An Introduction to Support Vector Machine

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

Outline

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

Linear Discriminant Function

- g(x) is a linear function:

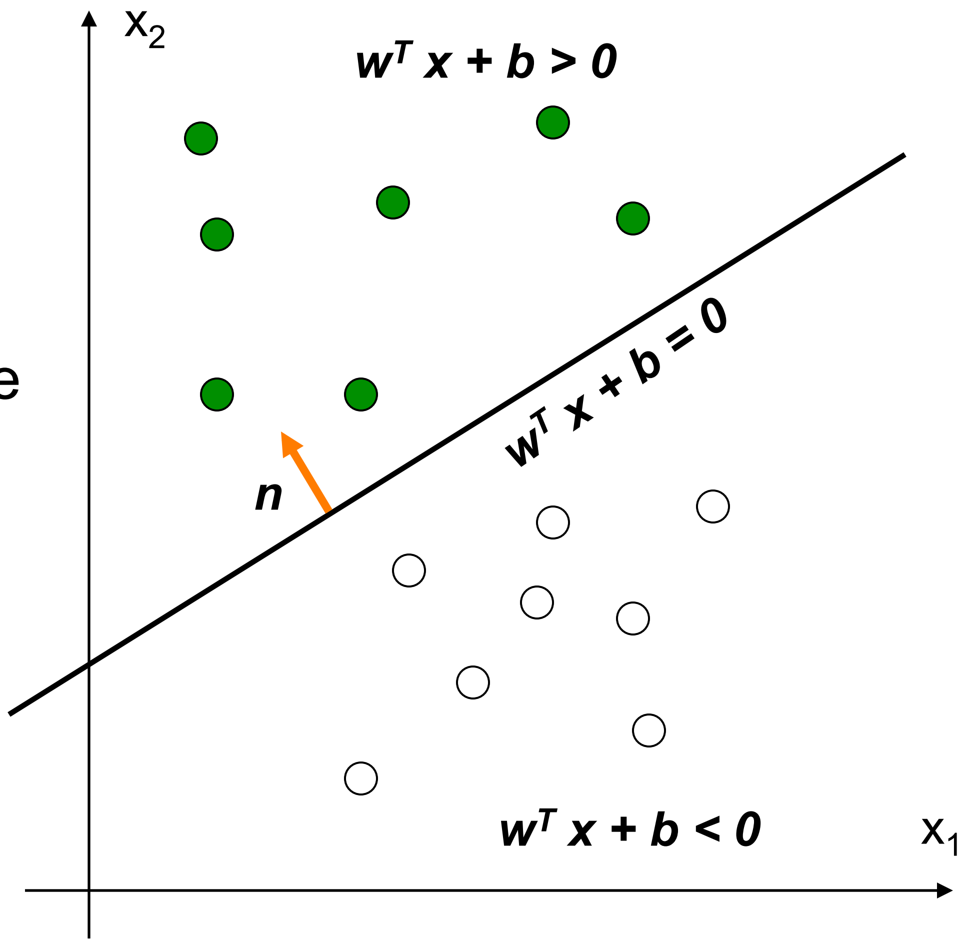
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$

- A hyper-plane in the feature space

$$\boldsymbol{w}^T \boldsymbol{x} + b = 0$$

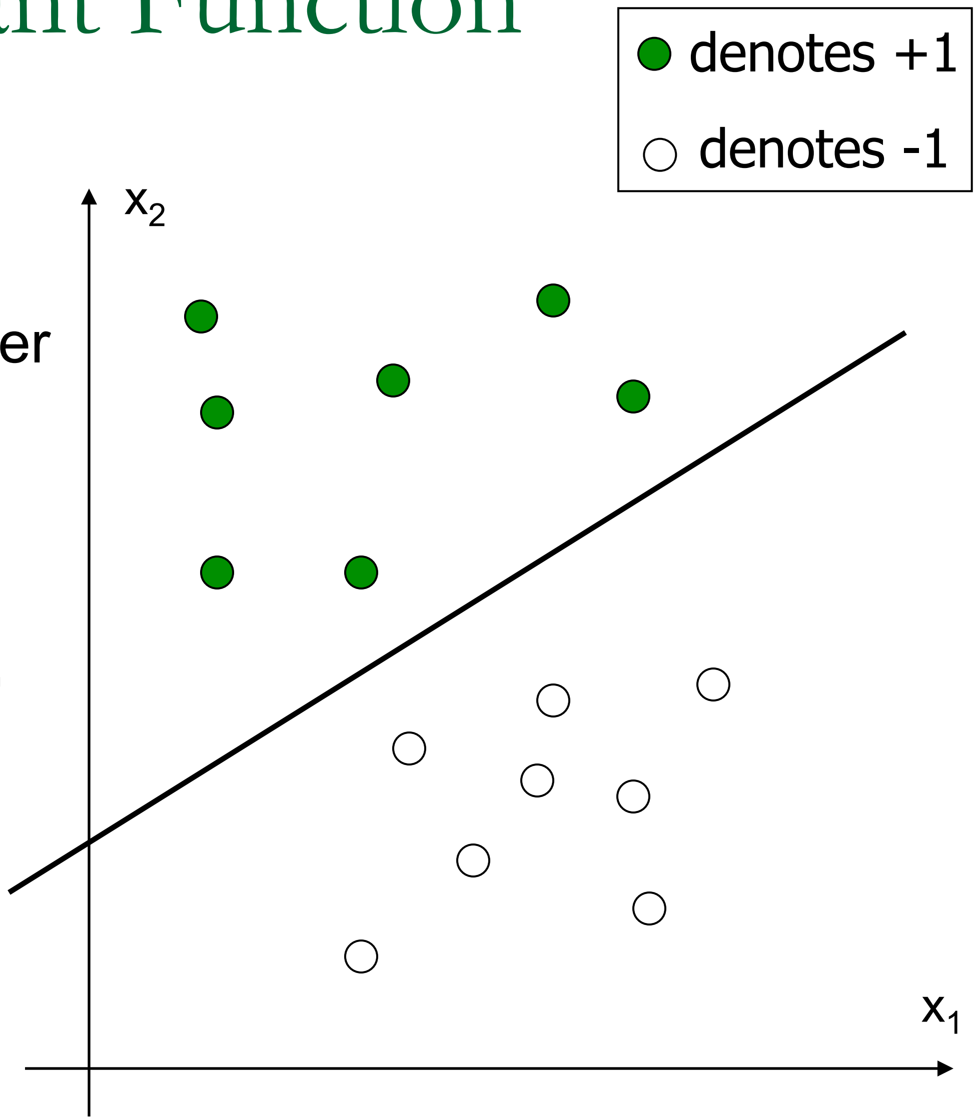
- (Unit-length) normal vector of the hyper-plane:

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



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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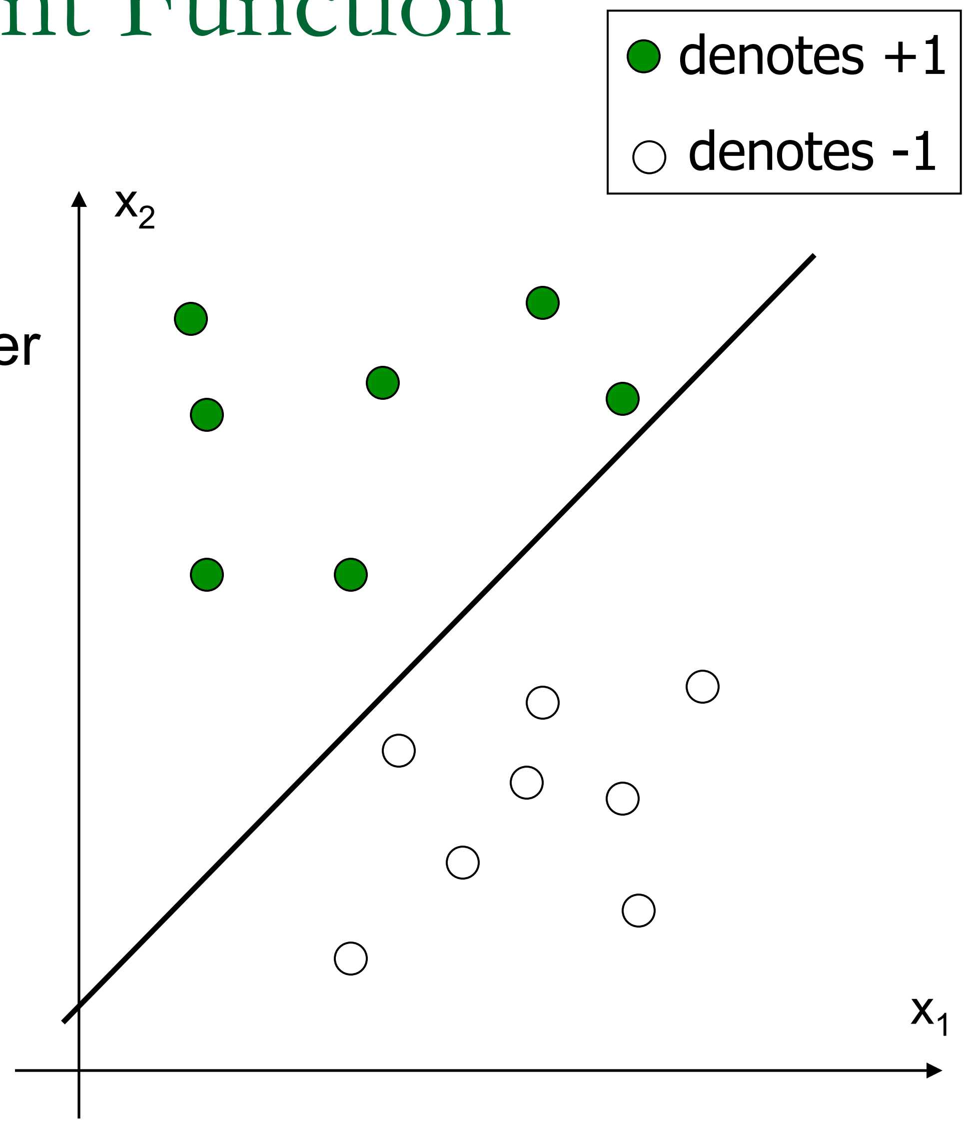

