

Classification

Industrial AI Lab.
Prof. Seungchul Lee
Yunseob Hwang, Juwon Na

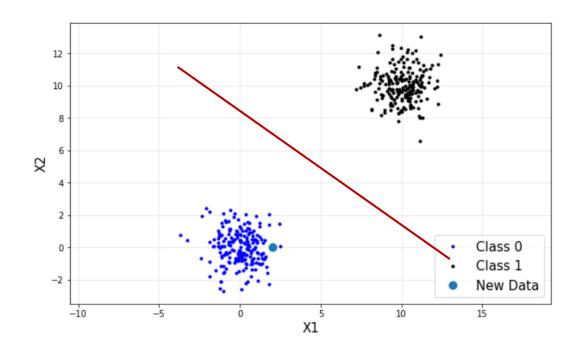


Classification

- We will learn
 - Perceptron
 - Logistic regression

To find

 a classification boundary





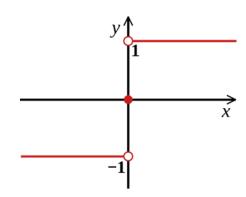


• For input
$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$
 'attributes of a customer'

• Weights
$$\omega = \begin{bmatrix} \omega_1 \\ \vdots \\ \omega_d \end{bmatrix}$$

$$\text{Approve credit if } \sum_{i=1}^d \omega_i x_i > \text{threshold},$$

$$\text{Deny credit if } \sum_{i=1}^d \omega_i x_i < \text{threshold.}$$

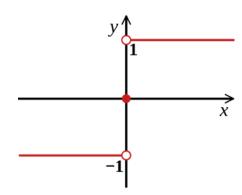


$$h(x) = ext{sign}\left(\left(\sum_{i=1}^d \omega_i x_i
ight) - ext{threshold}
ight) = ext{sign}\left(\left(\sum_{i=1}^d \omega_i x_i
ight) + \omega_0
ight)$$

$$h(x) = ext{sign}\left(\left(\sum_{i=1}^d \omega_i x_i
ight) - ext{threshold}
ight) = ext{sign}\left(\left(\sum_{i=1}^d \omega_i x_i
ight) + \omega_0
ight)$$

• Introduce an artificial coordinate $x_0 = 1$:

$$h(x) = \mathrm{sign}\left(\sum_{i=0}^d \omega_i x_i
ight)$$



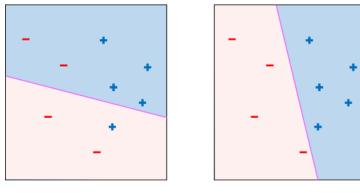
In a vector form, the perceptron implements

$$h(x) = \mathrm{sign}\left(\omega^T x
ight)$$

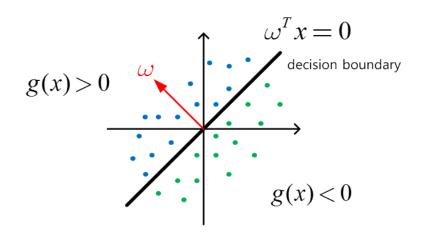
• Works for linearly separable data

Hyperplane

- Separates a D-dimensional space into two half-spaces
- Defined by an outward pointing normal vector
- $-\omega$ is orthogonal to any vector lying on the hyperplane
- Assume the hyperplane passes through origin, $\omega^T x = 0$ with $x_0 = 1$



Linearly separable data

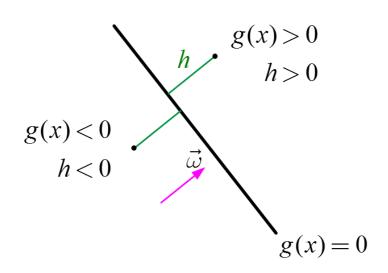


Sign

Sign with respect to a line

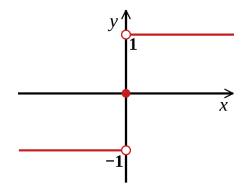
$$\omega = \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_1 x_1 + \omega_2 x_2 + \omega_0 = \omega^T x + \omega_0$$

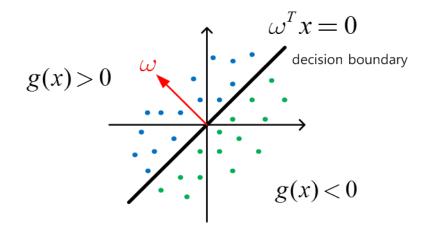
$$\omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix}, \quad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_0 + \omega_1 x_1 + \omega_2 x_2 = \omega^T x$$



