Fourth Industrial Summer School

Day 5

Discriminant Classification

Session Objectives

- ✓ Discriminative Classification
  - Linear Discriminant Analysis
    - How it works
    - Python Example
    - Try it your self
  - Support Vector Machines(SVM)
    - Hard Margin
    - Soft Margin
    - Kernel tricks
  - Hands on
- ✓ Semi-supervised Learning
  - When to use
  - Python Example
  - Hands on

Linear Discriminant analysis

- Linear Discriminant analysis or LDA is a classification method
- Developed in 1936 by R. A. Fisher
- It is a mathematically robust and often produces models whose accuracy is as good as complex ones.

Main idea

- The main idea of LDA is to reduce the dimensionality of the data while considering maximum separability.
- This is not similar to PCA that reduces the dimensionality while focusing on a dimension with the most variations.
- Linear Discriminant Analysis (LDA) is like PCA, but it focuses on maximizing the separability among known classes.

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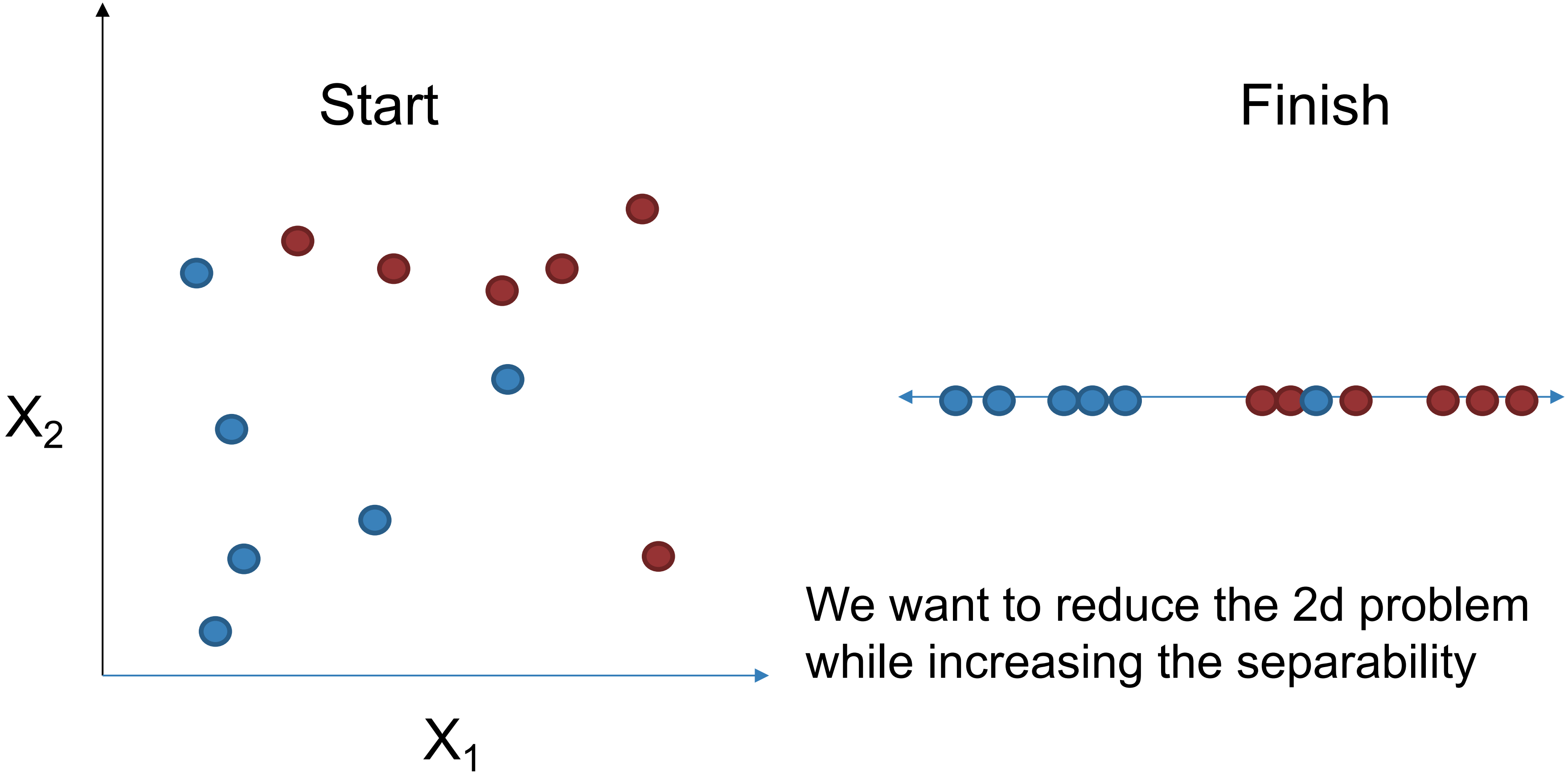

We want to reduce the 2d problem while increasing the separability

What is the best way to do that?

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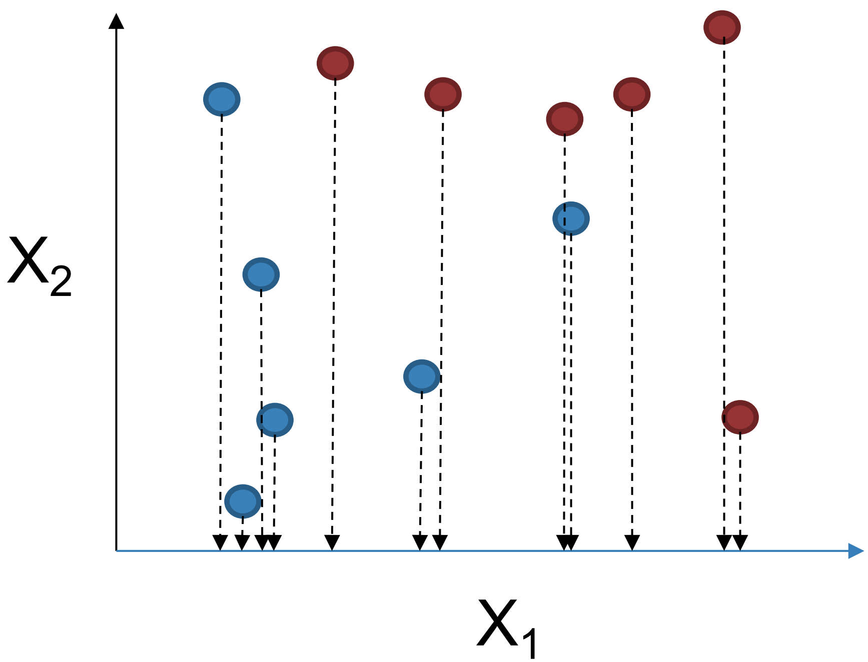
- One option is to ignore X_2 and focus on X_1



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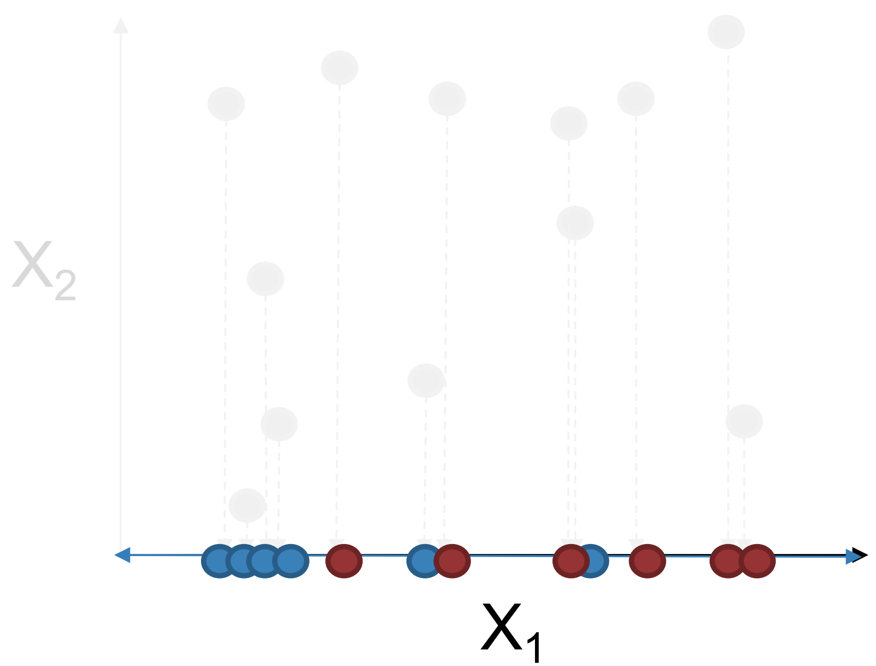

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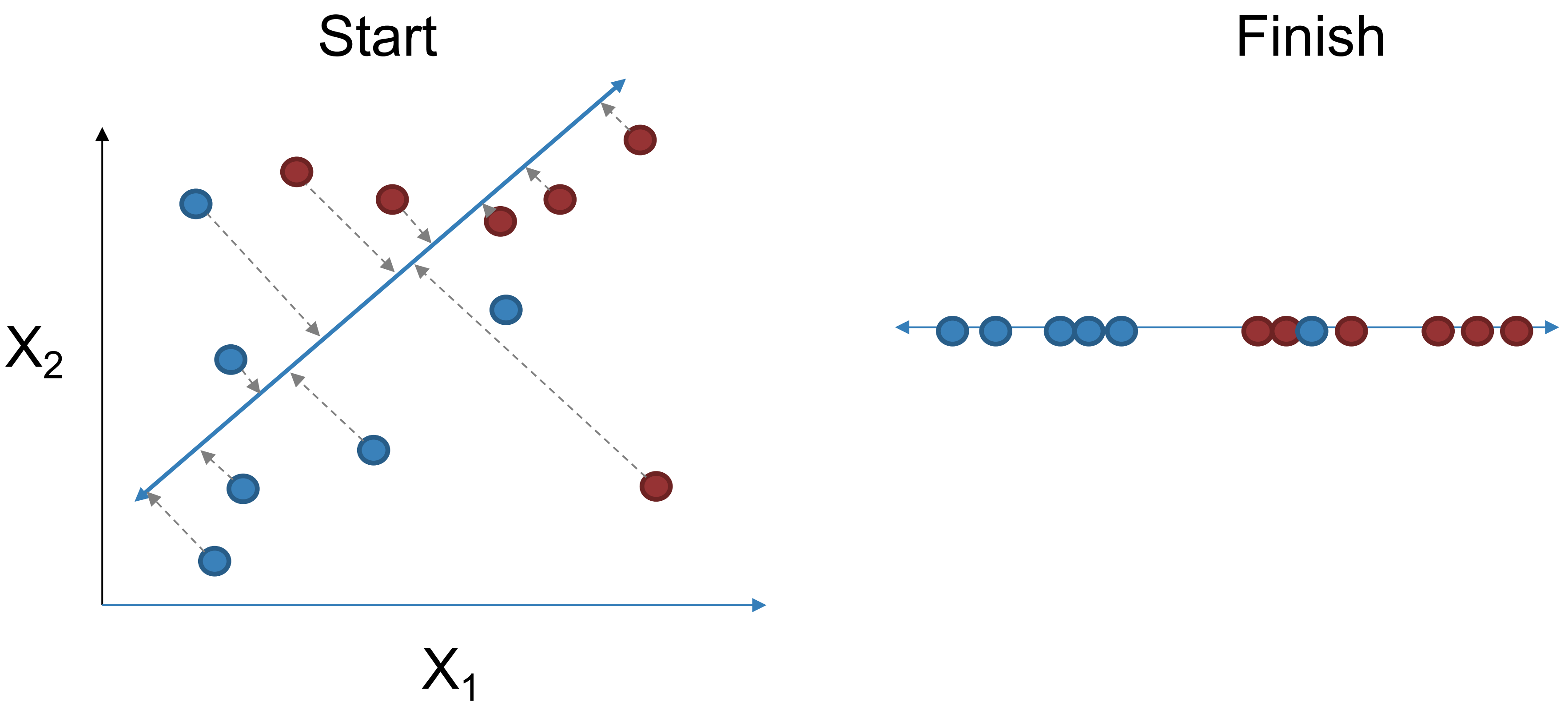

