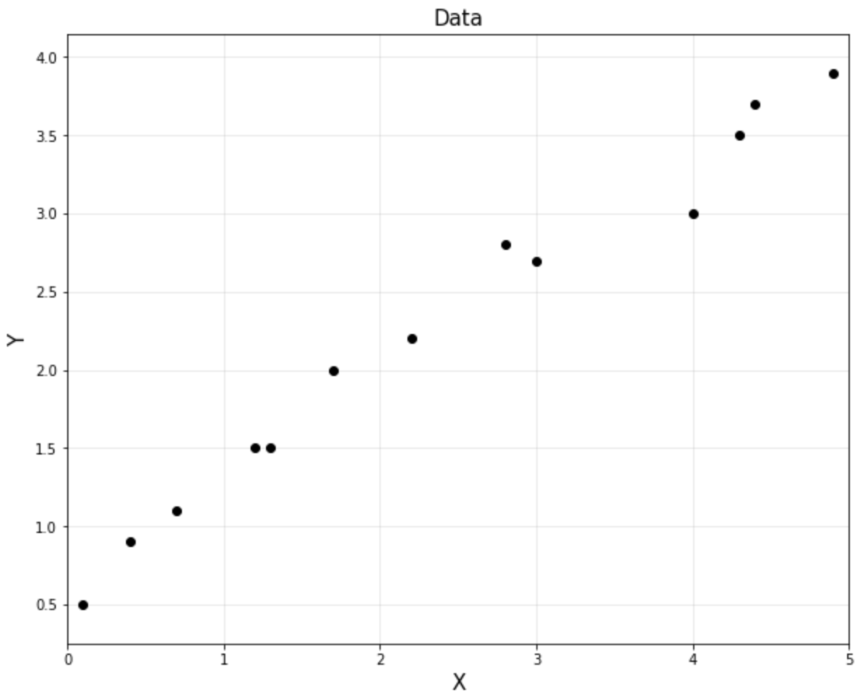
Machine Learning

Industrial AI Lab.
Prof. Seungchul Lee

Regression

Assumption: Linear Model

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

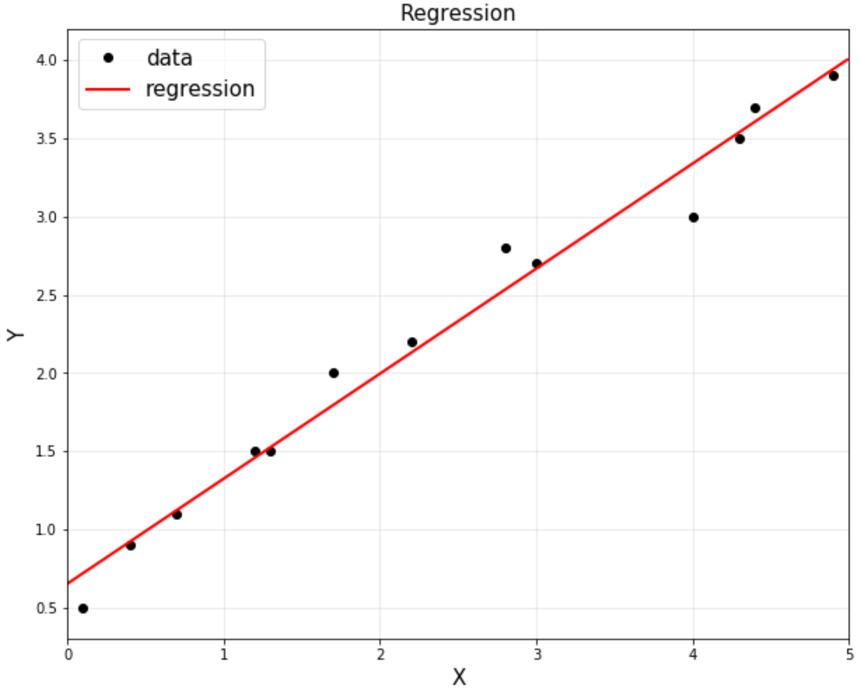


- In many cases, a linear model is used to predict y_i

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

Assumption: Linear Model

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

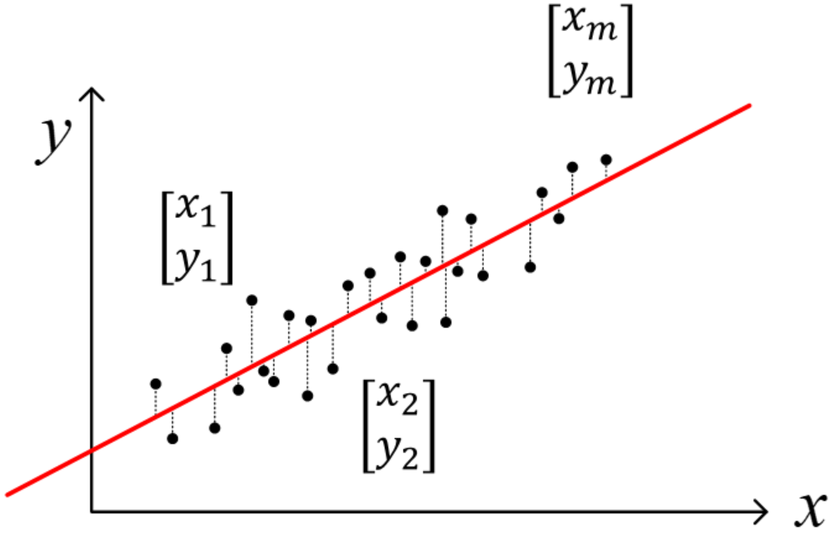


- In many cases, a linear model is used to predict y_i

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

Linear Regression

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



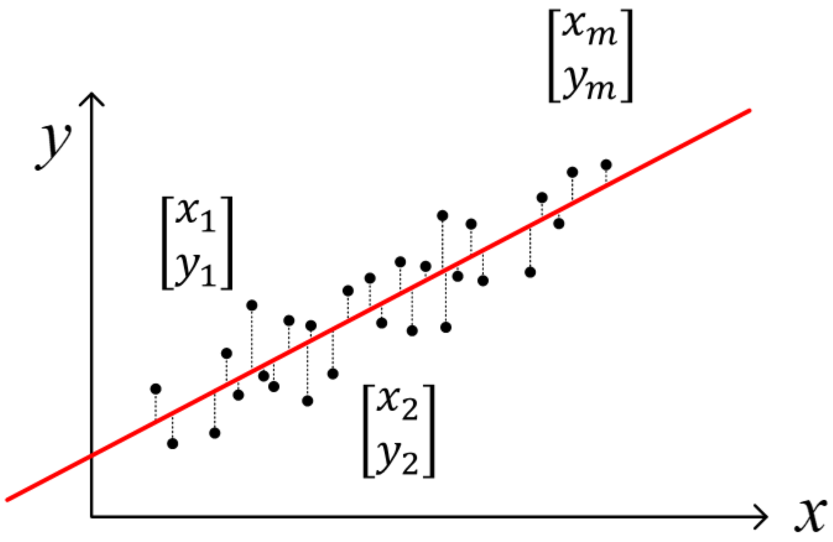
$$\text{Given} \begin{cases} x_i : \text{inputs} \\ y_i : \text{outputs} \end{cases}, \text{Find } \theta_0 \text{ and } \theta_1$$

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

- $\hat{y}_i$: 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

$$\hat{y}_i = \theta_0 + \theta_1 x_i \qquad \text{such that} \qquad \min_{\theta_0, \theta_1} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2$$

