线性回归与线性分类

Linear Regression and Linear Classification

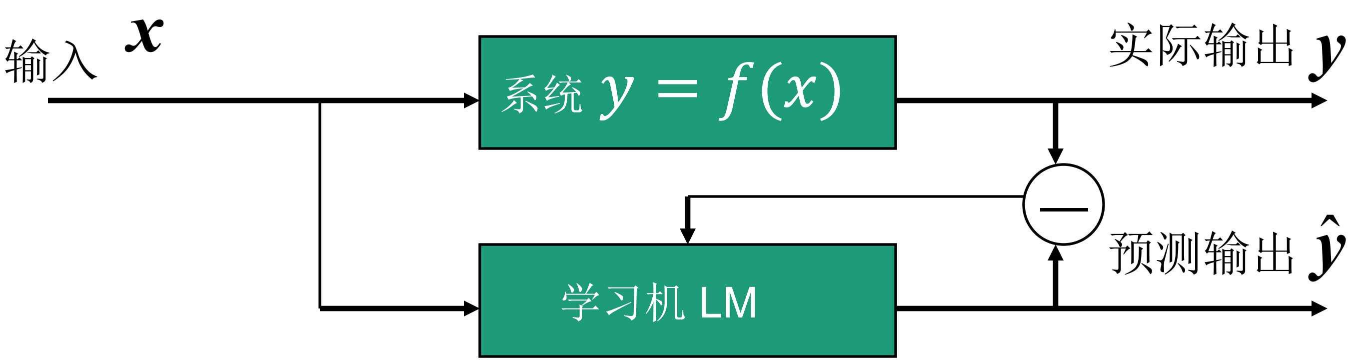
洪 波

Dept. of Biomedical Engineering

Tsinghua University

机器学习
Machine Learning

未知函数，未知分类器



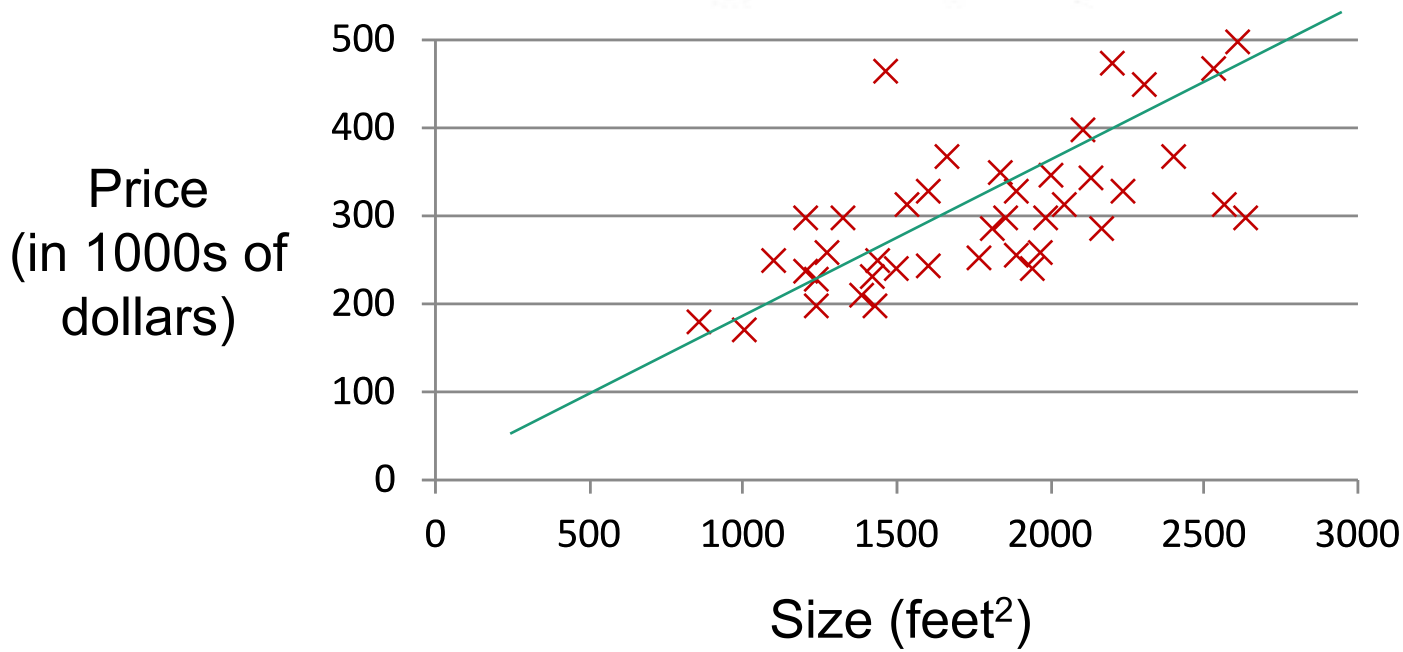
函数逼近，模式分类

“学习材料”：一组观测样本　$(x_1, y_1), (x_1, y_1), \cdots, (x_n, y_n)$

Linear Regression 线性回归

Linear Regression (Housing Prices Prediction)

$$h_\theta(x) = \theta_0 + \theta_1 x$$



Regression Problem: Predict real-valued output

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Parameter optimization

Training Set

Size in feet^2 (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
…	…

Hypothesis: $$h_\theta(x) = \theta_0 + \theta_1 x$$

θ_i's: Parameters

How to choose θ_i's ?

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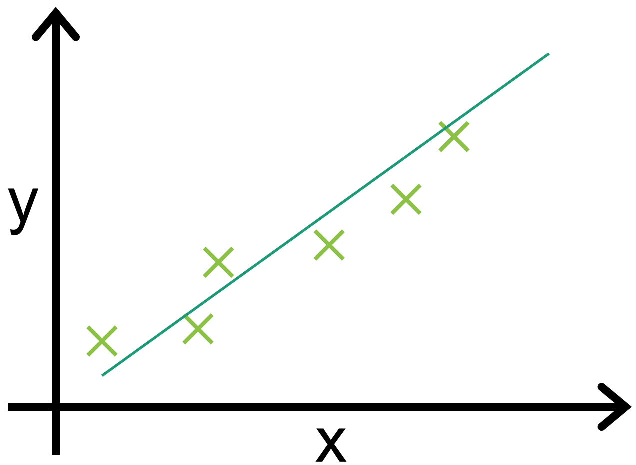
Cost Function 代价函数/目标函数



Choose θ_0, θ_1 so that $h_\theta(x)$ is close to y for our training examples (x, y)

代价函数 $$J(\boldsymbol{\theta}) = J(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1) = \frac{1}{2m}\sum_{i=1}^{m}(h(\boldsymbol{x}^{(i)}) - \boldsymbol{y}^{(i)})^2$$

简化模型 – 只考虑一个参数 θ_1

Hypothesis:

$$h_\theta(x) = \theta_0 + \theta_1 x$$

Parameters:

$$\theta_0, \theta_1$$

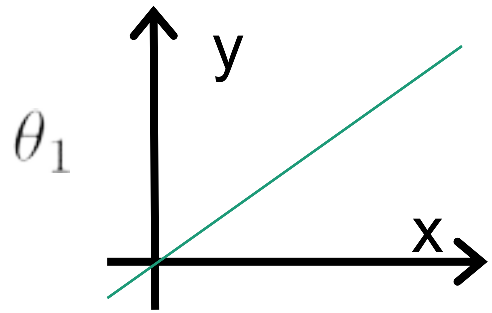
Cost Function:

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Goal: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

<u>Simplified</u>

$$h_\theta(x) = \theta_1 x$$



$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$\underset{\theta_1}{\text{minimize}}\ J(\theta_1)$

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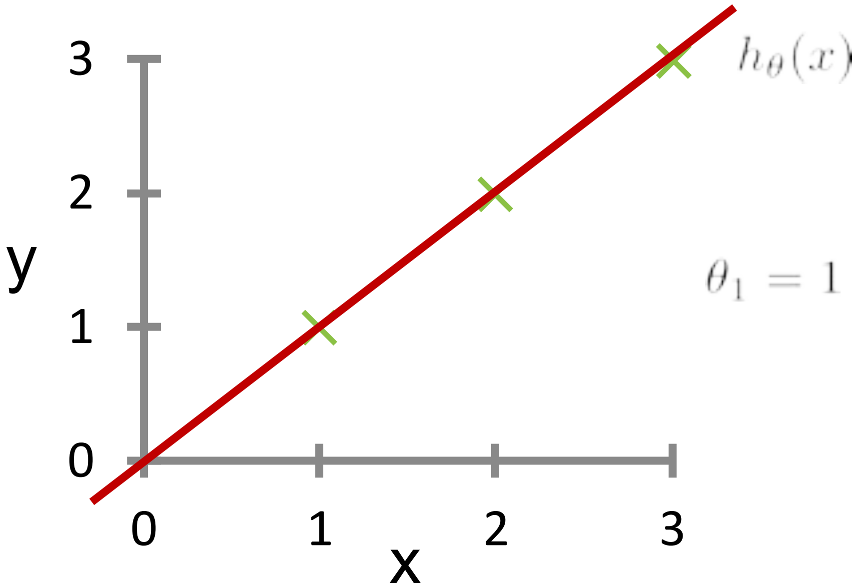
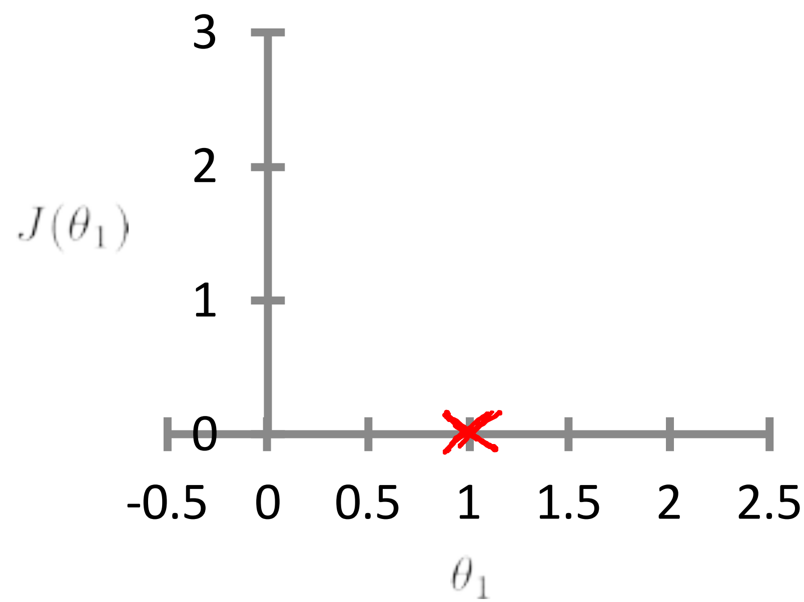
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)

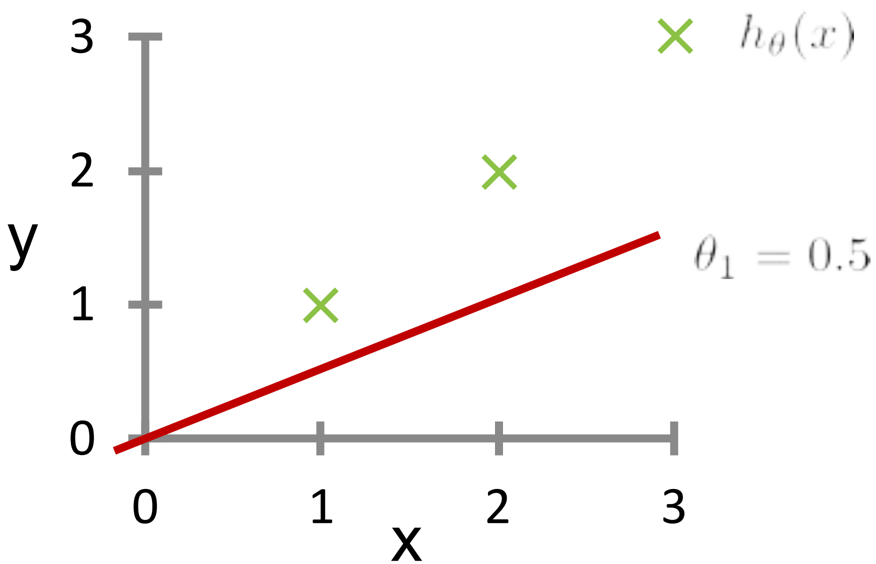


$$J(\theta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Modified from Andrew Ng ML

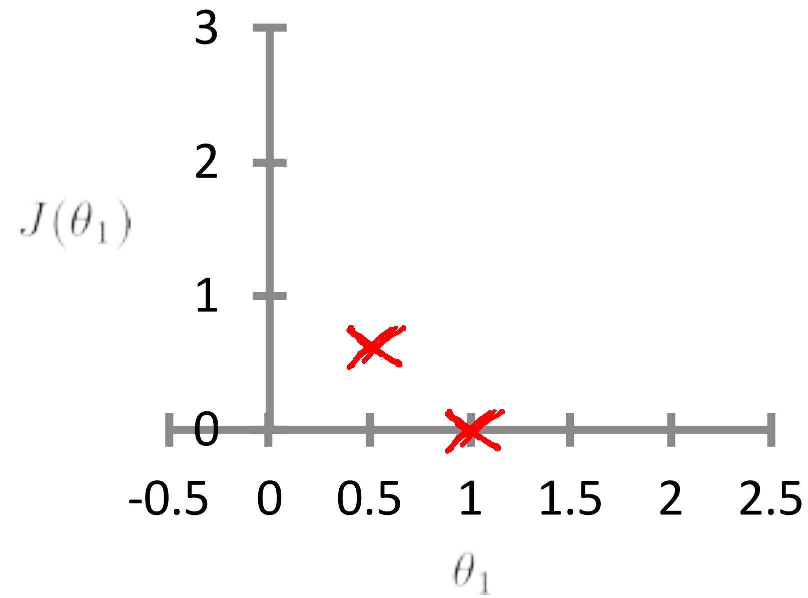
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)

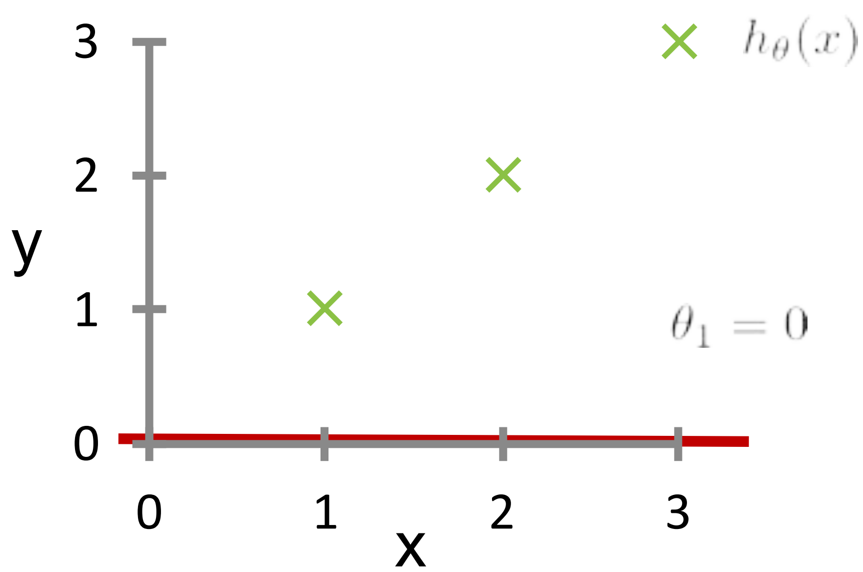


$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Modified from Andrew Ng ML

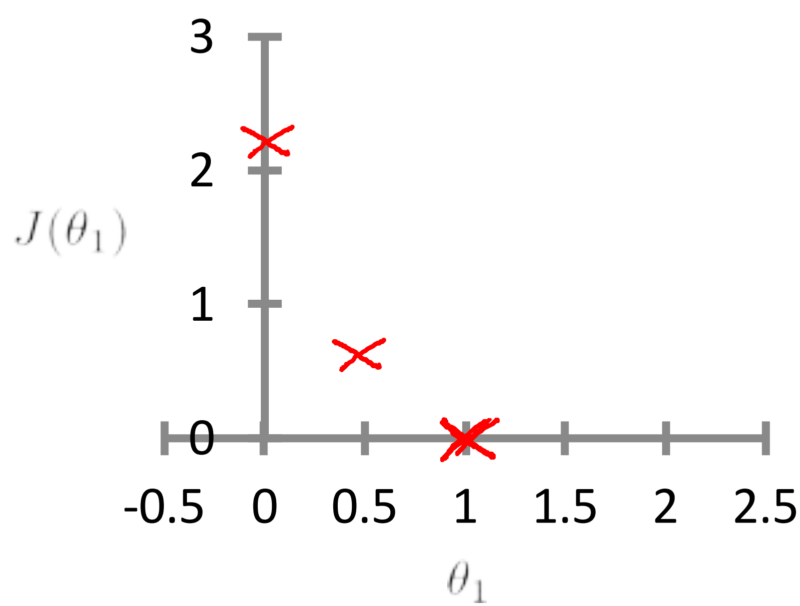
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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回到两个参数的情况 θ_0, θ_1

模型假设: $h_\theta(x) = \theta_0 + \theta_1 x$

模型参数: θ_0, θ_1

代价函数: $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

优化目标: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

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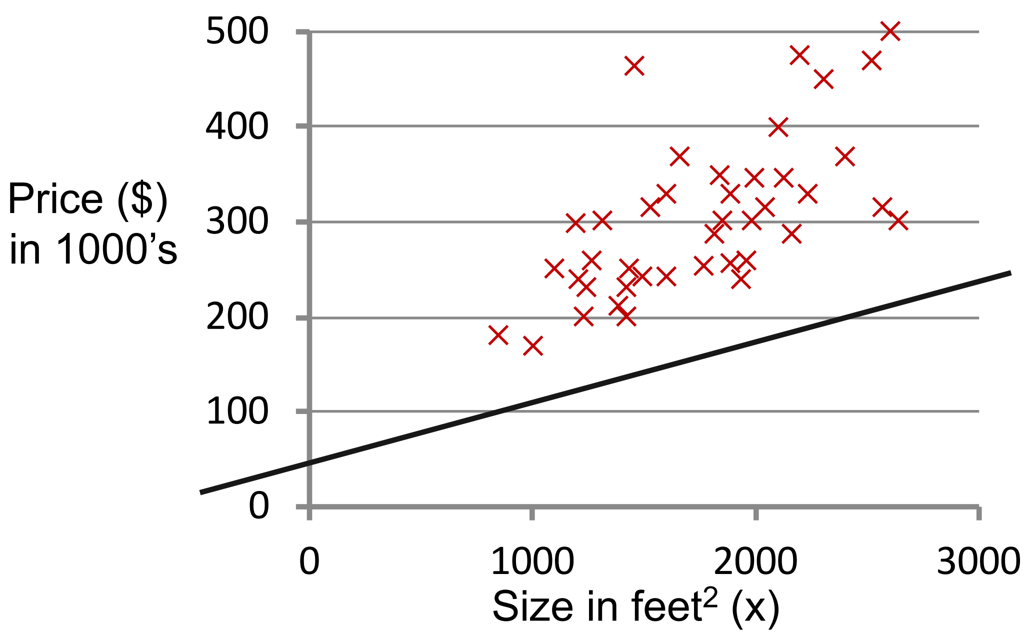
代价函数什么样？

$h_\theta(x)$

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



$$h_\theta(x) = 50 + 0.06x$$

$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

?

