Supervised Learning

without Scikit Learn

by Prof. Seungchul Lee
Industrial AI Lab
http://isystems.unist.ac.kr/
POSTECH

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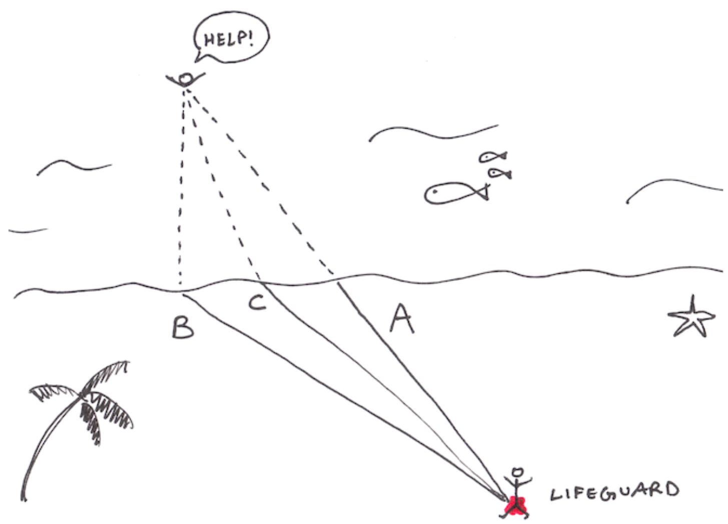
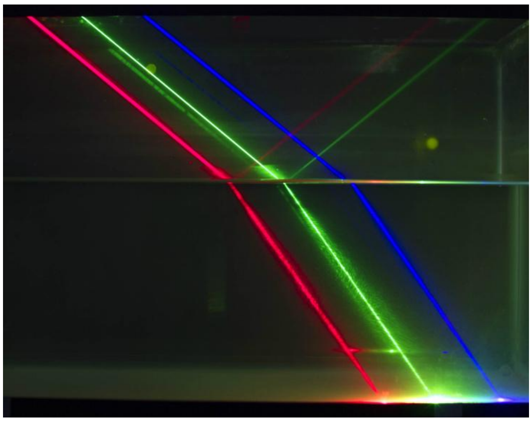
1. Optimization

- an important tool in 1) engineering problem solving and 2) decision science
- peolple optimize
- nature optimizes



(source: http://nautil.us/blog/to-save-drowning-people-ask-yourself-what-would-light-do (http://nautil.us/blog/to-save-drowning-people-ask-yourself-what-would-light-do))

3 key components

1. objective
2. decision variable or unknown
3. constraints

Procedures

1. The process of identifying objective, variables, and constraints for a given problem is known as "modeling"
2. Once the model has been formulated, optimization algorithm can be used to find its solutions.

In mathematical expression

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0, \qquad i = 1, \cdots, m \end{aligned}$$

Remarks) equivalent

$$\begin{aligned} \min_{x} f(x) \quad & \leftrightarrow \quad \max_{x} -f(x) \\ g_i(x) \leq 0 \quad & \leftrightarrow \quad -g_i(x) \geq 0 \\ h(x) = 0 \quad & \leftrightarrow \quad \begin{cases} h(x) \leq 0 & \text{and} \\ h(x) \geq 0 \end{cases} \end{aligned}$$

The good news: for many classes of optimization problems, people have already done all the "hardwork" of developing numerical algorithms

$$
\begin{array}{rl}
\max_x & x_1 + x_2 \\
\text{subject to} & 2x_1 + x_2 \leq 29 \\
& x_1 + 2x_2 \leq 25 \\
& x_1 \geq 2 \\
& x_2 \geq 5
\end{array}
\quad \Longrightarrow \quad
\begin{array}{rl}
\min_x & -\begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
\text{subject to} & \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leq \begin{bmatrix} 29 \\ 25 \end{bmatrix} \\
& \begin{bmatrix} 2 \\ 5 \end{bmatrix} \leq \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leq \begin{bmatrix} \\ \end{bmatrix}
\end{array}
$$

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import cvxpy as cvx

f = np.array([[1, 1]])
A = np.array([[2, 1], [1, 2]])
b = np.array([[29], [25]])
lb = np.array([[2], [5]])

x = cvx.Variable(2,1)
obj = cvx.Minimize(-f*x)
const = [A*x <= b, lb <= x]

prob = cvx.Problem(obj, const).solve()

print (x.value)
```

```
[[11.]
 [ 7.]]
```

2. Linear Regression

Begin by considering linear regression (easy to extend to more comlex predictions later on)

Given $\begin{cases} x_i : \text{inputs} \\ y_i : \text{outputs} \end{cases}$, find θ_1 and θ_2

$$
x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \approx \hat{y}_i = \theta_1 x_i + \theta_2
$$

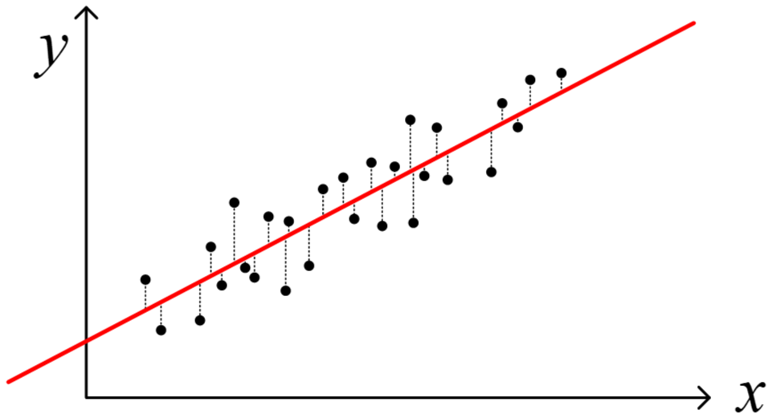
- $\hat{y}_i$: predicted output

- $\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$: Model parameters

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

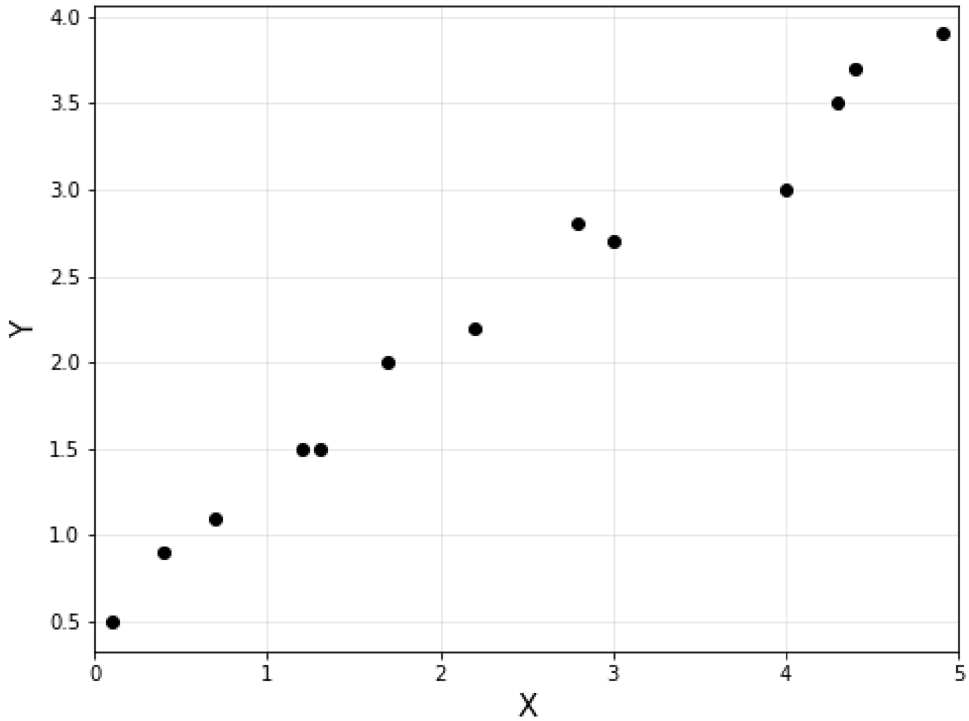
- In many cases, a linear model to predict y_i can be used

$$\hat{y}_i = \theta_1 x_i + \theta_2 \quad \text{such that} \quad \min_{\theta_1, \theta_2} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2$$



In [2]:

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

# 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)

# to plot
plt.figure(figsize=(10, 6))
plt.plot(x, y, 'ko', label="data")
plt.xlabel('X', fontsize=15)
plt.ylabel('Y', fontsize=15)
plt.axis('scaled')
plt.grid(alpha=0.3)
plt.xlim([0, 5])
plt.show()
```



Use CVXPY optimization (least squared)

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

$$
\begin{aligned}
\hat{y}_i &= \begin{bmatrix} x_i & 1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \\
&= \begin{bmatrix} x_i \\ 1 \end{bmatrix}^T \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \quad, \qquad \text{feature vector } \phi(x_i) = \begin{bmatrix} x_i \\ 1 \end{bmatrix} \\
&= \phi^T(x_i)\theta
\end{aligned}
$$

