An Introduction of Support Vector Machine

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Review: What We've Learned So Far

- Bayesian Decision Theory
- Maximum-Likelihood & Bayesian Parameter Estimation
- Nonparametric Density Estimation
  - Parzen-Window, k_n-Nearest-Neighbor
- K-Nearest Neighbor Classifier
- Decision Tree Classifier

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 textbook

V. Vapnik

Outline

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

Discriminant Function

- Chapter 2.4: the classifier is said to assign a feature vector *x* to class w_i if

$$g_i(\mathbf{x}) > g_j(\mathbf{x}) \qquad \text{for all } \quad j \neq i$$

- For two-category case, $g(\mathbf{x}) \equiv g_1(\mathbf{x}) - g_2(\mathbf{x})$

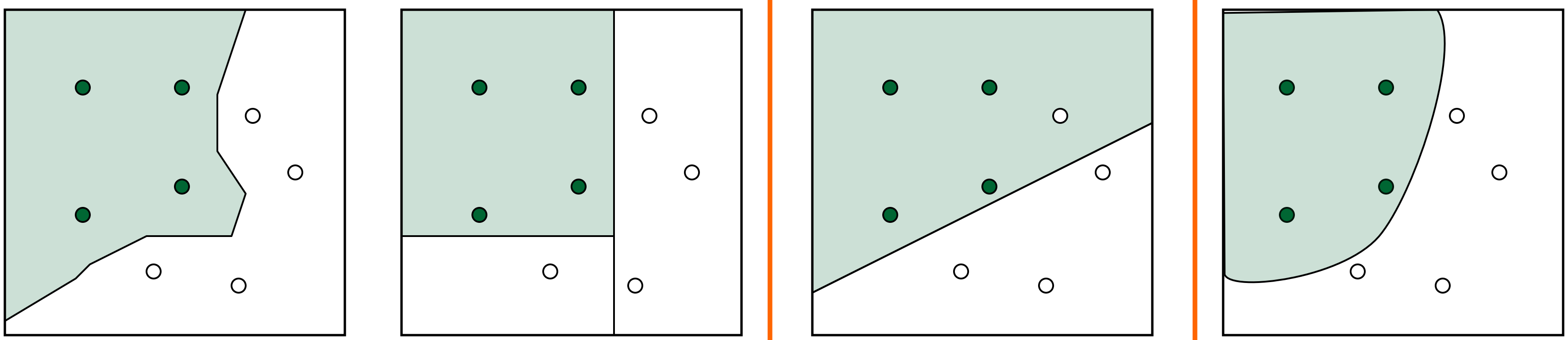
$$\text{Decide } \omega_1 \text{ if } g(\mathbf{x}) > 0; \text{ otherwise decide } \omega_2$$

- An example we've learned before:
  - Minimum-Error-Rate Classifier

$$g(\mathbf{x}) \equiv p(\omega_1 \,|\, \mathbf{x}) - p(\omega_2 \,|\, \mathbf{x})$$

Discriminant Function

- It can be arbitrary functions of *x*, such as:



Nearest Neighbor

Decision Tree

Linear Functions

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

Nonlinear Functions

Linear Discriminant Function

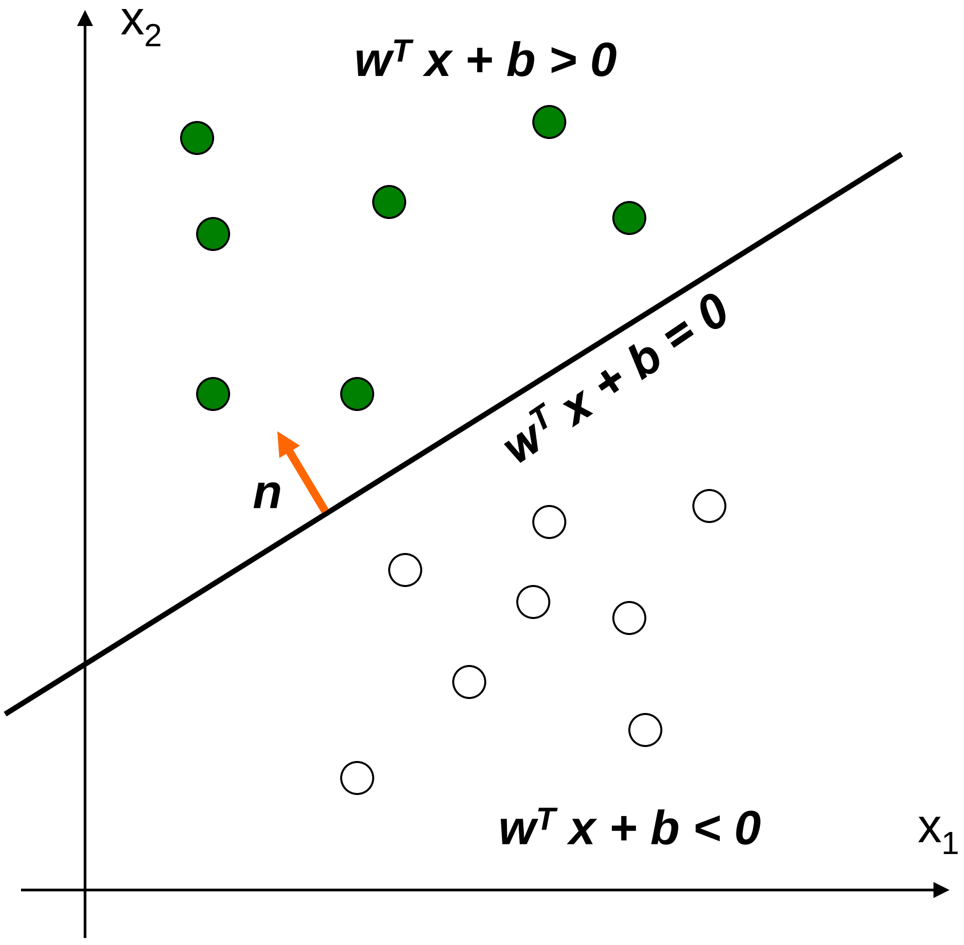
- g(x) is a linear function:

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

- A hyper-plane in the feature space

- (Unit-length) normal vector of the hyper-plane:

