Support Vector Machine

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Classification (Linear)

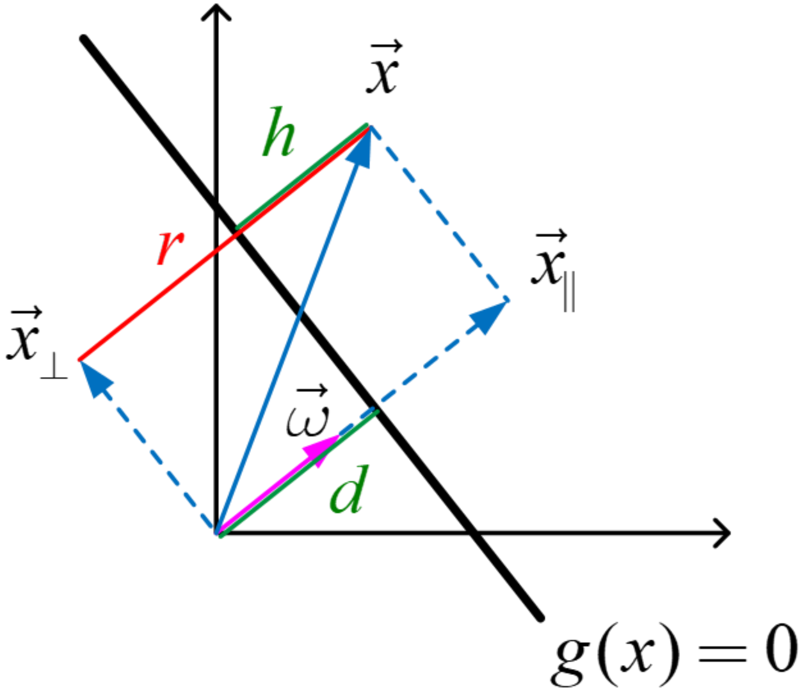
- Autonomously figure out which category (or class) an unknown item should be categorized into

- 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)

Distance from a Line

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

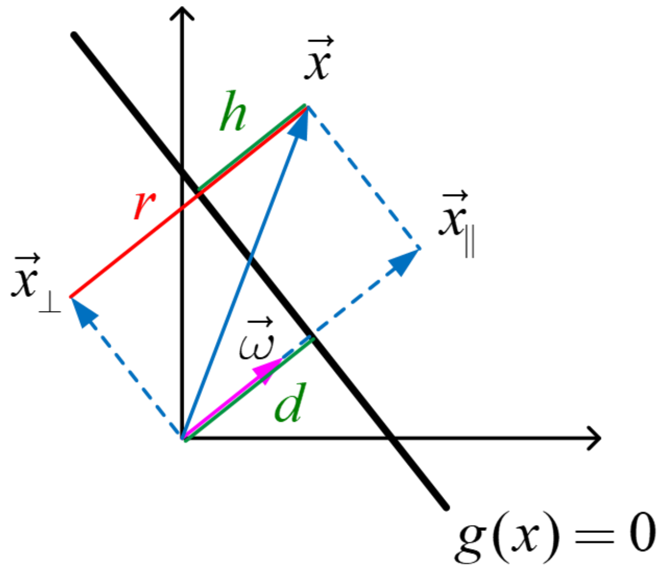


ω

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

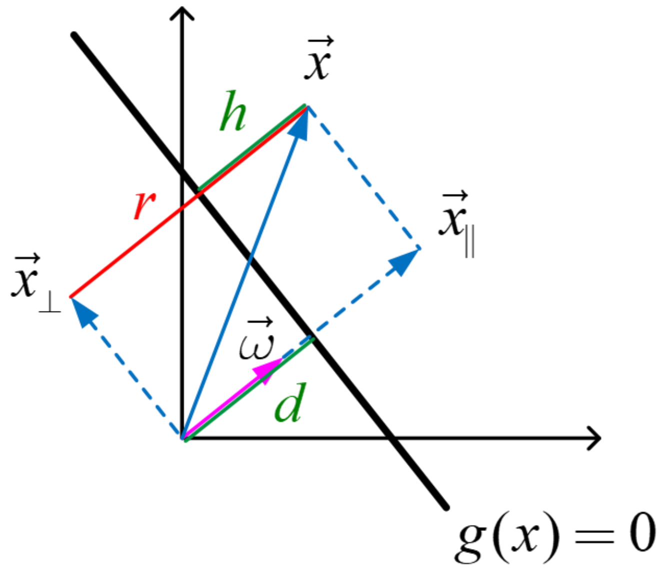
$$g(\vec{p}) = g(\vec{q}) = 0 \quad \Rightarrow \quad \omega_0 + \omega^T \vec{p} = \omega_0 + \omega^T \vec{q} = 0$$
$$\Rightarrow \quad \omega^T (\vec{p} - \vec{q}) = 0$$

$$\therefore \ \omega : \text{normal to the line (orthogonal)}$$
$$\Longrightarrow \ \text{tells the direction of the line}$$



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)



$$g(x) = \omega_0 + \omega^T x = 0$$

$$\Rightarrow \omega_0 + \omega^T d\frac{\omega}{\|\omega\|} = \omega_0 + d\frac{\omega^T \omega}{\|\omega\|} = \omega_0 + d\|\omega\| = 0$$

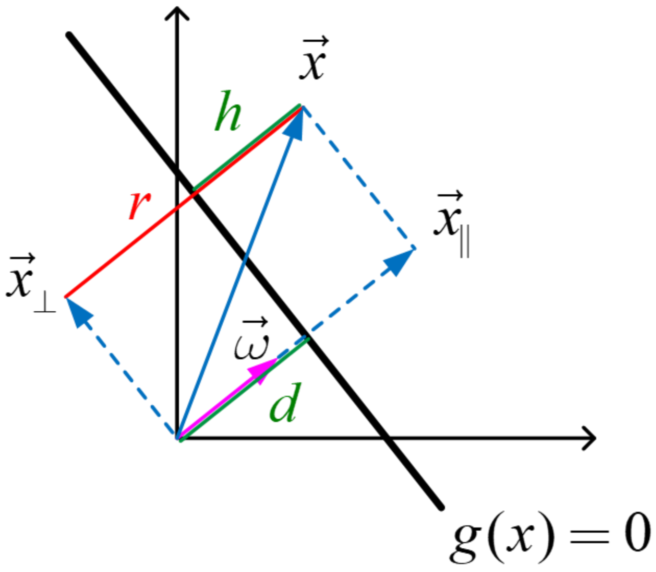
$$\therefore d = -\frac{\omega_0}{\|\omega\|}$$

