Support Vector Machines

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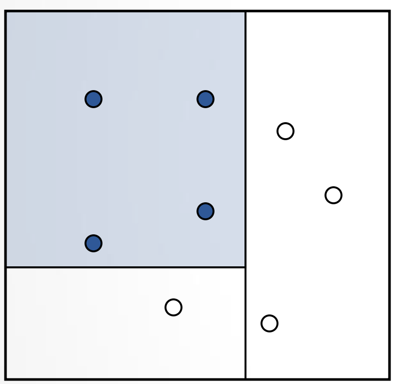
What We have Learned So Far?

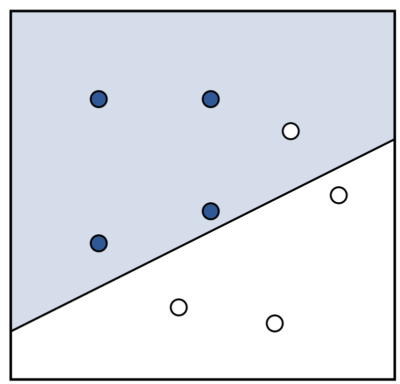
1. Decision Trees
2. Naïve Bayes
3. Linear Regression
4. Logistic Regression
5. Perceptron
6. Neural networks
7. K-Nearest Neighbors

- **Which of the above are linear and which are not?**
- **(1) (6) and (7) are non-linear**
    - **(2) is linear under certain restrictions**

Decision Surfaces

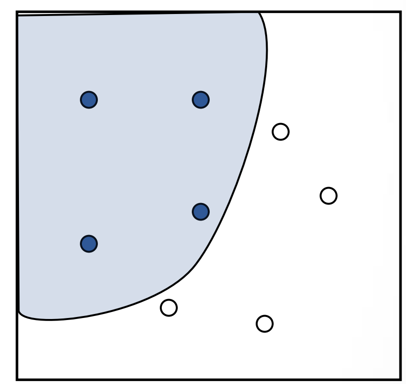


Decision Tree



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

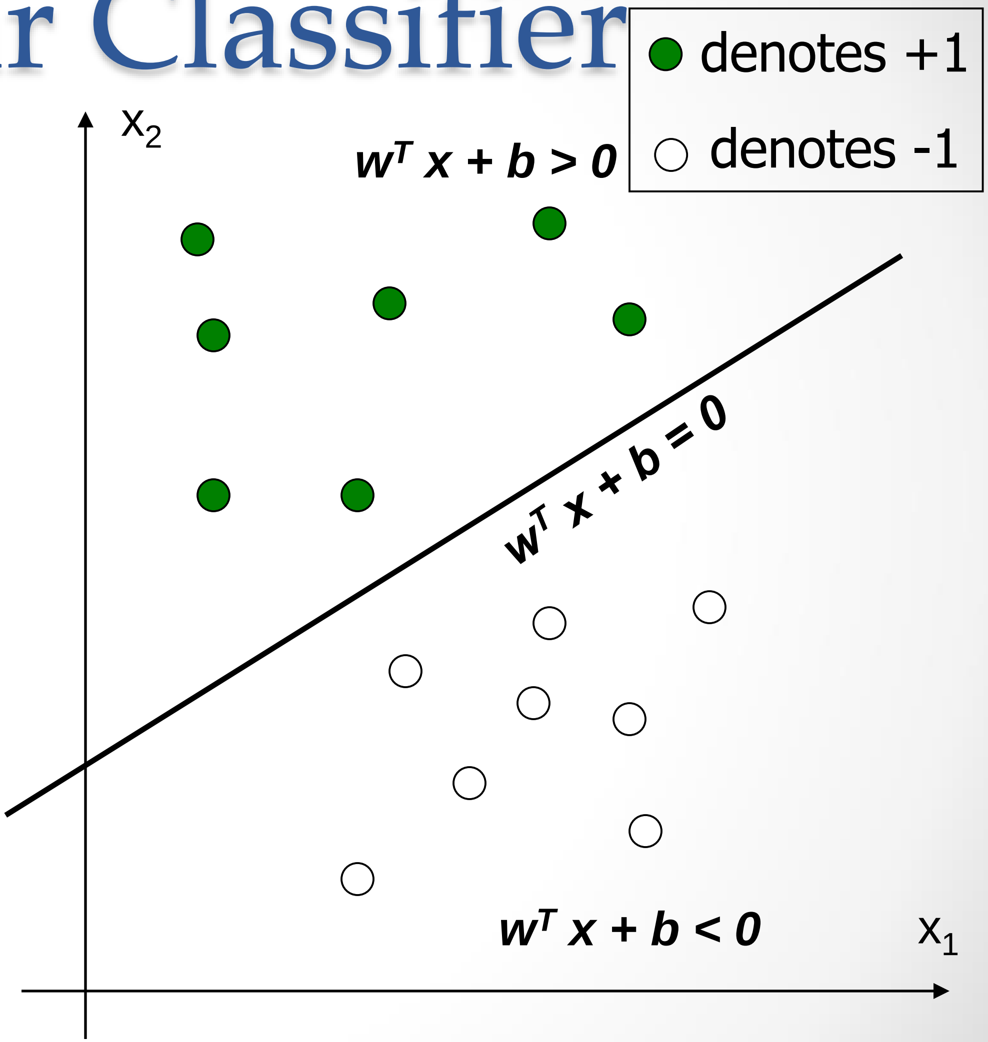
- Linear Discriminant Function
- Large Margin Linear Classifier
- Nonlinear SVM: The Kernel Trick
- SVM for Regression
- SMO Algorithm