How to Find ω

- All data in class 1 (y = 1)
 - -g(x) > 0
- All data in class 0 (y = -1)
 - -g(x)<0





Perceptron Algorithm

• The perceptron implements

$$h(x) = ext{sign}\left(\omega^T x
ight)$$

Given the training set

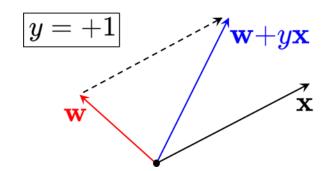
$$(x_1,y_1),(x_2,y_2),\cdots,(x_N,y_N) \quad ext{where } y_i \in \{-1,1\}$$

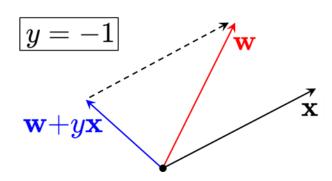
1) pick a misclassified point

$$\text{sign}\left(\omega^T x_n\right) \neq y_n$$

2) and update the weight vector

$$\omega \leftarrow \omega + y_n x_n$$





Perceptron Algorithm

- Why perceptron updates work?
- Let's look at a misclassified positive example $(y_n = +1)$
 - Perceptron (wrongly) thinks $\omega_{old}^T x_n < 0$
 - Updates would be

$$\omega_{new} = \omega_{old} + y_n x_n = \omega_{old} + x_n$$

$$\omega_{new}^T x_n = (\omega_{old} + x_n)^T x_n = \omega_{old}^T x_n + x_n^T x_n$$

– Thus $\omega_{new}^T x_n$ is less negative than $\omega_{old}^T x_n$

Iterations of Perceptron

- 1. Randomly assign ω
- 2. One iteration of the PLA (perceptron learning algorithm)

$$\omega \leftarrow \omega + yx$$

where (x, y) is a misclassified training point

3. At iteration $i = 1, 2, 3, \dots$, pick a misclassified point from

$$(x_1,y_1),(x_2,y_2),\cdots,(x_N,y_N)$$

- 4. And run a PLA iteration on it
- 5. That's it!

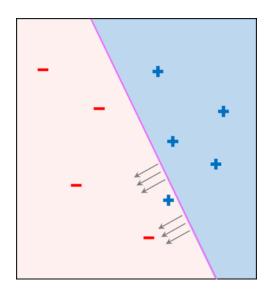
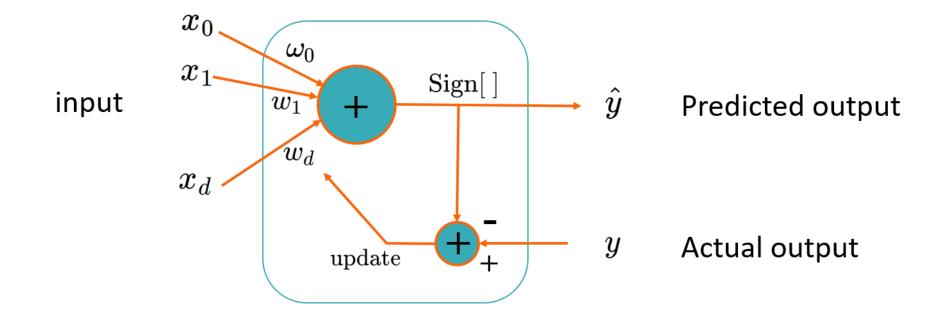


Diagram of Perceptron





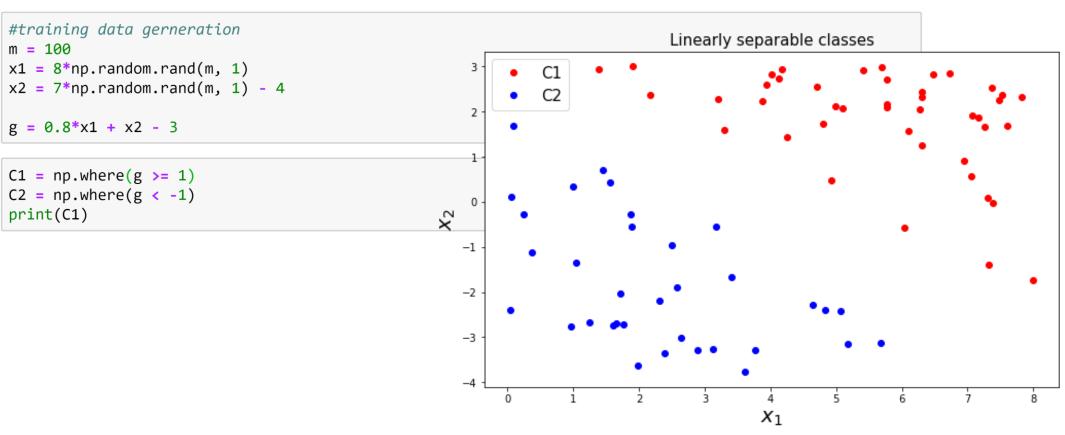
Perceptron Loss Function

$$L(\omega) = \sum_{n=1}^m \max\left\{0, -y_n\cdot\left(\omega^T x_n
ight)
ight\}$$

