Machine Learning

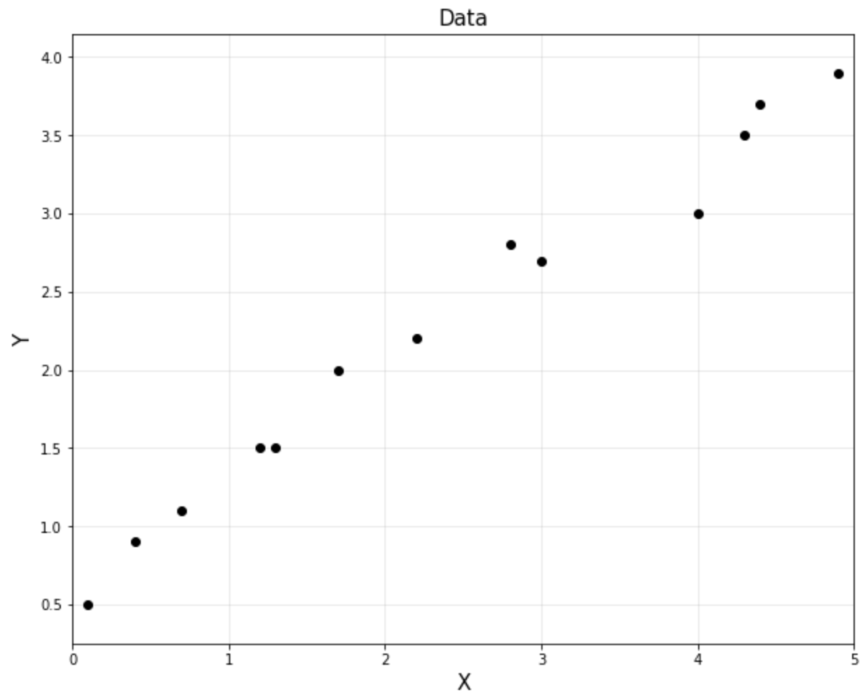
Industrial AI Lab.

Prof. Seungchul Lee

Regression

Assumption: Linear Model

$$\hat{y}_i = f(x_i\,;\theta) \;\; \text{in general}$$

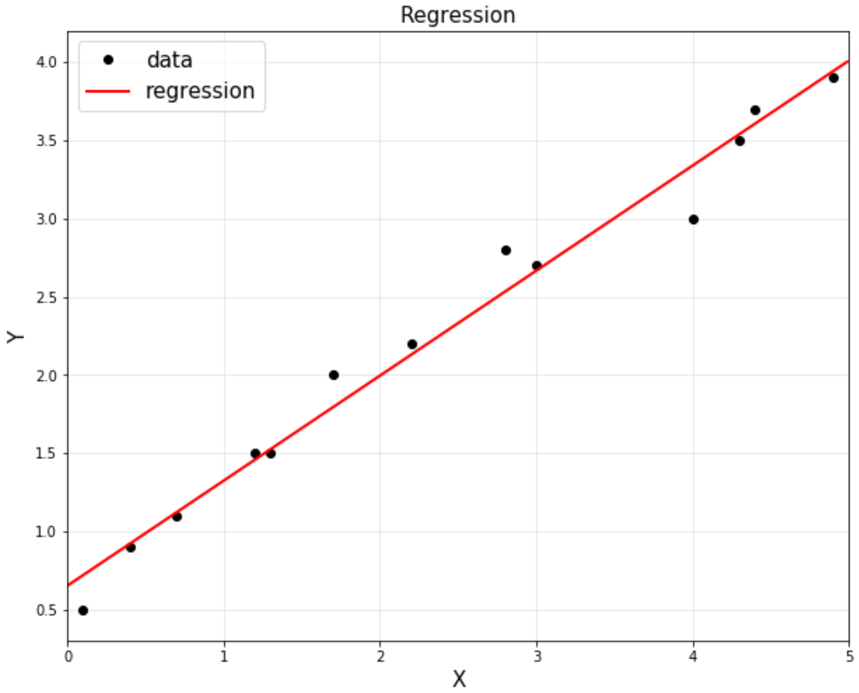


- In many cases, a linear model is used to predict y_i

$$\hat{y}_i = \theta_1 x_i + \theta_2$$

Assumption: Linear Model

$$\hat{y}_i = f(x_i\,;\theta) \text{ in general}$$



- In many cases, a linear model is used to predict y_i

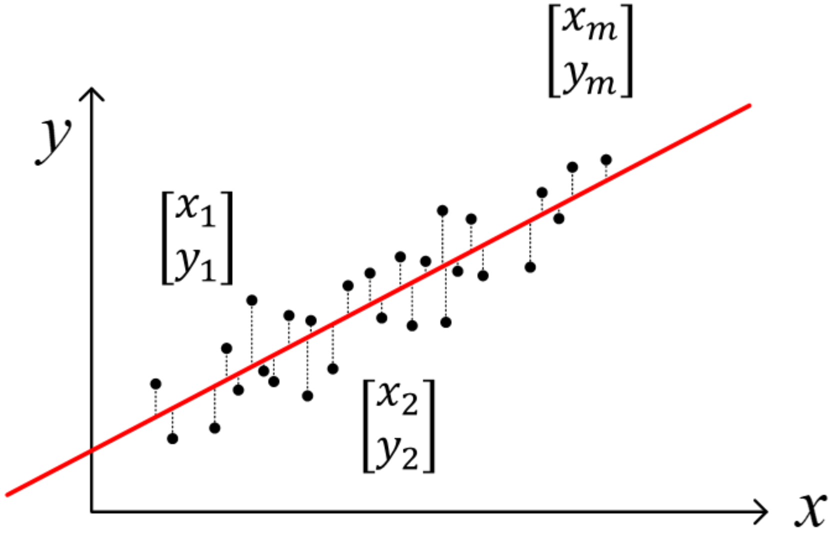
$$\hat{y}_i = \theta_1 x_i + \theta_2$$

Linear Regression

- $\hat{y}_i = f(x_i, \theta)$ in general
- In many cases, a linear model is assumed to predict y_i

$$\text{Given} \begin{cases} x_i : \text{inputs} \\ y_i : \text{outputs} \end{cases}$$, Find θ_0 and θ_1

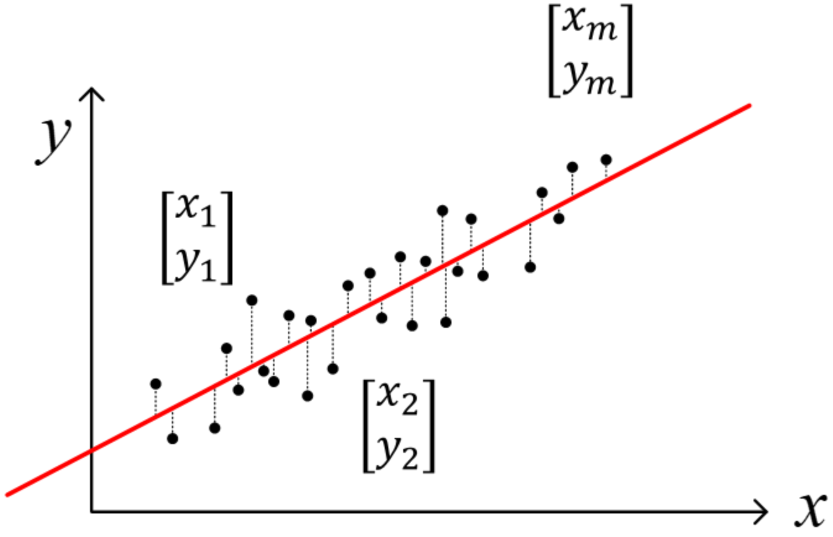
$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \approx \hat{y}_i = \theta_0 + \theta_1 x_i$$



- $\hat{y}_i$: predicted output
- $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$: model parameters

Linear Regression as Optimization

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \approx \hat{y}_i = \theta_0 + \theta_1 x_i$$



- How to find model parameters $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$
- Optimization problem

$$\hat{y}_i = \theta_0 + \theta_1 x_i \qquad \text{such that} \qquad \boxed{}$$

Re-cast Problem as Least Squares

- For convenience, we define a function that maps inputs to feature vectors, ϕ

$$
\begin{aligned}
\hat{y}_i &= \theta_0 + x_i\theta_1 = 1 \cdot \theta_0 + x_i\theta_1 \\
&= \begin{bmatrix} 1 & x_i \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \\
&= \begin{bmatrix} 1 \\ x_i \end{bmatrix}^T \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \\
&= \phi^T(x_i)\theta
\end{aligned}
$$

$$
\text{feature vector } \phi(x_i) = \begin{bmatrix} 1 \\ x_i \end{bmatrix}
$$

$$
\Phi = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_m \end{bmatrix} = \begin{bmatrix} \phi^T(x_1) \\ \phi^T(x_2) \\ \vdots \\ \phi^T(x_m) \end{bmatrix} \implies \hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_m \end{bmatrix} = \Phi\theta
$$