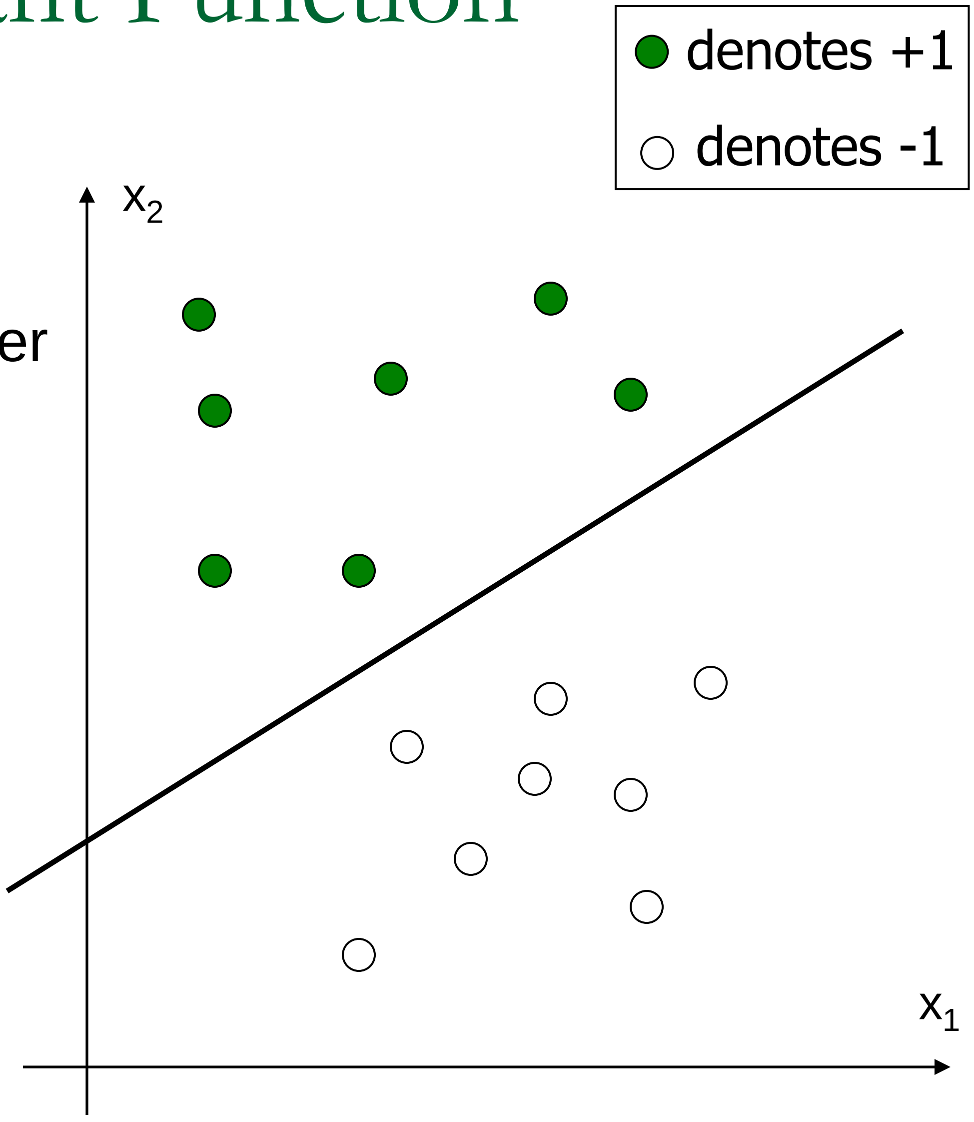
$$\mathbf{n} = \frac{\mathbf{w}}{\|\mathbf{w}\|}$$



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!



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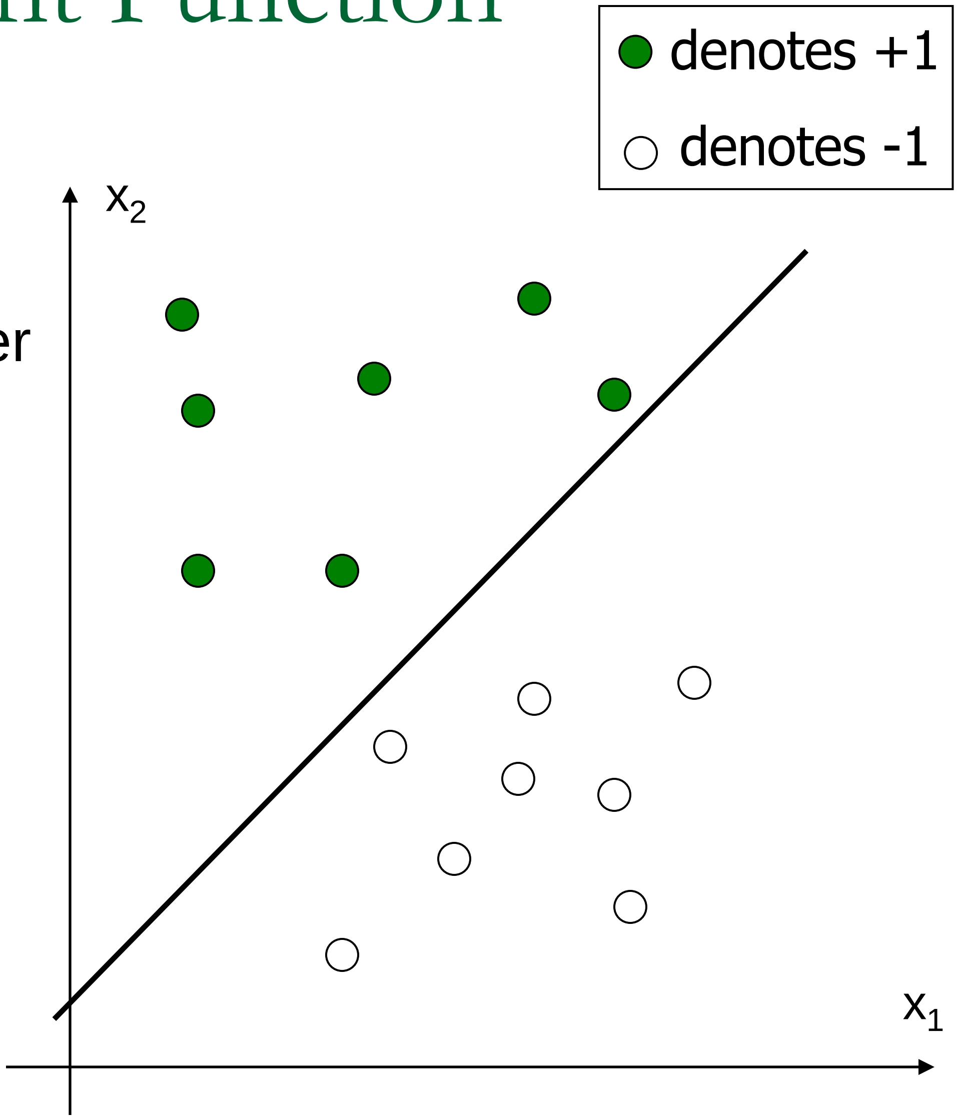