Linear Discriminant Function or a Linear Classifier

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

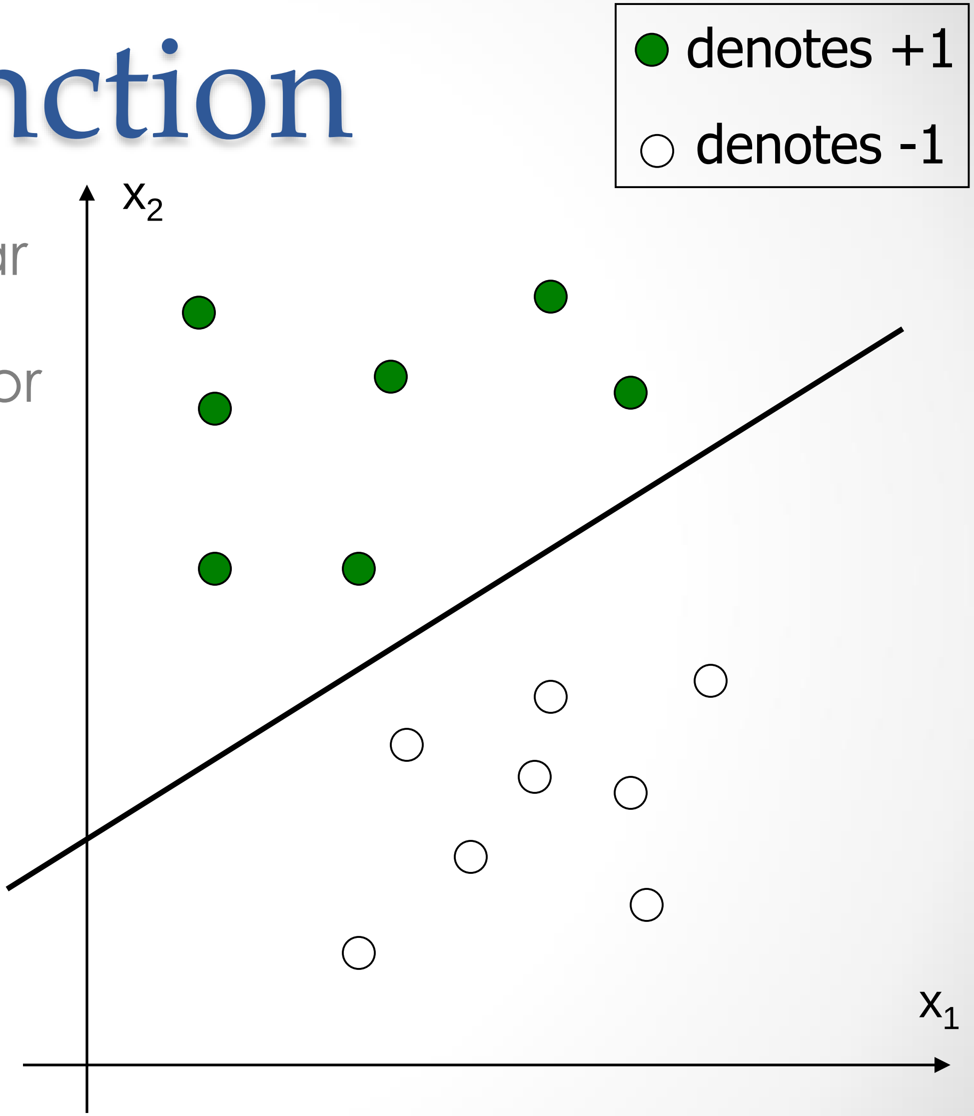
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$

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



Linear Discriminant Function

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



- Infinite number of answers!

Linear Discriminant Function

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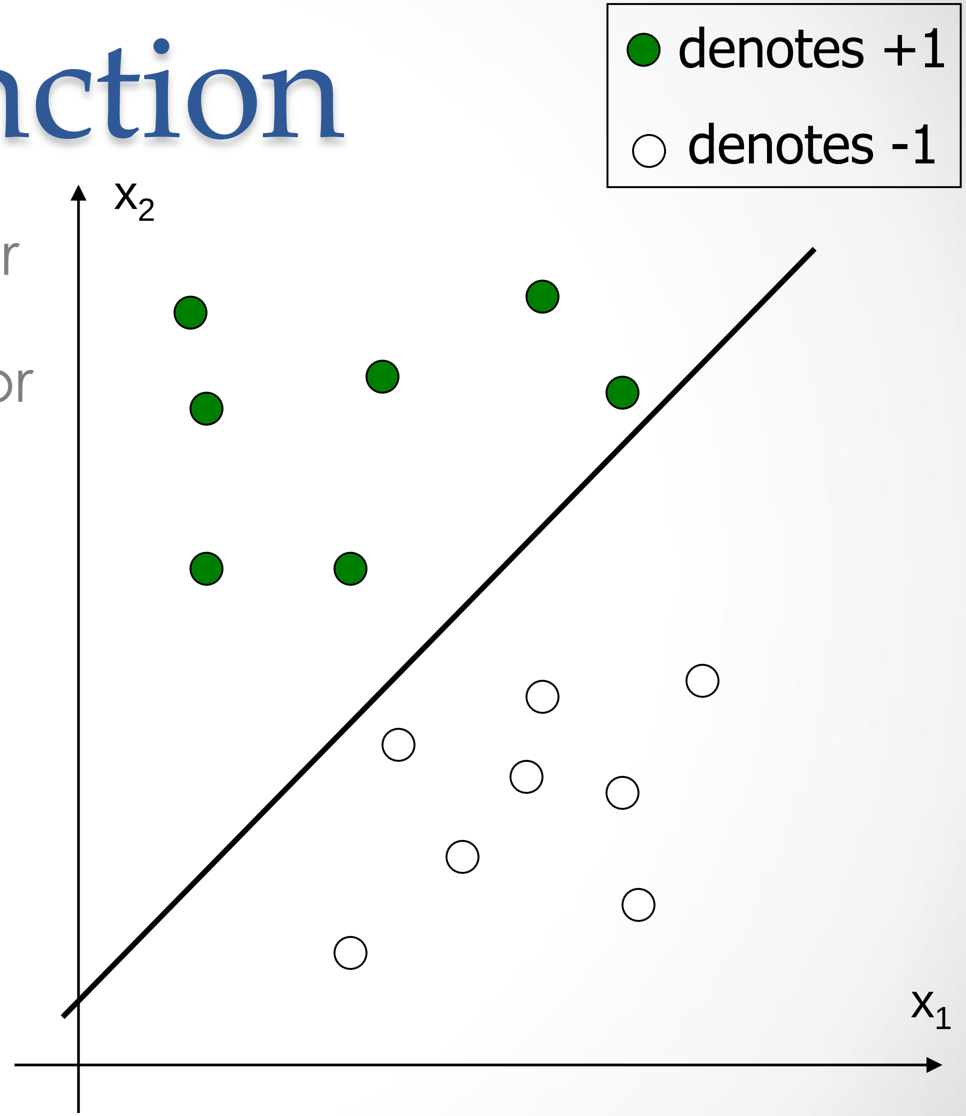

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Linear Discriminant Function