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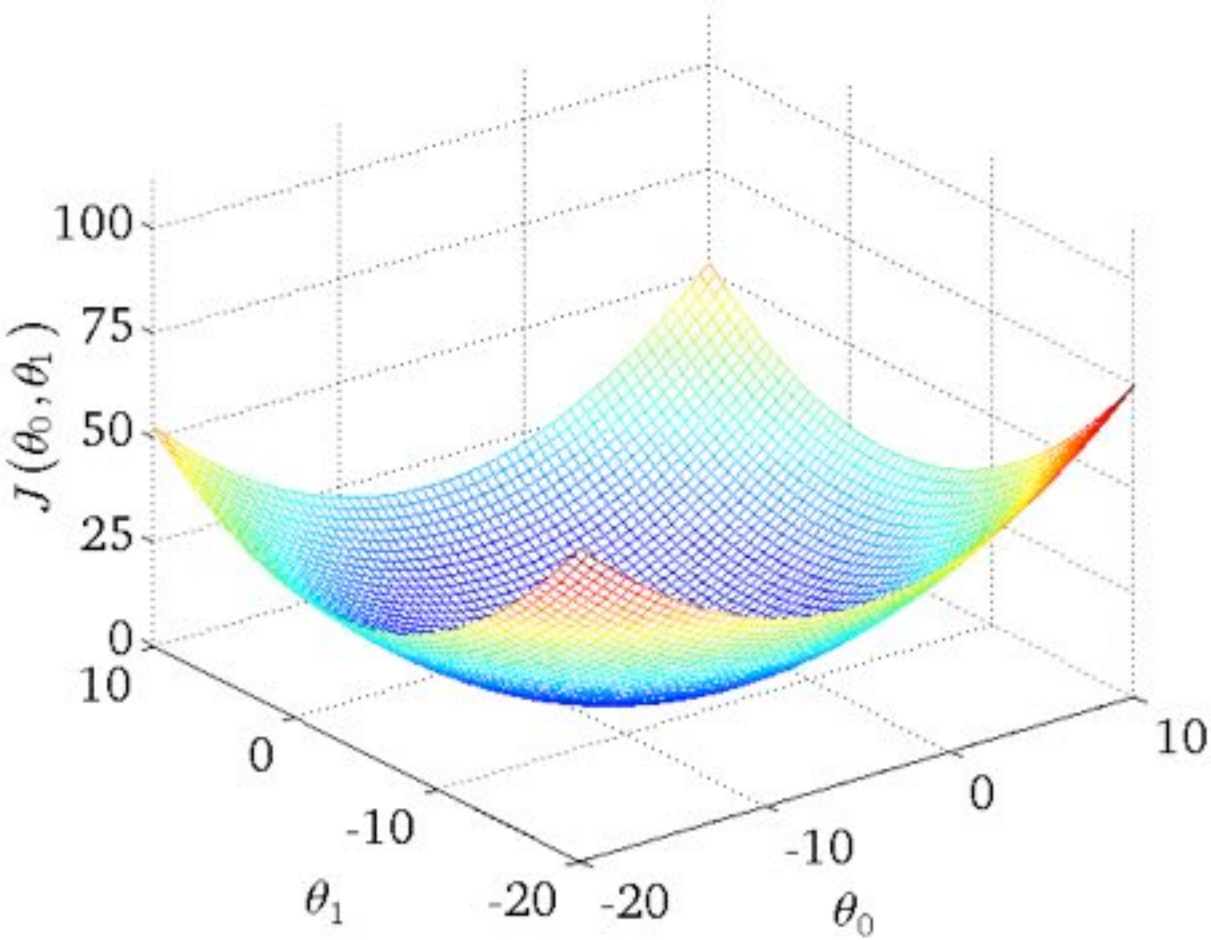
代价函数



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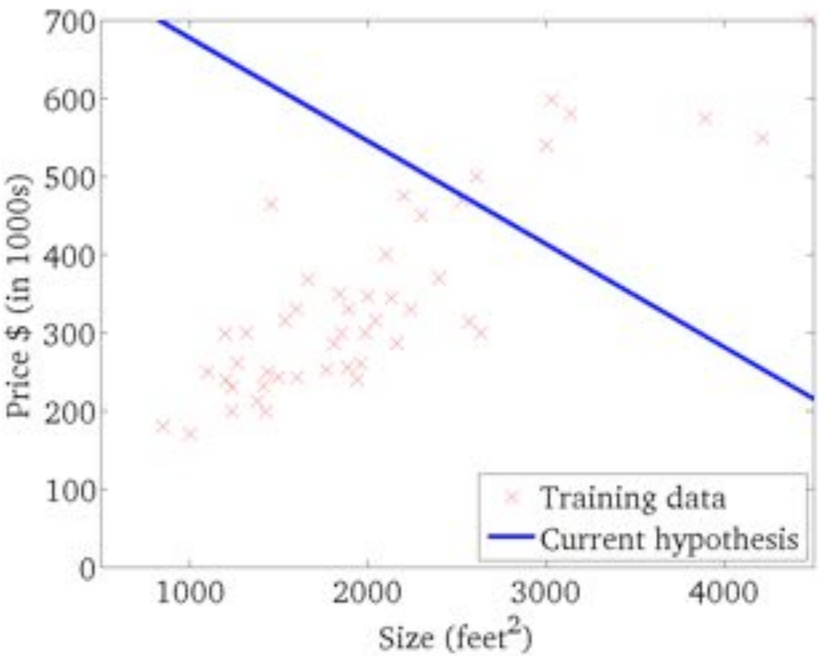
代价函数与模型参数

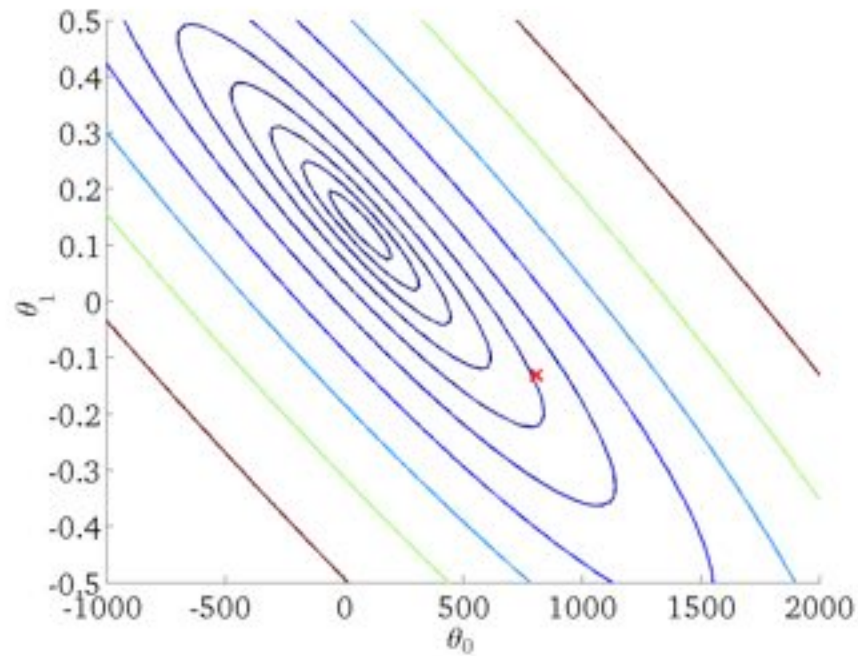
$$h_\theta(x)$$

(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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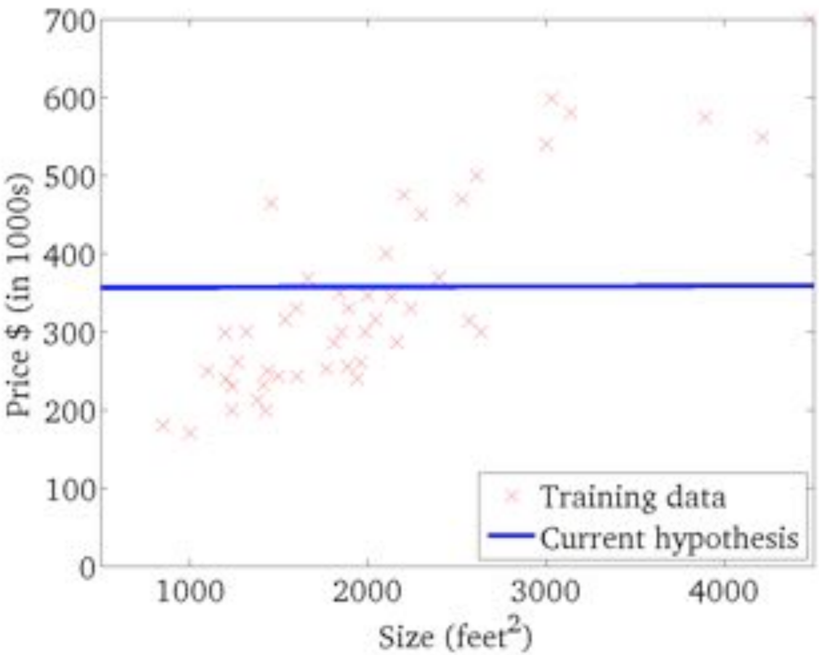
代价函数与模型参数

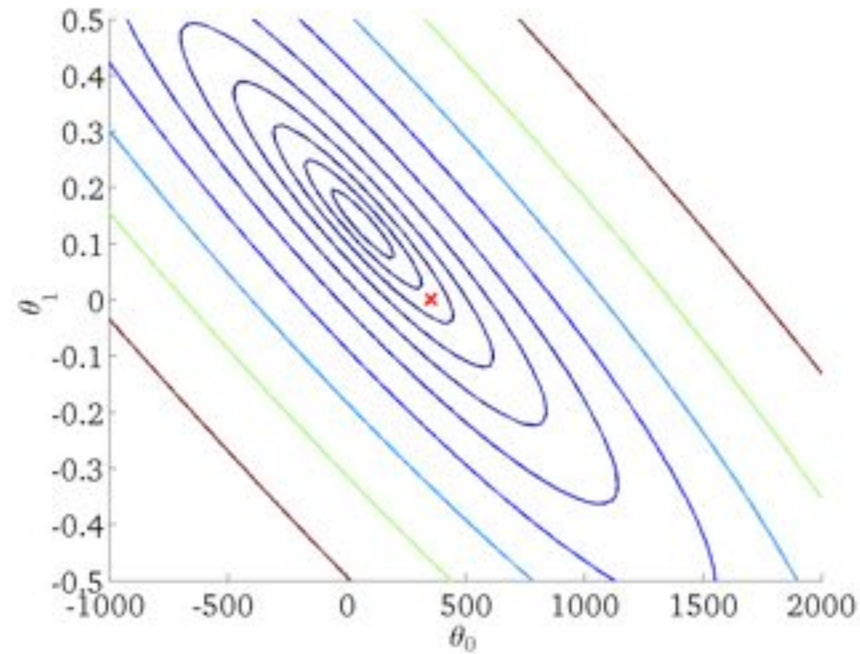
$h_\theta(x)$

(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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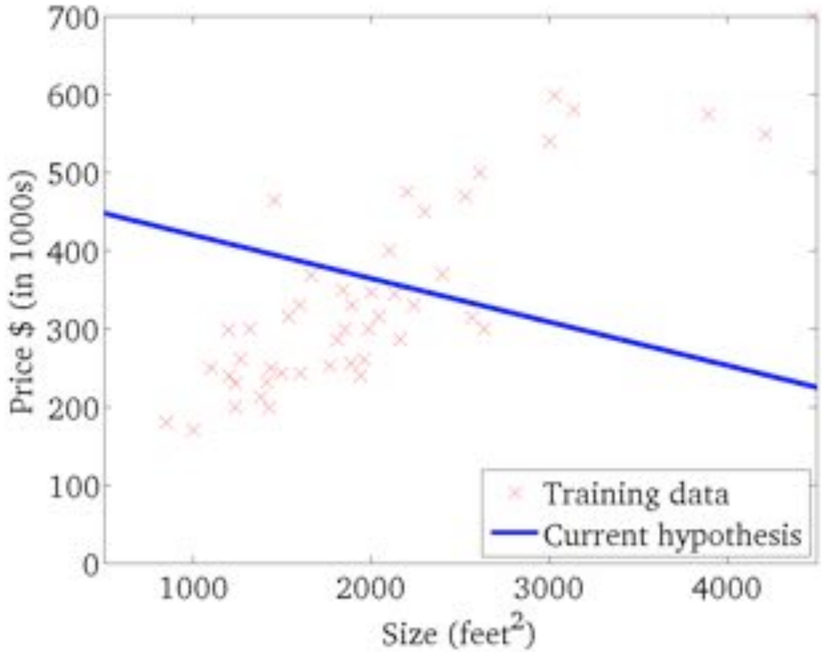
代价函数与模型参数

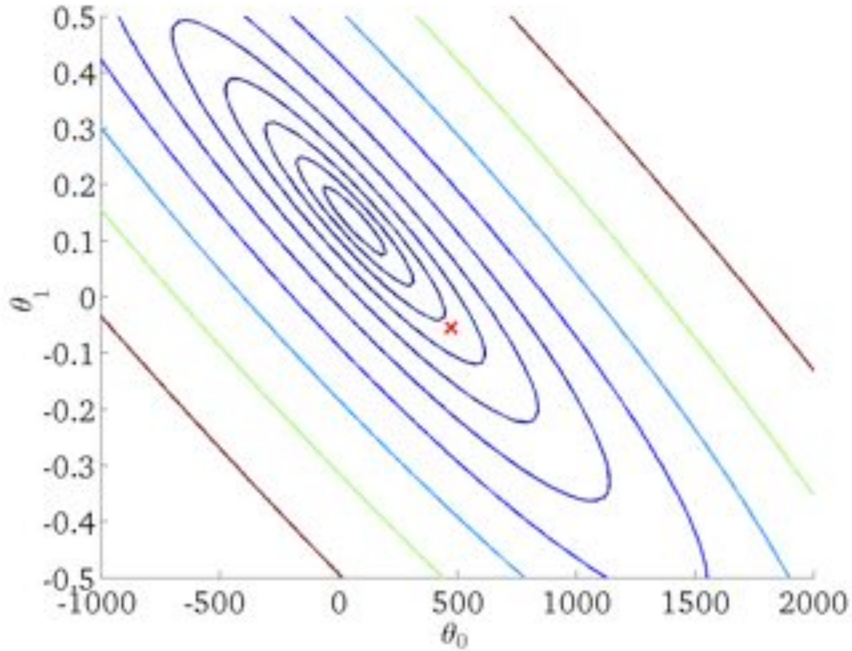
$$h_\theta(x)$$

(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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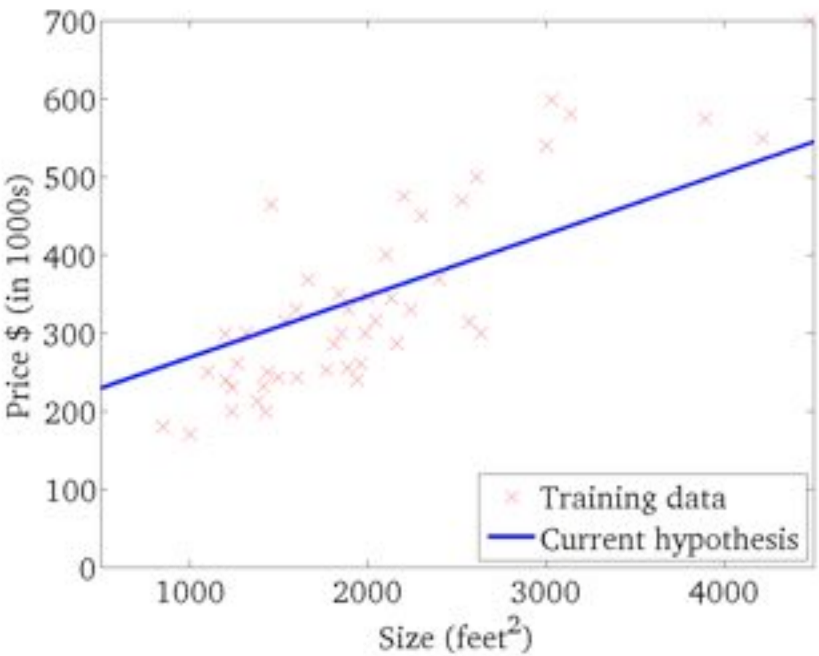
代价函数与模型参数