Optimization

$$\min_{\theta_0,\theta_1} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2 = \min_{\theta} \|\Phi\theta - y\|_2^2 \qquad \left(\text{same as } \min_{x} \|Ax - b\|_2^2\right)$$

$$\text{solution } \theta^* = \boxed{}$$

- Scalar Objective: $J = \|Ax - y\|^2$

$$\begin{aligned} J(x) &= (Ax - y)^T (Ax - y) \\ &= \left(x^T A^T - y^T\right)(Ax - y) \\ &= x^T A^T A x - x^T A^T y - y^T A x + y^T y \end{aligned}$$

$$\begin{aligned} \frac{\partial J}{\partial x} &= A^T A x + \left(A^T A\right)^T x - A^T y - \left(y^T A\right)^T \\ &= 2A^T A x - 2A^T y = 0 \end{aligned}$$

$$\implies \left(A^T A\right) x = A^T y$$

$$\therefore \quad x^* = \left(A^T A\right)^{-1} A^T y$$

y	$\frac{\partial y}{\partial x}$
Ax	A^T
$x^T A$	A
$x^T x$	$2x$
$x^T A x$	$Ax + A^T x$

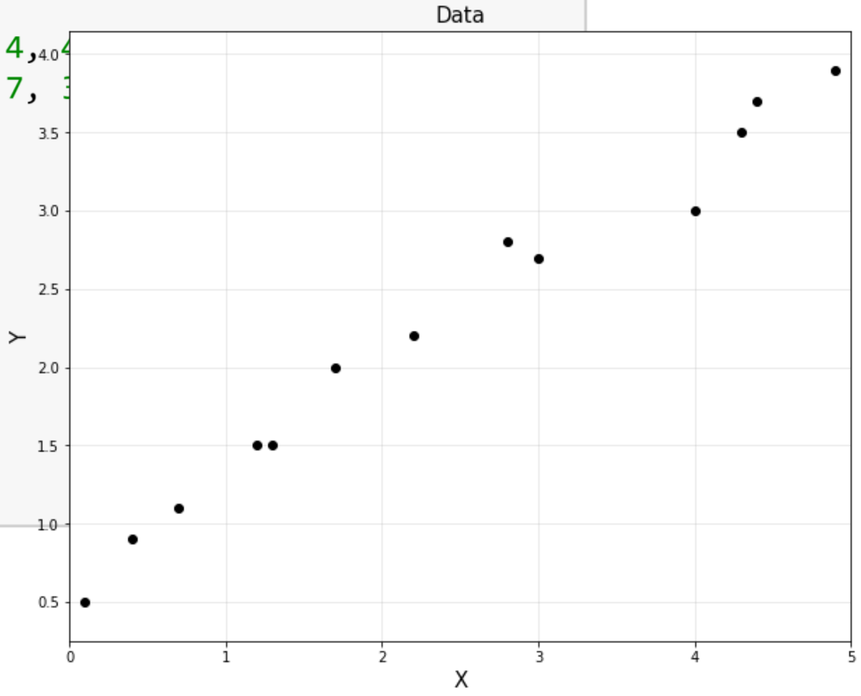
Solve using Linear Algebra

- known as *least square*

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

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

```
# data points in column vector [input, output]
x = np.array([0.1, 0.4, 0.7, 1.2, 1.3, 1.7, 2.2, 2.8, 3.0, 4.0, 4.3, 4.4,
y = np.array([0.5, 0.9, 1.1, 1.5, 1.5, 2.0, 2.2, 2.8, 2.7, 3.0, 3.5, 3.7,

plt.figure(figsize=(10,8))
plt.plot(x,y,'ko')
plt.title('Data', fontsize=15)
plt.xlabel('X', fontsize=15)
plt.ylabel('Y', fontsize=15)
plt.axis('equal')
plt.grid(alpha=0.3)
plt.xlim([0, 5])
plt.show()
```

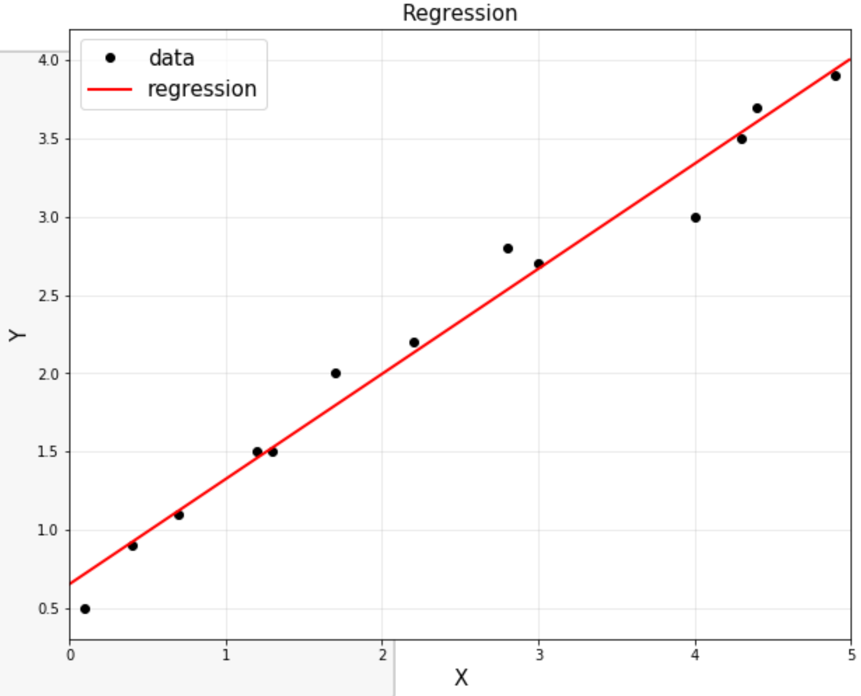


Solve using Linear Algebra

```
m = y.shape[0]
#A = np.hstack([x, np.ones([m, 1])])
A = np.hstack([x**0, x])
A = np.asmatrix(A)

theta = (A.T*A).I*A.T*y

print('theta:\n', theta)
```

```
theta:
 [[0.65306531]
 [0.67129519]]
```