Re-cast Problem as Least Squares

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

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

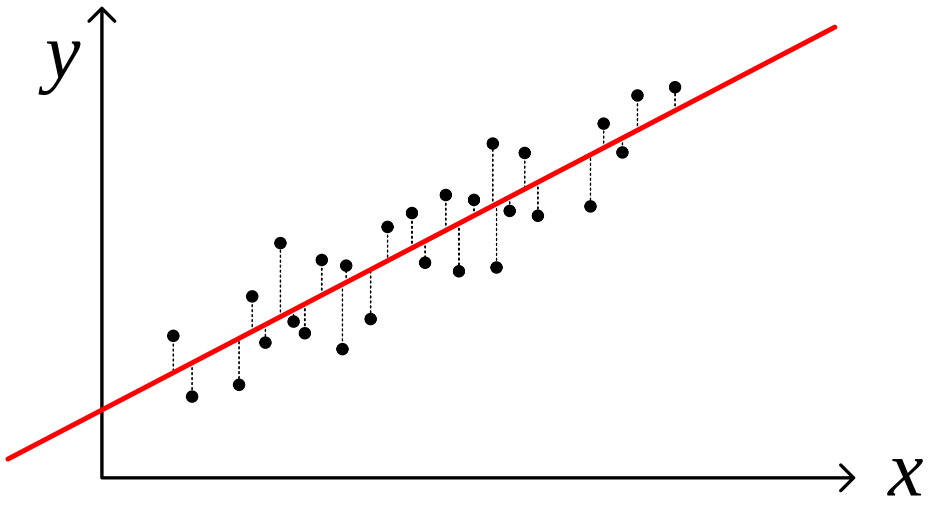
$$
\text{feature vector } \phi(x_i) = \begin{bmatrix} 1 \\ x_i \end{bmatrix}
$$

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

Optimization

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

$$\text{solution } \theta^* = (\Phi^T\Phi)^{-1}\Phi^T y$$



Optimization: Note

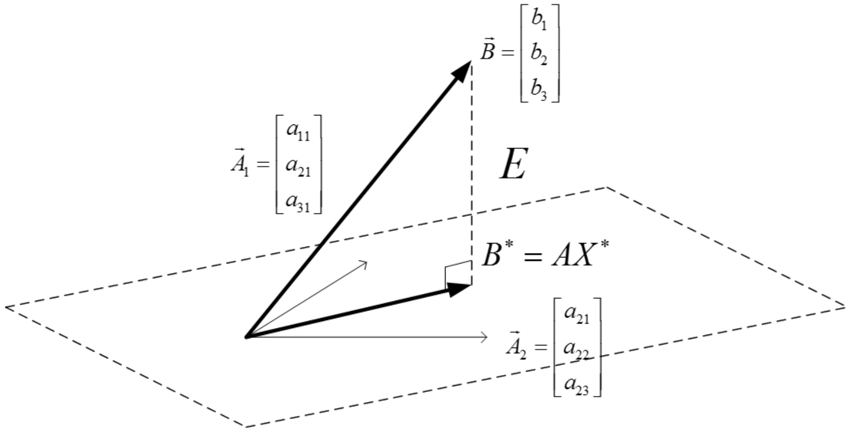
$$\begin{array}{ccccc} \text{input} & & \text{feature} & & \text{predicted output} \\ x_i & \rightarrow & \begin{bmatrix} 1 \\ x_i \end{bmatrix} & \rightarrow & \hat{y}_i \end{array}$$

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_m \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

$$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ \vec{A}_1 & \vec{A}_2 & \vec{x} & \vec{B} \end{array}$$

over-determined or
projection

$$A(=\Phi) = \left[\vec{A}_1 \ \vec{A}_2\right]$$



the same principle in a higher dimension

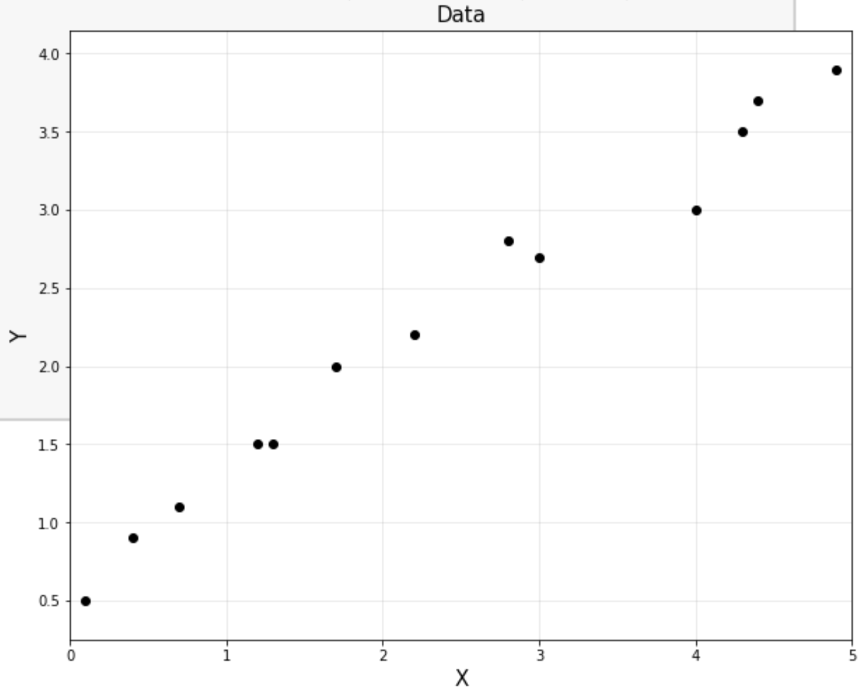
Solve using Linear Algebra

- 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, 4.9]).reshape(-1, 1)
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, 3.9]).reshape(-1, 1)

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()
```



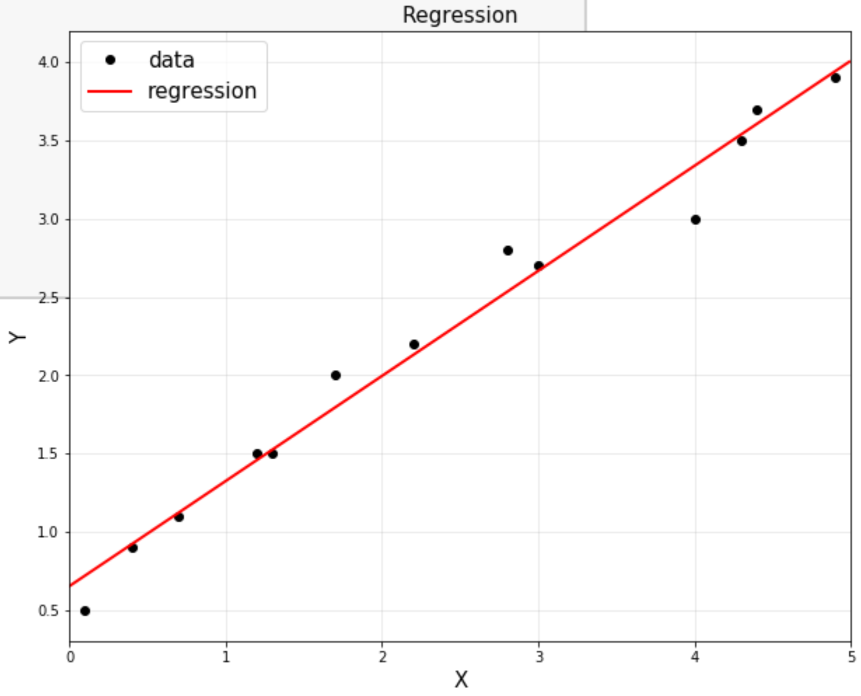
Solving using Linear Algebra

```python
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]]
```

Solving using Linear Algebra

```
# 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: Regression

```python
from sklearn import linear_model
```

