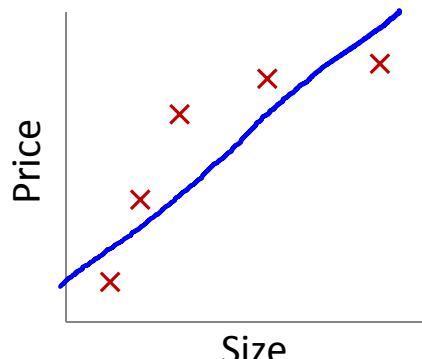


Machine Learning

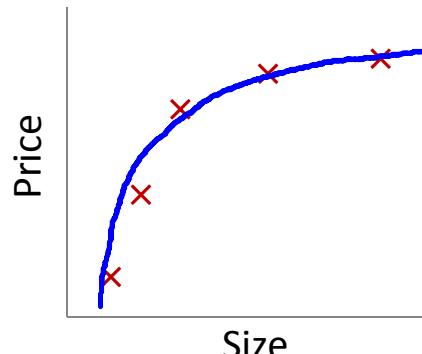
Regularization

The problem of overfitting

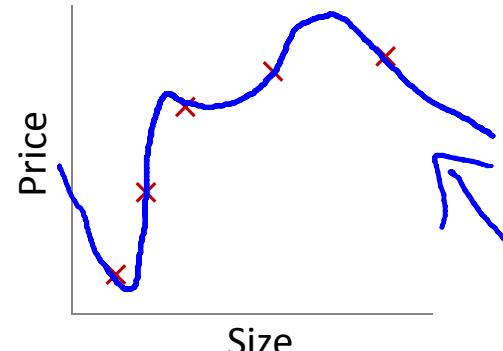
Example: Linear regression (housing prices)



$\rightarrow \theta_0 + \theta_1 x$
"Underfit" "High bias"



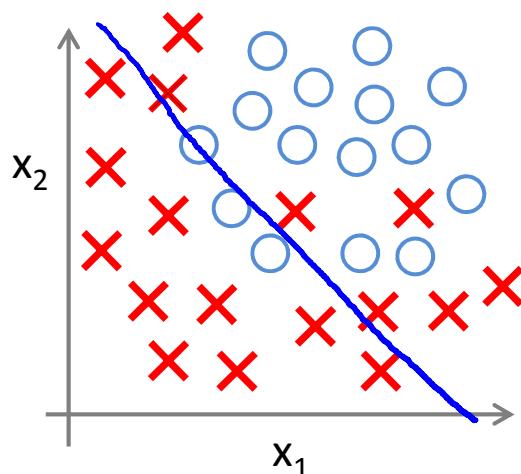
$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2$
"Just right"



$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$
"Overfit" "High variance"

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

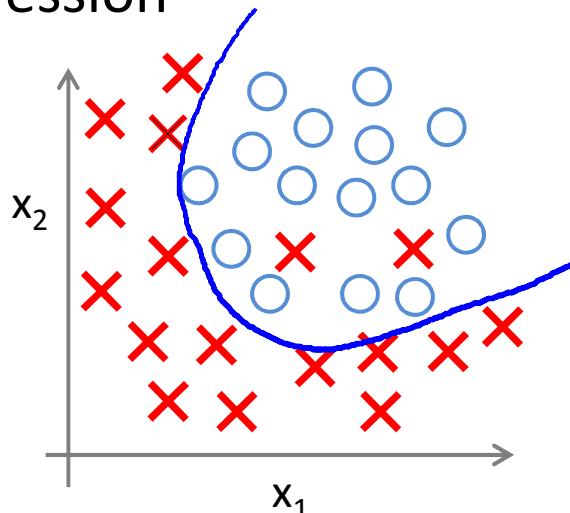


$$\rightarrow h_\theta(x) = g(\underline{\theta_0 + \theta_1 x_1 + \theta_2 x_2})$$

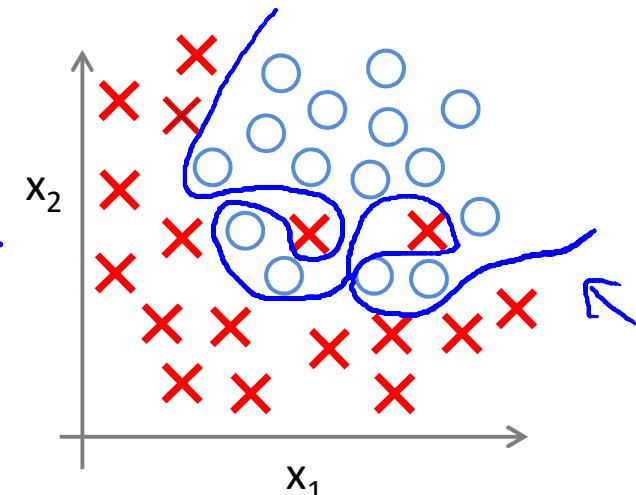
(g = sigmoid function)