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- LDA is doing that reduction by utilizing the information of all dimensions. It finds a new dimension that satisfies two conditions
  - Maximizing the distance between the classes centroids

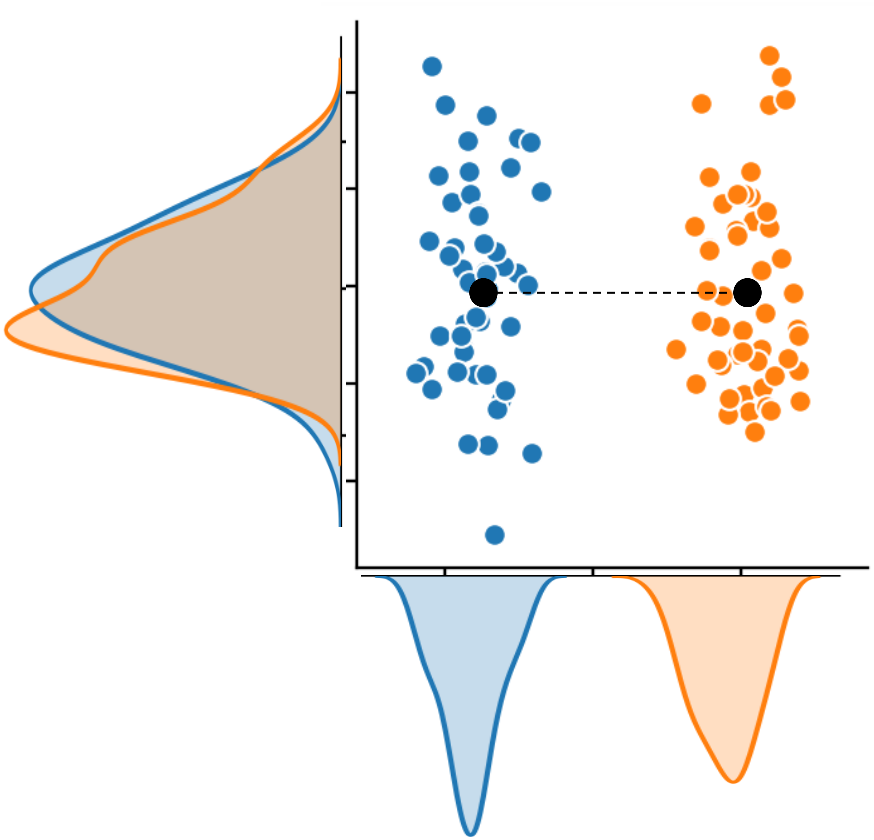
$$d = (\mu_1 - \mu_2)^2$$

  - Minimizing the speared within each class.

$$Sw = s_1^2 + s_2^2$$

Assessing Discrimination of the model

- One way to assess the effectiveness of the discrimination is to compute the Mahalanobis distance between the groups!



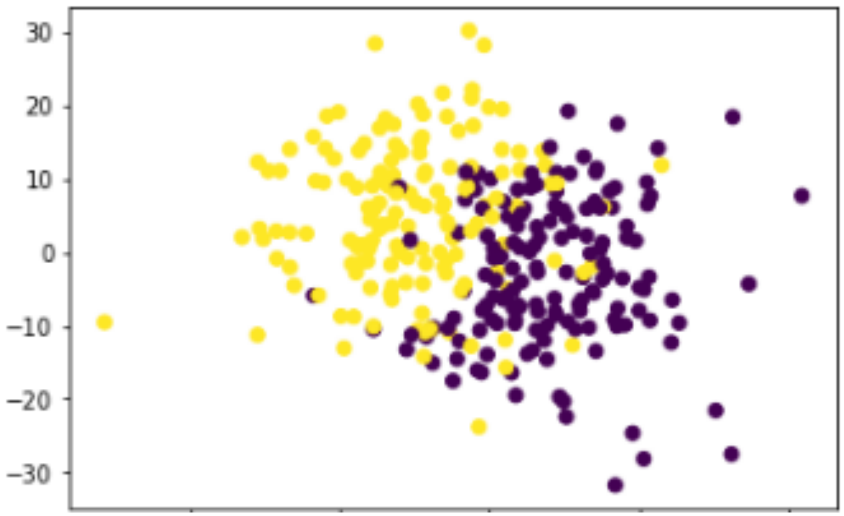
LDA in steps

1. Compute the frequency of each class $p(c_1), p(c_2)$
2. Compute the mean of each group $\mu_1,\ \mu_2$
3. Compute the covariance matrix of each group $\Sigma_1,\ \Sigma_2$
4. Compute the pooled covariance matrix: $\Sigma_p = \frac{1}{n_1+n_2}(n_1\Sigma_1 + n_2\Sigma_2)$
5. Compute the inverse of Σ_p^{-1}
6. Compute the linear combination parameters: $\beta = \Sigma_p^{-1}(\mu_1 - \mu_2)$
7. Apply the decision rule on the new data to classify

$$D(X) = \begin{cases} Class\ 1: & \beta^T\left(x - \left(\frac{\mu_1 + \mu_2}{2}\right)\right) > \log\left(\frac{p(c_1)}{p(c_2)}\right) \\ Class\ 2: & \beta^T\left(x - \left(\frac{\mu_1 + \mu_2}{2}\right)\right) \leq \log\left(\frac{p(c_1)}{p(c_2)}\right) \end{cases}$$

Example(Make data)

```
import matplotlib.pyplot as plt
from sklearn import datasets
X, y = datasets.make_blobs(n_samples=300, centers=2, #will define classes
                           n_features=20, cluster_std=10,
                           random_state =6)
plt.scatter(X[:,0], X[:,1], c=y)
plt.show()
```



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```
# making some dataa (Linearly separable)
import matplotlib.pyplot as plt
from sklearn import datasets
X, y = datasets.make_blobs(n_samples=300, centers=2, #will define classes
                           n_features=20, cluster_std=10,
                           random_state =6)
plt.scatter(X[:,0], X[:,1], c=y)
plt.show()
```

Example (Split data)

```
# Split the data into training and test
from sklearn.model_selection import train_test_split
X2, X_test, y2, y_test = train_test_split(X, y, test_size=0.1, shuffle=True)
X_train, X_Validate, y_train, y_Validate = train_test_split(X2, y2, test_size=0.2, shuffle=True)

print('Training set shape:', X_train.shape,
      '\nValidatation set shape:', X_Validate.shape,
      '\nTesting set shape:', X_test.shape )
```

```
Training set shape: (216, 20)
Validatation set shape: (54, 20)
Testing set shape: (30, 20)
```

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```
# Split the data into training and test
from sklearn.model_selection import train_test_split
X2, X_test, y2, y_test = train_test_split(X, y, test_size=0.1, shuffle=True)
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print('Training set shape:', X_train.shape,
      '\nValidatation set shape:', X_Validate.shape,
      '\nTesting set shape:', X_test.shape )
```

Example(LDA)

```
# Linear Discriminant Analysis
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis

# Using it as classifier, I don't need to specify parameters
lda = LinearDiscriminantAnalysis(n_components=2).fit(X_train, y_train)

print('Train accuracy:%0.2f'% lda.score(X_train, y_train))
print('Validation accuracy:%0.2f'% lda.score(X_Validate, y_Validate))
print('Tesing accuracy:%0.2f'% lda.score(X_test, y_test))
```

```
Train accuracy:0.98
Validation accuracy:0.93
Tesing accuracy:0.93
```

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```
# Linear Discriminant Analysis
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis

# Using it as classifier, I don't need to specify parameters
lda = LinearDiscriminantAnalysis(n_components=2).fit(X_train, y_train)

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print('Tesing accuracy:%0.2f'% lda.score(X_test, y_test))
```
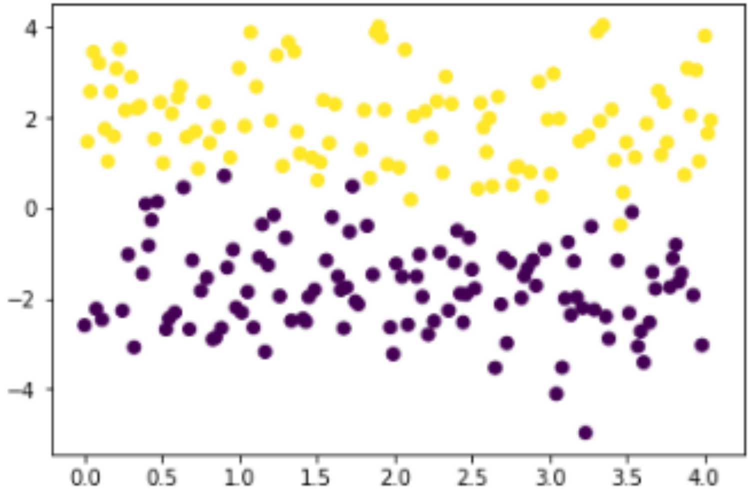

Example (Feature Reduction)

```
# in case of two classes: show how it separates the two classes
newX = lda.transform(X_train)
newX.shape
plt.scatter(np.linspace(0,max(newX),len(newX)), newX, c=y_train )
plt.show()
```



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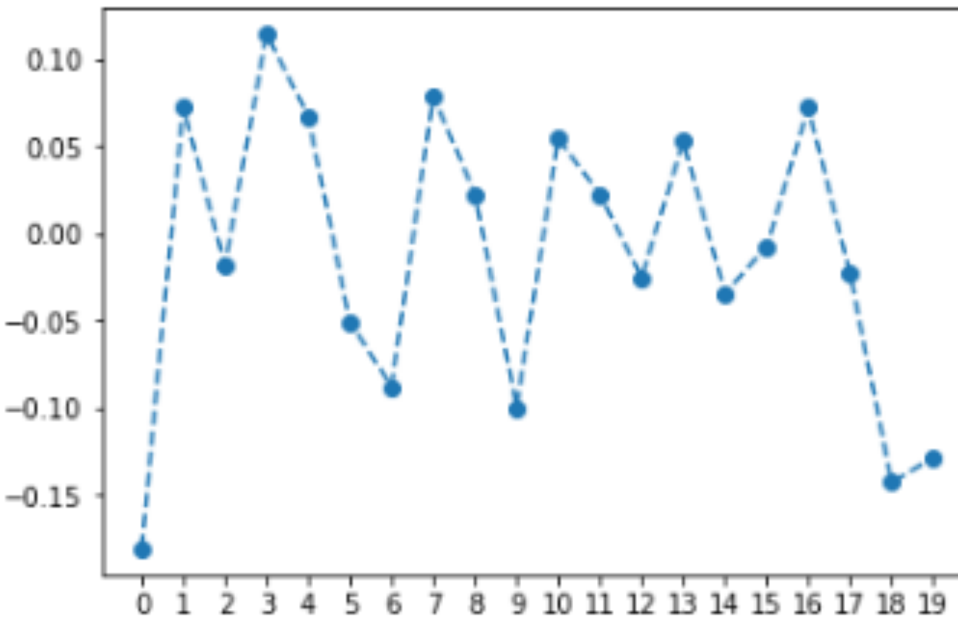
```
# in case of two classes: show how it separates the two classes

