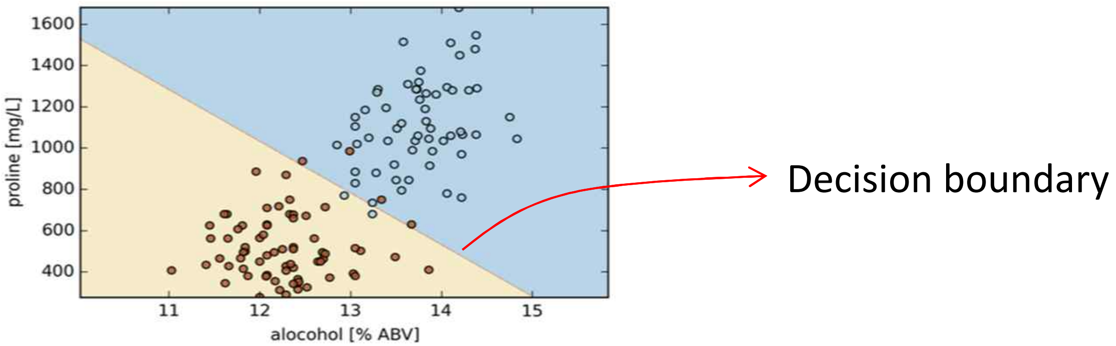
SUPPORT VECTOR MACHINE

Classification

- **Task: given X, predict Y**
  - Labeled data (X & Y)
  - “Predict class label (Y)”



Binary classification

SVM - Introduction

- SVMs provide a learning technique for classification

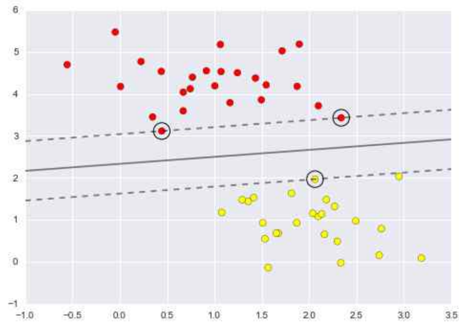
- Solution provided SVM is
  - Theoretically elegant
  - Computationally Efficient
  - Very effective in many large practical problems

- It has a simple geometrical interpretation in a high-dimensional feature space that is nonlinearly related to input space

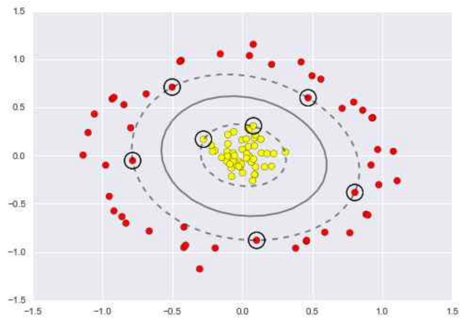
- By using kernels all computations keep simple.

Content

1. Linear SVM
2. Linear SVM: non-separable case



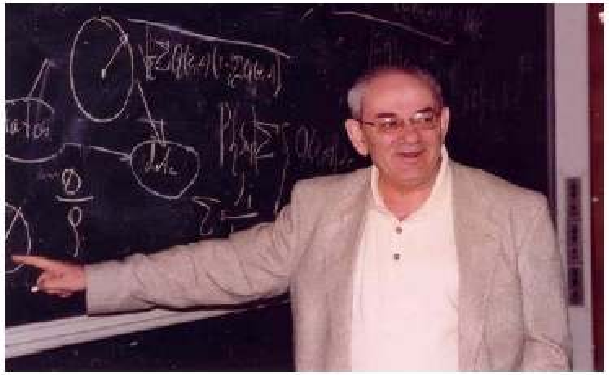
3. Non-linear SVM
   – Kernel trick



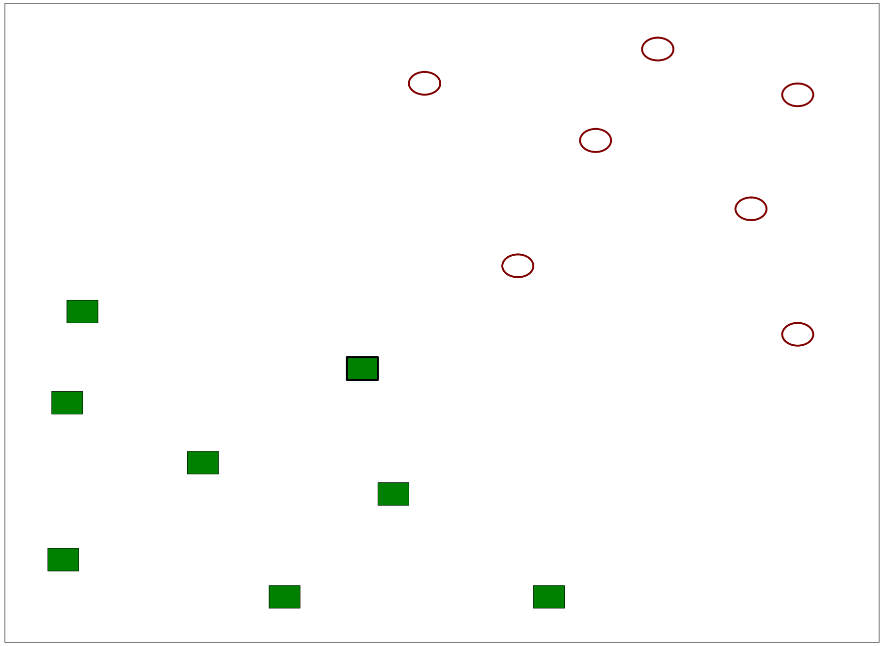
History

- The Study on Statistical Learning Theory was started in the 1960s by Vapnik
- Support Vector Machine is a practical learning method based on Statistical Learning Theory
- A simple SVM could beat a sophisticated neural networks with elaborate features in a handwriting recognition task.
- Now deep neural networks could beat SVM