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

Model parameter estimation

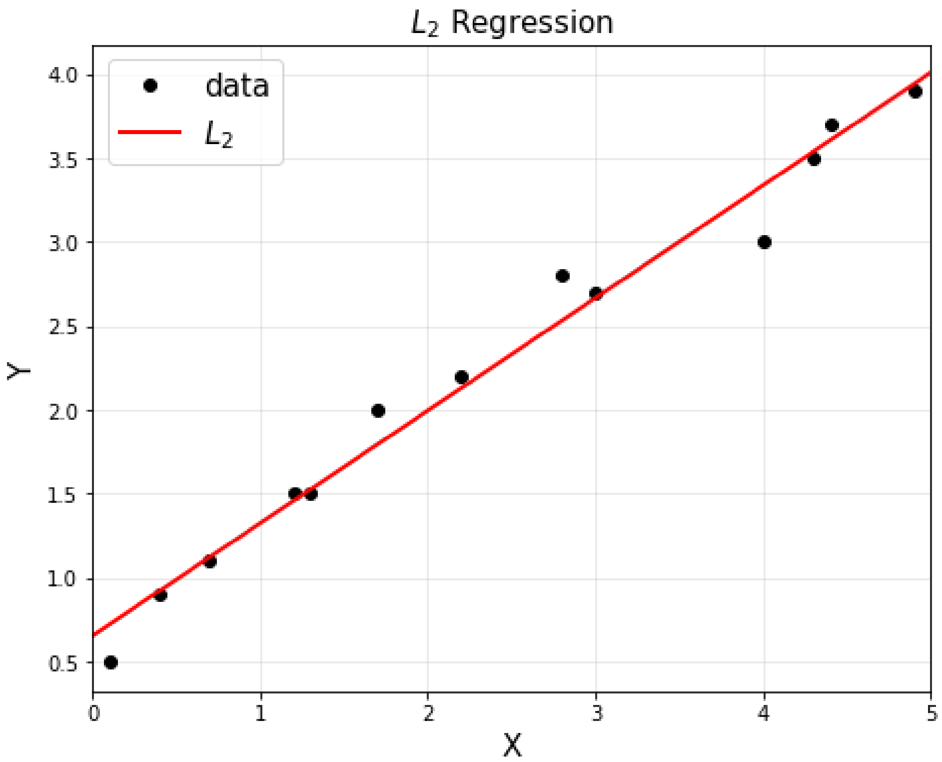
$$
\min_{\theta} \; \lVert \hat{y} - y \rVert_2 = \min_{\theta} \; \lVert \Phi\theta - y \rVert_2
$$

In [3]:

```python
import cvxpy as cvx

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

theta2 = cvx.Variable(2, 1)
obj = cvx.Minimize(cvx.norm(A*theta2-y, 2))
cvx.Problem(obj,[]).solve()

print('theta:\n', theta2.value)
```

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

In [4]:
```
# to plot
plt.figure(figsize=(10, 6))
plt.title('$L_2$ 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)
theta2 = theta2.value
yp = theta2[0,0]*xp + theta2[1,0]

plt.plot(xp, yp, 'r', linewidth=2, label="$L_2$")
plt.legend(fontsize=15)
plt.axis('scaled')
plt.grid(alpha=0.3)
plt.xlim([0, 5])
plt.show()
```



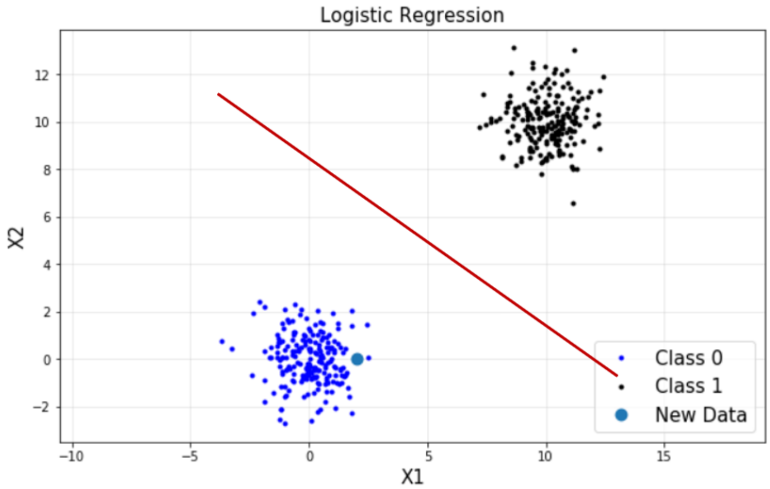
3. Classification (Linear)

- Figure out, autonomously, which category (or class) an unknown item should be categorized into
- Number of categories / classes
  - Binary: 2 different classes
  - Multiclass: more than 2 classes
- Feature
  - The measurable parts that make up the unknown item (or the information you have available to categorize)

- Perceptron: make use of sign of data
  - Discuss it later

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

- To find a classification boundary

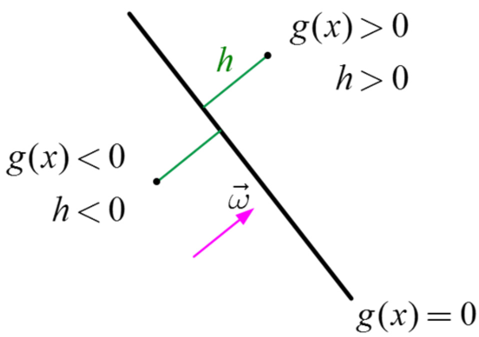


Sign

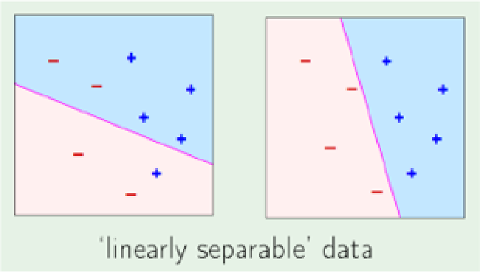
- Sign with respect to a line

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

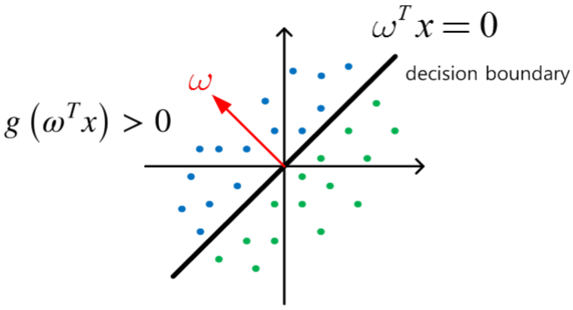
$$\omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix}, \qquad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \implies g(x) = \omega_0 + \omega_1 x_1 + \omega_2 x_2 = \omega^T x$$



Perceptron



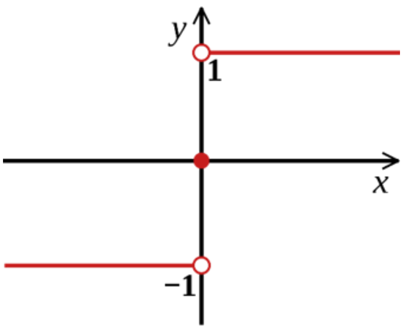
- Hyperplane
  - Separates a D-dimensional space into two half-spaces
  - Defined by an outward pointing normal vector
  - ω is orthogonal to any vector lying on the hyperplane



How to find ω

- All data in class 1
  - $g(\omega^T x) > 0$

- All data in class 0
  - $g(\omega^T x) < 0$



Perceptron Algorithm

The perceptron implements

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

Given the training set

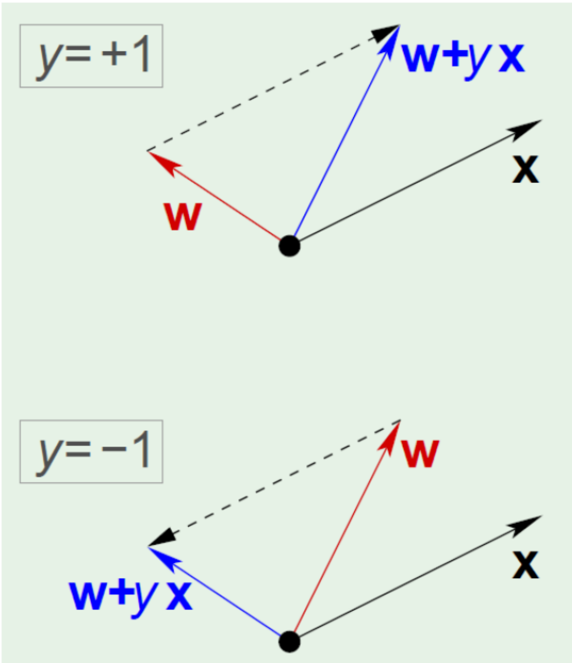
$$(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N) \quad \text{where } y_i \in \{-1, 1\}$$

1) pick a misclassified point

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

2) and update the weight vector

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



- 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 $\omega_{old}^T x_n$

In [5]:
```
import numpy as np
import matplotlib.pyplot as plt

% matplotlib inline
```

In [6]:
```
#training data gerneration
m = 100
x1 = 8*np.random.rand(m, 1)
x2 = 7*np.random.rand(m, 1) - 4

g0 = 0.8*x1 + x2 - 3
g1 = g0 - 1
g2 = g0 + 1
```