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

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

```python
reg.coef_
```

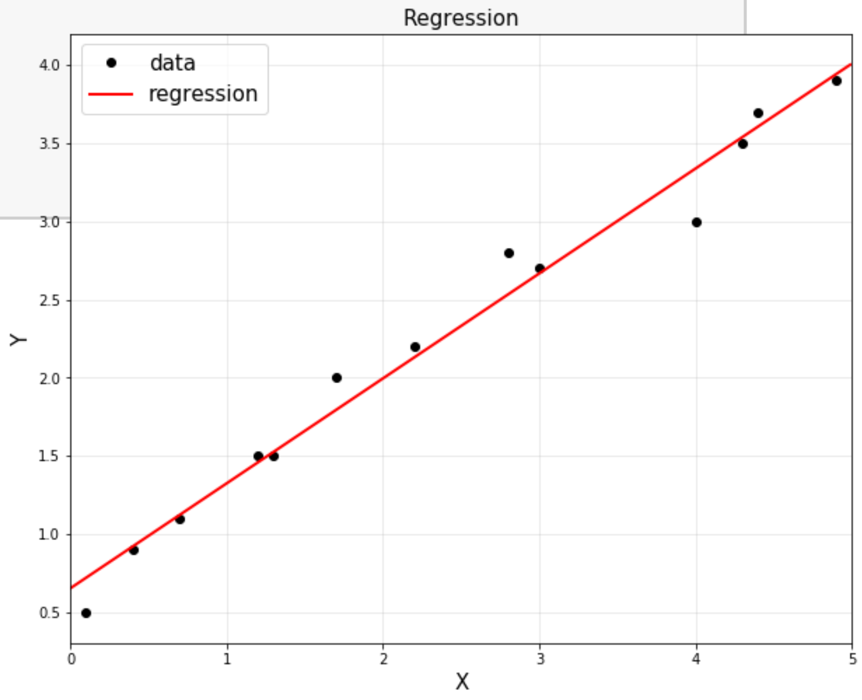
```
array([[0.67129519]])
```

```python
reg.intercept_
```