Distance from a Line: h

- for any vector of x

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

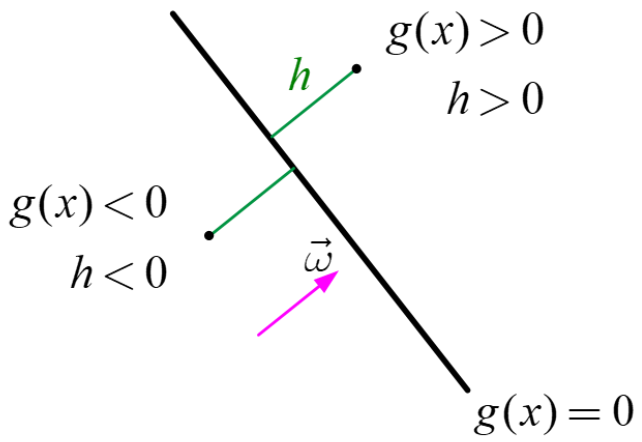
$$\omega^T x = \omega^T\left(x_\perp + r\frac{\omega}{||\omega||}\right) = r\frac{\omega^T\omega}{||\omega||} = r||\omega||$$

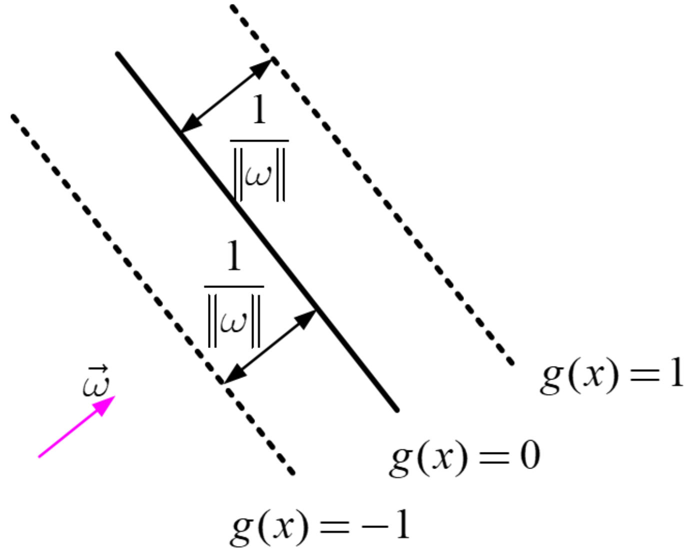


$$\begin{aligned} g(x) &= \omega_0 + \omega^T x \\ &= \omega_0 + r||\omega|| \qquad (r = d + h) \\ &= \omega_0 + (d+h)||\omega|| \\ &= \omega_0 + \left(-\frac{\omega_0}{||\omega||} + h\right)||\omega|| \\ &= h||\omega|| \end{aligned}$$

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

Distance from a Line: h

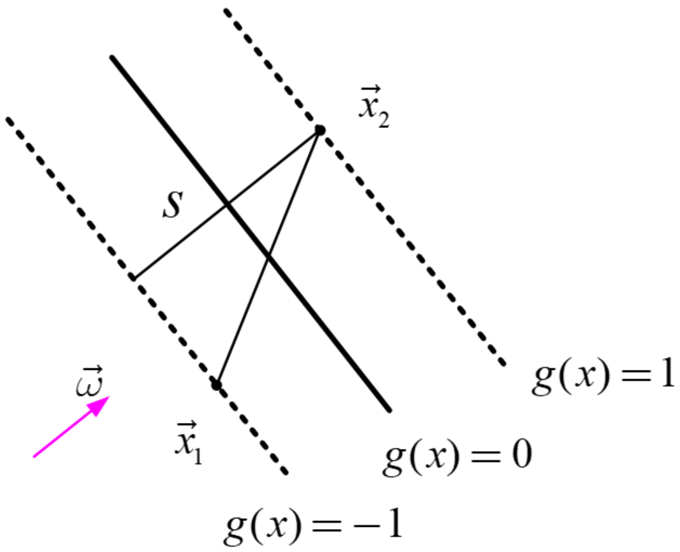




$$h = \frac{g(x)}{\|\omega\|}$$

Distance from a Line: h

- Another method to find a distance between $g(x) = 1$ and $g(x) = -1$
- Suppose $g(x_1) = -1$ and $g(x_2) = 1$



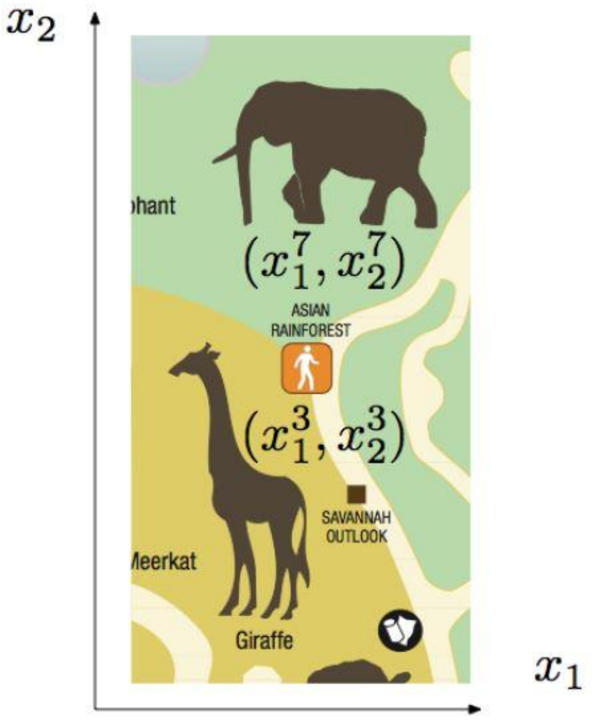
$$\begin{aligned} \omega_0 + \omega^T x_1 &= -1 \\ \omega_0 + \omega^T x_2 &= 1 \end{aligned} \implies \omega^T (x_2 - x_1) = 2$$

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

Illustrative Example

- Binary classification
  - C_1 and C_0
- Features
  - The coordinate of the unknown animal i in the zoo

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



Hyperplane

- Is it possible to distinguish between C_1 and C_0 by its coordinates on a map of the zoo?