Vladimir Vapnik



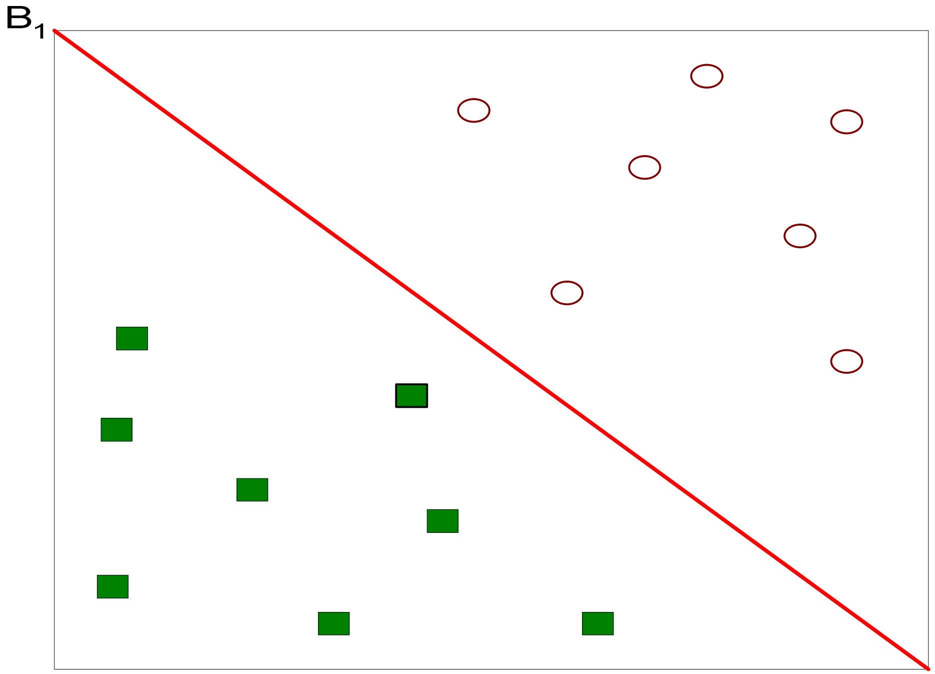
Support Vector Machines



Two dimensional training data

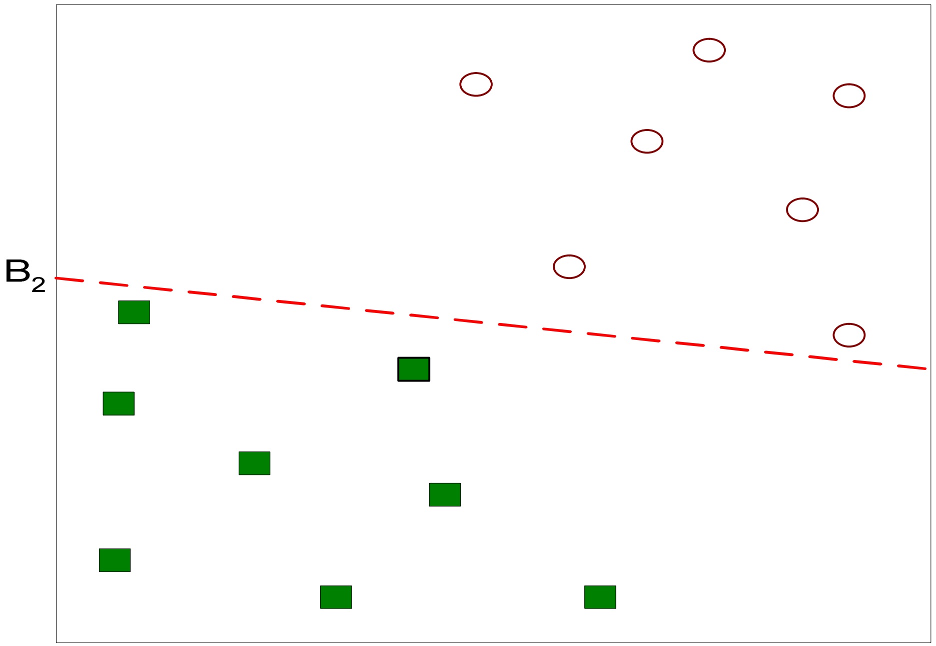
- Find a linear hyperplane (decision boundary) that will separate the data