- Loss = 0 on examples where perceptron is correct, i.e., $y_n \cdot (\omega^T x_n) > 0$
- Loss > 0 on examples where perceptron is misclassified, i.e., $y_n \cdot (\omega^T x_n) < 0$

- Note:
 - $-\operatorname{sign}(\omega^T x_n) \neq y_n$ is equivalent to $y_n \cdot (\omega^T x_n) < 0$

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```





• Unknown parameters ω

$$g(x)=\omega_0+\omega^Tx=\omega_0+\omega_1x_1+\omega_2x_2=0$$

$$\omega = egin{bmatrix} \omega_0 \ \omega_1 \ \omega_2 \end{bmatrix}$$

$$y = egin{bmatrix} y^{(1)} \ y^{(2)} \ y^{(3)} \ dots \ y^{(m)} \end{bmatrix}$$

```
X1 = np.hstack([np.ones([C1.shape[0],1]), x1[C1], x2[C1]])
X2 = np.hstack([np.ones([C2.shape[0],1]), x1[C2], x2[C2]])
X = np.vstack([X1, X2])
y = np.vstack([np.ones([C1.shape[0],1]), -np.ones([C2.shape[0],1])])
X = np.asmatrix(X)
y = np.asmatrix(y)
```

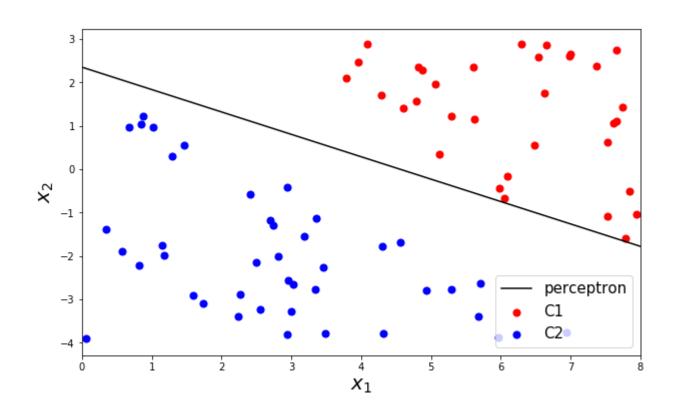
$$\omega = \left[egin{array}{c} \omega_0 \ \omega_1 \ \omega_2 \end{array}
ight]$$

 $\omega \leftarrow \omega + yx$ where (x, y) is a misclassified training point

$$g(x) = \omega_0 + \omega^T x = \omega_0 + \omega_1 x_1 + \omega_2 x_2 = 0$$
 $\implies x_2 = -rac{\omega_1}{\omega_2} x_1 - rac{\omega_0}{\omega_2}$

```
x1p = np.linspace(0,8,100).reshape(-1,1)
x2p = - w[1,0]/w[2,0]*x1p - w[0,0]/w[2,0]

plt.figure(figsize=(10, 6))
plt.scatter(x1[C1], x2[C1], c='r', s=50, label='C1')
plt.scatter(x1[C2], x2[C2], c='b', s=50, label='C2')
plt.plot(x1p, x2p, c='k', label='perceptron')
plt.xlim([0,8])
plt.xlabel('$x_1$', fontsize = 20)
plt.ylabel('$x_2$', fontsize = 20)
plt.legend(loc = 1, fontsize = 15)
plt.show()
```





Perceptron using Scikit-Learn

```
X1 = np.hstack([x1[C1], x2[C1]])
X2 = np.hstack([x1[C2], x2[C2]])
X = np.vstack([X1, X2])

y = np.vstack([np.ones([C1.shape[0],1]), -np.ones([C2.shape[0],1])])
```

```
from sklearn import linear_model

clf = linear_model.Perceptron(tol=1e-3)
clf.fit(X, np.ravel(y))
```

```
clf.predict([[3, -2]])
```

$$x = egin{bmatrix} \left(x^{(1)}
ight)^T \ \left(x^{(2)}
ight)^T \ \left(x^{(3)}
ight)^T \ dots \ \left(x^{(3)}
ight)^T \end{bmatrix} = egin{bmatrix} x_1^{(1)} & x_2^{(1)} \ x_1^{(2)} & x_2^{(2)} \ x_1^{(3)} & x_2^{(3)} \ dots \ \left(x_1^{(m)} & x_2^{(m)} \
ight) \end{bmatrix}$$

$$y = egin{bmatrix} y^{(1)} \ y^{(2)} \ y^{(3)} \ dots \ y^{(m)} \end{bmatrix}$$



The Best Hyperplane Separator?