# To transform any new data into LDA space, use .transform(data)
newX = lda.transform(X_train)

plt.scatter(np.linspace(0,max(newX),len(newX)), newX, c=y_train )
plt.show()
```

Feature Contribution

```
# data properties
# The large the coef of a feature, the more important its role in the discrimination
plt.plot(np.arange(0,lda.coef_.size), lda.coef_[0], 'o--')
plt.xticks(np.arange(0,lda.coef_.size))
plt.show()
```



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# data properties
# The large the coef of a feature, the more important its role in the discrimination
plt.plot(np.arange(0,lda.coef_.size), lda.coef_[0], 'o--')
plt.xticks(np.arange(0,lda.coef_.size))
plt.show()

Try it out

- You may generate more features say 50 and experiment LDA
- Increase number of classes
- Increase the cluster std
- Try different data shapes (circles or moons)

Pros and Cons

- Derived Linearity rather than assumed
- Considers the ratio (between groups SS)/(within groups SS) as large as possible.
- Can play a role in feature selection by looking on the coefficients

- Assumes conditional densities of clusters are approximately normal.
- Coefficients may not indicate Feature Significance in case of more than two outcomes problems.

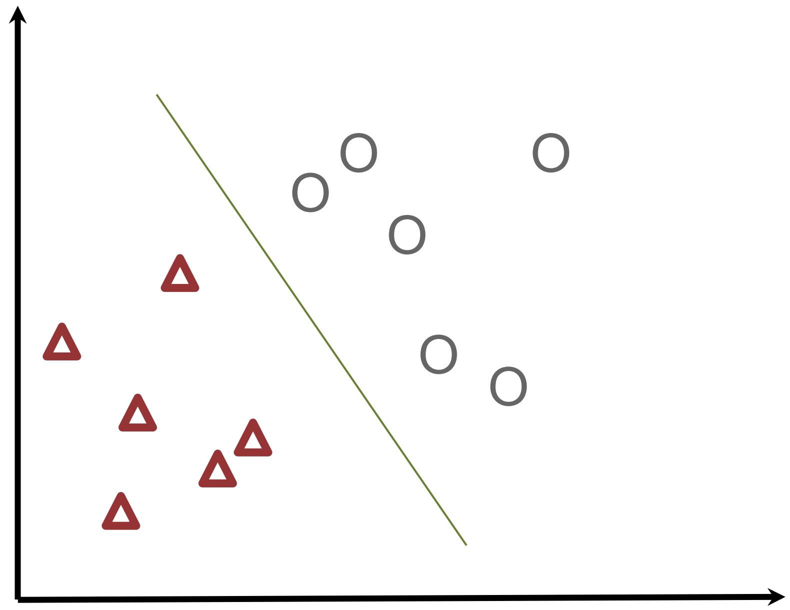
Support Vector Machines

Introduction: history

- SVM was first introduced in **1963** by V. Vapnik and A. Chervonenkis
- It dose really well with linear decision surfaces
- It becomes popular because of its success in modeling many machine learning problems, after its generalization in **1992** by Vapnik et. al (kernel trick)
- The basic idea is to separate a two class data points using a line (in 2-d space)

How it works?

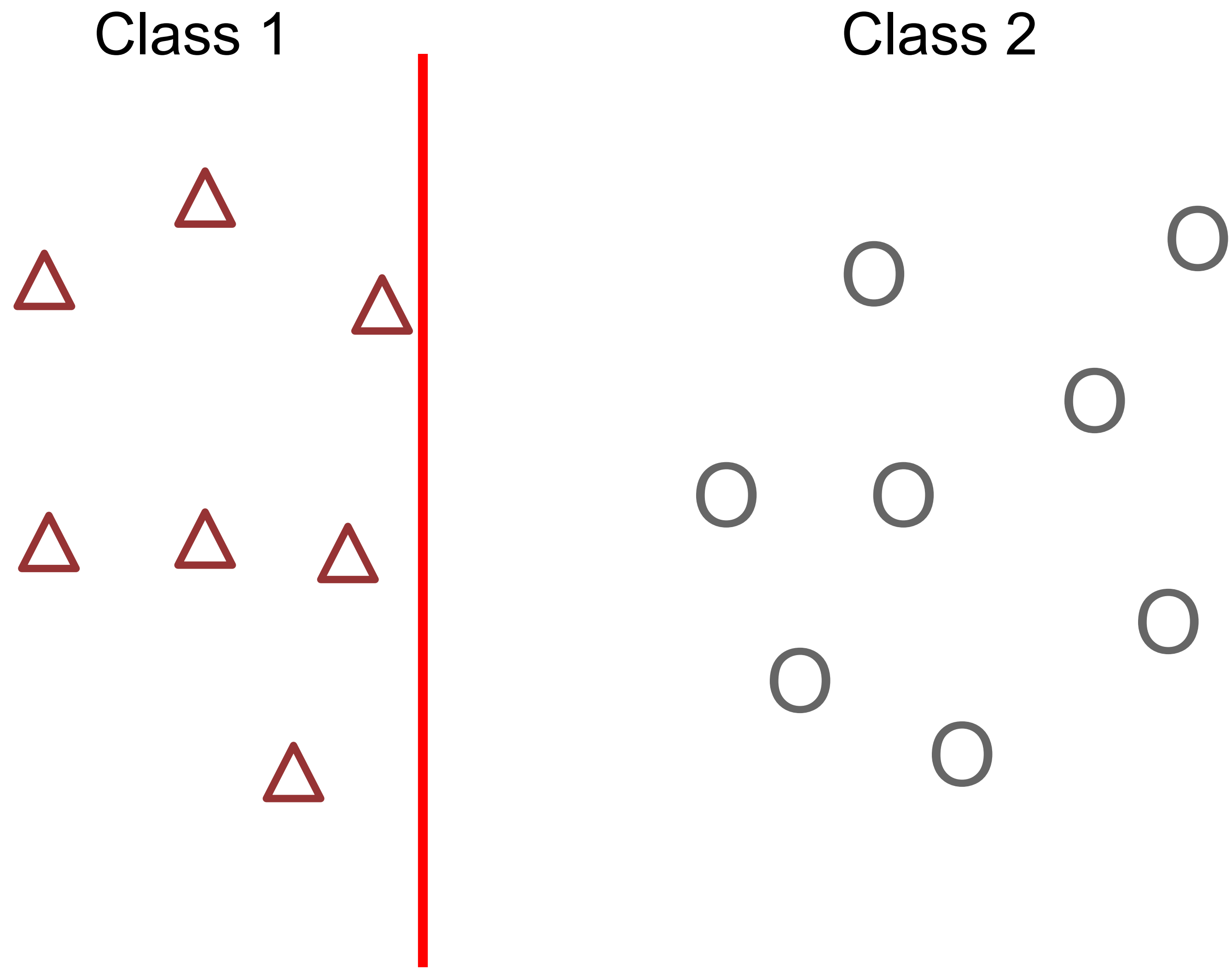
- Assume linear separability for now (and relax this later)



- Given such data points, we want to draw a line that separates the two classes.

$$w_1x_1 + w_2x_2 + b = 0$$