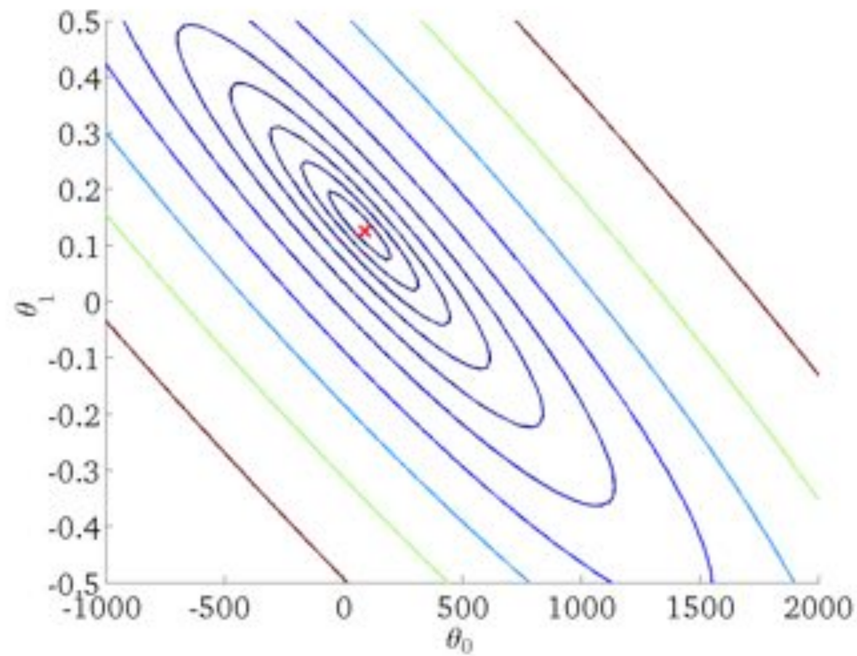
$h_\theta(x)$

(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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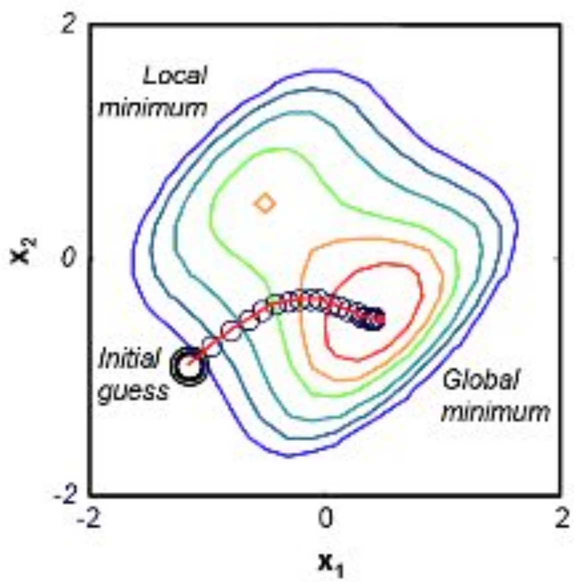
Gradient descent 梯度下降算法

$$J(\theta) = J(\theta_0, \theta_1) = \frac{1}{2m}\sum_{i=1}^{m}(h(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})^2$$



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

$$\theta_0 = \theta_0 - \frac{\alpha}{m}\sum_{i=1}^{m}\left(h(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)}\right)$$

$$\theta_1 = \theta_1 - \frac{\alpha}{m}\sum_{i=1}^{m}\left(\left(h(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)}\right)x_i\right)$$

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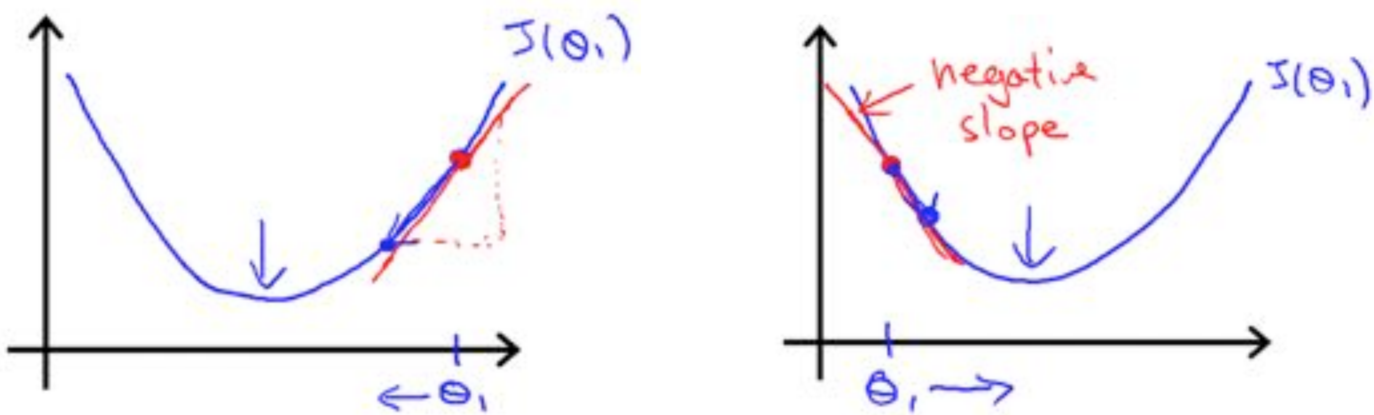
Gradient descent 梯度下降算法

repeat until convergence {

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

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

}



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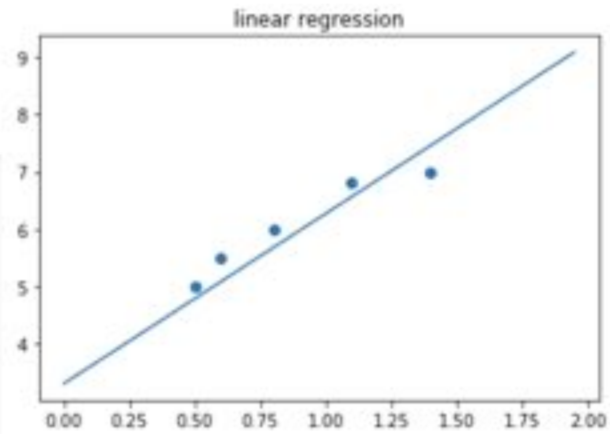
线性回归算法Python实现

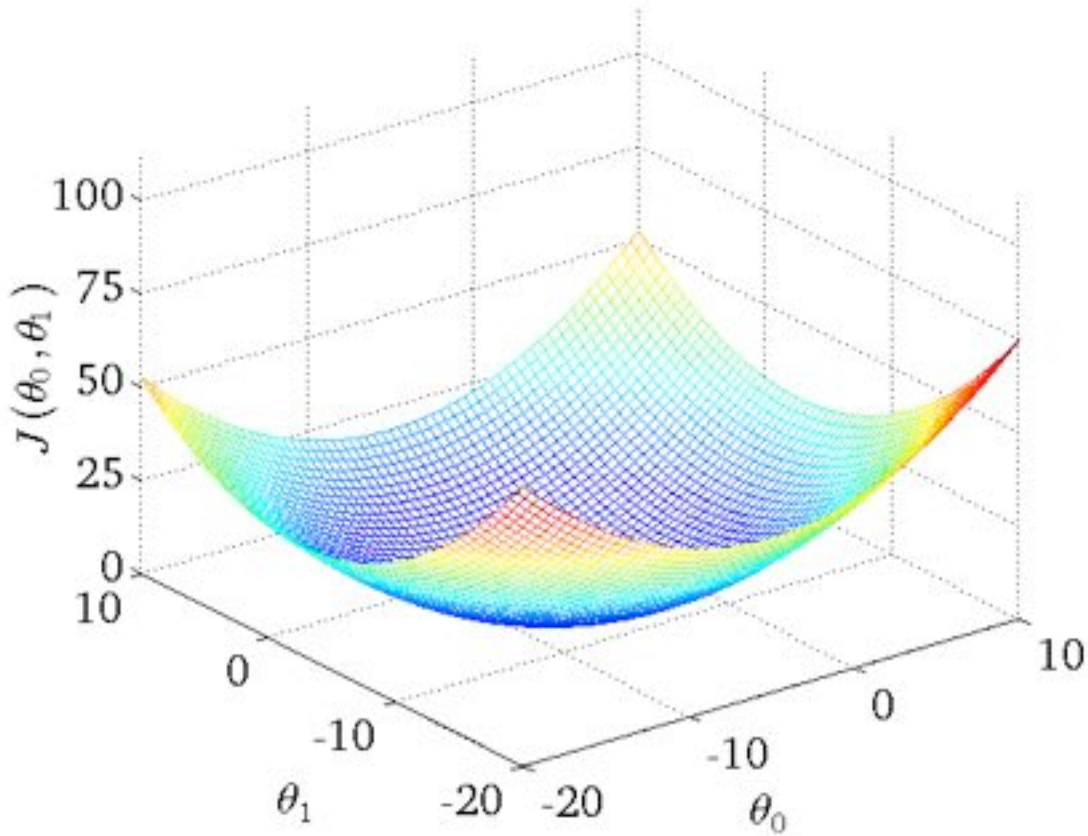
Algorithm for Linear Regression

```
import numpy as np
wheat_and_bread = np.array([[0.5,5],[0.6,5.5],[0.8,6],[1.1,6.8],[1.4,7]])
sample_x=wheat_and_bread[:,0]
sample_y=wheat_and_bread[:,1]
def step_gradient(b_current, m_current, points, learningRate):
    b_gradient = 0
    m_gradient = 0
    N = float(len(points))
    for i in range(0, points.shape[0]):
        x = points[i][0]
        y = points[i][1]
        b_gradient += -(2/N) * (y - ((m_current * x) + b_current))
        m_gradient += -(2/N) * x * (y - ((m_current * x) + b_current))
    new_b = b_current - (learningRate * b_gradient)
    new_m = m_current - (learningRate * m_gradient)
    return [new_b, new_m]
def compute_value(b,m,point):
    return m*point+b
range_x=np.arange(0,2,0.05)
def gradient_descent_runner(points, starting_b, starting_m, learning_rate, num_iterations):
    b = starting_b
    m = starting_m
    plt.ion()
    for i in range(num_iterations):
        b, m = step_gradient(b, m, points, learning_rate)
        plt.cla()
        plt.scatter(sample_x,sample_y)
        plt.plot(range_x,compute_value(b,m,range_x))
        plt.pause(0.01)
    plt.ioff()
    plt.title('linear regression')
    plt.show()

    #return [b, m]
gradient_descent_runner(wheat_and_bread, 1, 1, 0.01, 100)
```



Convex Optimization 凸优化问题



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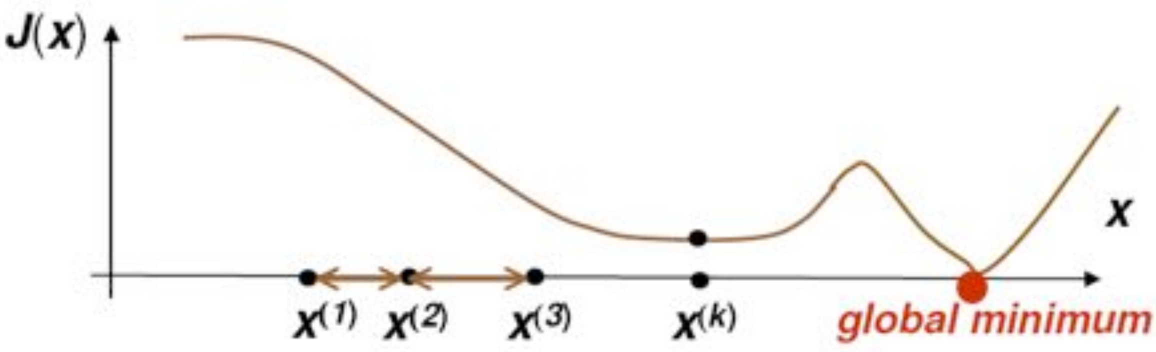
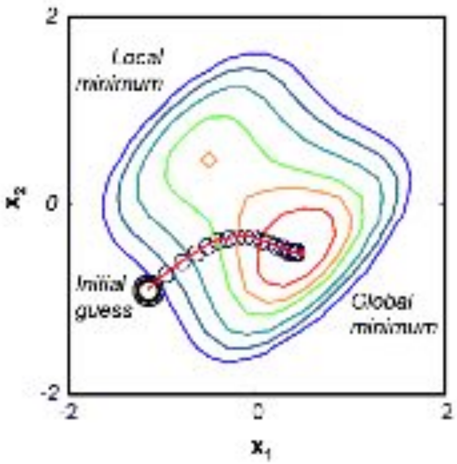
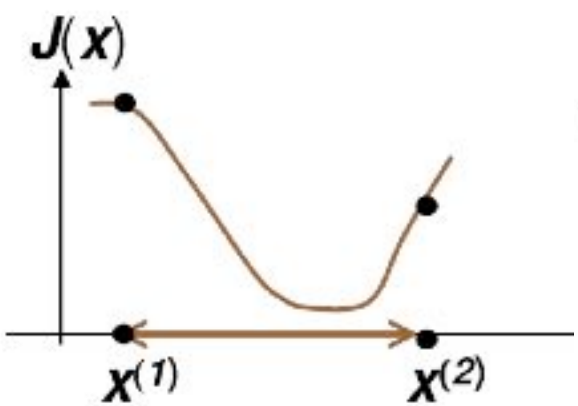
梯度下降法的两个问题