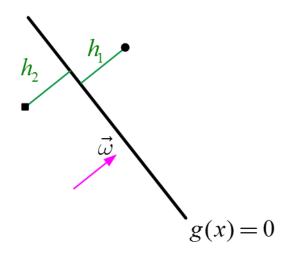
- Perceptron finds one of the many possible hyperplanes separating the data if one exists
- Of the many possible choices, which one is the best?
- Utilize distance information
- Intuitively we want the hyperplane having the maximum margin
- Large margin leads to good generalization on the test data
 - we will see this formally when we discuss Support Vector Machine (SVM)
- Utilize distance information from all data samples
 - We will see this formally when we discuss the logistic regression
- Perceptron will be shown to be a basic unit for neural networks and deep learning later

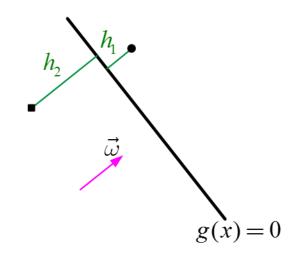


Logistic Regression



Using Distances





$$|h_1|+|h_2|$$

$$|h_1|\cdot |h_2|$$

$$|h_1|+|h_2|$$

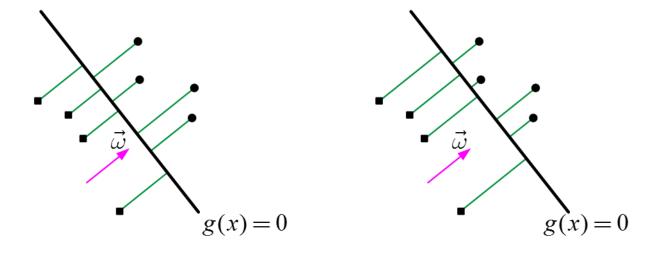
$$|h_1|\cdot |h_2|$$

$$rac{|h_1|+|h_2|}{2} \geq \sqrt{|h_1|\cdot|h_2|} \qquad ext{equal iff} \quad |h_1|=|h_2|$$

equal iff
$$|h_1| = |h_2|$$

Using all Distances

• basic idea: to find the decision boundary (hyperplane) of $g(x) = \omega^T x = 0$ such that maximizes $\prod_i |h_i| \to \text{optimization}$

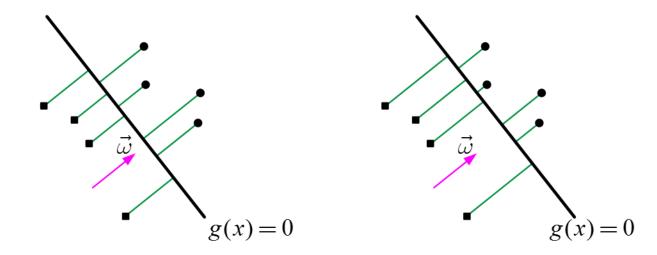


Inequality of arithmetic and geometric means

$$rac{x_1+x_2+\cdots+x_m}{m} \geq \sqrt[m]{x_1\cdot x_2\dots x_m}$$

and that equality holds if and only if $x_1 = x_2 = \cdots = x_m$

Using all Distances

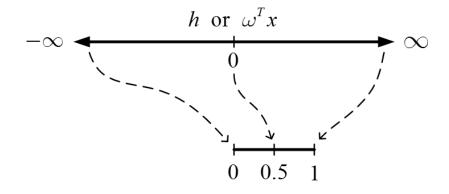


• Roughly speaking, this optimization of $\max \prod_i |h_i|$ tends to position a hyperplane in the middle of two classes

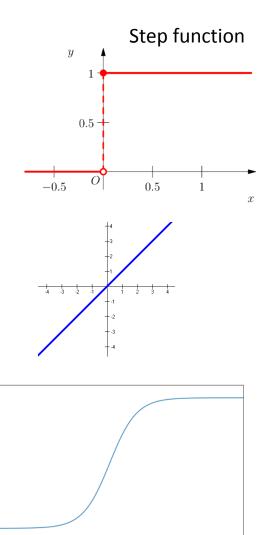
$$h = rac{g(x)}{\|\omega\|} = rac{\omega^T x}{\|\omega\|} \sim \omega^T x$$