Contd.



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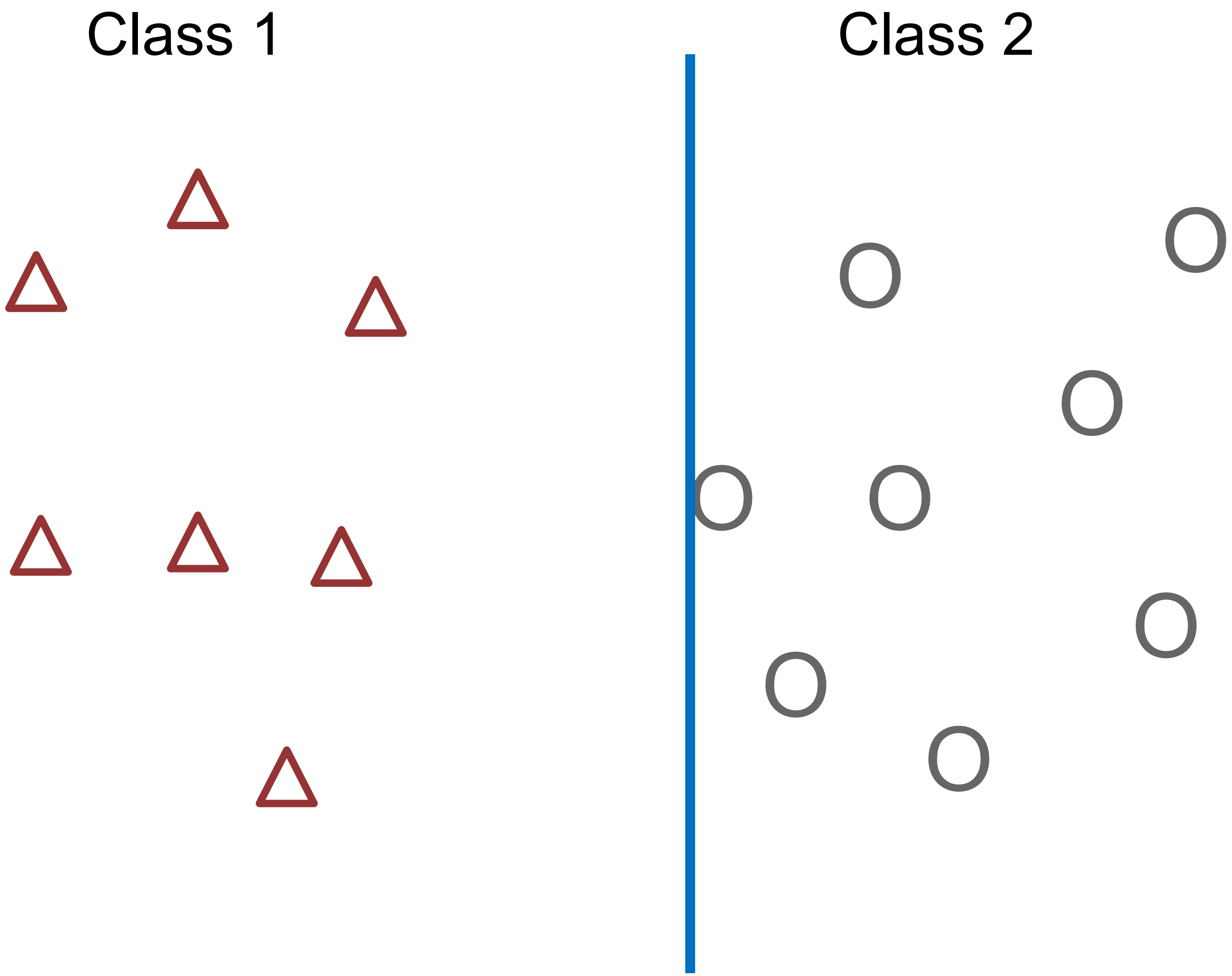

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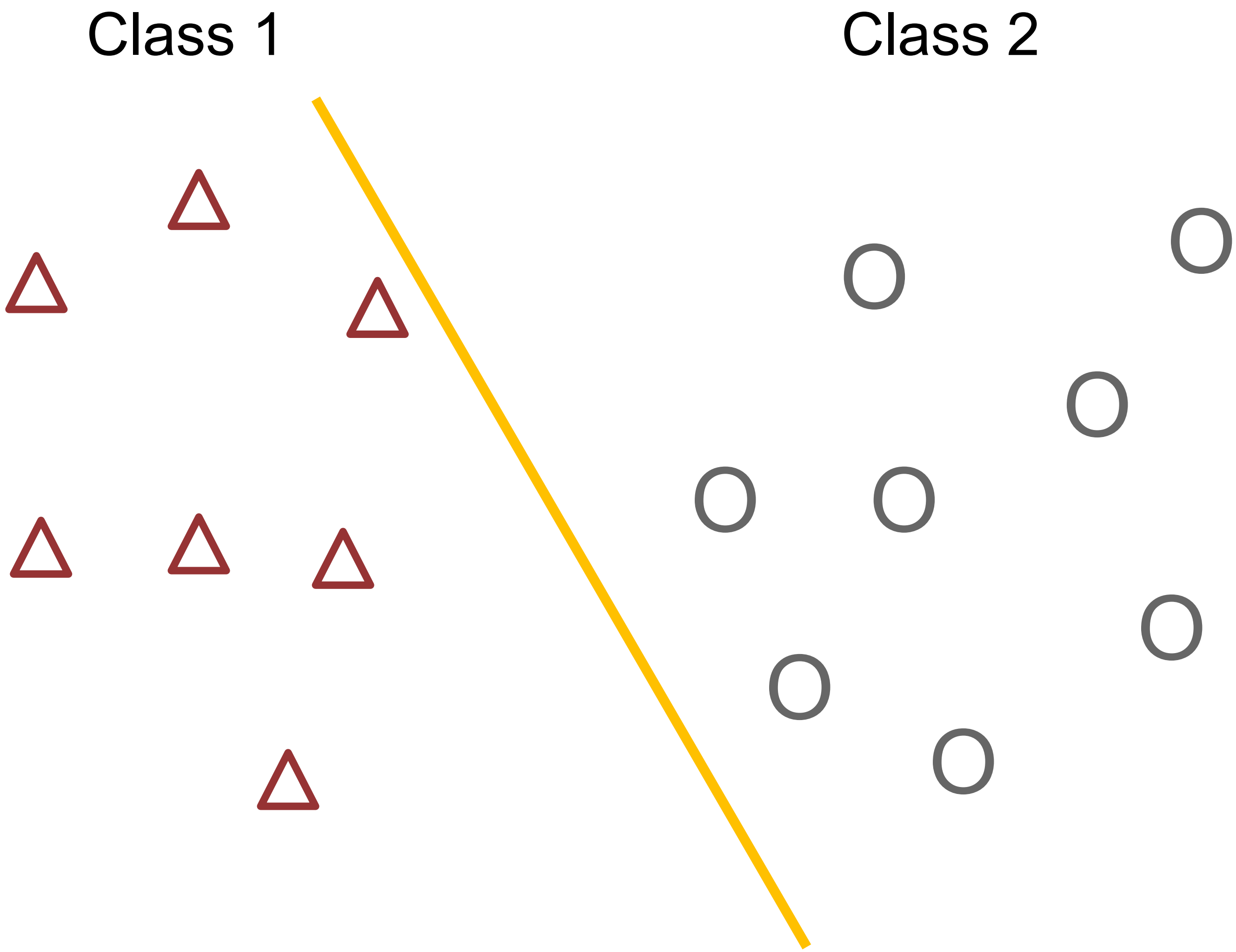
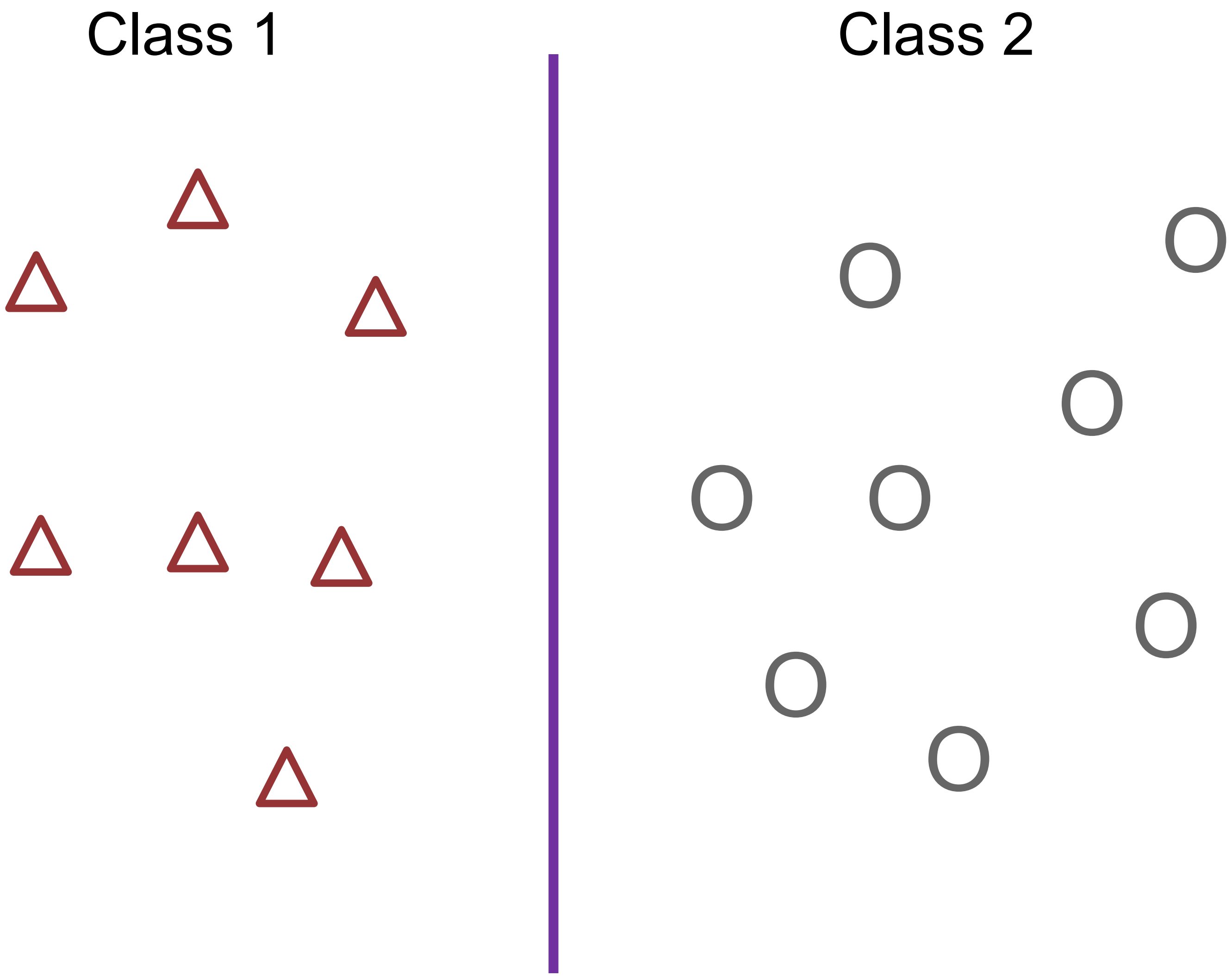


Optimal decision boundary

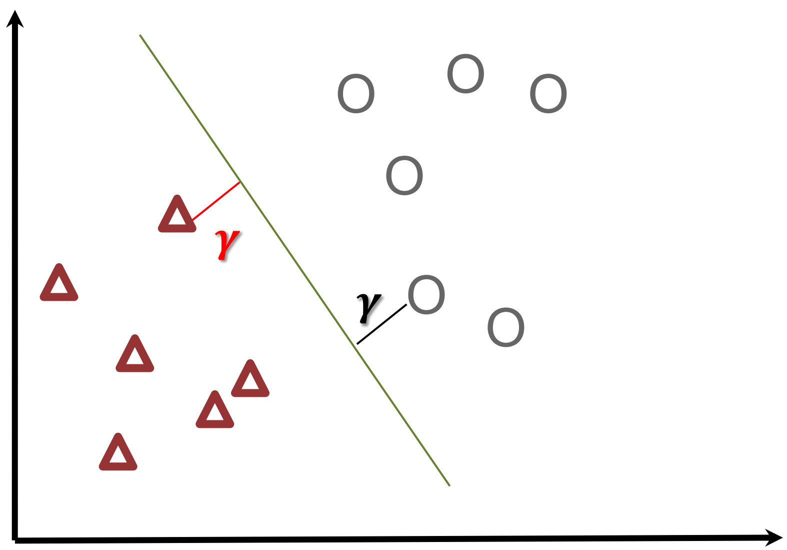


Optimal decision boundary

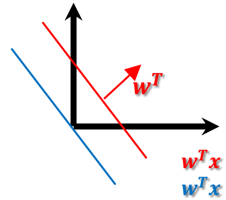
We're looking for a hyperplane that best separates the classes

How it works?

- Instead, we want to maximize the margin. In other words, we want to have a decision boundary far away from both classes as possible!

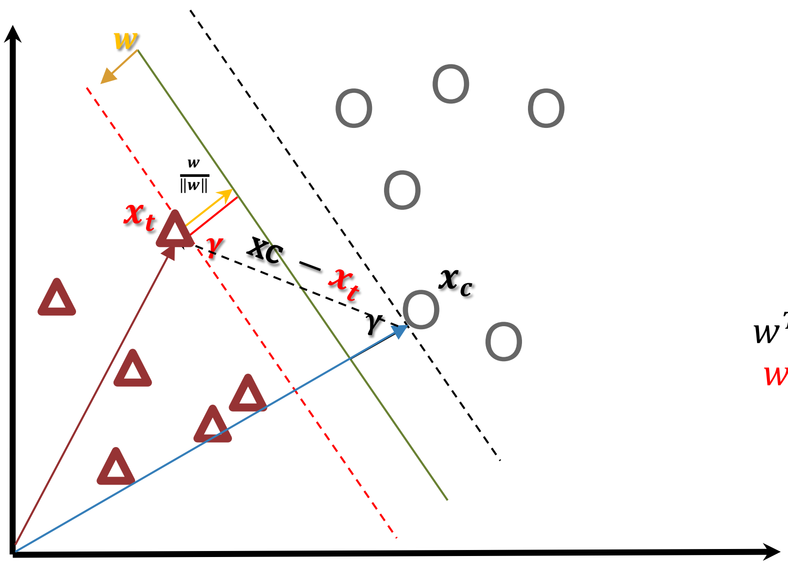


Define a margin



$w^T x + b = 0$, equate b=0
$w^T x = 0$, hence w is ⊥ on x

- SVM wants to maximize the margin between classes γ



$w^T x_c + b \geq +1$
$w^T x_t + b \leq -1$

***max γ*:**

$$(x_c - x_t) . \frac{w}{\|w\|}$$

$$(w. x_c - w. x_t) \frac{1}{\|w\|}$$

$$((1\text{-b}) - (\text{-1-b})) \frac{1}{\|w\|} = \frac{2}{\|w\|}$$

$$\max \frac{2}{\|w\|} \approx min\|w\| \approx \min \frac{1}{2} \|w\|^2$$

- So maximizing the margin γ, implicitly minimizing the vector **w**
- **Note both constraints have to be achieved.**

$$\max \gamma \approx \min \frac{1}{2} \|w\|^2 \ \ under \ y_i (w. x_i + b) \geq \ +1,$$

Hard margin

- To find the extremum, partial derivative is computed with respect to w and b
  - $\frac{\delta L}{\delta w}$: $w = \sum_{i=1}^{n} \alpha_i y_i x_i$
  - $\frac{\delta L}{\delta b}$: $\sum_{i=1}^{n} \alpha_i y_i = 0$
- By plug the value of w back in the Lagrangain function and simplify:

$$maximize: \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \, y_i y_j x_i^t . x_j$$

Subject to: $\sum_{i=1}^{n} \alpha_i y_i = 0, \;\; \alpha_i \geq \; 0 \; \forall i$

- Now if you want to make predictions just use:

$$\left(\sum_{i=1}^{n} \alpha_i y_i x_i . \boldsymbol{u}_i + b \right) \geq 1 \, , then\ circles\ otherwise\ triagnles$$

Example: SVM