1. 如果不是凸优化问题，不能保证全局最优，会落入局部极值点

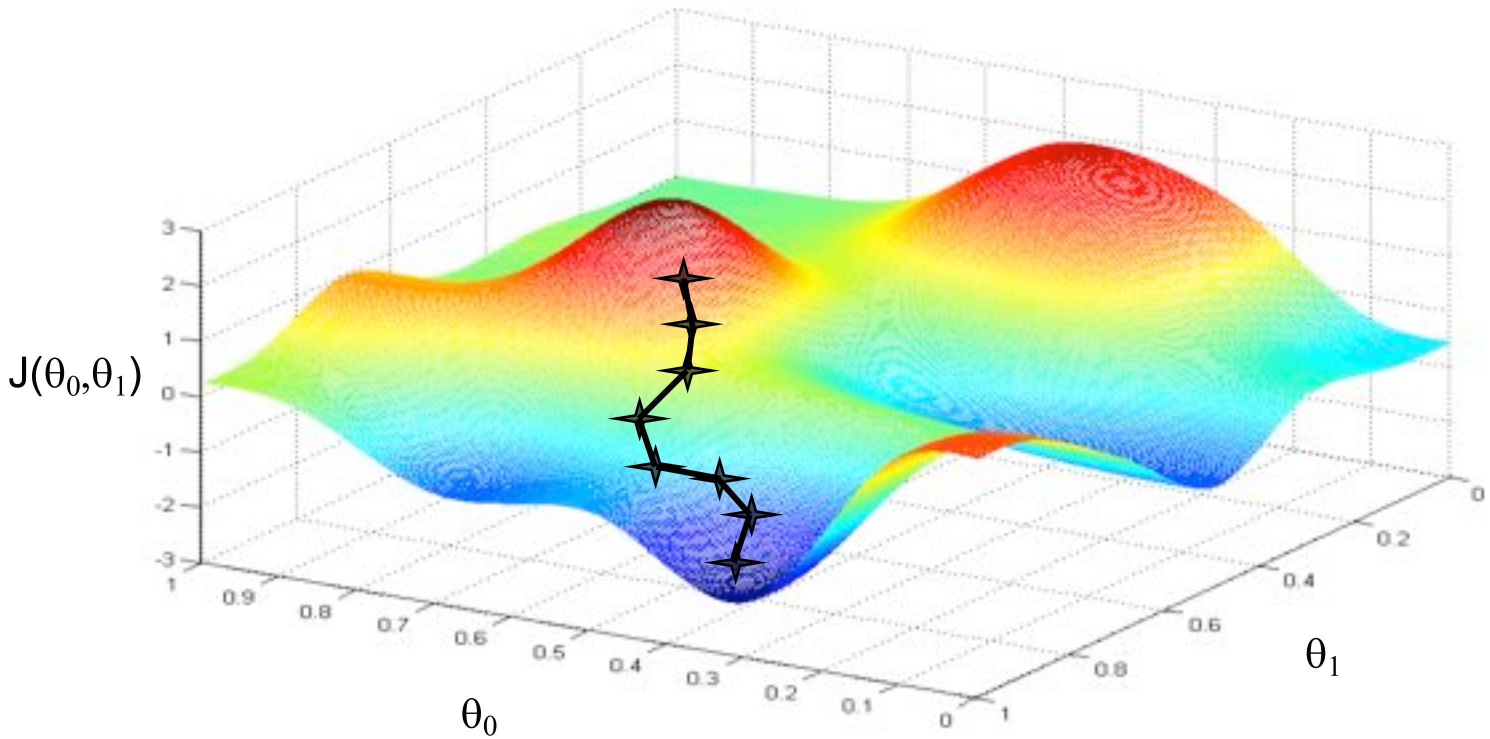




2. 学习率η不能太大，太小也不好



寻优结果对初始值的敏感性



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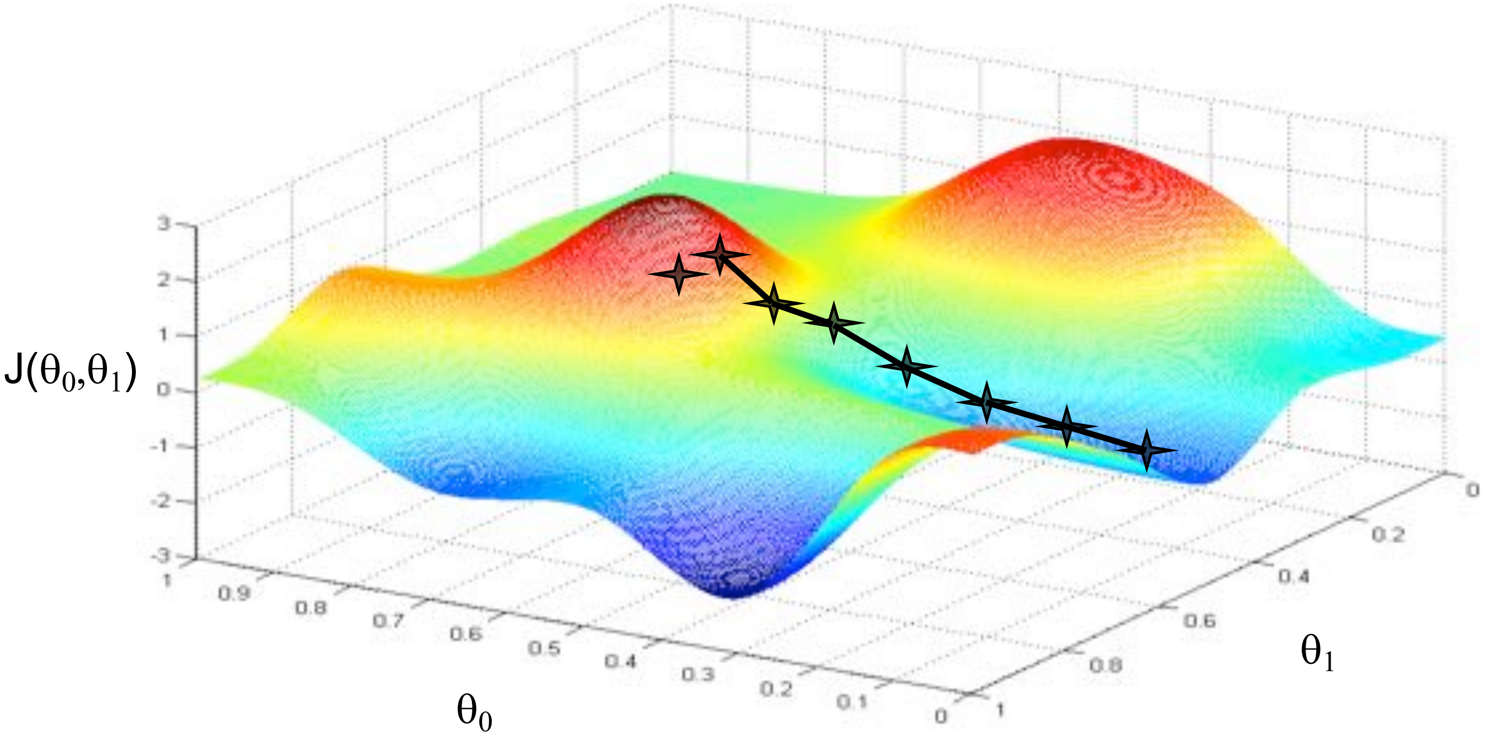
寻优结果对初始值的敏感性



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寻优算法 Advanced Optimization algorithm

Given θ, we have code that can compute

- $J(\theta)$
- $\frac{\partial}{\partial\theta_j}J(\theta)$ (for $j = 0, 1, \ldots, n$)

Optimization algorithms:

- Gradient descent
  梯度下降
- Conjugate gradient
  共轭梯度
- BFGS/L-BFGS
  拟牛顿法

Advantages:

- No need to manually pick α
- Often faster than gradient descent.

Disadvantages:

- More complex

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多变量问题 Multiple features (variables)

Size (feet^2)	Number of bedrooms	Number of floors	Age of home (years)	Price ($1000)
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

Notation:

n = number of features

$x^{(i)}$ = input (features) of i^{th} training example.

$x_j^{(i)}$ = value of feature j in i^{th} training example.

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多变量线性回归

$$h_{\theta}(x)=\theta_0+\theta_1x_1+\theta_2x_2+\cdots+\theta_nx_n$$

$$h_{\theta}(x)=\begin{bmatrix}\theta_0 & \theta_1 & \cdots & \theta_n\end{bmatrix}\begin{bmatrix}x_0\\x_1\\\vdots\\x_n\end{bmatrix}=\theta^{\mathrm{T}}x$$

$$h_{\theta}(X)=X\theta$$

样本维数n

$$X=\begin{bmatrix}x_0^{(1)} & x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)}\\x_0^{(2)} & x_1^{(2)} & x_2^{(2)} & \cdots & x_n^{(2)}\\\vdots & \vdots & \vdots & \ddots & \vdots\\x_0^{(m)} & x_1^{(m)} & x_2^{(m)} & \cdots & x_n^{(m)}\end{bmatrix},\theta=\begin{bmatrix}\theta_0\\\theta_1\\\theta_2\\\vdots\\\theta_n\end{bmatrix}$$

样本个数m

在scikit-learn中，训练样本就是用m×n维的矩阵来表达的

多维情况的代价函数和梯度下降算法

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

$$\Downarrow$$

$$J(\boldsymbol{\theta})=\frac{1}{2m}(\boldsymbol{X\theta}-\vec{\boldsymbol{y}})^{\mathrm{T}}(\boldsymbol{X\theta}-\vec{\boldsymbol{y}})$$

$$\boldsymbol{\theta}_j=\boldsymbol{\theta}_j-\alpha\frac{\partial}{\partial\boldsymbol{\theta}_j}J(\boldsymbol{\theta})$$

$$\boldsymbol{\theta}_j=\boldsymbol{\theta}_j-\frac{\alpha}{m}\sum_{i=1}^{m}\left(\left(h(\boldsymbol{x}^{(i)})-\boldsymbol{y}^{(i)}\right)\boldsymbol{x}_j^{(i)}\right)$$

算法伪代码

Hypothesis: $h_\theta(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$

Parameters: $\theta_0, \theta_1, \ldots, \theta_n$

Cost function:

$$J(\theta_0, \theta_1, \ldots, \theta_n) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Gradient descent:

Repeat $\{$

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \ldots, \theta_n)$$

$\}$ (simultaneously update for every $j = 0, \ldots, n$)

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梯度下降：从单变量到多变量

Previously (n=1):

Repeat {

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

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

(simultaneously update θ_0, θ_1)

}

New algorithm $(n \geq 1)$:

Repeat {

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

(simultaneously update for θ_j
$j = 0, \ldots, n$)

}

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

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

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

$\ldots$

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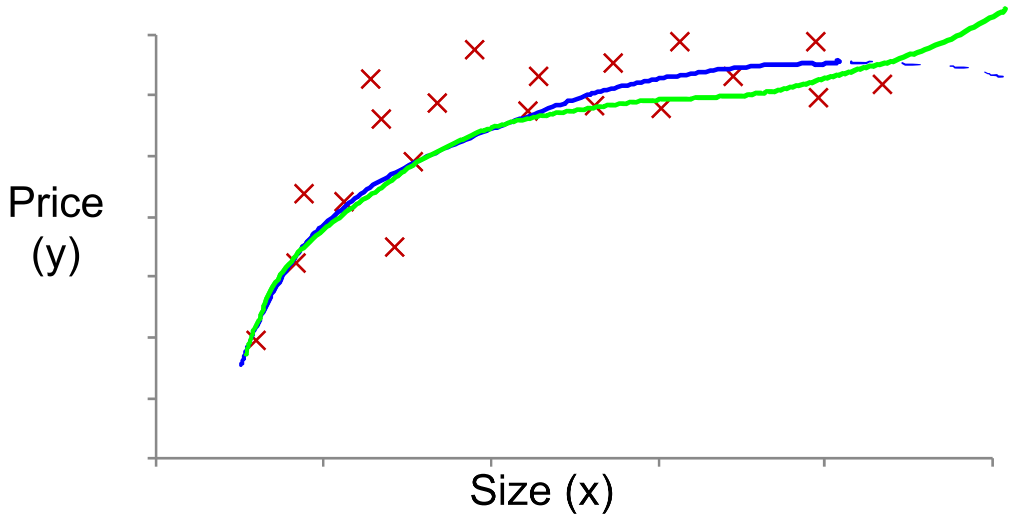
多项式回归 Polynomial regression



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

$$\boxed{\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3}$$

$$\begin{aligned} h_\theta(x) &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 \\ &= \theta_0 + \theta_1 (size) + \theta_2 (size)^2 + \theta_3 (size)^3 \end{aligned}$$

$$\begin{aligned} x_1 &= (size) \\ x_2 &= (size)^2 \\ x_3 &= (size)^3 \end{aligned}$$

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示例：房价预测

·CRIM：城镇人均犯罪率。

·ZN：城镇超过25，000平方英尺的住宅区域的占地比例。

·INDUS：城镇非零售用地占地比例。

·CHAS：是否靠近河边，1为靠近，0为远离。

·NOX：一氧化氮浓度。

·RM：每套房产的平均房间个数。

·AGE：在1940年之前就盖好，且业主自住的房子的比例。

·DIS：与波士顿市中心的距离。

·RAD：周边高速公道的便利性指数。

·TAX：每10，000美元的财产税率。

·PTRATIO：小学老师的比例。

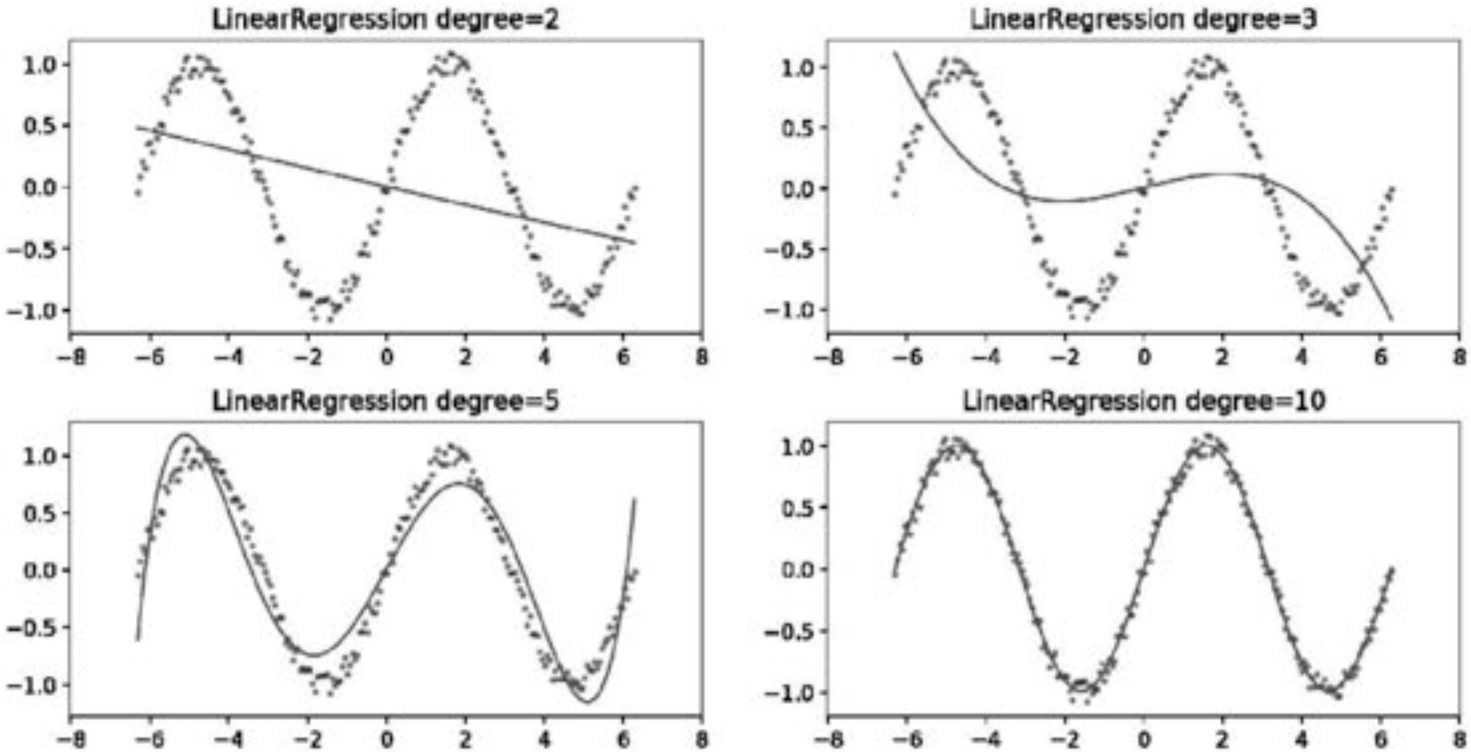
·B：城镇黑人的比例。

·LSTAT：地位较低的人口比例。

（506，13）

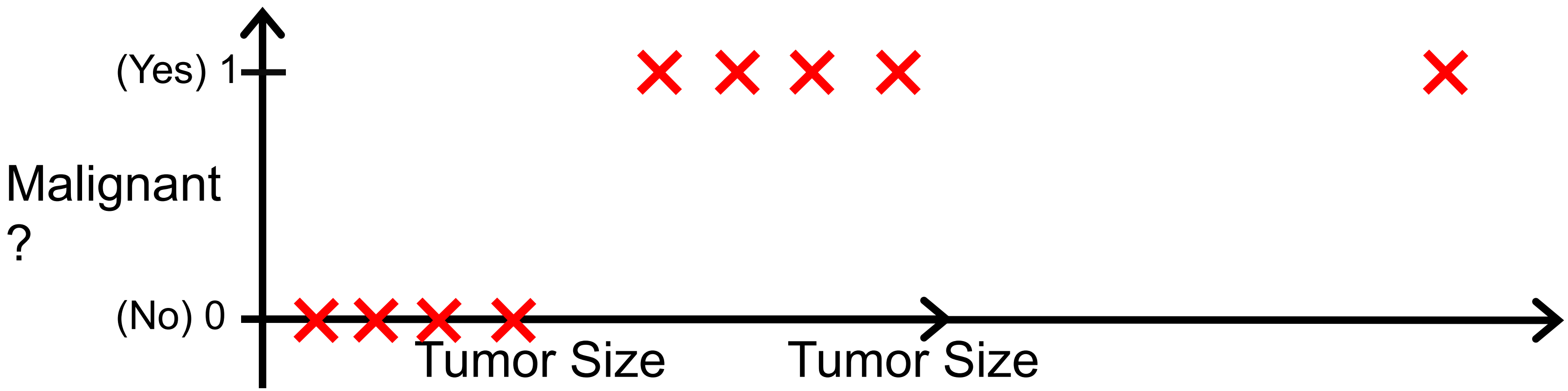
```
from sklearn.datasets import load_boston
boston = load_boston()
X = boston.data
y = boston.target
X.shape
```

示例：多项式拟合正弦函数



Logistic Regression 分类器

从回归到分类



Threshold classifier output $h_\theta(x)$ at 0.5:

If $h_\theta(x) \geq 0.5$, predict "y = 1"

If $h_\theta(x) < 0.5$, predict "y = 0"