Sigmoid Function

• We link or squeeze $(-\infty, +\infty)$ to (0, 1) for several reasons:



$$\sigma(z) = rac{1}{1 + e^{-z}} \implies \sigma\left(\omega^T x
ight) = rac{1}{1 + e^{-\omega^T x}}$$



Sigmoid Function

- $\sigma(z)$ is the sigmoid function, or the logistic function
 - Logistic function always generates a value between 0 and 1
 - Crosses 0.5 at the origin, then flattens out

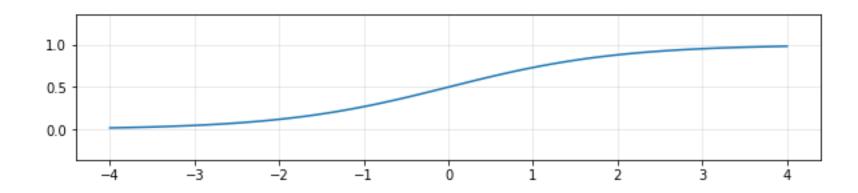
```
# plot a sigmoid function

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

z = np.linspace(-4,4,100)
s = 1/(1 + np.exp(-z))

plt.figure(figsize=(10,2))
plt.plot(z, s)
plt.xlim([-4, 4])
plt.axis('equal')
plt.grid(alpha = 0.3)
plt.show()
```

$$\sigma(z) = rac{1}{1 + e^{-z}} \implies \sigma(\omega^T x) = rac{1}{1 + e^{-\omega^T x}}$$



Sigmoid Function

- Benefit of mapping via the logistic function
 - Monotonic: same or similar optimization solution
 - Continuous and differentiable: good for gradient descent optimization
 - Probability or confidence: can be considered as probability

$$P\left(y=+1\mid x,\omega
ight)=rac{1}{1+e^{-\omega^{T}x}}\;\;\in\;\left[0,1
ight]$$

- Probability that the label is +1

$$P(y = +1 \mid x; \omega)$$

Probability that the label is 0

$$P\left(y=0\mid x\,;\omega
ight)=1-P\left(y=+1\mid x\,;\omega
ight)$$

Goal: We Need to Fit ω to Data

• For a single data point (x, y) with parameters ω

$$egin{aligned} P\left(y = +1 \mid x \, ; \omega
ight) &= h_{\omega}(x) = \sigma\left(\omega^T x
ight) \ P\left(y = 0 \mid x \, ; \omega
ight) &= 1 - h_{\omega}(x) = 1 - \sigma\left(\omega^T x
ight) \end{aligned}$$

It can be compactly written as

$$P(y \mid x; \omega) = (h_{\omega}(x))^{y} (1 - h_{\omega}(x))^{1-y}$$

• For m training data points, the likelihood function of the parameters:

$$egin{aligned} \mathscr{L}(\omega) &= P\left(y^{(1)}, \cdots, y^{(m)} \mid x^{(1)}, \cdots, x^{(m)} ; \omega
ight) \ &= \prod_{i=1}^m P\left(y^{(i)} \mid x^{(i)} ; \omega
ight) \ &= \prod_{i=1}^m \left(h_\omega\left(x^{(i)}
ight)
ight)^{y^{(i)}} \left(1 - h_\omega\left(x^{(i)}
ight)
ight)^{1-y^{(i)}} \qquad \left(\sim \prod_i \lvert h_i
vert
ight) \end{aligned}$$

Goal: We Need to Fit ω to Data

$$egin{aligned} \mathscr{L}(\omega) &= P\left(y^{(1)}, \cdots, y^{(m)} \mid x^{(1)}, \cdots, x^{(m)} \; ; \omega
ight) \ &= \prod_{i=1}^m P\left(y^{(i)} \mid x^{(i)} \; ; \omega
ight) \ &= \prod_{i=1}^m \left(h_\omega\left(x^{(i)}
ight)
ight)^{y^{(i)}} \left(1 - h_\omega\left(x^{(i)}
ight)
ight)^{1-y^{(i)}} \qquad \left(\sim \prod_i \lvert h_i
vert
ight) \end{aligned}$$

It would be easier to work on the log likelihood.

$$\ell(\omega) = \log \mathscr{L}(\omega) = \sum_{i=1}^m y^{(i)} \log h_\omega \left(x^{(i)}
ight) + \left(1 - y^{(i)}
ight) \log \left(1 - h_\omega \left(x^{(i)}
ight)
ight)$$