```
from sklearn import svm
X, y = datasets.make_blobs(n_samples=300, centers=2, #will define classes
                           n_features=20, cluster_std=1,
                           random_state =6)

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, shuffle=True)
svmL= svm.SVC(kernel='linear',
              C=1e20,
              tol= 1e-3,
              max_iter = 1000,
              random_state=None).fit(X_train, y_train)
svmL.score(X_test,y_test )
```

```
1.0
```

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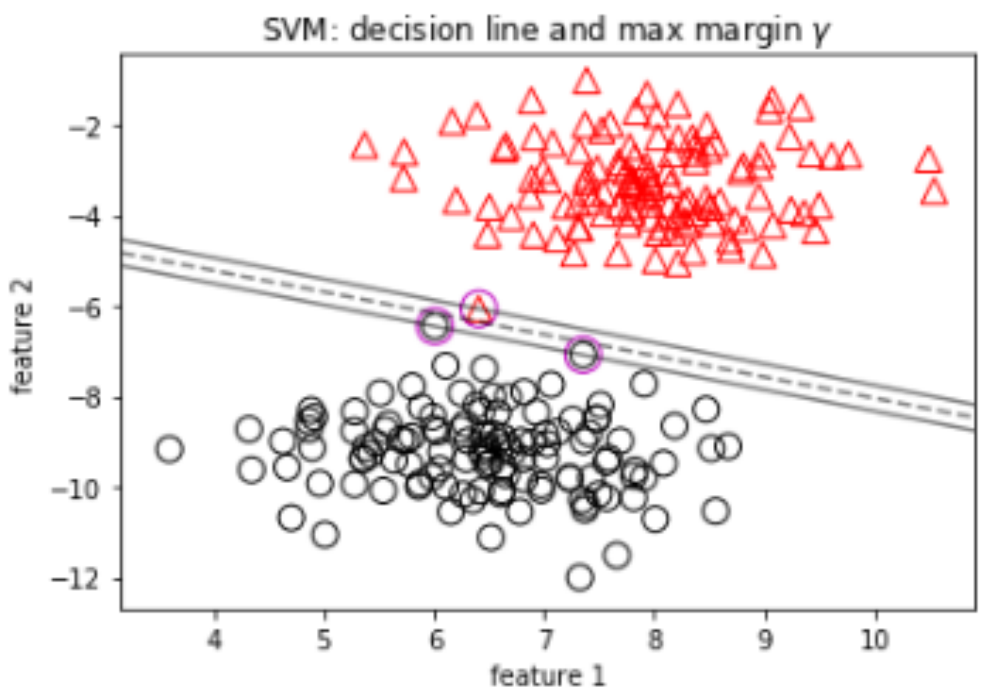
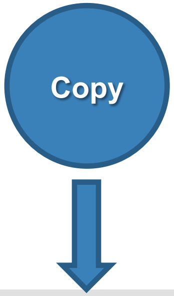
svmL.score(X_test,y_test )
```

Example: SVM(hard margin)

```
plot_SVM_decisionline2(svmL, X_train, y_train)
```





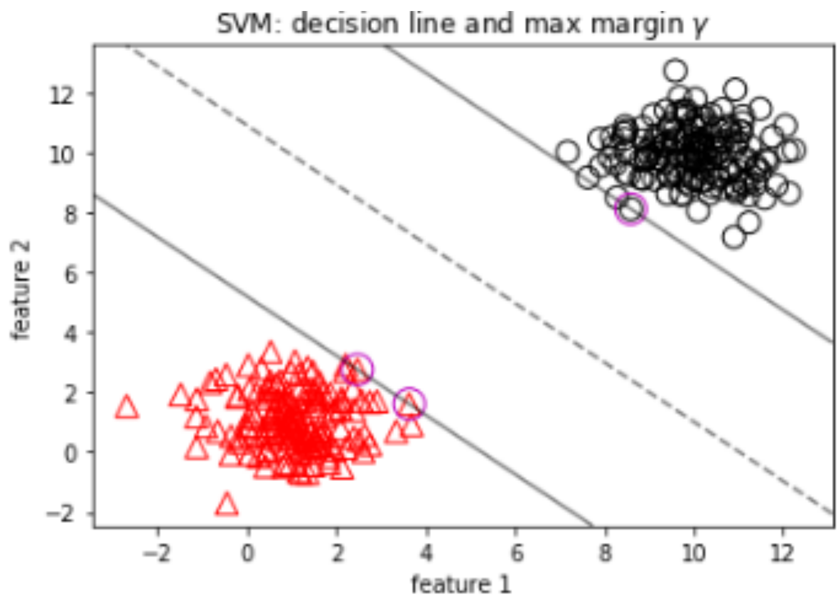

```
plot_SVM_decisionline2(svmL, X_train, y_train)
```

Example: SVM(hard margin)

```
X, y = datasets.make_blobs(n_samples=300, centers=[[1,1], [10,10]],
                           n_features=2, cluster_std=1,
                           random_state =6)

# train the model on this new data
svmL.fit(X,y )

plot_SVM_decisionline2(svmL, X, y)
```



What if one point landed in the other class

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```
X, y = datasets.make_blobs(n_samples=300, centers=[[1,1], [10,10]],
                           n_features=2, cluster_std=1,
                           random_state =6)

# train the model on this new data
svmL.fit(X,y )

plot_SVM_decisionline2(svmL, X, y)
```

Example: SVM(hard margin)

```
# get a list of indecies of class 1
ind= np.where(y==1)[0] # tuple
y[ind[np.random.randint(10)]] = 0

# train the model on this new data
svmL.fit(X,y )

plot_SVM_decisionline2(svmL, X, y)
```

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```
# get a list of indecies of class 1
ind= np.where(y==1)[0] # tuple
y[ind[np.random.randint(10)]] = 0

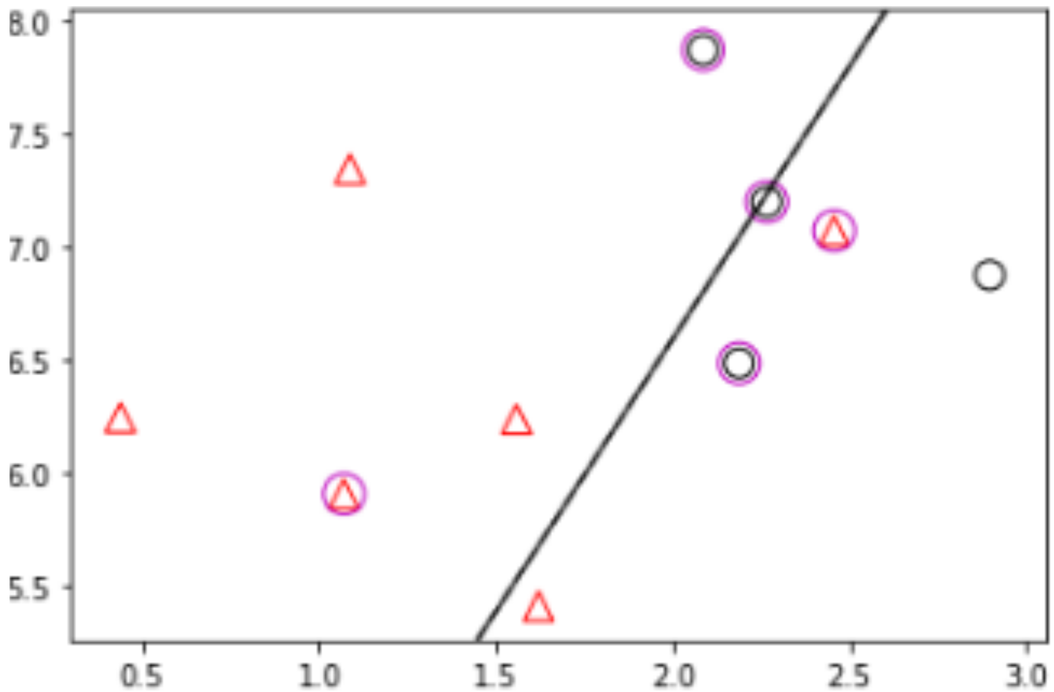
# train the model on this new data
svmL.fit(X,y )

plot_SVM_decisionline2(svmL, X, y)
```

SVM
Soft-Margin

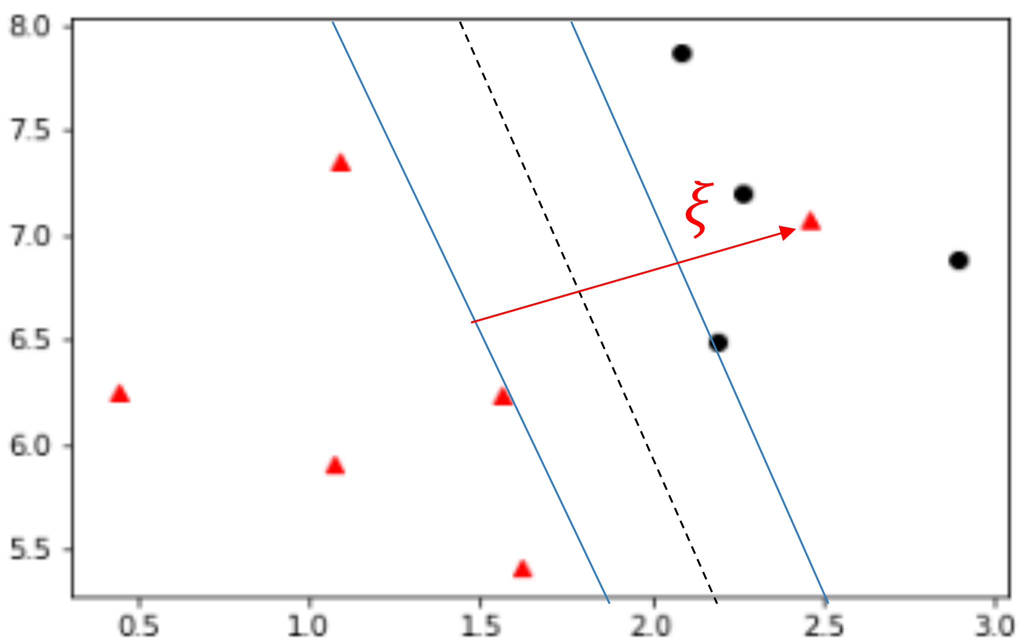
Soft Margin

- In reality, datasets suffer overlapping between class samples.
- Using SVM with Hard-margin optimization won't work!