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

Scikit-Learn: Regression

```python
# 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

Classification

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

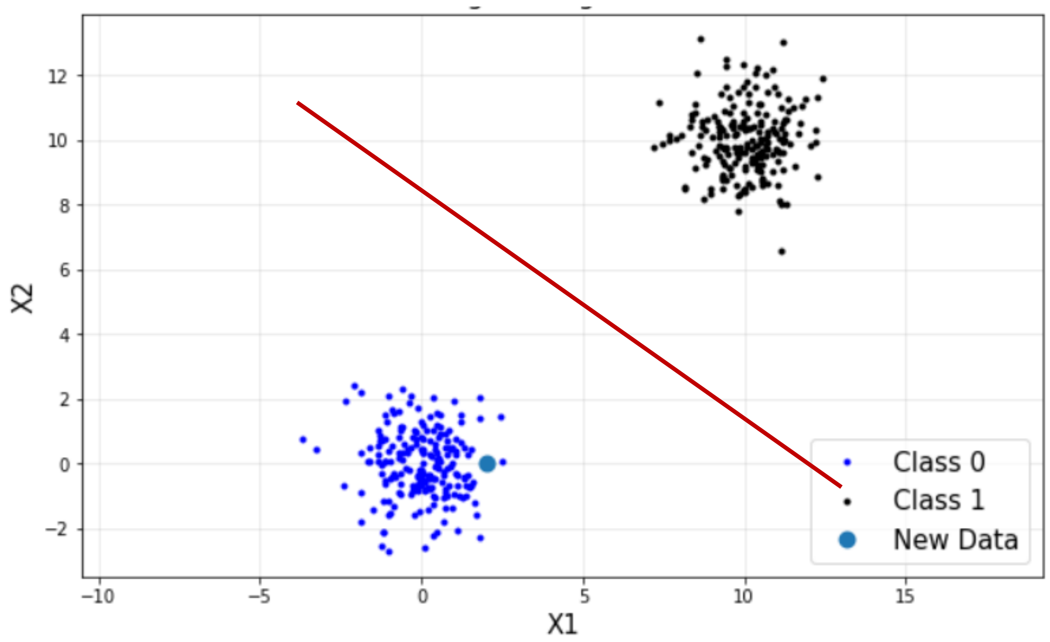
- Start with a binary class problem
  - Later look at multiclass classification problem, although this is just an extension of binary classification

- We could use linear regression
  - Then, threshold the classifier output (i.e. anything over some value is yes, else no)
  - linear regression with thresholding seems to work

Classification

- We will learn
  - Perceptron
  - Logistic regression

- To find a classification boundary

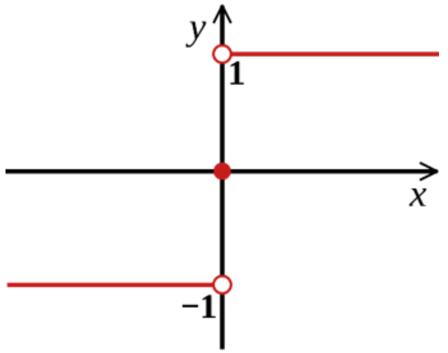


Perceptron

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

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

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



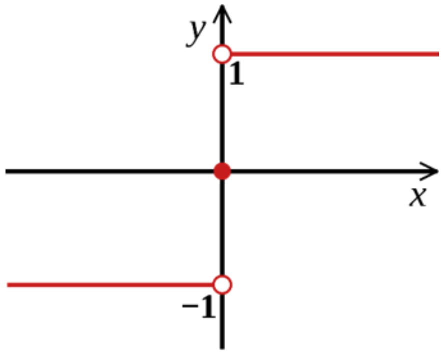
$$h(x) = \text{sign}\left(\left(\sum_{i=1}^{d} \omega_i x_i\right) - \text{threshold}\right) = \text{sign}\left(\left(\sum_{i=1}^{d} \omega_i x_i\right) + \omega_0\right)$$

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 $x_0 = 1$:

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



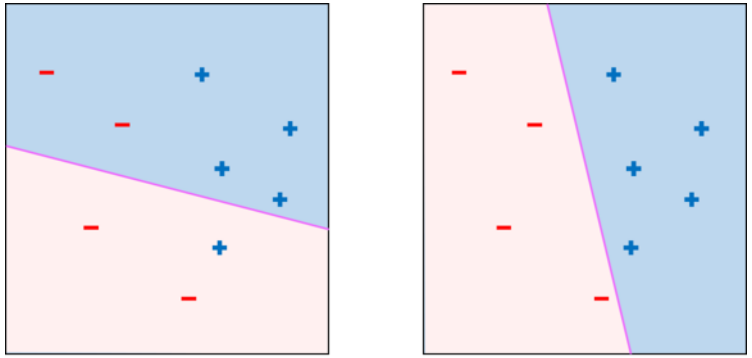
- In a vector form, the perceptron implements

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

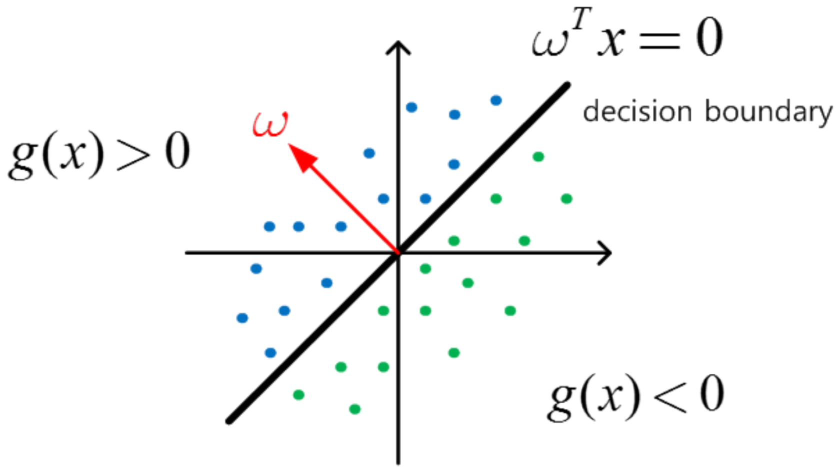
Perceptron

- Linearly separable data

- Hyperplane
  - Separates a D-dimensional space into two half-spaces
  - Defined by an outward pointing normal vector