• The logistic regression problem can be solved as a (convex) optimization problem:

$$\hat{\omega} = rg \max_{\omega} \ell(\omega)$$

• Again, it is an optimization problem

Logistic Regression using GD



Gradient Descent for Logistic Regression

• To use the gradient descent method, we need to find the derivative of it

$$abla \ell(\omega) = \left[egin{array}{c} rac{\partial \ell(\omega)}{\partial \omega_1} \ dots \ rac{\partial \ell(\omega)}{\partial \omega_n} \end{array}
ight]$$

• We need to compute $\frac{\partial \ell(\omega)}{\partial \omega_j}$

$$\ell(\omega) = \log \mathscr{L}(\omega) = \sum_{i=1}^m y^{(i)} \log h_\omega \left(x^{(i)}
ight) + \left(1 - y^{(i)}
ight) \log \left(1 - h_\omega \left(x^{(i)}
ight)
ight)$$

Gradient Descent for Logistic Regression

$$\ell(\omega) = \log \mathscr{L}(\omega) = \sum_{i=1}^m y^{(i)} \log h_\omega \left(x^{(i)}
ight) + \left(1 - y^{(i)}
ight) \log \left(1 - h_\omega \left(x^{(i)}
ight)
ight)$$

• Think about a single data point with a single parameter ω for the simplicity.

$$\frac{\partial}{\partial \omega} [y \log(\sigma) + (1 - y) \log(1 - \sigma)]$$

$$= y \frac{\sigma'}{\sigma} + (1 - y) \frac{-\sigma}{1 - \sigma}$$

$$= \left(\frac{y}{\sigma} - \frac{1 - y}{1 - \sigma}\right) \sigma'$$

$$= \frac{y - \sigma}{\sigma(1 - \sigma)} \sigma'$$

$$= \frac{y - \sigma}{\sigma(1 - \sigma)} \sigma(1 - \sigma)x$$

$$= (y - \sigma)x$$

• For m training data points with parameters ω

$$\frac{\partial \ell(\omega)}{\partial \omega_i} = \sum_{i=1}^m \left(y^{(i)} - h_\omega \left(x^{(i)} \right) \right) x_j^{(i)} \quad \overset{\text{vectorization}}{=} \quad \left(y - h_\omega(x) \right)^T x_j = x_j^T \left(y - h_\omega(x) \right)$$

Gradient Descent for Logistic Regression

$$\omega = \left[egin{array}{c} \omega_0 \ \omega_1 \ \omega_2 \end{array}
ight], \qquad x = \left[egin{array}{c} 1 \ x_1 \ x_2 \end{array}
ight]$$

$$X = egin{bmatrix} \left(x^{(1)}
ight)^T \ \left(x^{(2)}
ight)^T \ \left(x^{(3)}
ight)^T \end{bmatrix} = egin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \ 1 & x_1^{(2)} & x_2^{(2)} \ 1 & x_1^{(3)} & x_2^{(3)} \ dots & dots & dots \end{bmatrix}$$

$$y = egin{bmatrix} y^{(1)} \ y^{(2)} \ y^{(3)} \ dots \end{bmatrix}$$

- Maximization problem
- Be careful on matrix shape

$$rac{\partial \ell(\omega)}{\partial \omega_j} = \sum_{i=1}^m \left(y^{(i)} - h_\omega \left(x^{(i)}
ight)
ight) x_j^{(i)}$$

$$\stackrel{\text{vectorization}}{=} \quad \left(y - h_{\omega}(x)\right)^{T} x_{j} = x_{j}^{T} \left(y - h_{\omega}(x)\right)$$

$$abla \ell(\omega) = egin{bmatrix} rac{\partial \ell(\omega)}{\partial \omega_0} \ rac{\partial \ell(\omega)}{\partial \omega_1} \ rac{\partial \ell(\omega)}{\partial \omega_2} \end{bmatrix} = X^T \left(y - h_\omega(x)
ight) = X^T \left(y - \sigma(X\omega)
ight)$$

$$\omega \leftarrow \omega - \eta \left(-\nabla \ell(\omega) \right)$$

Logistic Regression in Python

```
# datat generation

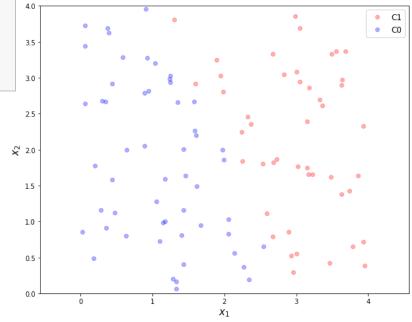
m = 100
w = np.array([[-6], [2], [1]])
X = np.hstack([np.ones([m,1]), 4*np.random.rand(m,1), 4*np.random.rand(m,1)])

w = np.asmatrix(w)
X = np.asmatrix(X)

y = 1/(1 + np.exp(-X*w)) > 0.5

C1 = np.where(y == True)[0]
C0 = np.where(y == False)[0]

y = np.empty([m,1])
y[C1] = 1
y[C0] = 0
```