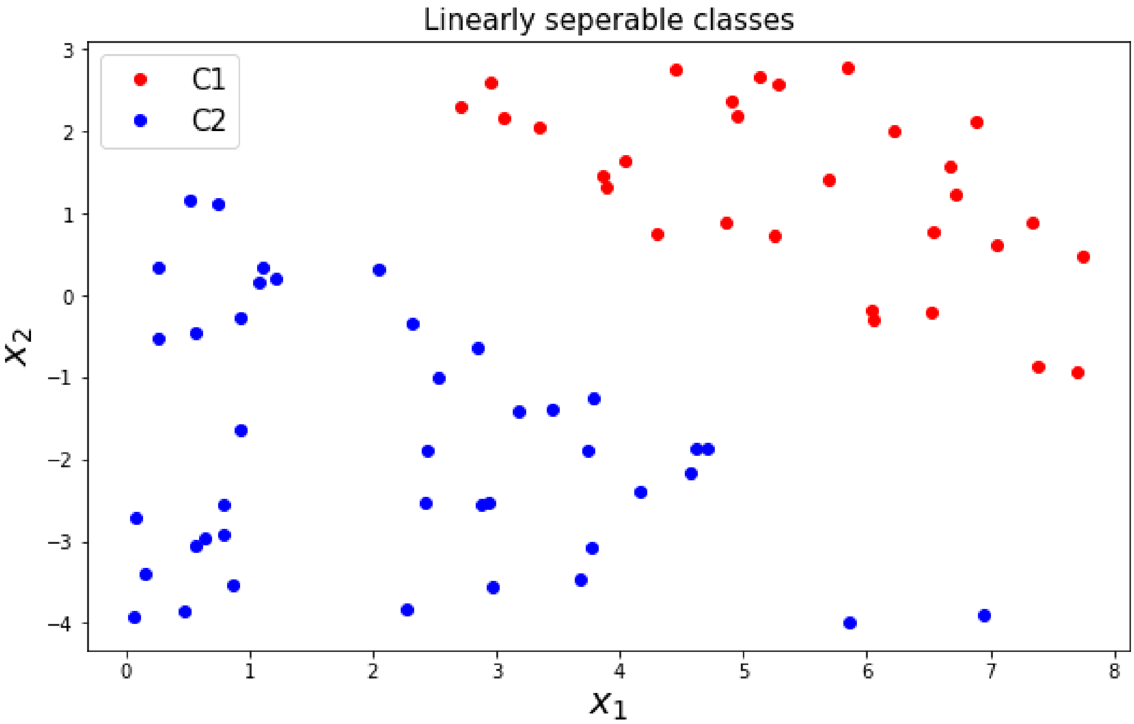
In [7]:
```
C1 = np.where(g1 >= 0)
C2 = np.where(g2 < 0)
print(C1)
```

```
(array([ 0,  2,  4,  5,  6,  7, 10, 17, 22, 24, 25, 27, 28, 30, 31, 38, 51,
       52, 53, 56, 57, 61, 62, 64, 70, 78, 85, 86, 89, 98], dtype=int64), a
rray([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0], dtype=int64))
```

In [8]:
```
C1 = np.where(g1 >= 0)[0]
C2 = np.where(g2 < 0)[0]
print(C1.shape)
print(C2.shape)
```

```
(30,)
(41,)
```

In [9]:
```
plt.figure(figsize=(10, 6))
plt.plot(x1[C1], x2[C1], 'ro', label='C1')
plt.plot(x1[C2], x2[C2], 'bo', label='C2')
plt.title('Linearly seperable classes', fontsize=15)
plt.legend(loc='upper left', fontsize=15)
plt.xlabel(r'$x_1$', fontsize=20)
plt.ylabel(r'$x_2$', fontsize=20)
plt.show()
```



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

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

In [10]:

```
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)
```

$$\omega = \begin{bmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{bmatrix}$$

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

where (x, y) is a misclassified training point

In [11]:

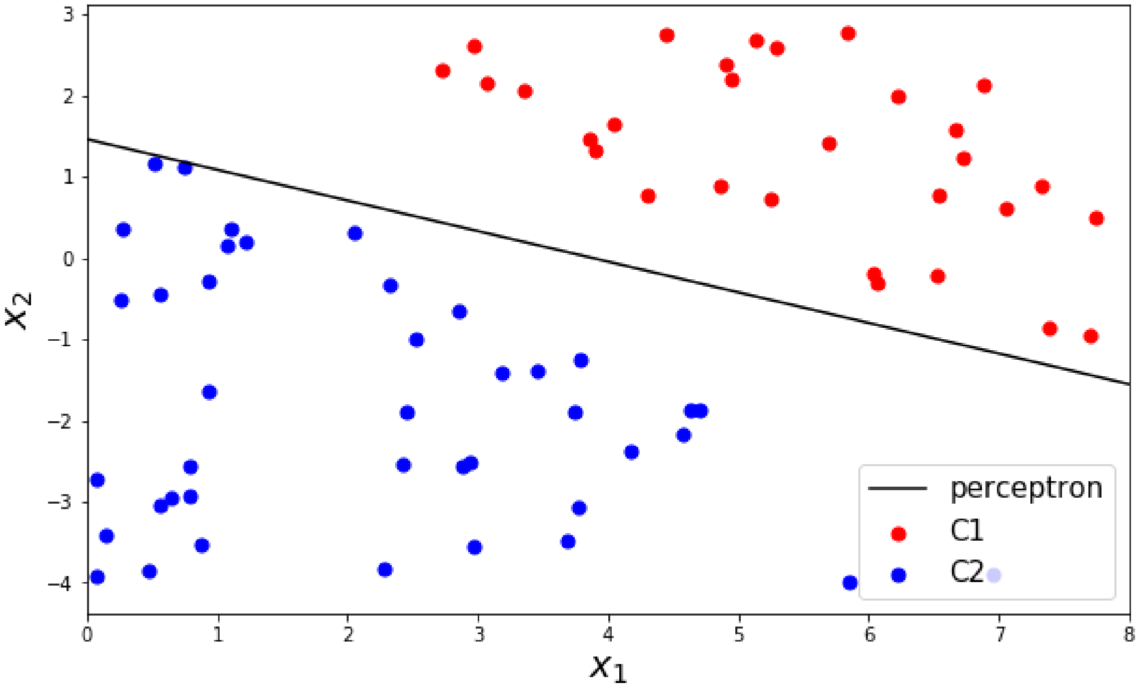
```
w = np.ones([3,1])
w = np.asmatrix(w)

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)
```

```
[[-13.        ]
 [  3.35733863]
 [  8.90909811]]
```

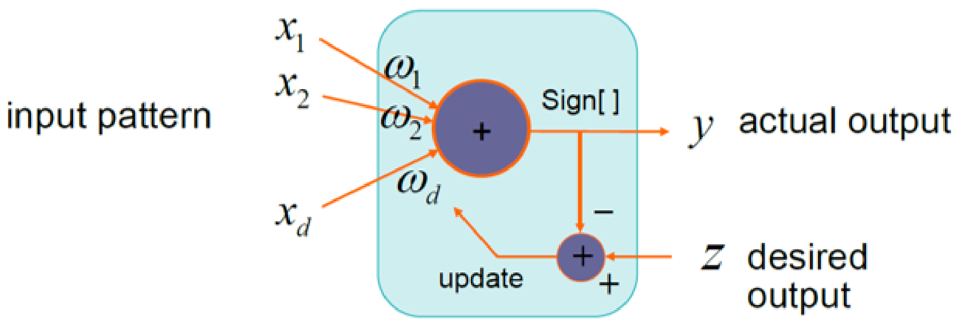
$$\begin{aligned} g(x) &= \omega^T x + \omega_0 = \omega_1 x_1 + \omega_2 x_2 + \omega_0 = 0 \\ \implies x_2 &= -\frac{\omega_1}{\omega_2} x_1 - \frac{\omega_0}{\omega_2} \end{aligned}$$

Not a unique solution

In [12]:
```
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 = 4, fontsize = 15)
plt.show()
```