Soft Margin

- To cope with this issue, the constraints are relaxed by introducing a slack variable ξ controlled by a weight parameter C
- The optimization and constraints becomes:
  - $\min \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi_i$
  - $y_i(w^T x + b) \geq 1 - \xi\,, \quad \xi \geq 0$



Soft Margin

- By solving the new optimization problem using Lagrange multiplier :
- The partial derivatives are computed with respect to w, b and ξ
  - $\frac{\delta L}{\delta w}$: $w = \sum_{i=1}^{n} \alpha_i y_i x_i$
  - $\frac{\delta L}{\delta b}$: $\sum_{i=1}^{n} \alpha_i y_i = 0$
  - $\frac{\delta L}{\delta \xi}$: $\sum_{i=1}^{n} C - \alpha_i - \beta_i, \quad C = \alpha_i + \beta_i, \quad \beta_i = C - \alpha_i$

$$maximize: \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \, y_i y_j x_i^t . x_j$$

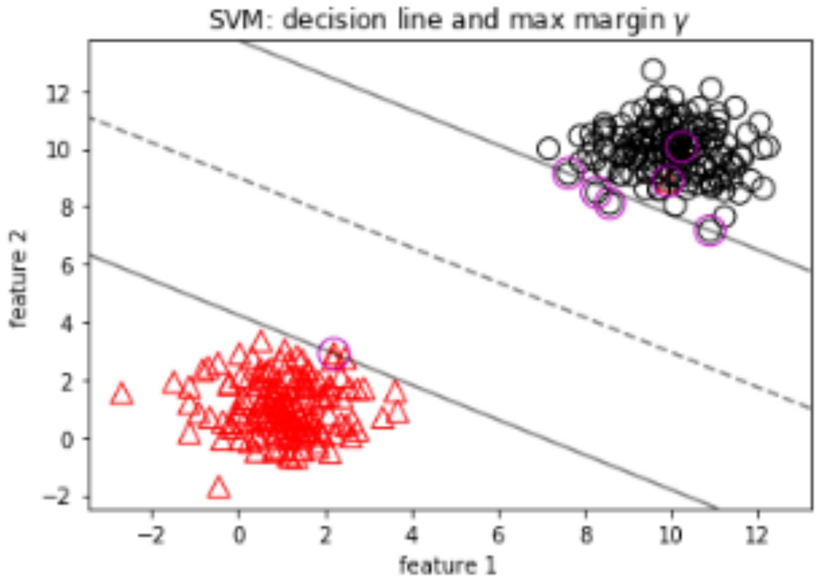
.

Example: SVM(hard margin)

```
svmL= svm.SVC(kernel='linear',
              C=0.3,
              tol= 1e-3,
              max_iter = 1000,
              random_state=None).fit(X_train, y_train)

# train the model on this new data
svmL.fit(X,y )

plot_SVM_decisionline2(svmL, X, y)
```



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# train the model on this new data
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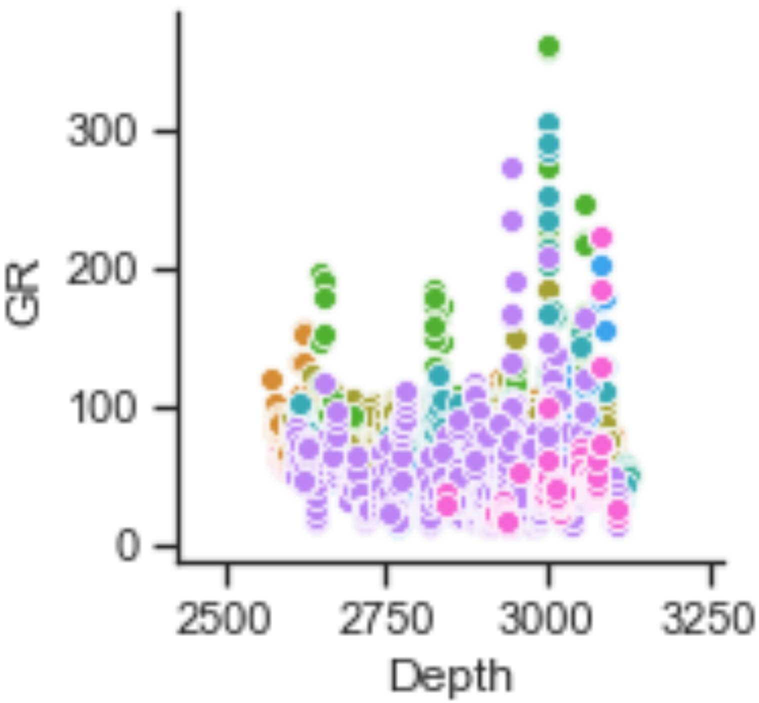
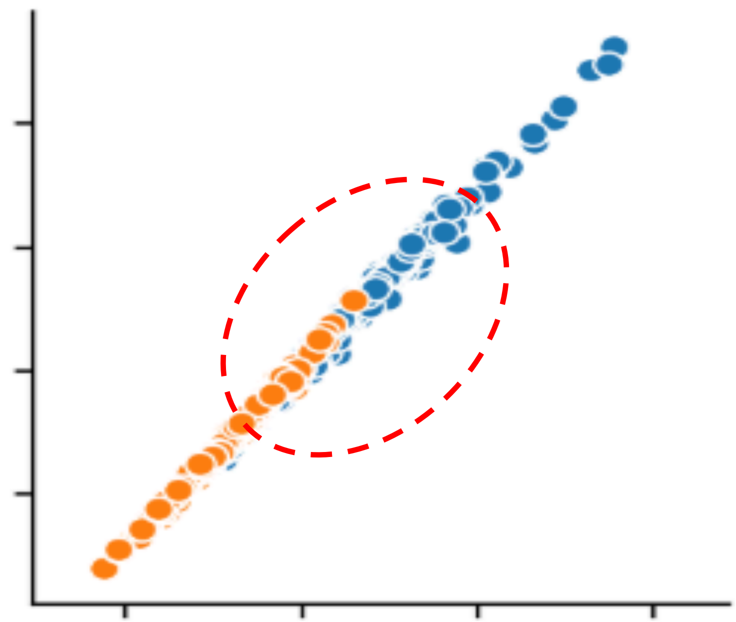
plot_SVM_decisionline2(svmL, X, y)

Real problems

- Real problems are not linearly separable in nature.
- For example, Facies dataset or Cancer dataset (Scikit learn)

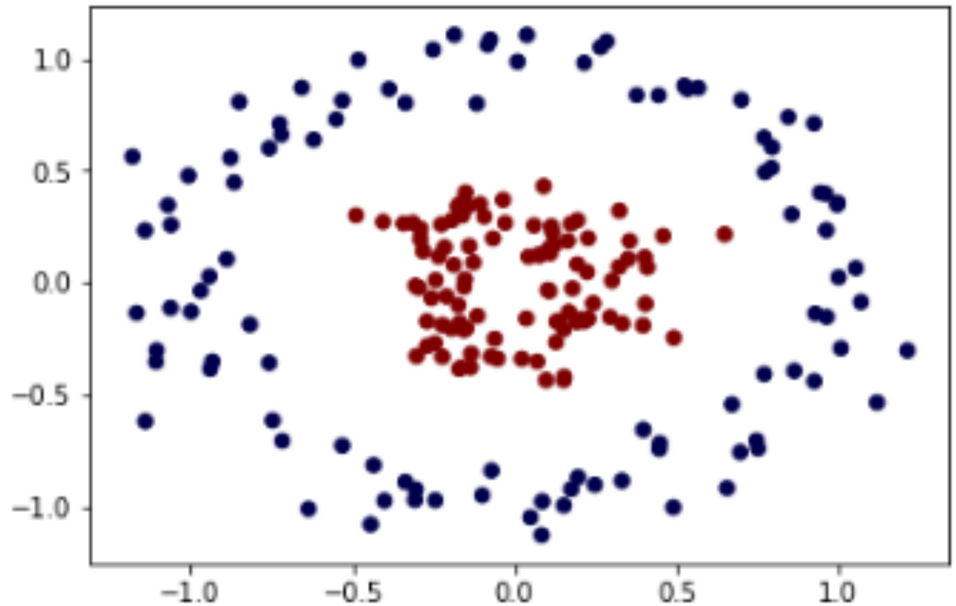




Kernel Trick

Kernel Trick

- Kernel trick is a data transformation that allow non-linearly separable data becomes separable in the another dimension.



Kernel Trick

$$maximize: \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j \, y_i y_j x_i^t . x_j$$

- The dot-product is targeted to transform the data.

$$K(x_i, x_j) = \phi(x_i).\phi(x_j)$$

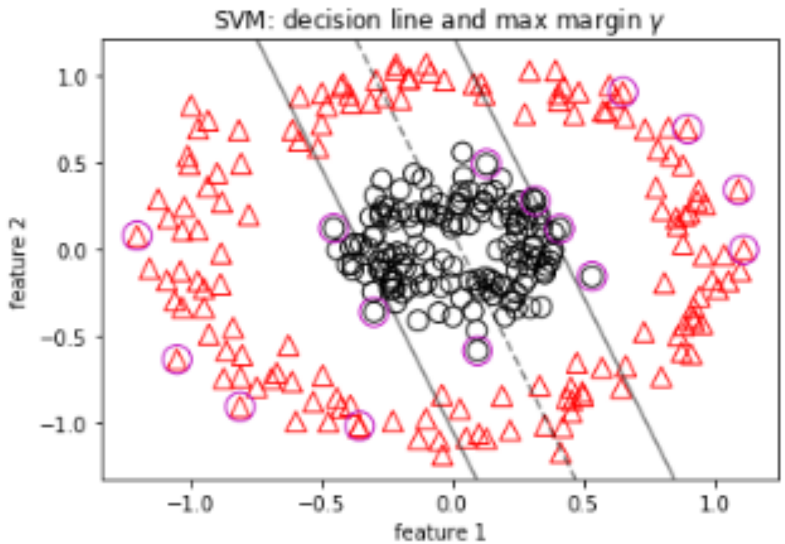
- Common Kernels are:
  - Polynomial $(\boldsymbol{x_i}.\boldsymbol{x_j})^{\boldsymbol{n}}$
  - Radial Basis Function (RBF) $\mathbf{e}^{-\frac{|x_i - x_j|}{2\sigma^2}}$, depends on the value of sigma
  - Sigmoid-like: $\mathbf{tanh}(\mathbf{c}\mathbf{x_i^T}\mathbf{x_j} + \mathbf{h})$

Example: SVM(linear)

```
# Try linear SVM on Circles dataset
svmL= svm.SVC(kernel='linear',
              C=1e20,
              tol= 1e-3,
              max_iter = 1000,
              random_state=None).fit(Xc, yc)

# train the model on this new data
svmL.fit(Xc,yc )

plot_SVM_decisionline2(svmL, Xc, yc)
```



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svmL= svm.SVC(kernel='linear',
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        tol= 1e-3,
        max_iter = 1000,
        random_state=None).fit(Xc, yc)