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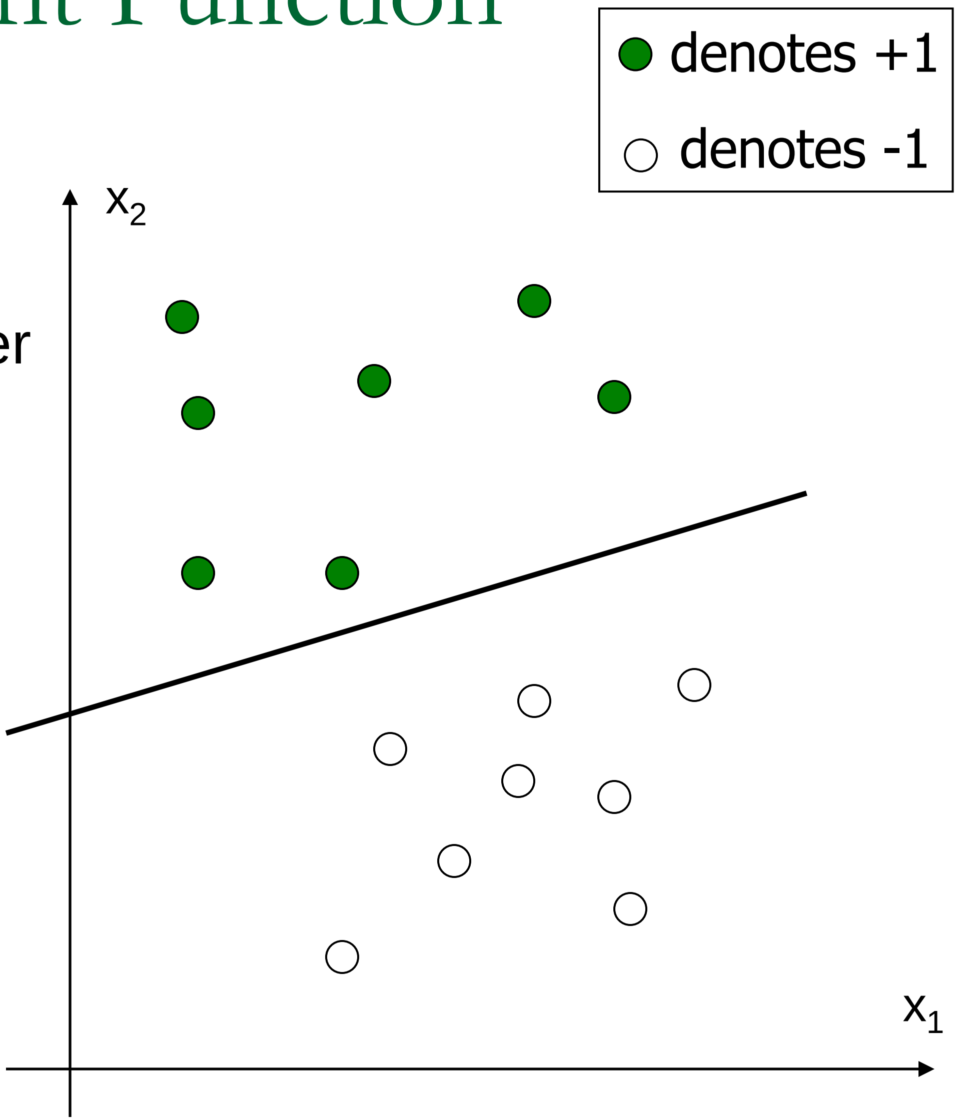
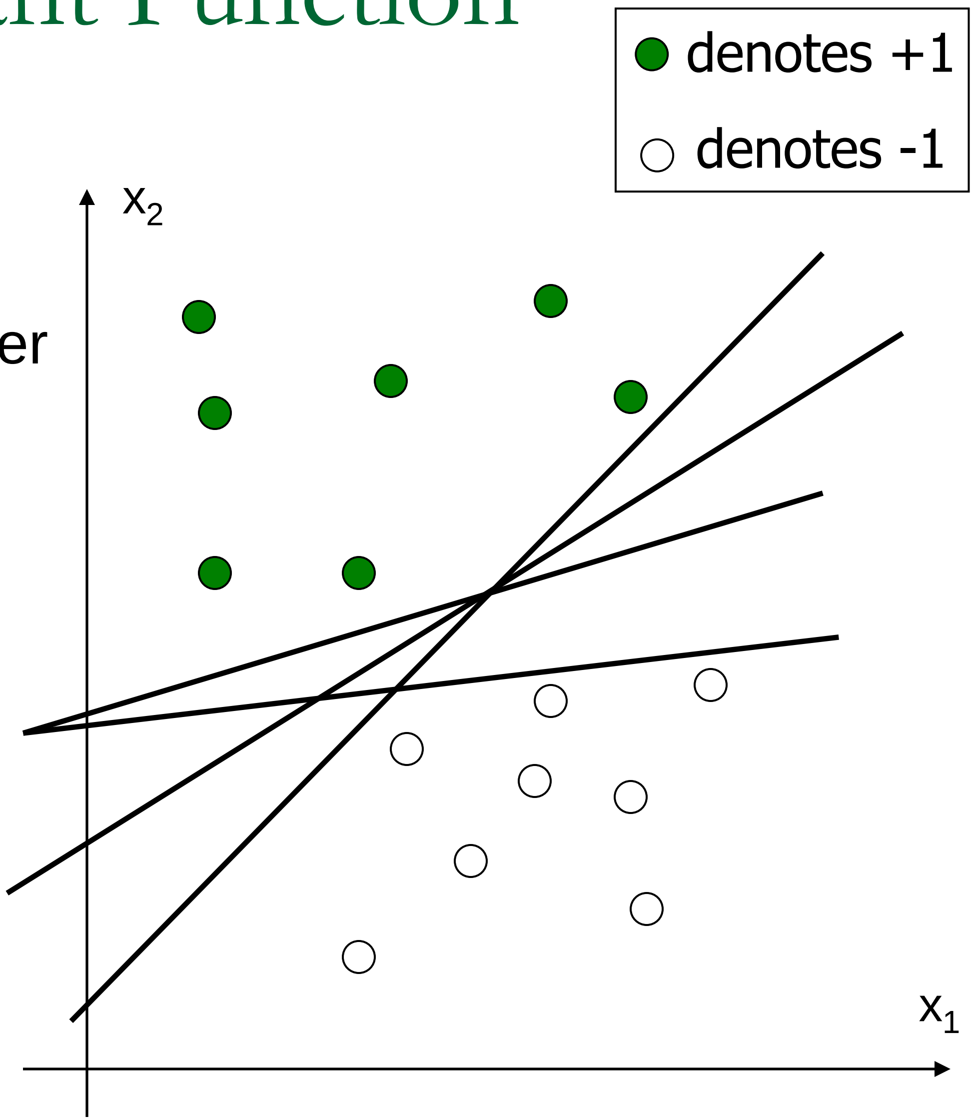