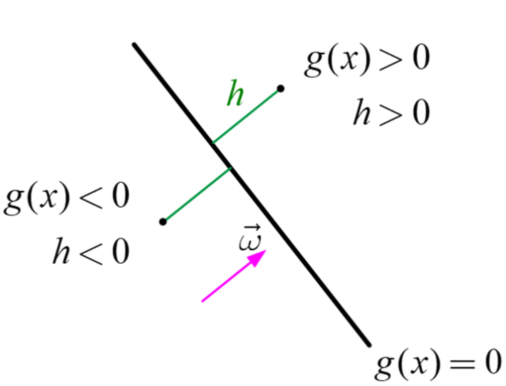


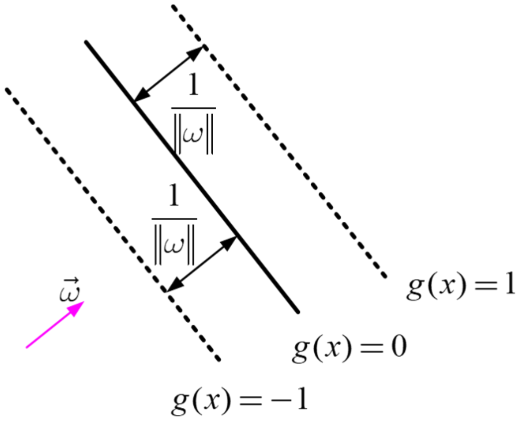
Perceptron

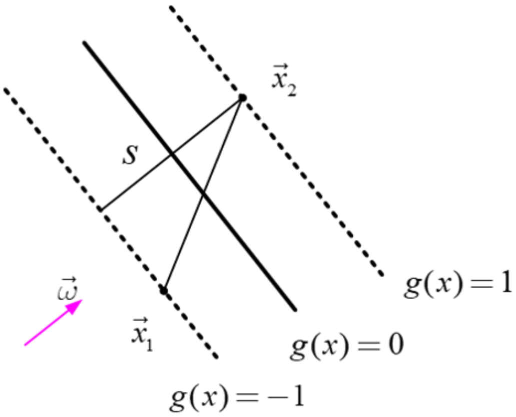


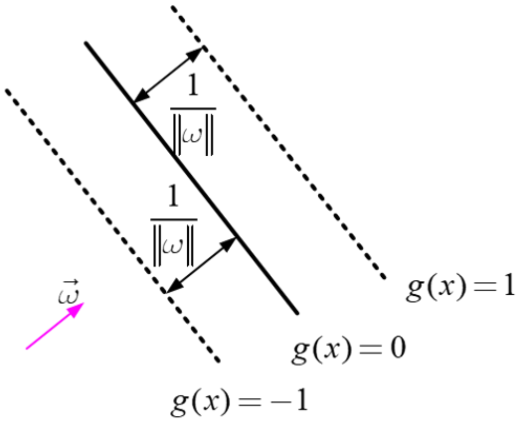
3.1. Distance

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









- Find a distance between $g(x) = -1$ and $g(x) = 1$

suppose $g(x_1) = -1,\ g(x_2) = 1$

$$\begin{aligned} \omega^T x_1 + \omega_0 &= -1 \\ \omega^T x_2 + \omega_0 &= 1 \end{aligned} \quad \Longrightarrow \quad \omega^T (x_2 - x_1) = 2$$

$$s = \left\langle \frac{\omega}{\|\omega\|}, x_2 - x_1 \right\rangle = \frac{1}{\|\omega\|} \omega^T (x_2 - x_1) = \frac{2}{\|\omega\|}$$

3.2. Illustrative Example

- Binary classification: C_1 and C_2

- Features: the coordinate of ith data

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

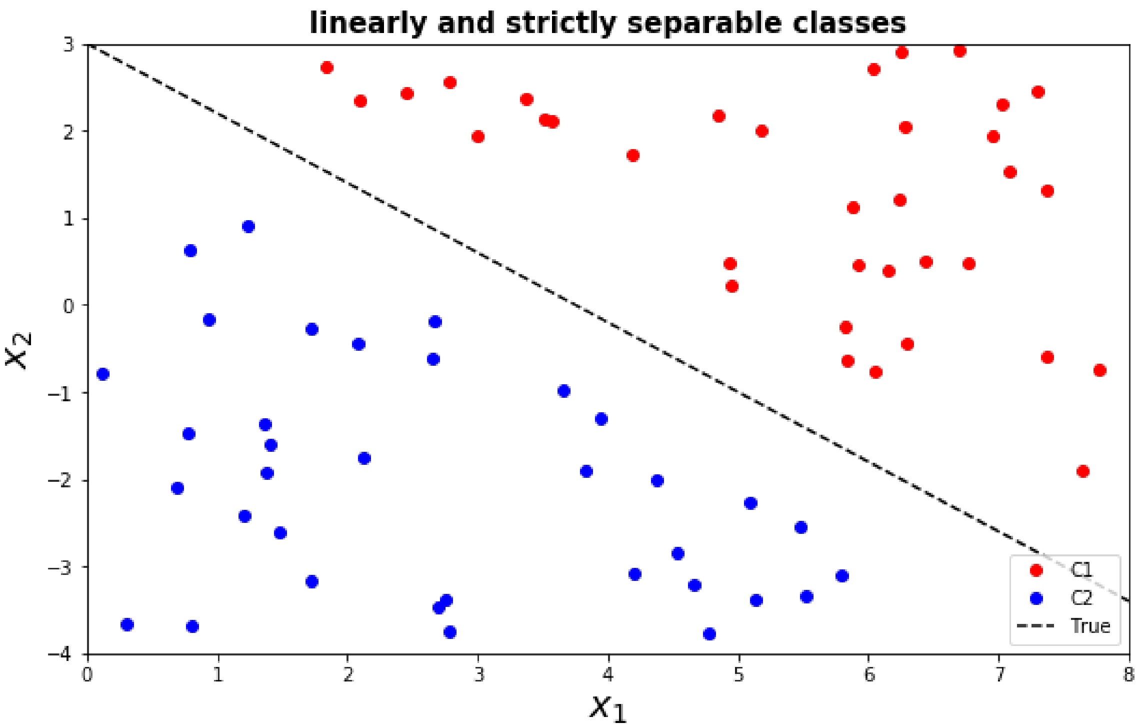
- Is it possible to distinguish between C_1 and C_2 by its coordinates?

- We need to find a separating hyperplane (or a line in 2D)

$$\begin{aligned} \omega_1 x_1 + \omega_2 x_2 + \omega_0 &= 0 \\ \begin{bmatrix} \omega_1 & \omega_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \omega_0 &= 0 \\ \omega^T x + \omega_0 &= 0 \end{aligned}$$

In [13]:
```
import numpy as np
import matplotlib.pyplot as plt

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

g0 = 0.8*x1 + x2 - 3
g1 = g0 - 1
g2 = g0 + 1

C1 = np.where(g1 >= 0)[0]
C2 = np.where(g2 < 0)[0]
```

In [14]:
```
xp = np.linspace(0,8,100).reshape(-1,1)
ypt = -0.8*xp + 3

plt.figure(figsize=(10, 6))
plt.plot(x1[C1], x2[C1], 'ro', label='C1')
plt.plot(x1[C2], x2[C2], 'bo', label='C2')
plt.plot(xp, ypt, '--k', label='True')
plt.title('linearly and strictly separable classes', fontweight = 'bold', fo
ntsize = 15)
plt.xlabel('$x_1$', fontsize = 20)
plt.ylabel('$x_2$', fontsize = 20)
plt.legend(loc = 4)
plt.xlim([0, 8])
plt.ylim([-4, 3])
plt.show()
```



- Given:
  - Hyperplane defined by ω and ω_0
  - Animals coordinates (or features) x

- Decision making:

$$\omega^T x + \omega_0 > 0 \implies x \text{ belongs to } C_1$$
$$\omega^T x + \omega_0 < 0 \implies x \text{ belongs to } C_2$$

- Find ω and ω_0 such that x given $\omega^T x + \omega_0 = 0$

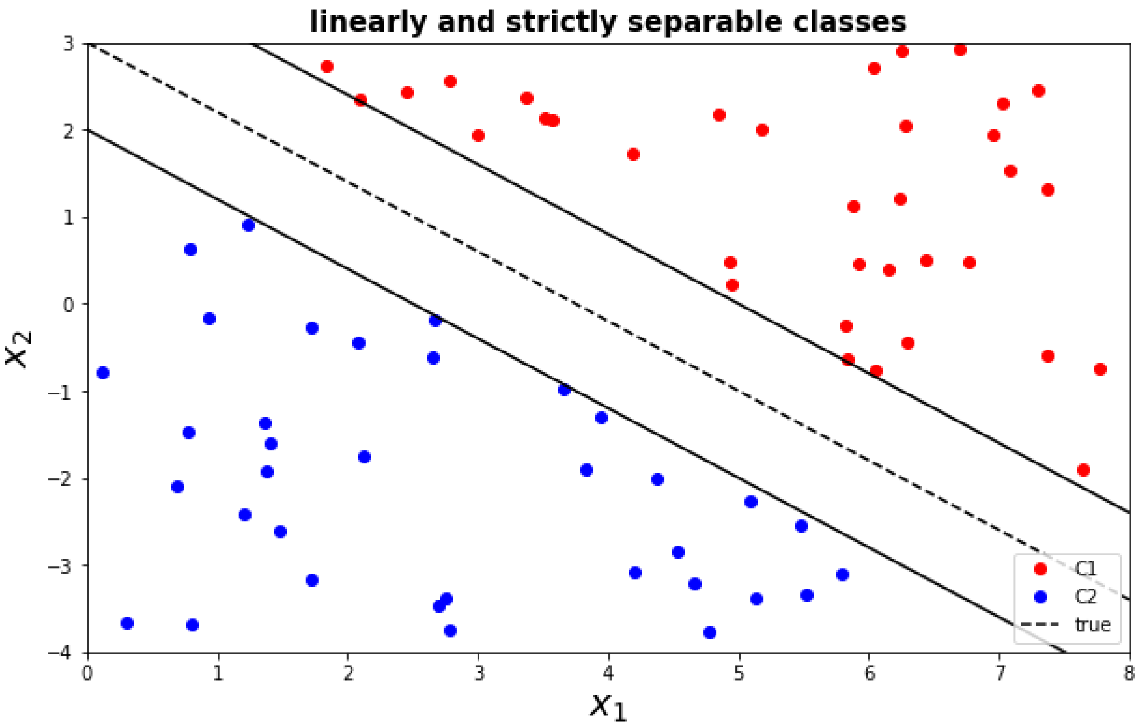
  or

- Find ω and ω_0 such that $x \in C_1$ given $\omega^T x + \omega_0 > 1$ and $x \in C_2$ given $\omega^T x + \omega_0 < -1$

$$\begin{aligned} &\omega^T x + \omega_0 > b \\ \iff &\frac{\omega^T}{b} x + \frac{\omega_0}{b} > 1 \\ \iff &\omega'^T x + \omega'_0 > 1 \end{aligned}$$