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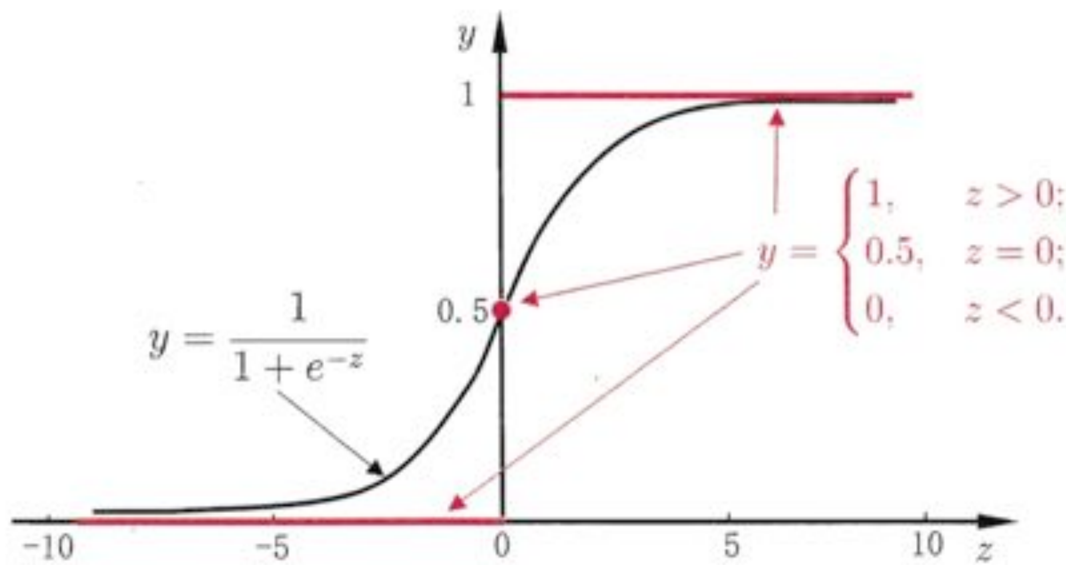
对数几率回归模型 Logistic Regression Model

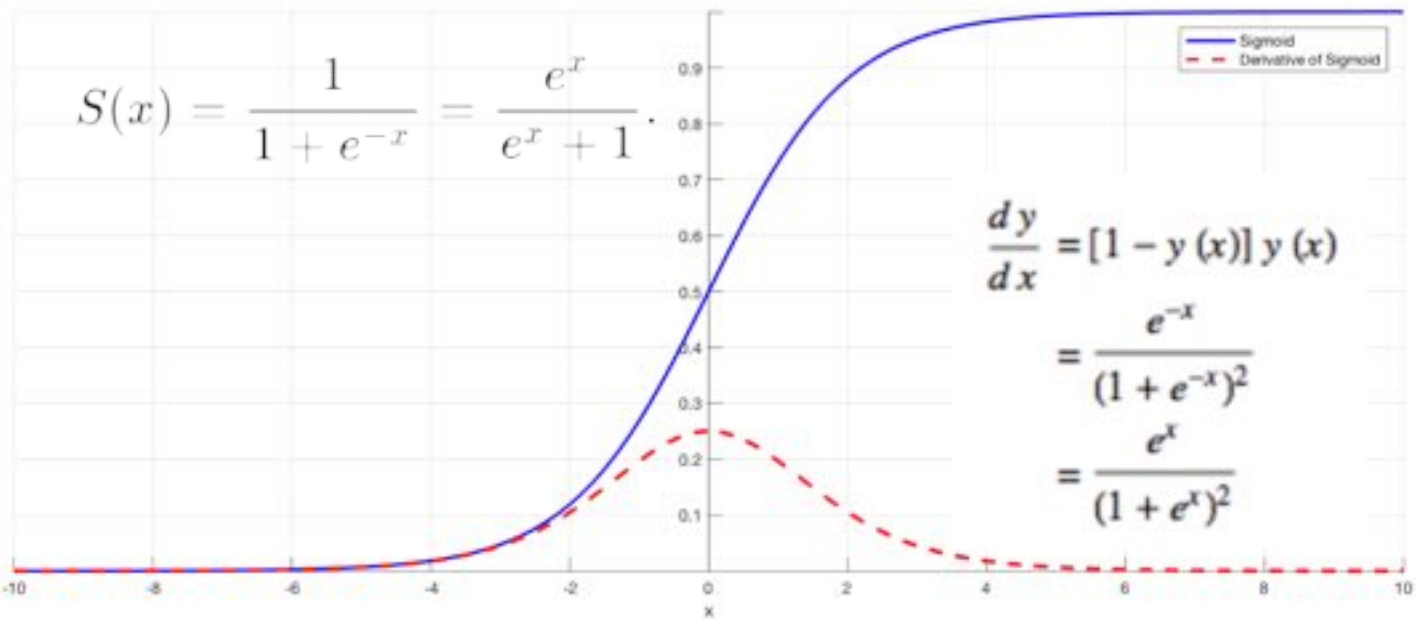
$$h_\theta(x) = \theta^T x \quad \Rightarrow \quad h_{\boldsymbol{\theta}}(x) = g(z) = g(\boldsymbol{\theta}^{\mathrm{T}} x) = \frac{1}{1+\mathrm{e}^{-\boldsymbol{\theta}^{\mathrm{T}} x}}$$

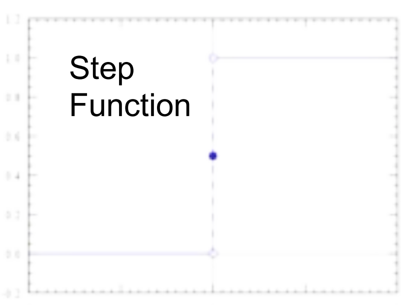
Sigmoid function
Logistic function

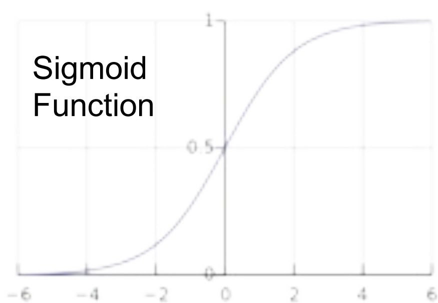


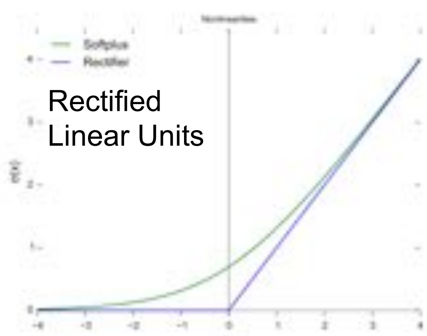
Modified from 周志华

Sigmoid function and beyond









https://github.com/Kulbear/deep-learning-nano-foundation/wiki/ReLU-and-Softmax-Activation-Functions

模型输出的含义
Interpretation of Hypothesis Output

$h_\theta(x)$ = estimated probability that y = 1 on input x

Example: If $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$

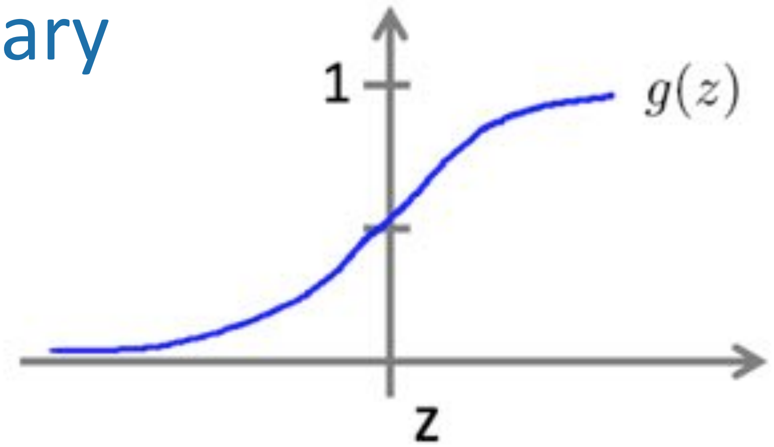
$h_\theta(x) = 0.7$ 70% 概率是恶性肿瘤

Probability that y = 1, given x, parameterized by θ

$$P(y=0|x;\theta) + P(y=1|x;\theta) = 1$$
$$P(y=0|x;\theta) = 1 - P(y=1|x;\theta)$$

Modified from Andrew Ng ML

决策边界 Decision boundary



Logistic regression

$$h_\theta(x) = g(\theta^T x)$$

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

Suppose predict "$y = 1$" if $h_\theta(x) \geq 0.5$

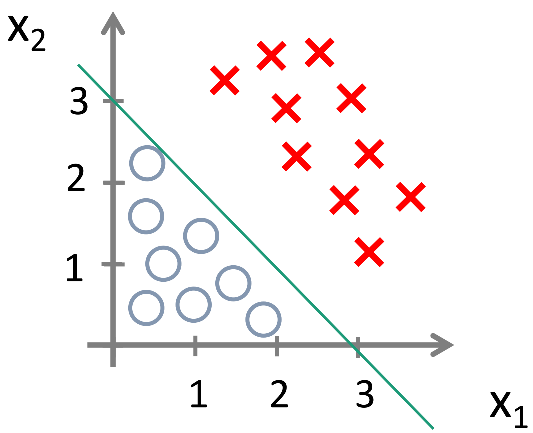
$$\theta^T X \geq 0$$

predict "$y = 0$" if $h_\theta(x) < 0.5$

$$\theta^T X < 0$$

Modified from Andrew Ng ML

决策边界 Decision boundary

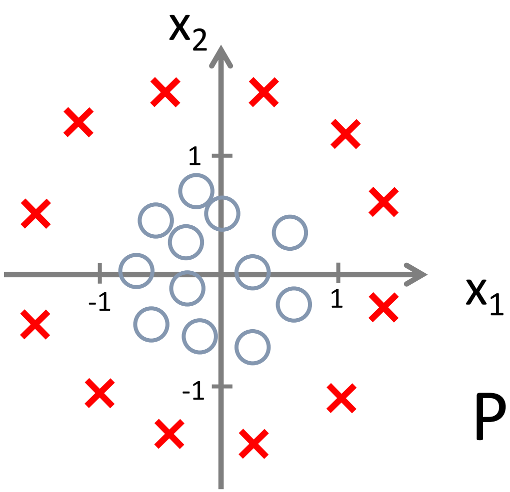


$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

Predict “$y = 1$“ if $-3 + x_1 + x_2 \geq 0$

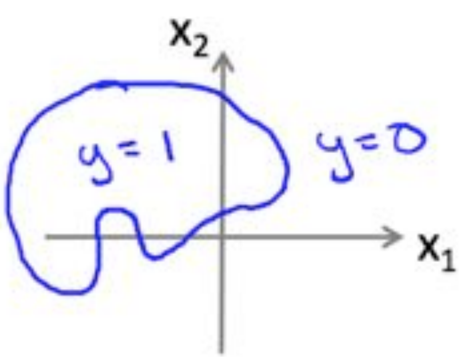
Modified from Andrew Ng ML

非线性决策边界
Non-linear decision boundaries



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

Predict "$y = 1$" if $-1 + x_1^2 + x_2^2 \geq 0$



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

Modified from Andrew Ng ML

优化问题 Optimization

Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$

m examples $\quad x \in \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_n \end{bmatrix} \quad x_0 = 1, y \in \{0, 1\}$

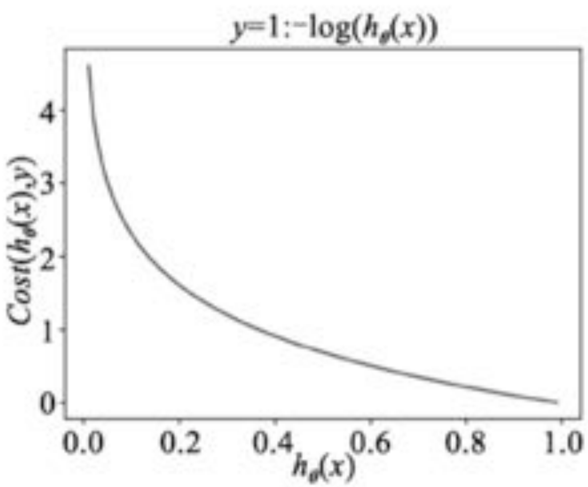
$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

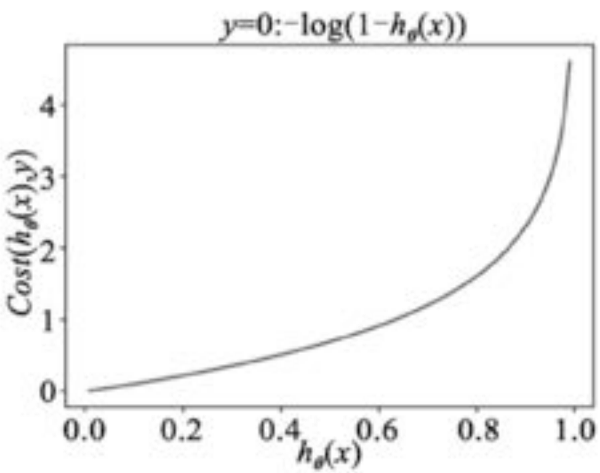
How to choose parameters θ ?

Modified from Andrew Ng ML

代价函数 Cost Function 😆

$$\mathrm{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$





当y=1时，随着$\boldsymbol{h_\theta}$ (x) 的值（预测为1的概率）越来越**大**，预测值越来越接近真实值，其成本越来越小。

当y=0时，随着$\boldsymbol{h_\theta}$ (x) 的值（预测为0的概率）越来越**大**，预测值越来越偏离真实值，其成本越来越大。

Modified from Andrew Ng ML

代价函数 Cost Function

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

$$\mathrm{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

由于是离散值，当y=1时，1-y=0，上式的后半部分为0；当y=0时，上式的前半部分为0。因此下式与分开表达的成本计算公式等价。

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

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

Modified from Andrew Ng ML

寻优算法：梯度下降法 Gradient Descent

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

Want $\min_\theta J(\theta)$:

Repeat $\{$

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

(simultaneously update all θ_j)

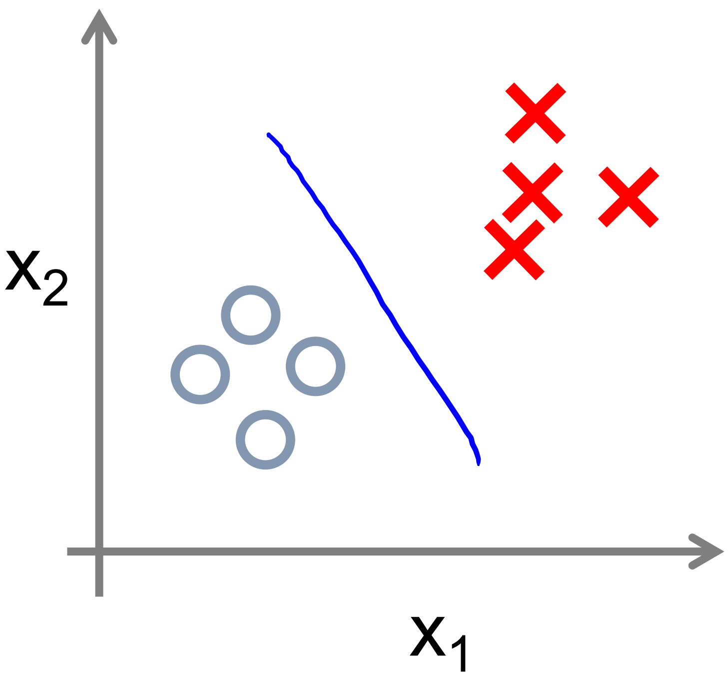
$\}$

Algorithm looks identical to linear regression!