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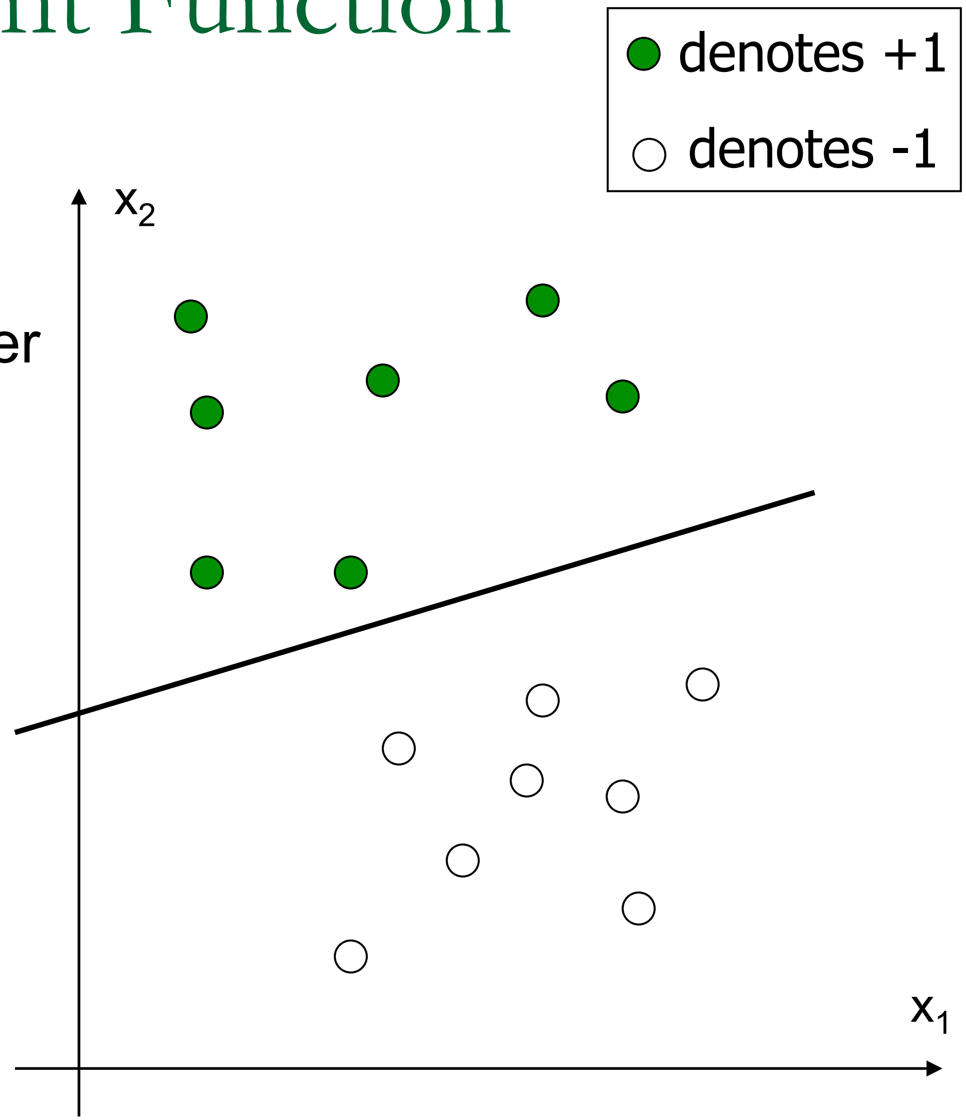
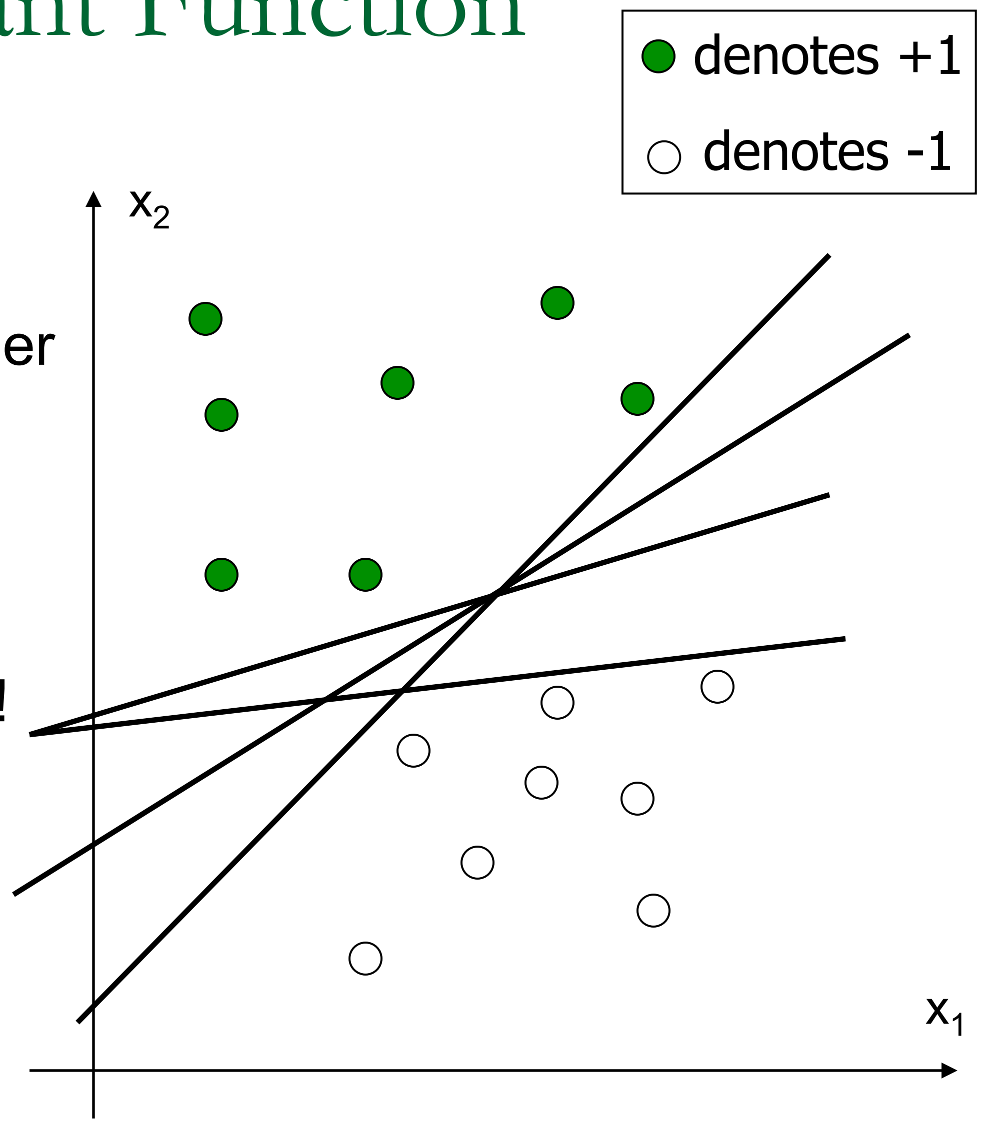


