CSE 4621
Machine Learning

Lecture 6

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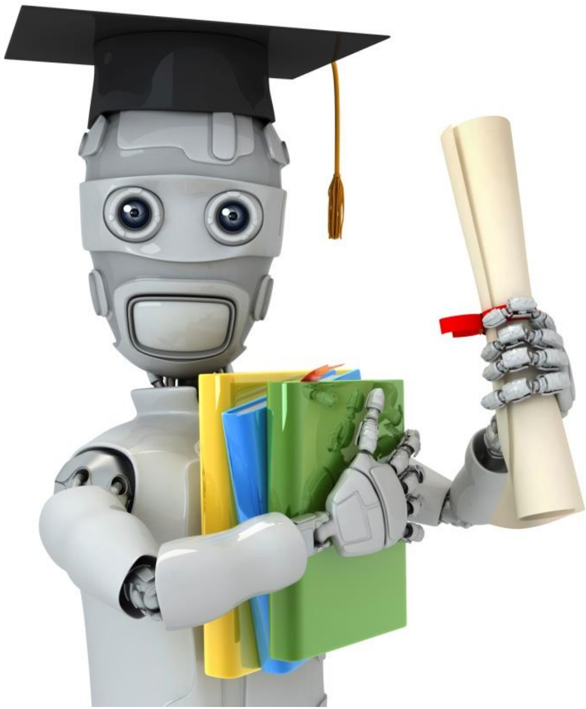


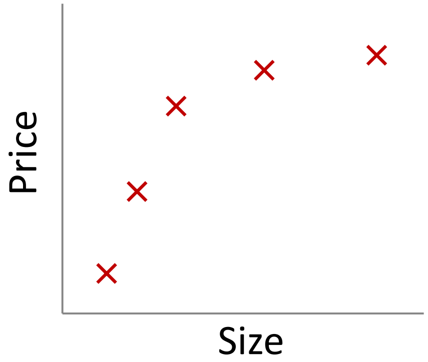
Machine Learning

Regularization

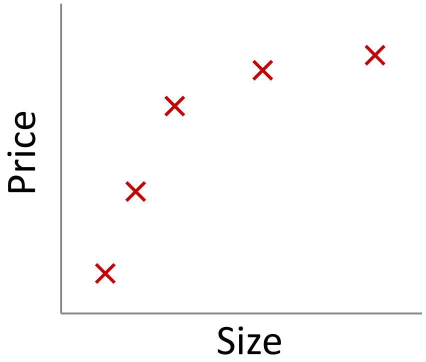
The problem of overfitting

Source & Special Thanks to Andrew Ng (Coursera) Machine Learning Course

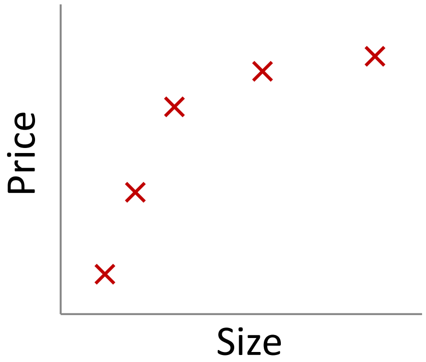
Example: Linear regression (housing prices)



$$\theta_0 + \theta_1 x$$



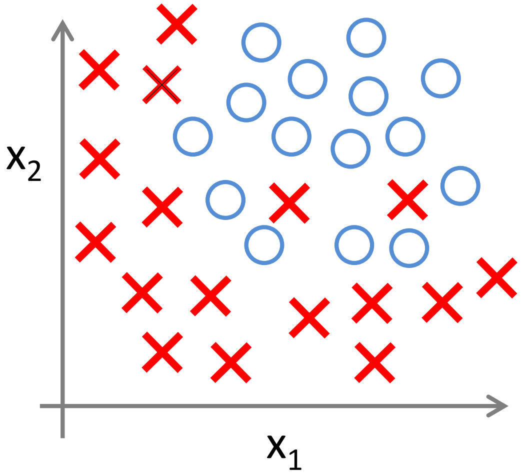
$$\theta_0 + \theta_1 x + \theta_2 x^2$$



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

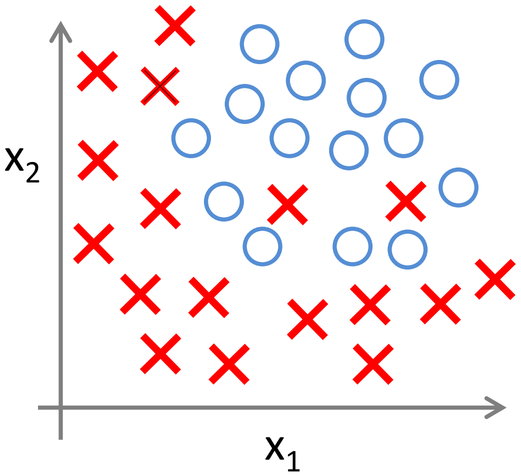
Overfitting: If we have too many features, the learned hypothesis may fit the training set very well ($J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$), but fail to generalize to new examples (predict prices on new examples).