Support Vector Machines



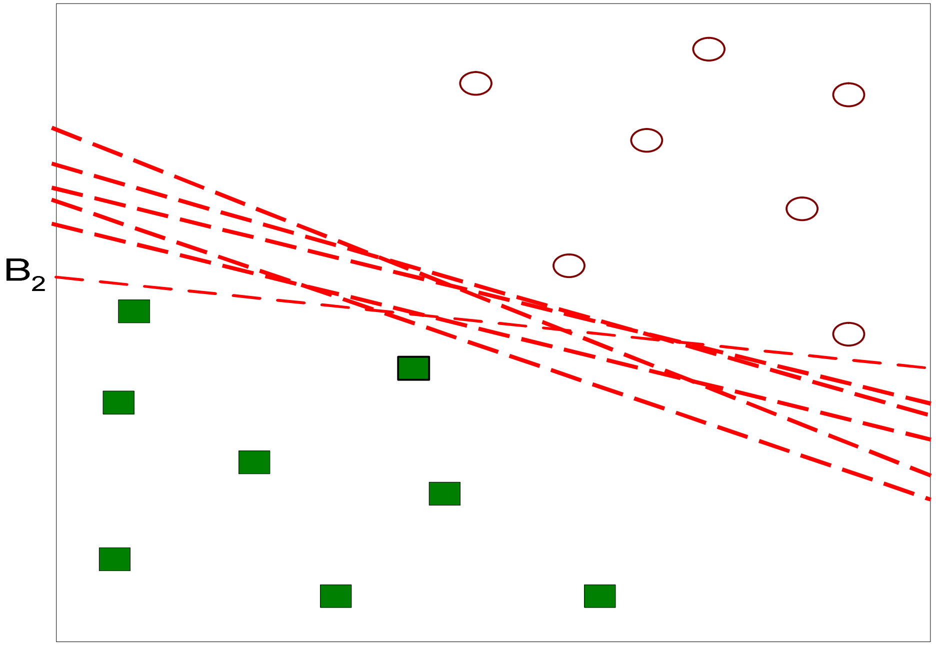
- One Possible Solution

Support Vector Machines



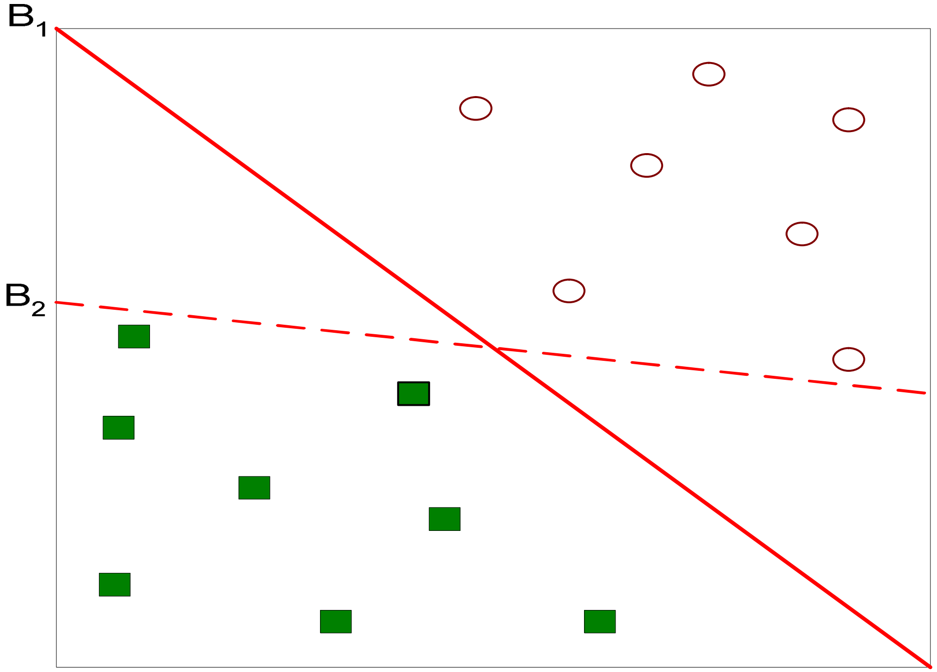
- Another possible solution

Support Vector Machines



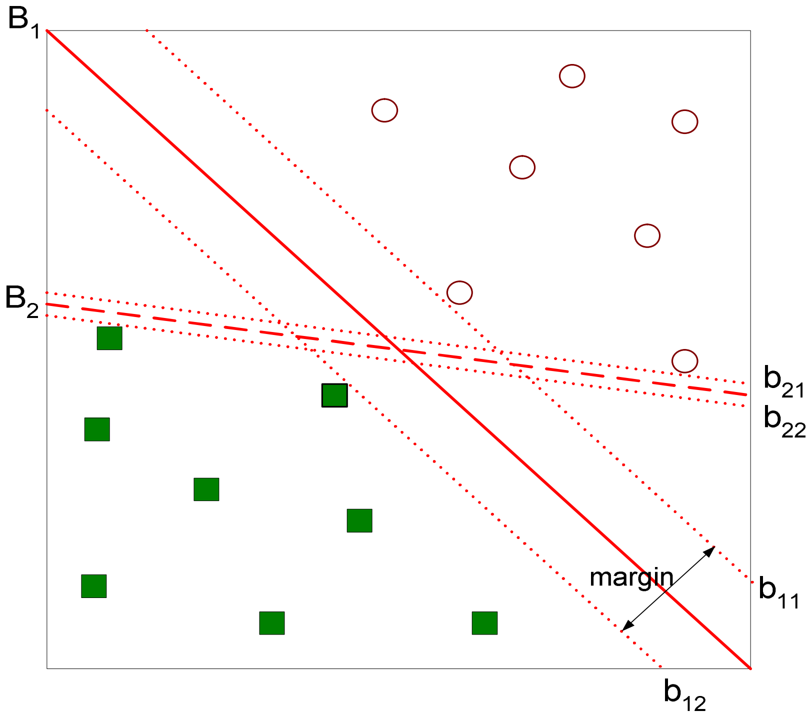
- Other possible solutions

Support Vector Machines



- Which one is better? B1 or B2?
- How do you define better?

Support Vector Machines



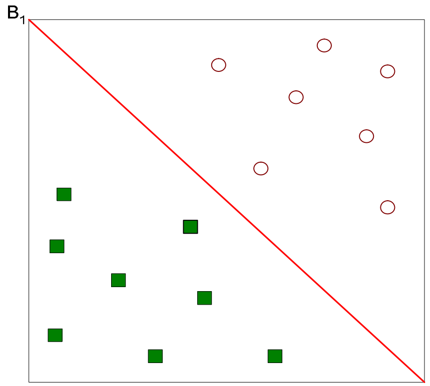
- Find hyperplane maximizes the margin => B1 is better than B2

Linear SVM: Separable case

- Linear decision boundary

- Consider a binary classification problem consisting of N training samples ($\mathbf{x}_i$,y_i), i=1,…,N where
  - $\mathbf{x}_i=(x_{i1},x_{i2},\ldots,x_{id})^T$: the attributes
  - y_i : class labels (either -1 or 1)
  - Decision boundary: $\mathbf{w} \cdot \mathbf{x} + b = 0$

    (or $w_1x_1+\ldots+ w_dx_d+b=0$)

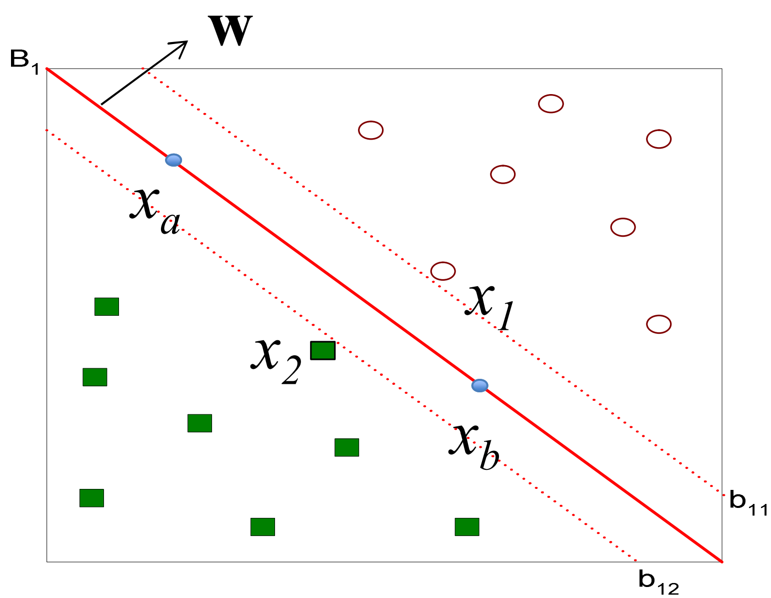


Linear Classifier

$$\mathbf{w} \cdot \mathbf{x_a} + b = 0$$
$$\mathbf{w} \cdot \mathbf{x_b} + b = 0$$
$$\Rightarrow \mathbf{w} \cdot (\mathbf{x_a} - \mathbf{x_b}) = 0$$

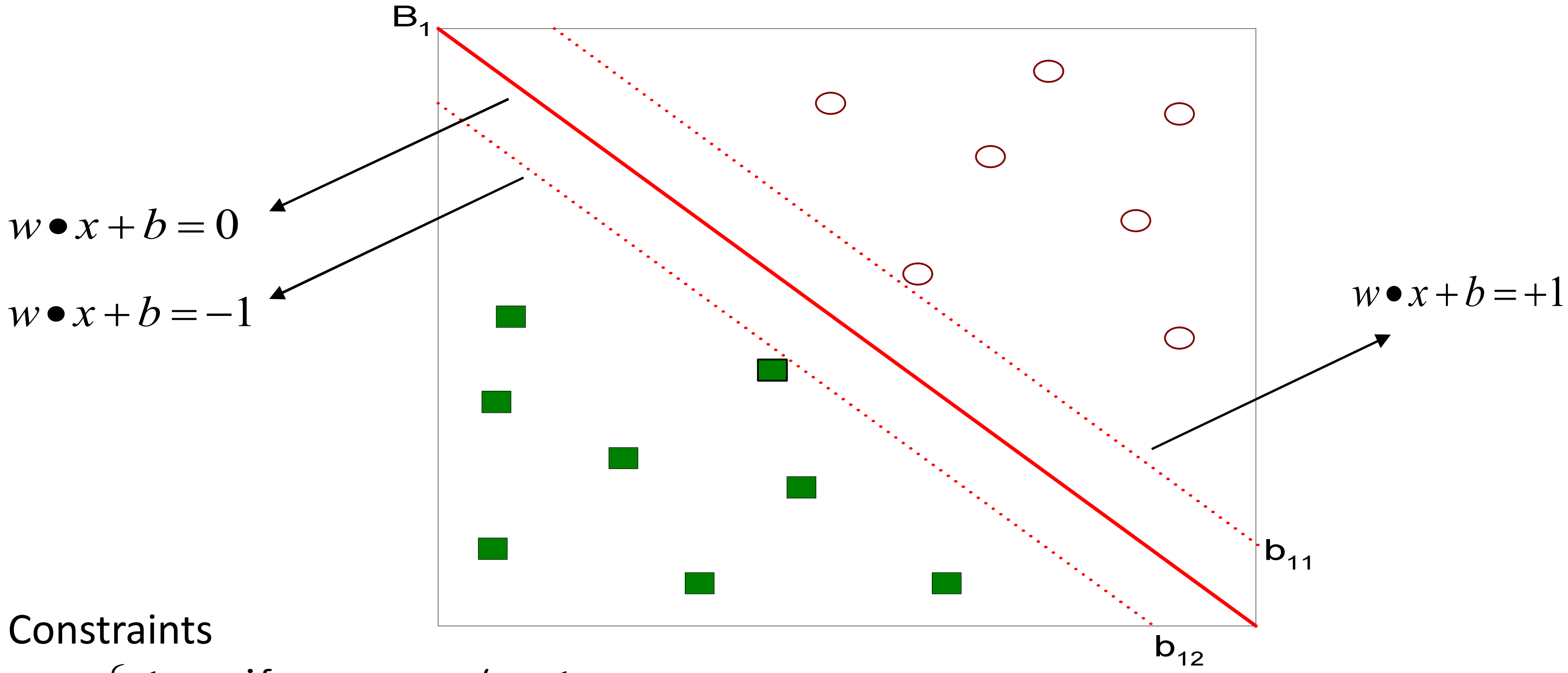
One possible linear classifier:

$$y = \begin{cases} 1 & \text{if } \mathrm{w} \bullet \mathrm{x} + \mathrm{b} > 0 \\ -1 & \text{if } \mathrm{w} \bullet \mathrm{x} + \mathrm{b} < 0 \end{cases}$$



$$\mathbf{w} \cdot \mathbf{x} + b = 0$$

Linear SVM

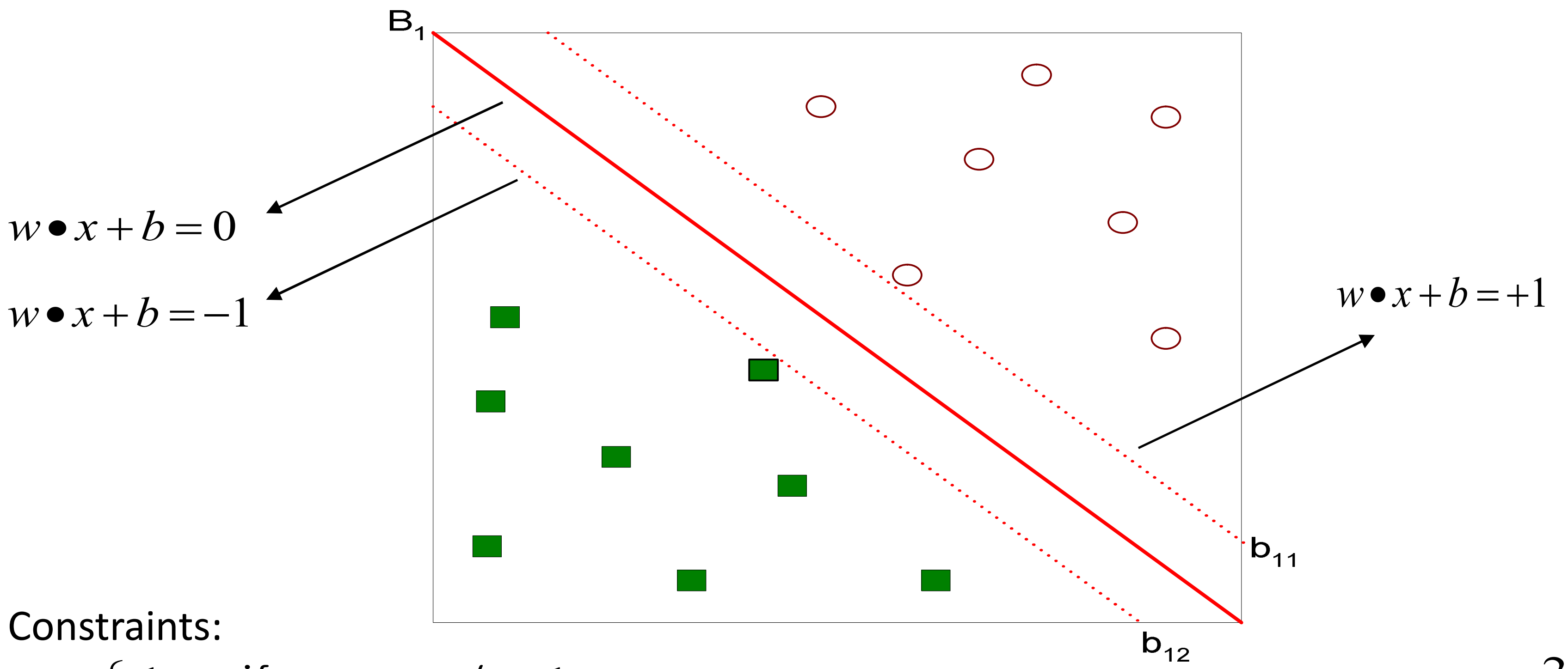


Constraints

$$y_i = \begin{cases} 1 & \text{if } w \bullet x_i + b \geq 1 \\ -1 & \text{if } w \bullet x_i + b \leq -1 \end{cases}$$

Margin $=$

Linear SVM



Constraints:

$$y_i = \begin{cases} 1 & \text{if } w \bullet x_i + b \geq 1 \\ -1 & \text{if } w \bullet x_i + b \leq -1 \end{cases}$$

Objective: Maximize $\text{Margin} = \dfrac{2}{\|w\|}$

Learning linear SVM

- Training phase: estimate the parameters w and b from the training data
- Objective: maximize margin
- Constraints:

$$\mathbf{w} \cdot \mathbf{x_i} + b \geq 1 \text{ if } y_i = 1$$
$$\mathbf{w} \cdot \mathbf{x_i} + b \leq -1 \text{ if } y_i = -1$$

$$y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1, i = 1, ..., N$$

Optimization problem

- We want to maximize: $\text{Margin} = \dfrac{2}{\|\vec{w}\|^2}$
  - Which is equivalent to minimizing: $L(w) = \dfrac{\|\vec{w}\|^2}{2}$
  - But subjected to the following constraints:

$$y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1, i = 1, ..., N$$

- This is a constrained (convex) optimization problem
  - Numerical approaches to solve it (e.g., quadratic programming)
  - Lagrange multiplier method:

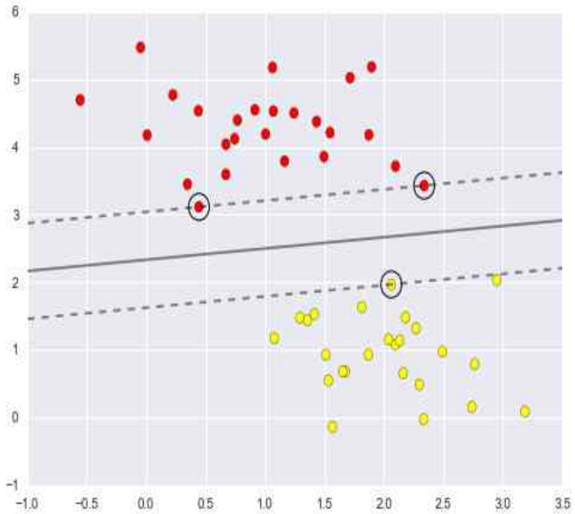
Linear SVM

- Test phase
  - Once the parameters of the decision boundary are found, a test instance z is classified as follows:

$$f(z) = 1 \text{ if } \mathbf{w} \cdot \mathbf{z} + b \geq 0$$
$$f(z) = -1 \text{ otherwise}$$

Example – linear SVM

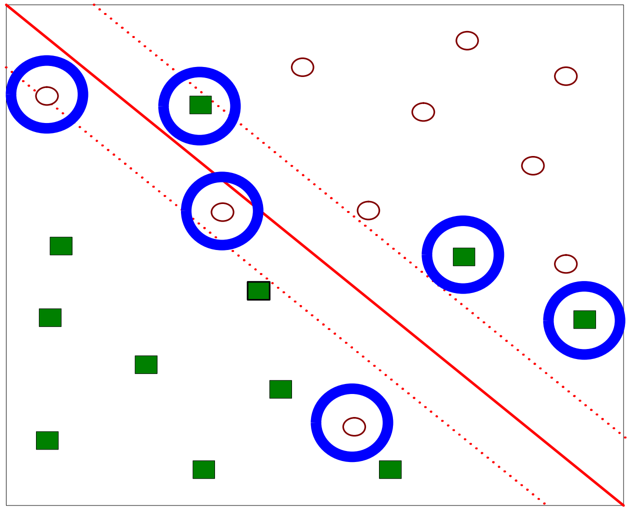
```
from sklearn.svm import SVC # "Support vector classifier"

# create SVM classifier
model = SVC(kernel='linear’)

# train the model using the training data
model.fit(Xtrain, ytrain)

# predict the label for test dataset
Ypred = model.predict(Xtest)
```



https://jakevdp.github.io/PythonDataScienceHandbook/05.07-support-vector-machines.html

Linear SVM: non-separable case

- What if the problem is not linearly separable?