Logistic Regression in Python

```
# be careful with matrix shape

def h(x,w):
    return 1/(1 + np.exp(-x*w))
```

```
alpha = 0.0001
w = np.zeros([3,1])

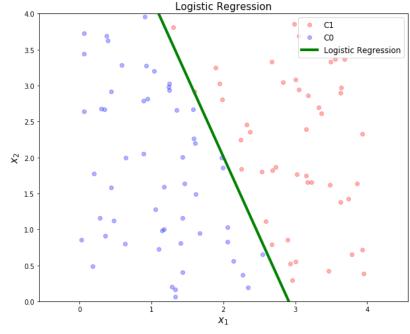
for i in range(1000):
    df = -X.T*(y - h(X,w))
    w = w - alpha*df

print(w)
```

$$h_{\omega}(x) = h(x\,;\omega) = \sigma\left(\omega^T x
ight) = rac{1}{1 + e^{-\omega^T x}}$$

$$abla \ell(\omega) = egin{bmatrix} rac{\partial \ell(\omega)}{\partial \omega_0} \ rac{\partial \ell(\omega)}{\partial \omega_1} \ rac{\partial \ell(\omega)}{\partial \omega_2} \end{bmatrix} = X^T \left(y - h_\omega(x)
ight) = X^T \left(y - \sigma(X\omega)
ight)$$

$$\omega \leftarrow \omega - \eta \left(-\nabla \ell(\omega) \right)$$



Logistic Regression using Scikit-Learn

```
X = X[:,1:3]
X.shape
```

```
from sklearn import linear_model

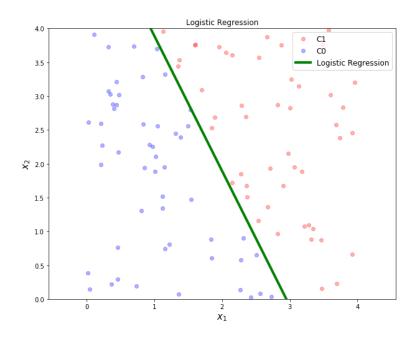
clf = linear_model.LogisticRegression(solver='lbfgs')
clf.fit(X,np.ravel(y))
```

```
w0 = clf.intercept_[0]
w1 = clf.coef_[0,0]
w2 = clf.coef_[0,1]

xp = np.linspace(0,4,100).reshape(-1,1)
yp = - w1/w2*xp - w0/w2
```

$$\omega = \left[egin{array}{c} \omega_1 \ \omega_2 \end{array}
ight], \qquad \omega_0, \qquad x = \left[egin{array}{c} x_1 \ x_2 \end{array}
ight]$$

$$X = egin{bmatrix} \left(x^{(1)}
ight)^T \ \left(x^{(2)}
ight)^T \ \left(x^{(3)}
ight)^T \ dots \end{bmatrix} = egin{bmatrix} x_1^{(1)} & x_2^{(1)} \ x_1^{(2)} & x_2^{(2)} \ x_1^{(3)} & x_2^{(3)} \ dots & dots \end{bmatrix}, \qquad y = egin{bmatrix} y^{(1)} \ y^{(2)} \ y^{(3)} \ dots \end{bmatrix}$$





Multiclass Classification



Multiclass Classification

- Generalization to more than 2 classes is straightforward
 - one vs. all (one vs. rest)
 - one vs. one
- Using the softmax function instead of the logistic function
 - (refer to <u>UFLDL Tutorial</u>)
 - see them as probability

$$P\left(y=k\mid x,\omega
ight)=rac{\exp\left(\omega_{k}^{T}x
ight)}{\sum_{k}\exp\left(\omega_{k}^{T}x
ight)}\in\left[0,1
ight]$$

• We maintain a separator weight vector ω_k for each class k

Softmax function

- We maintain a separator weight vector ω_k for each class k
- Using the softmax function instead of the logistic function
 - see them as probability

$$P\left(y=k\mid x,\omega
ight)=rac{\exp\left(\omega_{k}^{T}x
ight)}{\sum_{k}\exp\left(\omega_{k}^{T}x
ight)}\in\left[0,1
ight]$$