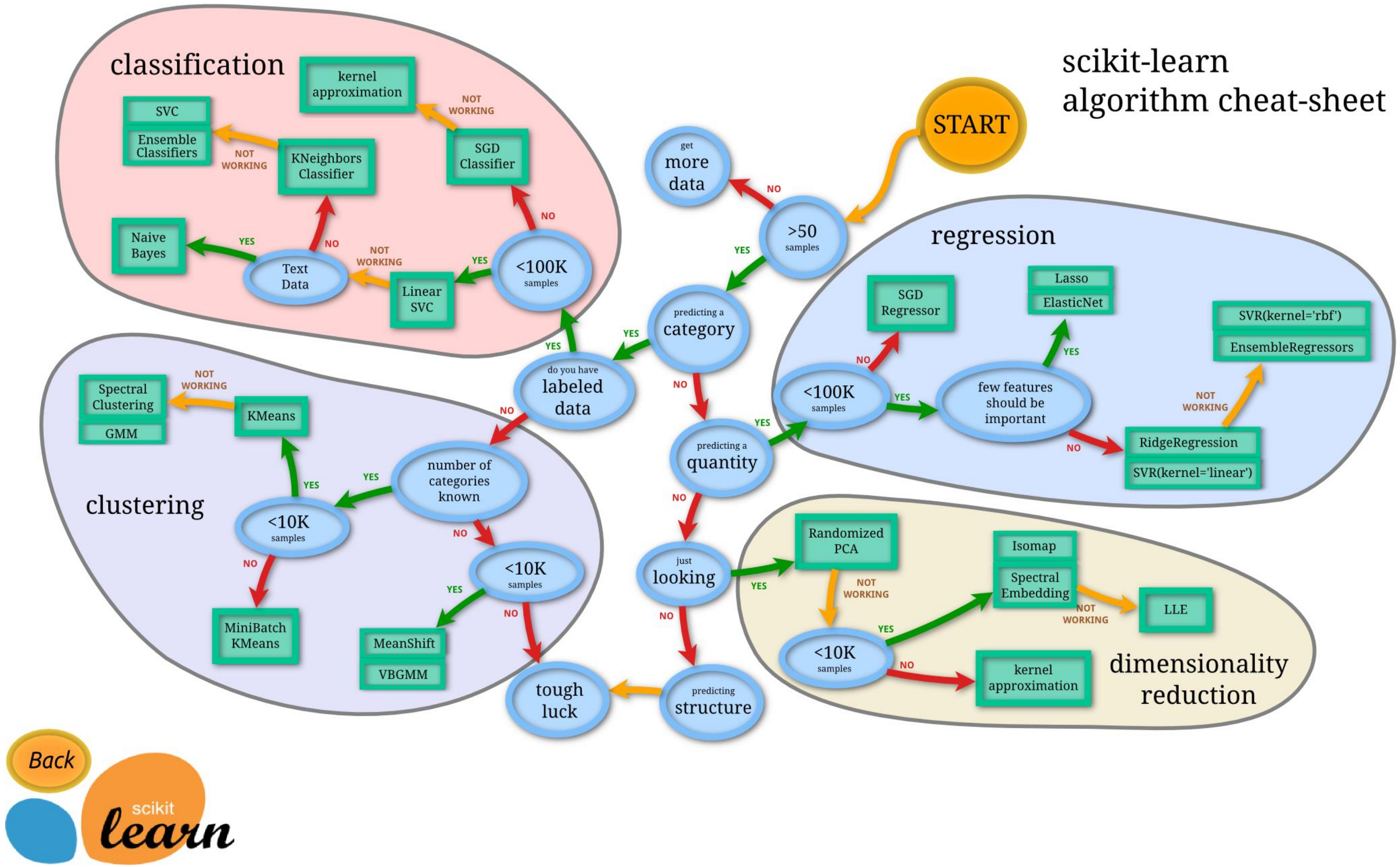
```
# to plot
plt.figure(figsize=(10, 8))
plt.title('Regression', fontsize=15)
plt.xlabel('X', fontsize=15)
plt.ylabel('Y', fontsize=15)
plt.plot(x, y, 'ko', label="data")

# to plot a straight line (fitted line)
xp = np.arange(0, 5, 0.01).reshape(-1, 1)
yp = theta[0,0] + theta[1,0]*xp

plt.plot(xp, yp, 'r', linewidth=2, label="regression")
plt.legend(fontsize=15)
plt.axis('equal')
plt.grid(alpha=0.3)
plt.xlim([0, 5])
plt.show()
```



Scikit-Learn

- Machine Learning in Python
- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license
- https://scikit-learn.org/stable/index.html#

Scikit-Learn



Scikit-Learn: Regression

```
from sklearn import linear_model
```

```
reg = linear_model.LinearRegression()
reg.fit(x, y)
```

```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
         normalize=False)
```

```
reg.coef_
```

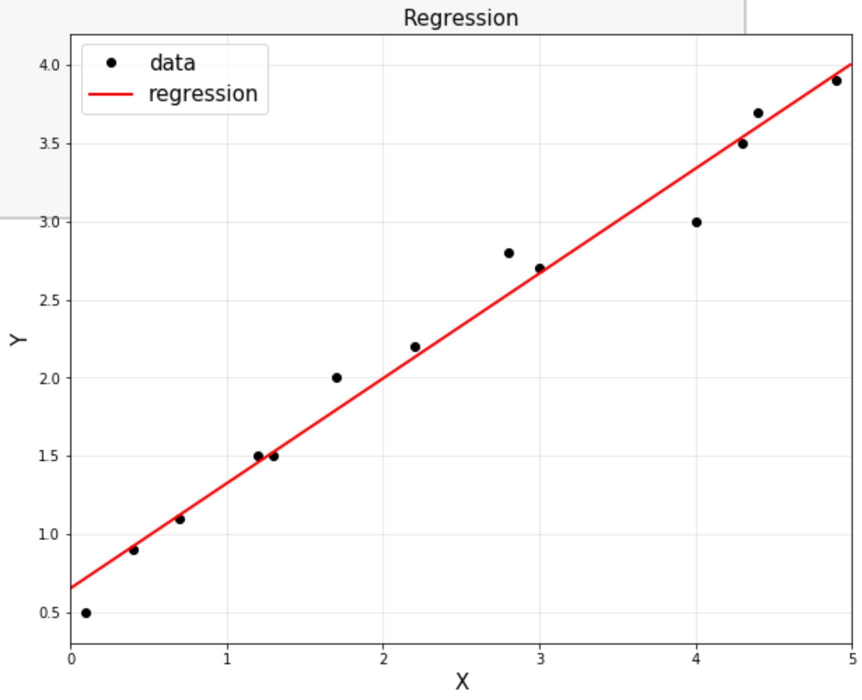
```
array([[0.67129519]])
```

```
reg.intercept_
```

```
array([0.65306531])
```

Scikit-Learn: Regression

```
# to plot
plt.figure(figsize=(10, 8))
plt.title('Regression', fontsize=15)
plt.xlabel('X', fontsize=15)
plt.ylabel('Y', fontsize=15)
plt.plot(x, y, 'ko', label="data")

# to plot a straight line (fitted line)
plt.plot(xp, reg.predict(xp), 'r', linewidth=2, label="regression")
plt.legend(fontsize=15)
plt.axis('equal')
plt.grid(alpha=0.3)
plt.xlim([0, 5])
plt.show()
```



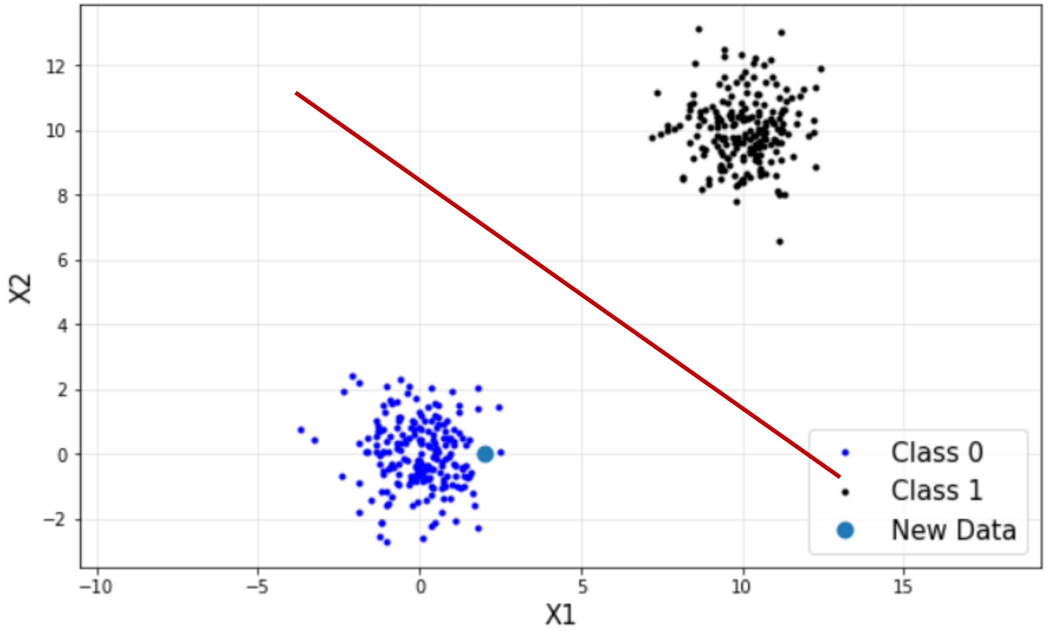
Classification: Perceptron

Classification

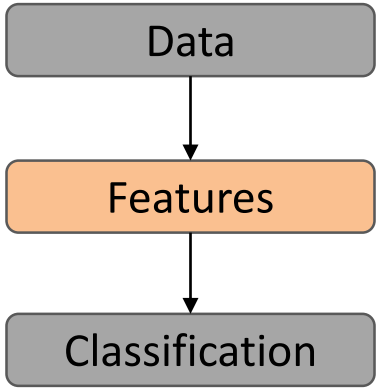
- Where y is a discrete value
  - Develop the classification algorithm to determine which class a new input should fall into

