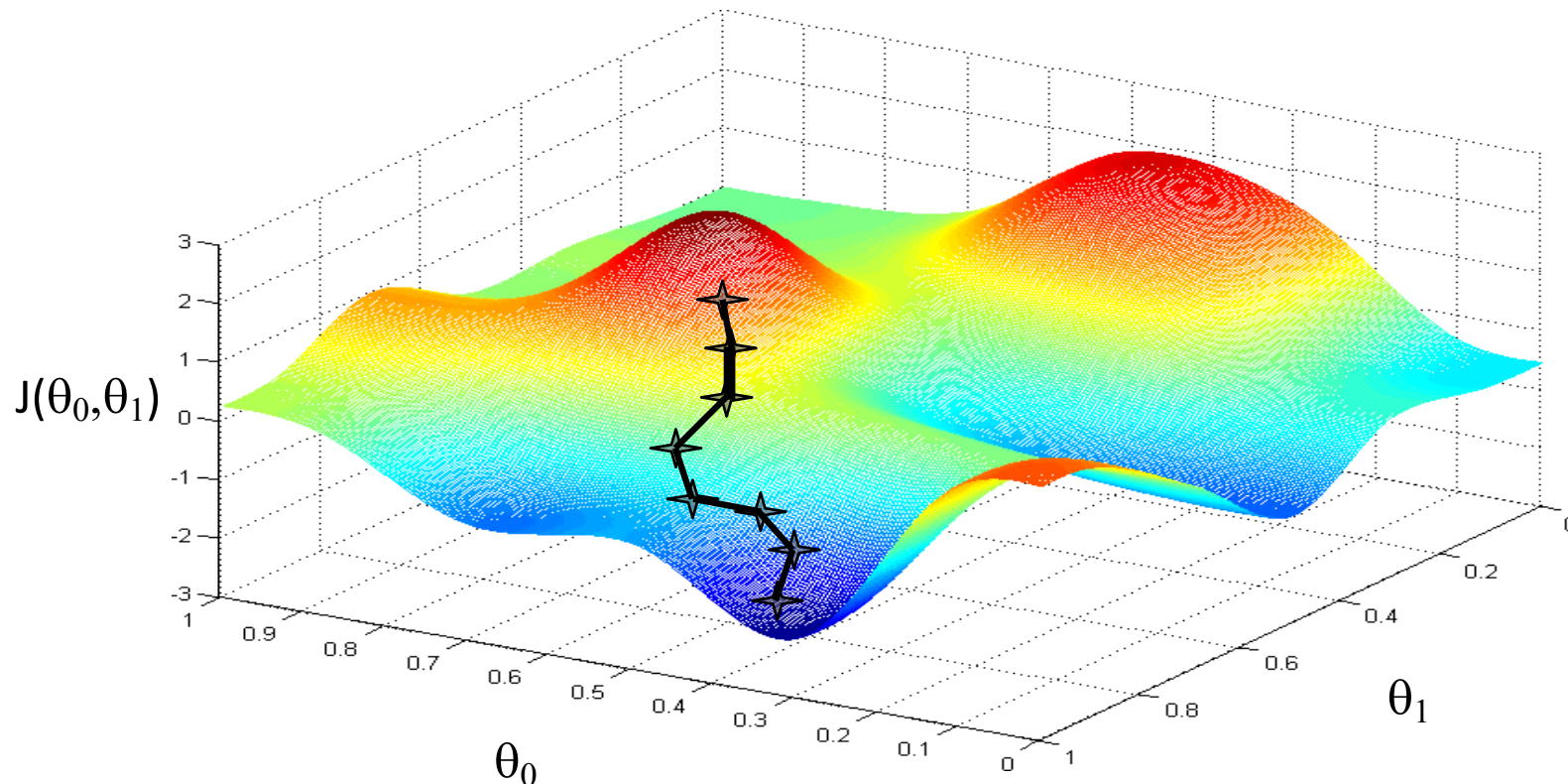
Basic Search Procedure

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



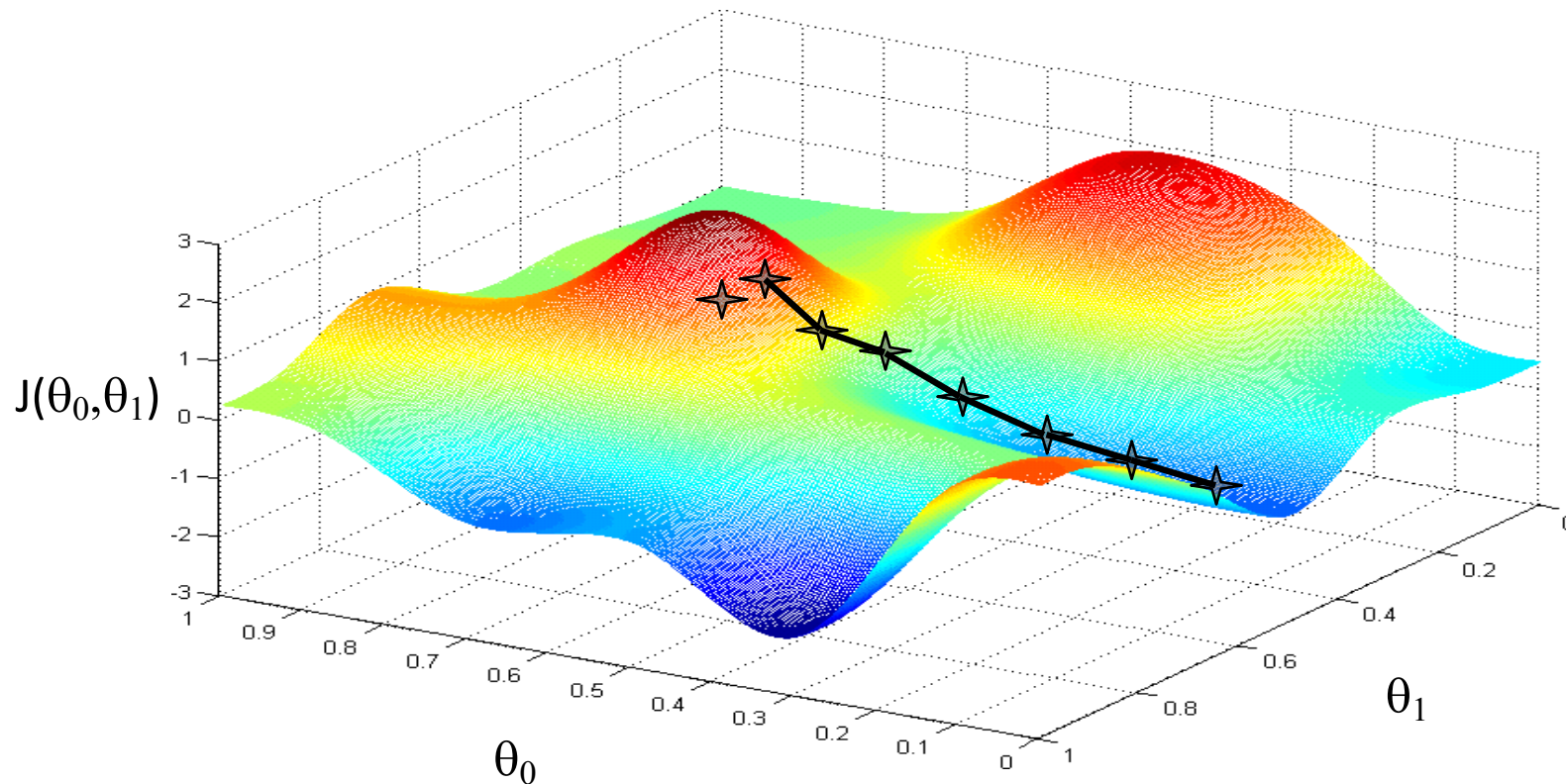
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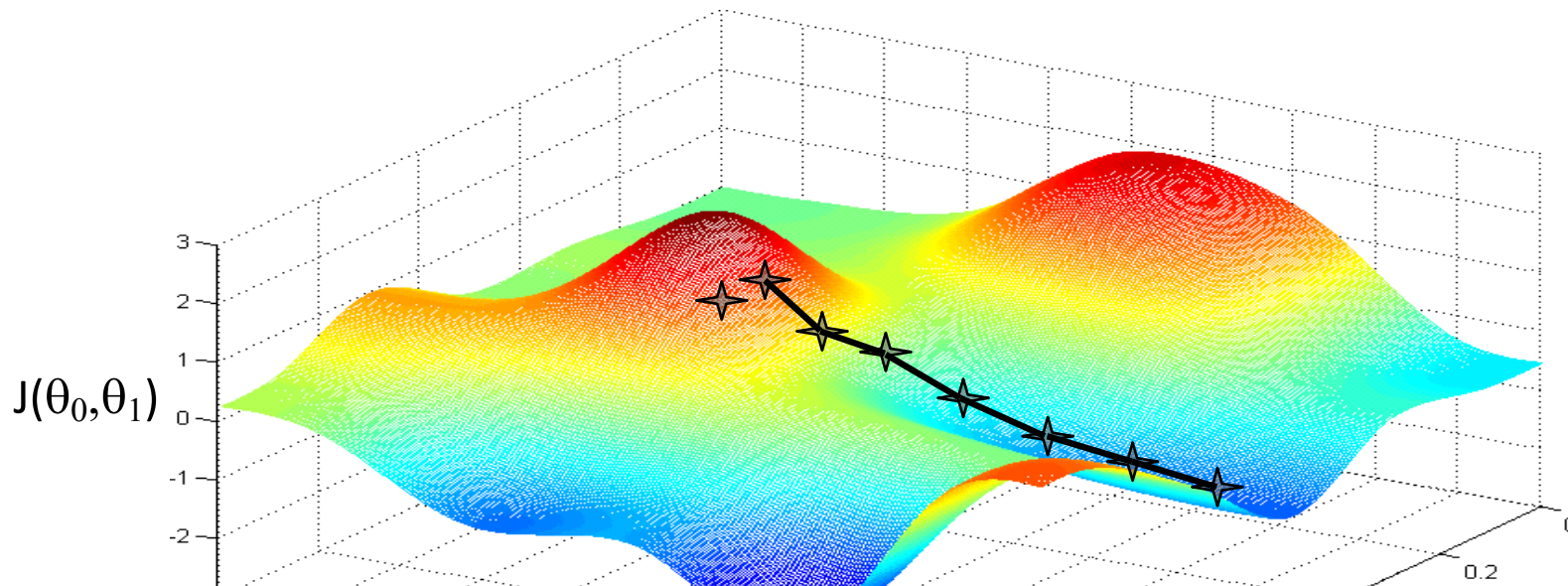
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Basic Search Procedure