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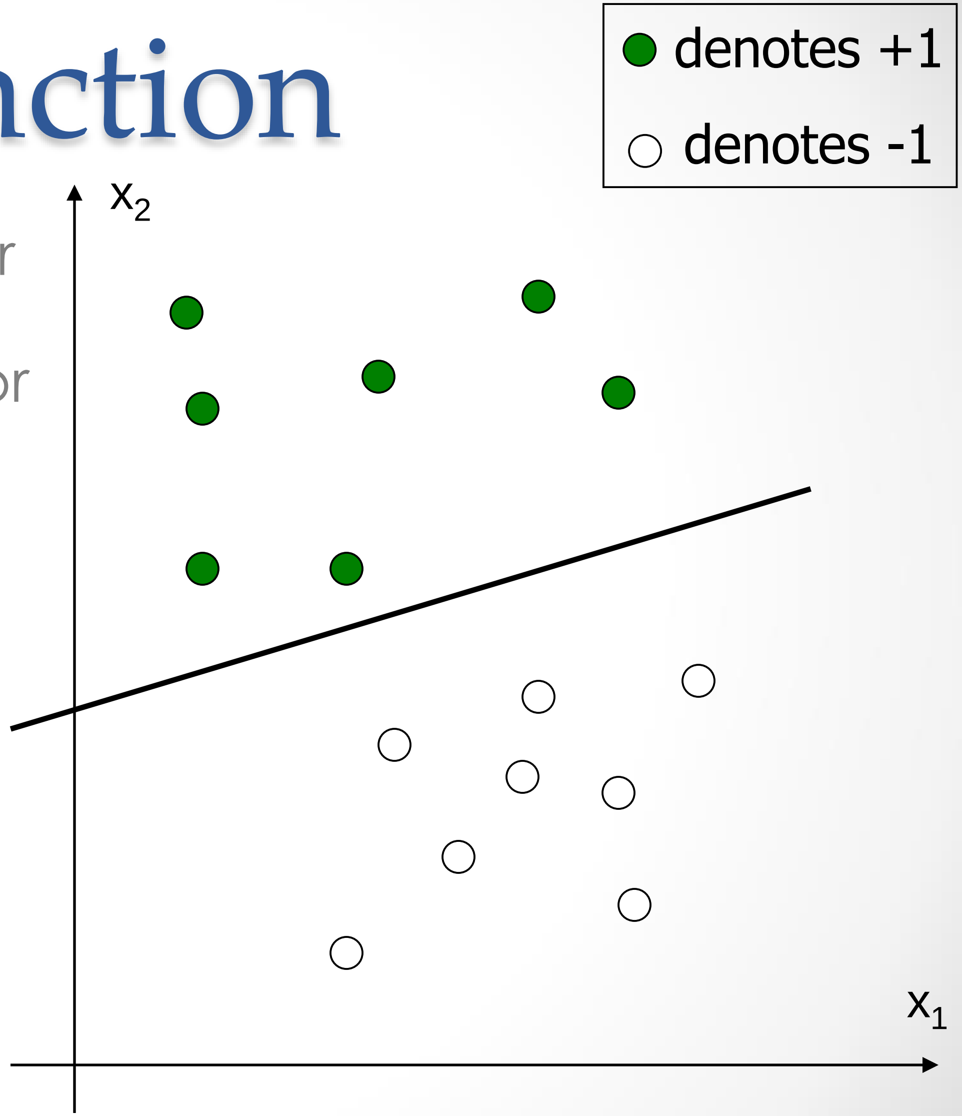
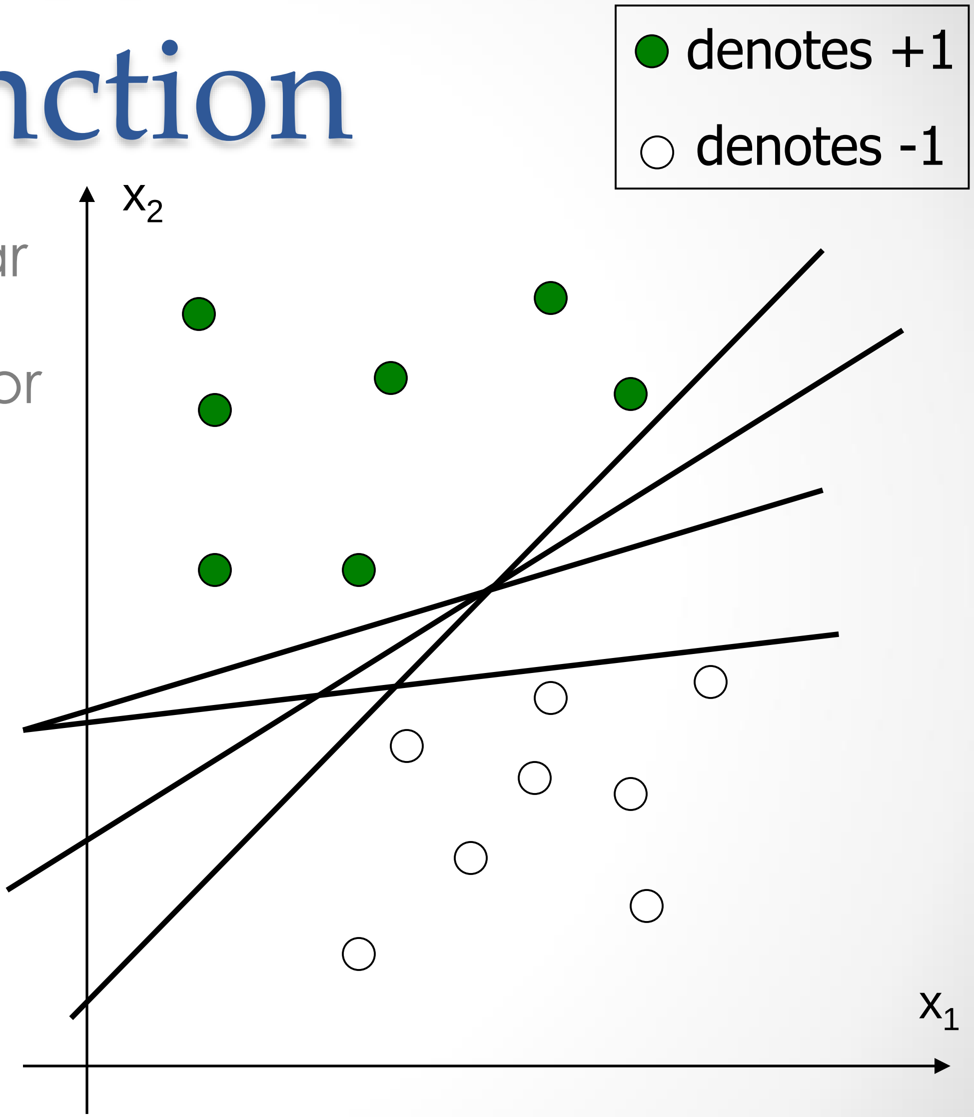