- We will learn
  - Perceptron
  - Logistic regression

- To find a classification boundary



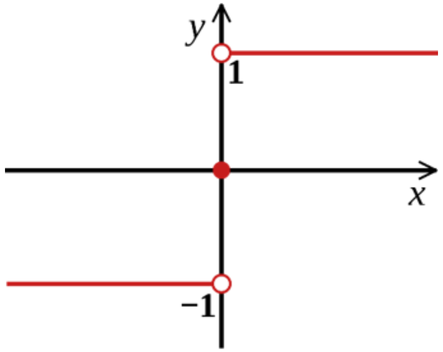
Perceptron



- For input $x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$ 'attributes of a customer'
- Weights $\omega = \begin{bmatrix} \omega_1 \\ \vdots \\ \omega_d \end{bmatrix}$

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

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



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

Perceptron

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

- Introduce an artificial coordinate $x_0 = 1$:

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

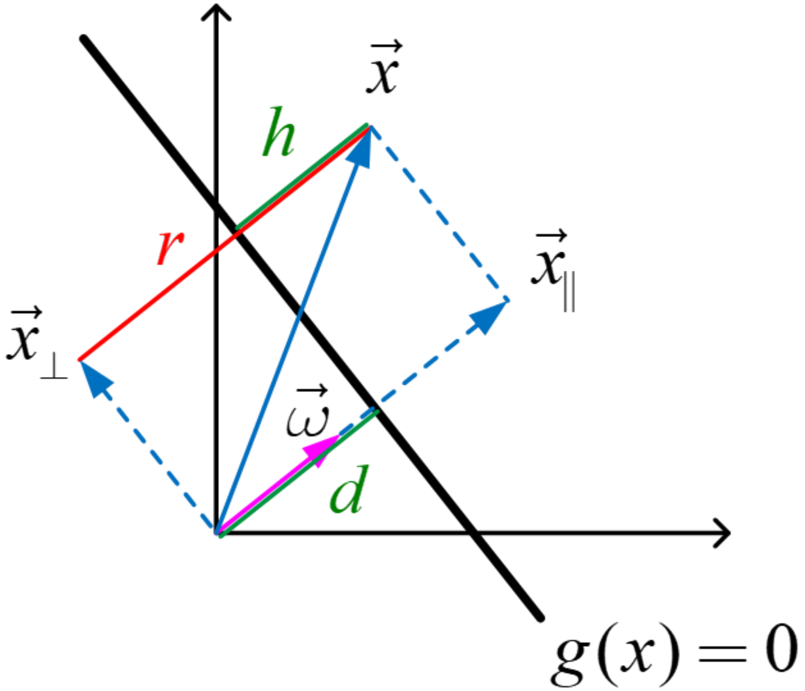
- In a vector form, the perceptron implements

$$h(x) = \text{sign}\left(\omega^T x\right)$$

- Let's see geometrical meaning of perceptron

Distance from a Line

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

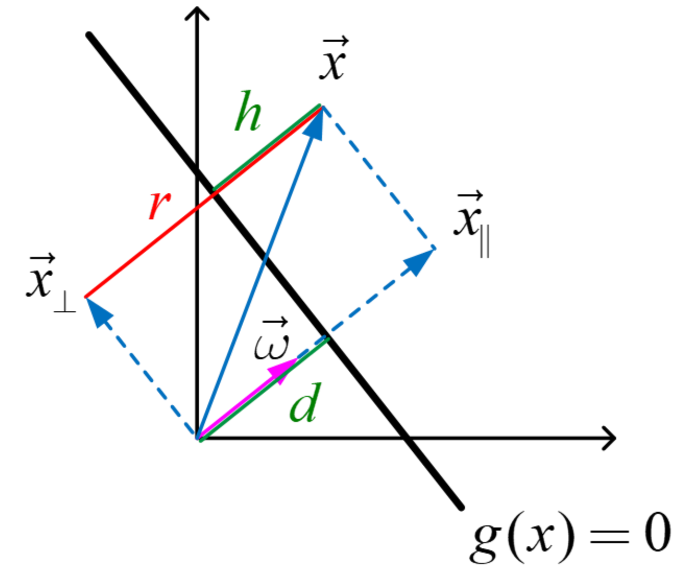


$\boldsymbol{\omega}$

- If $\vec{p}$ and $\vec{q}$ are on the decision line

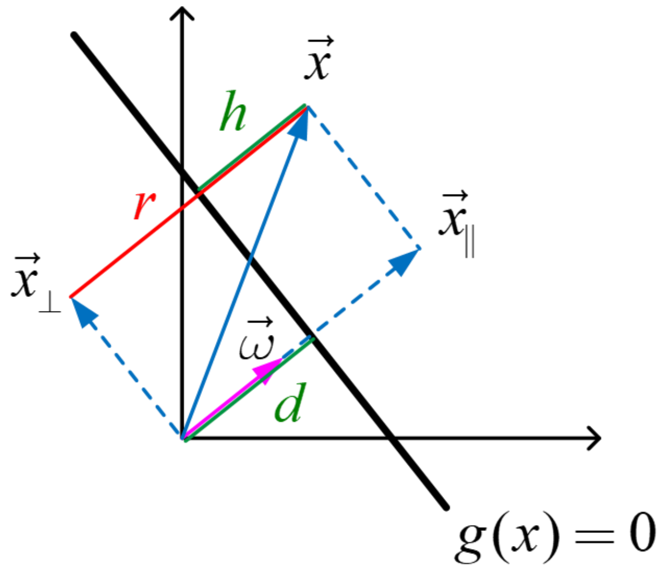
$\therefore\ \omega$: normal to the line (orthogonal)

$\Longrightarrow$ tells the direction of the line



Signed Distance d

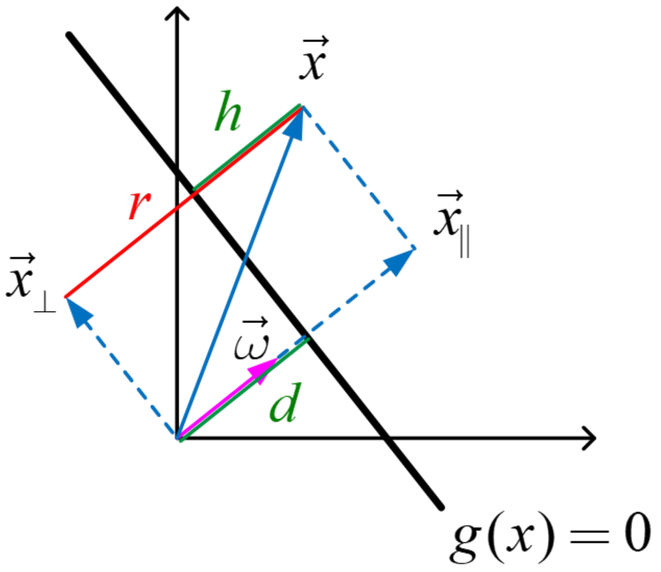
- If x is on the line and $x = d\frac{\omega}{\|\omega\|}$ (where d is a normal distance from the origin to the line)



Distance from a Line: h

- for any vector of x

$$x = x_\perp + r\frac{\omega}{\|\omega\|}$$



$$\therefore\ h = \frac{g(x)}{\|\omega\|} \implies \text{orthogonal signed distance from the line}$$

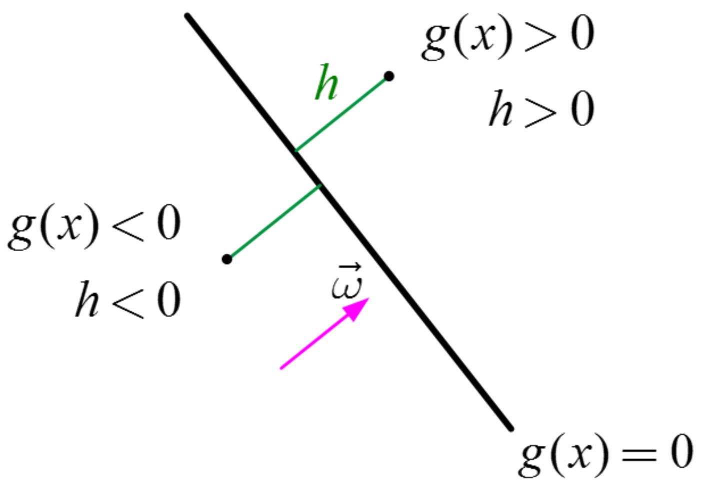
Sign

$$\therefore\ h = \frac{g(x)}{\|\omega\|} \implies \text{orthogonal signed distance from the line}$$