Linear Discriminant Function

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

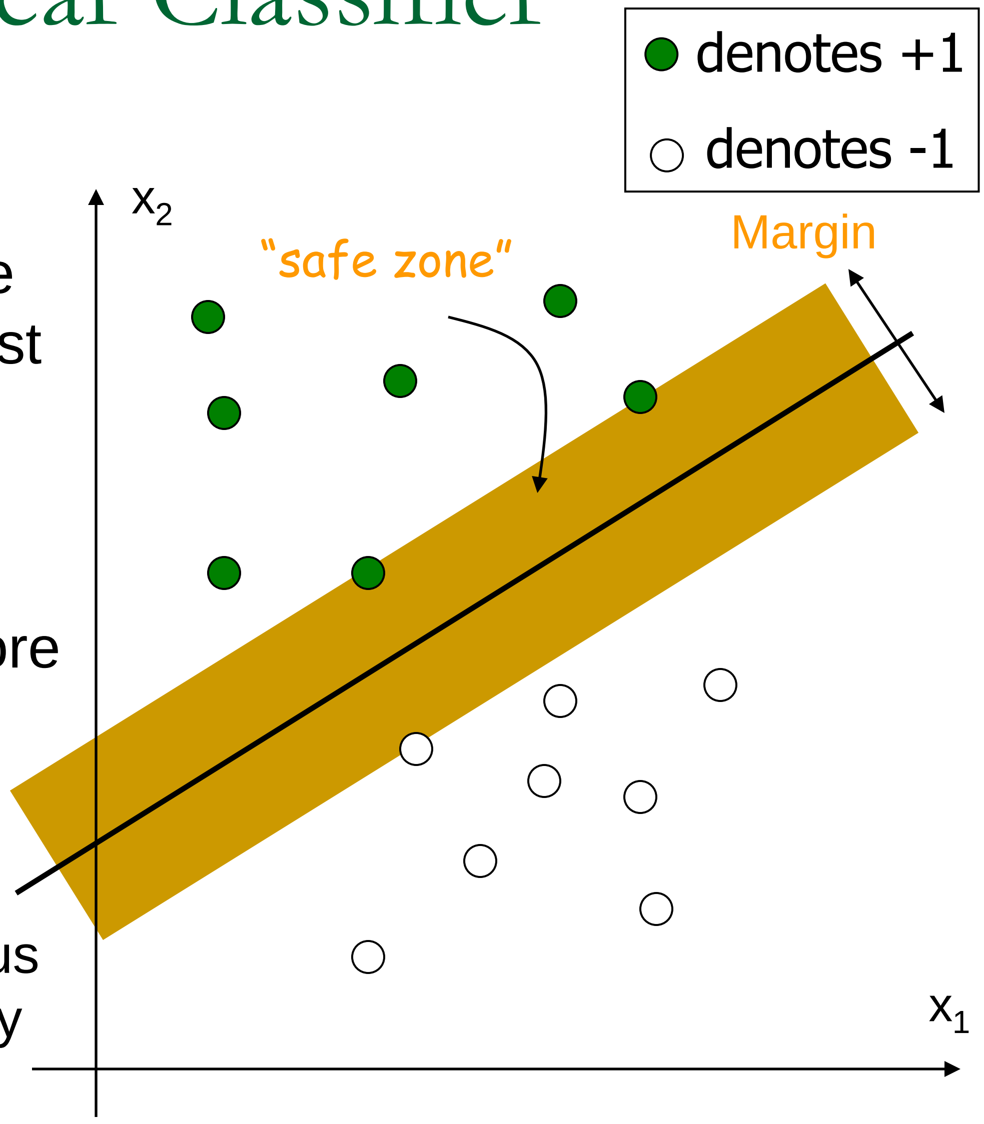
- Infinite number of answers!

- 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?
  - Robust to outliners and thus strong generalization ability



Large Margin Linear Classifier

- Given a set of data points:

$\{(\mathbf{x}_i, y_i)\},\ i = 1, 2, \cdots, n$, where

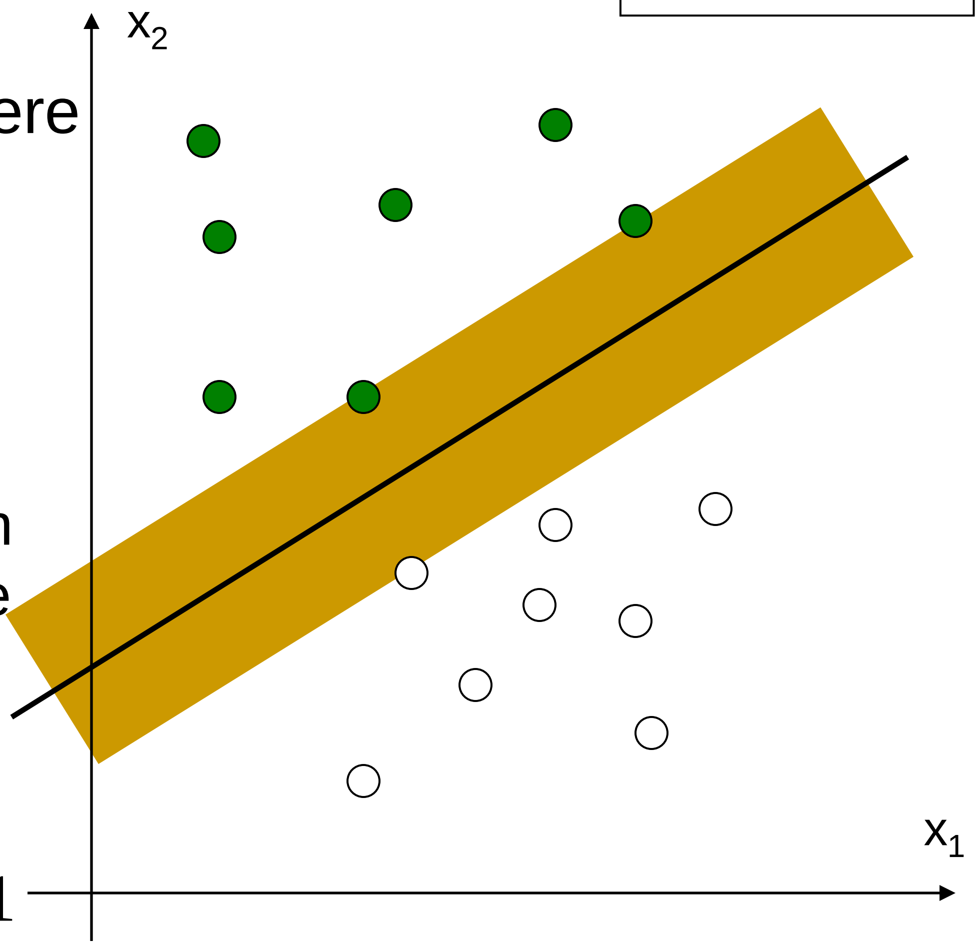
$$\text{For } y_i = +1,\quad \mathbf{w}^T \mathbf{x}_i + b > 0$$