"Underfit"



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



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

"Overfit"

Addressing overfitting:

x_1 = size of house

x_2 = no. of bedrooms

x_3 = no. of floors

x_4 = age of house

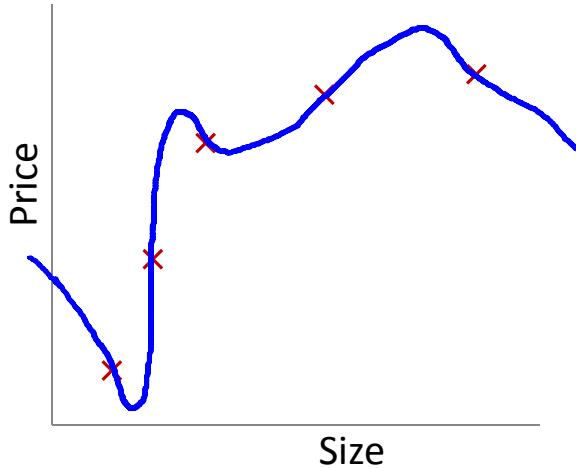
x_5 = average income in neighborhood

x_6 = kitchen size

:

:

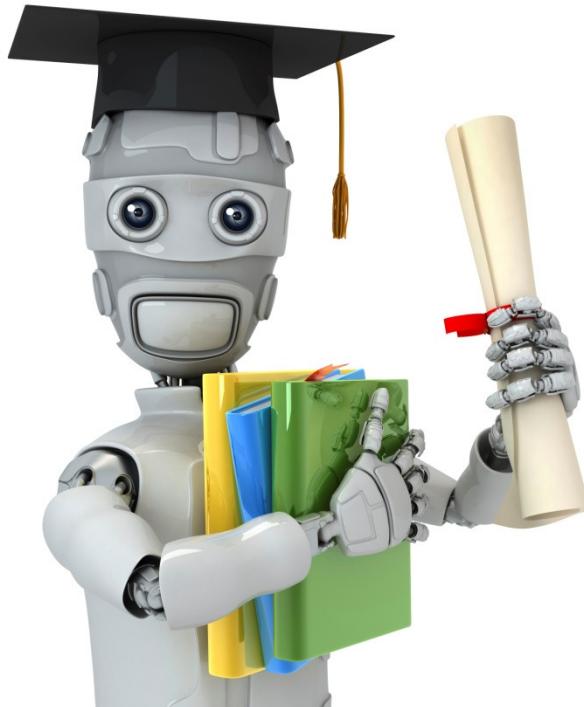
x_{100}



Addressing overfitting:

Options:

1. Reduce number of features.
 - — Manually select which features to keep.
 - — Model selection algorithm (later in course).
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 .

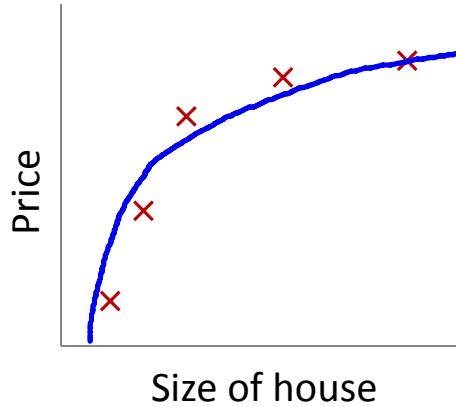


Machine Learning

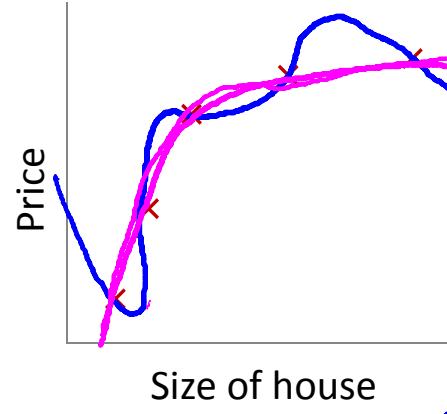
Regularization

Cost function

Intuition



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



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

Suppose we penalize and make θ_3, θ_4 really small.

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

$$\underline{\theta_3 \approx 0}$$

$$\underline{\theta_4 \approx 0}$$

Regularization.