- Sign with respect to a line

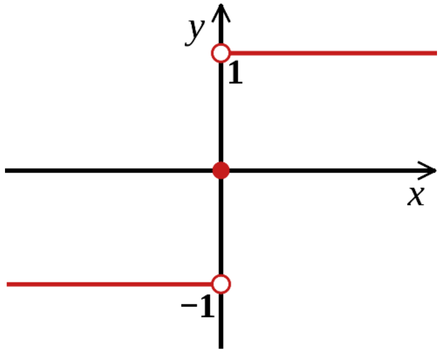
$$\omega = \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_1 x_1 + \omega_2 x_2 + \omega_0 = \omega^T x + \omega_0$$

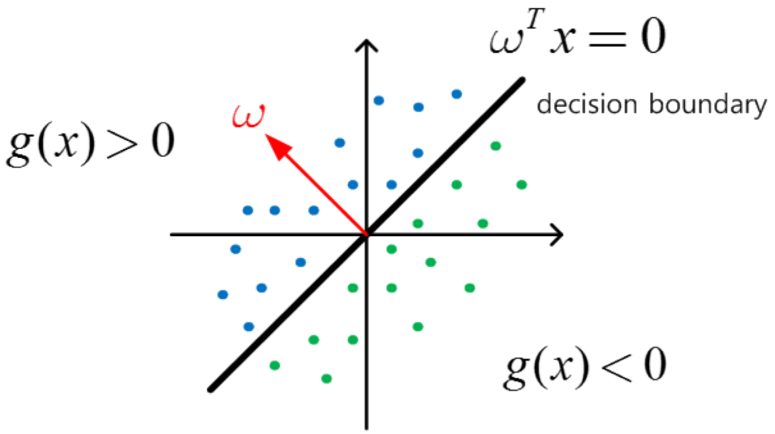
$$\omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix}, \quad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_0 + \omega_1 x_1 + \omega_2 x_2 = \omega^T x$$



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

$$h(x) = \text{sign}\left(\omega^T x\right)$$

- Given the training set

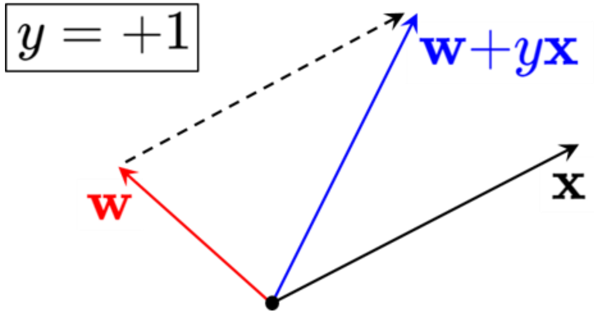
$$(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N) \quad \text{where } y_i \in \{-1, 1\}$$

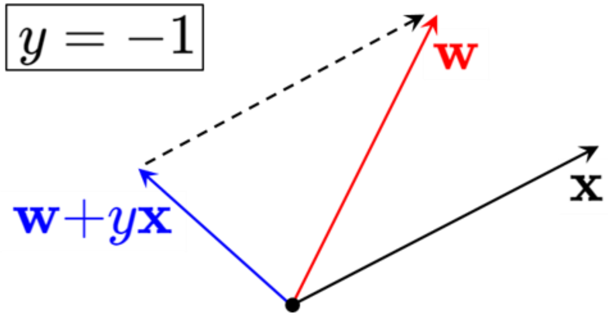
1) pick a misclassified point

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

2) and update the weight vector

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





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 $t = 1,2,3, \cdots$, 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!

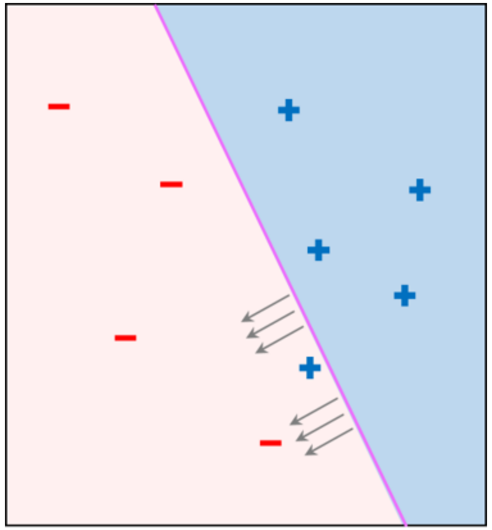
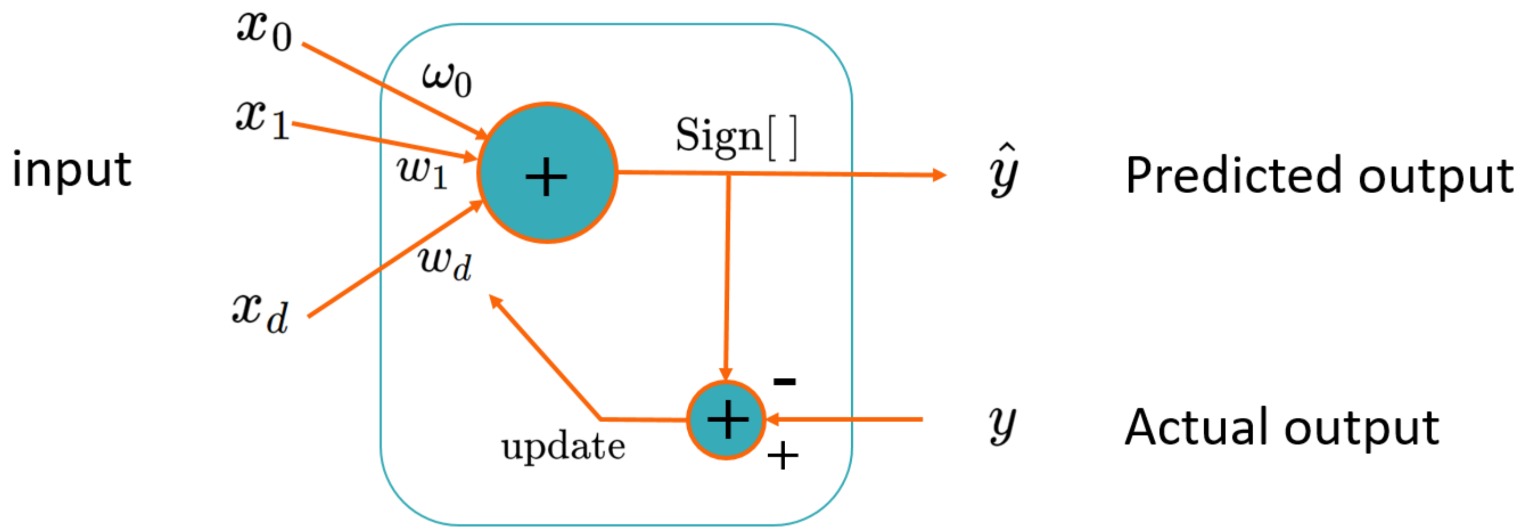