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



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

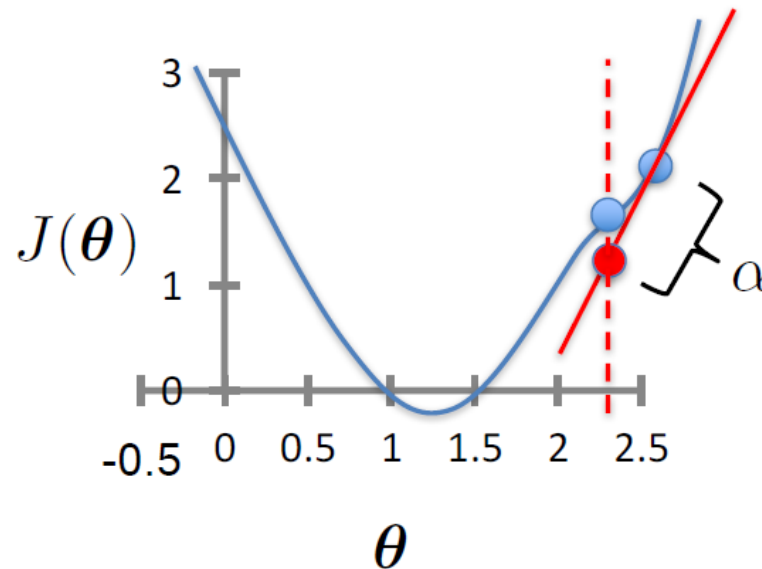
Gradient Descent

- Initialize θ
- Repeat until convergence

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

simultaneous update
for $j = 0 \dots d$

learning rate (small)
e.g., $\alpha = 0.05$



Gradient Descent

- Initialize θ
- Repeat until convergence

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

simultaneous update
for $j = 0 \dots d$

For Linear Regression:

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

Gradient Descent

- Initialize θ
- Repeat until convergence

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

simultaneous update
for $j = 0 \dots d$

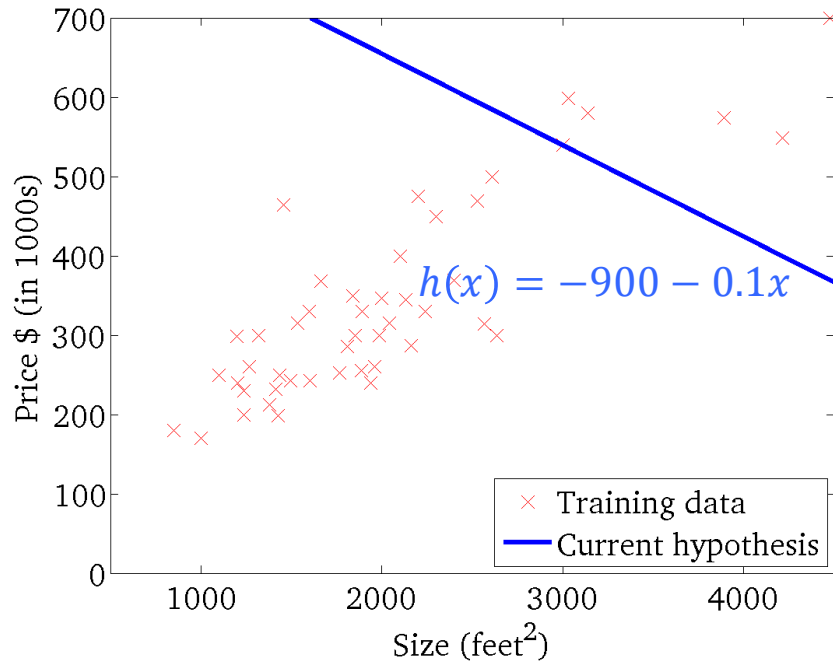
- To achieve simultaneous update
 - At the start of each GD iteration, compute $h_{\theta}(\mathbf{x}^{(i)})$
 - Use this stored value in the update step loop
- Assume convergence when $\|\theta_{new} - \theta_{old}\|_2 < \epsilon$

$$\text{L2 norm: } \|\mathbf{v}\|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \dots + v_{|\mathbf{v}|}^2}$$