  - ω 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

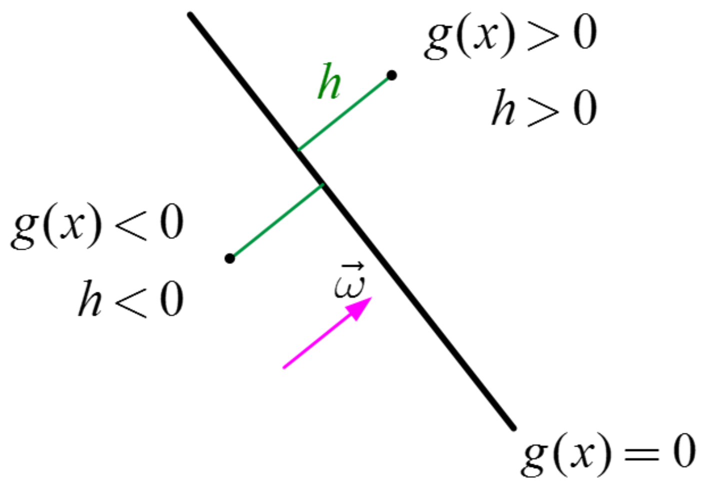


Sign

- Sign with respect to a line

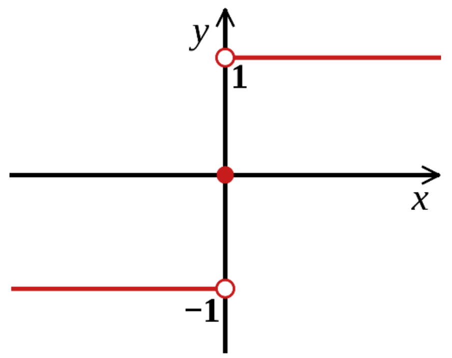
$$\omega = \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_1 x_1 + \omega_2 x_2 + \omega_0 = \omega^T x + \omega_0$$

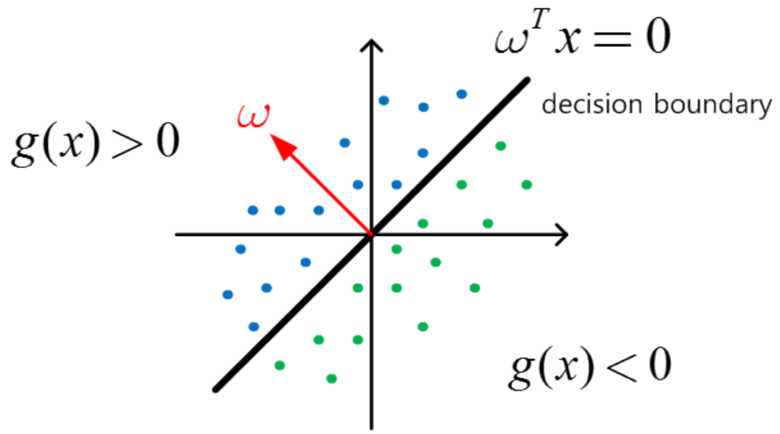
$$\omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix}, \quad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_0 + \omega_1 x_1 + \omega_2 x_2 = \omega^T x$$



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

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

- Given the training set

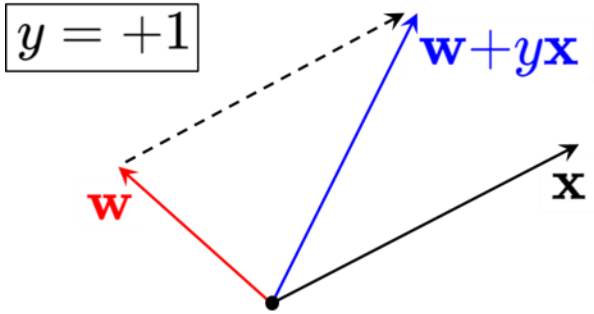
$$(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N) \quad \text{where } y_i \in \{-1, 1\}$$

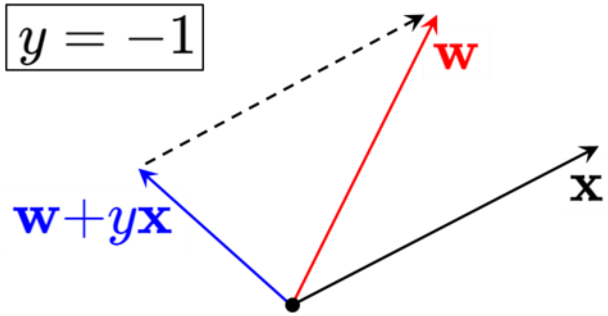
1) pick a misclassified point

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

2) and update the weight vector

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





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)

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

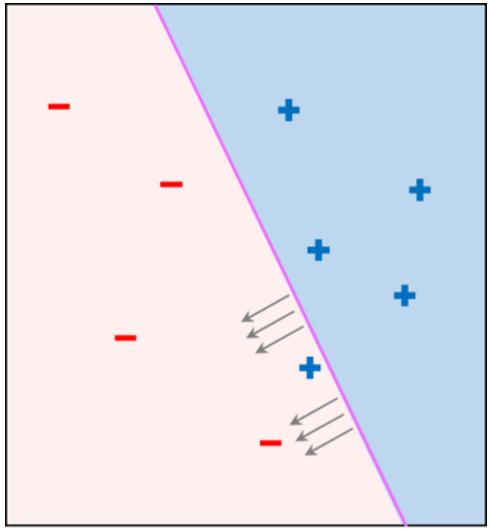
   where (x, y) is a misclassified training point

3. At iteration $t = 1,2,3,\cdots$, pick a misclassified point from

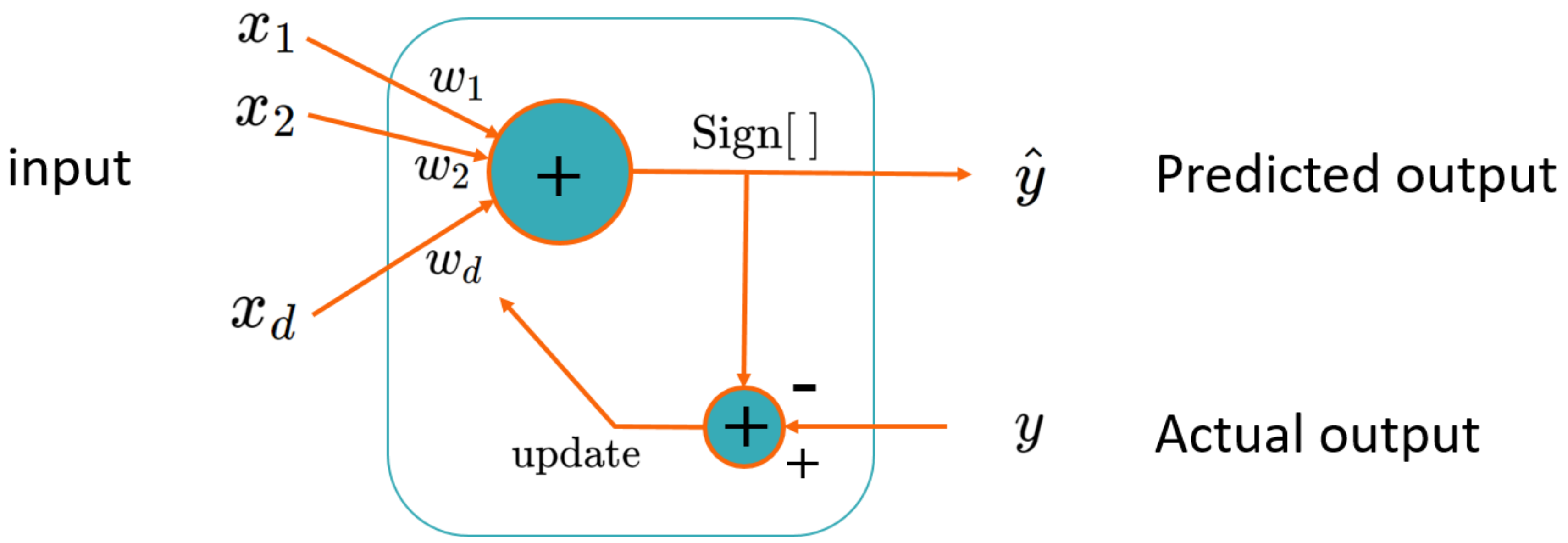
$$(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)$$

4. And run a PLA iteration on it

5. That's it!



Perceptron

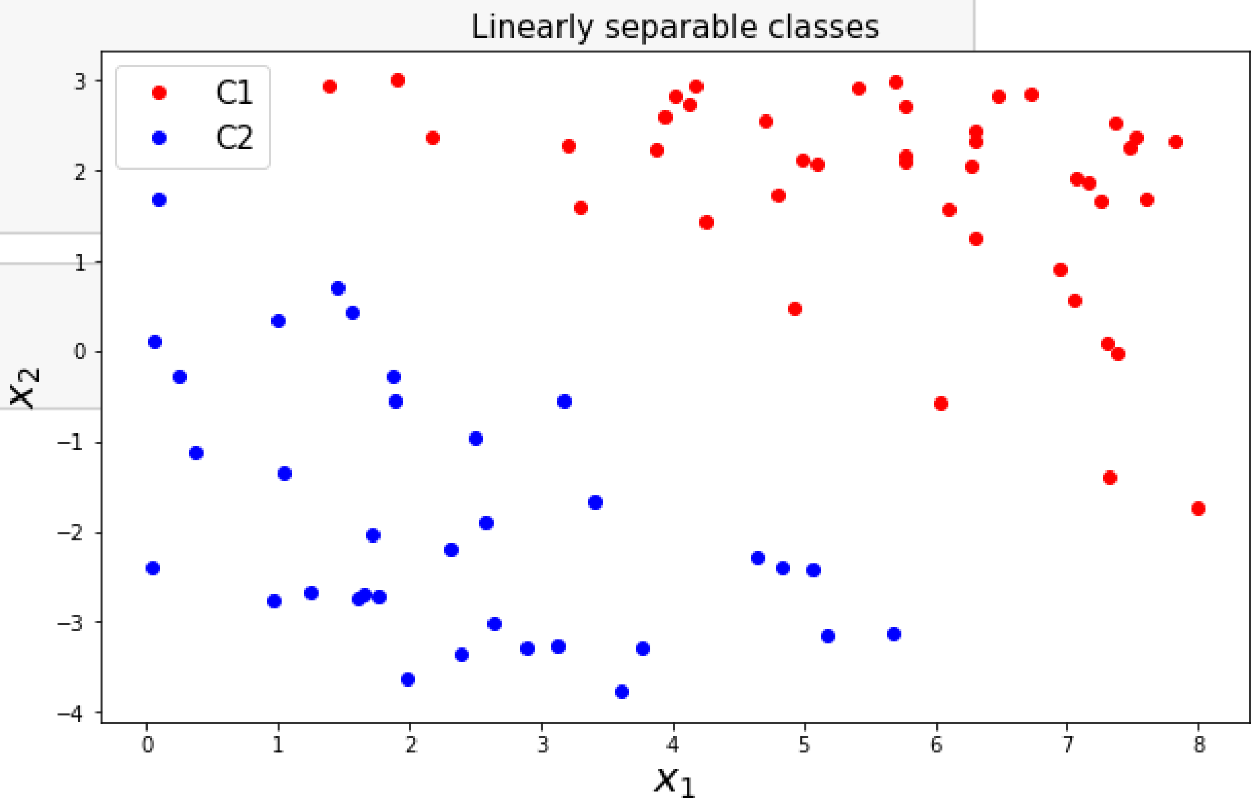

input
x_1
x_2
x_d
w_1
w_2
w_d
+
Sign[ ]
$\hat{y}$
Predicted output
-
+
+
update
y
Actual output

Python Example