Linear Discriminant Function

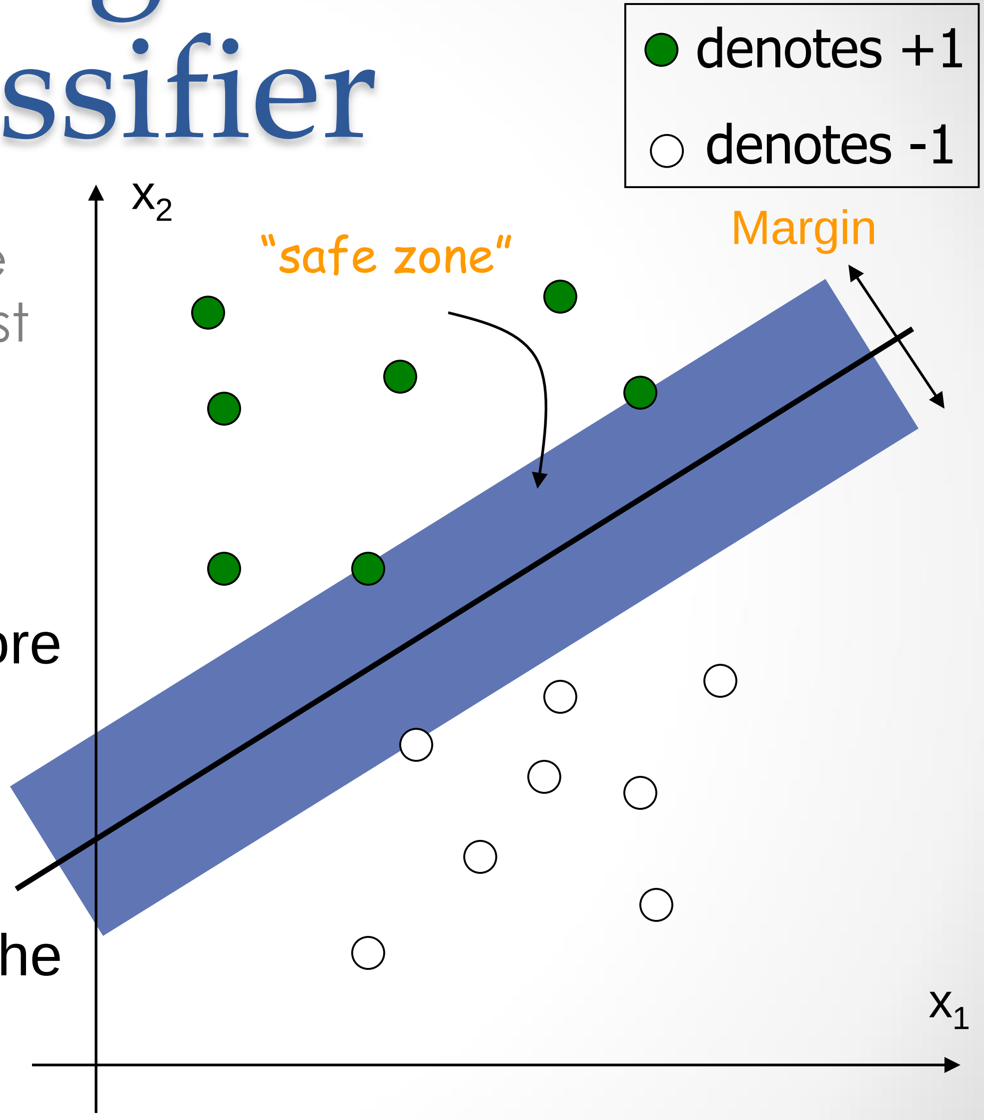
- How would you classify these points using a linear discriminant function in order to minimize the error rate?



- Infinite number of answers!
- Which one is the best?