$$\text{For } y_i = -1,\quad \mathbf{w}^T \mathbf{x}_i + b < 0$$

- With a scale transformation on both *w* and *b*, the above is equivalent to

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

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



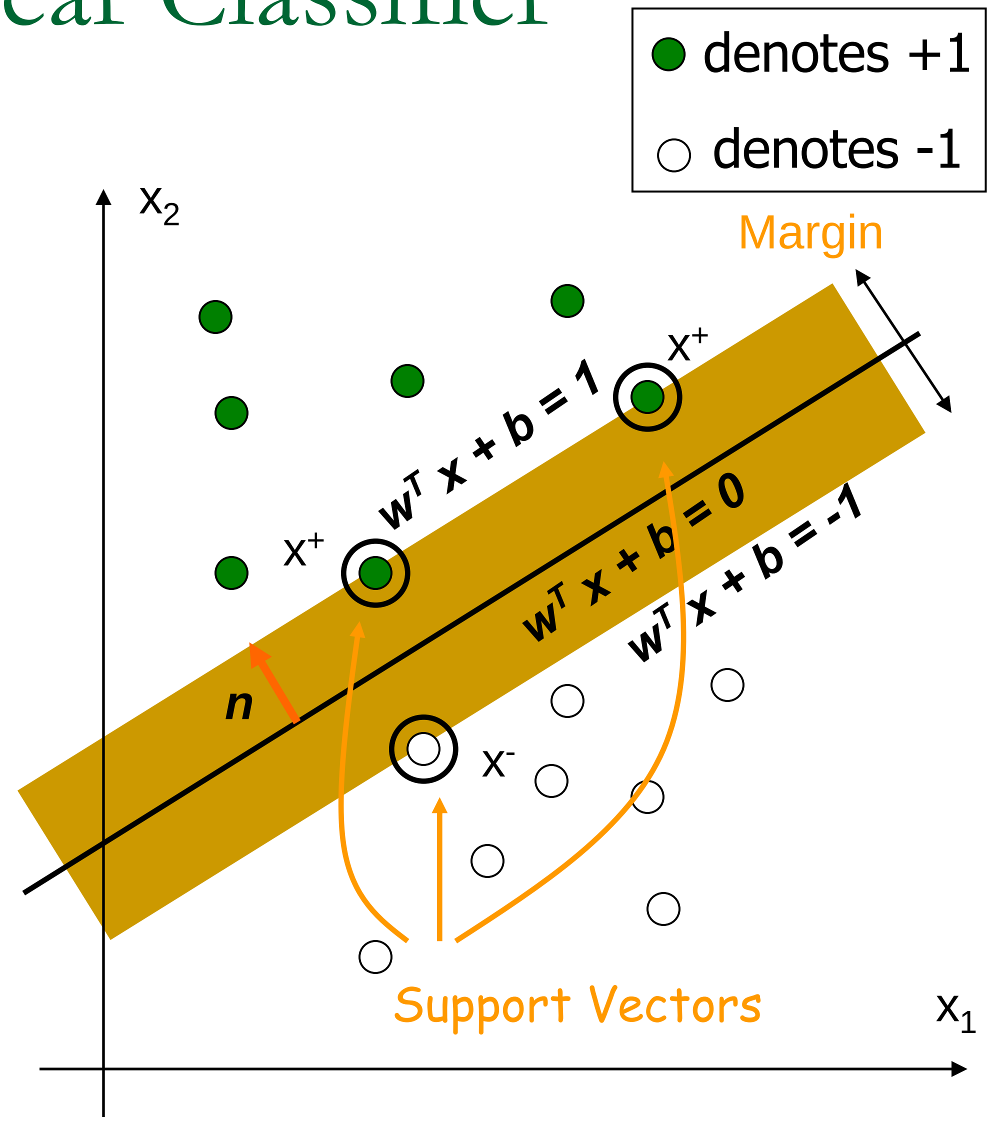
Large Margin Linear Classifier

- We know that

$$\mathbf{w}^T\mathbf{x}^+ + b = 1$$
$$\mathbf{w}^T\mathbf{x}^- + b = -1$$

- The margin width is:

$$M = (\mathbf{x}^+ - \mathbf{x}^-)\cdot\mathbf{n}$$
$$= (\mathbf{x}^+ - \mathbf{x}^-)\cdot\frac{\mathbf{w}}{\|\mathbf{w}\|} = \frac{2}{\|\mathbf{w}\|}$$