- Same problem if strictly separable

In [15]:
```
#  see how data are generated
xp = np.linspace(0,8,100).reshape(-1,1)
ypt = -0.8*xp + 3

plt.figure(figsize=(10, 6))
plt.plot(x1[C1], x2[C1], 'ro', label='C1')
plt.plot(x1[C2], x2[C2], 'bo', label='C2')
plt.plot(xp, ypt, '--k', label='true')
plt.plot(xp, ypt-1, '-k')
plt.plot(xp, ypt+1, '-k')
plt.title('linearly and strictly separable classes', fontweight = 'bold', fo
ntsize = 15)
plt.xlabel('$x_1$', fontsize = 20)
plt.ylabel('$x_2$', fontsize = 20)
plt.legend(loc = 4)
plt.xlim([0, 8])
plt.ylim([-4, 3])
plt.show()
```



3.2.1. Optimization Formulation 1

- $n\ (=2)$ features
- $m = N + M$ data points in training set

$$x^{(i)} = \begin{bmatrix} x_1^{(i)} \\ x_2^{(i)} \end{bmatrix} \text{ with } \omega = \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix} \qquad \text{or} \qquad x^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \\ x_2^{(i)} \end{bmatrix} \text{ with } \omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix}$$

- N belongs to C_1 in training set
- M belongs to C_2 in training set
- ω and ω_0 are the unknown variables

$$
\begin{aligned}
\text{minimize} \quad & \text{something} \\
\text{subject to} \quad & \begin{cases} \omega^T x^{(1)} + \omega_0 \geq 1 \\ \omega^T x^{(2)} + \omega_0 \geq 1 \\ \quad \vdots \\ \omega^T x^{(N)} + \omega_0 \geq 1 \end{cases} \\
& \begin{cases} \omega^T x^{(N+1)} + \omega_0 \leq -1 \\ \omega^T x^{(N+2)} + \omega_0 \leq -1 \\ \quad \vdots \\ \omega^T x^{(N+M)} + \omega_0 \leq -1 \end{cases}
\end{aligned}
$$

or

$$
\begin{aligned}
\text{minimize} \quad & \text{something} \\
\text{subject to} \quad & \begin{cases} \omega^T x^{(1)} \geq 1 \\ \omega^T x^{(2)} \geq 1 \\ \quad \vdots \\ \omega^T x^{(N)} \geq 1 \end{cases} \\
& \begin{cases} \omega^T x^{(N+1)} \leq -1 \\ \omega^T x^{(N+2)} \leq -1 \\ \quad \vdots \\ \omega^T x^{(N+M)} \leq -1 \end{cases}
\end{aligned}
$$

Code (CVXPY)

$$
X_1 = \begin{bmatrix} \left(x^{(1)}\right)^T \\ \left(x^{(2)}\right)^T \\ \vdots \\ \left(x^{(N)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(N)} & x_2^{(N)} \end{bmatrix}
$$

$$
X_2 = \begin{bmatrix} \left(x^{(N+1)}\right)^T \\ \left(x^{(N+2)}\right)^T \\ \vdots \\ \left(x^{(N+M)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(N+1)} & x_2^{(N+1)} \\ 1 & x_1^{(N+2)} & x_2^{(N+2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(N+M)} & x_2^{(N+M)} \end{bmatrix}
$$

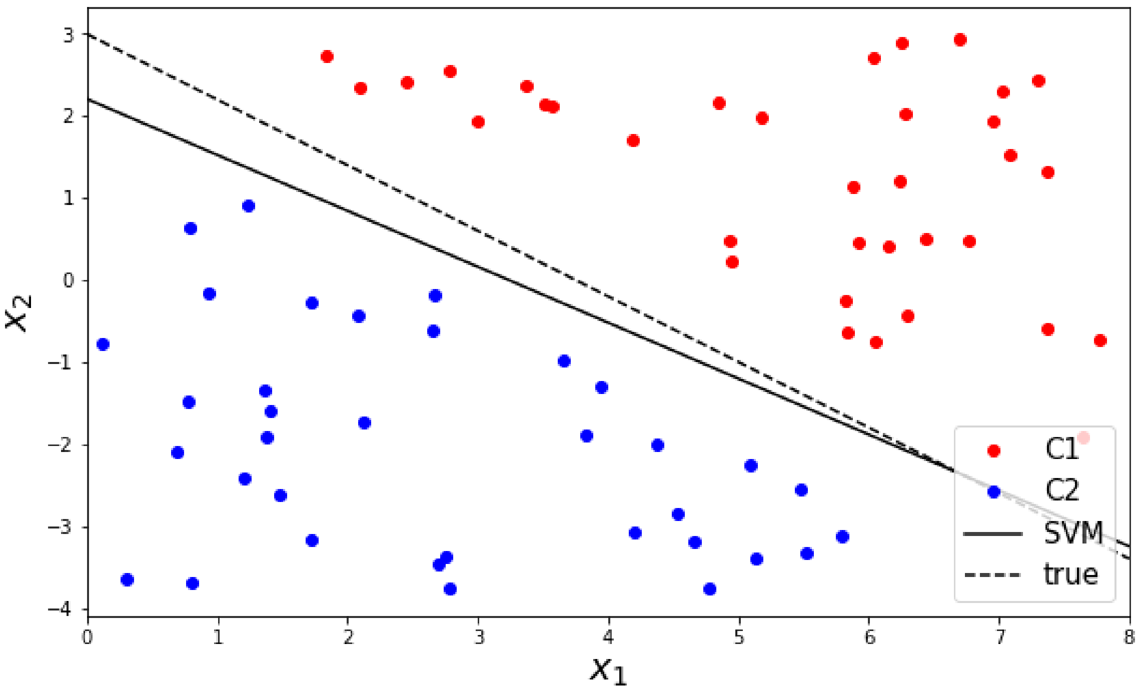
$$
\begin{aligned}
\text{minimize} \quad & \text{something} \\
\text{subject to} \quad & X_1 \omega \geq 1 \\
& X_2 \omega \leq -1
\end{aligned}
$$

$$
\begin{aligned}
\text{minimize} \quad & \text{something} \\
\text{subject to} \quad & X_1 \omega \geq 1 \\
& X_2 \omega \leq -1
\end{aligned}
$$

In [16]:
```
# CVXPY using simple classification
import cvxpy as cvx

N = C1.shape[0]
M = C2.shape[0]

X1 = np.hstack([np.ones([N,1]), x1[C1], x2[C1]])
X2 = np.hstack([np.ones([M,1]), x1[C2], x2[C2]])

X1 = np.asmatrix(X1)
X2 = np.asmatrix(X2)
```

In [17]:
```
w = cvx.Variable(3,1)
obj = cvx.Minimize(1)
const = [X1*w >= 1, X2*w <= -1]
prob = cvx.Problem(obj, const).solve()

w = w.value
```