Example: Logistic regression

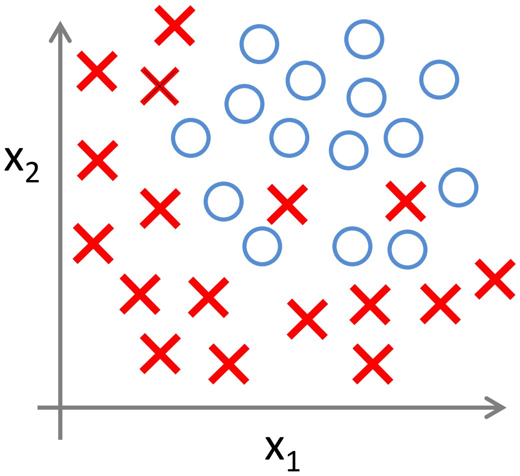


$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

(g = sigmoid function)



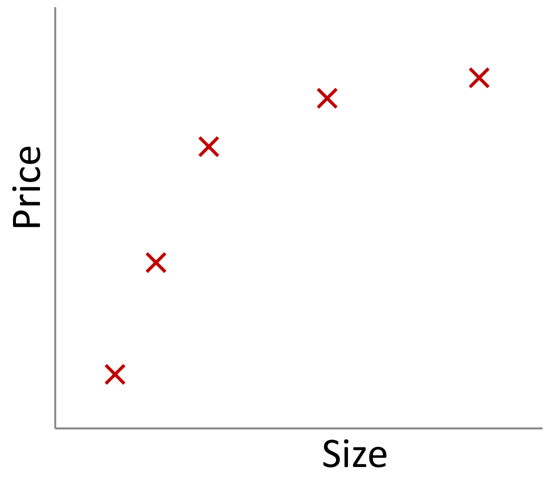
$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 \\ + \theta_3 x_1^2 + \theta_4 x_2^2 \\ + \theta_5 x_1 x_2)$$



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 \\ + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 \\ + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$$

Addressing overfitting:

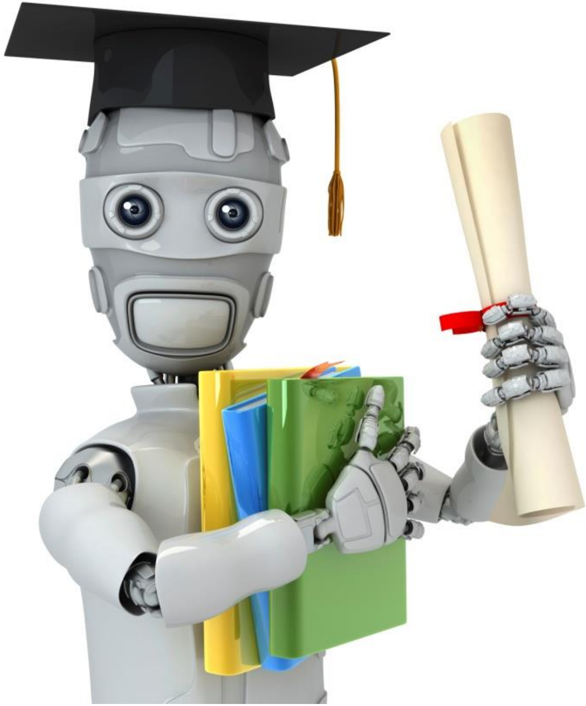
$x_1 =$ size of house
$x_2 =$ no. of bedrooms
$x_3 =$ no. of floors
$x_4 =$ age of house
$x_5 =$ average income in neighborhood
$x_6 =$ kitchen size
$\vdots$
x_{100}



Addressing overfitting:

Options:

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.