Diagram of Perceptron



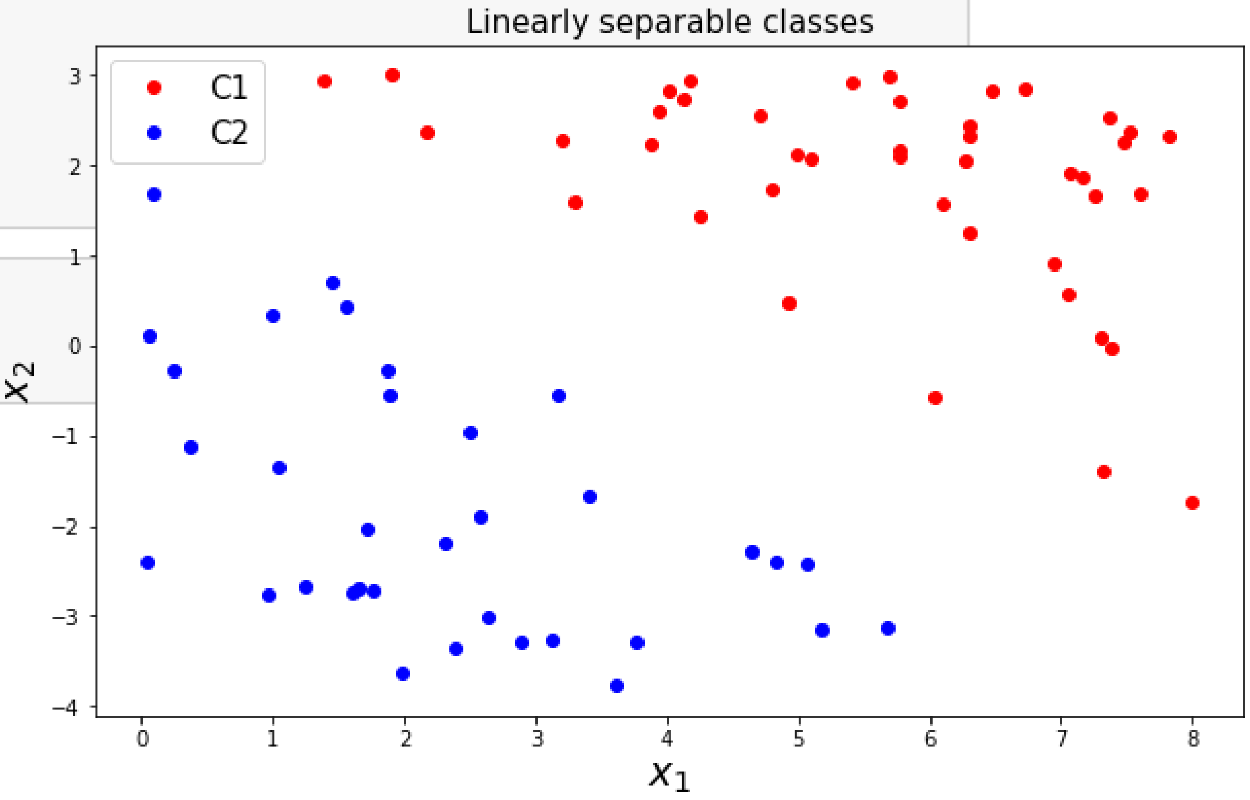
- Perceptron will be shown to be a basic unit for neural networks and deep learning later

Perceptron Algorithm in Python

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

```
#training data gerneration
m = 100
x1 = 8*np.random.rand(m, 1)
x2 = 7*np.random.rand(m, 1) - 4

g = 0.8*x1 + x2 - 3
```

```
C1 = np.where(g >= 1)
C2 = np.where(g < -1)
print(C1)
```



Perceptron Algorithm in Python

- Unknown parameters ω

$$g(x) = \omega_0 + \omega^T x = \omega_0 + \omega_1 x_1 + \omega_2 x_2 = 0$$

$$\omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} \qquad x = \begin{bmatrix} \left(x^{(1)}\right)^T \\ \left(x^{(2)}\right)^T \\ \left(x^{(3)}\right)^T \\ \vdots \\ \left(x^{(m)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ 1 & x_1^{(3)} & x_2^{(3)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(m)} & x_2^{(m)} \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

```python
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)
```

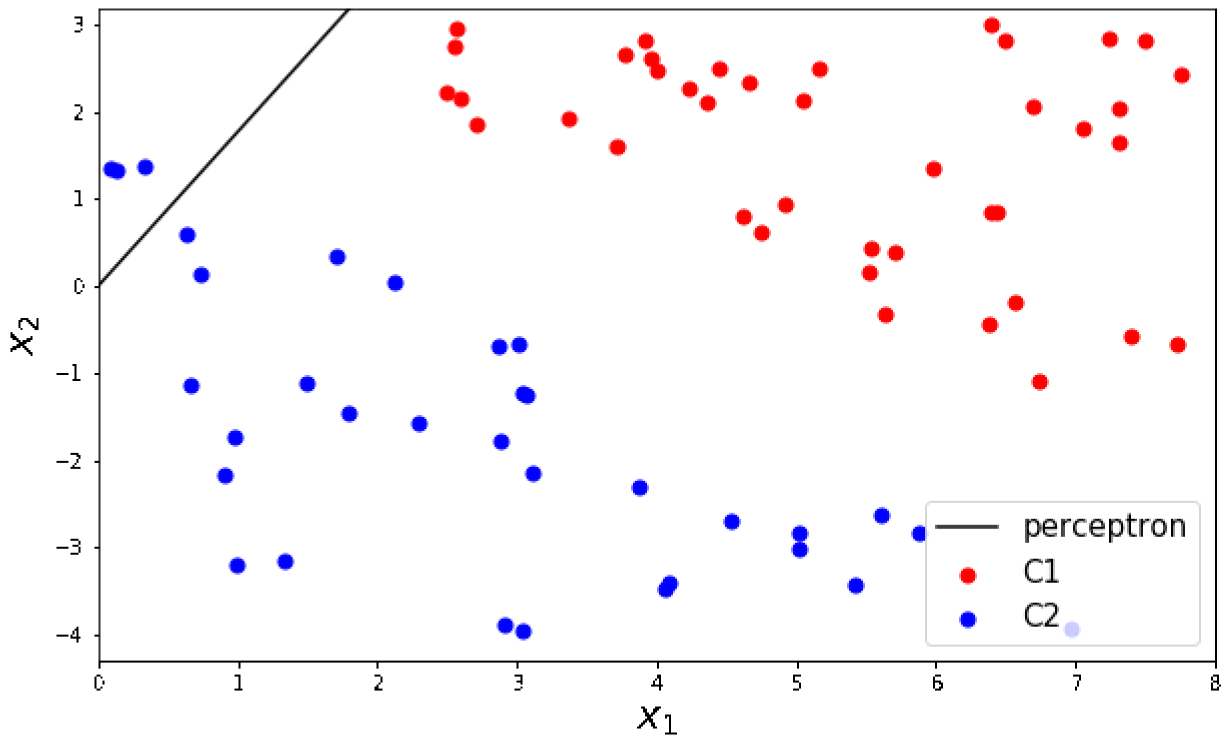
Perceptron Algorithm in Python

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

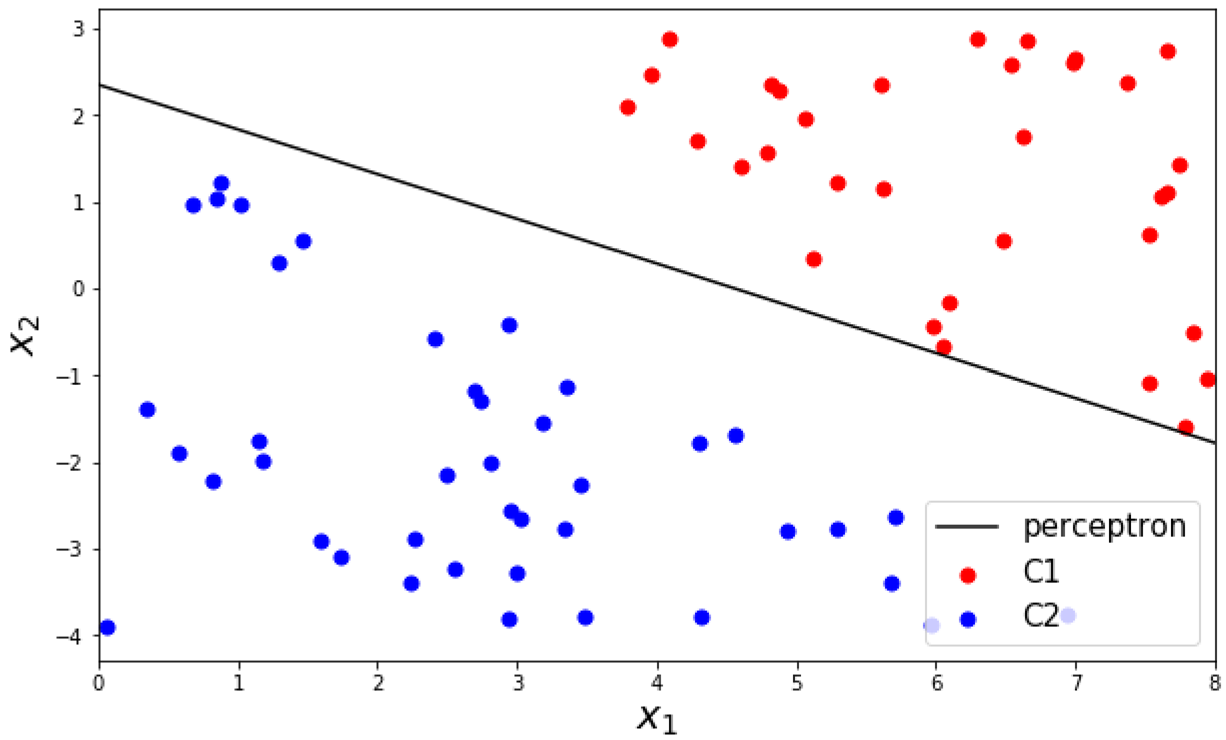
$\omega \leftarrow \omega + yx$ where (x, y) is a misclassified training point

```
w = np.ones([3,1])
w = np.asmatrix(w)

n_iter = y.shape[0]
for k in range(n_iter):
    for i in range(n_iter):
        if y[i,0] != np.sign(X[i,:]*w)[0,0]:
            w += y[i,0]*X[i,:].T

print(w)
```