Gradient Descent

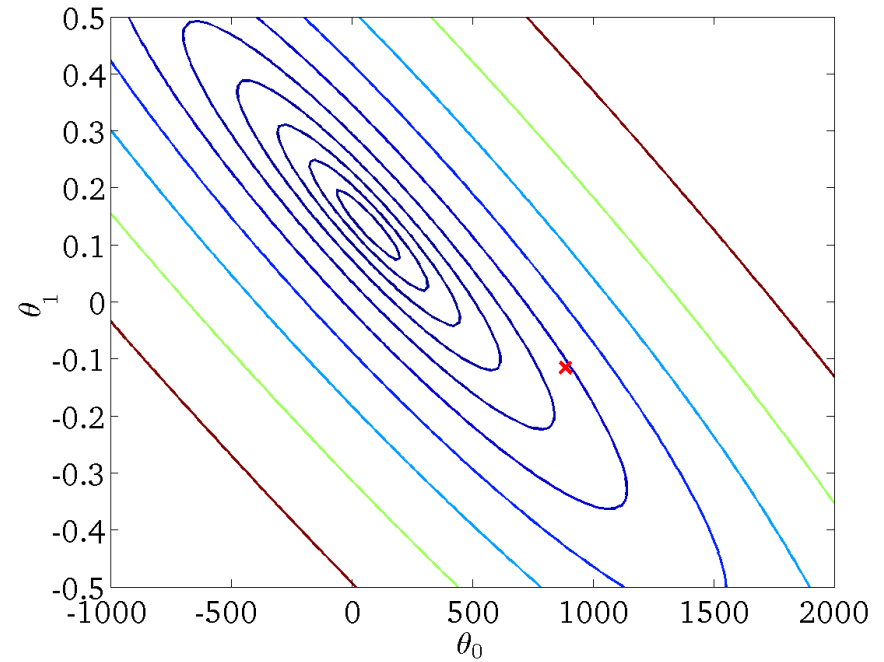
$$h_{\theta}(x)$$

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



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

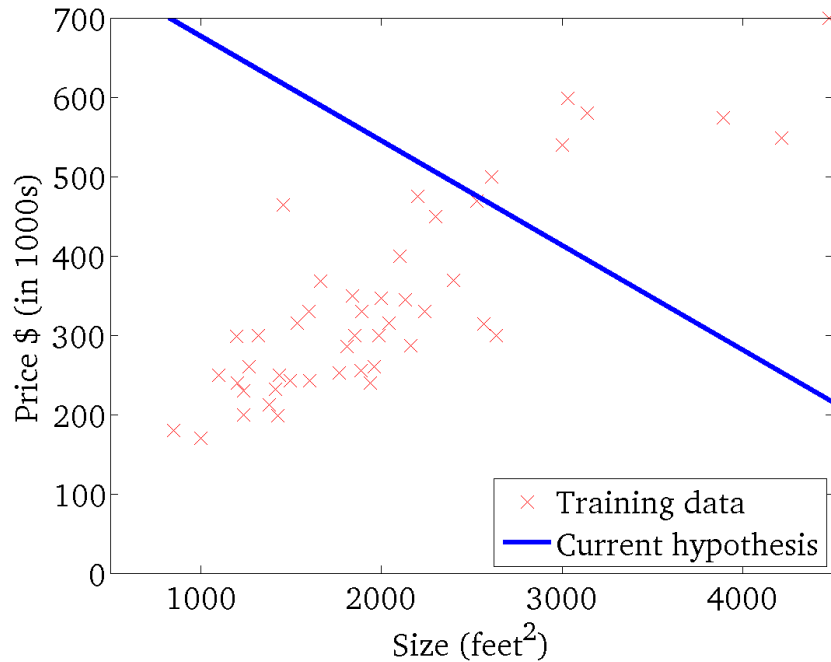
(function of the parameter(θ_0, θ_1))



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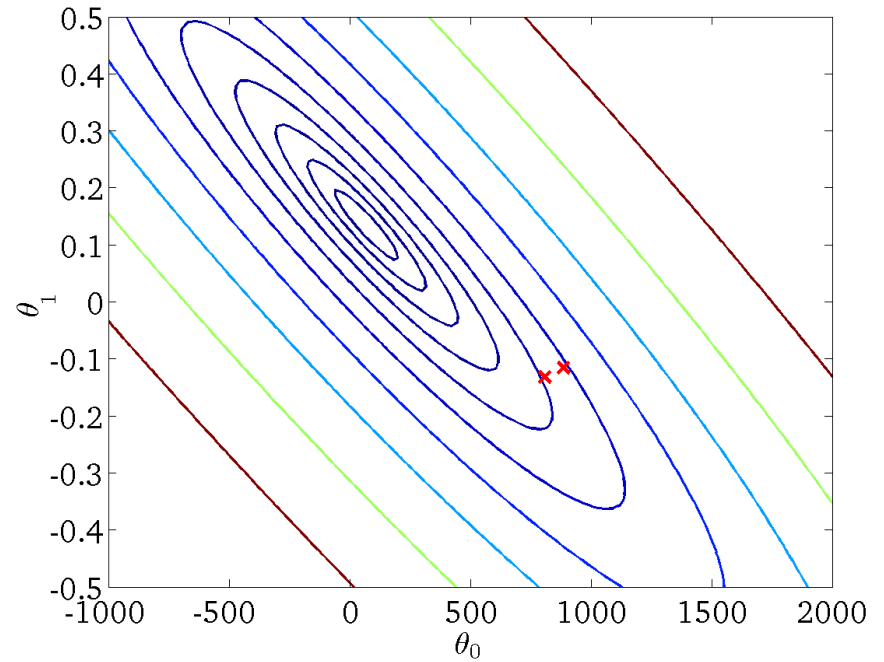
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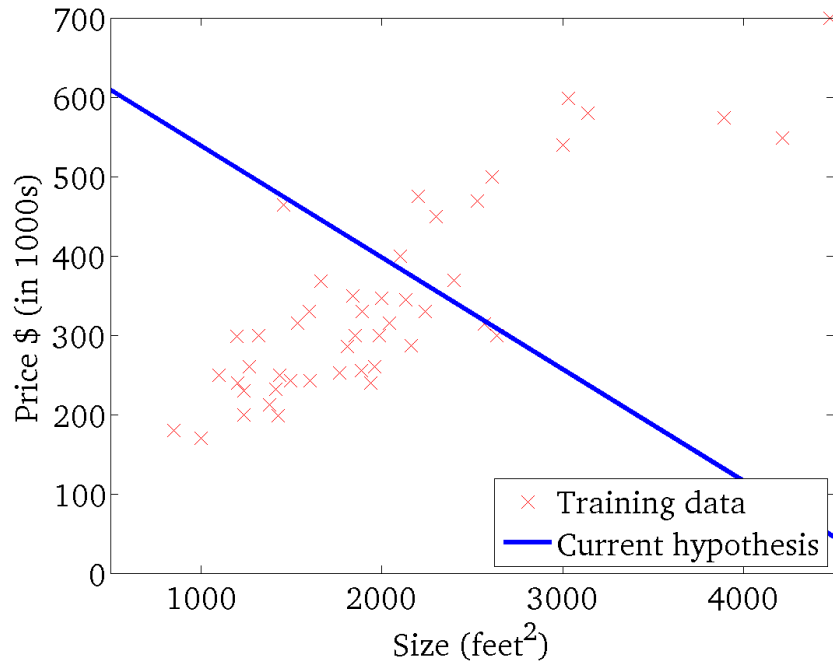
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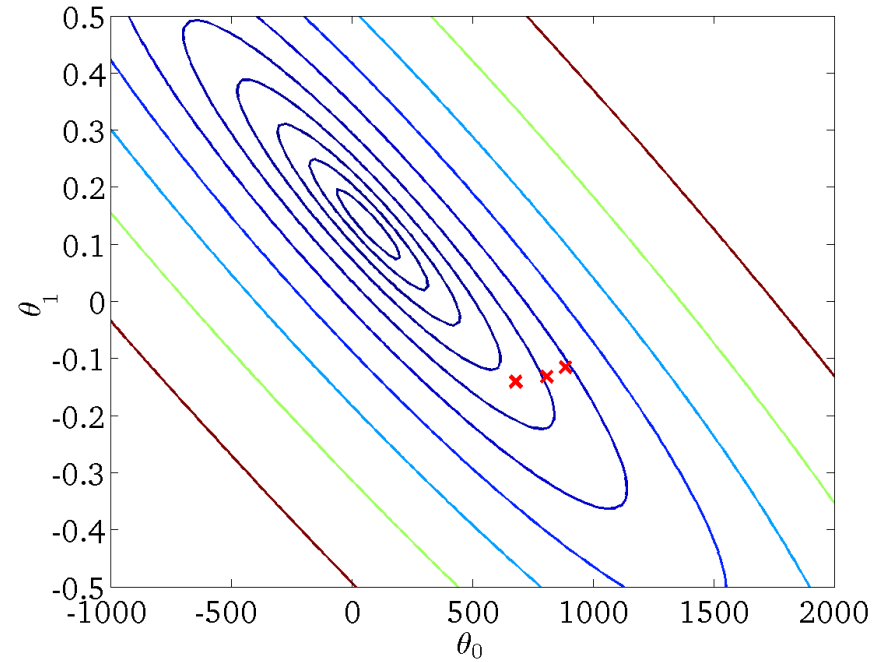
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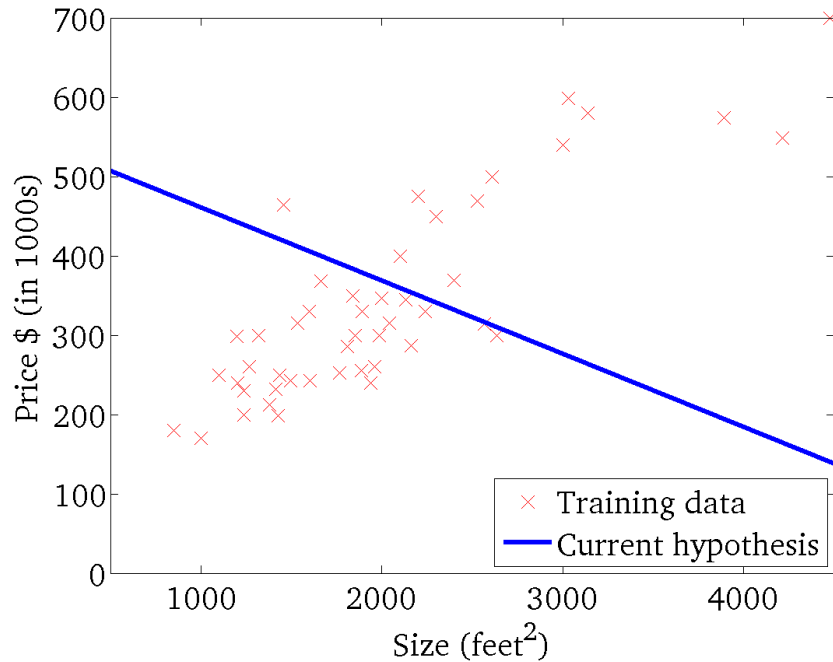
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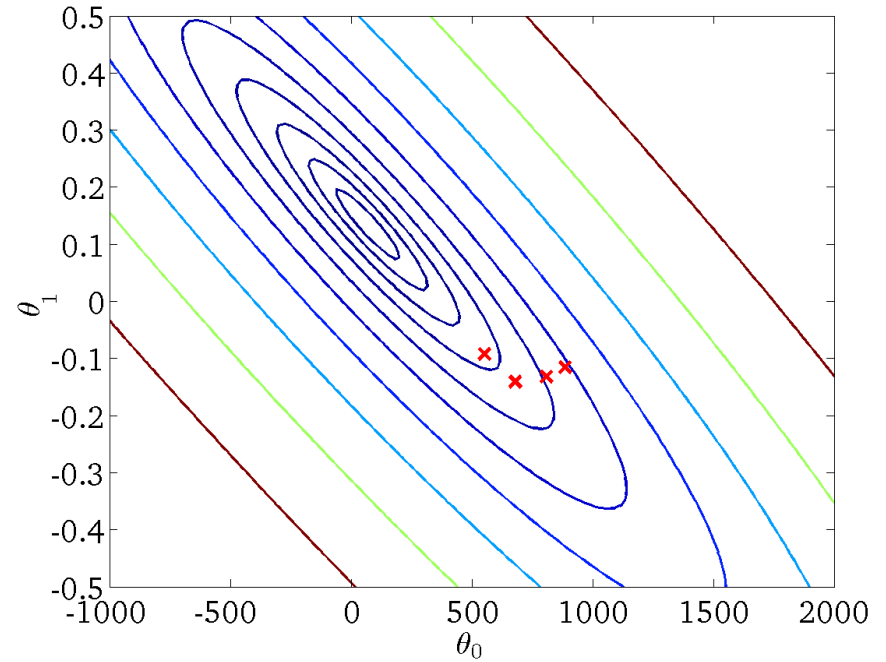
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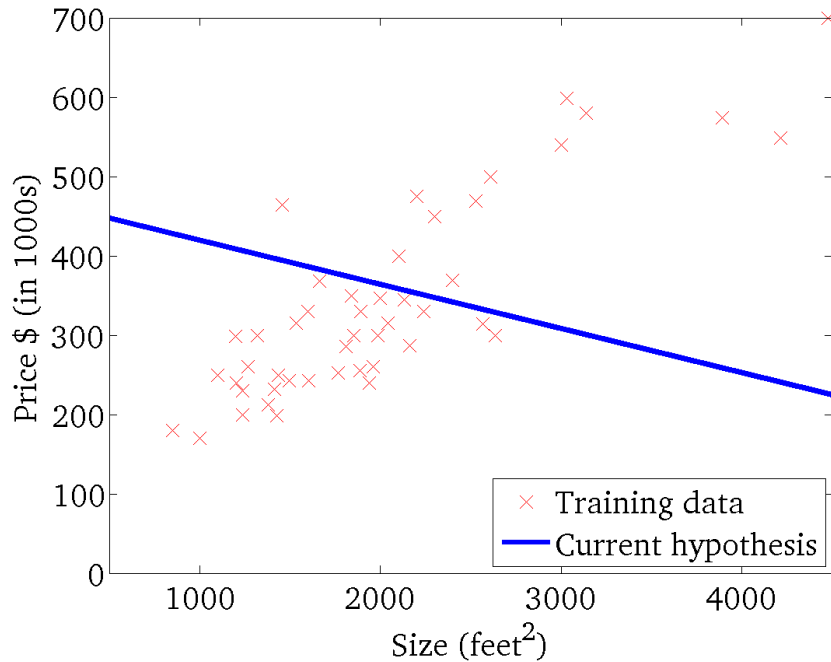
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Gradient Descent

