Regularization

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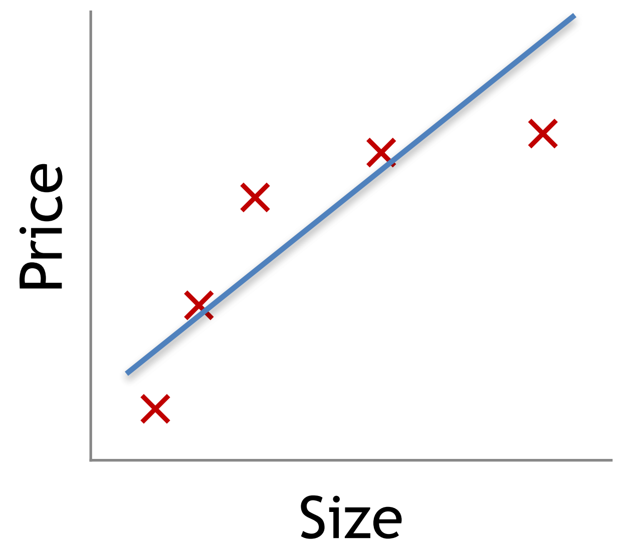
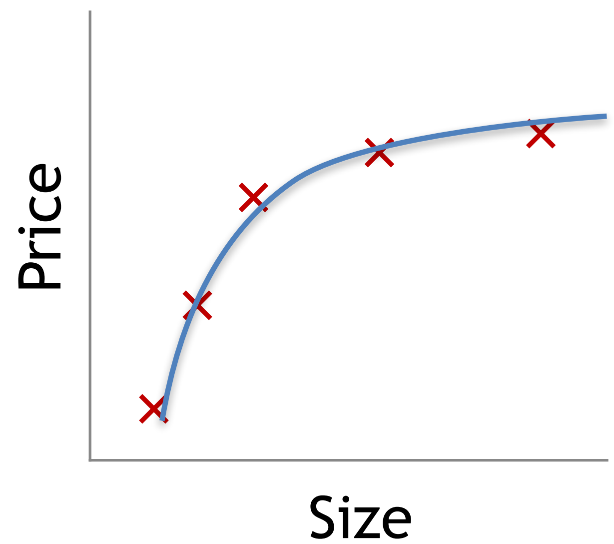
Regularization

The problem of overfitting

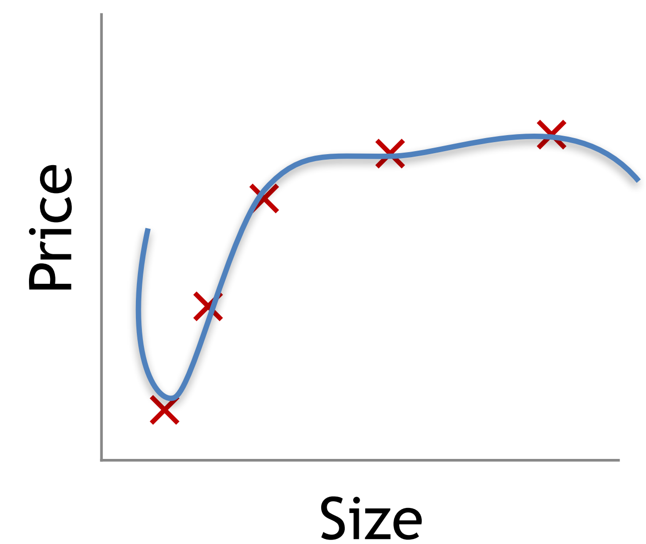
Example: Linear regression (housing prices)



