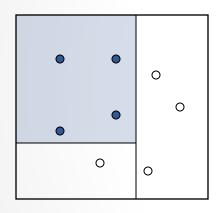
Support Vector Machines

Vibhav Gogate
The University of Texas at dallas

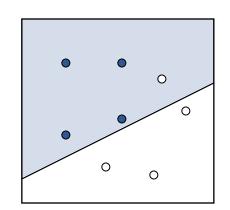
What We have Learned So Far?

- 1. Decision Trees
- 2. Naïve Bayes
- 3. Linear Regression
- 4. Logistic Regression
- 5. Perceptron
- 6. Neural networks
- Which of the above are linear and which are not?
- (1) (2) and (6) are non-linear

Decision Surfaces

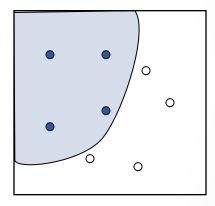


Decision Tree



Linear Functions

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$



Nonlinear Functions (Neural nets)

Today: Support Vector Machine (SVM)

- A classifier derived from statistical learning theory by Vapnik, et al. in 1992
- SVM became famous when, using images as input, it gave accuracy comparable to neural-network with hand-designed features in a handwriting recognition task
- Currently, SVM is widely used in object detection & recognition, content-based image retrieval, text recognition, biometrics, speech recognition, etc.
- Also used for regression (will not cover today)
- Chapter 5.1, 5.2, 5.3, 5.11 (5.4*) in Bishop
- SVM tutorial (start reading from Section 3)

V. Vapnik

Outline

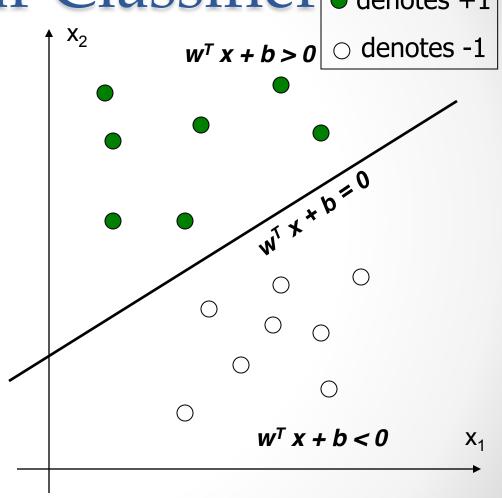
- Linear Discriminant Function
- Large Margin Linear Classifier
- Nonlinear SVM: The Kernel Trick
- Demo of SVM

Linear Discriminant Function or a Linear Classifier odenotes +1

 Given data and two classes, learn a function of the form:

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$

- A hyper-plane in the feature space
- Decide class=1 if g(x)>0 and class=-1 otherwise



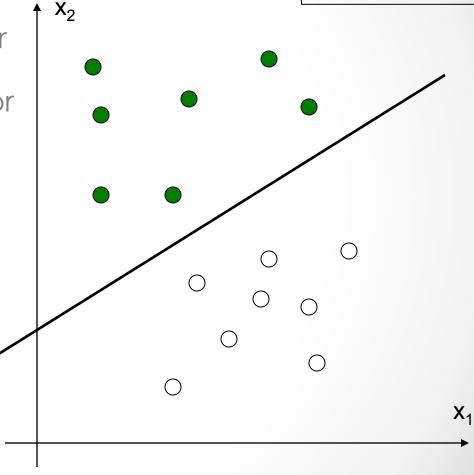
Function

denotes +1

○ denotes -1

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!



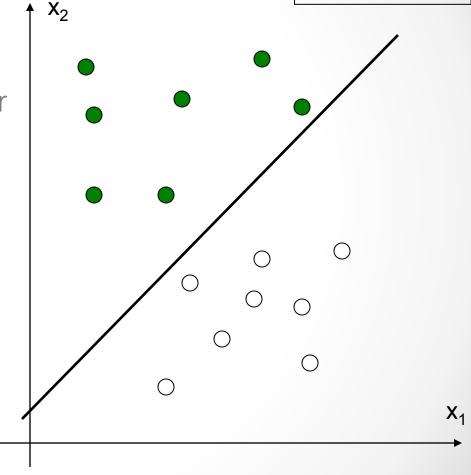
Function

denotes +1

denotes -1

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!