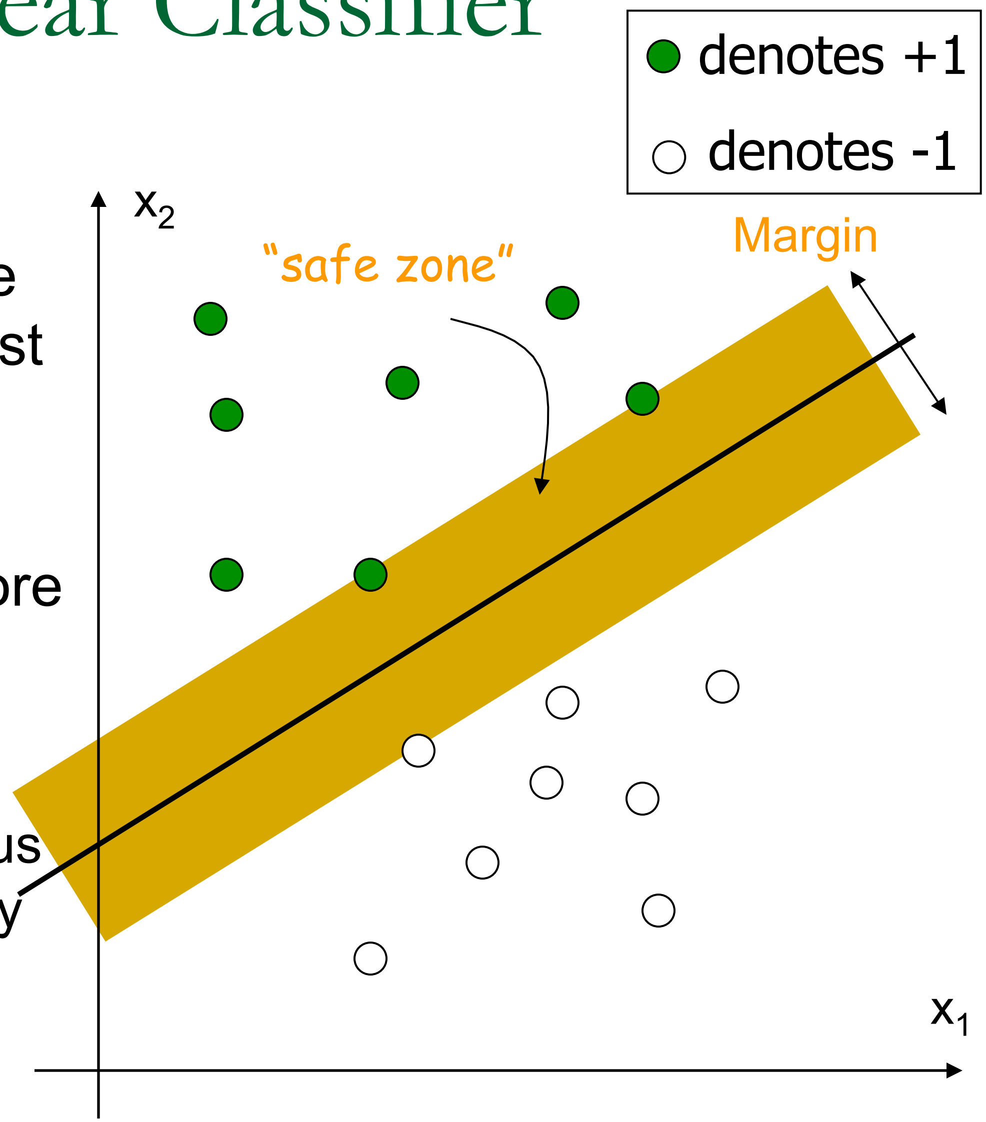
Linear Discriminant Function



- 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
  - Good according to PAC (Probably Approximately Correct) theory.

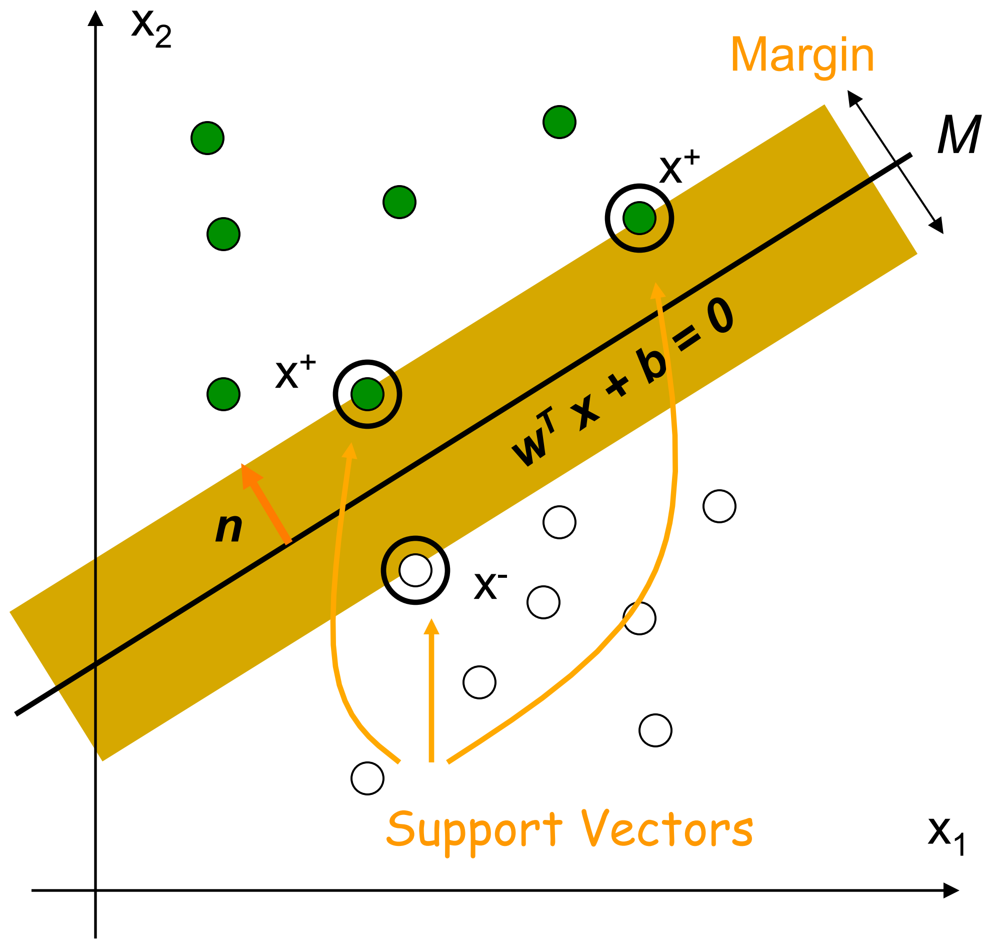


Maximum Margin Classification

- Distance from point $\mathbf{x}_i$ to the hyperplane is:

$$r = \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|}$$

- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** *M* of the classifier is the distance between support vectors on both sides.
- Only support vectors matter; other training points are ignorable.