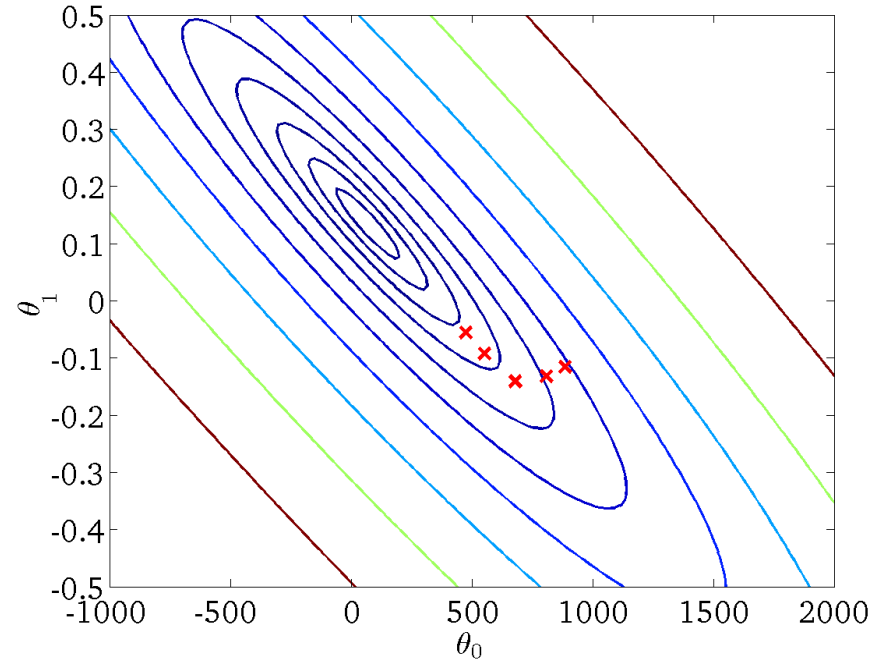
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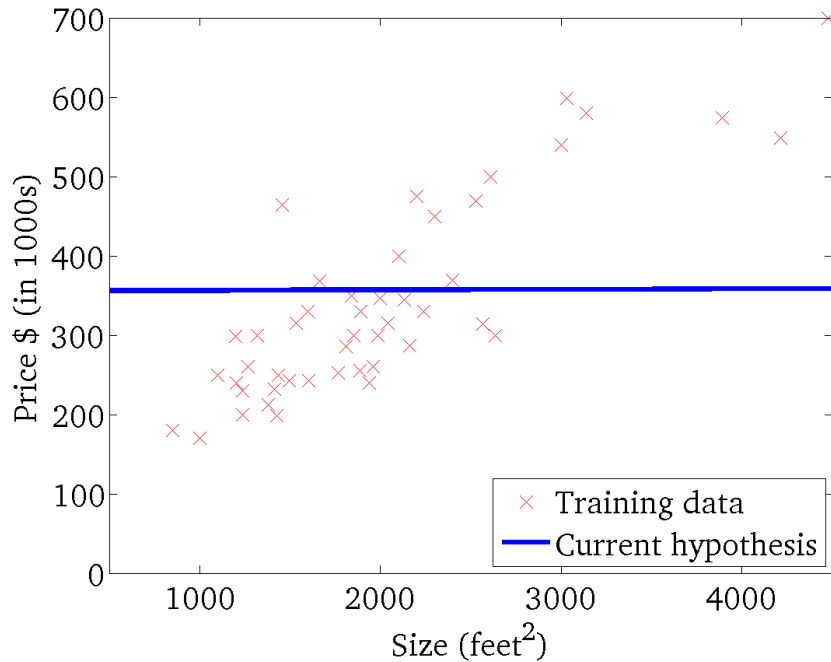
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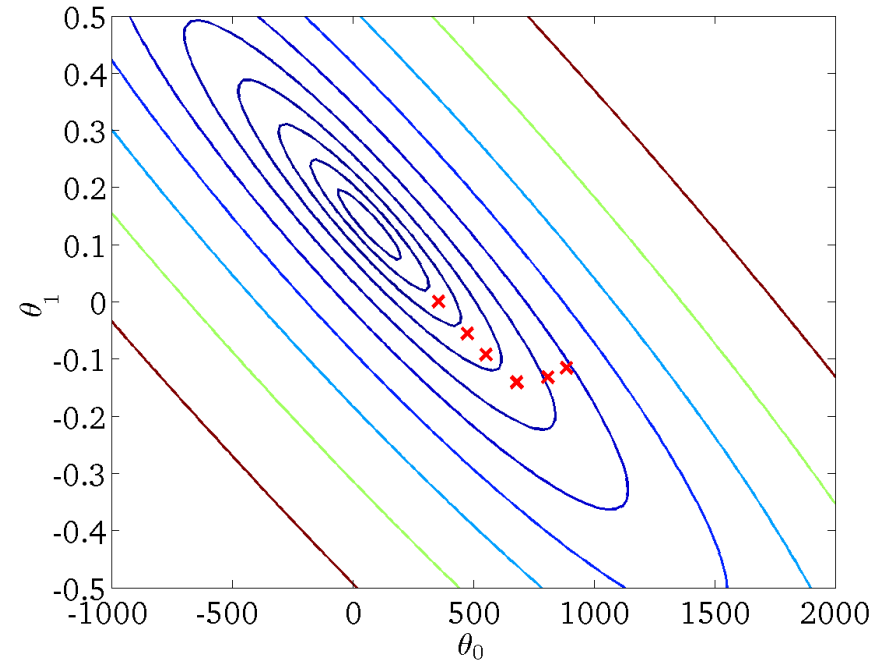
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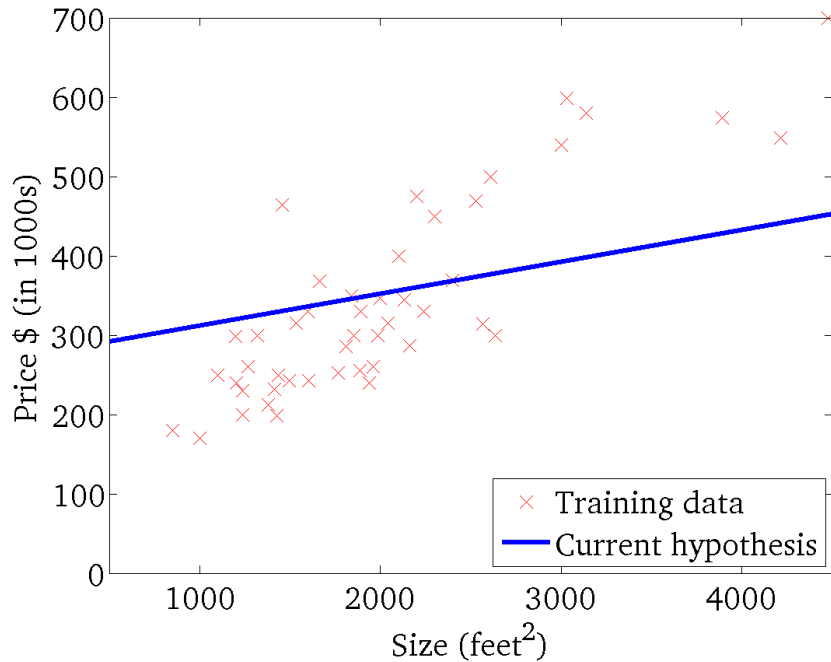
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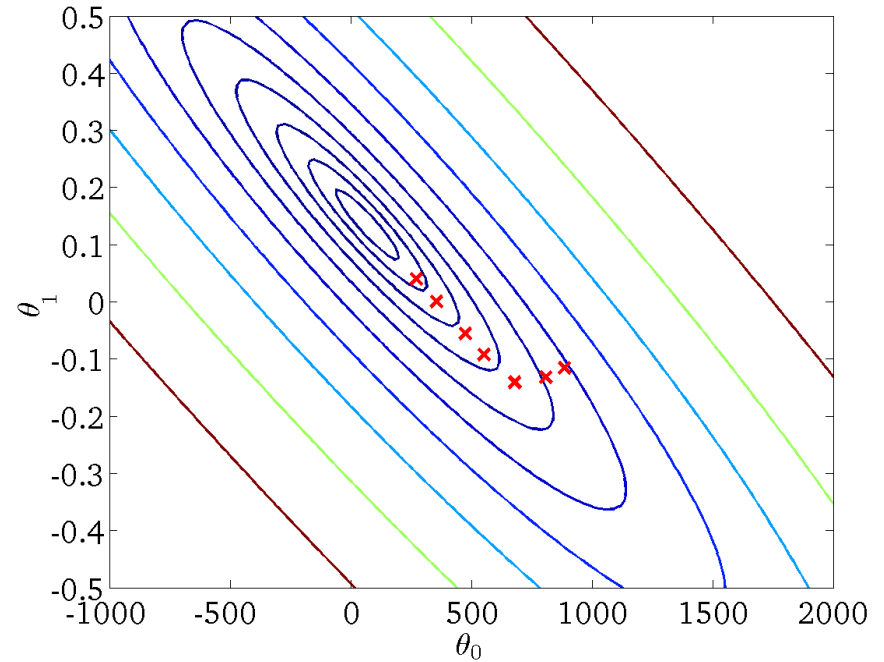