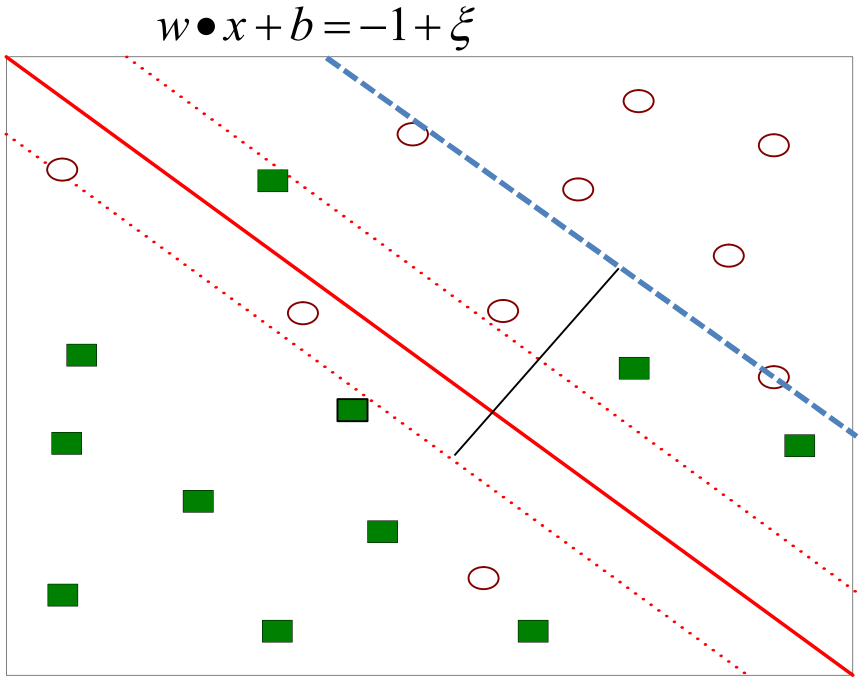
Use a soft margin approach

Slack variables for non-separable data

Relax the constraints

$$\mathbf{w} \cdot \mathbf{x_i} + b \geq 1 - \xi \text{ if } y_i = 1$$
$$\mathbf{w} \cdot \mathbf{x_i} + b \leq -1 + \xi \text{ if } y_i = -1$$

minimize $L(w) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i\right)^k$



Linear SVM: non-separable case

- What if the problem is not linearly separable?
  - Introduce slack variables
    - Need to minimize: $$L(w) = \frac{\| \vec{w} \|^2}{2} + C \left(\sum_{i=1}^{N} \xi_i \right)^k$$
    - Subject to: $$f(\vec{x}_i) = \begin{cases} 1 & \text{if } \vec{\mathrm{w}} \bullet \vec{\mathrm{x}}_\mathrm{i} + \mathrm{b} \geq 1 - \xi_\mathrm{i} \\ -1 & \text{if } \vec{\mathrm{w}} \bullet \vec{\mathrm{x}}_\mathrm{i} + \mathrm{b} \leq -1 + \xi_\mathrm{i} \end{cases}$$
    - *C, k*: user-specified parameters

Tuning hyper-parameter

- C for soft margin
  - Large C: margin is hard
  - Smaller C: margin is soft

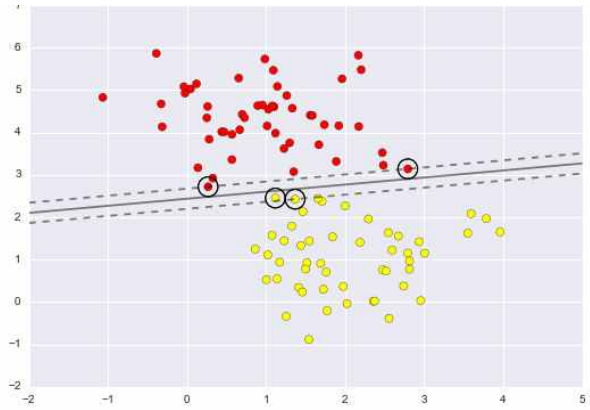
$$\mathbf{w} \cdot \mathbf{x_i} + b \geq 1 - \xi \text{ if } y_i = 1$$
$$\mathbf{w} \cdot \mathbf{x_i} + b \leq -1 + \xi \text{ if } y_i = -1$$

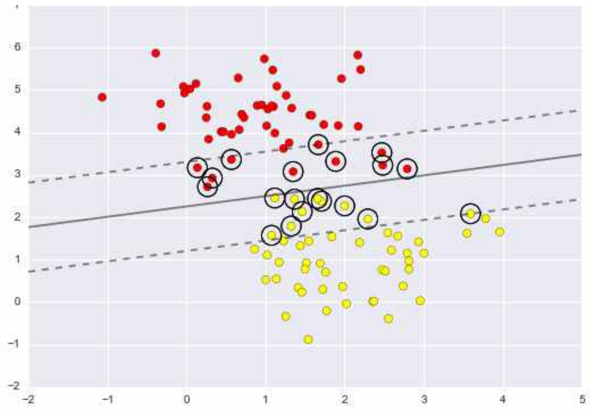
minimize $L(w) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i\right)^k$

```
model = SVC(kernel='linear', C=10.0)
```

```
model = SVC(kernel='linear', C=0.1)
```