$\theta_0 + \theta_1 x$



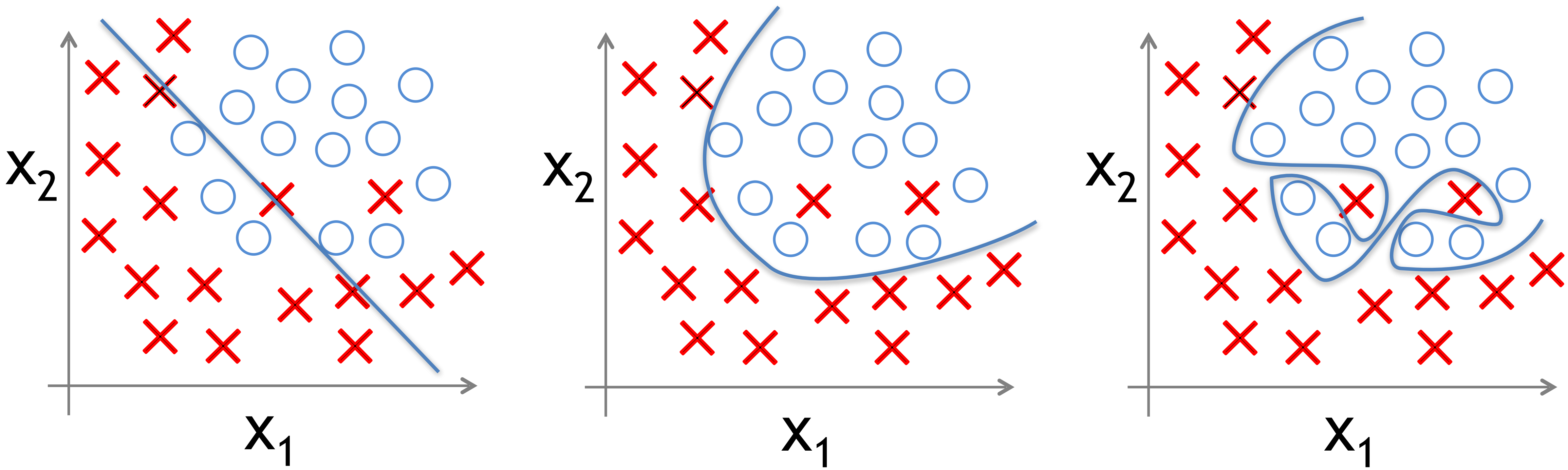
$\theta_0 + \theta_1 x + \theta_2 x^2$



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

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



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

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

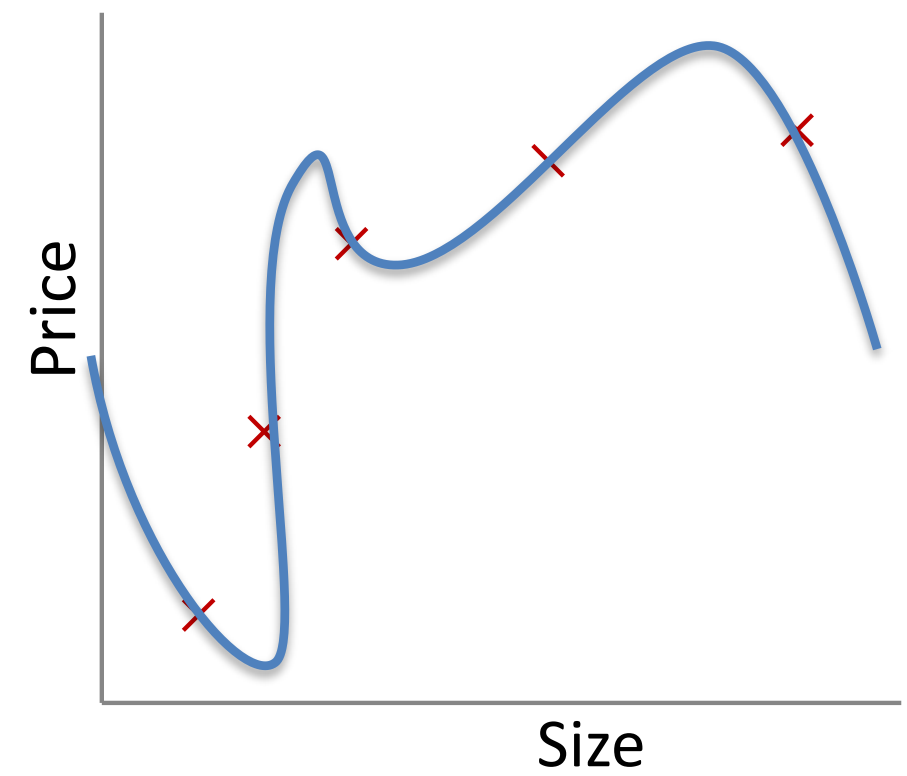
$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2$
$+\theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2$
$+\theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$