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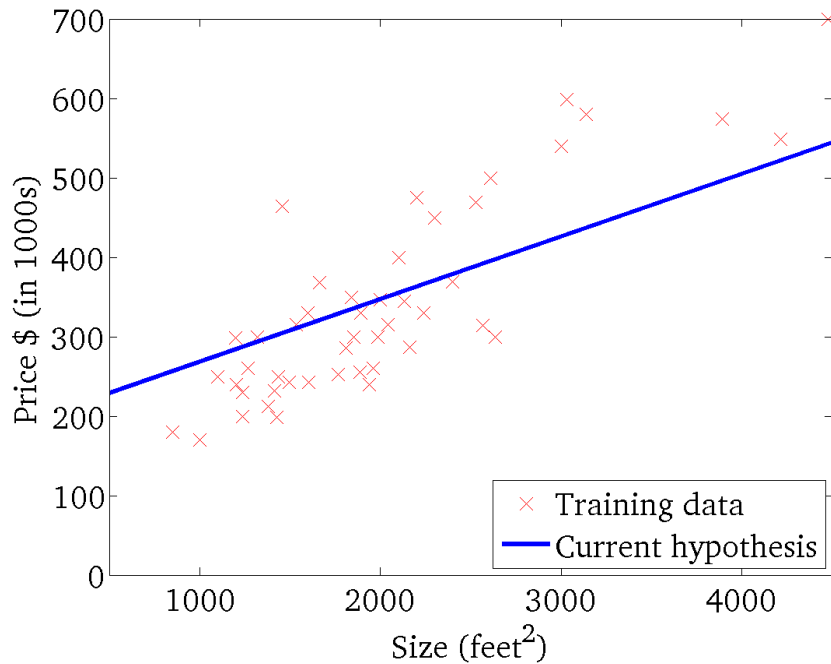
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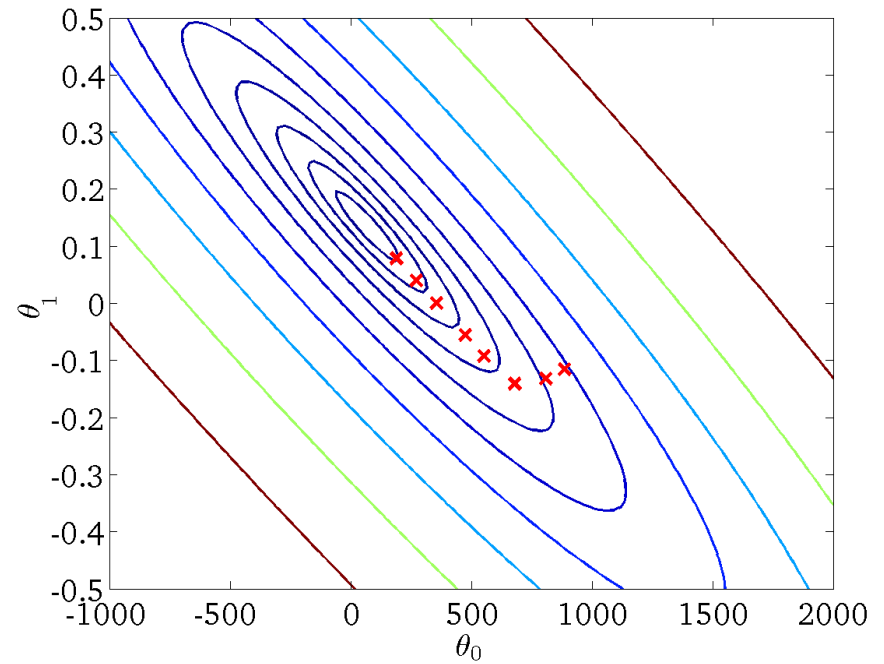
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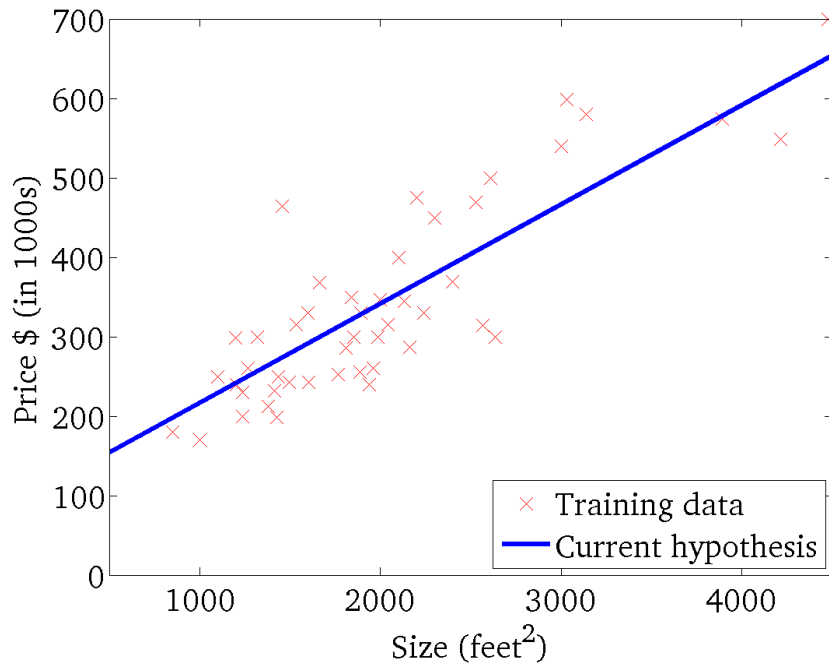
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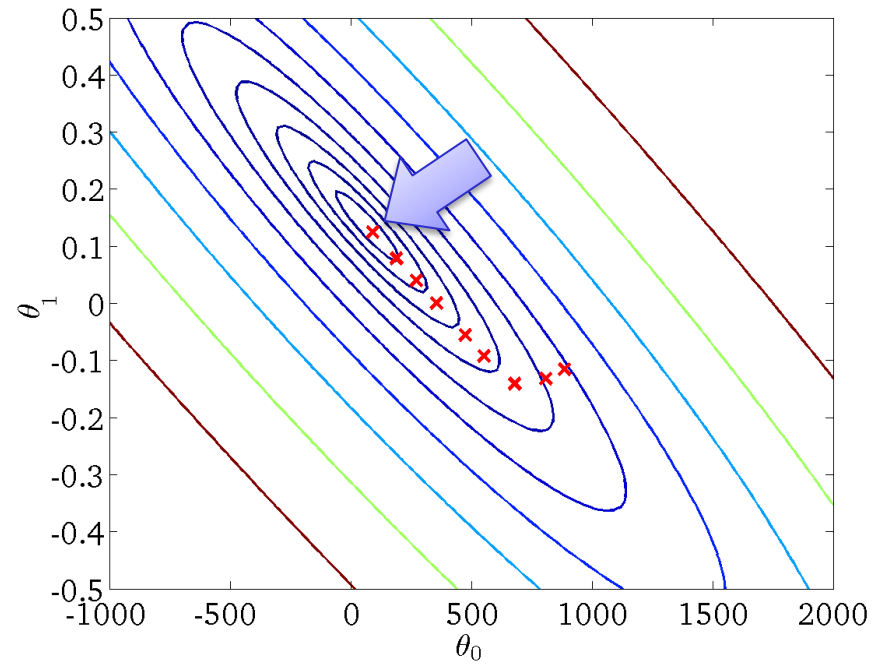
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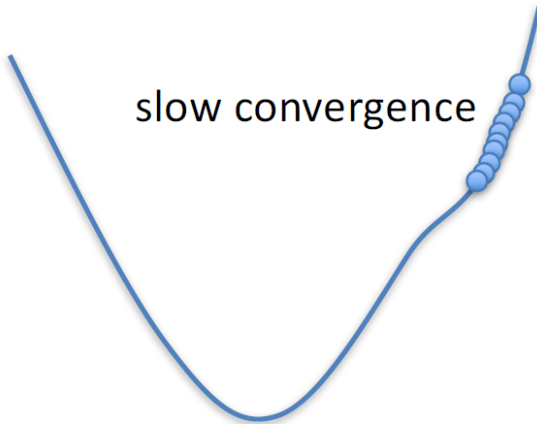
$$J(\theta_0, \theta_1)$$