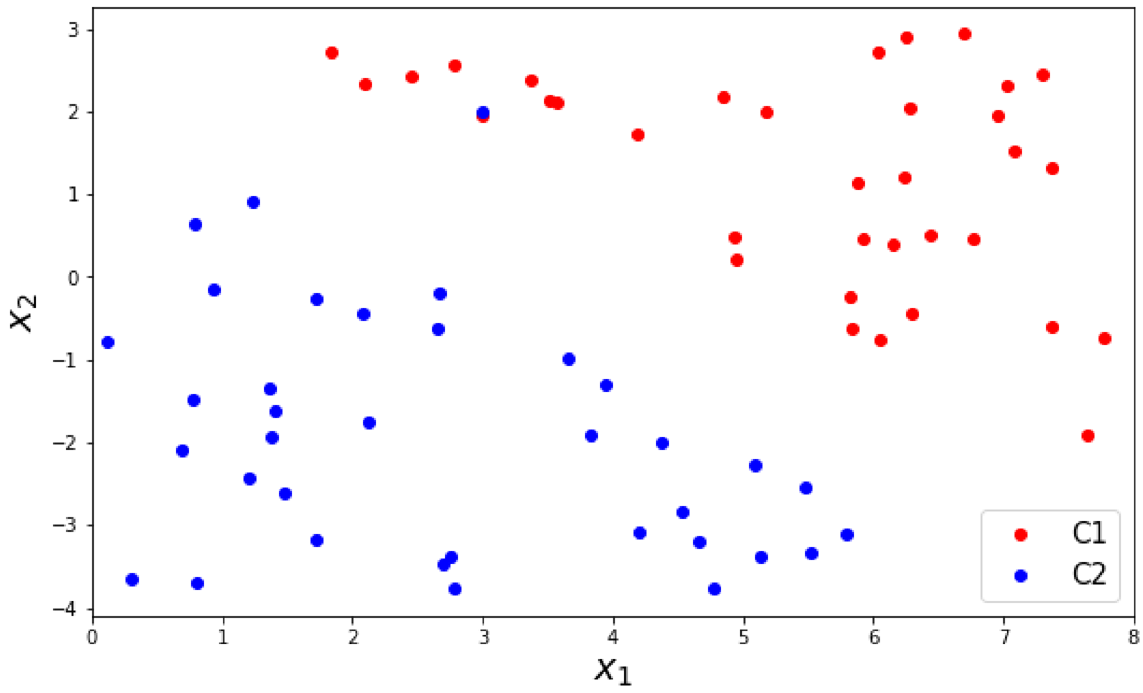
In [18]:
```
xp = np.linspace(0,8,100).reshape(-1,1)
yp = - w[1,0]/w[2,0]*xp - w[0,0]/w[2,0]

plt.figure(figsize=(10, 6))
plt.plot(X1[:,1], X1[:,2], 'ro', label='C1')
plt.plot(X2[:,1], X2[:,2], 'bo', label='C2')
plt.plot(xp, yp, 'k', label='SVM')
plt.plot(xp, ypt, '--k', label='true')
plt.xlim([0,8])
plt.xlabel('$x_1$', fontsize = 20)
plt.ylabel('$x_2$', fontsize = 20)
plt.legend(loc = 4, fontsize = 15)
plt.show()
```



3.2.2. Outlier

- Note that in the real world, you may have noise, errors, or outliers that do not accurately represent the actual phenomena
- Non-separable case
- No solutions (hyperplane) exist
  - We will allow some training examples to be misclassified !
  - but we want their number to be minimized

In [19]:
```
X1 = np.hstack([np.ones([N,1]), x1[C1], x2[C1]])
X2 = np.hstack([np.ones([M,1]), x1[C2], x2[C2]])

outlier = np.array([1, 3, 2]).reshape(-1,1)
X2 = np.vstack([X2, outlier.T])

X1 = np.asmatrix(X1)
X2 = np.asmatrix(X2)

plt.figure(figsize=(10, 6))
plt.plot(X1[:,1], X1[:,2], 'ro', label='C1')
plt.plot(X2[:,1], X2[:,2], 'bo', label='C2')
plt.xlim([0,8])
plt.xlabel('$x_1$', fontsize = 20)
plt.ylabel('$x_2$', fontsize = 20)
plt.legend(loc = 4, fontsize = 15)
plt.show()
```



$$\begin{aligned} \text{minimize} \quad & \text{something} \\ \text{subject to} \quad & X_1 \omega \geq 1 \\ & X_2 \omega \leq -1 \end{aligned}$$

In [20]:
```
w = cvx.Variable(3,1)
obj = cvx.Minimize(1)
const = [X1*w >= 1, X2*w <= -1]
prob = cvx.Problem(obj, const).solve()

print(w.value)
```

```
None
```

- No solutions (hyperplane) exist
- We will allow some training examples to be misclassified !
- but we want their number to be minimized

3.2.3. Optimization Formulation 2

- $n \; (=2)$ features
- $m = N + M$ data points in a training set

$$x^i = \begin{bmatrix} 1 \\ x_1^{(i)} \\ x_2^{(i)} \end{bmatrix} \quad \text{with } \omega = \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} \qquad \begin{array}{rl} \text{minimize} & \text{something} \\ \text{subject to} & X_1 \omega \geq 1 \\ & X_2 \omega \leq -1 \end{array}$$

- N belongs to C_1 in training set
- M belongs to C_2 in training set
- ω and ω_0 are the variables (unknown)

- For the non-separable case, we relex the above constraints
- Need slack variables u and v where all are positive

The optimization problem for the non-separable case

$$\begin{aligned} \text{minimize} \quad & \sum_{i=1}^{N} u_i + \sum_{i=1}^{M} v_i \\ \text{subject to} \quad & \begin{cases} \omega^T x^{(1)} \geq 1 - u_1 \\ \omega^T x^{(2)} \geq 1 - u_2 \\ \quad\quad \vdots \\ \omega^T x^{(N)} \geq 1 - u_N \end{cases} \\ & \begin{cases} \omega^T x^{(N+1)} \leq -(1 - v_1) \\ \omega^T x^{(N+2)} \leq -(1 - v_2) \\ \quad\quad \vdots \\ \omega^T x^{(N+M)} \leq -(1 - v_M) \end{cases} \\ & \begin{cases} u \geq 0 \\ v \geq 0 \end{cases} \end{aligned}$$

- Expressed in a matrix form

$$X_1 = \begin{bmatrix} \left(x^{(1)}\right)^T \\ \left(x^{(2)}\right)^T \\ \vdots \\ \left(x^{(N)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(N)} & x_2^{(N)} \end{bmatrix}$$

$$X_2 = \begin{bmatrix} \left(x^{(N+1)}\right)^T \\ \left(x^{(N+2)}\right)^T \\ \vdots \\ \left(x^{(N+M)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(N+1)} & x_2^{(N+1)} \\ 1 & x_1^{(N+2)} & x_2^{(N+2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(N+M)} & x_2^{(N+M)} \end{bmatrix}$$

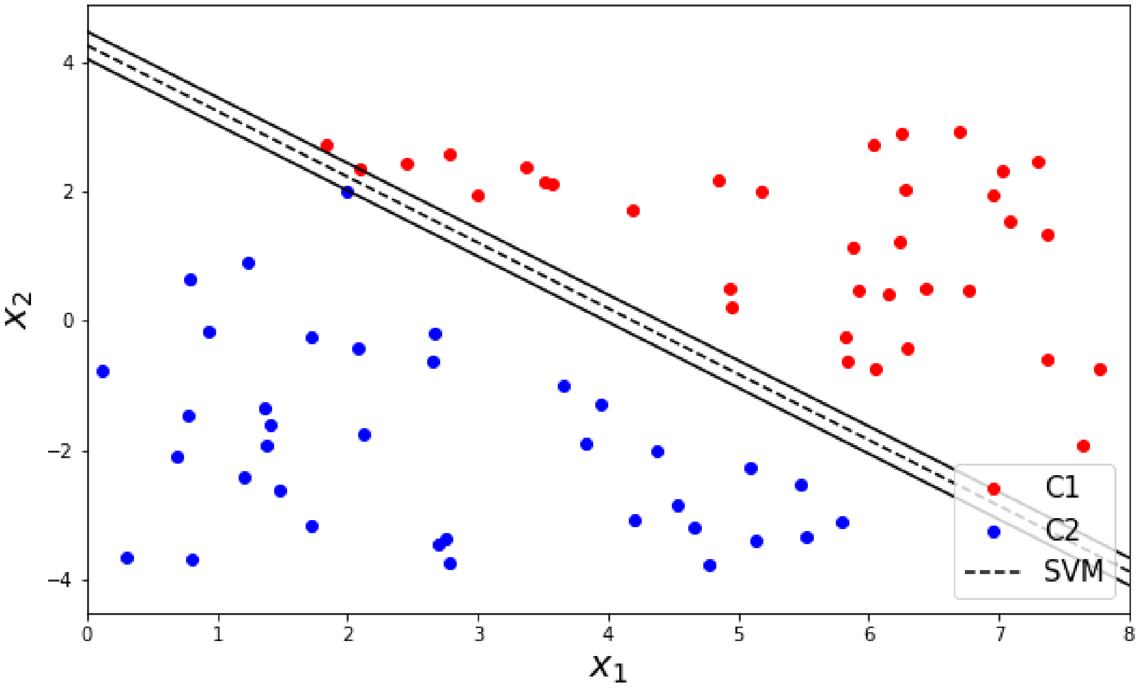
$$u = \begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix}$$

$$v = \begin{bmatrix} v_1 \\ \vdots \\ v_M \end{bmatrix}$$

$$\begin{aligned} \text{minimize} \quad & 1^T u + 1^T v \\ \text{subject to} \quad & X_1 \omega \geq 1 - u \\ & X_2 \omega \leq -(1 - v) \\ & u \geq 0 \\ & v \geq 0 \end{aligned}$$

```
In [21]: 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]])

         outlier = np.array([1, 2, 2]).reshape(-1,1)
         X2 = np.vstack([X2, outlier.T])

         X1 = np.asmatrix(X1)
         X2 = np.asmatrix(X2)

         N = X1.shape[0]
         M = X2.shape[0]

         w = cvx.Variable(3,1)
         u = cvx.Variable(N,1)
         v = cvx.Variable(M,1)
         obj = cvx.Minimize(np.ones((1,N))*u + np.ones((1,M))*v)
         const = [X1*w >= 1-u, X2*w <= -(1-v), u >= 0, v >= 0 ]
         prob = cvx.Problem(obj, const).solve()

         w = w.value
```