Large Margin Linear Classifier

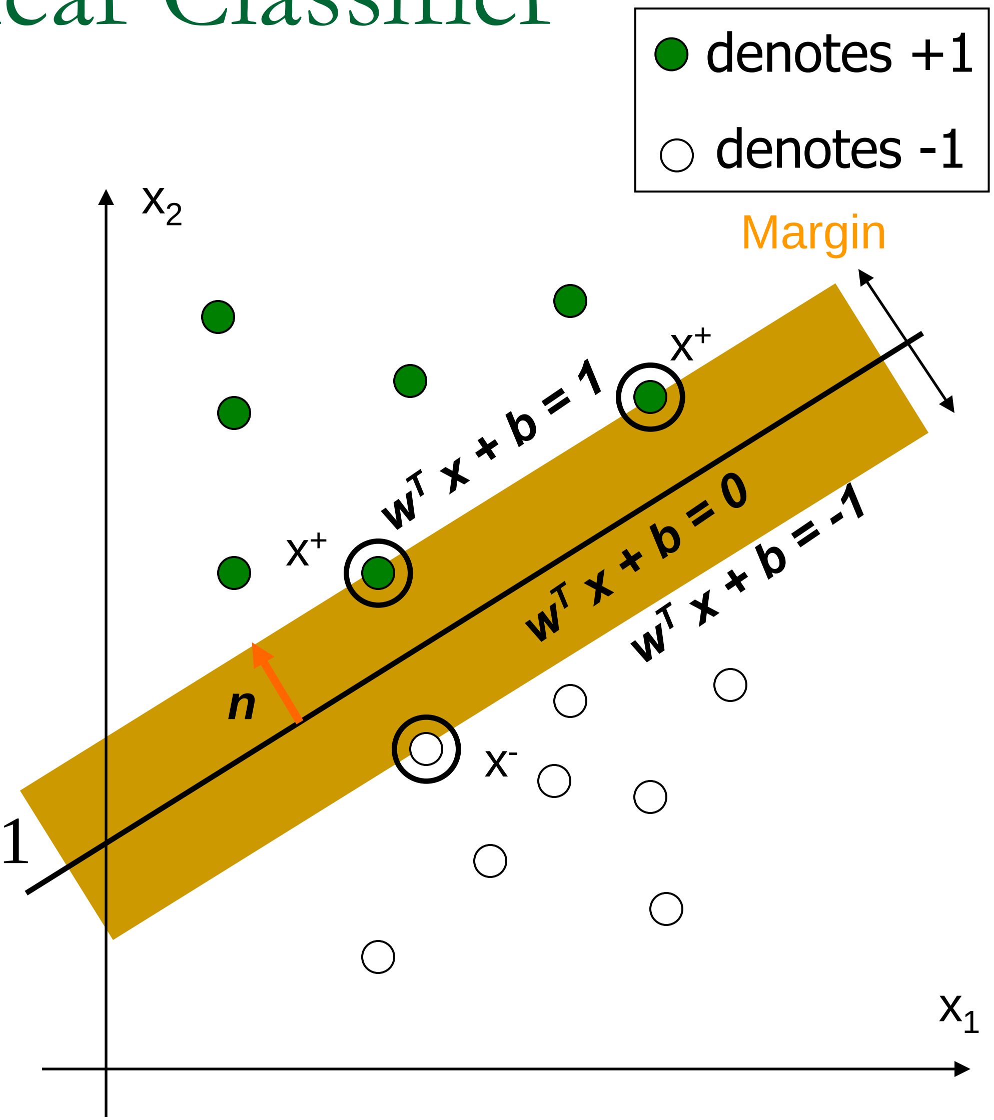
- Formulation:

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

such that

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

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



Large Margin Linear Classifier

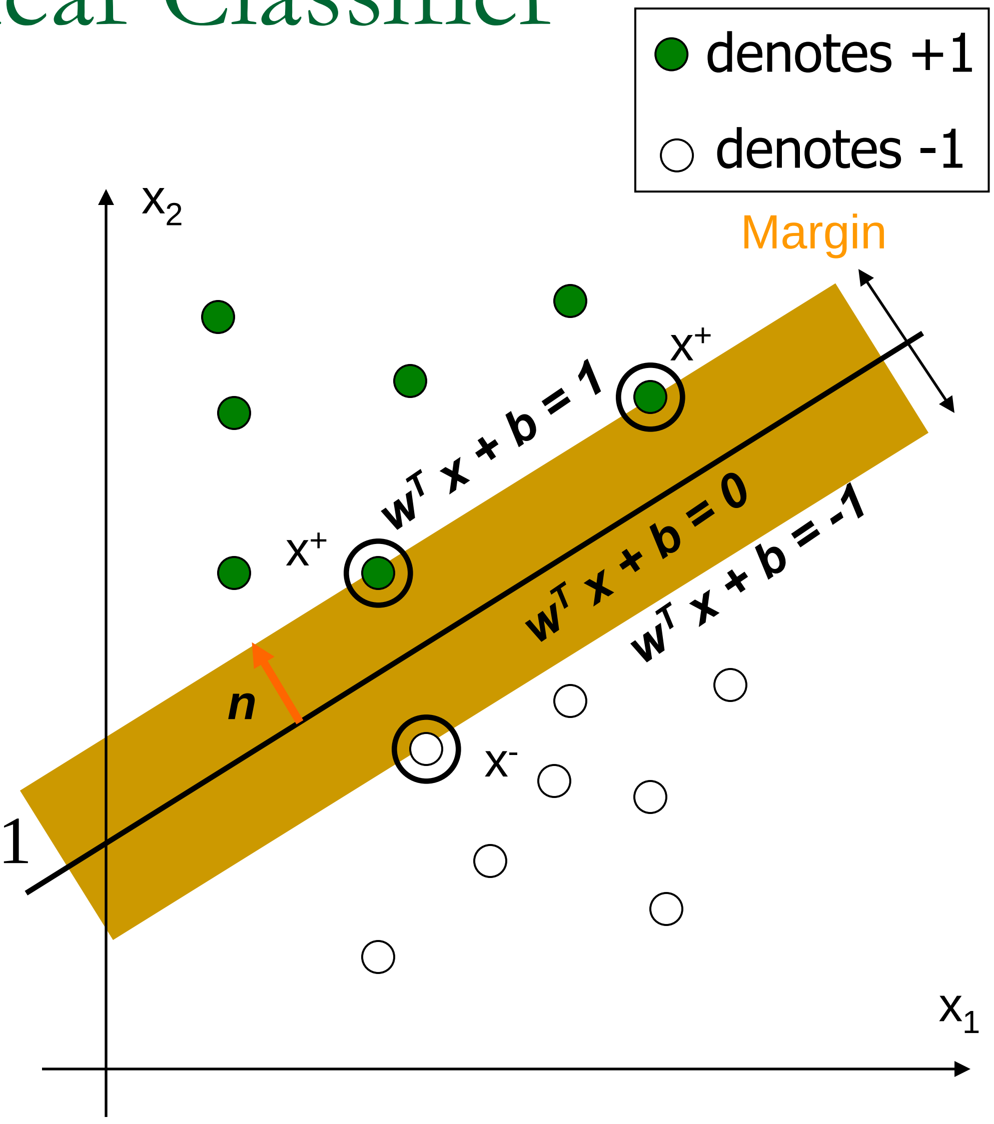
- Formulation:

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

such that

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

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



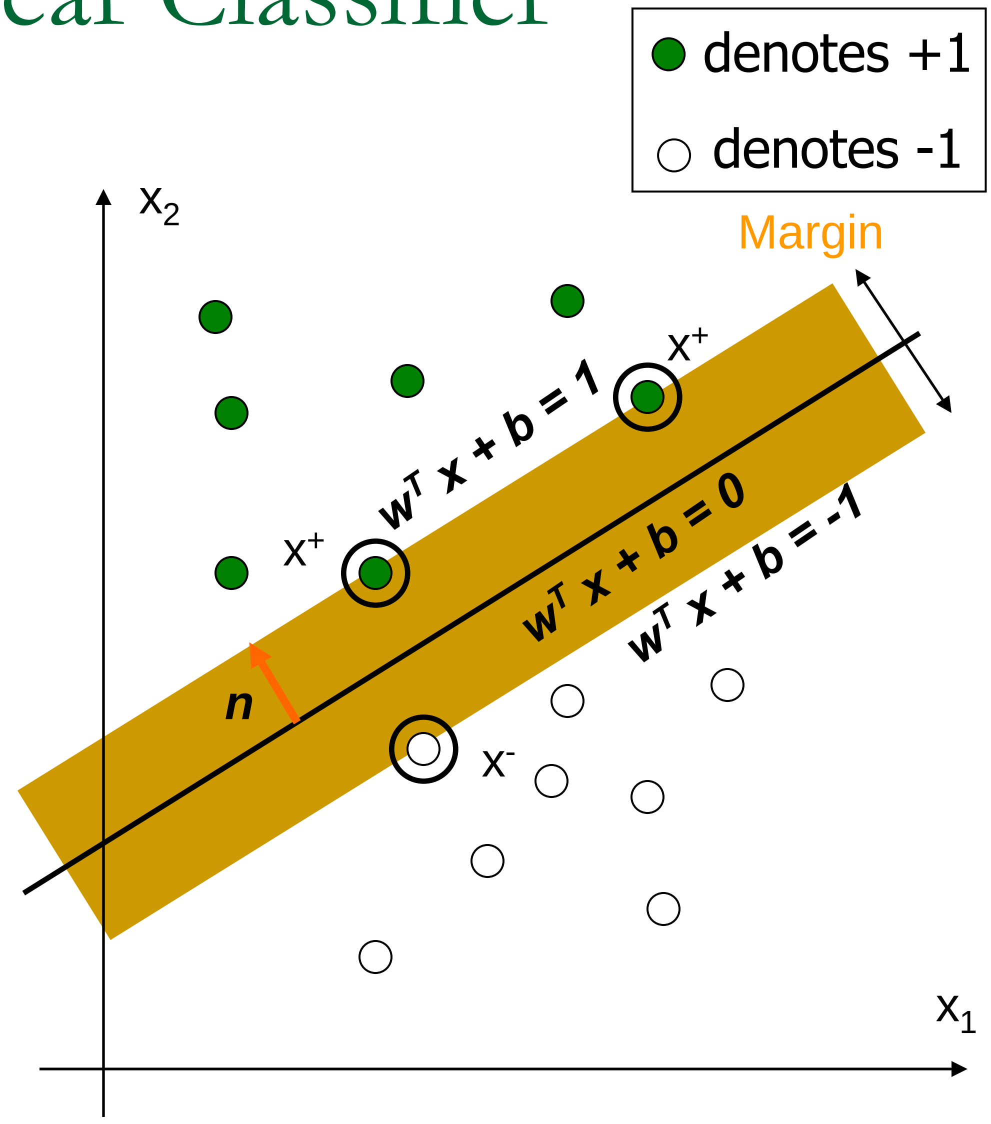
Large Margin Linear Classifier

- Formulation:

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

such that

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



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

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

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

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

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

Solving the Optimization Problem

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

s.t. $\alpha_i \geq 0$

Lagrangian Dual Problem

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

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

Solving the Optimization Problem

- From KKT condition, we know:

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

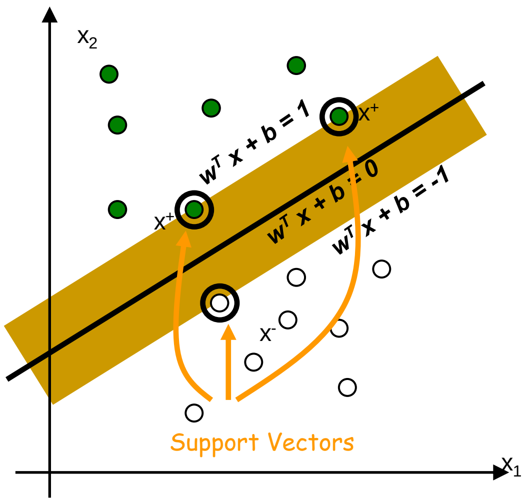
- Thus, only support vectors have $\alpha_i \neq 0$

- 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:

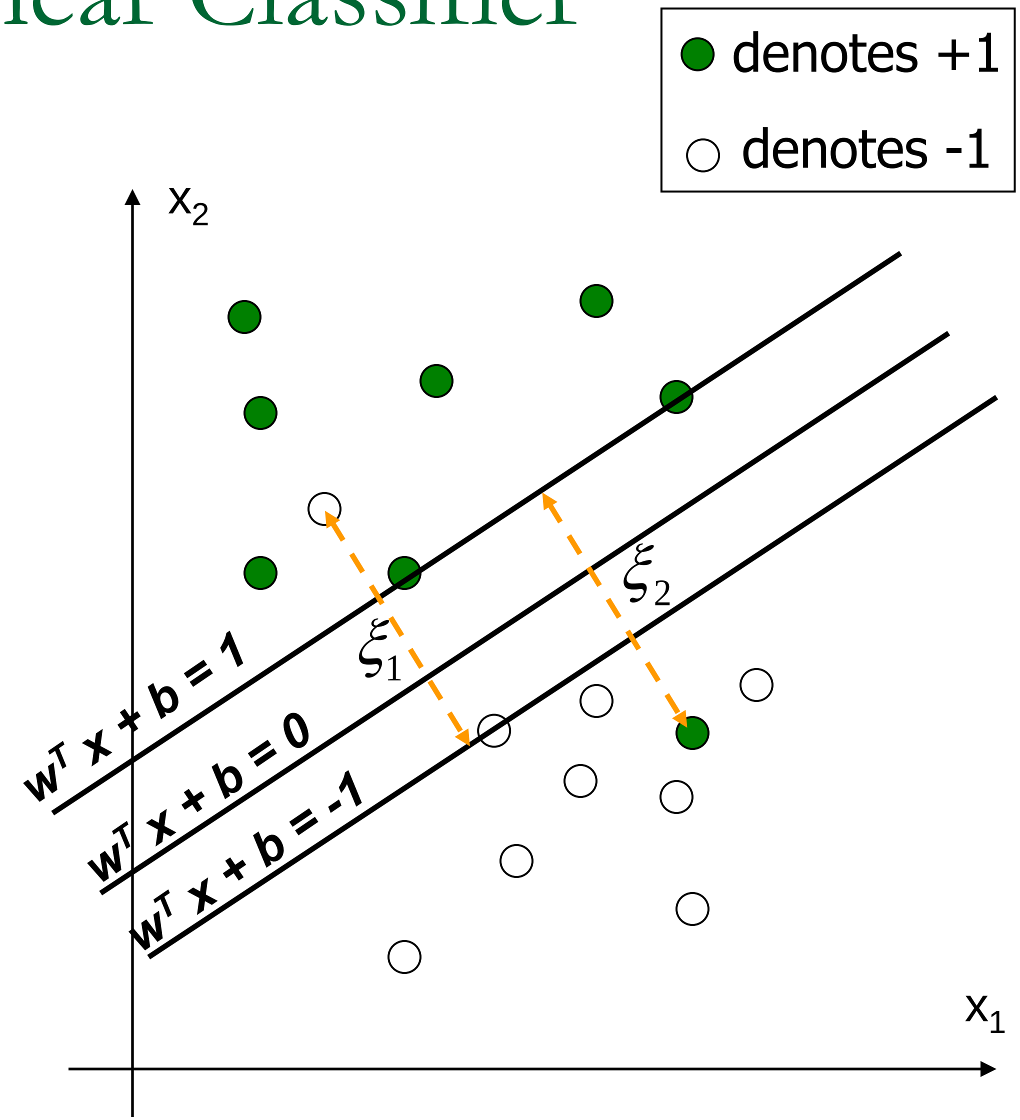
$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = \sum_{i \in \mathrm{SV}} \alpha_i \mathbf{x}_i^T \mathbf{x} + b$$