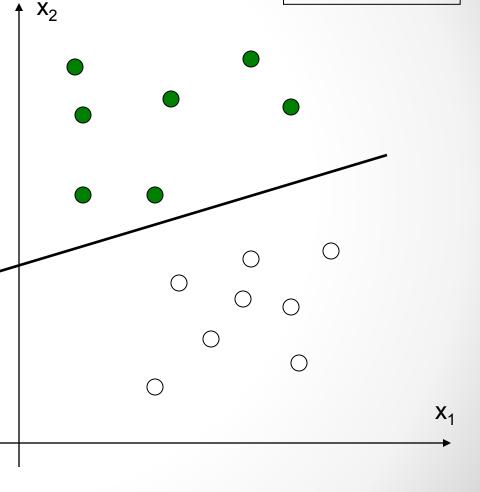
Function

denotes +1

○ denotes -1

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!



Function

 X_2

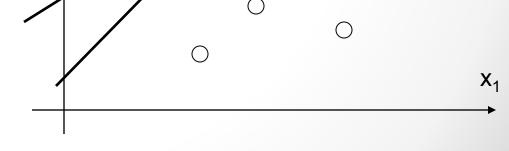
denotes +1

odenotes -1

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!

Which one is the best?



Large Margin Linear

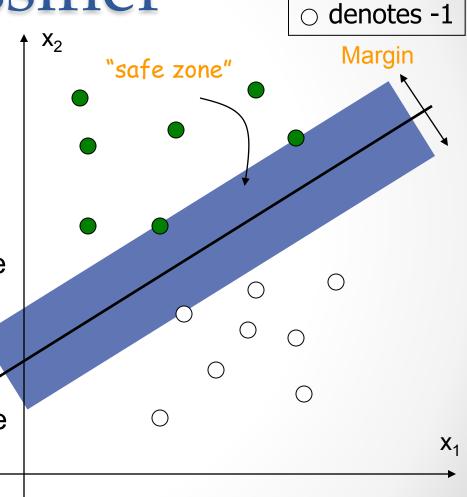
Odenotes +1

Classifier

 The linear discriminant function (classifier) with the maximum margin is the best

 Margin is defined as the width that the boundary could be increased by before hitting a data point

- Why it is the best?
 - The larger the margin the better generalization
 - Robust to outliers



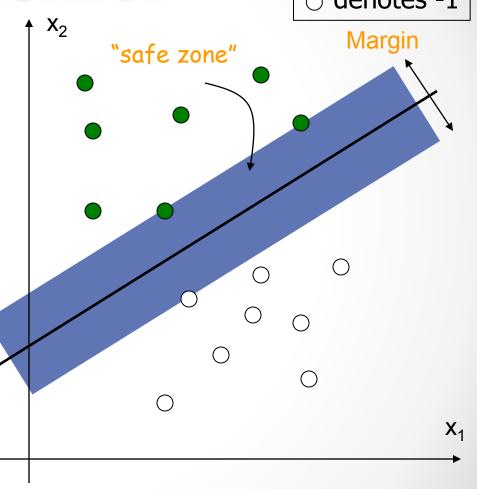
Classifier

- denotes +1
- denotes -1

- Aim: Learn a large margin classifier.
- Given a set of data points, define:

For
$$y_i = +1$$
, $\mathbf{w}^T \mathbf{x}_i + b \ge 1$
For $y_i = -1$, $\mathbf{w}^T \mathbf{x}_i + b \le -1$

 Give an algebraic expression for the width of the margin.



Algebraic Expression for Width of a Margin

Given 2 parallel lines with equations

$$ax + by + c_1 = 0$$

and

$$ax + by + c_2 = 0$$

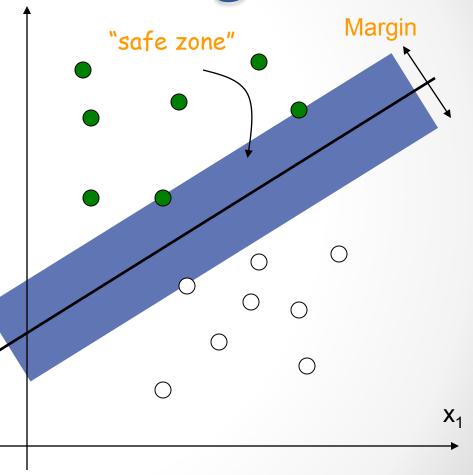
the distance between them is given by:

$$d = \frac{|c_2 - c_1|}{\sqrt{a^2 + b^2}}$$

Our lines in 2-D are:

$$w_1x_1 + w_2x_2 + b - 1 = 0$$
 and $w_1x_1 + w_2x_2 + b + 1 = 0$

Distance =
$$\frac{|b-1-b-1|}{\sqrt{w_1^2 + w_2^2}} = \frac{2}{||\mathbf{w}||}$$



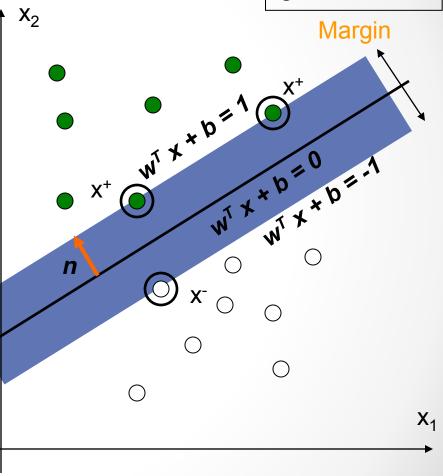
Classifier

- denotes +1
- denotes -1

- Aim: Learn a large margin classifier
- Mathematical Formulation: maximize $\frac{2}{\|\mathbf{w}\|}$

For
$$y_i = +1$$
, $\mathbf{w}^T \mathbf{x}_i + b \ge 1$

For
$$y_i = -1$$
, $\mathbf{w}^T \mathbf{x}_i + b \le -1$



Classifier

denotes +1

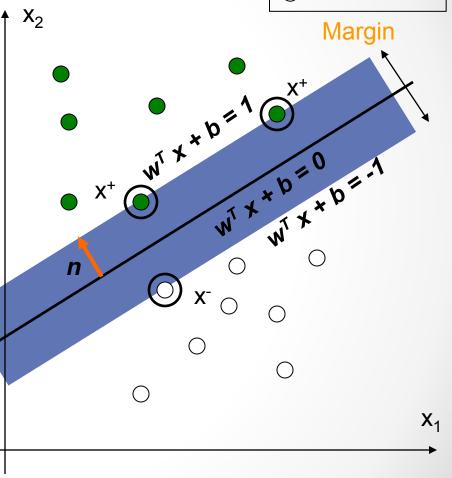
○ denotes -1

Formulation:

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2$$

For
$$y_i = +1$$
, $\mathbf{w}^T \mathbf{x}_i + b \ge 1$

For
$$y_i = -1$$
, $\mathbf{w}^T \mathbf{x}_i + b \le -1$



Classifier

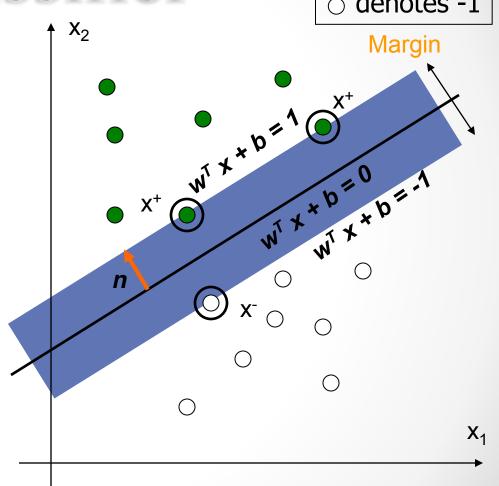
denotes +1

denotes -1

Formulation:

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2$$

$$y_i(\mathbf{w}^T\mathbf{x}_i+b) \ge 1$$



Quadratic programming with linear constraints

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2$$

s.t.
$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \ge 1$$

Lagrangian Function



minimize
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left(y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$

s.t.
$$\alpha_i \geq 0$$

minimize
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left(y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$

s.t.
$$\alpha_i \geq 0$$

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \qquad \mathbf{w} = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i$$

$$\frac{\partial L_p}{\partial b} = 0 \qquad \sum_{i=1}^n \alpha_i y_i = 0$$

minimize
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left(y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$

s.t.
$$\alpha_i \geq 0$$

Lagrangian Dual Problem



maximize
$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

s.t.
$$\alpha_i \ge 0$$
 , and $\sum_{i=1}^n \alpha_i y_i = 0$

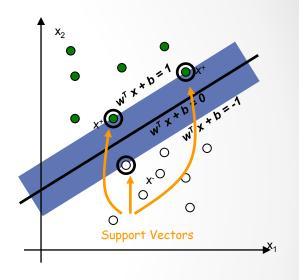
From the equations, we can prove that: (KKT conditions):

$$\alpha_i \left(y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \right) = 0$$

- Thus, only support vectors have $\alpha_i \neq 0$
- The solution has the form:

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = \sum_{i \in SV} \alpha_i y_i \mathbf{x}_i$$

get *b* from $y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1 = 0$, where \mathbf{x}_i is support vector



The linear discriminant function is:

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{i \in SV} \alpha_i \mathbf{x}_i^T \mathbf{x} + b$$

- Notice it relies on a dot product between the test point x and the support vectors x_i
- Also keep in mind that solving the optimization problem involved computing the dot products x_i^Tx_j between all pairs of training points

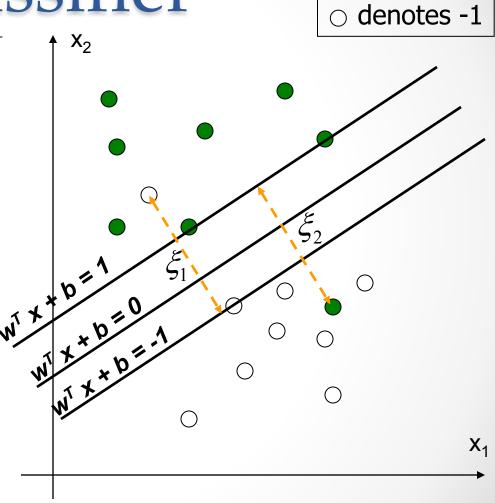
Large Margin Linear

otherwise denotes +1

Classifier

 What if data is not linear separable? (noisy data, outliers, etc.)

 Slack variables ξ_i can be added to allow misclassification of difficult or noisy data points



Large Margin Linear Classifier

Formulation:

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i$$

such that

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \ge 1 - \xi_i$$
$$\xi_i \ge 0$$

Parameter C can be viewed as a way to control over-fitting.

Large Margin Linear Classifier

Formulation: (Lagrangian Dual Problem)

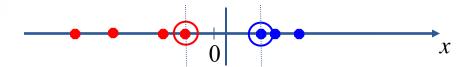
maximize
$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$0 \le \alpha_i \le C$$

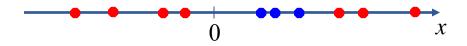
$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

Non-linear SVMs

Datasets that are linearly separable with noise work out great:



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



- Kernel Trick!!!
 - SVM = Linear SVM + Kernel Trick

Kernel Trick Motivation

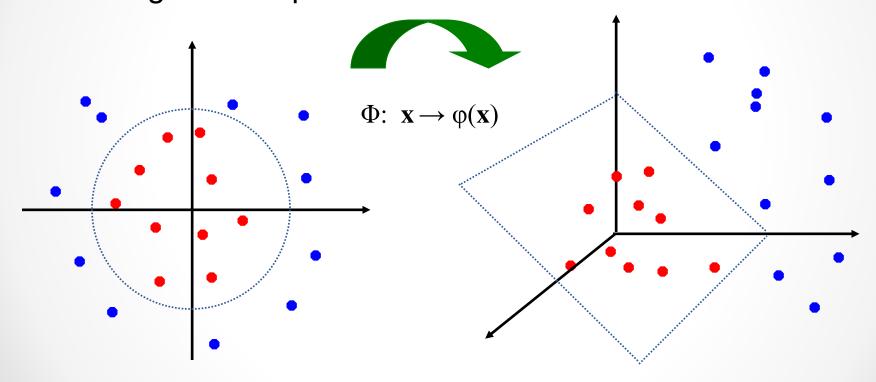
- Linear classifiers are well understood, widely-used and efficient.
- How to use linear classifiers to build non-linear ones?
- Neural networks: Construct non-linear classifiers by using a network of linear classifiers (perceptrons).