Small values for parameters

$$\theta_0, \theta_1, \dots, \theta_n$$

- “Simpler” hypothesis
- Less prone to overfitting

$$\theta_3, \theta_4$$

$\uparrow \approx 0$

Housing:

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

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

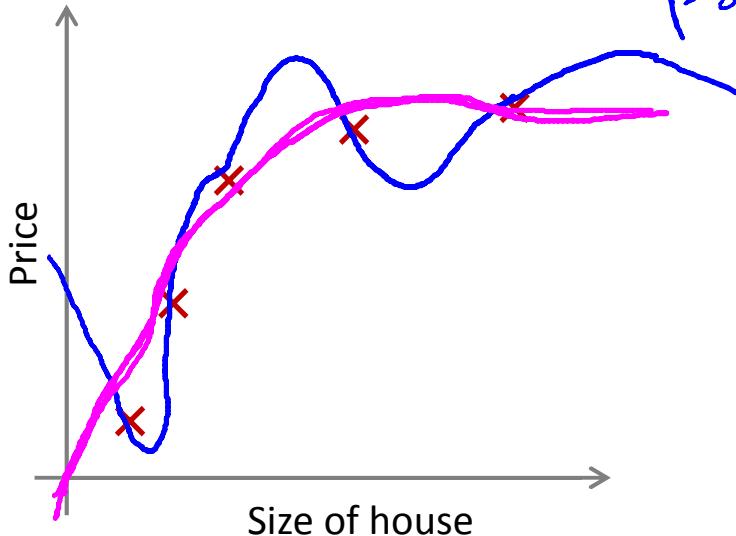
~~$\theta_1, \theta_2, \theta_3, \dots, \theta_{100}$~~

Regularization.

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

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

regularization parameter



In regularized linear regression, we choose θ to minimize

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

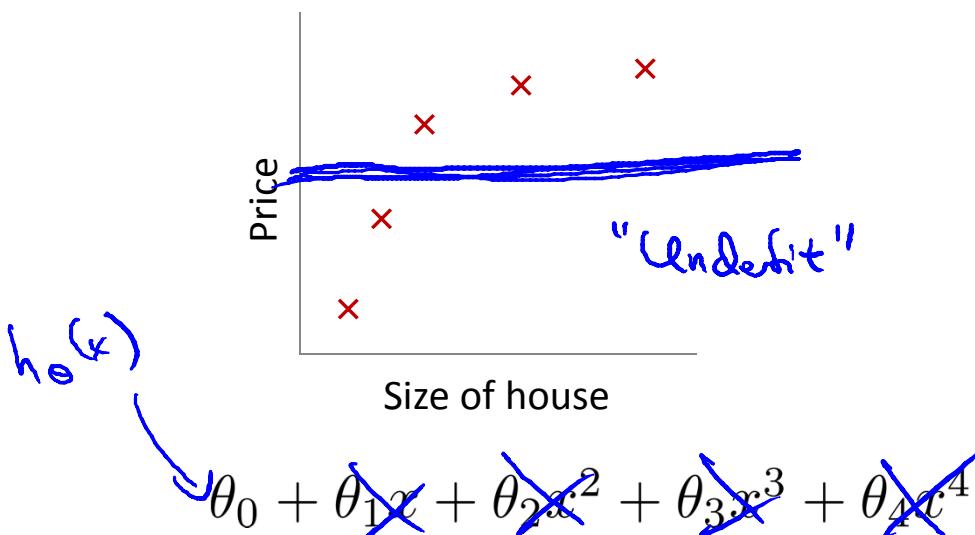
What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?

- Algorithm works fine; setting λ to be very large can't hurt it
- Algorithm fails to eliminate overfitting.
- Algorithm results in underfitting. (Fails to fit even training data well).
- Gradient descent will fail to converge.

In regularized linear regression, we choose θ to minimize

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

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

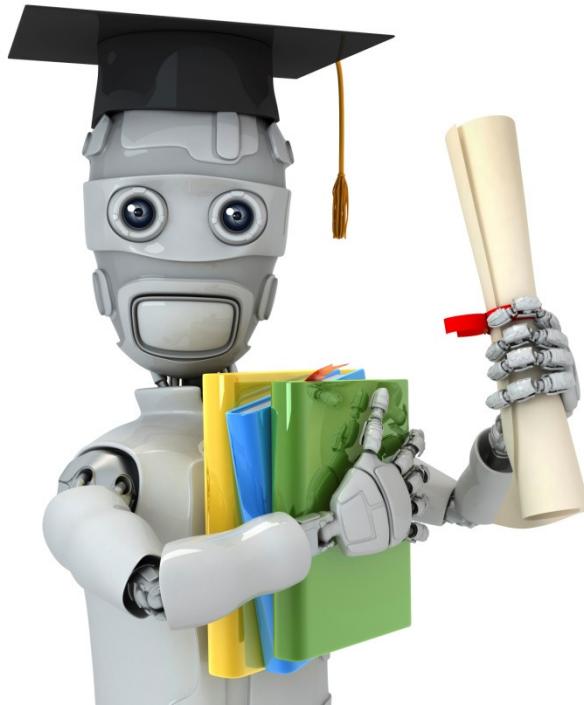


$$\underline{\theta}_1, \underline{\theta}_2, \underline{\theta}_3, \underline{\theta}_4$$

$$\theta_1 \approx 0, \theta_2 \approx 0$$

$$\theta_3 \approx 0, \theta_4 \approx 0$$

$$h_\theta(x) = \underline{\theta}_0$$



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 {

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

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

$$\begin{aligned} \theta_j &:= \theta_j - \boxed{\alpha} \left[\frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right] \\ &\quad (j = \cancel{0}, 1, 2, 3, \dots, n) \end{aligned}$$