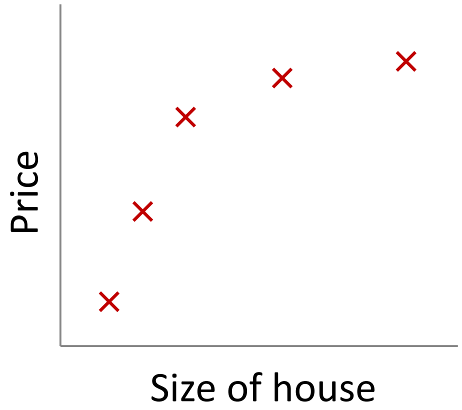


Machine Learning

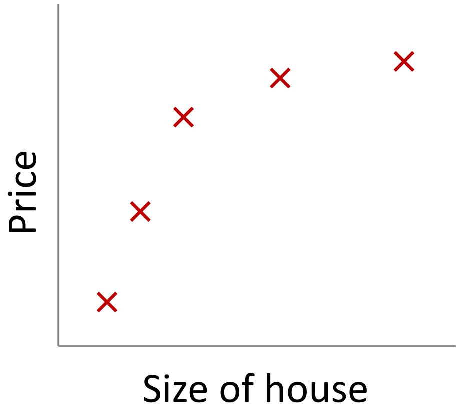
Regularization

Cost function

Intuition



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



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

Suppose we penalize and make θ_3, θ_4 really small.

$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Regularization.

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

- "Simpler" hypothesis
- Less prone to overfitting

Housing:

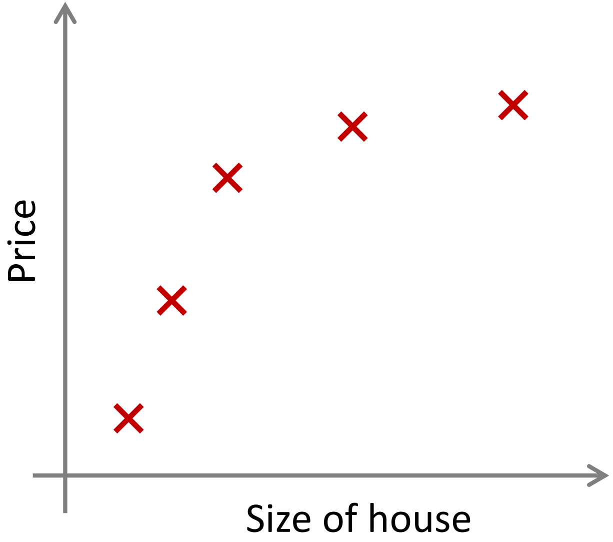
- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

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

Regularization.

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

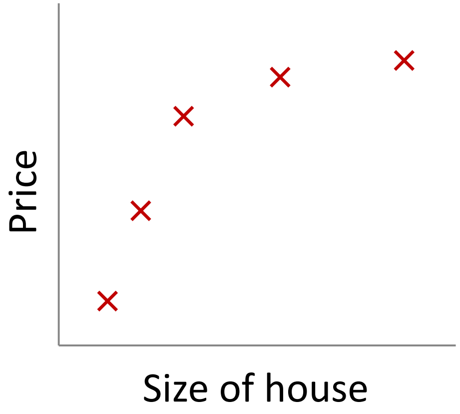
$$\min_\theta J(\theta)$$



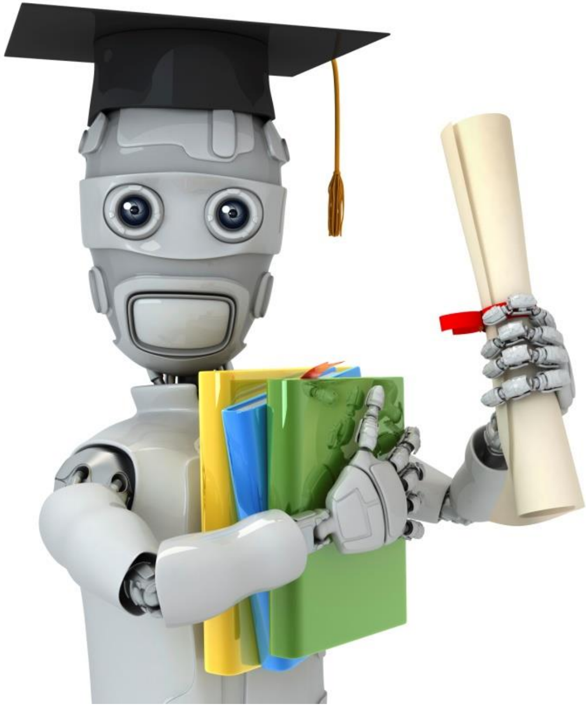
In regularized linear regression, we choose θ to minimize

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

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?