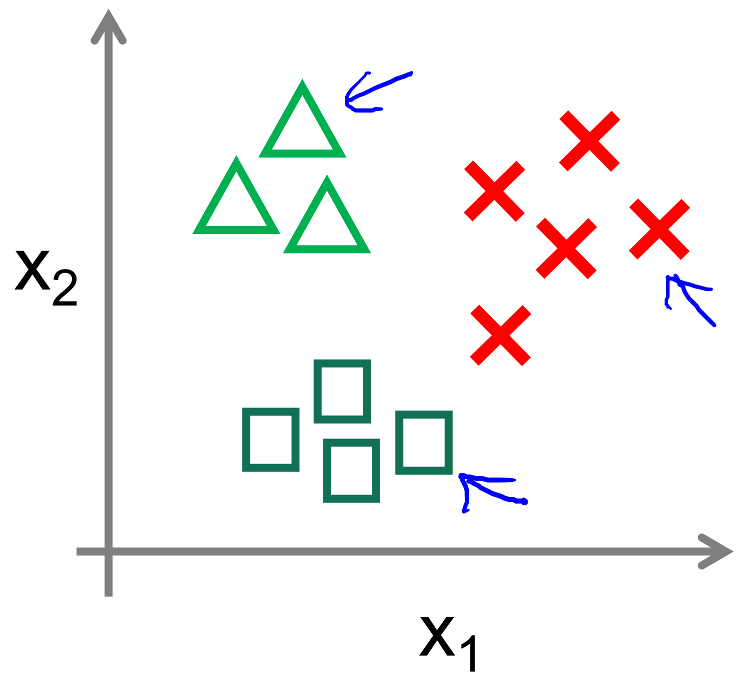
Modified from Andrew Ng ML

多分类问题 Multi-class classification

Binary classification:

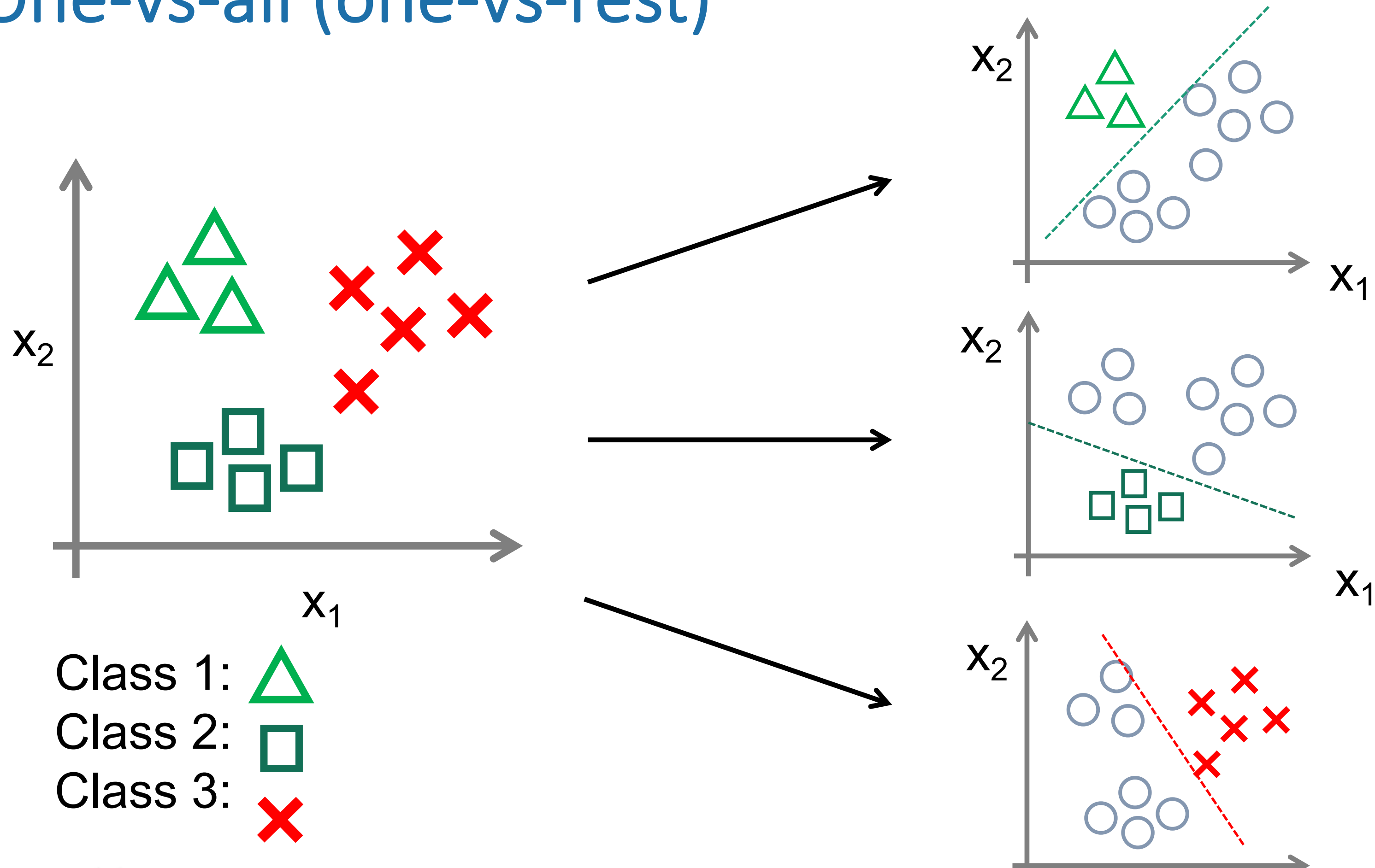


Multi-class classification:



Modified from Andrew Ng ML

One-vs-all (one-vs-rest)



$$h_\theta^{(i)}(x) = P(y = i | x; \theta) \qquad (i = 1, 2, 3)$$

$$\boxed{\max_i h_\theta^{(i)}(x)}$$

Modified from Andrew Ng ML

示例：乳腺癌检测

·radius：半径，即病灶中心点离边界的平均距离。

·texture：纹理，灰度值的标准偏差。

·perimeter：周长，即病灶的大小。

·area：面积，也是反映病灶大小的一个指标。

·smoothness：平滑度，即半径的变化幅度。

·compactness：密实度，周长的平方除以面积的商，再减1，即 $\frac{perimeter^2}{area} - 1$。

·concavity：凹度，凹陷部分轮廓的严重程度。

·concave points：凹点，凹陷轮廓的数量。

·symmetry：对称性。

·fractal dimension：分形维度。

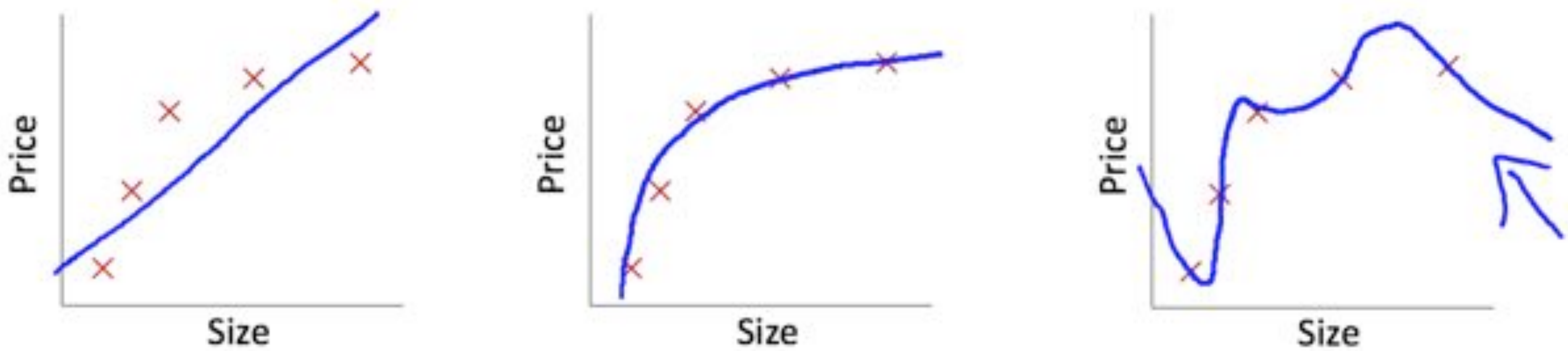
```
# 载入数据
from sklearn.datasets import load_breast_cancer

cancer = load_breast_cancer()
X = cancer.data
y = cancer.target
print('data shape: {0}; no. positive: {1}; no. negative: {2}'.format(
    X.shape, y[y==1].shape[0], y[y==0].shape[0]))
print(cancer.data[0])
```

上述代码输出结果如下：

```
data shape: (569, 30); no. positive: 357; no. negative: 212
[  1.79900000e+01   1.03800000e+01   1.22800000e+02   1.00100000e+03
   1.18400000e-01   2.77600000e-01   3.00100000e-01   1.47100000e-01
   2.41900000e-01   7.87100000e-02   1.09500000e+00   9.05300000e-01
   8.58900000e+00   1.53400000e+02   6.39900000e-03   4.90400000e-02
   5.37300000e-02   1.58700000e-02   3.00300000e-02   6.19300000e-03
   2.53800000e+01   1.73300000e+01   1.84600000e+02   2.01900000e+03
   1.62200000e-01   6.65600000e-01   7.11900000e-01   2.65400000e-01
   4.60100000e-01   1.18900000e-01]
```

Overfitting and Regularization
过拟合与正则化

Example: Linear regression (housing prices)

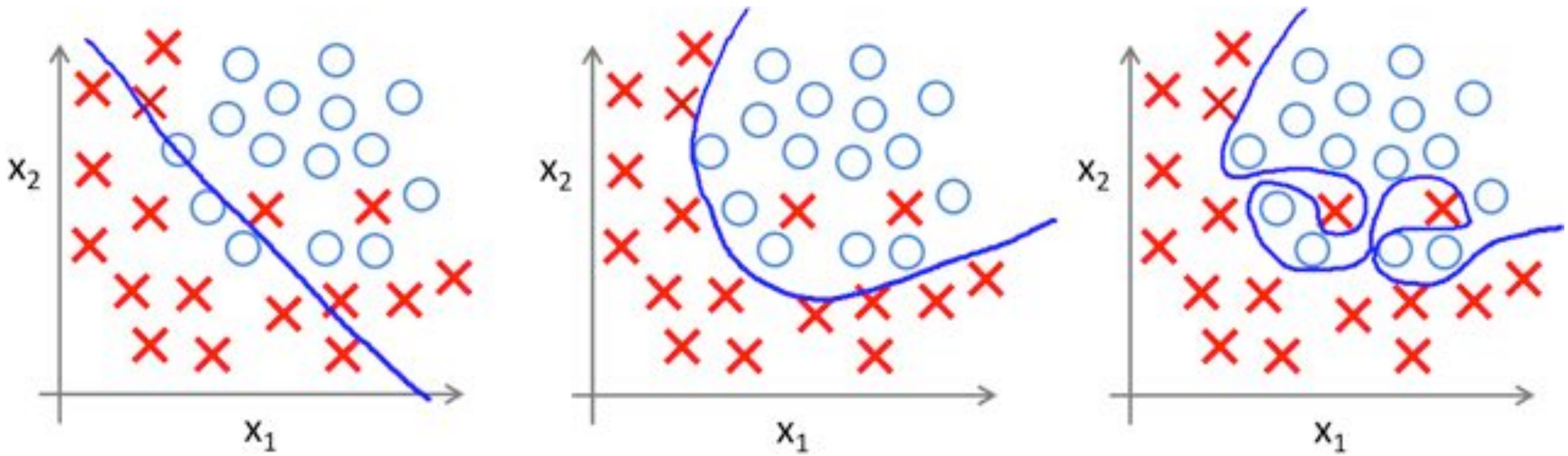


$\theta_0 + \theta_1 x$ $\qquad$ $\theta_0 + \theta_1 x + \theta_2 x^2$ $\qquad$ $\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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).

Modified from Andrew Ng ML

Example: Logistic regression



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

(g = sigmoid function)

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

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

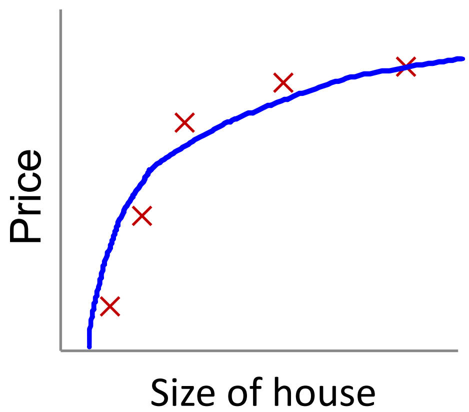
Modified from Andrew Ng ML

如何解决过拟合问题？

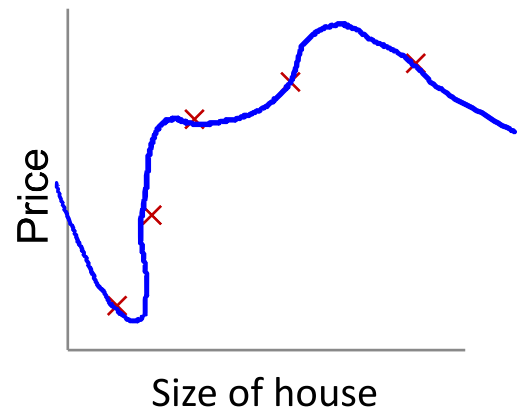
1. Reduce number of features
   - Manually select which features to keep.
   - Model selection algorithm (later in course).
2. Regularization 正则化
   - Keep all the features, but reduce magnitude/values of parameters θ_j.
   - Works well when we have a lot of features, each of which contributes a bit to predicting y.

Modified from Andrew Ng ML

正则化 Regularization



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



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

Suppose we penalize and make θ_3, θ_4 really small.

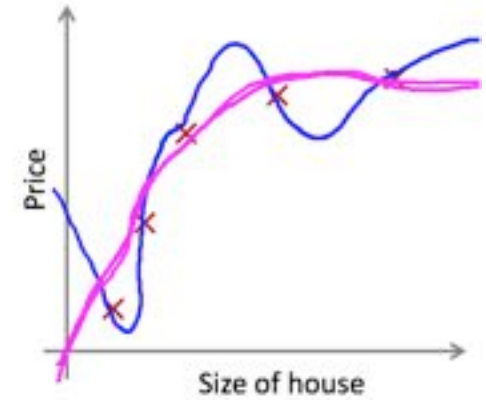
$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Modified from Andrew Ng ML

正则化 Regularization

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

– "Simpler" hypothesis
– Less prone to overfitting



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

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

正则项

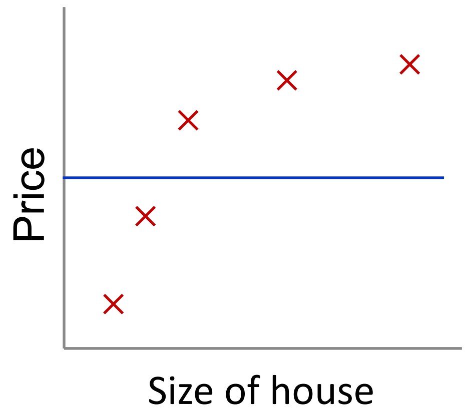
Modified from Andrew Ng ML

过度正则化导致欠拟合

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



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

Modified from Andrew Ng ML

线性回归的正则化梯度下降算法

Linear regression - Gradient descent with regularization

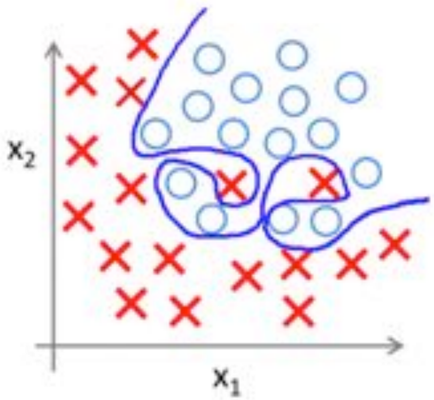
代价函数 $J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$

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

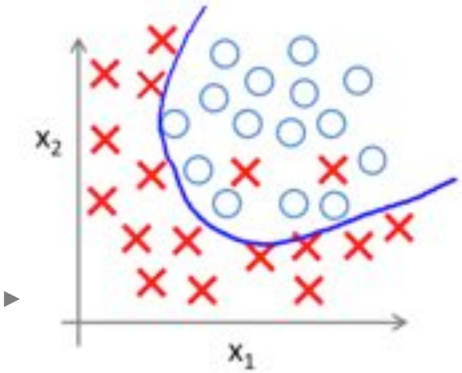
$$\theta_j = \theta_j - \alpha \boxed{\frac{1}{m}\sum_{i=1}^{m}\left[\left(\left(h(x^{(i)}) - y^{(i)}\right)x_j^{(i)}\right) + \frac{\lambda}{m}\theta_j\right]}$$

$$\theta_j = \theta_j\underline{(1 - \alpha\frac{\lambda}{m})} - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(\left(h(x^{(i)}) - y^{(i)}\right)x_j^{(i)}\right)$$

对数几率回归的正则化
Logistic regression with regularization



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



代价函数

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

正则化

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

Modified from Andrew Ng ML

对数几率回归的正则化梯度下降算法

代价函数

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

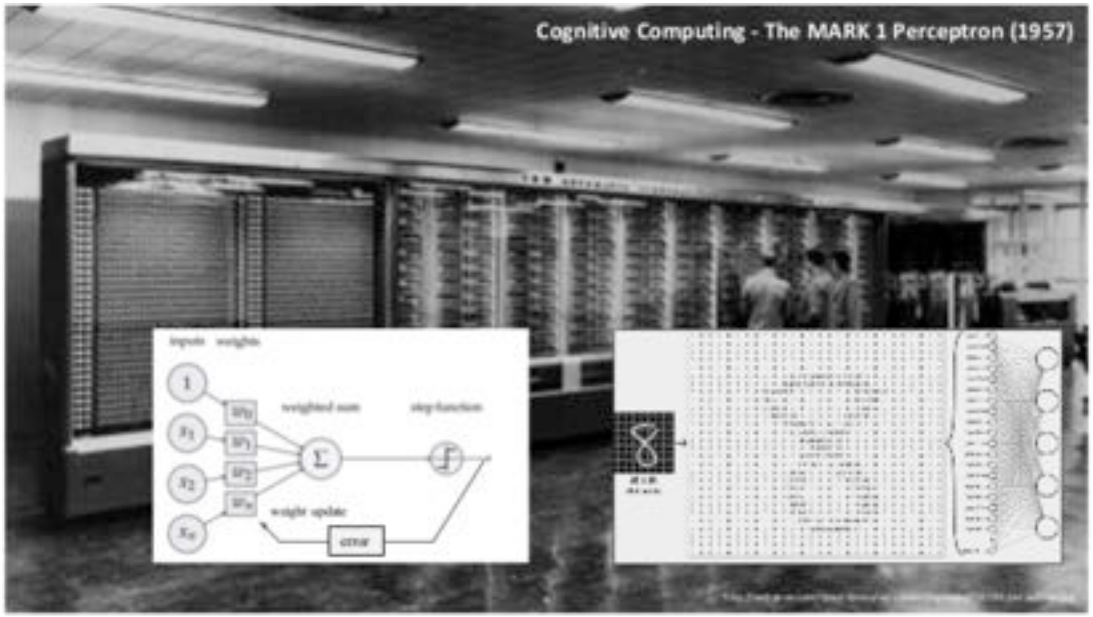
梯度 $\frac{\partial J(\theta)}{\partial \theta_j}$