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

$$\omega_0 + \omega_1 x_1 + \omega_2 x_2 = 0$$

$$\omega_0 + \begin{bmatrix} \omega_1 & \omega_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0$$

$$\omega_0 + \omega^T x = 0$$

Decision Making

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

- Decision making:

$$
\begin{aligned}
\omega_0 + \omega^T x > 0 &\implies x \text{ belongs to } C_1 \\
\omega_0 + \omega^T x < 0 &\implies x \text{ belongs to } C_0
\end{aligned}
$$

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

Decision Boundary or Band

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

or

- Find ω and ω_0 such that
  - $x \in C_1$ given $\omega_0 + \omega^T x > 1$ and
  - $x \in C_0$ given $\omega_0 + \omega^T x < -1$

$$\omega_0 + \omega^T x > b, \quad (b > 0)$$

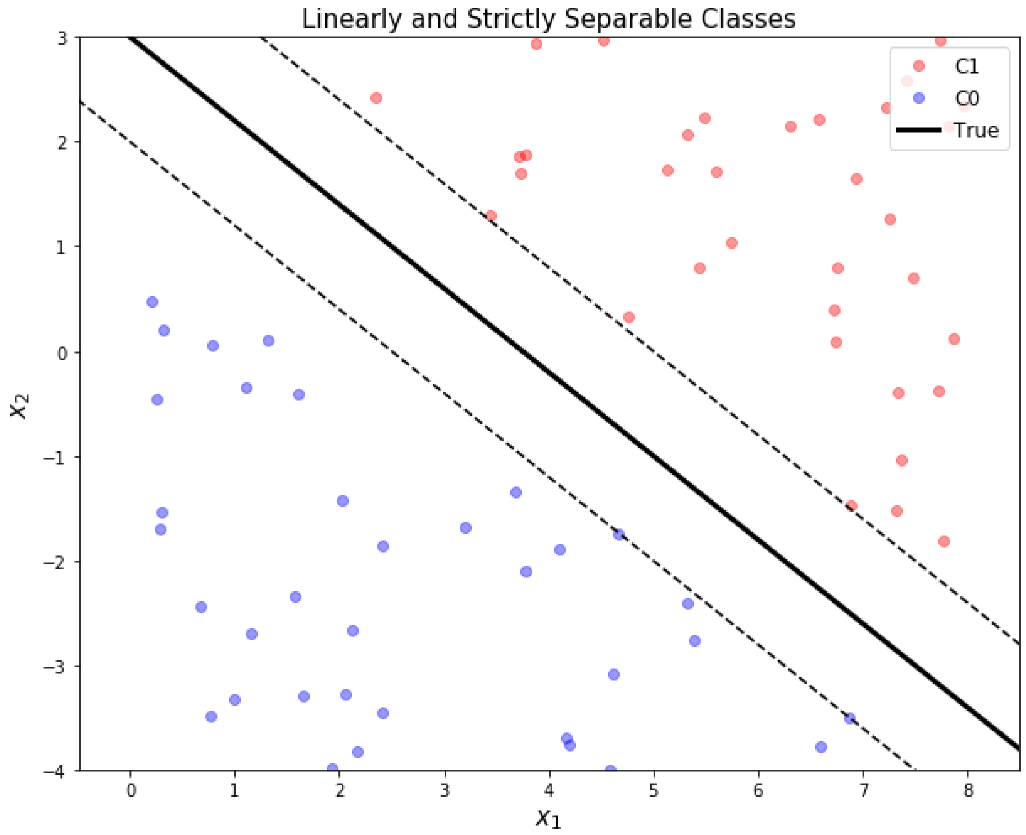
$$\Longleftrightarrow \frac{\omega_0}{b} + \frac{\omega^T}{b} x > 1$$

$$\Longleftrightarrow \omega_0' + \omega'^T x > 1$$

Data Generation for Classification

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

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

C1 = np.where(g1 >= 0)[0]
C0 = np.where(g0 < 0)[0]

xp = np.linspace(-1,9,100).reshape(-1,1)
ypt = -0.8*xp + 3
```

```
#  see how data are generated
xp = np.linspace(-1,9,100).reshape(-1,1)
ypt = -0.8*xp + 3