# train the model on this new data
svmL.fit(Xc,yc )

plot_SVM_decisionline2(svmL, Xc, yc)
```
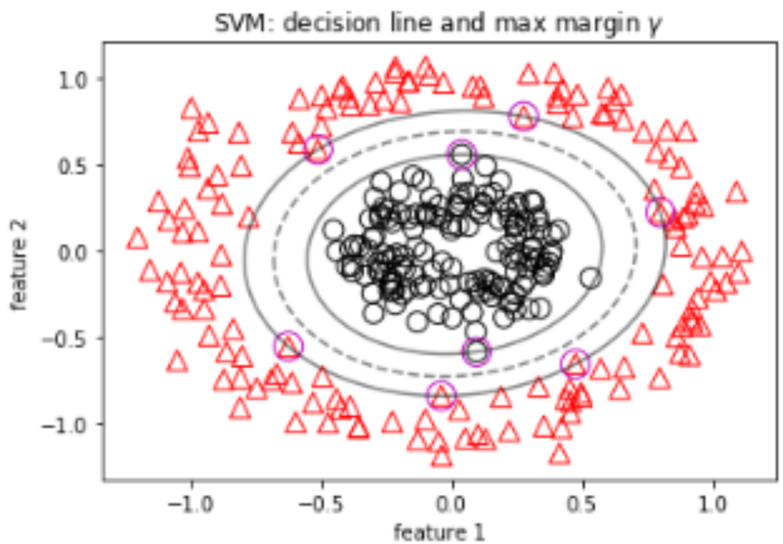

Example: SVM(linear)

```
# Try RBF SVM on Circles dataset
svmL= svm.SVC(kernel='rbf',
              gamma =0.2,
              C=1e20,
              tol= 1e-3,
              max_iter = 1000,
              random_state=None).fit(Xc, yc)

# train the model on this new data
svmL.fit(Xc,yc )

plot_SVM_decisionline2(svmL, Xc, yc)
```



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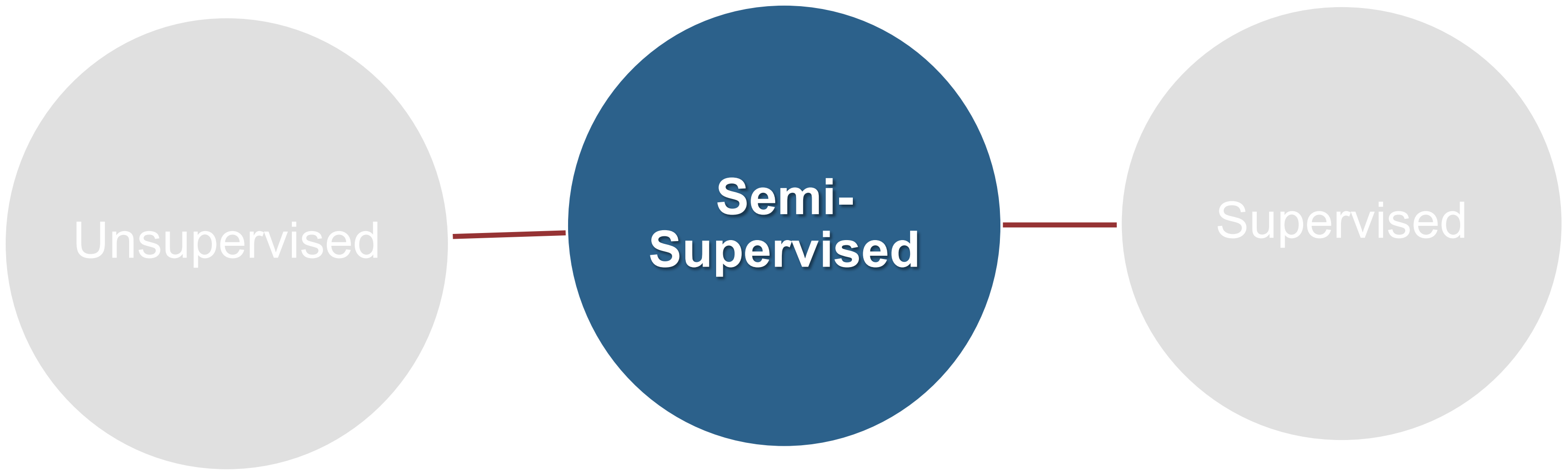
```
# Try RBF SVM on Circles dataset
svmL= svm.SVC(kernel='rbf',
        gamma =0.2,
        C=1e20,
        tol= 1e-3,
        max_iter = 1000,
        random_state=None).fit(Xc, yc)

# train the model on this new data
svmL.fit(Xc,yc )

plot_SVM_decisionline2(svmL, Xc, yc)
```

Semi-Supervised

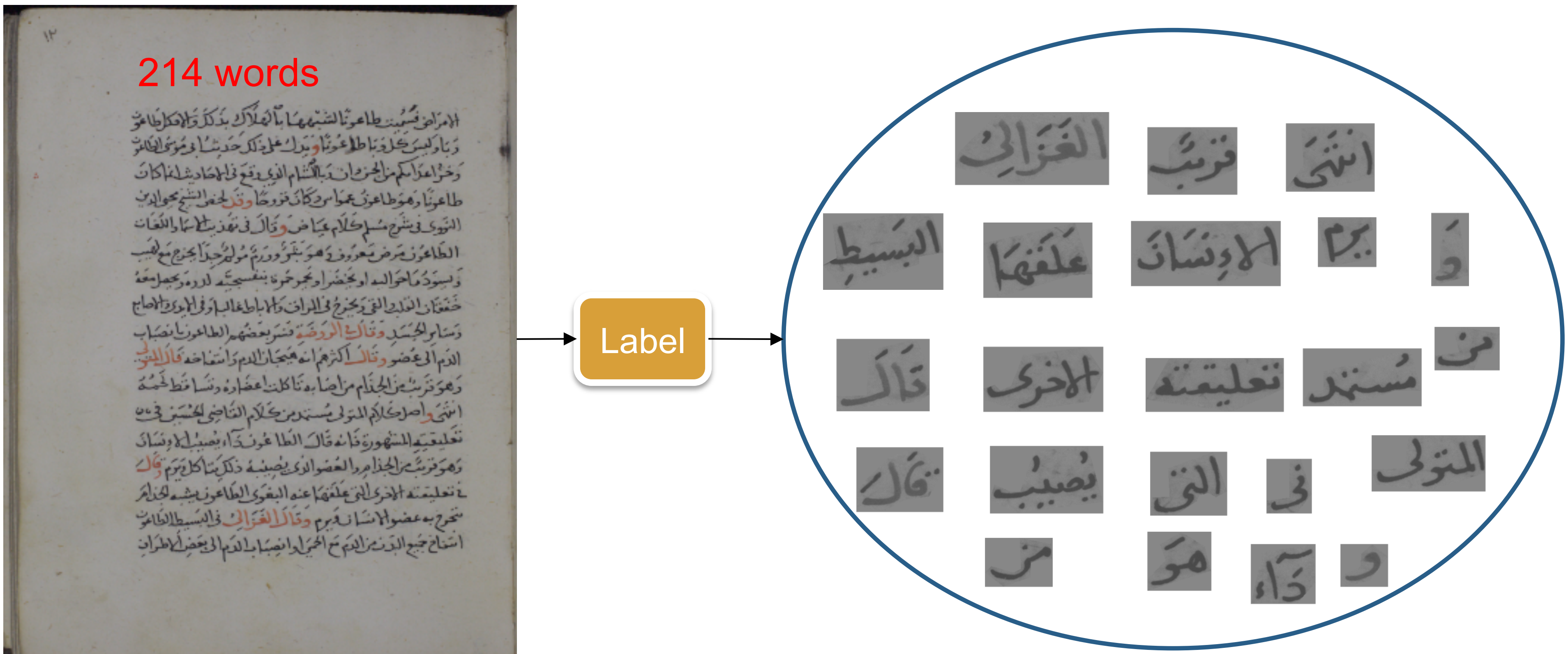
Introduction

- Semi-supervised is a middle ground between supervised and un-supervised.
- It means we have some sort of labeled and unlabeled data.
- Labeled data should help to understand the unlabeled data



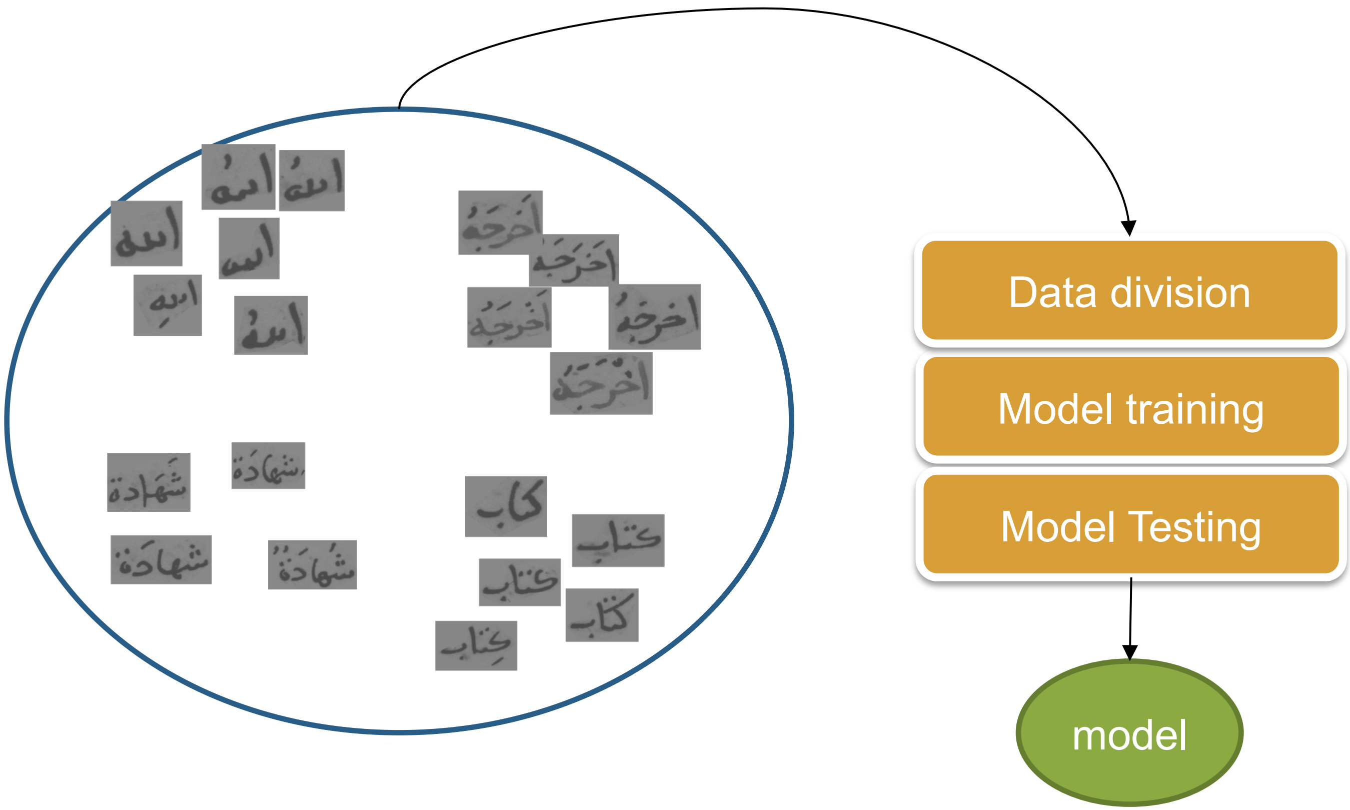
Example

- One example of semi-supervised learning is **Pseudo-labeling**.
- Suppose you have a large unlabeled dataset, and you want to label them for generating a good model for future predictions.



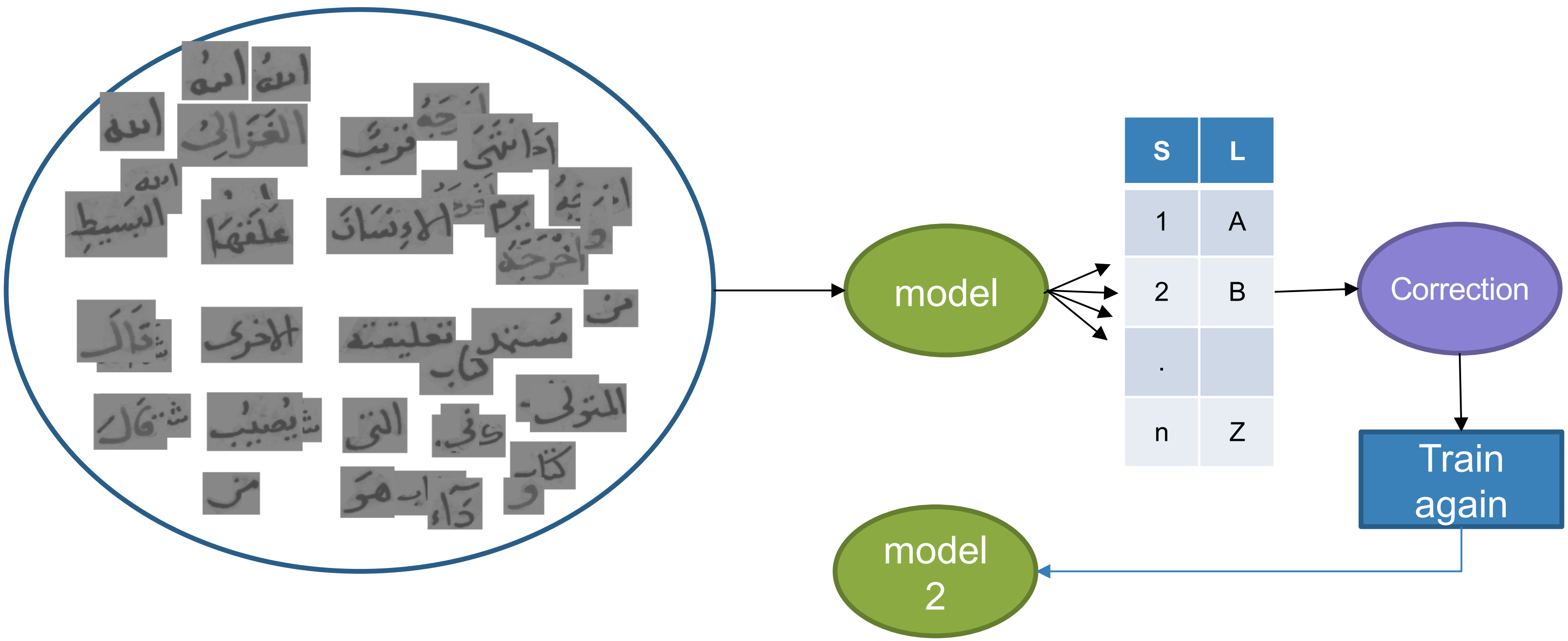
Pseudo-labeling

- Then, this labeled set is used to train and generate a machine model.



Pseudo-labeling

- Now, this model is used to label the larger dataset



Labeling

- Labeling is expensive and difficult

- Labeling is unreliable process
  - Such as Segmentation applications
  - May require experts to do that!

- Unlabeled data
  - Easy to obtain in large numbers
  - Ex. Sensors readings, text documents, images, etc.

Example