• For example,

$$P(y = 0 | x_0, \omega) = 0.87$$

$$0 P(y = 1 | x_0, \omega) = 0.01$$

$$P(y = 2 | x_0, \omega) = 0.12$$

Softmax regression

Logistic regression can be replaced with softmax function

$$P\left(y=+1\mid x,\omega
ight)=rac{1}{1+e^{-\omega^{T}x}}\;\;\in\;\left[0,1
ight]$$

$$p=rac{1}{1+e^{-\omega^Tx}}=rac{e^{\omega^Tx}}{e^{\omega^Tx}+1} \ 1-p=rac{e^{\omega^Tx}+1}{e^{\omega^Tx}+1}$$

$$\ell(\omega) = -\sum_{i=1}^{m} y^{(i)} \log h_{\omega} \left(x^{(i)} \right) + \left(1 - y^{(i)} \right) \log \left(1 - h_{\omega} \left(x^{(i)} \right) \right)$$

Logistic regression

$$P\left(y=k\mid x,\omega
ight)=rac{\exp\left(\omega_{k}^{T}x
ight)}{\sum_{k}\exp\left(\omega_{k}^{T}x
ight)}\in\left[0,1
ight]$$

Cross entropy

$$\ell(\omega) = -\sum_{i=1}^{m} y^{(i)} \log s_{\omega} \left(x^{(i)} \right)$$

Softmax regression

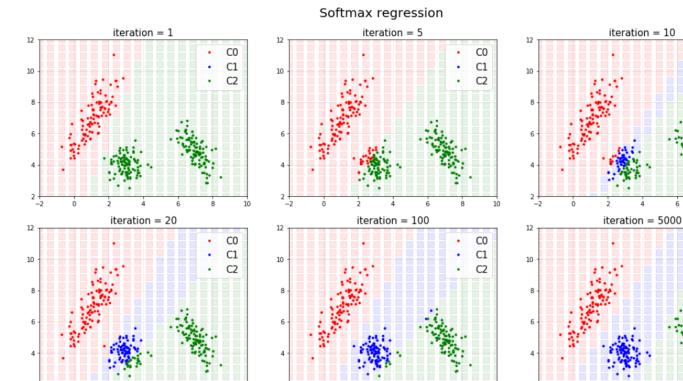
Softmax regression

```
def s(X, w):
    scores = np.dot(X, w)
    softmax = (np.exp(scores).T/np.sum(np.exp(scores), axis = 1)).T
    return softmax
```

$$P\left(y=k\mid x,\omega
ight)=rac{\exp\left(\omega_{k}^{T}x
ight)}{\sum_{k}\exp\left(\omega_{k}^{T}x
ight)}\in\left[0,1
ight]$$

```
alpha = 0.1
w = np.zeros([3,3])

losses = []
weights = []
for i in range(5000):
    loss = - 1/len(X)*np.sum(Y * s(X, w))
    df = - 1/len(X)*np.dot(X.T, (Y - s(X, w)))
    w = w - alpha*df
    losses.append(loss)
    weights.append(w)
```





C1

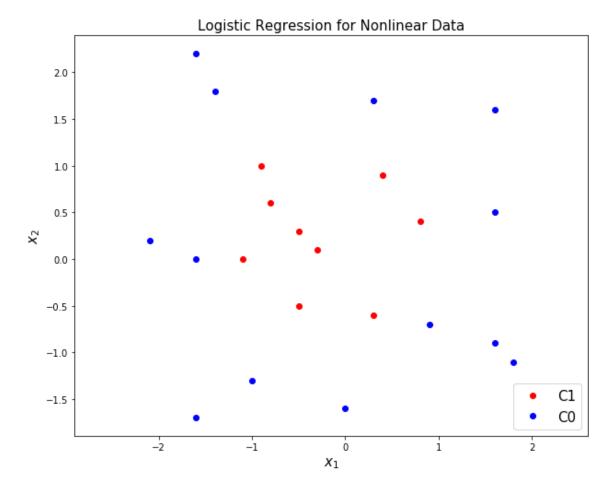
C1

Non-linear Classification



Non-linear Classification

- Same idea as non-linear regression: non-linear features
 - Explicit or implicit Kernel





Explicit Kernel

$$egin{aligned} x = egin{bmatrix} x_1 \ x_2 \end{bmatrix} &\implies z = \phi(x) = egin{bmatrix} rac{\sqrt{2}x_1}{\sqrt{2}x_2} \ x_1^2 \ \sqrt{2}x_1x_2 \ x_2^2 \end{bmatrix} \end{aligned}$$



Non-linear Classification