plt.figure(figsize=(10, 8))
plt.plot(x1[C1], x2[C1], 'ro', alpha = 0.4, label = 'C1')
plt.plot(x1[C0], x2[C0], 'bo', alpha = 0.4, label = 'C0')
plt.plot(xp, ypt, 'k', linewidth = 3, label = 'True')
plt.plot(xp, ypt-1, '--k')
plt.plot(xp, ypt+1, '--k')
plt.title('Linearly and Strictly Separable Classes', fontsize = 15)
plt.xlabel(r'$x_1$', fontsize = 15)
plt.ylabel(r'$x_2$', fontsize = 15)
plt.legend(loc = 1, fontsize = 12)
plt.axis('equal')
plt.xlim([0, 8])
plt.ylim([-4, 3])
plt.show()
```



Optimization Formulation 1

- $n\ (= 2)$ features
- N belongs to C_1 in training set
- M belongs to C_0 in training set
- $m = N + M$ data points in training set

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

or

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

- ω and ω_0 are the unknown variables

Optimization Formulation 1

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

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

CVXPY 1

$$\begin{aligned} \text{minimize} \quad & \text{something} \\ \text{subject to} \quad & X_1\omega \geq 1 \\ & X_0\omega \leq -1 \end{aligned}$$

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

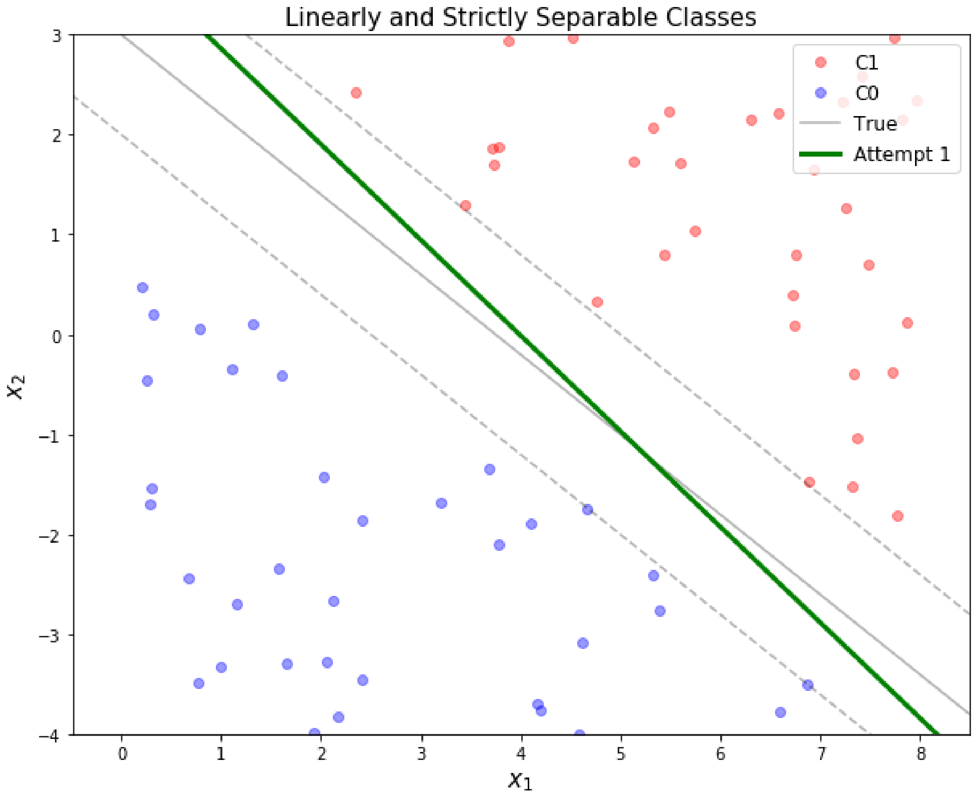
$$X_0 = \begin{bmatrix} \left(x^{(N+1)}\right)^T \\ \left(x^{(N+2)}\right)^T \\ \vdots \\ \left(x^{(N+M)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(N+1)} & x_2^{(N+1)} \\ 1 & x_1^{(N+2)} & x_2^{(N+2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(N+M)} & x_2^{(N+M)} \end{bmatrix}$$

```
import cvxpy as cvx

N = C1.shape[0]
M = C0.shape[0]

X1 = np.hstack([np.ones([N,1]), x1[C1], x2[C1]])
X0 = np.hstack([np.ones([M,1]), x1[C0], x2[C0]])

X1 = np.asmatrix(X1)
X0 = np.asmatrix(X0)
```

```
w = cvx.Variable([3,1])

obj = cvx.Minimize(1)
const = [X1*w >= 1, X0*w <= -1]
prob = cvx.Problem(obj, const).solve()

w = w.value
```

CVXPY 1

$$
\begin{aligned}
\text{minimize} \quad & \text{something} \\
\text{subject to} \quad & X_1\omega \geq 1 \\
& X_0\omega \leq -1
\end{aligned}
$$



Linear Classification: Outlier

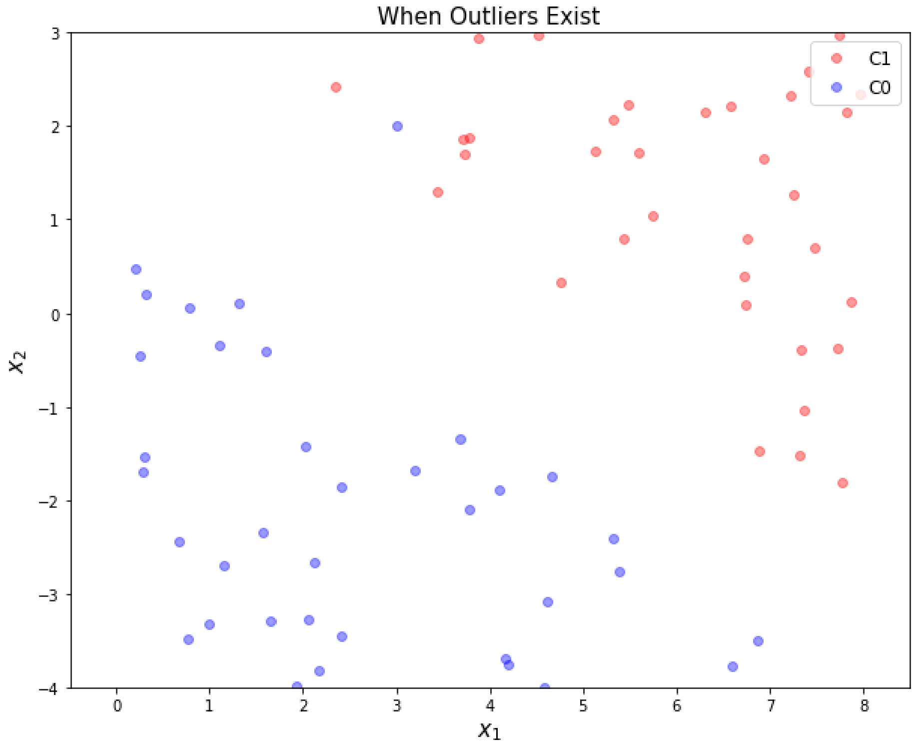
- Note that in the real world, you may have noise, errors, or outliers that do not accurately represent the actual phenomena

- Linearly non-separable case

Outliers