Large Margin Linear 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

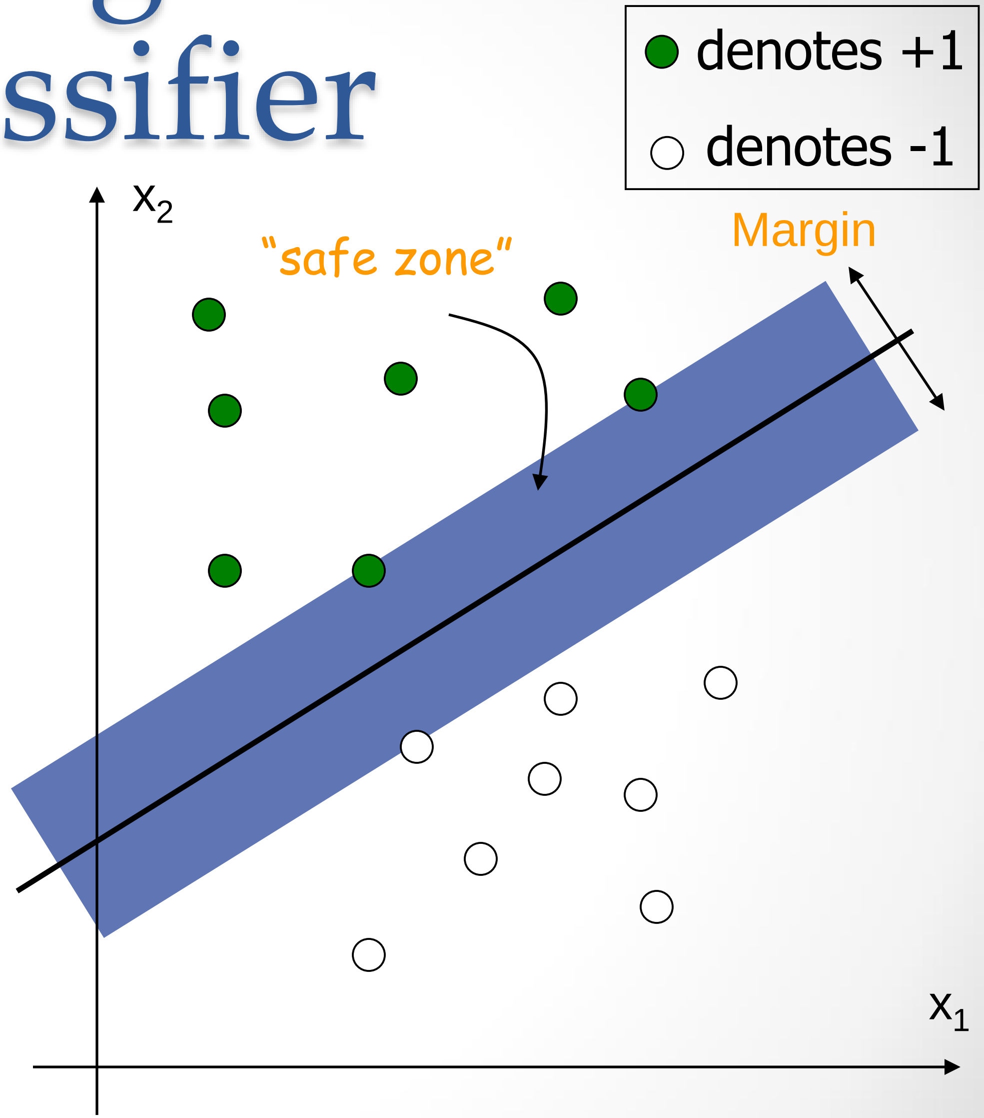
Large Margin Linear Classifier

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

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

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

- 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

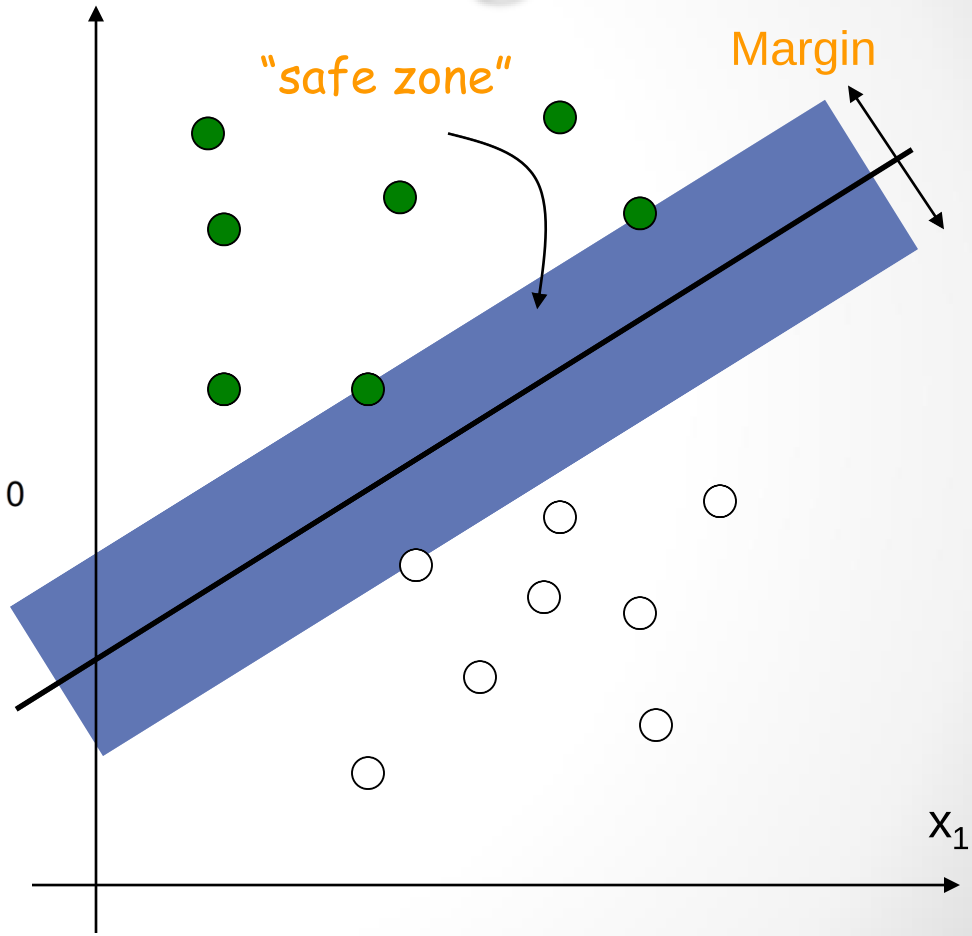
$$ax + by + c_2 = 0$$

the distance between them is given by:

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

Our lines in 2-D are:
$w_1 x_1 + w_2 x_2 + b - 1 = 0$ and $w_1 x_1 + w_2 x_2 + b + 1 = 0$

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



Large Margin Linear Classifier

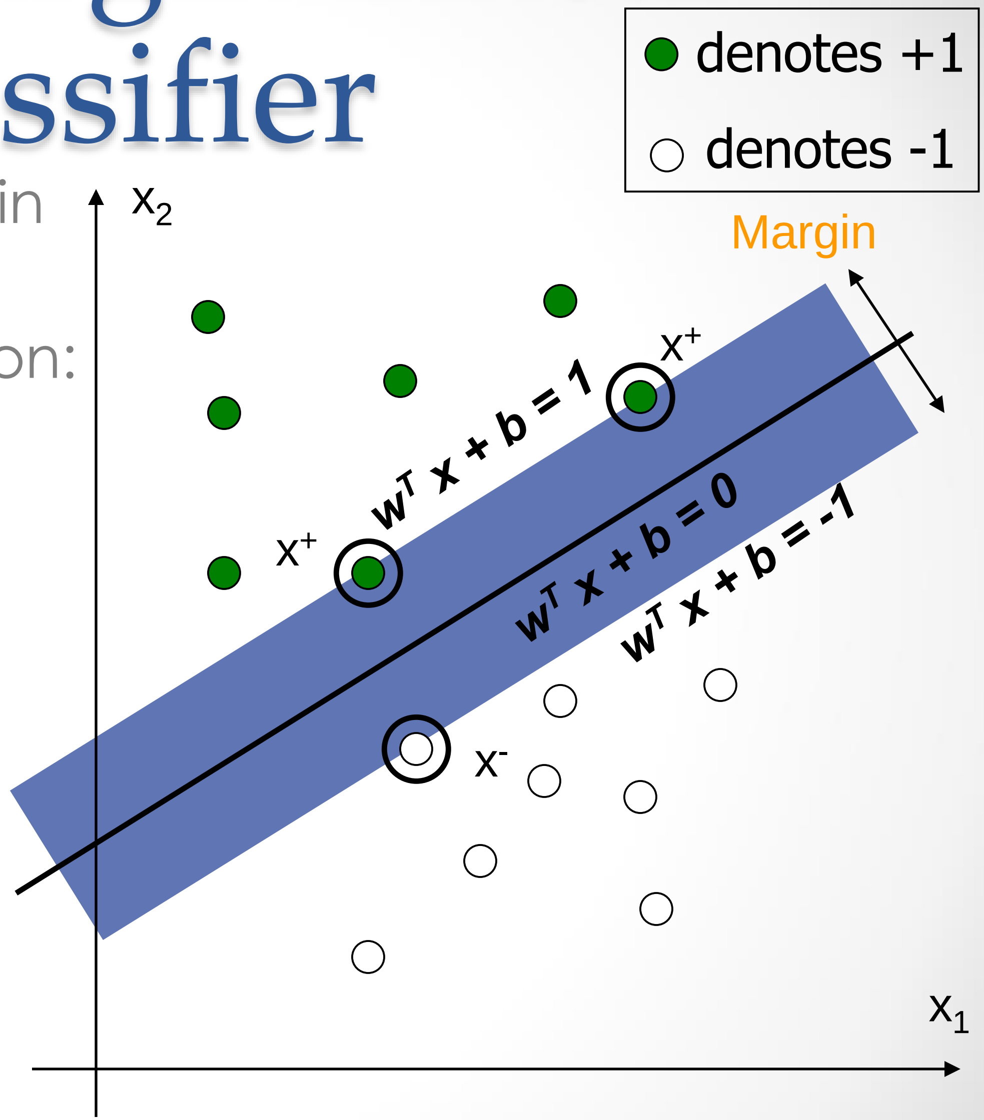
- Aim: Learn a large margin classifier
- Mathematical Formulation:

$$\text{maximize} \quad \frac{2}{\|\mathbf{w}\|}$$

such that

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

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



Common theme in machine learning:
LEARNING IS OPTIMIZATION

Large Margin Linear Classifier

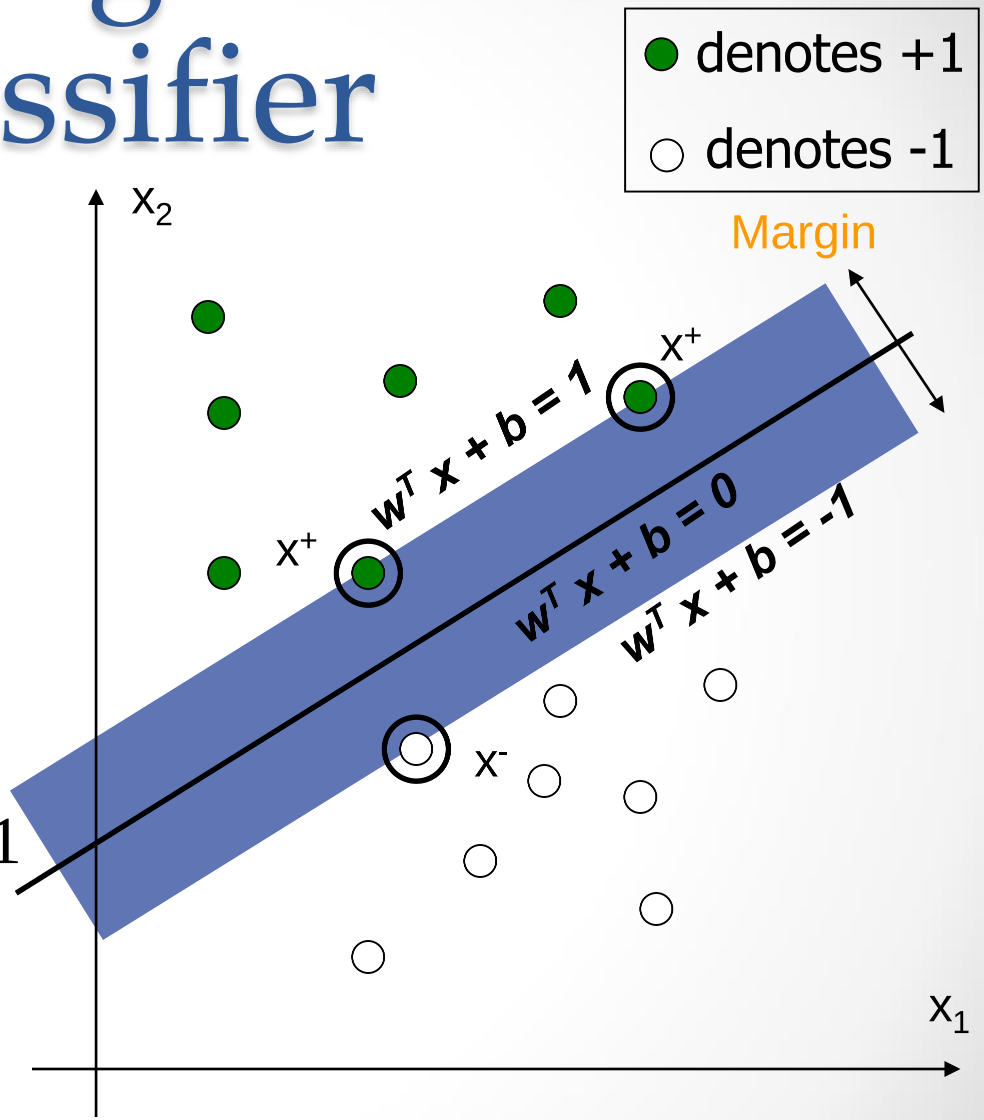
- Formulation:

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

such that

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

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



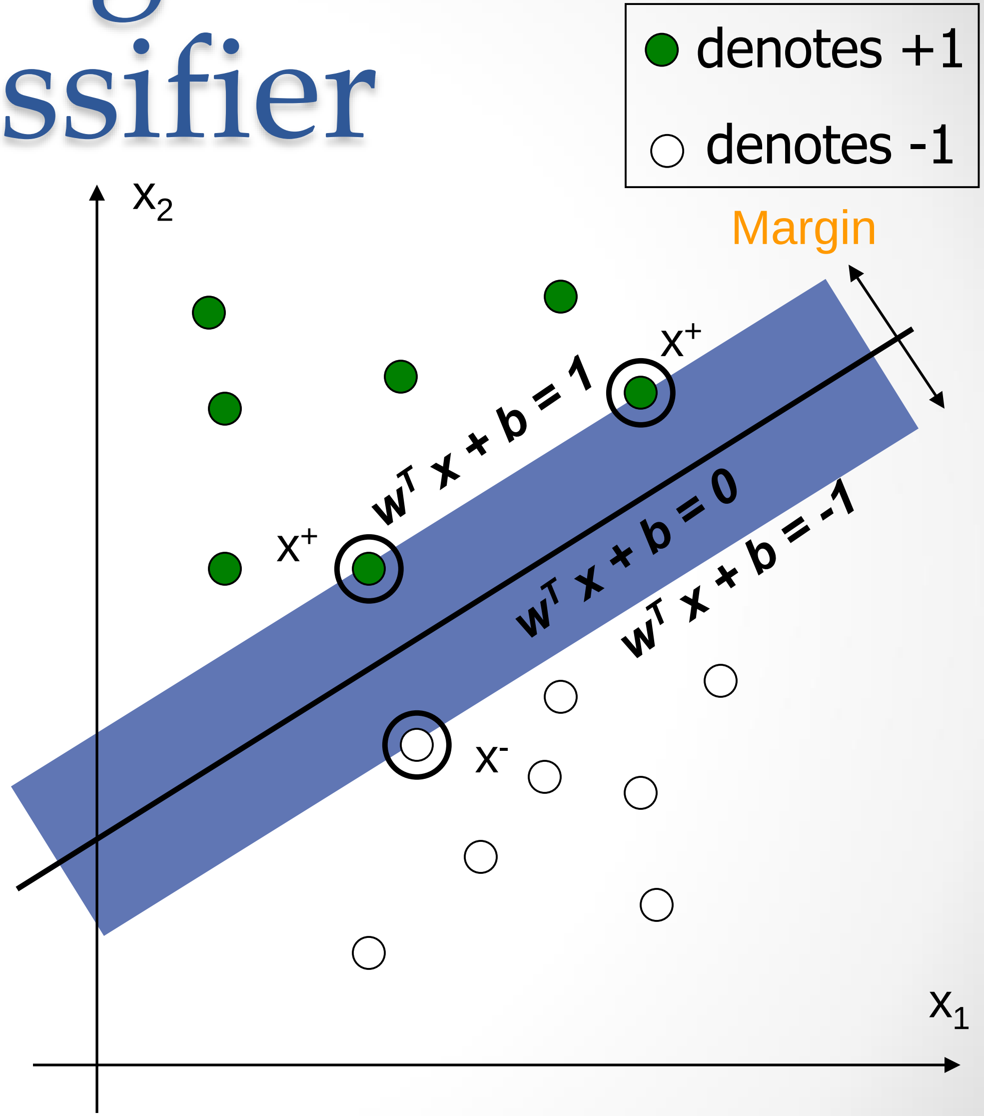
Large Margin Linear Classifier

- Formulation:

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

such that

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



Large Margin Linear Classifier

- Formulation:

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

such that

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

- This is a Quadratic programming problem with linear constraints
  - Off-the-shelf Software
- However, we will convert it to Lagrangian dual in order **to use the kernel trick!**

Lagrangian Duality

- The Lagrangian method is a general method for converting constrained optimization problems to unconstrained ones.
  - unconstrained optimization problems are easier
- When we have equality constraints, the transformation looks as follows

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & h_i(w) = 0, \quad i = 1, \ldots, l \end{aligned} \quad \Rightarrow \quad \mathcal{L}(w, \beta) = f(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

set $\mathcal{L}$'s partial derivatives to zero: $\dfrac{\partial \mathcal{L}}{\partial w_i} = 0; \quad \dfrac{\partial \mathcal{L}}{\partial \beta_i} = 0,$

solve for w and β.

Lagrangian Duality

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \le 0, \quad i = 1, \ldots, k \\ & h_i(w) = 0, \quad i = 1, \ldots, l. \end{aligned}$$

Lagrangian function

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Same as solving the primal problem

Not the same as solving the following dual problem

$$\min_w \max_{\alpha, \beta \,:\, \alpha_i \ge 0} \mathcal{L}(w, \alpha, \beta)$$

Let the optimal solution be

$$p^* = \min_w \max_{\alpha, \beta \,:\, \alpha_i \ge 0} \mathcal{L}(w, \alpha, \beta)$$

$$\max_{\alpha, \beta \,:\, \alpha_i \ge 0} \min_w \mathcal{L}(w, \alpha, \beta)$$

Let the optimal solution be

$$d^* = \max_{\alpha, \beta \,:\, \alpha_i \ge 0} \min_w \mathcal{L}(w, \alpha, \beta)$$

$$p^* \ge d^*$$

Solving the Optimization Problem

Quadratic programming with linear constraints

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

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

Lagrangian Function

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

$$\text{s.t.} \quad \alpha_i \geq 0$$

Solving the Optimization Problem

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

$$\text{s.t.} \quad \alpha_i \geq 0$$

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

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

Solving the Optimization Problem

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

$$\text{s.t.} \quad \alpha_i \geq 0$$

Lagrangian Dual Problem

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

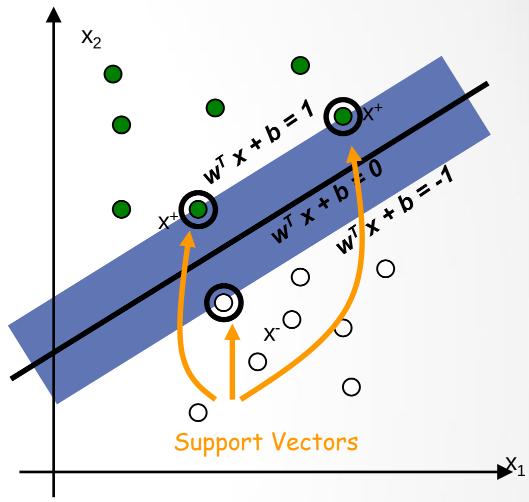
$$\text{s.t.} \quad \alpha_i \geq 0 \text{ , and } \sum_{i=1}^{n} \alpha_i y_i = 0$$

Solving the Optimization Problem

- 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:

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

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

where $\mathbf{x}_i$ is support vector

Solving the Optimization Problem

- The linear discriminant function is:

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

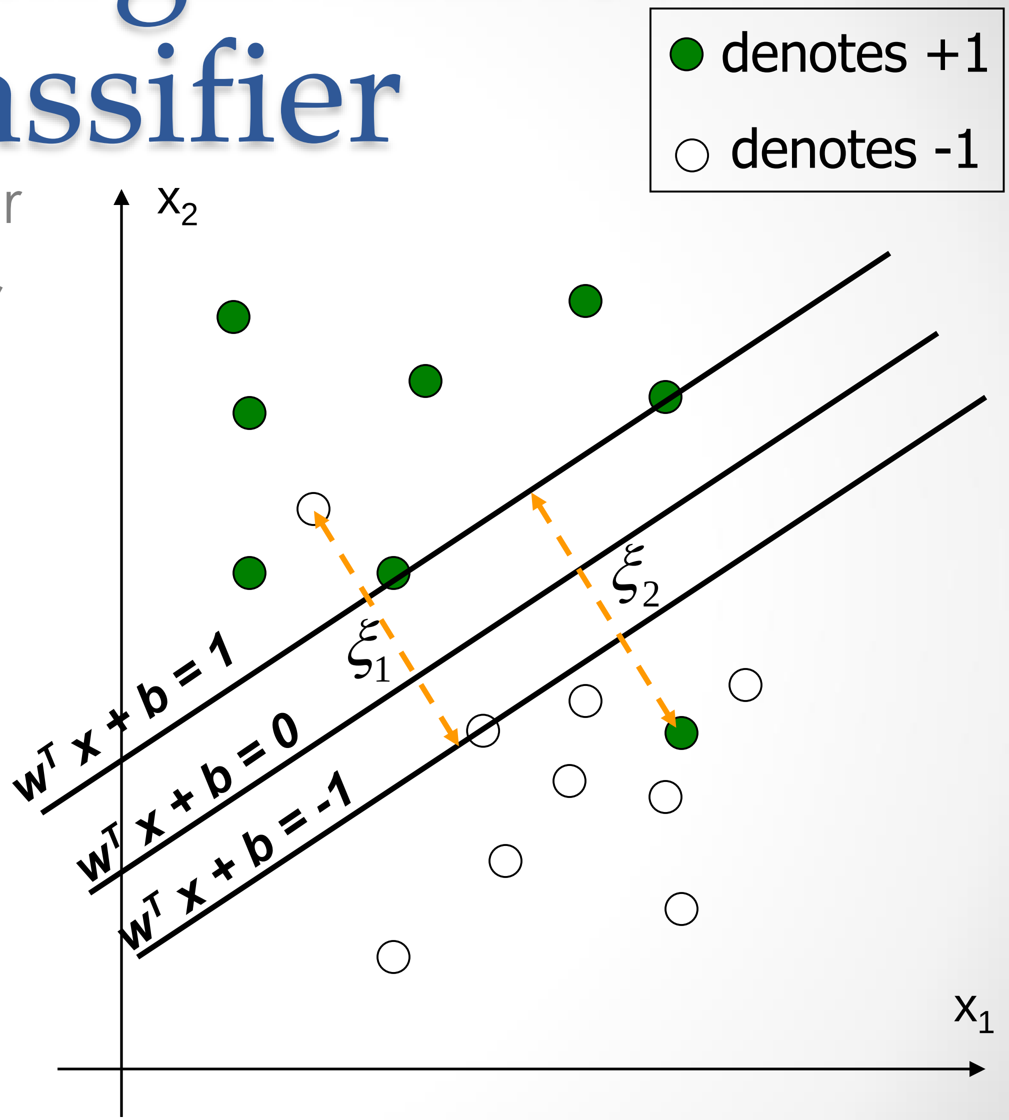
- Notice it relies on a *dot product* between the test point ***x*** and the support vectors $\boldsymbol{x}_i$