Perceptron Algorithm in Python



Perceptron Algorithm in Python



Scikit-Learn for Perceptron

```
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]])
```

```
array([-1.])
```

$$x = \begin{bmatrix} \left(x^{(1)}\right)^T \\ \left(x^{(2)}\right)^T \\ \left(x^{(3)}\right)^T \\ \vdots \\ \left(x^{(m)}\right)^T \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} \\ x_1^{(2)} & x_2^{(2)} \\ x_1^{(3)} & x_2^{(3)} \\ \vdots & \vdots \\ x_1^{(m)} & x_2^{(m)} \end{bmatrix}$$

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

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 from all data samples
  - We will see this formally when we discuss the logistic regression

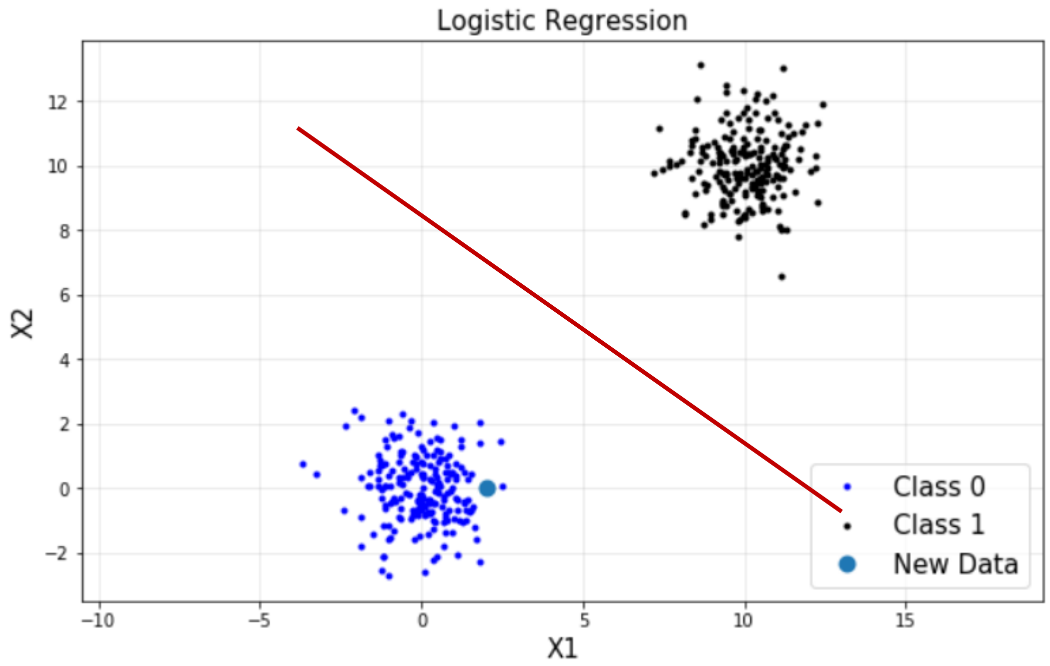
Classification: Logistic Regression

Classification: Logistic Regression

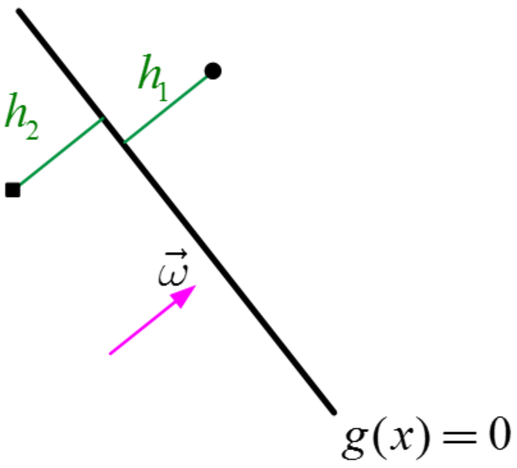
- Perceptron: make use of sign of data
- Logistic regression: make use of distance of data

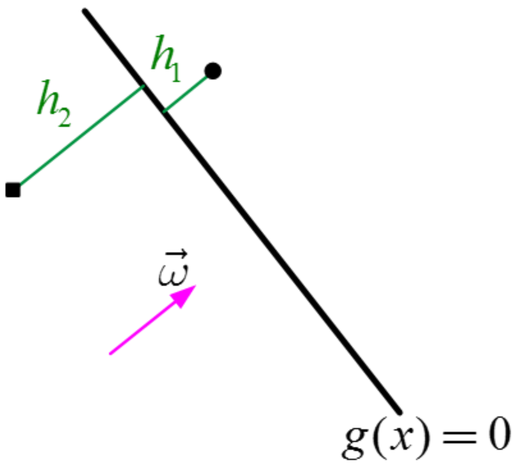
- Logistic regression is a classification algorithm
  - don't be confused from its name

- To find a classification boundary



Using Distances





$$|h_1| + |h_2|$$

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

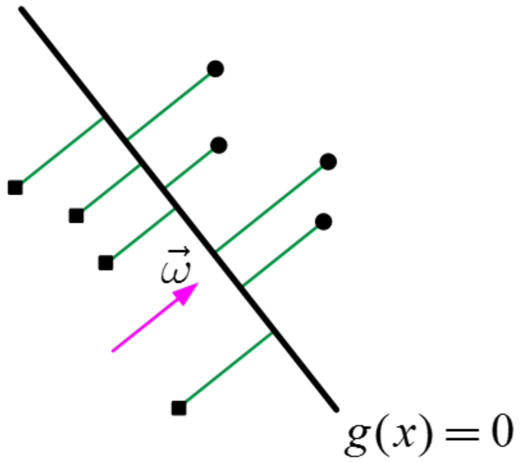
$$|h_1| + |h_2|$$

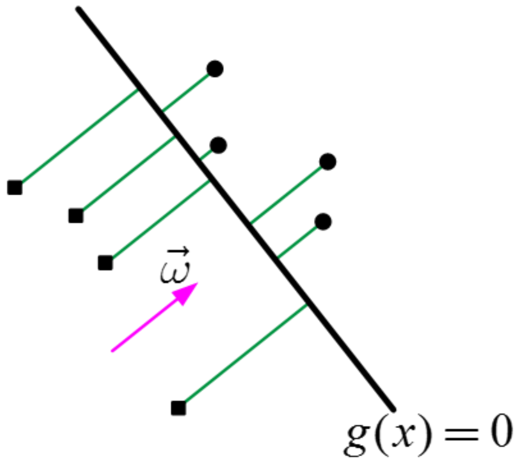
$$|h_1| \cdot |h_2|$$

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

Using all Distances

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



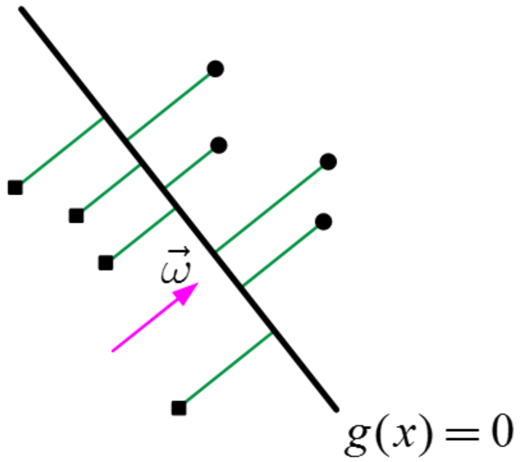


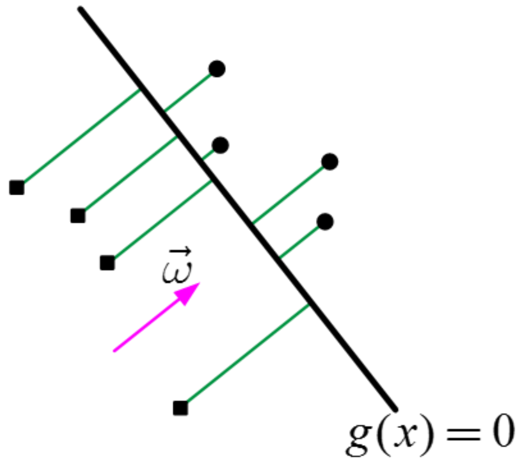
  – Inequality of arithmetic and geometric means