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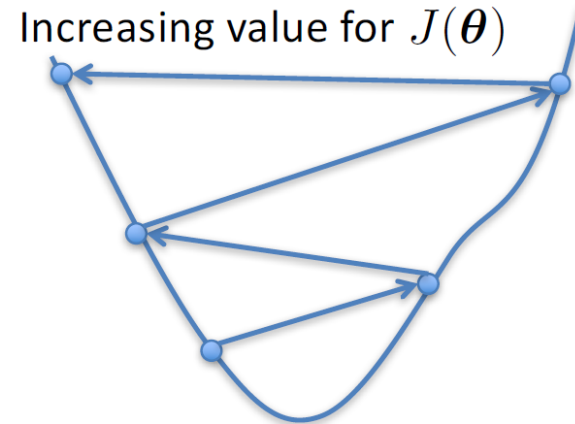


Choosing α

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

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:

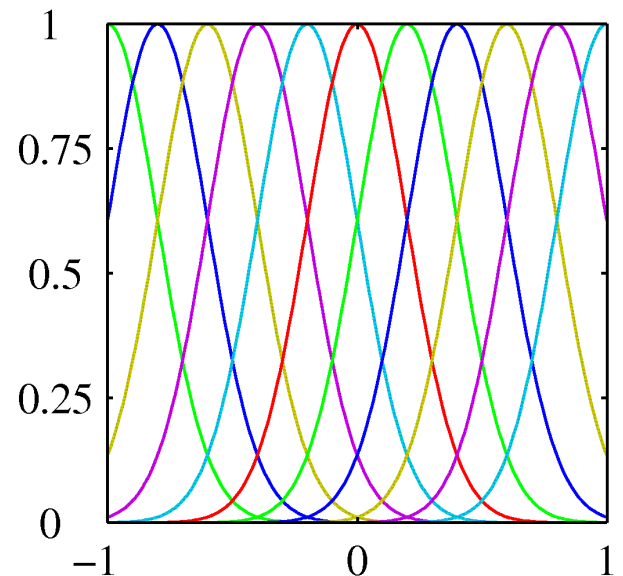
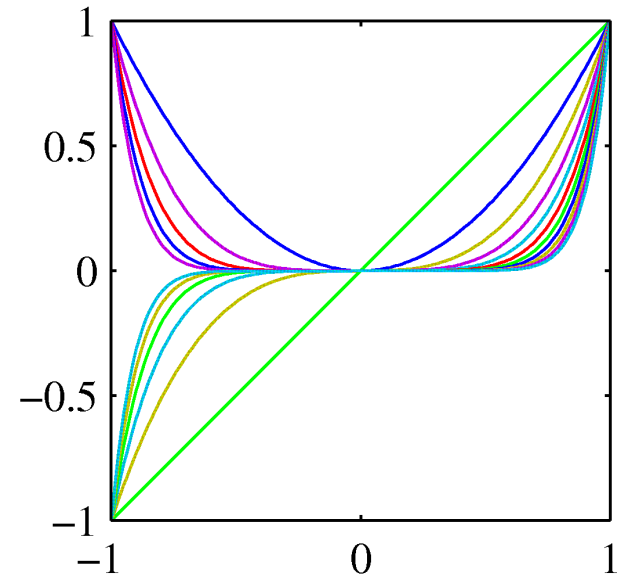
$$\phi_j(\mathbf{x}) = x_j$$