}

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

$$1 - \alpha \frac{\lambda}{m} < 1$$

$$0.99$$

$$\theta_j \times 0.99$$

$$\boxed{\theta_j^2}$$

Normal equation

$$\underline{X} = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \leftarrow \text{m} \times (n+1)$$

$$y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix} \uparrow \mathbb{R}^m$$

$$\rightarrow \min_{\theta} J(\theta) \quad \underline{\text{---}}$$

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

E.g. n=2 $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ $(n+1) \times (n+1)$

Non-invertibility (optional/advanced).

Suppose $m \leq n$, \leftarrow

(#examples) (#features)

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

non-invertible / singular

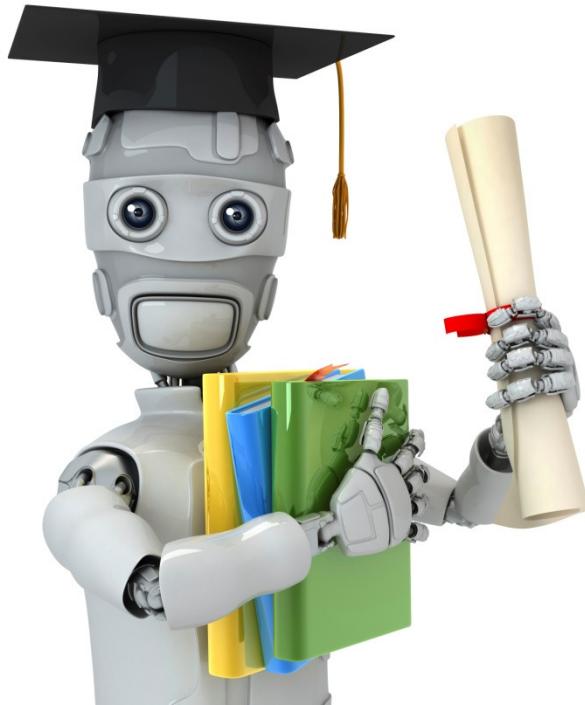
pinv

inv
R

If $\lambda > 0$,

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

invertible .

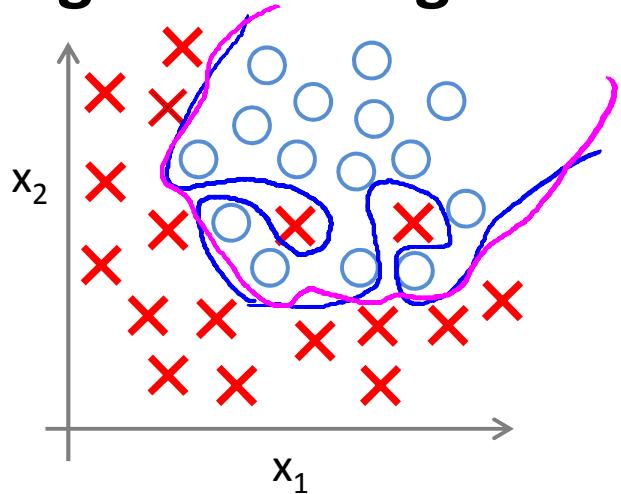


Machine Learning

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:

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

$\theta_1, \theta_2, \dots, \theta_n$

Gradient descent

Repeat {

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

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

$\underbrace{(j = \cancel{X}, 1, 2, 3, \dots, n)}_{\theta_1, \dots, \theta_n}$

}

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

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

Advanced optimization

f minunc (Q costFunction)
 $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$ theta(1) ←
theta(2) ←
theta(n+1) ←

→ function [jVal, gradient] = costFunction(theta)

jVal = [code to compute $J(\theta)$];

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

→ gradient (1) = [code to compute $\frac{\partial}{\partial \theta_0} J(\theta)$];

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

→ gradient (2) = [code to compute $\frac{\partial}{\partial \theta_1} J(\theta)$];

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

J(θ)

→ gradient (3) = [code to compute $\frac{\partial}{\partial \theta_2} J(\theta)$];

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

gradient (n+1) = [code to compute $\frac{\partial}{\partial \theta_n} J(\theta)$];