```
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)
```



Python Example

- 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)
```

Python Example

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

$\omega \leftarrow \omega + yx$ 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)
```

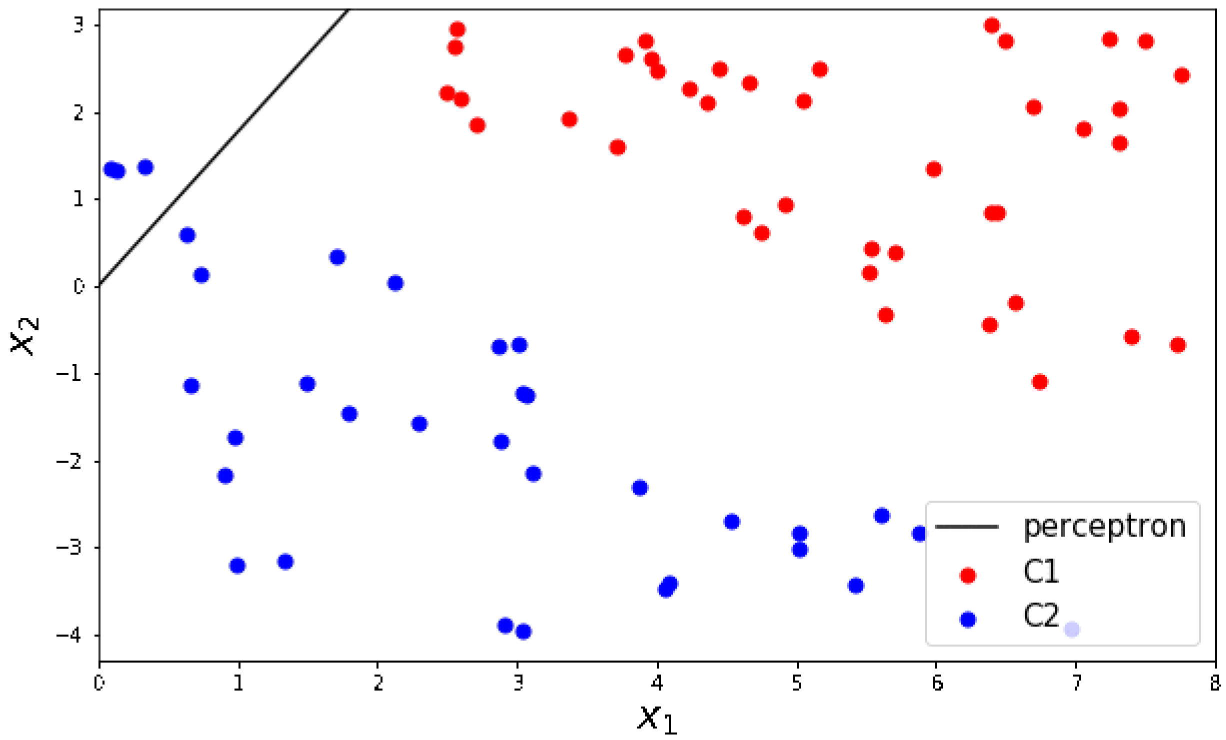
Python Example

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

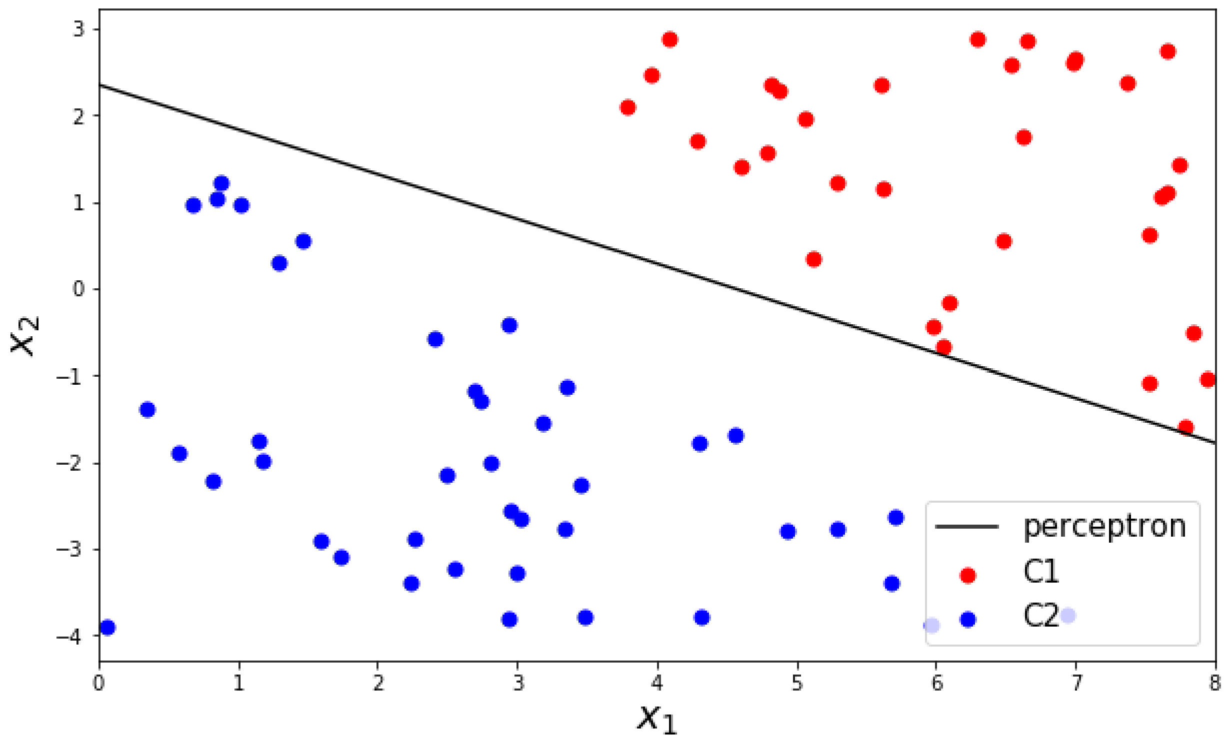
$$\Longrightarrow \quad x_2 = -\frac{\omega_1}{\omega_2} x_1 - \frac{\omega_0}{\omega_2}$$