Kernels:

- Map the problem from the input space to a new higher-dimensional space (called the feature space) by doing a non-linear transformation using a special function called the kernel.
- o Then use a linear model in this new high-dimensional feature space. The linear model in the feature space corresponds to a non-linear model in the input space.

Non-linear SVMs: Feature Space

General idea: the original input space can be mapped to some higher-dimensional feature space where the training set is separable:



Nonlinear SVMs: The Kernel Trick

With this mapping, our discriminant function is now:

$$g(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b = \sum_{i \in SV} \alpha_i \phi(\mathbf{x}_i)^T \phi(\mathbf{x}) + b$$

- No need to know this mapping explicitly, because we only use the dot product of feature vectors in both the training and test.
- A kernel function is defined as a function that corresponds to a dot product of two feature vectors in some expanded feature space:

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

Nonlinear SVMs: The Kernel Trick

An example:

2-dimensional vectors $\mathbf{x} = [x_1 \ x_2]$;

let
$$K(x_i,x_j)=(1 + x_i^T x_j)^2$$
,

Need to show that $K(x_i,x_j) = \varphi(x_i)^T \varphi(x_j)$:

$$\begin{split} K(\mathbf{x_i}, & \mathbf{x_j}) = (1 + \mathbf{x_i}^{\mathrm{T}} \mathbf{x_j})^2, \\ & = 1 + x_{i1}^2 x_{j1}^2 + 2 \ x_{i1} x_{j1} \ x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2 x_{i1} x_{j1} + 2 x_{i2} x_{j2} \\ & = [1 \ x_{i1}^2 \ \sqrt{2} \ x_{i1} x_{i2} \ x_{i2}^2 \ \sqrt{2} x_{i1} \ \sqrt{2} x_{i2}]^{\mathrm{T}} [1 \ x_{j1}^2 \ \sqrt{2} \ x_{j1} x_{j2} \ x_{j2}^2 \ \sqrt{2} x_{j1} \ \sqrt{2} x_{j2}] \\ & = \varphi(\mathbf{x_i})^{\mathrm{T}} \varphi(\mathbf{x_i}), \quad \text{where } \varphi(\mathbf{x}) = [1 \ x_{1}^2 \ \sqrt{2} \ x_{1} x_{2} \ x_{2}^2 \ \sqrt{2} x_{1} \ \sqrt{2} x_{2}] \end{split}$$

Nonlinear SVMs: The Kernel Trick

Examples of commonly-used kernel functions:

□ Linear kernel:
$$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$$

- □ Polynomial kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$
- Gaussian (Radial-Basis Function (RBF)) kernel:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2})$$

Sigmoid:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$$

In general, functions that satisfy Mercer's condition can be kernel functions.

Nonlinear SVM: Optimization

Formulation: (Lagrangian Dual Problem)

maximize
$$\sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$
such that
$$0 \le \alpha_{i} \le C$$

$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

The solution of the discriminant function is

$$g(\mathbf{x}) = \sum_{i \in SV} \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b$$

The optimization technique is the same.

Support Vector Machine: Algorithm

- 1. Choose a kernel function
- 2. Choose a value for C
- 3. Solve the quadratic programming problem (many software packages available)
- 4. Construct the discriminant function from the support vectors

Some Issues

- Choice of kernel
 - Gaussian or polynomial kernel is default
 - if ineffective, more elaborate kernels are needed
 - domain experts can give assistance in formulating appropriate similarity measures
- Choice of kernel parameters
 - e.g. σ in Gaussian kernel
 - σ is the distance between closest points with different classifications
 - In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.
- Optimization criterion Hard margin v.s. Soft margin
 - a lengthy series of experiments in which various parameters are tested

Summary: Support Vector Machine

- 1. Large Margin Classifier
 - Better generalization ability & less over-fitting
- 2. The Kernel Trick
 - Map data points to higher dimensional space in order to make them linearly separable.
 - Since only dot product is used, we do not need to represent the mapping explicitly.

Additional Resource

http://www.kernel-machines.org/

Demo of LibSVM

http://www.csie.ntu.edu.tw/~cjlin/libsvm/