C=10.0





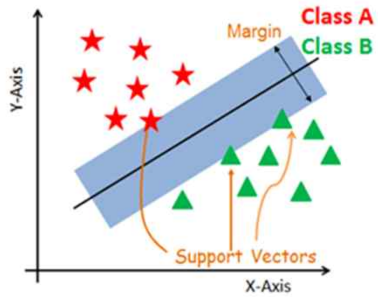
C=0.1

Linear SVM - summary

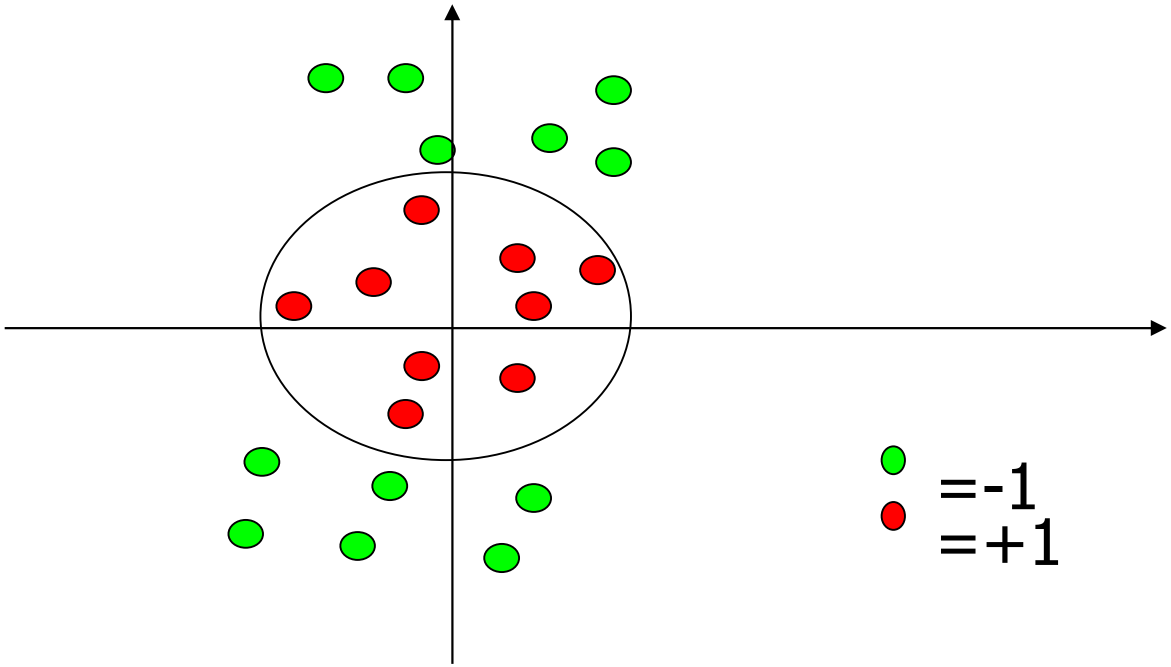
- Training phase: solve a constrained optimization problem to get the decision boundary (w and b)
  - Separable case
  - Non-separable case

- Test phase: given w, b

$$f(z) = 1 \text{ if } \mathbf{w} \cdot \mathbf{z} + b \geq 0$$
$$f(z) = -1 \text{ otherwise}$$



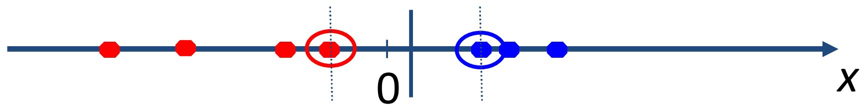
Problems with linear SVM



What if the decison function is not a linear?

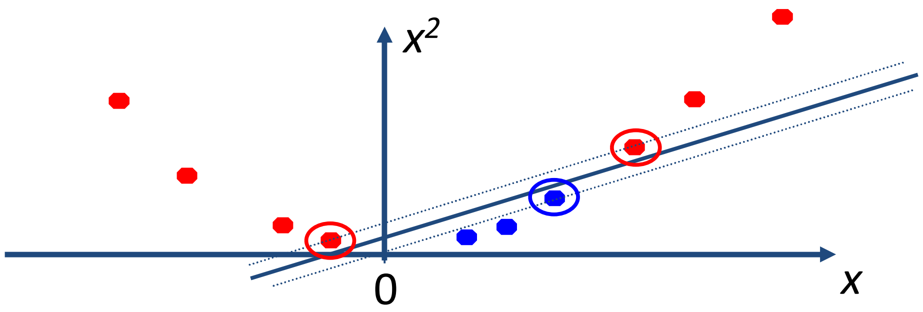
Non-linear SVMs

- Datasets that are linearly separable with some noise work out great:



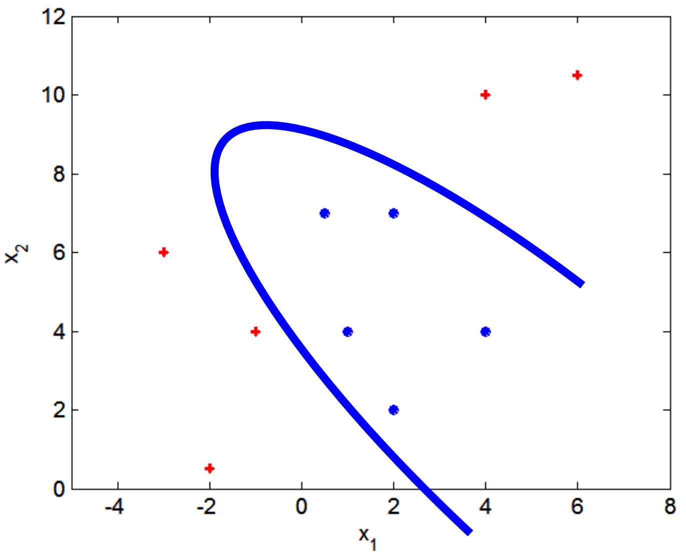
- But what are we going to do if the dataset is just too hard?

- How about… mapping data to a higher-dimensional space:



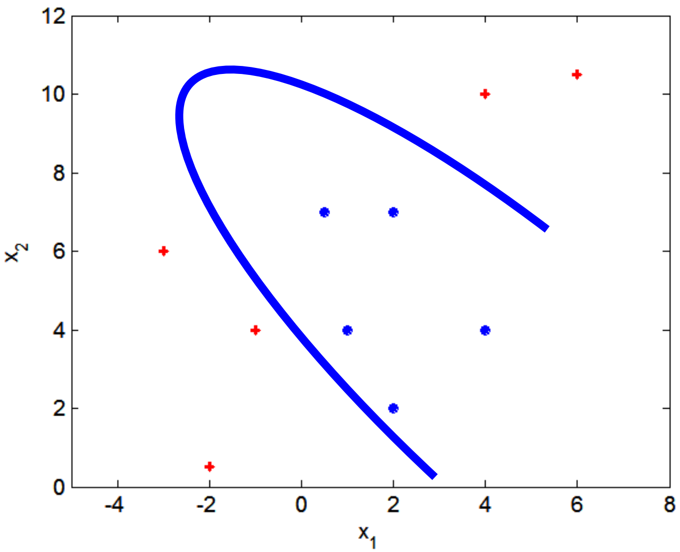
Nonlinear Support Vector Machines

- What if decision boundary is not linear?

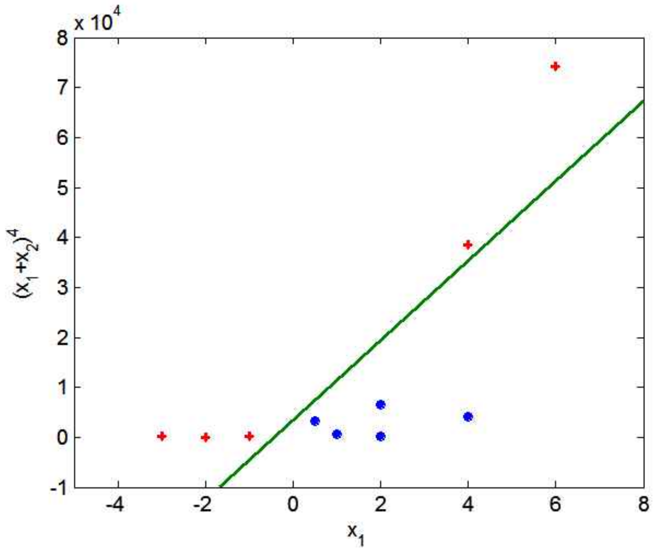


Nonlinear SVM

- Transform data into a new space so that a linear boundary can be used to separate the instance