- 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

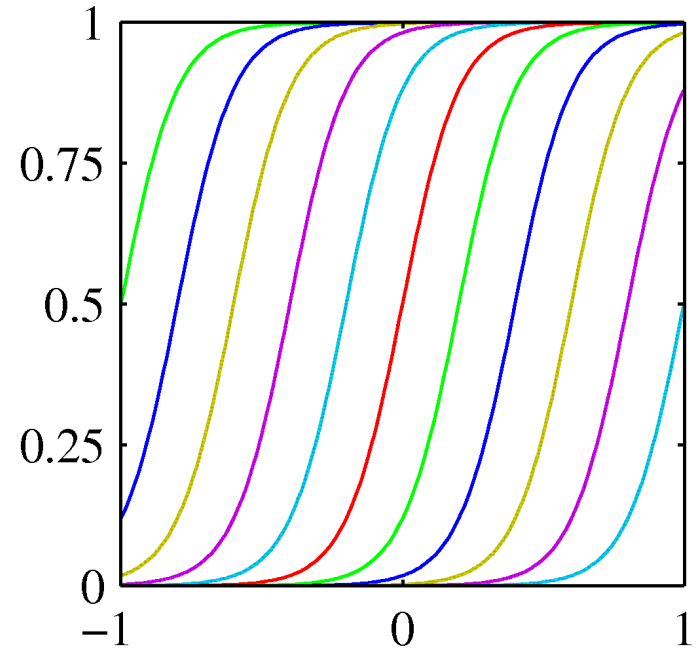
- Sigmoidal basis functions:

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

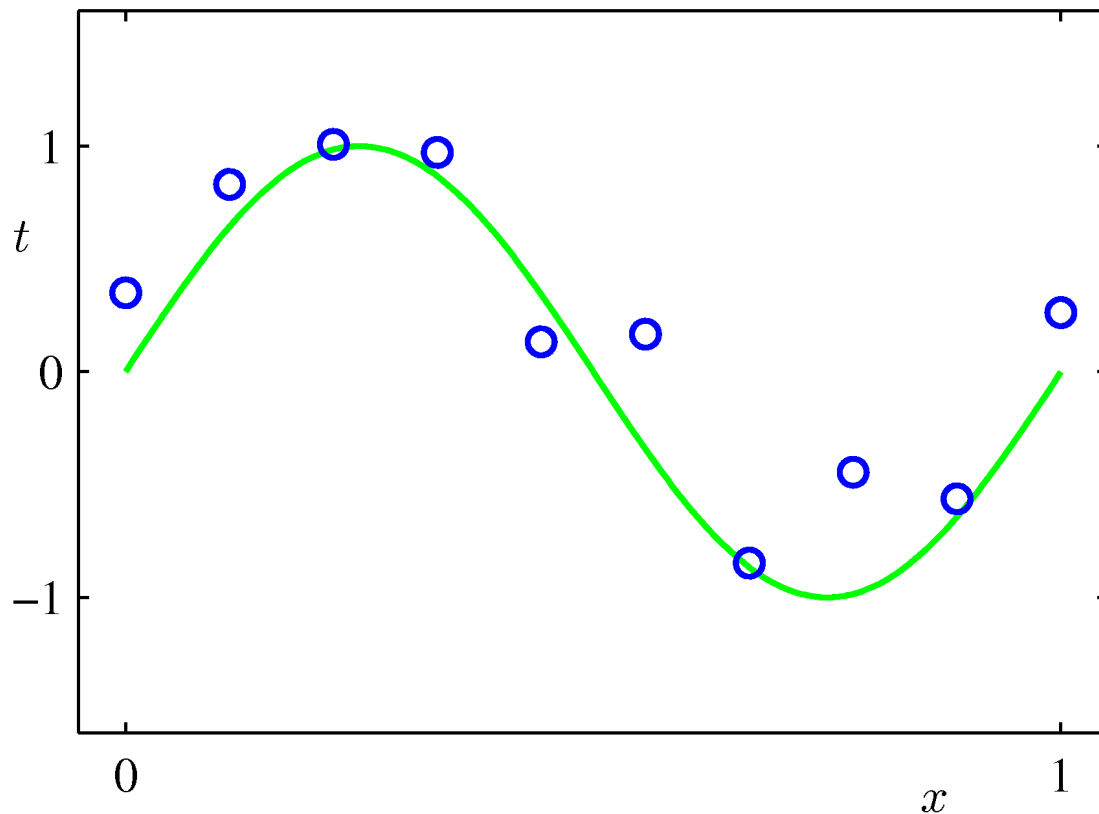
where

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

- 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



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

Linear Basis Function Models

- Basic Linear Model:

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

- Generalized Linear Model:


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

- 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

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: 

$$\begin{bmatrix} 1 \\ 6 \\ 3 \\ 4 \end{bmatrix}$$

- as opposed to a row vector:


$$[1 \quad 6 \quad 3 \quad 4]$$

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

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

Linear Algebra Concepts

- Transpose: reflect vector/matrix on line:

$$\begin{bmatrix} a \\ b \end{bmatrix}^T = [a \quad b] \quad \begin{bmatrix} a & b \\ c & d \end{bmatrix}^T = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

- Note: $(Ax)^T = x^T A^T$ (We'll define multiplication soon.)

- Vector norms:

- Norm of $\mathbf{v} = (v_1, \dots, v_k)$ is $(\sum_i |v_i|^p)^{\frac{1}{p}}$

- Common norms: L_1, L_2

- $L_{\text{infinity}} = \max_i |v_i|$

- Length of a vector \mathbf{v} is $L_2(\mathbf{v})$

Linear Algebra Concepts

- Vector dot product: $\mathbf{u} \cdot \mathbf{v} = (u_1 \ u_2) \cdot (v_1 \ v_2) = u_1 v_1 + u_2 v_2$

- Note: dot product of u with itself = $\text{length}(u)^2 = \|u\|_2^2$

- 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:

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v} = (u_1 \quad u_2) \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = u_1 v_1 + u_2 v_2$$

- Outer product:

$$\mathbf{u}\mathbf{v}^T = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} (v_1 \quad v_2) = \begin{pmatrix} u_1 v_1 & u_1 v_2 \\ u_2 v_1 & u_2 v_2 \end{pmatrix}$$

Vectorization

- Benefits of vectorization
 - More compact equations
 - Faster code (using optimized matrix libraries)

- Consider our model:

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

- Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \mathbf{x}^T = [1 \quad x_1 \quad \cdots \quad x_d]$$

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

Vectorization

- Consider our model for n instances:

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

- Let

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

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

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

Vectorization

- For the linear regression cost function:

$$\begin{aligned} J(\boldsymbol{\theta}) &= \frac{1}{2n} \sum_{i=1}^n (h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})^2 \\ &= \frac{1}{2n} \sum_{i=1}^n (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - \mathbf{y}^{(i)})^2 \\ &= \frac{1}{2n} \underbrace{(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^T}_{\mathbb{R}^{1 \times n}} \underbrace{(\underbrace{\mathbf{X}\boldsymbol{\theta}}_{\mathbb{R}^{n \times 1}} - \mathbf{y})}_{\mathbb{R}^{n \times 1}} \end{aligned}$$

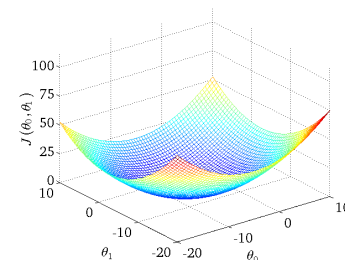
$\mathbb{R}^{n \times (d+1)}$
 $\mathbb{R}^{(d+1) \times 1}$

Let:

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

Closed Form Solution

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



$$\begin{aligned} J(\theta) &= \frac{1}{2n} (X\theta - y)^T (X\theta - y) \\ &\propto \theta^T X^T X \theta - \boxed{y^T X \theta} - \boxed{\theta^T X^T y} + y^T y \\ &\propto \theta^T X^T X \theta - 2\theta^T X^T y + y^T y \end{aligned}$$