Large Margin Linear Classifier

- Given a set of data points:

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

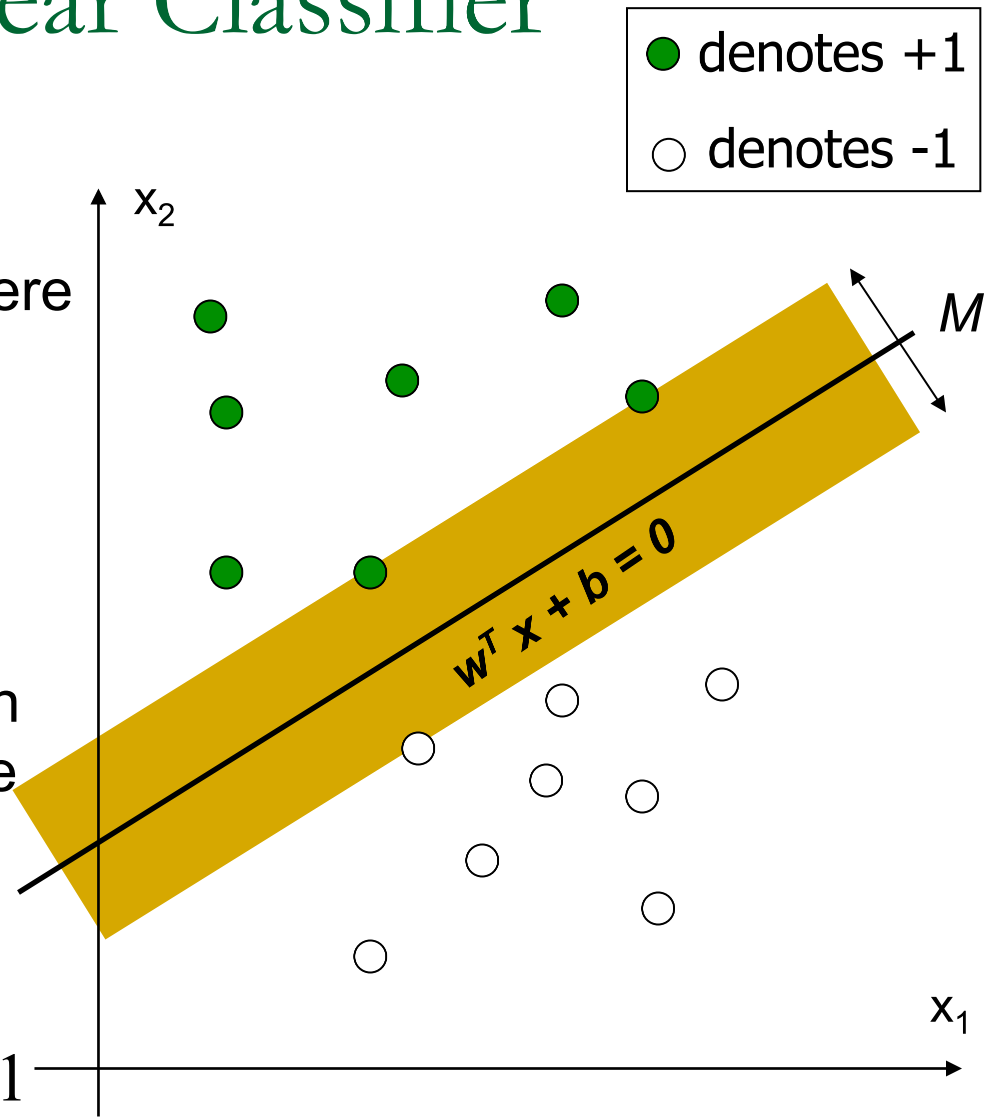
  $\boldsymbol{w}^T\mathbf{x}_i + b \geq M/2$ if $y_i = +1$