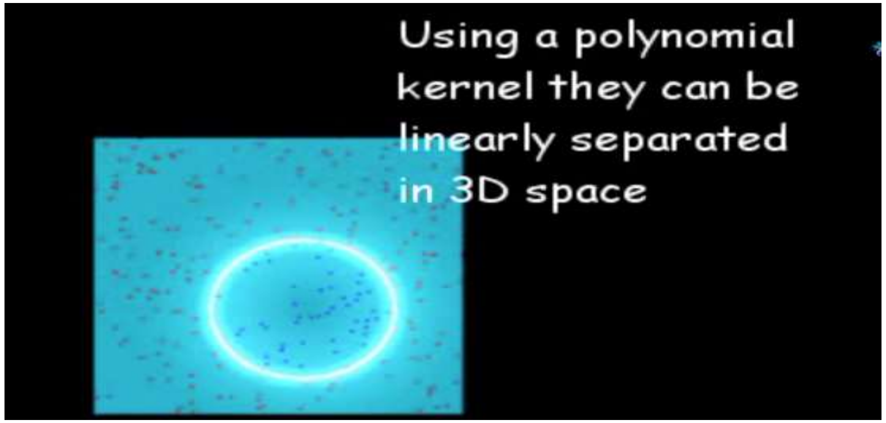


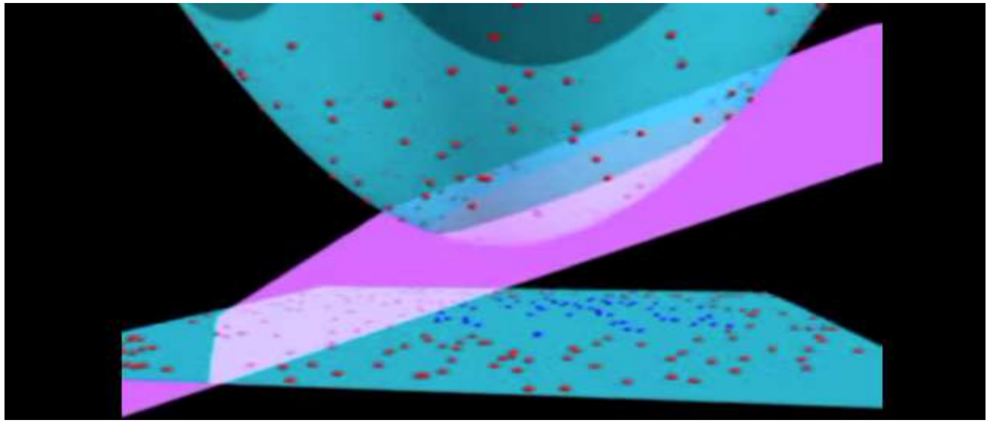
$$\mathbf{x} \rightarrow \mathbf{\Phi}(\mathbf{x})$$



SVM with polynomial kernel visualization

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





Issues in nonlinear SVM

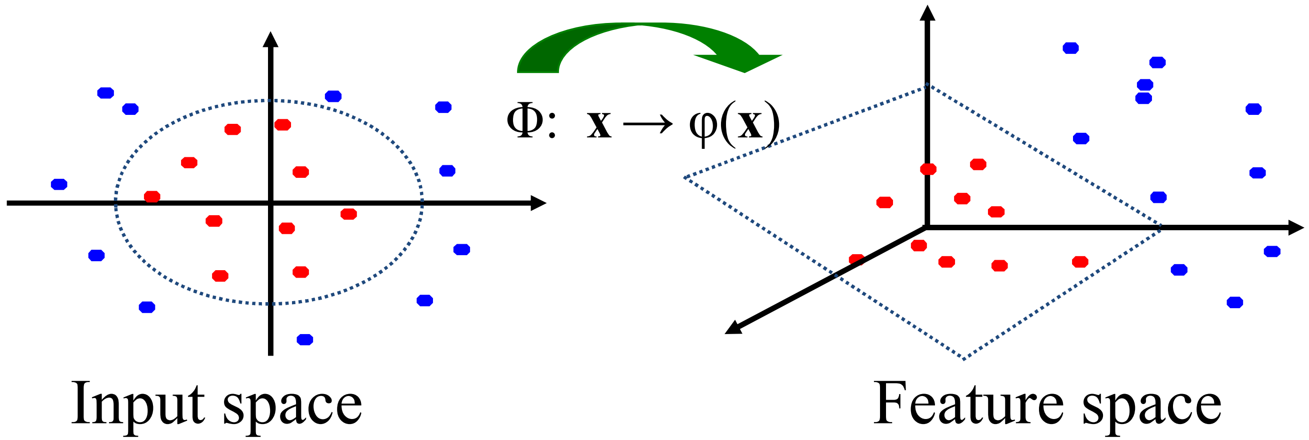
- It is not clear what type of mapping function to use

- Solving optimization problems in a high-dimensional space can be computationally expensive

➔ Use **Kernel Trick**

Extension to Non-linear Decision Boundary

- Possible problem of the transformation
  - High computation burden and hard to get a good estimate
- SVM solves these two issues simultaneously
  - Kernel tricks for efficient computation
  - Minimizing $||\mathbf{w}||^2$ can lead to a "good" classifier



Learning nonlinear SVM

- Training phase:
  - Need to minimize: $L(w) = \frac{\| w \|^2}{2}$
  - subject to $y_i(\mathbf{w} \cdot \mathbf{\Phi}(\mathbf{x_i}) + b) \geq 1, i = 1, ..., N$
- Test phase: for a new instance z,

$$f(z) = 1 \text{ if } \mathbf{w} \cdot \mathbf{\Phi}(\mathbf{z}) + b \geq 0$$
$$f(z) = -1 \text{ otherwise}$$

Kernel trick

$$\mathbf{w} \cdot \mathbf{\Phi}(\mathbf{z}) + b = \sum_{i=1}^{n} \lambda_i y_i \Phi(x_i) \cdot \mathbf{\Phi}(\mathbf{z}) + b$$

Dot product in a high-dimensional space…
A kind of similarity measure

- There may exist a kernel function K such that

$$K(\mathbf{u}, \mathbf{v}) = \mathbf{\Phi}(\mathbf{u})\mathbf{\Phi}(\mathbf{v})$$

  – The dot product in a the transformed space can be expressed in terms of a similarity in the original space
  – e.g. K(u,v) = (u • v + 1)^2 for $\mathbf{\Phi}(\mathbf{u}) = (u_1^2, u_2^2, \sqrt{2}u_1, \sqrt{2}u_2, 1)$

Example Transformation

- Define the kernel function *K* (**x**,**y**) as

$$K(\mathrm{x},\mathrm{y}) = (1 + x_1 y_1 + x_2 y_2)^2$$

- Consider the following transformation

$$\phi(\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1 x_2)$$

$$\phi(\left[\begin{smallmatrix} y_1 \\ y_2 \end{smallmatrix}\right]) = (1, \sqrt{2}y_1, \sqrt{2}y_2, y_1^2, y_2^2, \sqrt{2}y_1 y_2)$$

$$\begin{aligned} \langle \phi(\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]), \phi(\left[\begin{smallmatrix} y_1 \\ y_2 \end{smallmatrix}\right]) \rangle &= (1 + x_1 y_1 + x_2 y_2)^2 \\ &= K(\mathrm{x},\mathrm{y}) \end{aligned}$$

- The inner product can be computed by *K* without going through the map $\phi(.)$