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



Machine Learning

Regularization

Regularized linear regression

Regularized linear regression

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

$$\min_\theta J(\theta)$$

Gradient descent

Repeat $\{$

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

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

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

$\}$

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

Normal equation

$$X = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

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

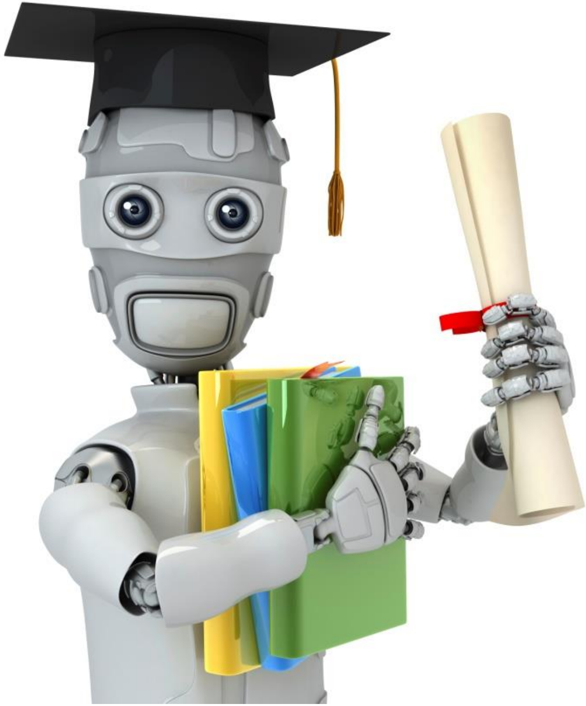
Non-invertibility (optional/advanced).

Suppose $m \leq n$,
(#examples) (#features)

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

If $\lambda > 0$,

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

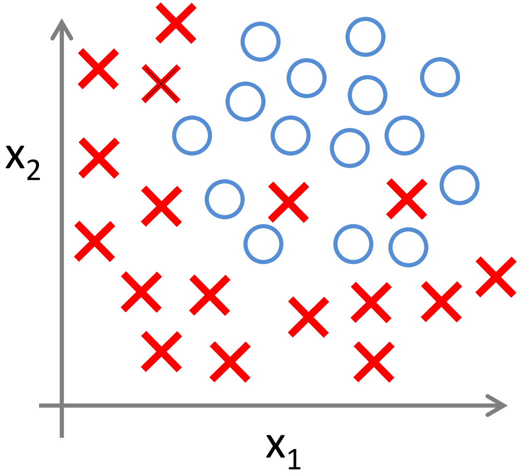


Machine Learning

Regularization

Regularized logistic regression

Regularized logistic regression.



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

$$J(\theta) = -\left[\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))\right]$$

Gradient descent

Repeat $\{$

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

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

$$(j = \cancel{0}, 1, 2, 3, \dots, n)$$

$\}$

L1 (Lasso) Regularization

- In L1 regularization, unimportant feature parameters shrink to zero.
  - Leads to sparse solution
- In Sparse solution majority of the input features have zero weights and very few features have non zero weights.
- L1 regularization does feature selection. It does this by assigning insignificant input features with zero weight and useful features with a non zero weight.

Cost Function

$$L(x,y) \equiv \sum_{i=1}^{n}(y_i - h_\theta(x_i))^2 + \boxed{\lambda \sum_{i=1}^{n}|\theta_i|}$$

Regularization Term

L2 (Ridge) Regularization

- L2 regularization forces the weights to be small but does not make them zero and gives non-sparse solution.
- L2 regularization is less likely than L1 to produce zero weight coefficients.
- Ridge regression performs better when all the input features influence the output.
- *L2 regularization is able to learn complex data patterns*

Cost Function

$$L(x,y) \equiv \sum_{i=1}^{n}(y_i - h_\theta(x_i))^2 + \boxed{\lambda \sum_{i=1}^{n} \theta_i^2}$$

Get Less than Perfect Solution!

- Regularization reduce the chances of overfitting because introducing λ makes us shift *away* from the very θ that was going to cause us overfitting problems.

- With Gradient Descent (for 1D feature space x)

$$\theta := \theta - (\theta^T \mathrm{x} - \mathrm{y})\,\mathrm{x} = \theta - D$$

Without Regularization

$$\theta := \begin{cases} \theta - (\theta^T \mathrm{x} - \mathrm{y})\,\mathrm{x} - \lambda, \mathrm{if}\ \theta > 0 \\ \theta - (\theta^T \mathrm{x} - \mathrm{y})\,\mathrm{x} + \lambda, \mathrm{if}\ \theta < 0 \end{cases}$$

L1 Regularization

$$\theta := \theta - (\theta^T \mathrm{x} - \mathrm{y})\,\mathrm{x} - \lambda\theta$$

L2 Regularization

Why?