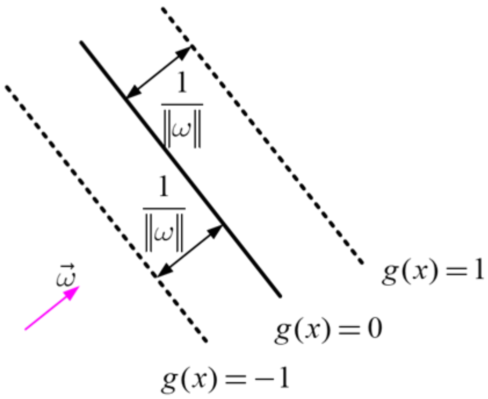
```
In [22]: xp = np.linspace(0,8,100).reshape(-1,1)
         yp = - w[1,0]/w[2,0]*xp - w[0,0]/w[2,0]

         plt.figure(figsize=(10, 6))
         plt.plot(X1[:,1], X1[:,2], 'ro', label='C1')
         plt.plot(X2[:,1], X2[:,2], 'bo', label='C2')
         plt.plot(xp, yp, '--k', label='SVM')
         plt.plot(xp, yp-1/w[2,0], '-k')
         plt.plot(xp, yp+1/w[2,0], '-k')
         plt.xlim([0,8])
         plt.xlabel('$x_1$', fontsize = 20)
         plt.ylabel('$x_2$', fontsize = 20)
         plt.legend(loc = 4, fontsize = 15)
         plt.show()
```



Further improvement

- Notice that hyperplane is not as accurately represent the division due to the outlier
- Can we do better when there are noise data or outliers?
- Yes, but we need to look beyond LP
- Idea: large margin leads to good generalization on the test data

3.3. Maximize Margin (Finally, it is Support Vector Machine)



- Distance (= margin)

$$\text{margin} = \frac{2}{\|\omega\|_2}$$

- Minimize $\|\omega\|_2$ to maximize the margin (closest samples from the decision line)

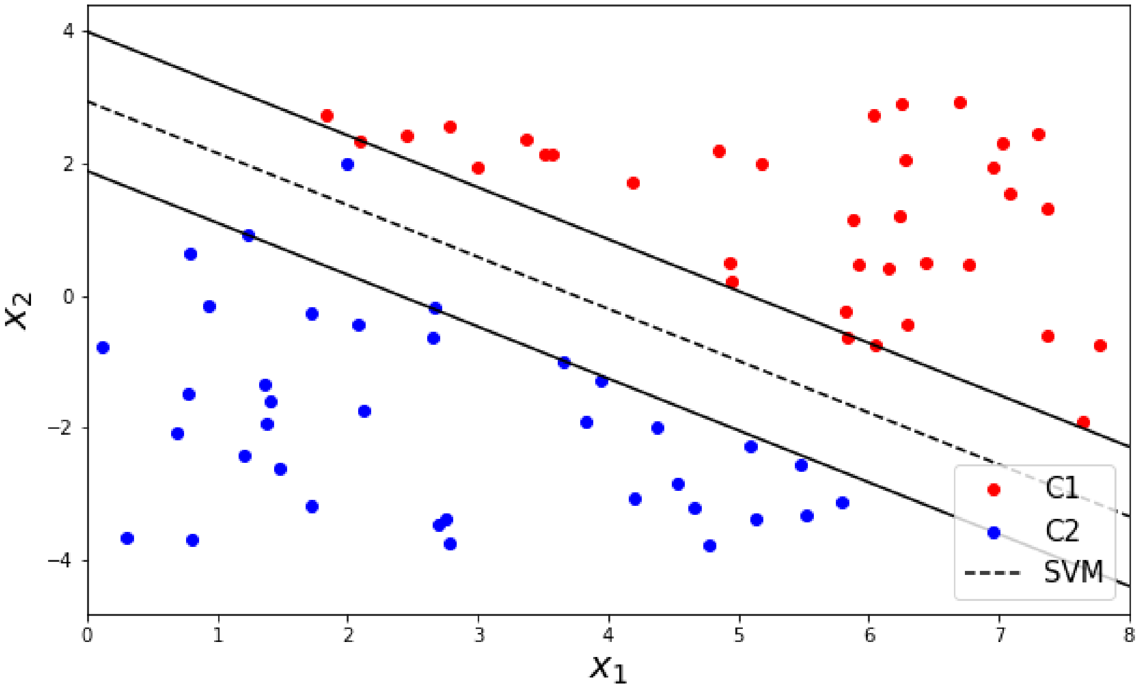
$$\text{maximize } \{\text{minimum distance}\}$$

- Use gamma (γ) as a weighting betwwen the followings:
  - Bigger margin given robustness to outliers
  - Hyperplane that has few (or no) errors

$$\begin{aligned}
\text{minimize} \quad & \|\omega\|_2 + \gamma(1^T u + 1^T v) \\
\text{subject to} \quad & X_1 \omega + \omega_0 \geq 1 - u \\
& X_2 \omega + \omega_0 \leq -(1 - v) \\
& u \geq 0 \\
& v \geq 0
\end{aligned}$$

In [23]:
```
g = 1
w = cvx.Variable(3,1)
u = cvx.Variable(N,1)
v = cvx.Variable(M,1)
obj = cvx.Minimize(cvx.norm(w,2) + g*(np.ones((1,N))*u + np.ones((1,M))*v))
const = [X1*w >= 1-u, X2*w <= -(1-v), u >= 0, v >= 0 ]
prob = cvx.Problem(obj, const).solve()

w = w.value
```

In [24]:
```
xp = np.linspace(0,8,100).reshape(-1,1)
yp = - w[1,0]/w[2,0]*xp - w[0,0]/w[2,0]

plt.figure(figsize=(10, 6))
plt.plot(X1[:,1], X1[:,2], 'ro', label='C1')
plt.plot(X2[:,1], X2[:,2], 'bo', label='C2')
plt.plot(xp, yp, '--k', label='SVM')
plt.plot(xp, yp-1/w[2,0], '-k')
plt.plot(xp, yp+1/w[2,0], '-k')
plt.xlim([0,8])
plt.xlabel('$x_1$', fontsize = 20)
plt.ylabel('$x_2$', fontsize = 20)
plt.legend(loc = 4, fontsize = 15)
plt.show()
```



3.4. Logistic Regression

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

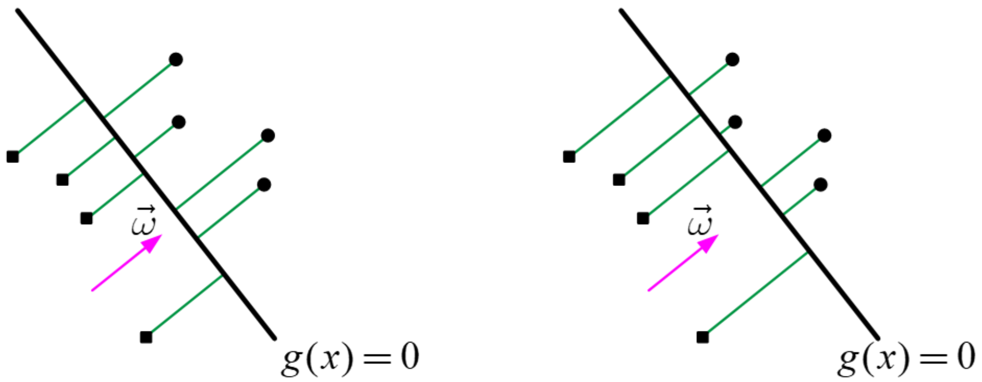
- Perceptron: make use of sign of data

- SVM: make use of margin (minimum distance)
  - Distance from a single data point

- We want to use distance information of ALL data points
  - logistic regression

Using 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

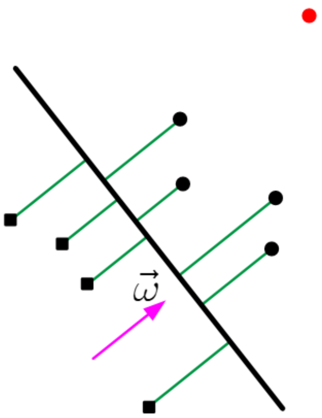


- Inequality of arithmetic and geometric means
$$\frac{x_1 + x_2 + \cdots + x_m}{m} \geq \sqrt[m]{x_1 \cdot x_2 \ldots x_m}$$
and that equality holds if and only if $x_1 = x_2 = \cdots = x_m$

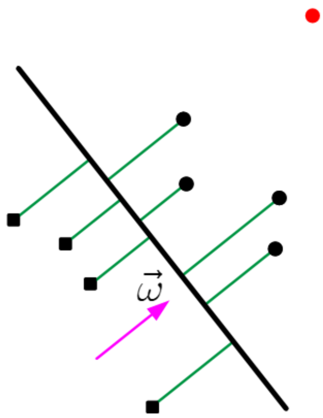
- Roughly speaking, this optimization of $\max \prod_i |h_i|$ tends to position a hyperplane in the middle of two classes
$$h = \frac{g(x)}{\|\omega\|} = \frac{\omega^T x}{\|\omega\|} \sim \omega^T x$$