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

$$\theta_j=\theta_j\underline{(1-\alpha\frac{\lambda}{m})}-\alpha\frac{1}{m}\sum_{i=1}^{m}\left(\left(h(x^{(i)})-y^{(i)}\right)x_j^{(i)}\right)$$

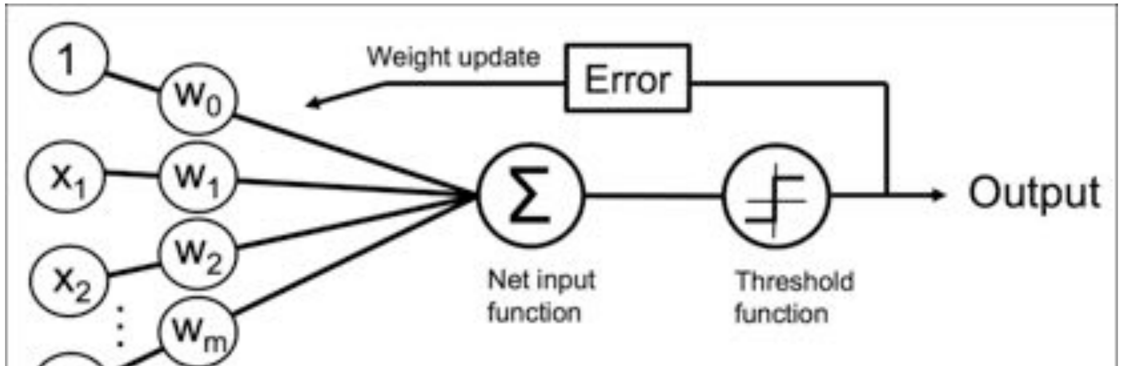
感知器Perceptron

感知机 Perceptron



Frank Rosenblatt, 1957

感知机 Perceptron



$$y = f(\sum_{i=1}^{m} \boldsymbol{w}_i \cdot \boldsymbol{x}_i) = f(\boldsymbol{W}^T \boldsymbol{X})$$

Frank Rosenblatt, 1957

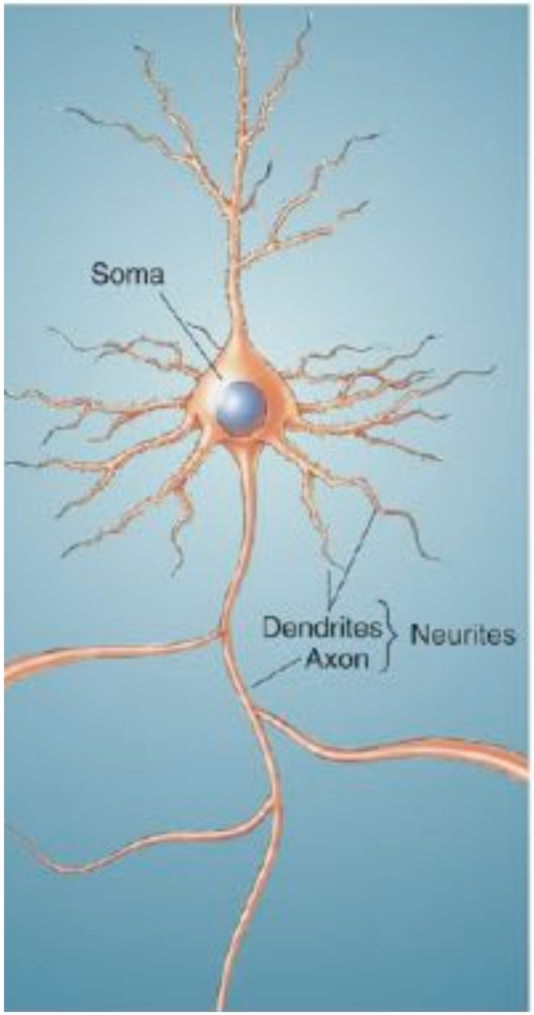
- Rosenblatt (1958) introduced the perceptron, the simplest form of neural network
- The perceptron is a single neuron with adjustable synaptic weights and a threshold activation function
- Rosenblatt also developed an error-correction rule to adapt these weights (the perceptron learning rule)
- He also proved that if the (two) classes were linearly separable, the algorithm would converge to a solution (the perceptron convergence theorem)

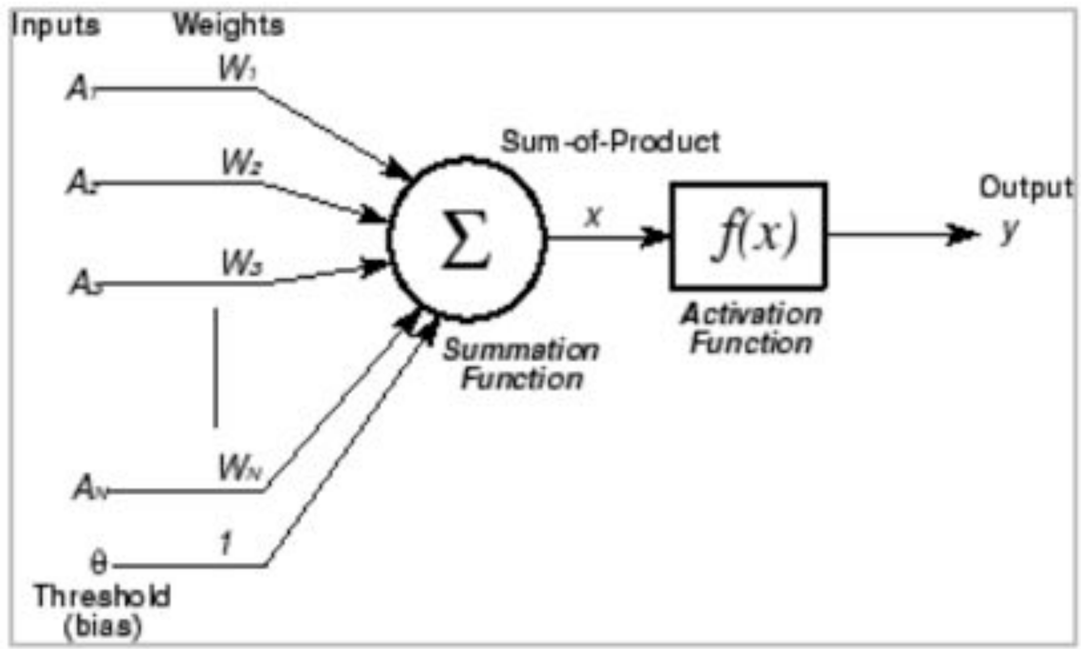
感知机 Perceptron

The perceptron, invented in the late 1950s, was considered a **paradigm shift**. For the first time, a machine could be taught to perform certain tasks using examples. This surprising invention was almost immediately followed by an equally surprising theoretical result, the perceptron convergence theorem, which states that a machine executing the perceptron algorithm can effectively produce a decision rule that is compatible with its training examples. A youthful wave of optimism took over the research community. Although it only dealt with a very specific category of tasks, namely pattern recognition tasks, the perceptron was widely publicized as the forerunner of more general learning machines.

Léon Bottou, 1988

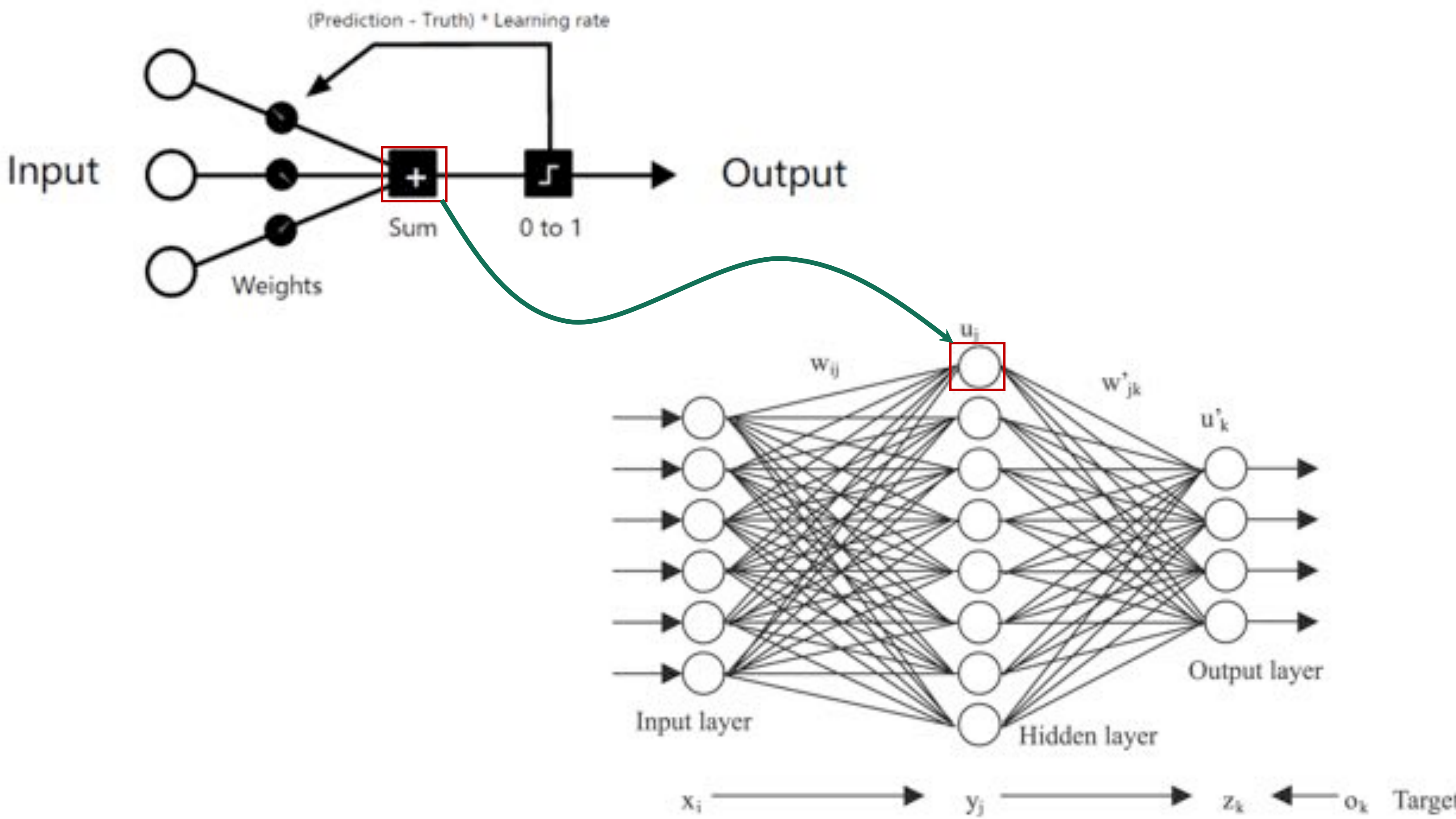
神经细胞的MP模型





McCulloch–Pitts 1943

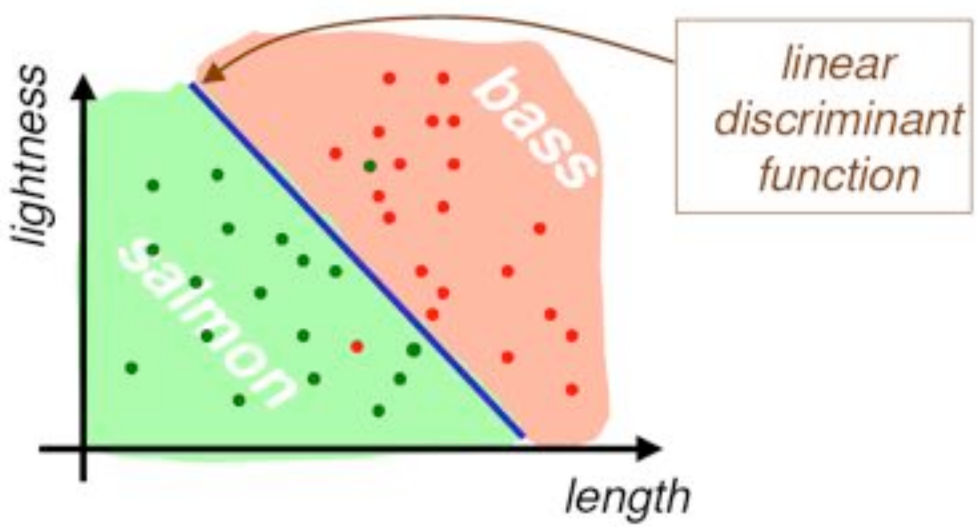
从感知机到神经网络


(Prediction - Truth) * Learning rate
Input
Output
Sum
0 to 1
Weights
u_j
w_{ij}
w'_{jk}
u'_k
Input layer
Hidden layer
Output layer
x_i
y_j
z_k
o_k
Target

线性分类器 Linear Classifier

- No probability distribution (no shape or parameters are known)
- Only labeled data available

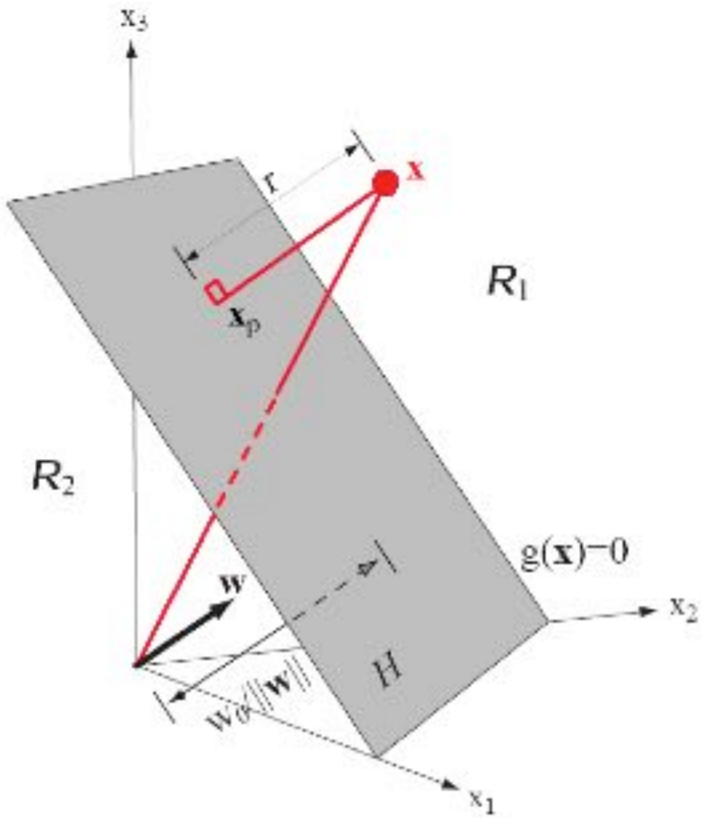
- The shape of discriminant functions is assumed to be linear



$$g(x) = w^T x + w_0 \Leftrightarrow \begin{cases} g(x) > 0 & x \in \omega_1 \\ g(x) < 0 & x \in \omega_2 \end{cases}$$

- **Need to estimate parameters of the linear function**

分类超平面 Hyperplane



$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0$$

$$\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

$$g(X) = W^{\mathrm{T}}(X_p + r\frac{W}{\|W\|}) + w_0 = W^{\mathrm{T}}X_p + w_0 + r\frac{W^{\mathrm{T}}W}{\|W\|} = r\|W\|$$

$$r = \frac{g(\mathbf{x})}{\|\mathbf{w}\|}$$

- The orientation of the surface is determined by the vector **w**
- The location of the surface is determined by the bias w_0
- **The discriminant function *g*(x) is proportional to the signed distance from x to the hyperplane**

线性判别函数的增广形式

$$g(x) = w^T x + w_0 \Leftrightarrow \begin{cases} g(x) > 0 & x \in \omega_1 \\ g(x) < 0 & x \in \omega_2 \end{cases}$$

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i = \sum_{i=0}^{d} w_i x_i$$

$$\mathbf{a} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix} = \begin{bmatrix} w_0 \\ \\ \mathbf{w} \\ \\ \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix} = \begin{bmatrix} 1 \\ \\ \mathbf{x} \\ \\ \end{bmatrix}$$