Kernel Trick

- K: kernel function
  - The kernel functions can be expressed as the dot product between two input vectors in some high-dimensional space
  - Computing the dot product using kernel functions is considerably cheaper than using the transformed attribute
  - We do not have to know the exact form of the mapping function Φ

Examples of Kernel Functions

- Polynomial kernel with degree *d*

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- Radial basis function (RBF) kernel with width σ

$$K(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x} - \mathbf{y}||^2/(2\sigma^2))$$

- Sigmoid with parameter κ and θ

$$K(\mathbf{x}, \mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$

Examples of Kernel Functions

- Polynomial kernel with degree *d*

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- Radial basis function kernel with width σ

$$K(\mathbf{x},\mathbf{y}) = \exp(-||\mathbf{x}-\mathbf{y}||^2/(2\sigma^2))$$

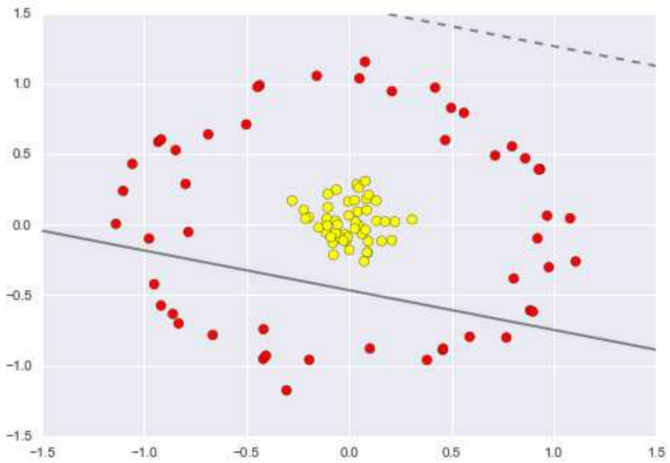
  – Closely related to radial basis function neural networks

- Sigmoid with parameter κ and θ

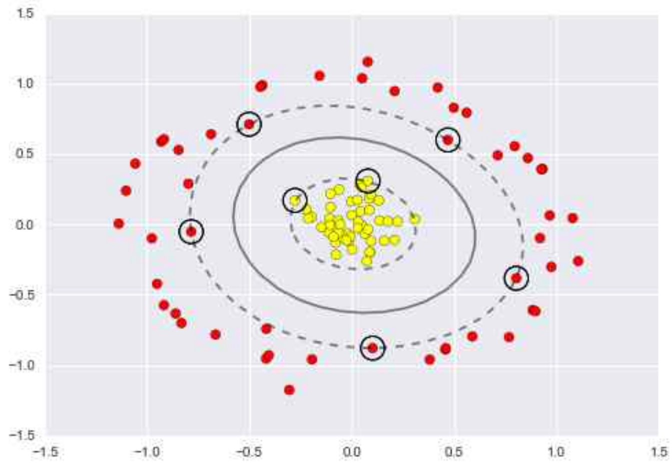
$$K(\mathbf{x},\mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$

Example - RBF

```
clf = SVC(kernel='linear')
clf.fit(X, y)
```

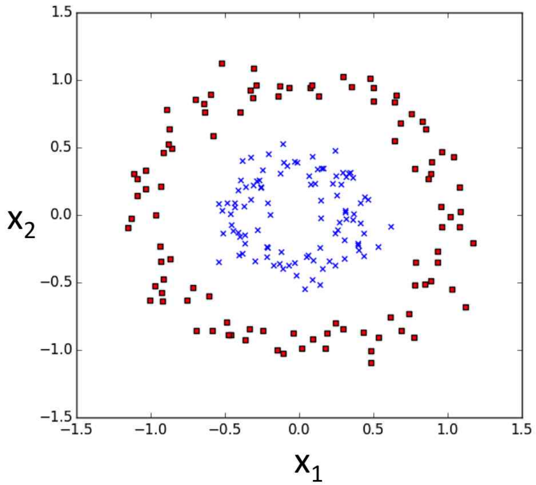



```
clf = SVC(kernel='rbf', C=1E6)
clf.fit(X, y)
```

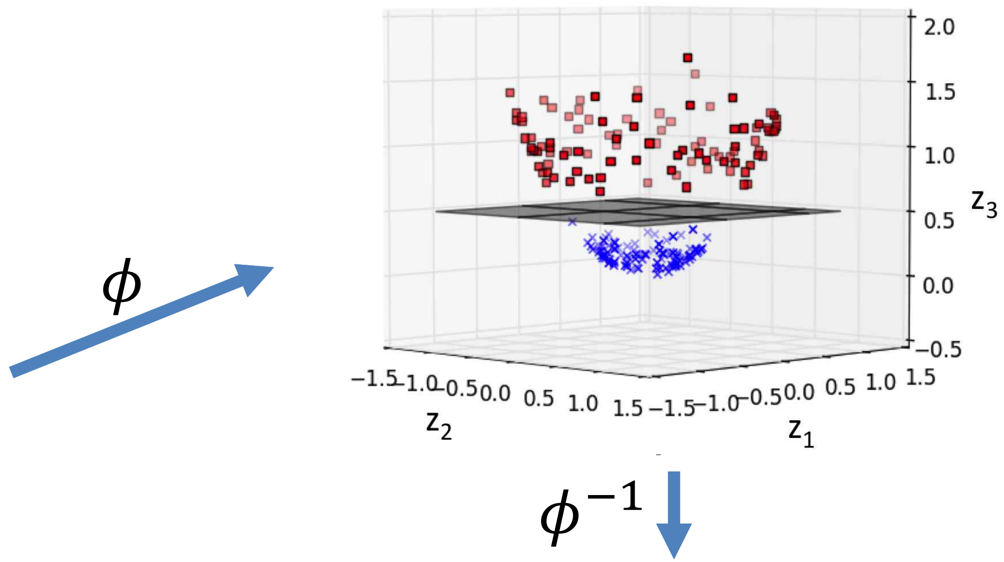


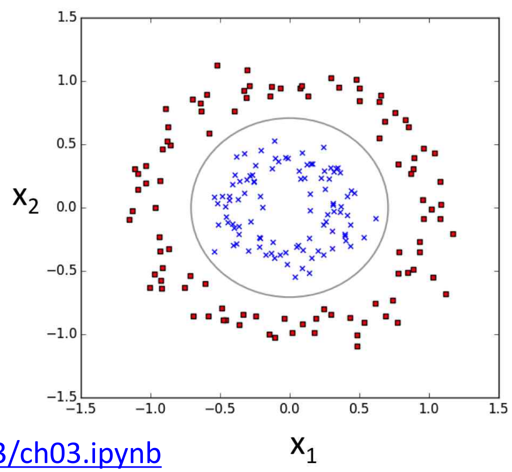
https://jakevdp.github.io/PythonDataScienceHandbook/05.07-support-vector-machines.html

Example



Non-linearly separable case





https://github.com/rasbt/python-machine-learning-book/blob/master/code/ch03/ch03.ipynb

SVM - summary

- Convex optimization problem in which efficient algorithms are available

- Maximizing margin of the decision boundary

- Attribute transformation to a high-dimensional space and kernel trick

- The user must still provide other parameters such as the type of kernel function and the cost function C for slack variables

- For binary classification. Can be extended to multi-class problems

Classification - Summary

- Classification algorithms discussed so far
  - KNN
  - Decision Tree
  - Random Forest
  - Support Vector Machine

Things to know

- What is done in training and test phase, respectively
- Time complexity
- Decision boundary
- Model parameters
- Hyper-parameters