```
w = cvx.Variable([3,1])

obj = cvx.Minimize(1)
const = [X1*w >= 1, X0*w <= -1]
prob = cvx.Problem(obj, const).solve()

print(w.value)
```

None



- No solutions (hyperplane) exist

- We have to allow some training examples to be misclassified !
- but we want their number to be minimized

Optimization Formulation 2

- n $(= 2)$ features
- N belongs to C_1 in training set
- M belongs to C_0 in training set
- $m = N + M$ data points in training set

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

$$\begin{aligned} \text{minimize} \quad & \text{something} \\ \text{subject to} \quad & X_1 \omega \geq 1 \\ & X_0 \omega \leq -1 \end{aligned}$$

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

Optimization Formulation 2

- The optimization problem for the non-separable case

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

Expressed in a Matrix Form

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

$$X_0 = \begin{bmatrix} \left(x^{(N+1)}\right)^T \\ \left(x^{(N+2)}\right)^T \\ \vdots \\ \left(x^{(N+M)}\right)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(N+1)} & x_2^{(N+1)} \\ 1 & x_1^{(N+2)} & x_2^{(N+2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(N+M)} & x_2^{(N+M)} \end{bmatrix}$$

$$u = \begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix} \qquad v = \begin{bmatrix} v_1 \\ \vdots \\ v_M \end{bmatrix}$$

$$\begin{array}{ll} \text{minimize} & 1^T u + 1^T v \\ \text{subject to} & X_1 \omega \geq 1 - u \\ & X_0 \omega \leq -(1 - v) \\ & u \geq 0 \\ & v \geq 0 \end{array}$$

$$\text{minimize} \quad \sum_{i=1}^{N} u_i + \sum_{i=1}^{M} v_i$$

$$\text{subject to} \quad \begin{cases} \omega^T x^{(1)} \geq 1 - u_1 \\ \omega^T x^{(2)} \geq 1 - u_2 \\ \quad \vdots \\ \omega^T x^{(N)} \geq 1 - u_N \end{cases}$$

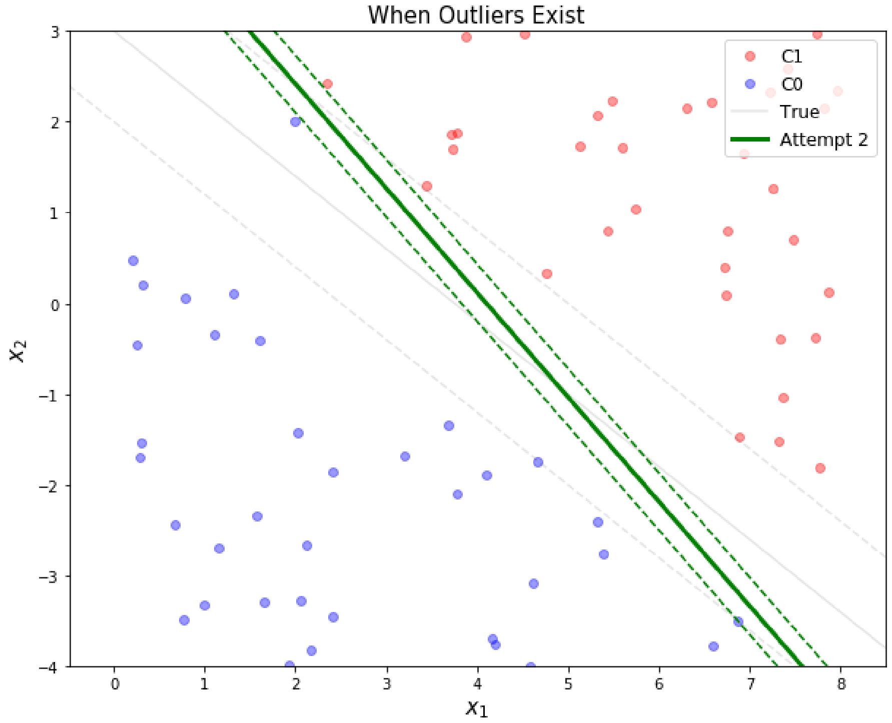
$$\begin{cases} \omega^T x^{(N+1)} \leq -(1 - v_1) \\ \omega^T x^{(N+2)} \leq -(1 - v_2) \\ \quad \vdots \\ \omega^T x^{(N+M)} \leq -(1 - v_M) \end{cases}$$

$$\begin{cases} u \geq 0 \\ v \geq 0 \end{cases}$$

CVXPY 2

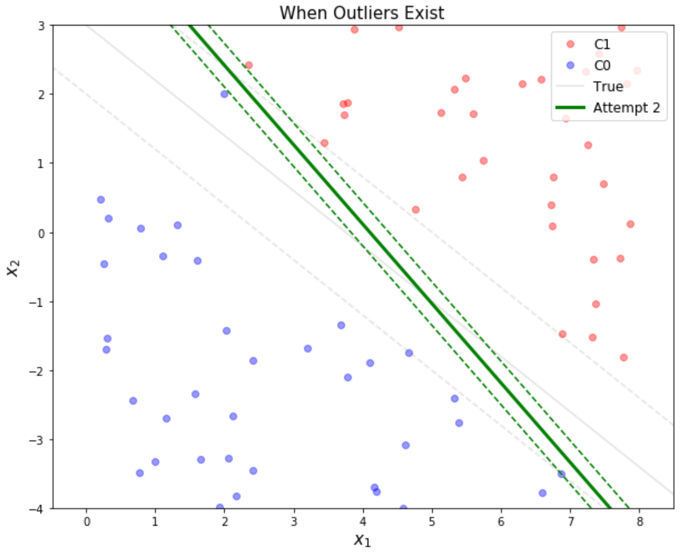
$$\begin{array}{ll} \text{minimize} & \text{something} \\ \text{subject to} & X_1\omega \geq 1 \\ & X_0\omega \leq -1 \end{array} \quad \Rightarrow \quad \begin{array}{ll} \text{minimize} & 1^T u + 1^T v \\ \text{subject to} & X_1\omega \geq 1 - u \\ & X_0\omega \leq -(1 - v) \\ & u \geq 0 \\ & v \geq 0 \end{array}$$