1×1

Take derivative and set equal to 0, then solve for θ :

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

$$(X^T X)\theta - X^T y = 0$$

$$(X^T X)\theta = X^T y$$

Closed Form Solution:

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

Closed Form Solution

- Can obtain θ by simply plugging X and y into

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

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

- If $X^T X$ 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

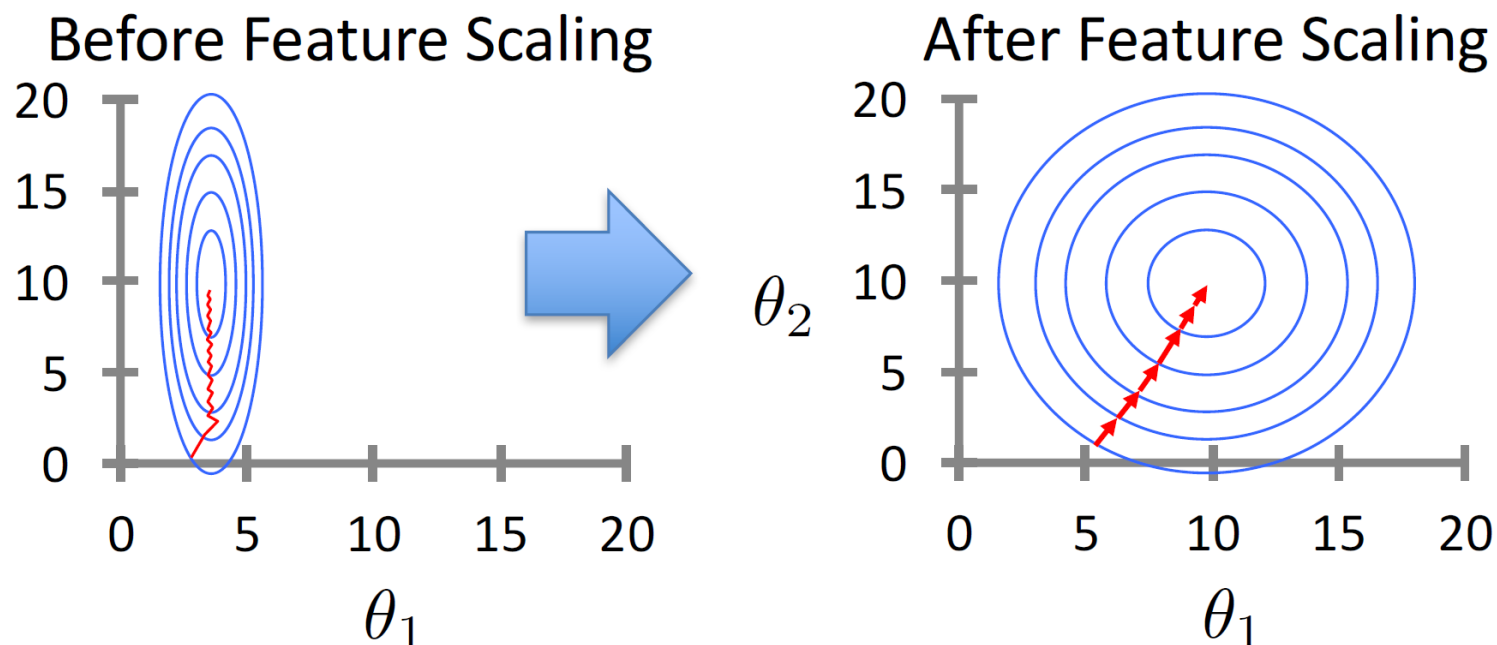
- Requires multiple iterations
- Need to choose α
- Works well when n is large
- Can support incremental learning

Closed Form Solution

- Non-iterative
- No need for α
- Slow if n is large
 - Computing $(X^T X)^{-1}$ is roughly $O(n^3)$

Improving Learning: Feature Scaling

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



- Makes gradient descent converge *much* faster

Feature Standardization

- Rescales features to have zero mean and unit variance

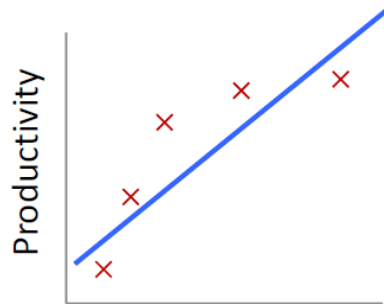
- Let μ_j be the mean of feature j : $\mu_j = \frac{1}{n} \sum_{i=1}^n x_j^{(i)}$

- Replace each value with:

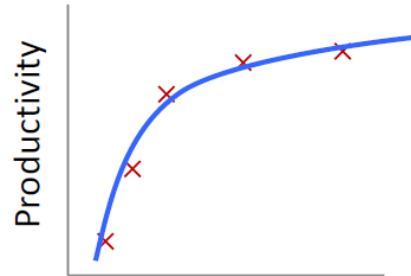
$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j} \quad \text{for } j = 1 \dots d \quad (\text{not } x_0!)$$

- 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

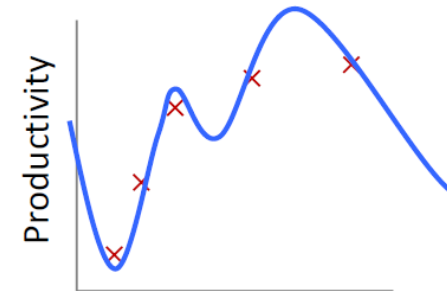
Quality of Fit



Time Spent
 $\theta_0 + \theta_1 x$
Underfitting
(high bias)



Time Spent
 $\theta_0 + \theta_1 x + \theta_2 x^2$
Correct fit



Time Spent
 $\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$
Overfitting
(high variance)

Overfitting:

- The learned hypothesis may fit the training set very well ($J(\theta) \approx 0$)
- ... 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

$$J(\boldsymbol{\theta}) = \underbrace{\frac{1}{2n} \sum_{i=1}^n (h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})^2}_{\text{model fit to data}} + \underbrace{\frac{\lambda}{2} \sum_{j=1}^d \theta_j^2}_{\text{regularization}}$$

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

Understanding Regularization

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

- 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:

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

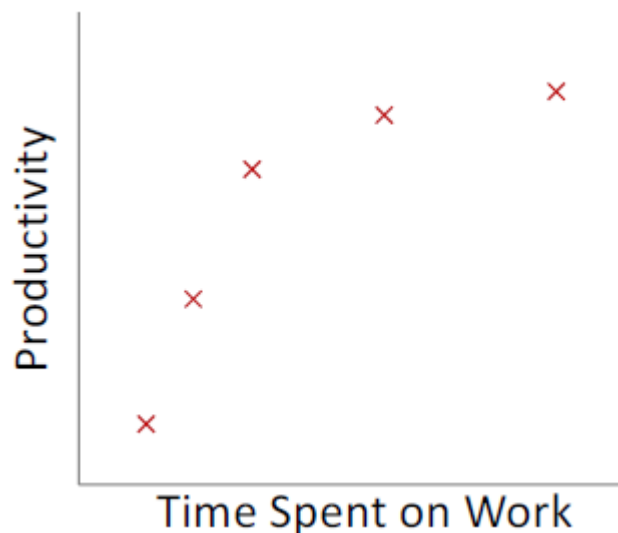
- L_2 regularization pulls coefficients toward 0

Understanding Regularization

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

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

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



Understanding Regularization

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

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

$$\theta_0 + \cancel{\theta_1}^0 x + \cancel{\theta_2}^0 x^2 + \cancel{\theta_3}^0 x^3 + \cancel{\theta_4}^0 x^4$$



Regularized Linear Regression

- Cost Function

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

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

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

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

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

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

regularization

Regularized Linear Regression

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

$$\begin{aligned}\theta_0 &\leftarrow \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^n (h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)}) \\ \theta_j &\leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^n (h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)}) x_j^{(i)} - \alpha \lambda \theta_j\end{aligned}$$

- We can rewrite the gradient step as:

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

Regularized Linear Regression

- To incorporate regularization into the closed form solution:

$$\theta = \left(X^T X + \lambda I \right)^{-1} X^T y$$

Regularized Linear Regression

- To incorporate regularization into the closed form solution:

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

- 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

Reference

- <https://www.seas.upenn.edu/~cis519>