- Introducing a penalty to the sum of the weights means that the model has to “distribute” its weights optimally, so naturally most of this “resource” will go to the simple features that explain most of the variance, with complex features getting small or zero weights.

$$\theta := \theta - (\theta^T \mathrm{x} - \mathrm{y})\,\mathrm{x} = \theta - D$$

Without Regularization

$$\theta := \begin{cases} \theta - \lambda / m - D, \text{if } \theta > 0 \\ \theta + \lambda / m - D, \text{if } \theta < 0 \end{cases}$$

L1 Regularization

$$\theta := \theta(1 - \lambda / m) - D$$

L2 Regularization

Example weights: $\hat{y} = 0.4561x_1 - 0.0007x_2 + 0.3251x_3 + 0.0009x_4 + 0.0001x_5 - 0.9142x_6 - 0.553$

Visual Interpretations

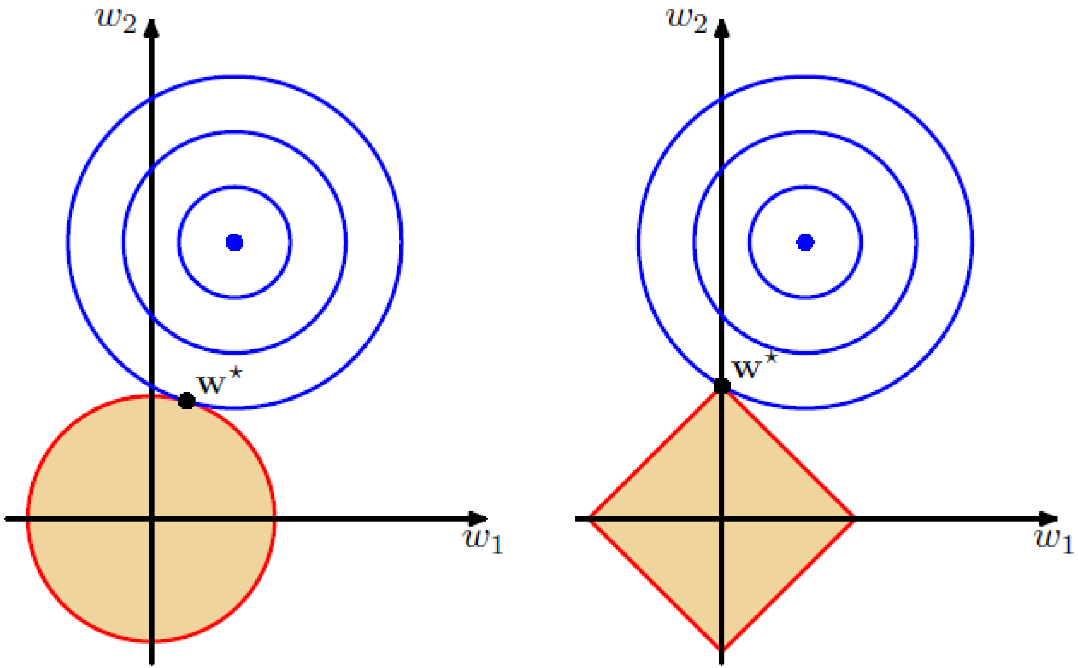
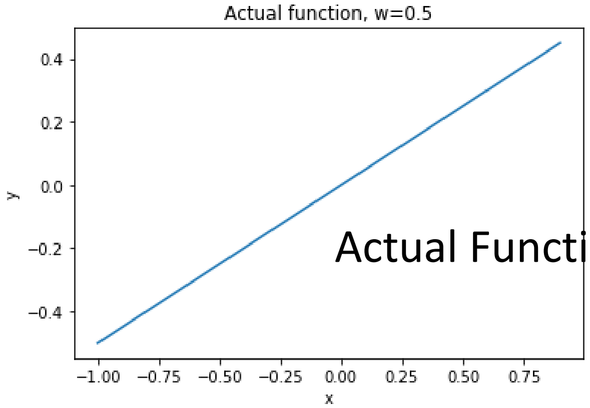


Figure 3.4 Plot of the contours of the unregularized error function (blue) along with the constraint region (3.30) for the quadratic regularizer $q = 2$ on the left and the lasso regularizer $q = 1$ on the right, in which the optimum value for the parameter vector $\mathbf{w}$ is denoted by $\mathbf{w}^\star$. The lasso gives a sparse solution in which $w_1^\star = 0$.

Visual Interpretations



Actual Function, y=0.5x