```
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, X0*w <= -(1-v), u >= 0, v >= 0 ]
prob = cvx.Problem(obj, const).solve()

w = w.value
```



Further Improvement

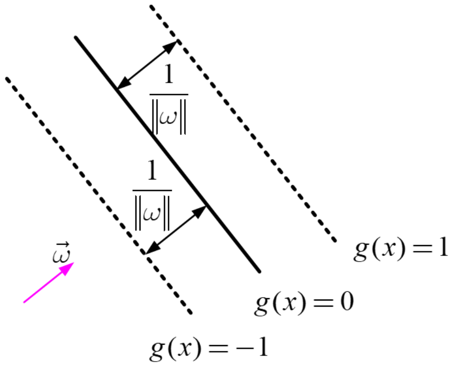
- Notice that hyperplane is not as accurately represent the division due to the outlier



- Can we do better when there are noise data or outliers?
- Yes, but we need to look beyond linear programming

- Idea: large margin leads to good generalization on the test data

Maximize Margin



- Finally, it is Support Vector Machine (SVM)
- 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 between the followings:
  - Bigger margin given robustness to outliers
  - Hyperplane that has few (or no) errors

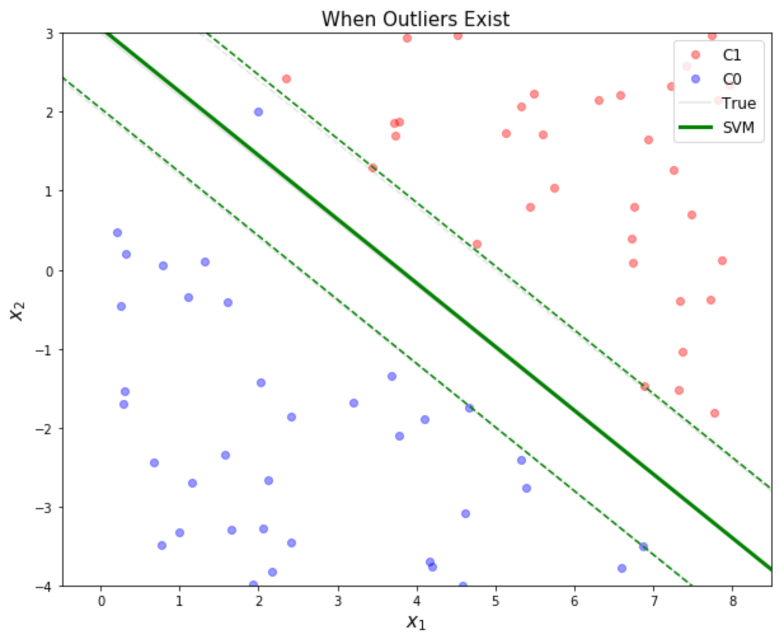
Support Vector Machine

$$\begin{aligned} \text{minimize} \quad & 1^T u + 1^T v \\ \text{subject to} \quad & X_1 \omega \geq 1 - u \\ & X_0 \omega \leq -(1 - v) \\ & u \geq 0 \\ & v \geq 0 \end{aligned}$$

$\Rightarrow$

$$\begin{aligned} \text{minimize} \quad & \|\omega\|_2 + \gamma(1^T u + 1^T v) \\ \text{subject to} \quad & X_1 \omega \geq 1 - u \\ & X_0 \omega \leq -(1 - v) \\ & u \geq 0 \\ & v \geq 0 \end{aligned}$$

```
g = 2

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, X0*w <= -(1-v), u >= 0, v >= 0 ]
prob = cvx.Problem(obj, const).solve()

w = w.value
```



Support Vector Machine

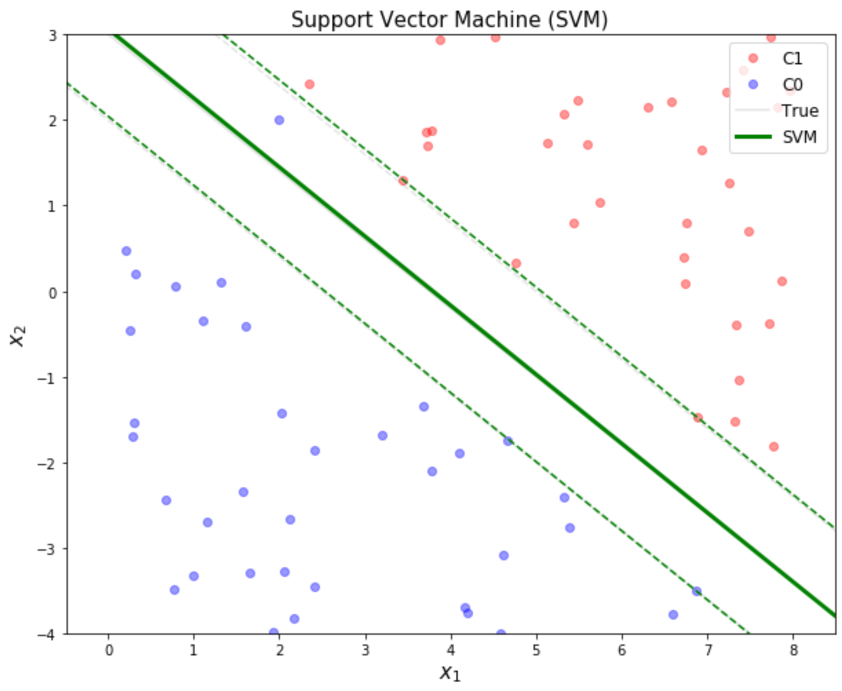
- In a more compact form

$$\begin{aligned} \text{minimize} \quad & \|\omega\|_2 + \gamma(1^T u + 1^T \upsilon) \\ \text{subject to} \quad & X_1 \omega \geq 1 - u \\ & X_0 \omega \leq -(1 - \upsilon) \\ & u \geq 0 \\ & \upsilon \geq 0 \end{aligned}$$

$$\begin{aligned} \omega^T x_n &\geq 1 \text{ for } y_n = +1 \\ \omega^T x_n &\leq -1 \text{ for } y_n = -1 \end{aligned} \iff y_n \cdot (\omega^T x_n) \geq 1$$

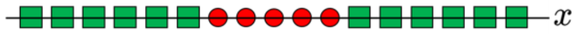
$$\begin{aligned} \text{minimize} \quad & \|\omega\|_2 + \gamma(1^T \xi) \\ \text{subject to} \quad & y_n \cdot (\omega^T x_n) \geq 1 - \xi_n \\ & \xi \geq 0 \end{aligned}$$