Augmented feature vector

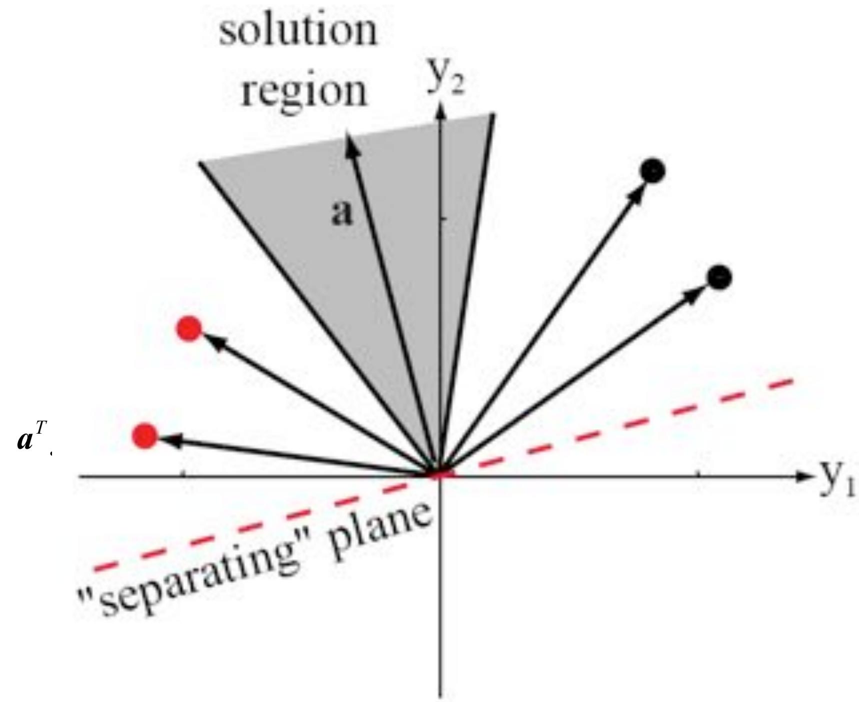
$$g(x) = a^T y \begin{cases} > 0 & x \in \omega_1 \\ < 0 & x \in \omega_2 \end{cases}$$

样本规范化 Normalization

$$g(x) = a^T y \begin{cases} > 0 & x \in \omega_1 \\ < 0 & x \in \omega_2 \end{cases}$$

$$y \leftarrow [-y] \quad \forall y \in \omega_2$$

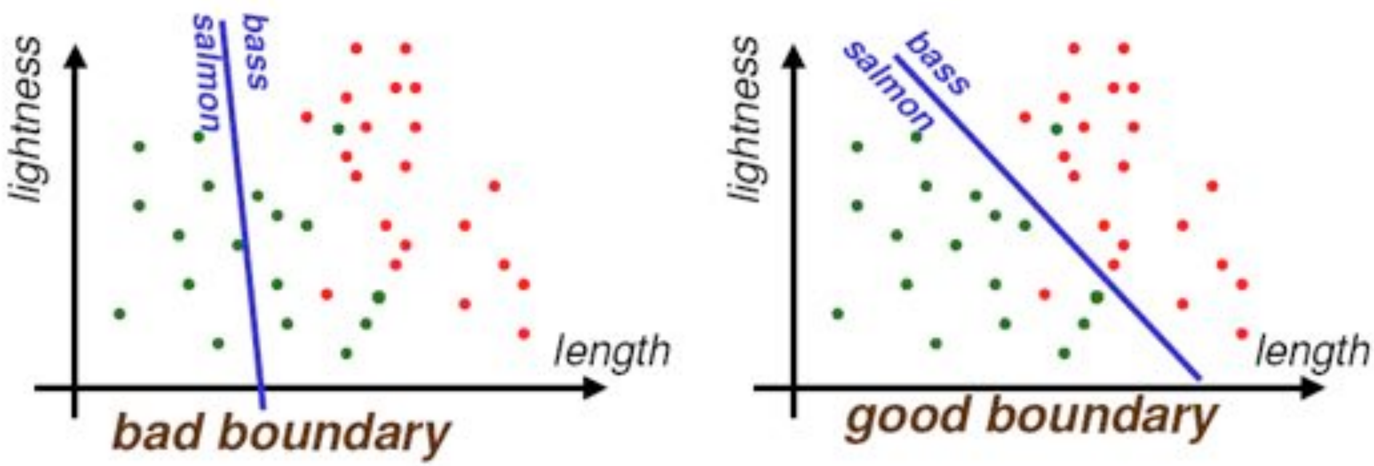
$$a^T y > 0 \quad \forall y$$



- 向量*a* 的取值范围如何确定？
- 怎样的*a*是最优的？

准则函数 Criterion Function

- **Which decision boundary is better（怎样的a是最优的）？**
- **The task is to find the best parameter of the line to separate the two classes with least error.**

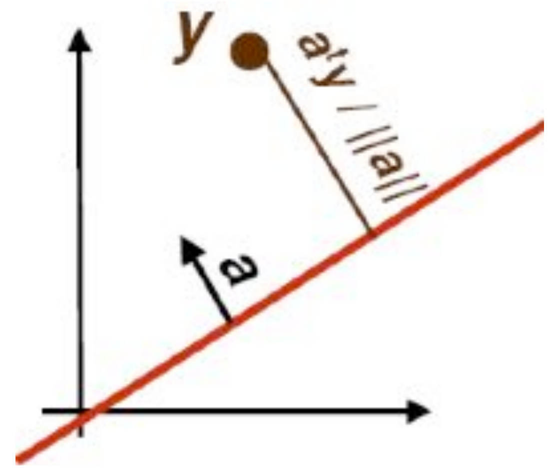


- **Need criterion function J(a) which is minimized when a is a solution vector**

感知器准则 Perceptron Rule

- 更好的选择: ***Perceptron*** criterion function

$$J_p(a) = \sum_{y \in Y_M} (-a^t y)$$



其中Y_M是错分样本集

$$Y_M(a) = \{ sample \ \ y_i \ \ s.t. \ \ a^t y_i < 0 \}$$

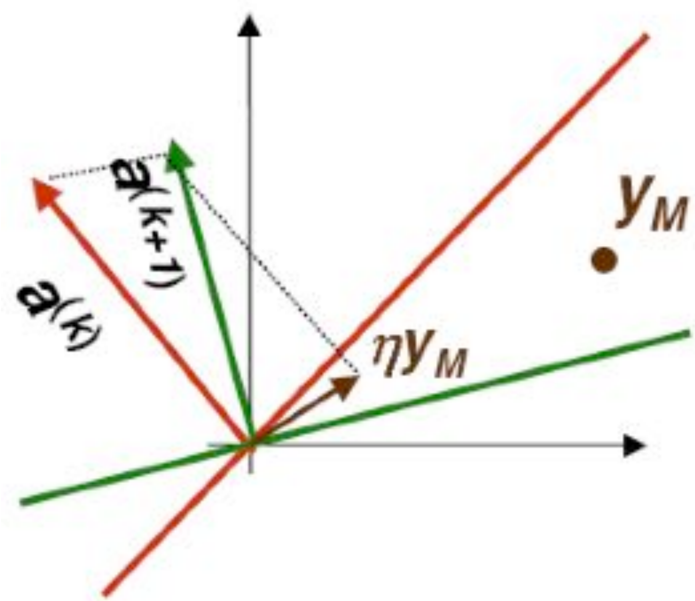
- $J_p(a)$ 是错分样本到决策面的距离之和的 $||a||$倍？
- $J_p(a)$是分段线性的，所以可用梯度下降法求解最小值

感知器准则下的梯度下降法

优化目标是最小化<u>错分样本</u>的负判决值之和

$$J_P(\mathbf{a}) = \sum_{y \in Y_M} \left(-\mathbf{a}^T y\right)$$

$$\nabla_a J_P(\mathbf{a}) = \sum_{y \in Y_M} (-y)$$



$$\mathbf{a}(k+1) = \mathbf{a}(k) + \eta \sum_{y \in Y_M(k)} y$$

Batch Update 成批更新

$$\mathbf{a}(k+1) = \mathbf{a}(k) + \eta \cdot y^k$$

Single-sample Update

单样本逐个更新

感知器准则算法伪代码

Batch Update

begin initialize $\mathbf{a}, \eta(\cdot)$, criterion $\theta, k = 0$

  do $k \leftarrow k + 1$

    $\mathbf{a} \leftarrow \mathbf{a} + \eta(k) \sum_{\mathbf{y} \in \mathcal{Y}_k} \mathbf{y}$

  until $\eta(k) \sum_{\mathbf{y} \in \mathcal{Y}_k} \mathbf{y} < \theta$

 return $\mathbf{a}$

end

Single-sample Update

begin initialize $\mathbf{a}, k = 0$

  do $k \leftarrow (k + 1) \mathrm{mod} n$

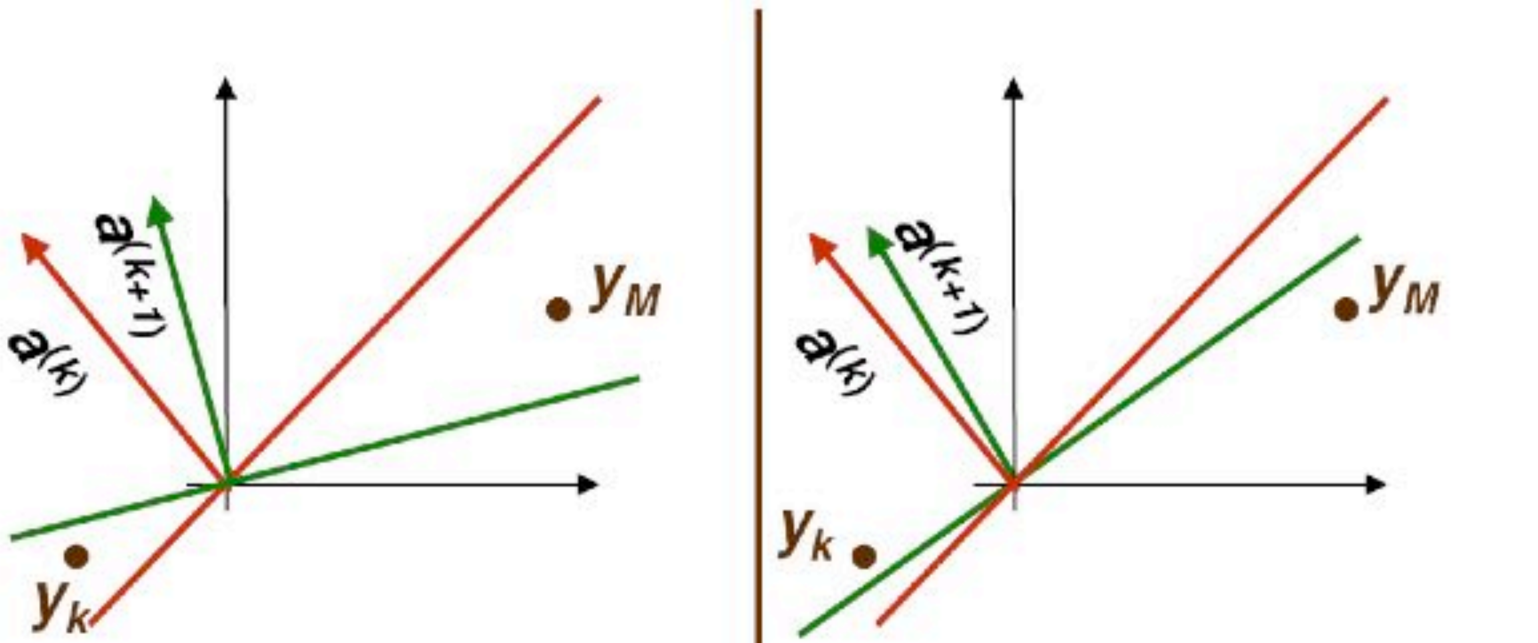
    if $\mathbf{y}_k$ is misclassified by $\mathbf{a}$ **then** $\mathbf{a} \leftarrow \mathbf{a} - \mathbf{y}_k$

  until all patterns properly classified

 return $\mathbf{a}$

end

Learning rate in single-sample update



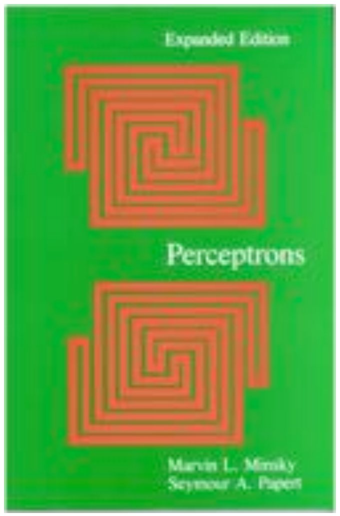
η is too large, previously correctly classified sample $\boldsymbol{y}_k$ is now misclassified

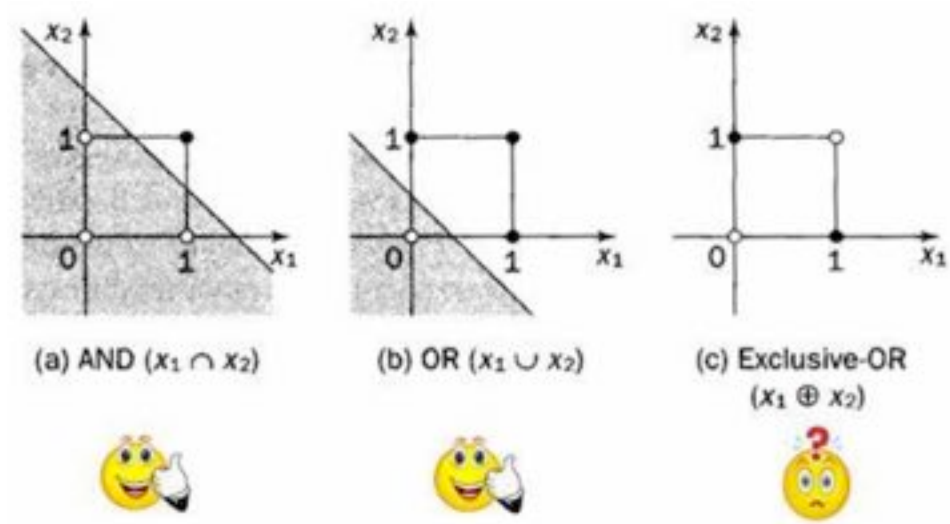
η is too small, $\boldsymbol{y}_M$ is still misclassified

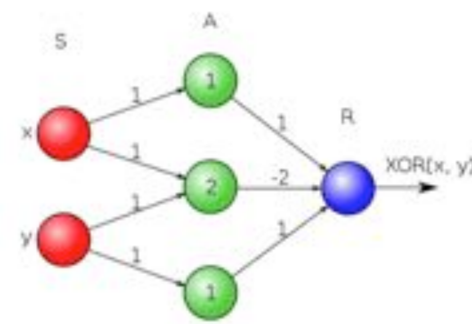
Perceptron Learning Algorithm: A Graphical Explanation Of Why It Works

https://towardsdatascience.com/perceptron-learning-algorithm-d5db0deab975

XOR problem killed Perceptron



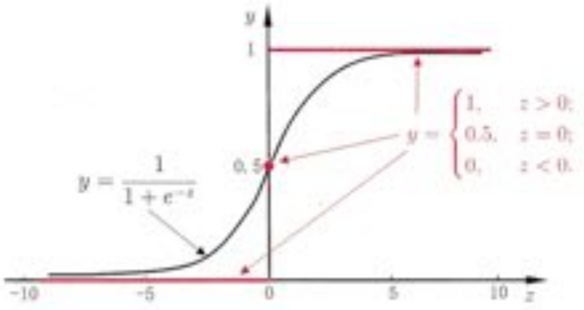




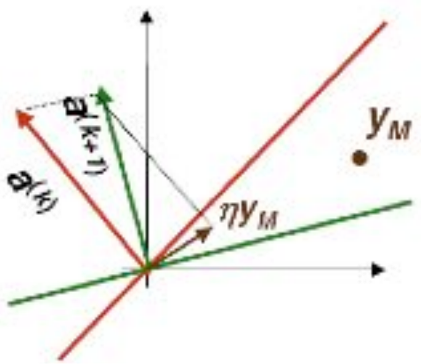
Minsky and Papert, 1969

总结：线性回归与线性分类

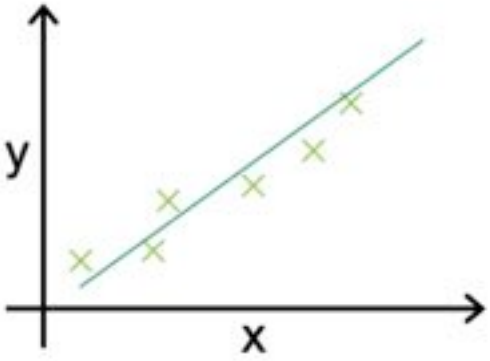
对数几率回归分类器
Logistic regression



感知机线性分类Perceptron



线性回归
Linear regression



机器学习的核心方法

- ☑ 模型选择 Model selection
- ☑ 代价函数 Cost function
- ☑ 优化算法 Optimization algorithm
- ☑ **正则化 Regularization**
- ☑ **核函数升维 Kernel trick**