- Also keep in mind that solving the optimization problem involved computing the dot products $\boldsymbol{x}_i^T \boldsymbol{x}_j$ between all pairs of training points

Large Margin Linear Classifier

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

- Slack variables ξ_i can be added to allow mis-classification of difficult or noisy data points



Large Margin Linear Classifier

- Formulation:

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

such that

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

$$\xi_i \geq 0$$

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

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

Without slack variables

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

Large Margin Linear Classifier

- Formulation: (Lagrangian Dual Problem)

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

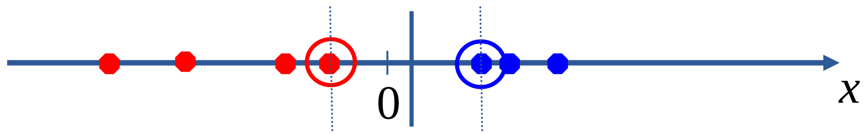
such that

$$0 \leq \alpha_i \leq C$$

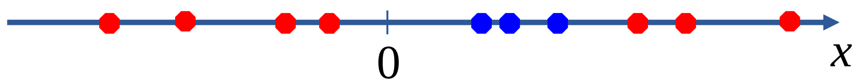
$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

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?



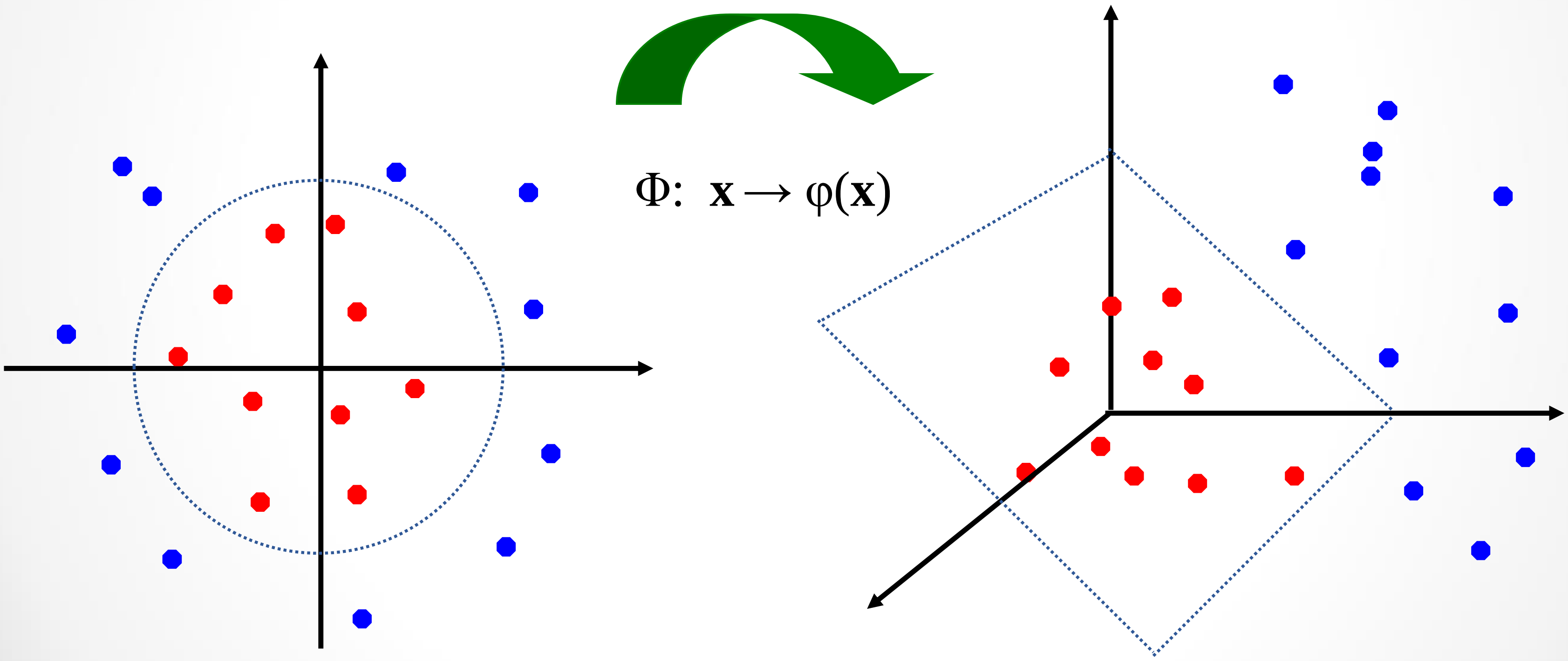
- Kernel Trick!!!
  - SVM = Linear SVM + Kernel Trick

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.
  - 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:



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Nonlinear SVMs: The Kernel Trick

- With this mapping, our discriminant function is now:

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

- 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 $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2$,

Need to show that $K(\mathbf{x}_i,\mathbf{x}_j) = \varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_j)$:

$$
\begin{aligned}
K(\mathbf{x}_i,\mathbf{x}_j)&=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2, \\
&= 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} \\
&= [1\ \ x_{i1}^2\ \ \sqrt{2}\, x_{i1}x_{i2}\ \ x_{i2}^2\ \ \sqrt{2}x_{i1}\ \ \sqrt{2}x_{i2}]^T [1\ \ x_{j1}^2\ \ \sqrt{2}\, x_{j1}x_{j2}\ \ x_{j2}^2\ \ \sqrt{2}x_{j1}\ \ \sqrt{2}x_{j2}] \\
&= \varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_j), \quad \text{where } \varphi(\mathbf{x}) = [1\ \ x_1^2\ \ \sqrt{2}\, x_1x_2\ \ x_2^2\ \ \sqrt{2}x_1\ \ \sqrt{2}x_2]
\end{aligned}
$$

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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:

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

  - 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: Kernel matrix should be positive semidefinite.

Nonlinear SVM: Optimization

- Formulation: (Lagrangian Dual Problem)

$$\text{maximize} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{such that} \quad 0 \le \alpha_i \le C$$

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

- The solution of the discriminant function is

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

- 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

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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/