```
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()
```

Python Example



Python Example



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]])
```

```
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
- 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)

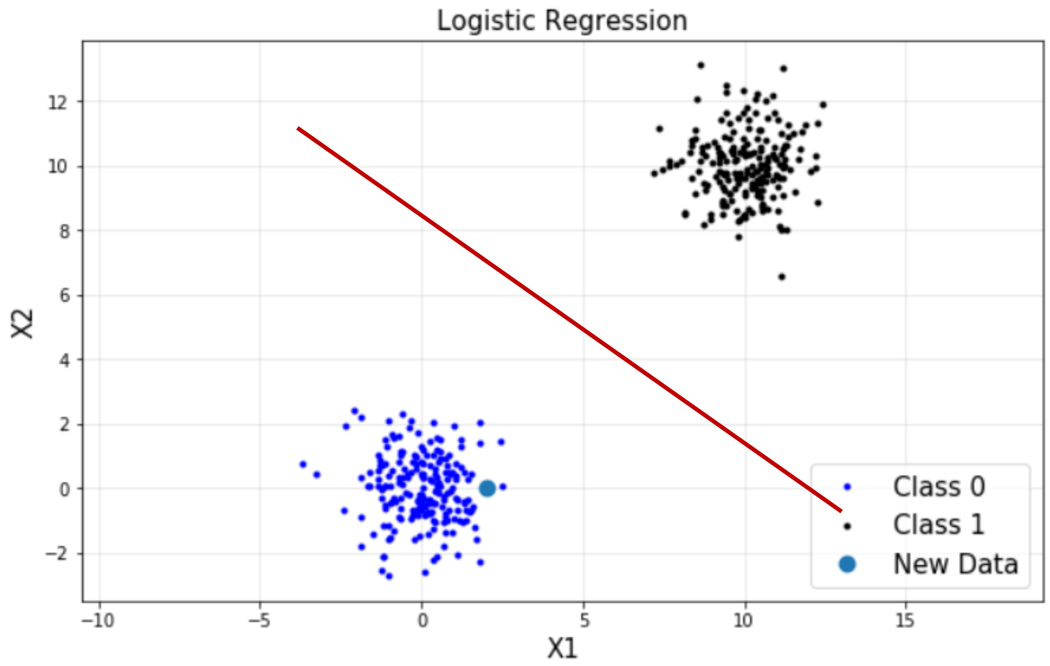
- Perceptron will be shown to be a basic unit for neural networks and deep learning later

Classification: Logistic Regression

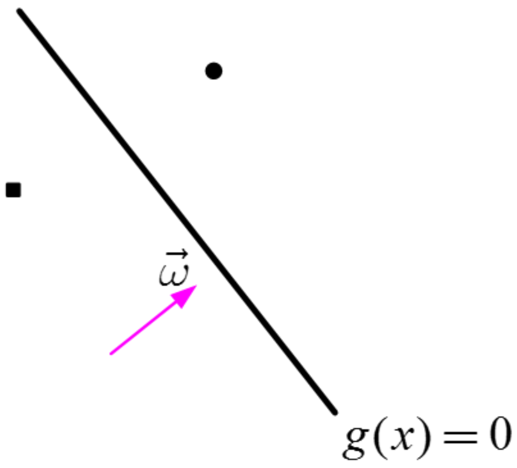
- Perceptron: make use of sign of data

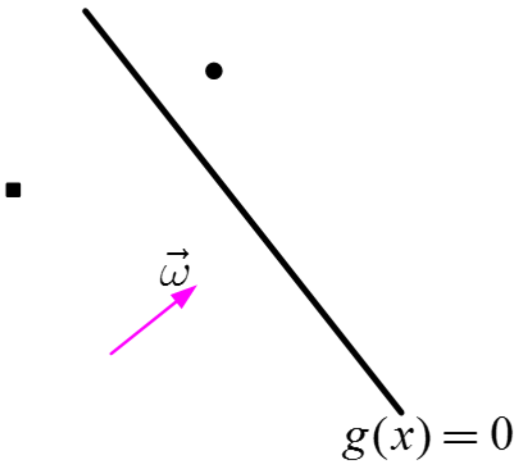
- Logistic regression is a classification algorithm
  - don't be confused from its name

- To find a classification boundary

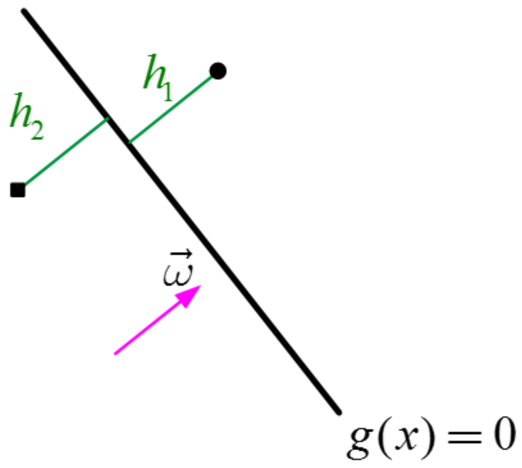


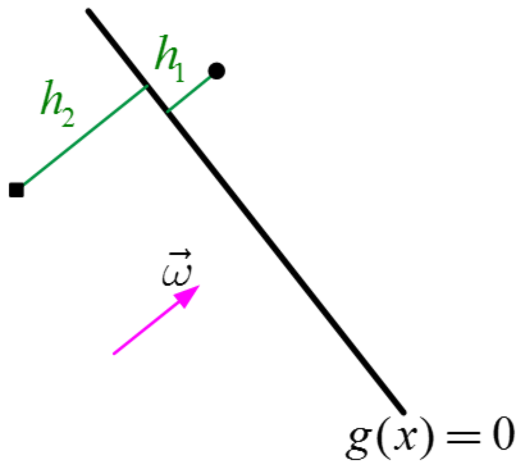
Using Distances





Using Distances





$$|h_1| + |h_2|$$

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

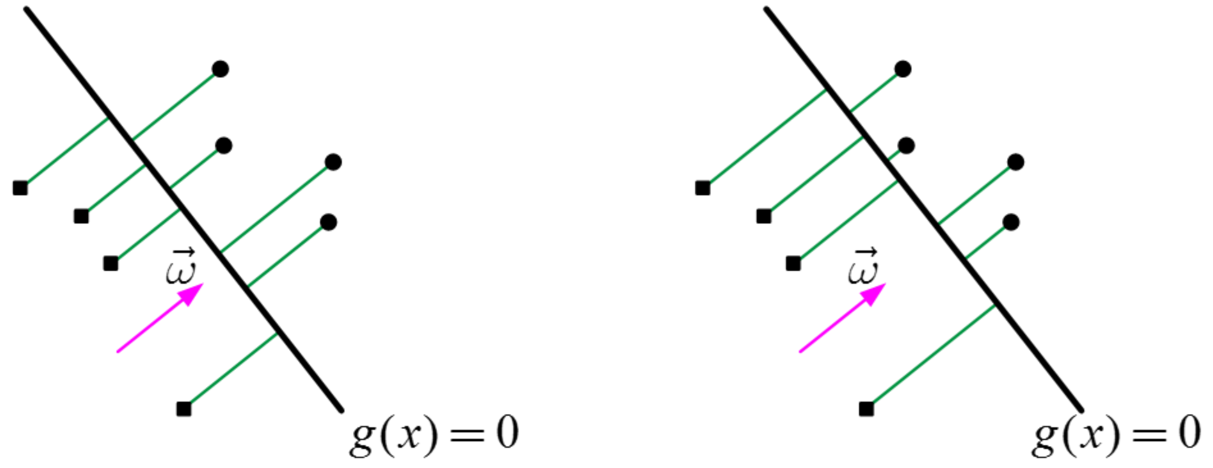
$$|h_1| + |h_2|$$

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

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

Using all Distances

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

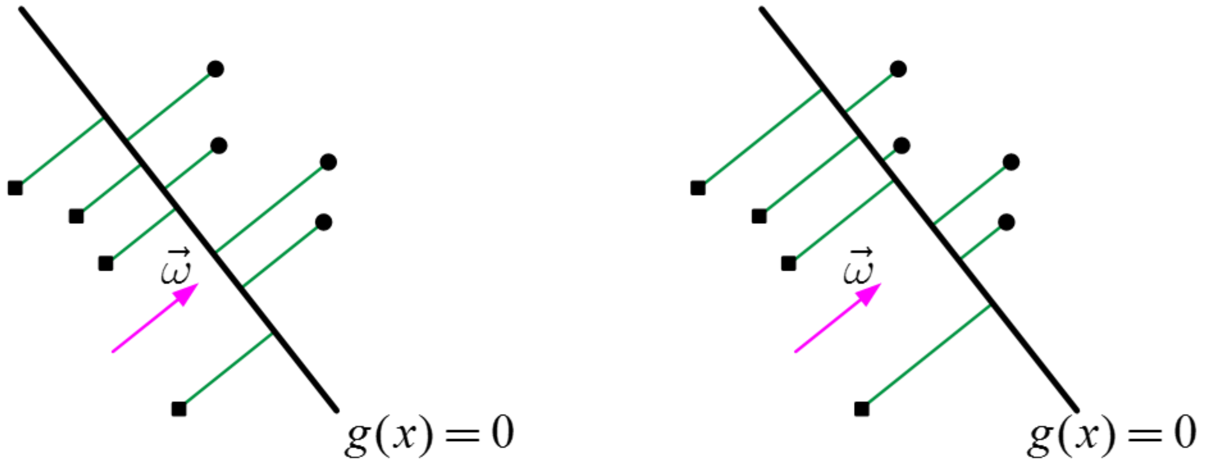


  – Inequality of arithmetic and geometric means

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

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

Using all Distances

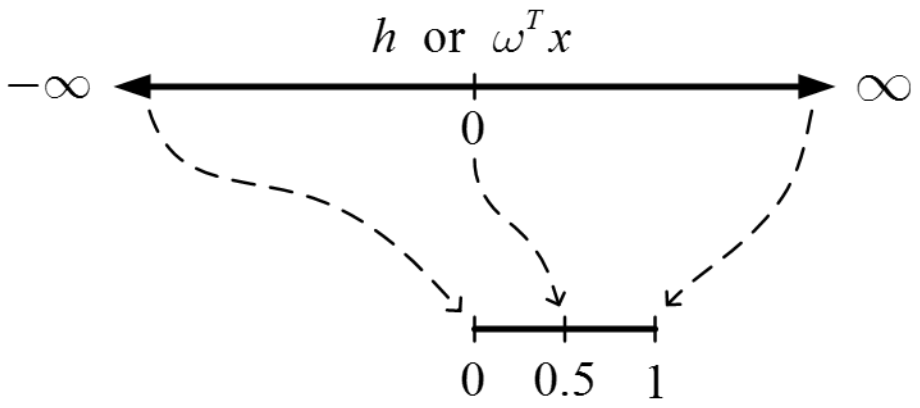


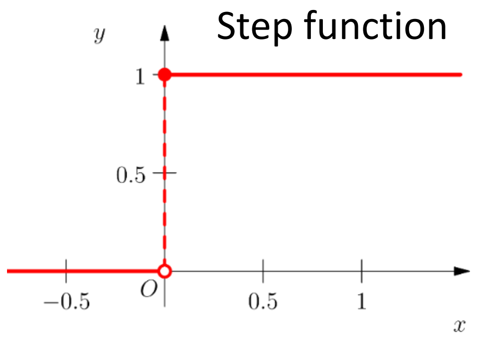
- Roughly speaking, this optimization of $\max \prod_i |h_i|$ tends to position a hyperplane in the middle of two classes

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

Sigmoid Function

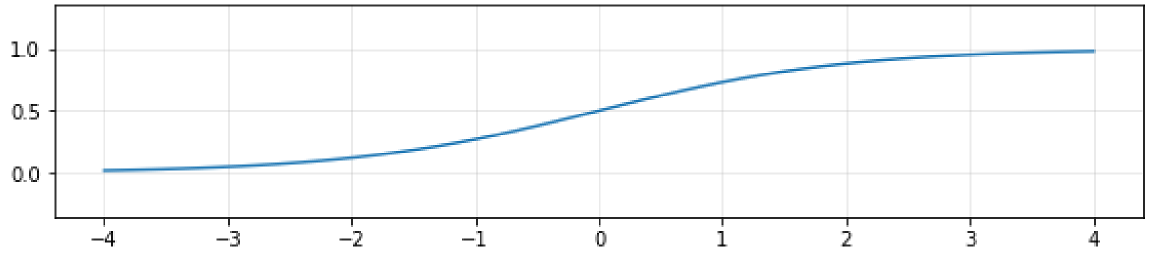
- We link or squeeze $(-\infty, +\infty)$ to $(0, 1)$ for several reasons:





- $\sigma(z)$ 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

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



Sigmoid Function

- The derivative of the sigmoid function satisfies

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

$$\sigma'(z) = \sigma(z)\,(1 - \sigma(z))$$

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

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

  - Probability that the label is $+1$

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

  - Probability that the label is 0

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

Goal: we need to fit ω to our data

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

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

- It can be 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:

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

- Again, it is an optimization problem

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.

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

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

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

Gradient Descent

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

$$\nabla \ell(\omega) = \begin{bmatrix} \frac{\partial \ell(\omega)}{\partial \omega_1} \\ \vdots \\ \frac{\partial \ell(\omega)}{\partial \omega_n} \end{bmatrix}$$

- We need to compute $\dfrac{\partial \ell(\omega)}{\partial \omega_j}$

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

Gradient Descent

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

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

$$\begin{aligned}
&\frac{\partial}{\partial \omega}[y \log(\sigma) + (1-y)\log(1-\sigma)] \\
&= y\frac{\sigma'}{\sigma} + (1-y)\frac{-\sigma}{1-\sigma} \\
&= \left(\frac{y}{\sigma} - \frac{1-y}{1-\sigma}\right)\sigma' \\
&= \frac{y-\sigma}{\sigma(1-\sigma)}\sigma' \\
&= \frac{y-\sigma}{\sigma(1-\sigma)}\sigma(1-\sigma)x \\
&= (y-\sigma)x
\end{aligned}$$

- For m training data points with parameters ω

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

Python Example

$$\omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix}, \qquad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}$$

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

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

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

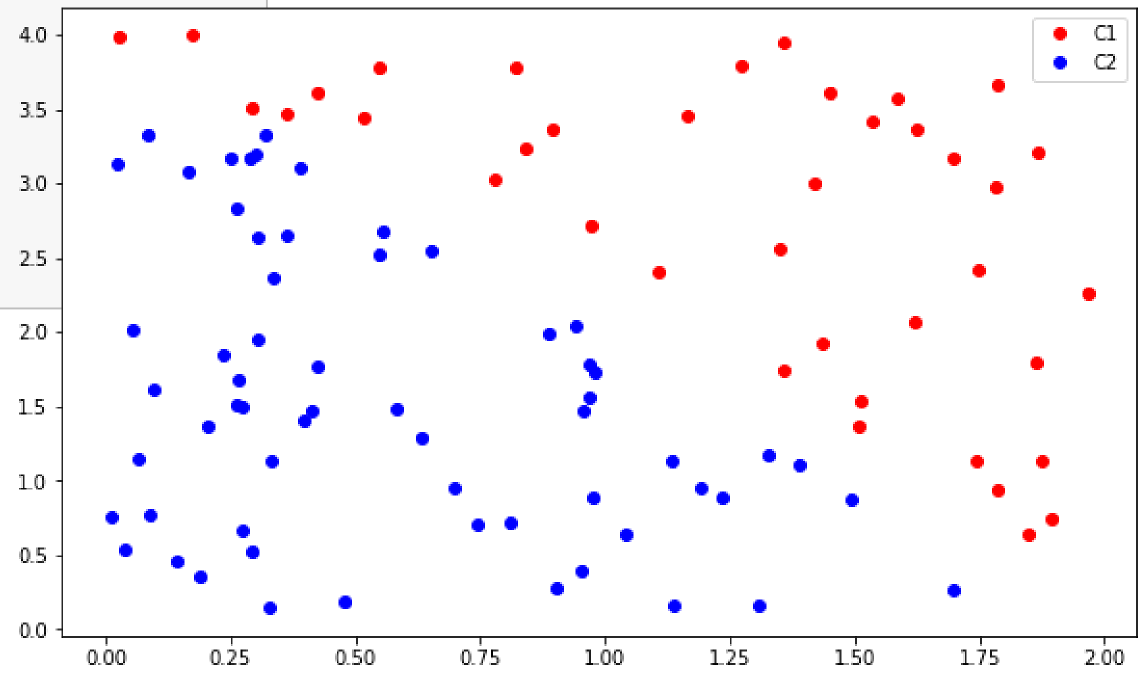
$$\overset{\text{vectorization}}{=} \quad (y - h_\omega(x))^T x_j = x_j^T \left(y - h_\omega(x)\right)$$

$$\nabla \ell(\omega) = \begin{bmatrix} \frac{\partial \ell(\omega)}{\partial \omega_0} \\ \frac{\partial \ell(\omega)}{\partial \omega_1} \\ \frac{\partial \ell(\omega)}{\partial \omega_2} \end{bmatrix} = X^T \left(y - h_\omega(x)\right) = X^T \left(y - \sigma(X\omega)\right)$$

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

Python Example