```python
# load label_propagation class
from sklearn.semi_supervised import label_propagation

# initialize a model
Prop_model = label_propagation.LabelPropagation(kernel='knn',

                                                )

Spread_model = label_propagation.LabelSpreading(kernel='rbf',
                                                gamma=0.3,
                                                )
#{'knn', 'rbf'} in case of rbf use gamma = value
```

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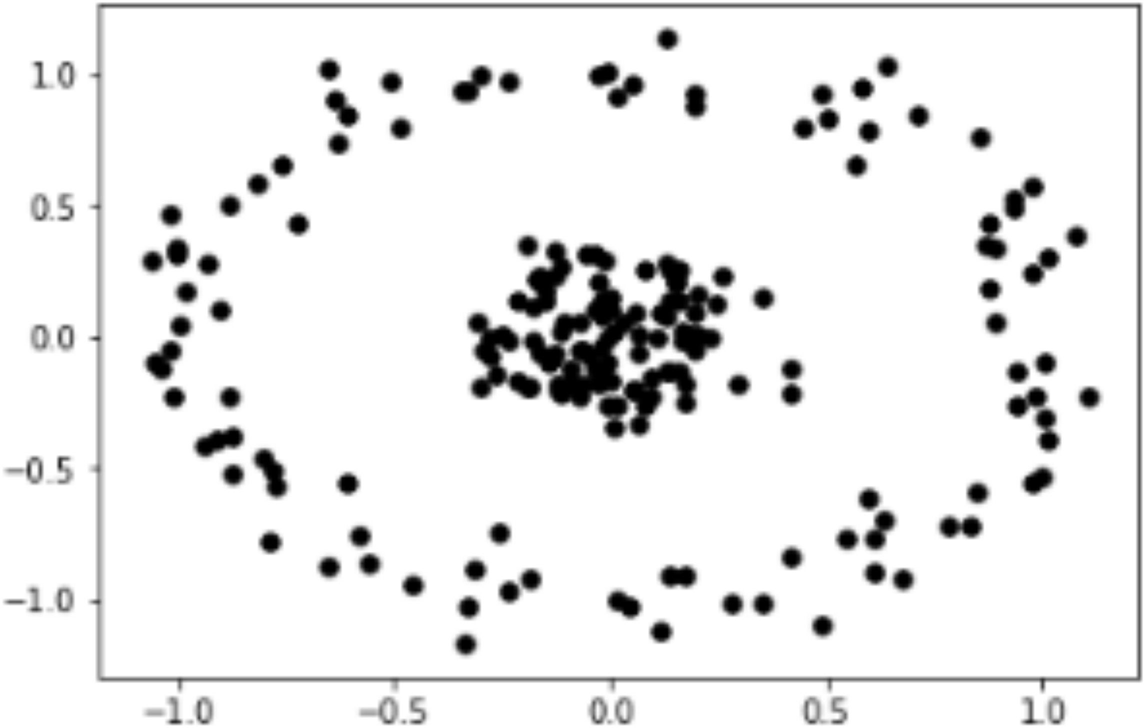
Example

```python
# let us use circles dataset
Xc, yc = make_circles( 200, factor=.2, noise=.1)
plt.scatter(Xc[:,0], Xc[:,1], c='k', s=30)
plt.show()
```



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Example

```python
# Changing labels to (unknown =-1)
rng = np.random.RandomState(42)
random_unlabeled = rng.rand(len(yc)) < 0.9
lbls = np.copy(yc)
lbls[random_unlabeled] = -1
```

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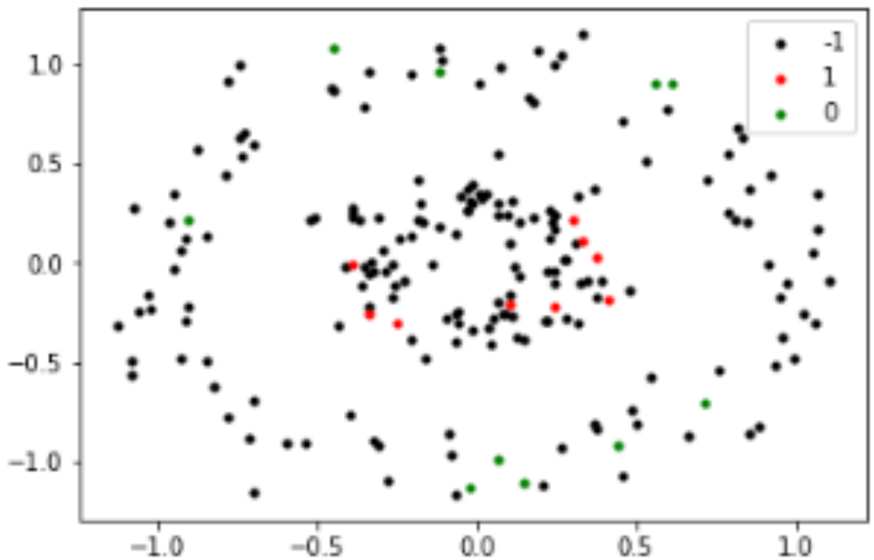
```python
# Changing labels to (unknown =-1)
rng = np.random.RandomState(42)
random_unlabeled = rng.rand(len(yc)) < 0.7
lbls = np.copy(yc)
lbls[random_unlabeled] = -1
```

Example

```
plt.scatter(Xc[lbls==-1,0], Xc[lbls==-1,1], c='k', s=10,facecolors='none', label='unlabel'  )
plt.scatter(Xc[lbls==1,0], Xc[lbls==1,1], c='r', s=10,facecolors='none' , label='1')
plt.scatter(Xc[lbls==0,0], Xc[lbls==0,1], c='g', s=10,facecolors='none' , label='0' )
plt.legend(labels=['-1', '1', '0'], loc=0)
plt.show()
```



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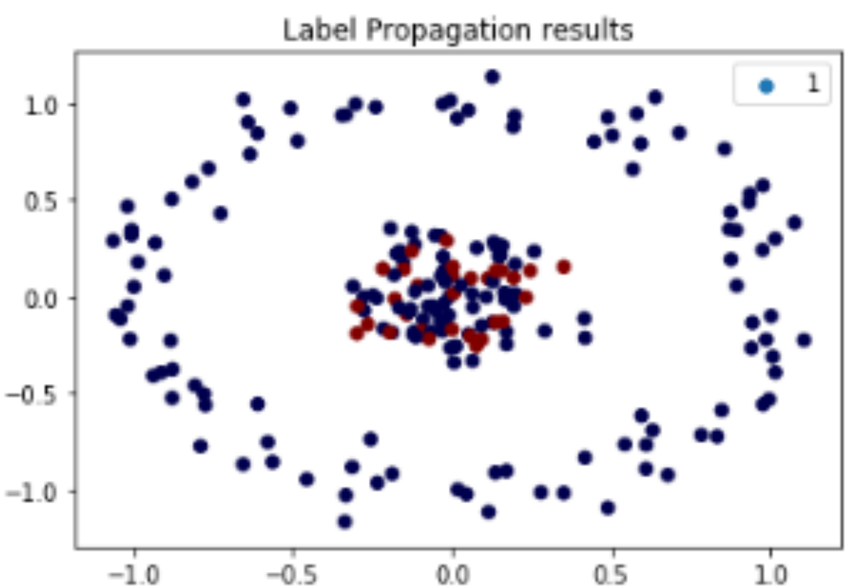
plt.show()
```

Example

```
Prop_model.fit(Xc, lbls)
prop_labels = Prop_model.transduction_
plt.scatter(Xc[:,0], Xc[:,1], c=prop_labels, s=30,facecolors='none',  cmap='seismic')
plt.legend(labels=['1', '0'], loc=0)
plt.title('Label Propagation results')
plt.show()
```



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Thank you