(g = sigmoid function)

$$g(z) = \frac{1}{1+e^{-z}}$$

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}



the problem gets harder as the number of features increases

Addressing overfitting

Options:

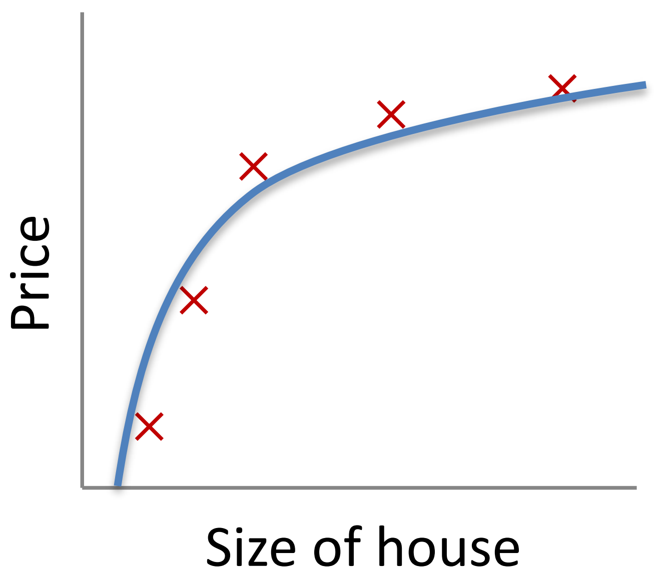
1. Reduce number of features
   - Manually select which features to keep
   - Model selection algorithm

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

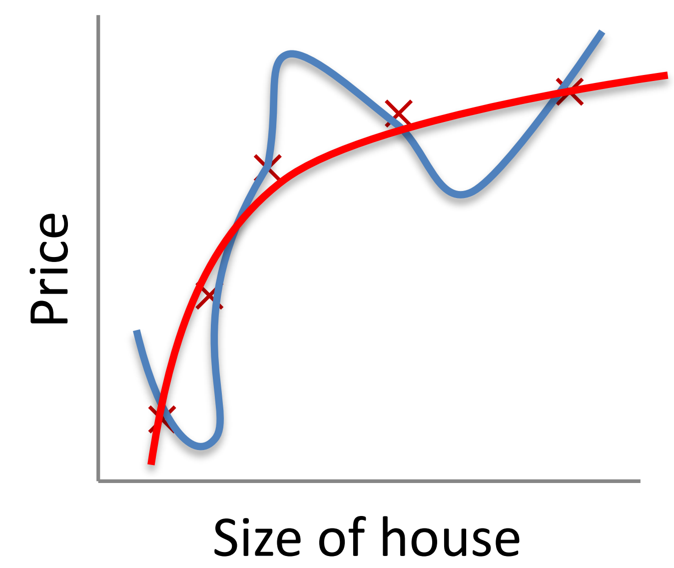
Regularization

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.

$$\min_{\theta} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2$$

$$\theta_3 \approx 0 \qquad \theta_4 \approx 0$$

Regularization

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

- "Simpler" hypothesis
- Less prone to overfitting

Housing:

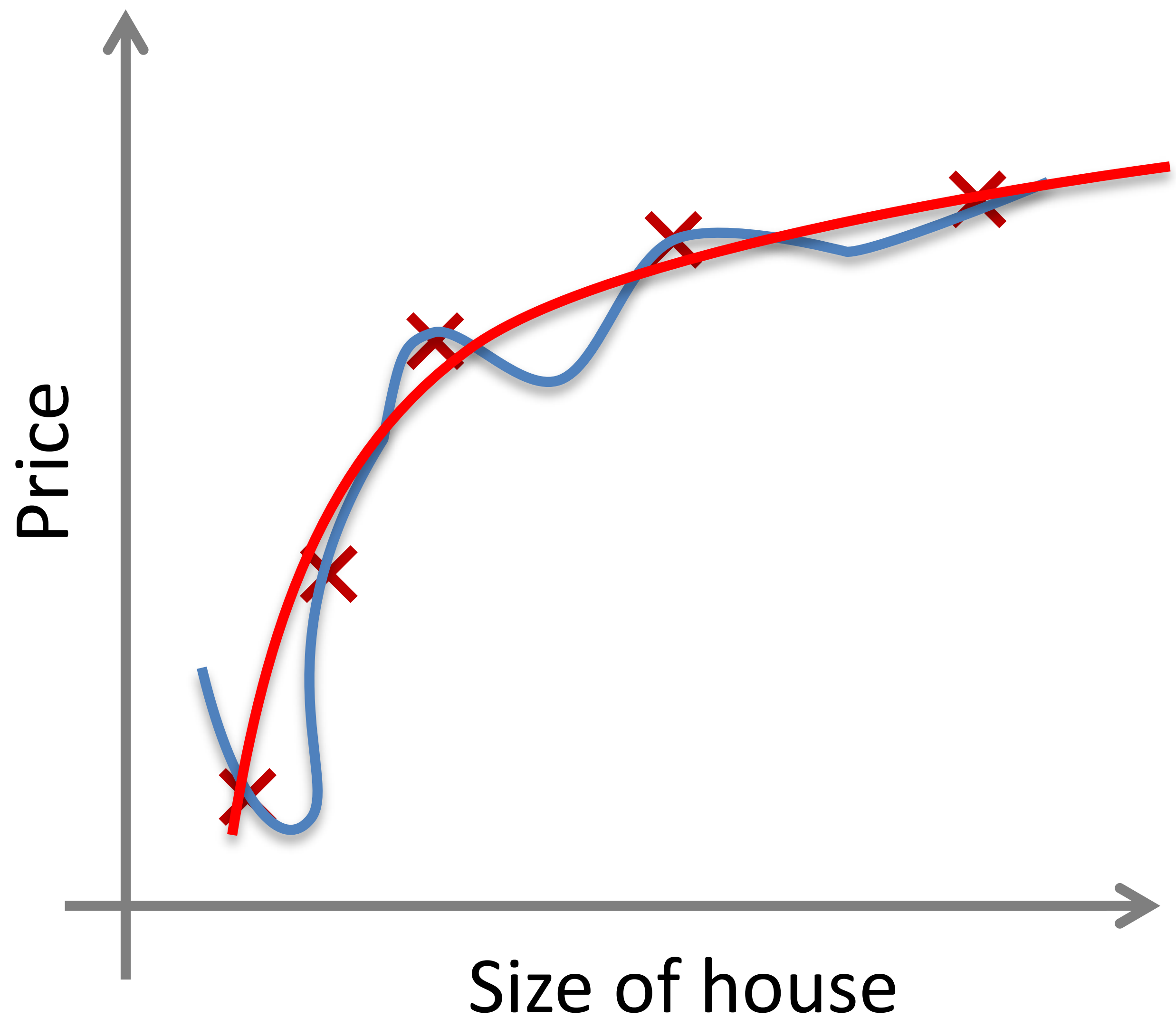
- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