```
X = np.vstack([X1, X0])
y = np.vstack([np.ones([N,1]), -np.ones([M,1])])

m = N + M

g = 2

w = cvx.Variable([3,1])
d = cvx.Variable([m,1])

obj = cvx.Minimize(cvx.norm(w,2) + g*(np.ones([1,m])*d))
const = [cvx.multiply(y, X*w) >= 1-d, d >= 0]
prob = cvx.Problem(obj, const).solve()

w = w.value
```



Classifying Non-linear Separable Data

- Consider the binary classification problem
  - each example represented by a single feature x
  - No linear separator exists for this data



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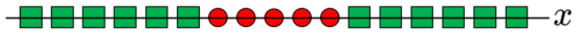
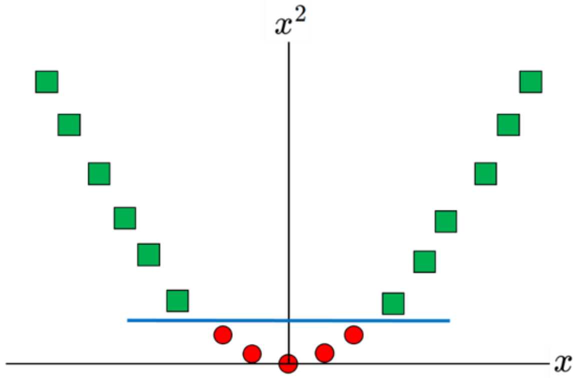


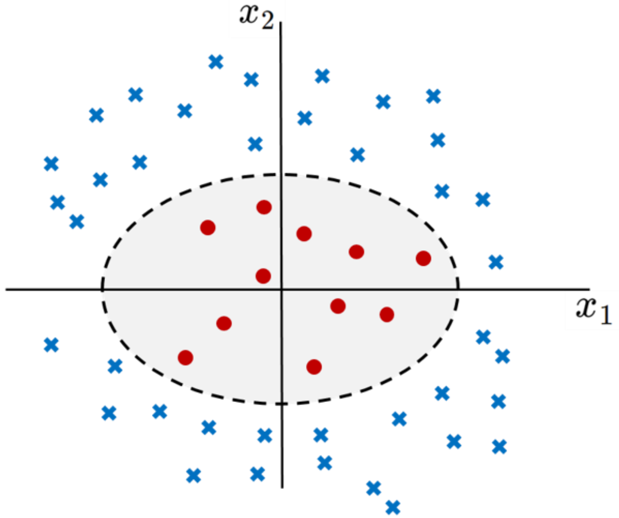
- Now map each example as $x \rightarrow \{x, x^2\}$
- Data now becomes linearly separable in the new representation

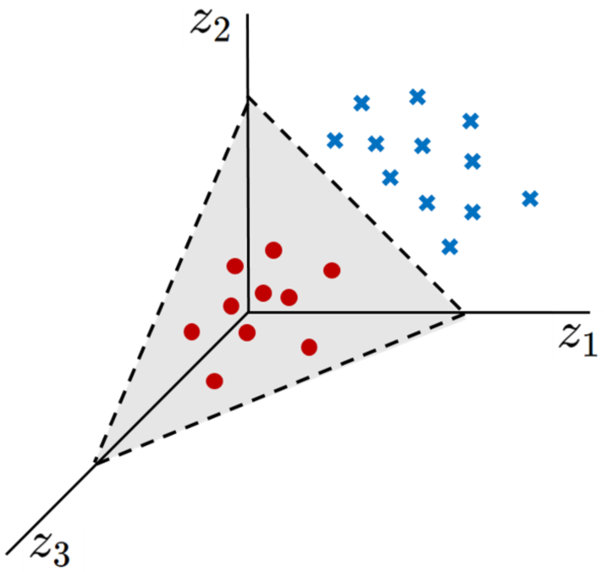


- Linear in the new representation = nonlinear in the old representation

Classifying Non-linear Separable Data

- Let's look at another example
  - Each example defined by a two features
  - No linear separator exists for this data $x = \{x_1, x_2\}$





- Now map each example as $x = \{x_1, x_2\} \rightarrow z = \left\{x_1^2, \sqrt{2}x_1x_2, x_2^2\right\}$
  - Each example now has three features (derived from the old representation)
- Data now becomes linear separable in the new representation

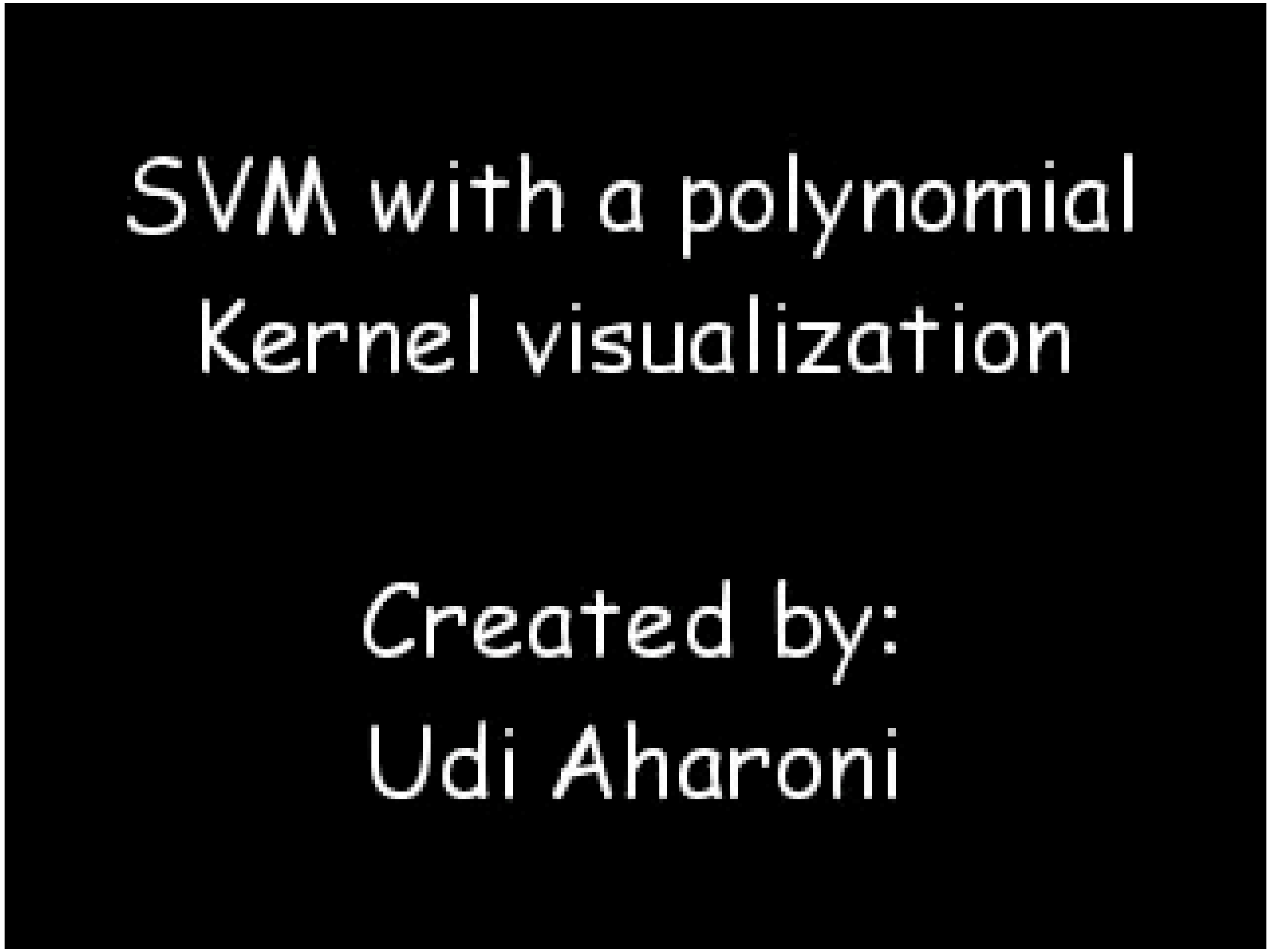
Kernel

- Often we want to capture nonlinear patterns in the data
  - nonlinear regression: input and output relationship may not be linear