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

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

$$\xi_i \geq 0$$

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

Large Margin Linear Classifier

- Formulation: (Lagrangian Dual Problem)

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

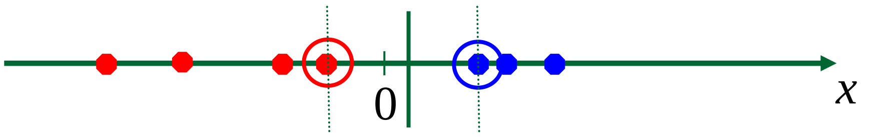
such that

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

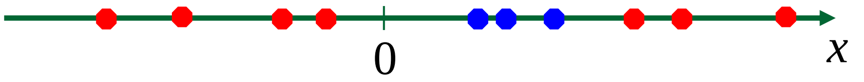
$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

Non-linear SVMs

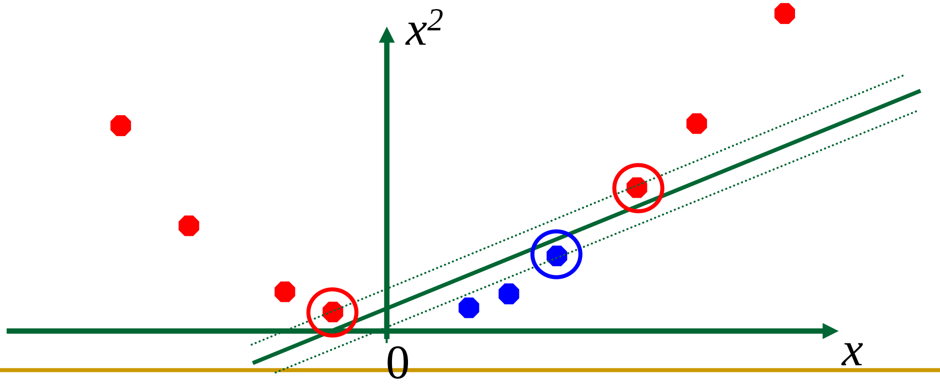
- Datasets that are linearly separable with noise work out great:



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



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



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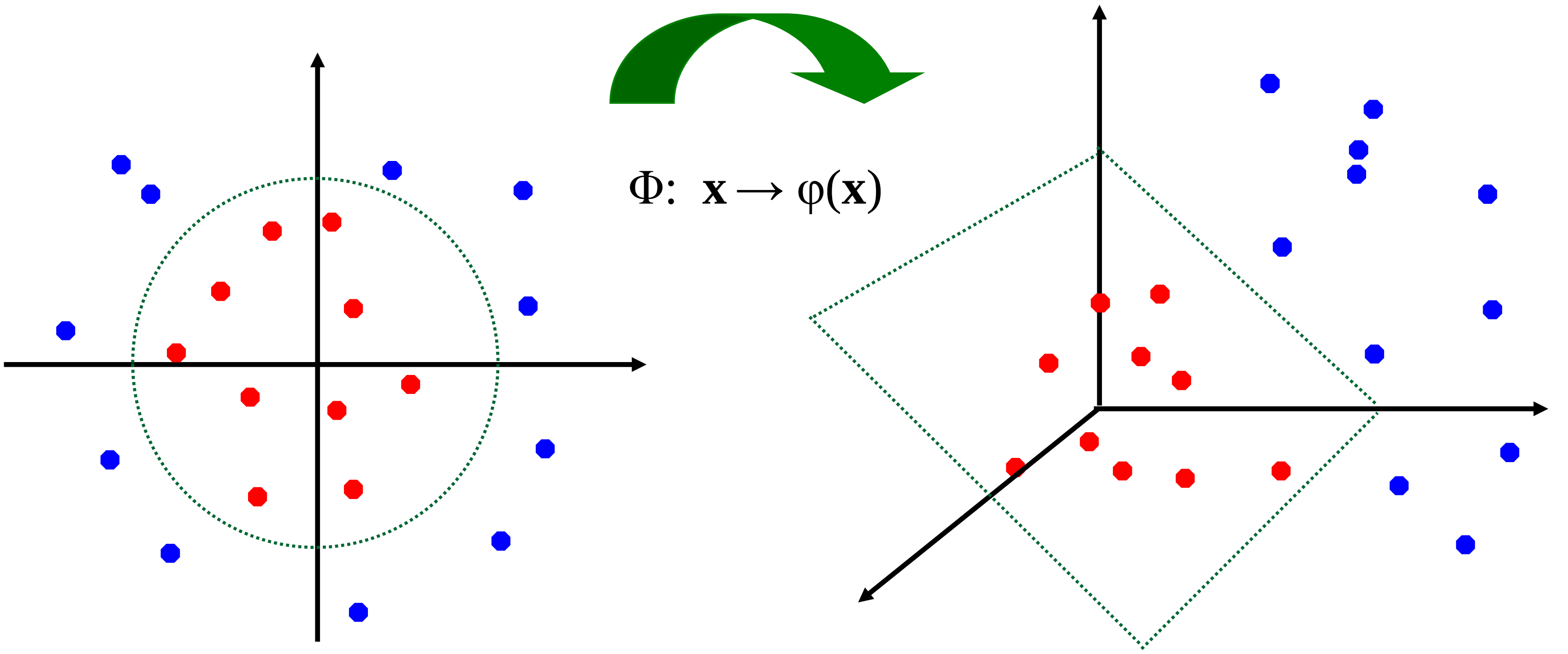
Non-linear SVMs: Feature Space

- 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 $K(\mathbf{x}_i,\mathbf{x}_j) = \varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_j)$:

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

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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.

Nonlinear SVM: Optimization

- Formulation: (Lagrangian Dual Problem)

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

such that

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

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

- The solution of the discriminant function is

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

- 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

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/