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

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

Using all Distances



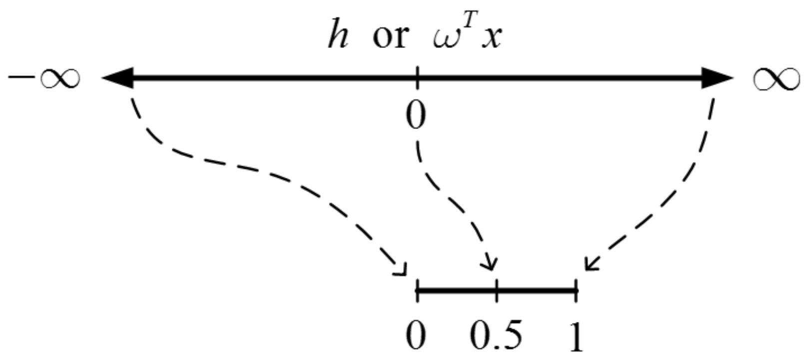


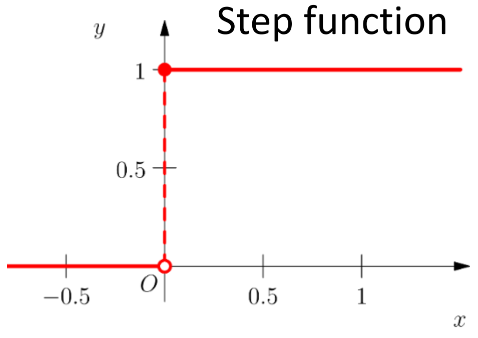
- Roughly speaking, this optimization of $\max \prod_i |h_i|$ tends to position a hyperplane in the middle of two classes

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

Sigmoid Function

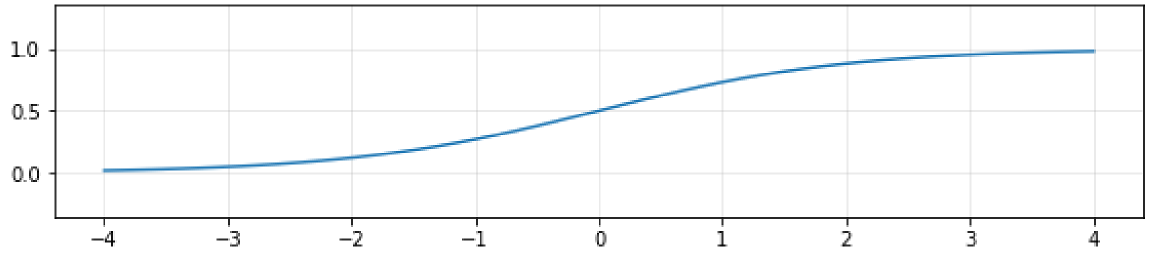
- We link or squeeze $(-\infty, +\infty)$ to $(0, 1)$ for several reasons:





- $\sigma(z)$ 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

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



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

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

  - Probability that the label is $+1$

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

  - Probability that the label is 0

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

Goal: we need to fit ω to our data

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

$$P\left(y=+1 \mid x ; \omega\right)=h_\omega(x)=\sigma\left(\omega^T x\right)$$
$$P\left(y=0 \mid x ; \omega\right)=1-h_\omega(x)=1-\sigma\left(\omega^T x\right)$$

- It can be compactly written as

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

$$\begin{aligned}
\mathscr{L}(\omega) &= P\left(y^{(1)}, \cdots, y^{(m)} \mid x^{(1)}, \cdots, x^{(m)} ; \omega\right) \\
&= \prod_{i=1}^{m} P\left(y^{(i)} \mid x^{(i)} ; \omega\right) \\
&= \prod_{i=1}^{m}\left(h_\omega\left(x^{(i)}\right)\right)^{y^{(i)}}\left(1-h_\omega\left(x^{(i)}\right)\right)^{1-y^{(i)}} \qquad \left(\sim \prod_{i}\left|h_i\right|\right)
\end{aligned}$$

Goal: we need to fit ω to our data

$$\begin{aligned}\mathscr{L}(\omega) &= P\left(y^{(1)}, \cdots, y^{(m)} \mid x^{(1)}, \cdots, x^{(m)} ; \omega\right) \\ &= \prod_{i=1}^{m} P\left(y^{(i)} \mid x^{(i)} ; \omega\right) \\ &= \prod_{i=1}^{m}\left(h_\omega\left(x^{(i)}\right)\right)^{y^{(i)}}\left(1-h_\omega\left(x^{(i)}\right)\right)^{1-y^{(i)}} \qquad \left(\sim \prod_{i} |h_i|\right)\end{aligned}$$

- It would be easier to work on the log likelihood.

$$\ell(\omega) = \boxed{}$$

cross-entropy later

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

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

- Again, it is an optimization problem

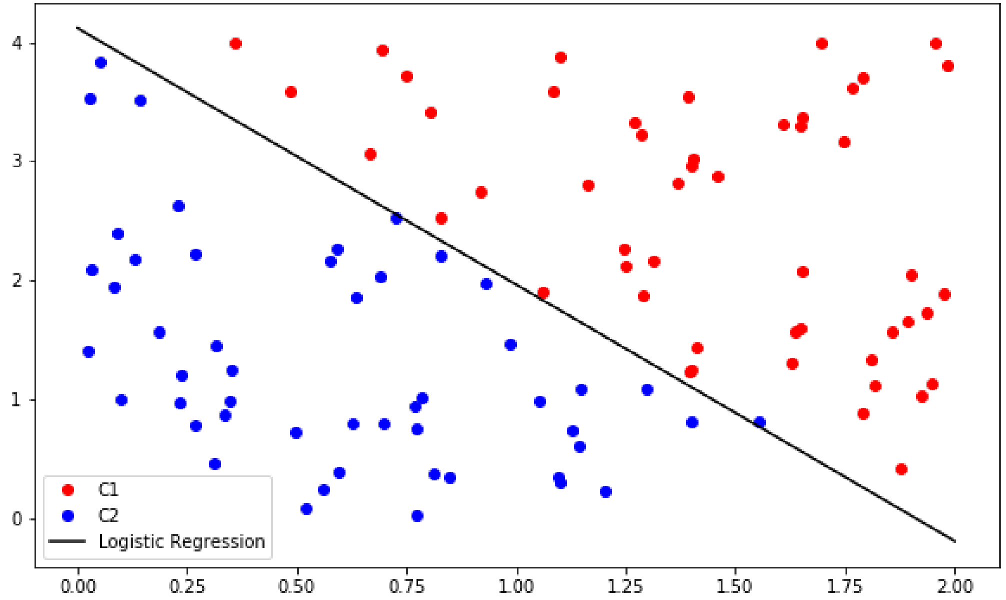
Scikit-Learn for Logistic Regression

$$\omega = \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix}, \qquad \omega_0, \qquad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$X = \begin{bmatrix} \left(x^{(1)}\right)^T \\ \left(x^{(2)}\right)^T \\ \left(x^{(3)}\right)^T \\ \vdots \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} \\ x_1^{(2)} & x_2^{(2)} \\ x_1^{(3)} & x_2^{(3)} \\ \vdots & \vdots \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \end{bmatrix}$$

```
from sklearn import linear_model

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

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

xp = np.linspace(0,2,100).reshape(-1,1)
yp = - w1/w2*xp - w0/w2

plt.figure(figsize = (10,6))
plt.plot(X[C1,0], X[C1,1], 'ro', label='C1')
plt.plot(X[C2,0], X[C2,1], 'bo', label='C2')
plt.plot(xp, yp, 'k', label='Logistic Regression')
plt.legend()
plt.show()
```



Multiclass Classification: Softmax

- 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
  - See them as probability

$$P\left(y=k \mid x, \omega\right)=\frac{\exp\left(\omega_k^T x\right)}{\sum_k \exp\left(\omega_k^T x\right)} \in [0,1]$$

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

  - Note: sigmoid function

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

Summary

- From parameter estimation of machine learning to optimization problems

Machine learning	**Optimization**
	Loss (or objective functions)
Regression	$\min_{\theta_1,\theta_2} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2$
Classification	$\ell(\omega) = \log \mathscr{L} = \log P(y \mid x, \omega) = \log \prod_{n=1}^{m} P(y_n \mid x_n, \omega) = \sum_{n=1}^{m} \log P(y_n \mid x_n, \omega)$