  - nonlinear classification: classes may note be separable by a linear boundary

- Linear models (e.g. linear regression, linear SVM) are note just rich enough
  - by mapping data to higher dimensions where it exhibits linear patterns
  - apply the linear model in the new input feature space
  - mapping = changing the feature representation

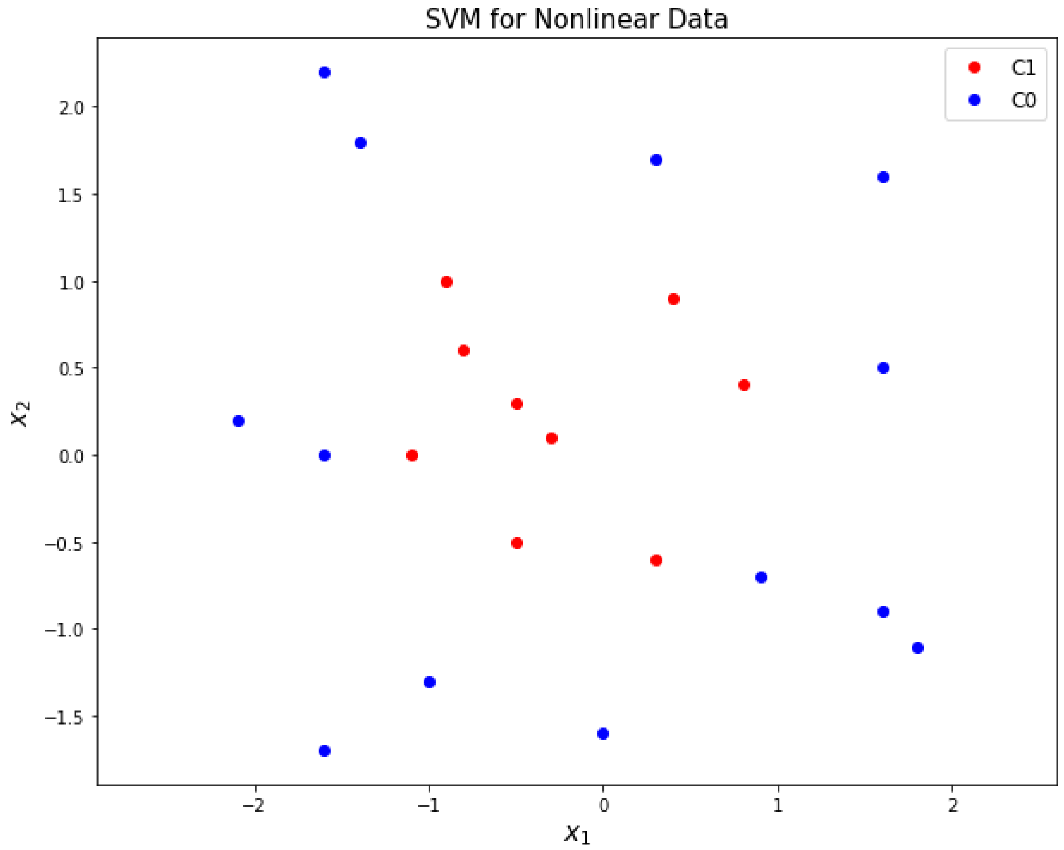
- Kernels: make linear model work in nonlinear settings

Nonlinear Classification



https://www.youtube.com/watch?v=3liCbRZPrZA

Classifying Non-linear Separable Data



POSTECH

Classifying Non-linear Separable Data

```
N = X1.shape[0]
M = X0.shape[0]

X = np.vstack([X1, X0])
y = np.vstack([np.ones([N,1]), -np.ones([M,1])])

X = np.asmatrix(X)
y = np.asmatrix(y)

m = N + M
Z = np.hstack([np.ones([m,1]), np.square(X[:,0]), np.sqrt(2)*np.multiply(X[:,0],X[:,1]), np.square(X[:,1])])

g = 10

w = cvx.Variable([4, 1])
d = cvx.Variable([m, 1])

obj = cvx.Minimize(cvx.norm(w, 2) + g*np.ones([1,m])*d)
const = [cvx.multiply(y, Z*w) >= 1-d, d>=0]
prob = cvx.Problem(obj, const).solve()

w = w.value
print(w)
```

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \Longrightarrow \quad z = \phi(x) = \begin{bmatrix} 1 \\ x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$$

$$\begin{aligned} \text{minimize} \quad & \|\omega\|_2 + \gamma(1^T\xi) \\ \text{subject to} \quad & y_n \cdot \left(\omega^T x_n\right) \geq 1 - \xi_n \\ & \xi \geq 0 \end{aligned}$$

Classifying Non-linear Separable Data