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

Regularization

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

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

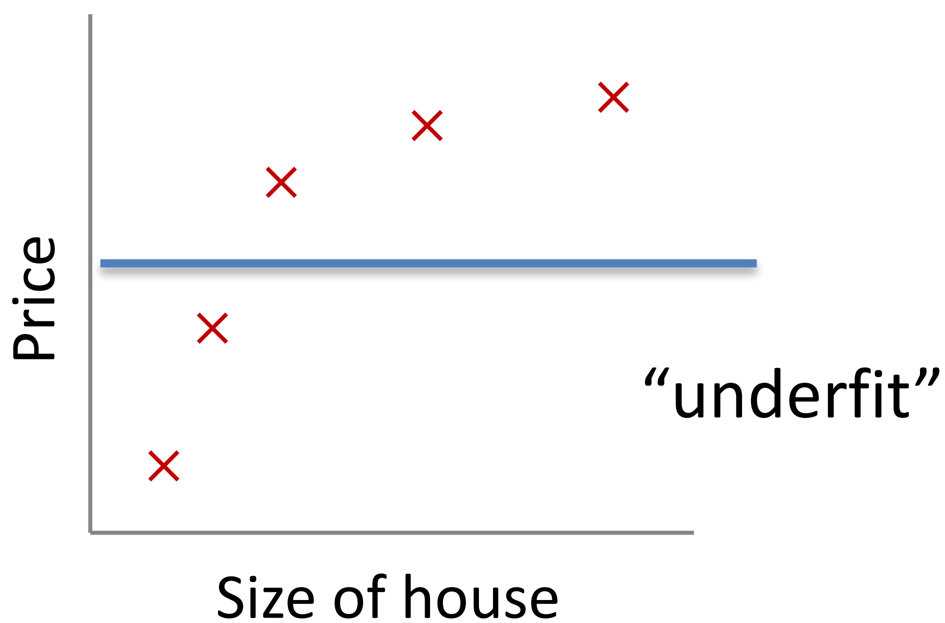


Regularization

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 $\lambda = 10^{10}$)?



$$\theta_1 \approx 0, \theta_2 \approx 0, \theta_3 \approx 0, \theta_4 \approx 0$$

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

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

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 $\{$

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

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

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

$\}$

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

Normal equation

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

$$m \times (n+1)$$

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

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

Non-invertibility

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

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

non-invertible

If $\lambda > 0$,

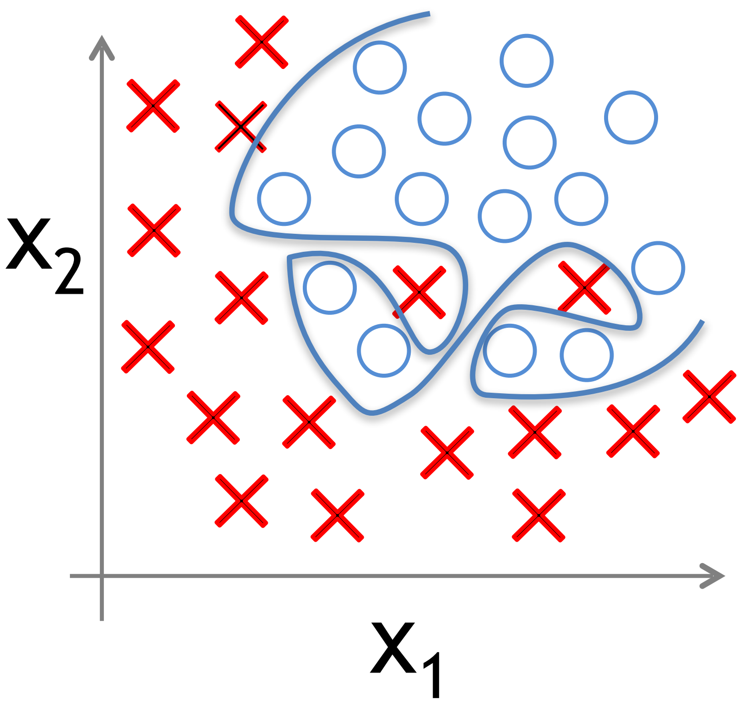
$$\theta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

invertible

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:

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

Gradient descent

Repeat $\{$

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

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

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

$\}$

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

Advanced optimization

```
def grad(theta, X, y):

    gradient[0] = [code to compute ∂/∂θ0 J(θ)]
```

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

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

```
    gradient[1] = [code to compute ∂/∂θ1 J(θ)]
```

$$\frac{\partial}{\partial\theta_1}J(\theta)$$

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

```
    gradient[2] = [code to compute ∂/∂θ2 J(θ)]
```

$$\frac{\partial}{\partial\theta_2}J(\theta)$$

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

⋮

```
    gradient[n] = [code to compute ∂/∂θn J(θ)]
```

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

```
    return gradient
```

```
def cost(theta, X, y):

      return jVal = code to compute J(θ)
```

$$J(\theta)$$

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