```python
# datat generation

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

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

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

C1 = np.where(y == True)[0]
C2 = np.where(y == False)[0]

y = np.empty([m,1])
y[C1] = 1
y[C2] = 0
y = np.asmatrix(y)
```



Python Example

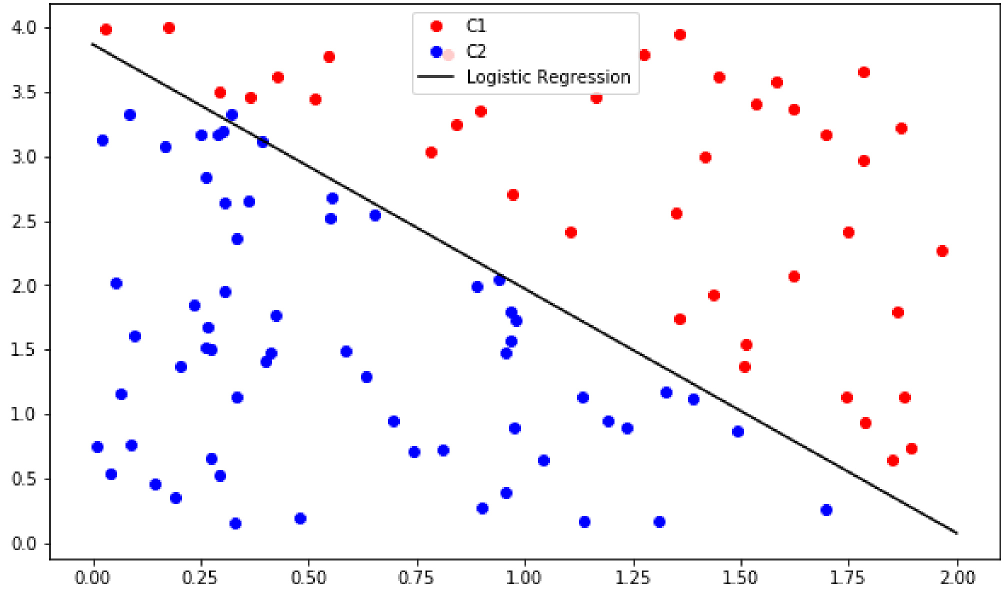
```python
# be careful with matrix shape

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

```python
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)
```

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

$$\nabla \ell(\omega) = \begin{bmatrix} \frac{\partial \ell(\omega)}{\partial \omega_0} \\ \frac{\partial \ell(\omega)}{\partial \omega_1} \\ \frac{\partial \ell(\omega)}{\partial \omega_2} \end{bmatrix} = X^T\left(y - h_\omega(x)\right) = X^T\left(y - \sigma(X\omega)\right)$$

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



Scikit-Learn

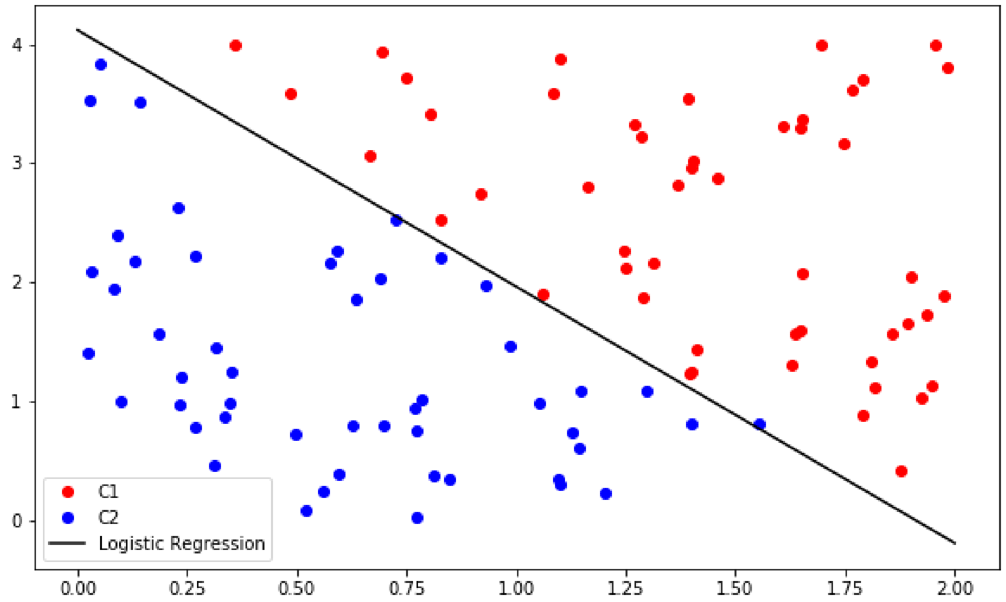
```
X = X[:,1:3]
```

```
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()
```

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

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



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

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

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	$$\begin{aligned} \ell(\omega) = \log \mathscr{L} = \log P(y \mid x, \omega) &= \log \prod_{n=1}^{m} P(y_n \mid x_n, \omega) \\ &= \sum_{n=1}^{m} \log P(y_n \mid x_n, \omega) \end{aligned}$$