Using all Distances with Outliers

- SVM vs. Logistic Regression



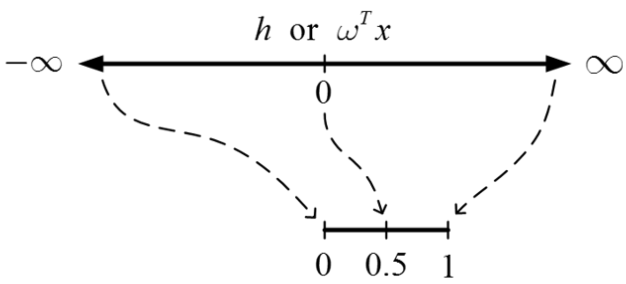
SVM

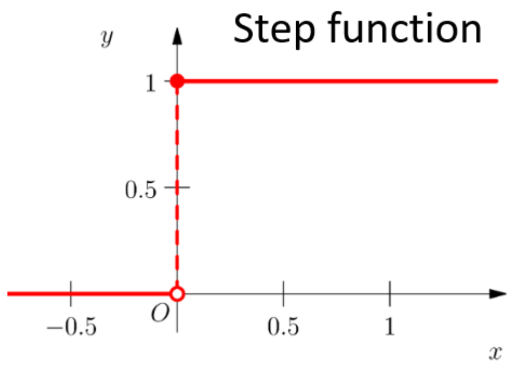


Logistic Regression

Sigmoid function

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

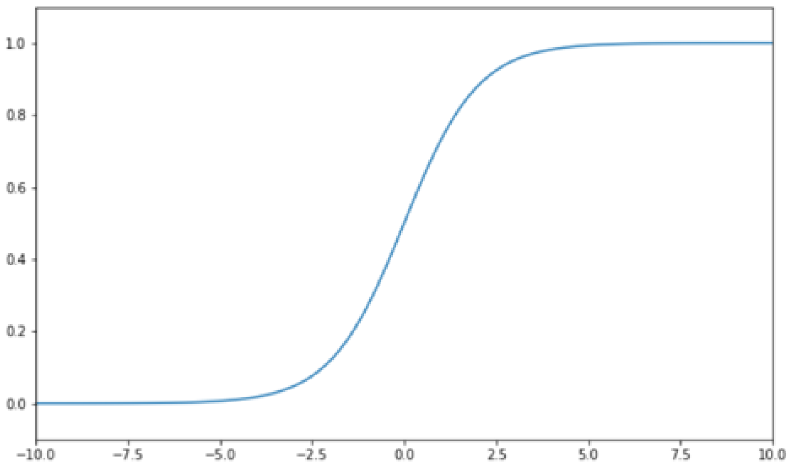




- If $\sigma(z)$ is the sigmoid function, or the logistic function

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

  - logistic function always generates a value between 0 and 1
  - Crosses 0.5 at the origin, then flattens out



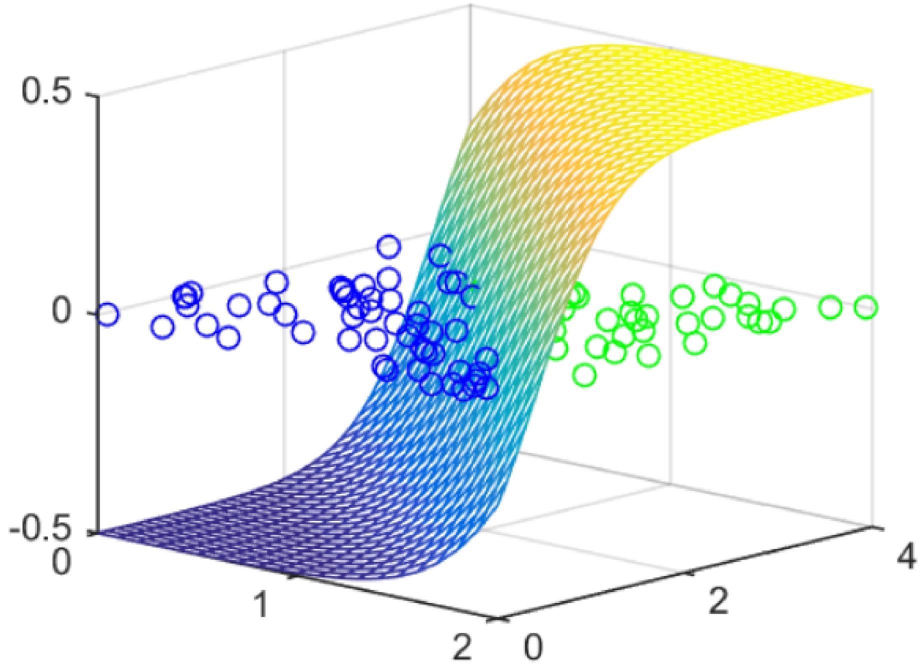
- Benefit of mapping via the logistic function
  - monotonic: same or similar optimziation solution
  - continuous and differentiable: good for gradient descent optimization
  - probability or confidence: can be considered as probability

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

- Goal: we need to fit ω to our data

$$\max \prod_i |h_i|$$

- Classified based on probability



In [25]:
```
m = 200

X0 = np.random.multivariate_normal([0, 0], np.eye(2), m)
X1 = np.random.multivariate_normal([10, 10], np.eye(2), m)

X = np.vstack([X0, X1])
y = np.vstack([np.zeros([m,1]), np.ones([m,1])])
```

In [26]:
```
from sklearn import linear_model

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

Out[26]:
```
LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=Tru
e,
          intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1,
          penalty='l2', random_state=None, solver='liblinear', tol=0.0001,
          verbose=0, warm_start=False)
```

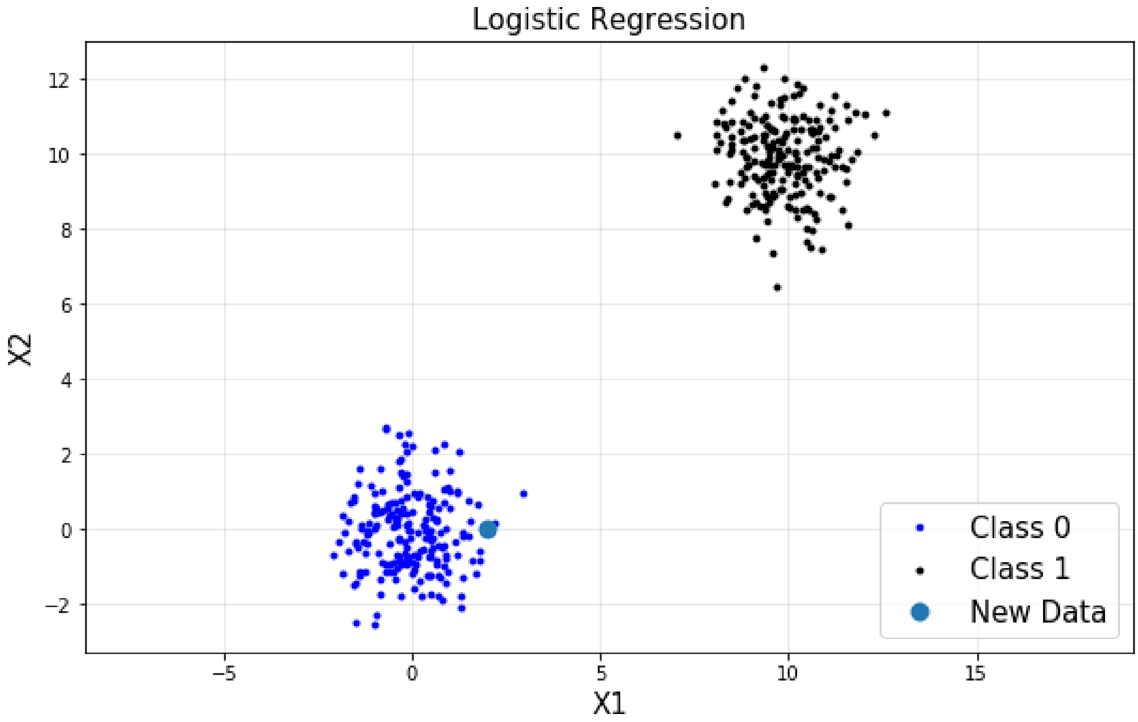
In [27]:
```
X_new = np.array([2, 0]).reshape(1, -1)
pred = clf.predict(X_new)

print(pred)
```

```
[0.]
```

In [28]:
```
pred = clf.predict_proba(X_new)

print(pred)
```

```
[[0.9407617 0.0592383]]
```

In [29]:
```
plt.figure(figsize=(10, 6))
plt.plot(X0[:,0], X0[:,1], '.b', label='Class 0')
plt.plot(X1[:,0], X1[:,1], '.k', label='Class 1')
plt.plot(X_new[0,0], X_new[0,1], 'o', label='New Data', ms=5, mew=5)

plt.title('Logistic Regression', fontsize=15)
plt.legend(loc='lower right', fontsize=15)
plt.xlabel('X1', fontsize=15)
plt.ylabel('X2', fontsize=15)
plt.grid(alpha=0.3)
plt.axis('equal')
plt.show()
```



In [30]:
```
%%javascript
$.getScript('https://kmahelona.github.io/ipython_notebook_goodies/ipython_no
tebook_toc.js')
```