  $\boldsymbol{w}^T\mathbf{x}_i + b \leq -M/2$ if $y_i = -1$

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

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

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



Large Margin Linear Classifier

- We know that

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

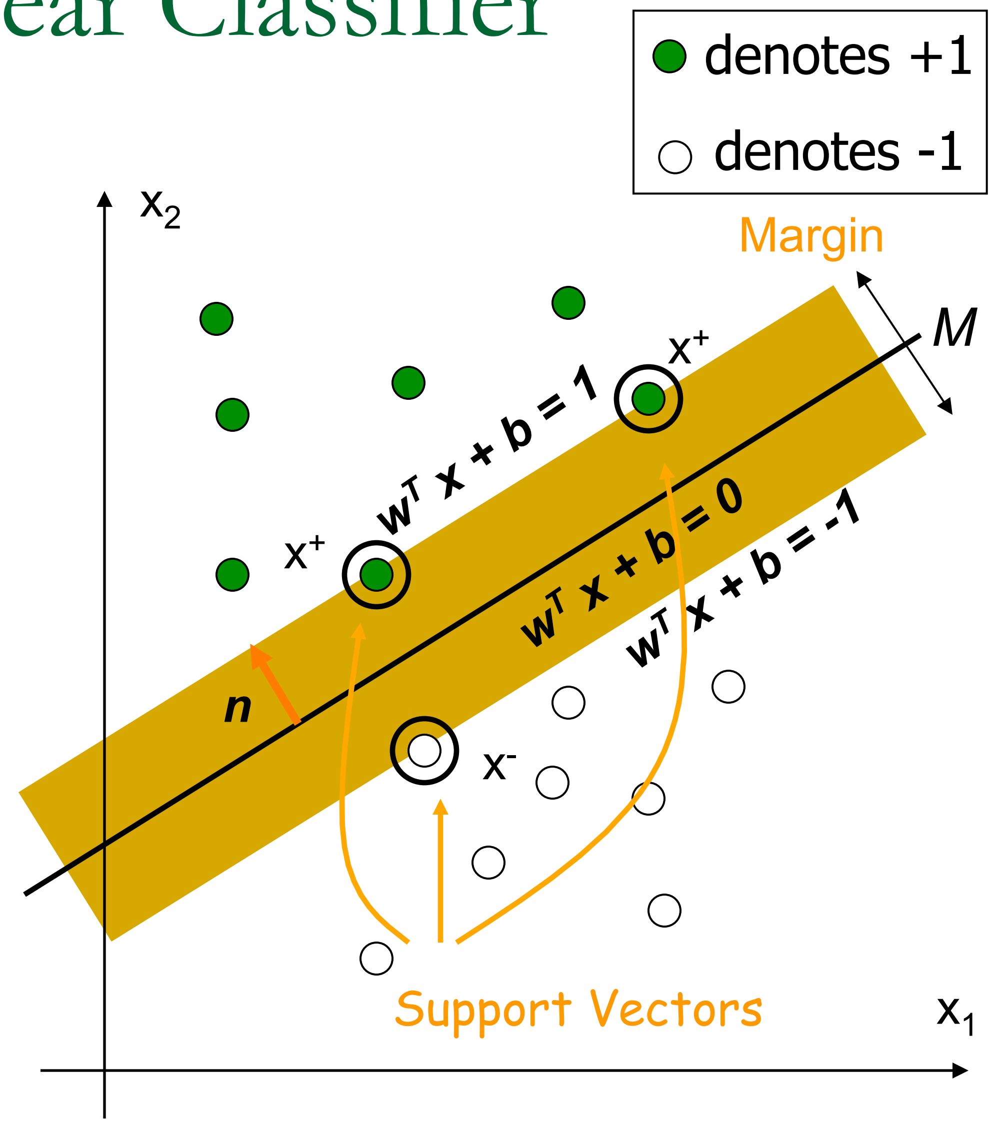
$$\mathbf{w}^T\mathbf{x}^- + b = -1$$

Thus $\mathbf{w}^T(\boldsymbol{x}^+ - \boldsymbol{x}^-) = 2$

- 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

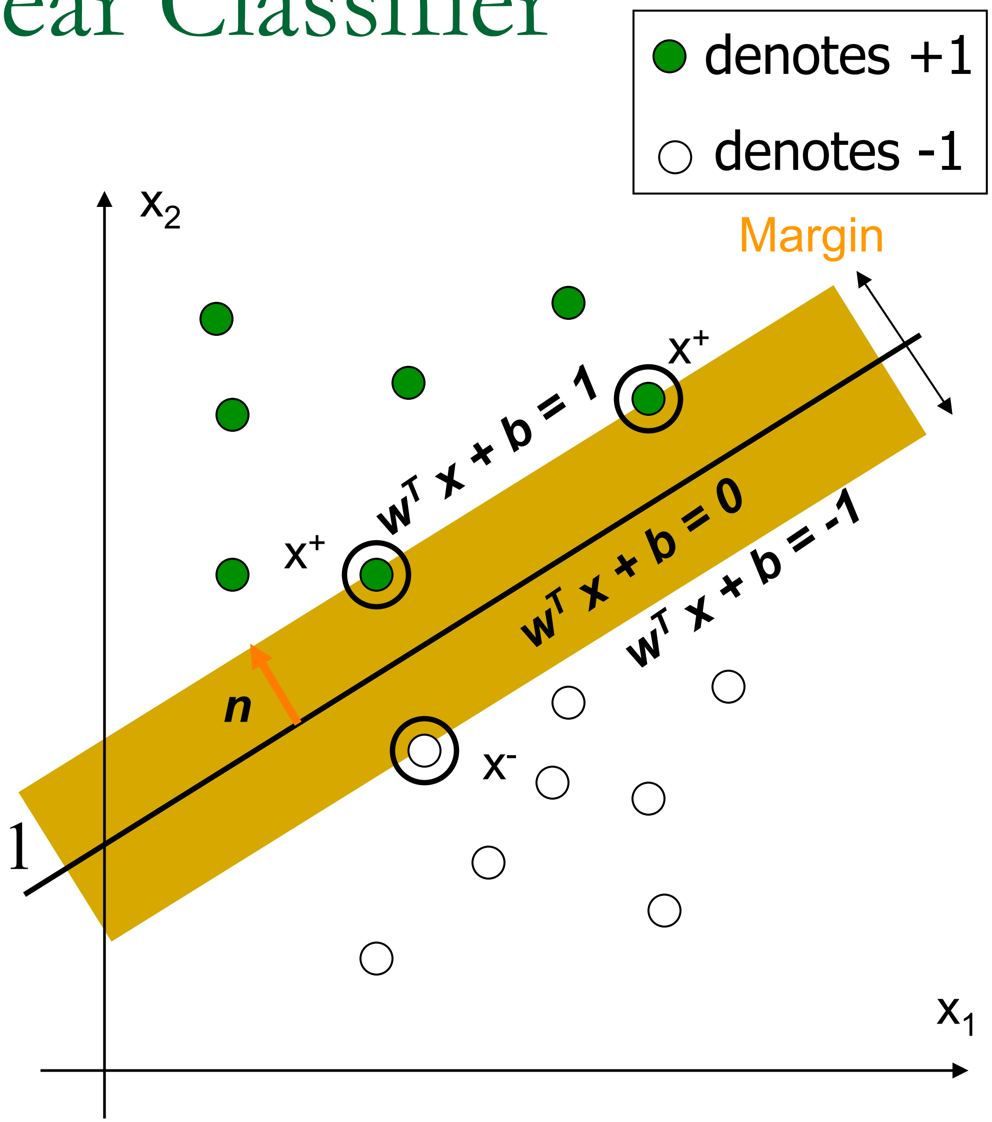
- Formulation:

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

such that

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

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



Large Margin Linear Classifier

- Formulation:

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

such that

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

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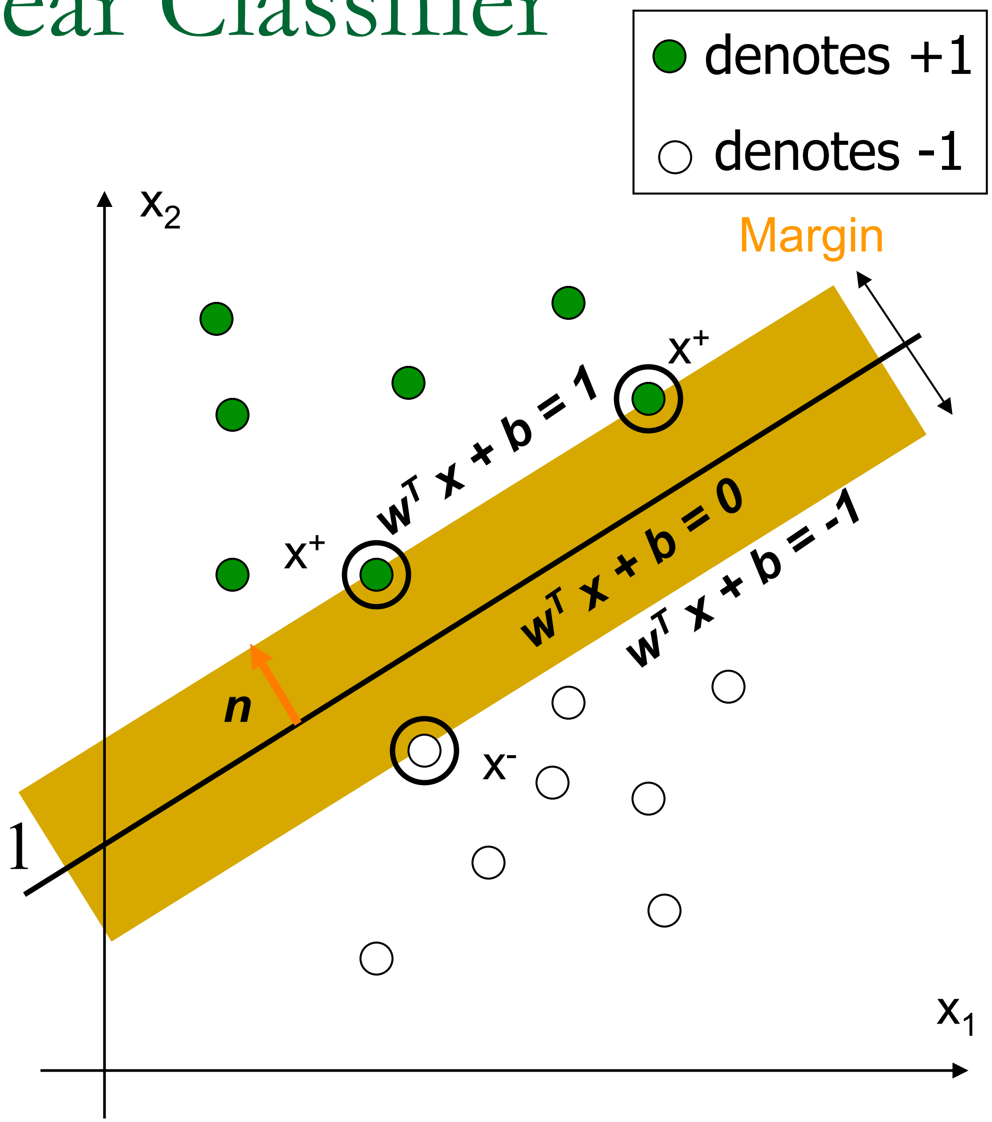


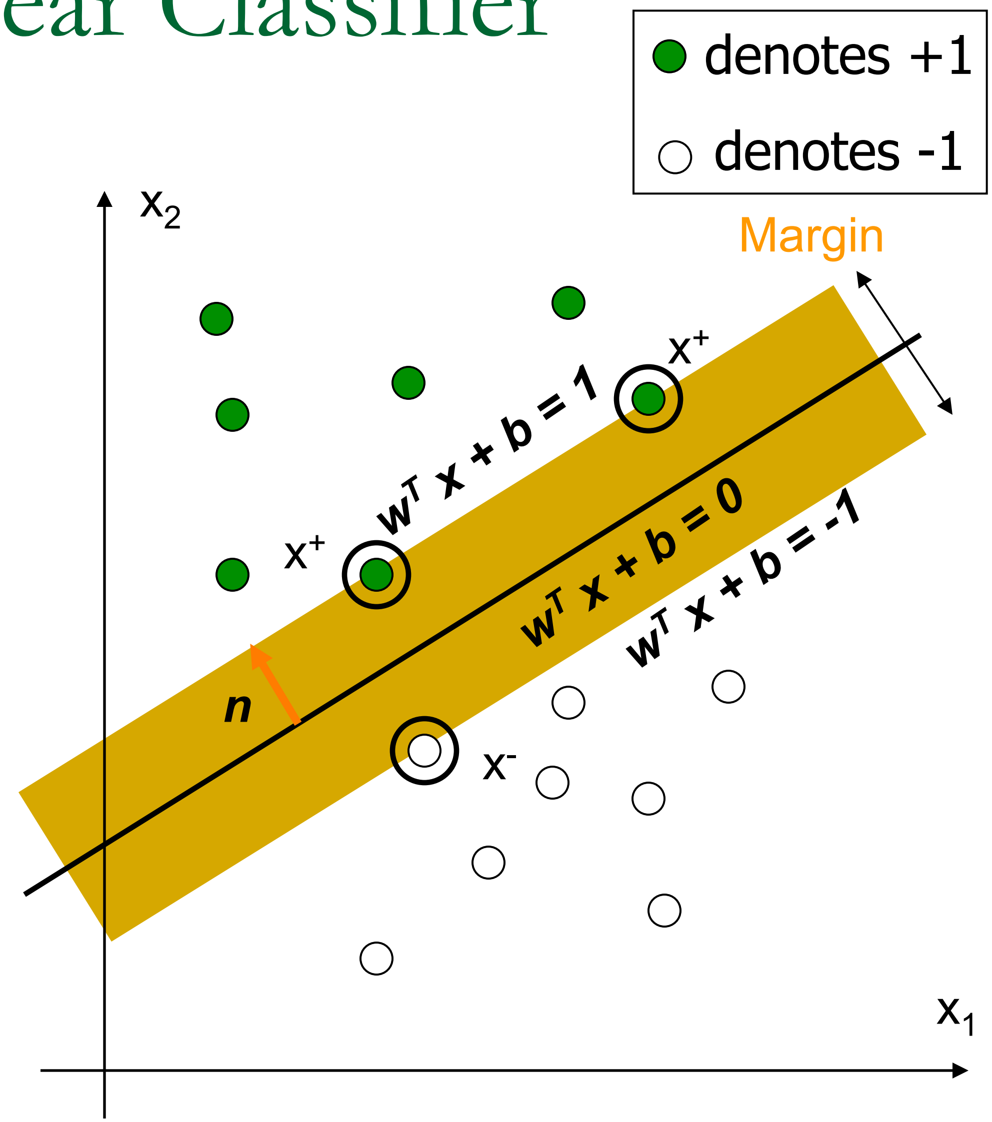
Large Margin Linear Classifier

- 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

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

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

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

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

Solving the Optimization Problem

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

s.t. $\alpha_i \geq 0$

Lagrangian Dual Problem

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

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

Solving the Optimization Problem

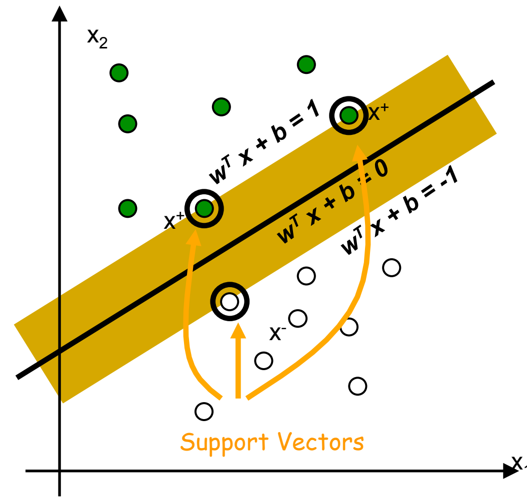
- From KKT (Karush–Kuhn–Tucker) condition, we know:

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

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

- The solution has the form:

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



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

where $\mathbf{x}_k$ is any support vector

Thus, $b = y_k - \Sigma\alpha_i y_i \mathbf{x}_i^T \mathbf{x}_k$ for any $\alpha_k > 0$

Solving the Optimization Problem

- The linear discriminant function is:

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

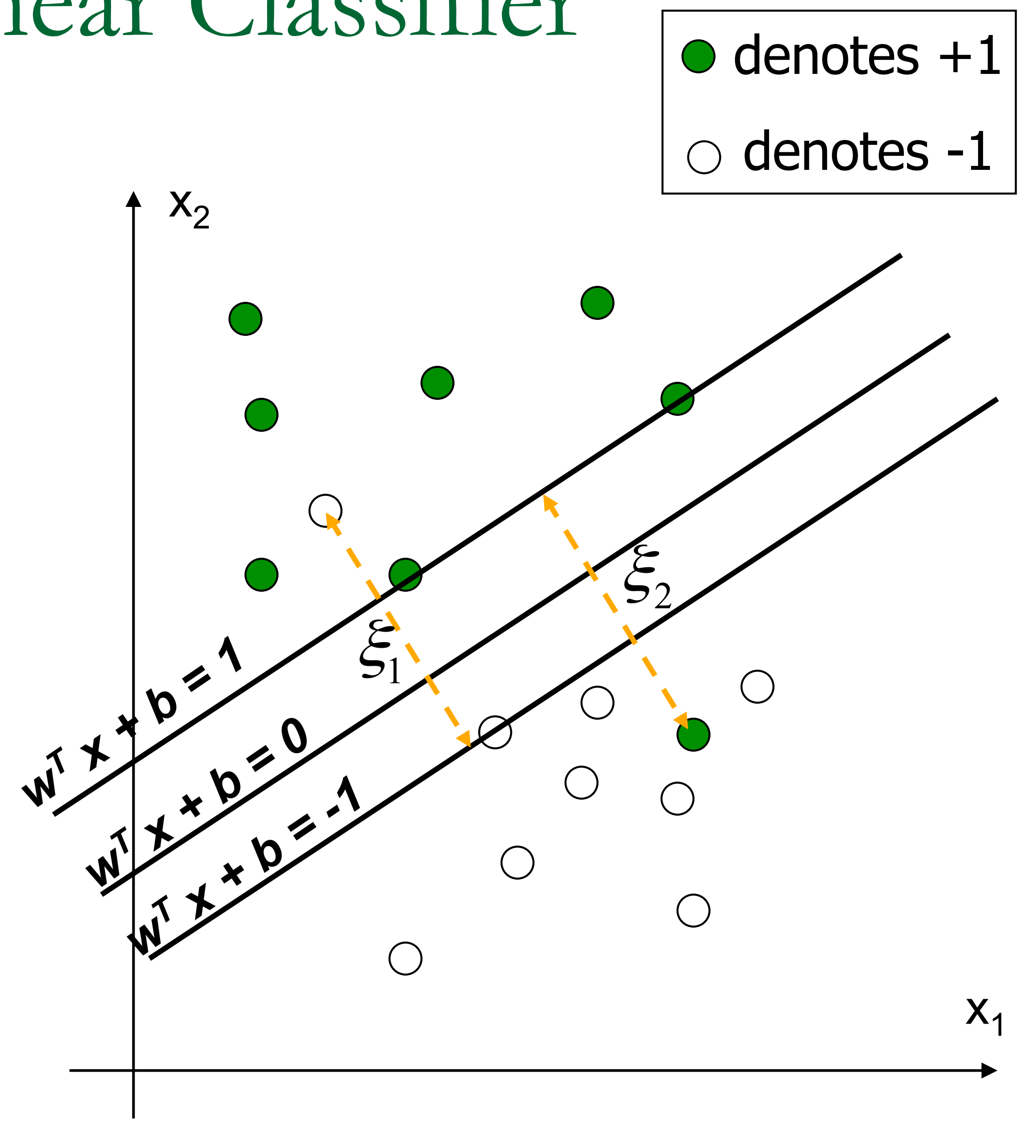
That is, no need to compute **w** explicitly for classification.

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

- Parameter *C* can be viewed as a way to control over-fitting: it "trades off" the relative importance of maximizing the margin and fitting the training data.
  - For large values of C, the optimization will choose a smaller-margin hyperplane if that hyperplane does a better job of getting all the training points classified correctly. Conversely, a very small value of C will cause the optimizer to look for a larger-margin separating hyperplane, even if that hyperplane misclassifies more points.

Solving the Optimization Problem

- 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

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

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

Solving the Optimization Problem

- Again, $\mathbf{x}_i$ with non-zero α_i will be support vectors.
- Solution to the dual problem is:

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

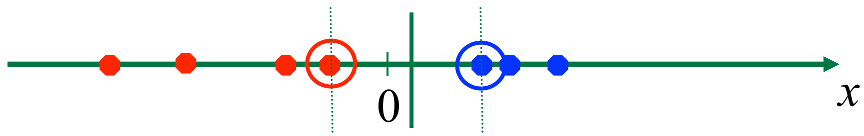
$b = y_k(1 - \xi_k) - \Sigma \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_k$ for any k s.t. $\alpha_k > 0$

Again, we don't need to compute **w** explicitly for classification:

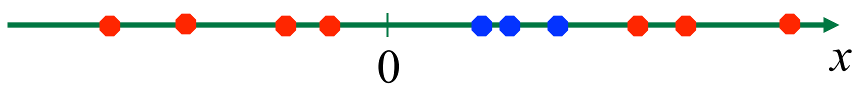
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{i \in \mathrm{SV}} \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

Non-linear SVMs

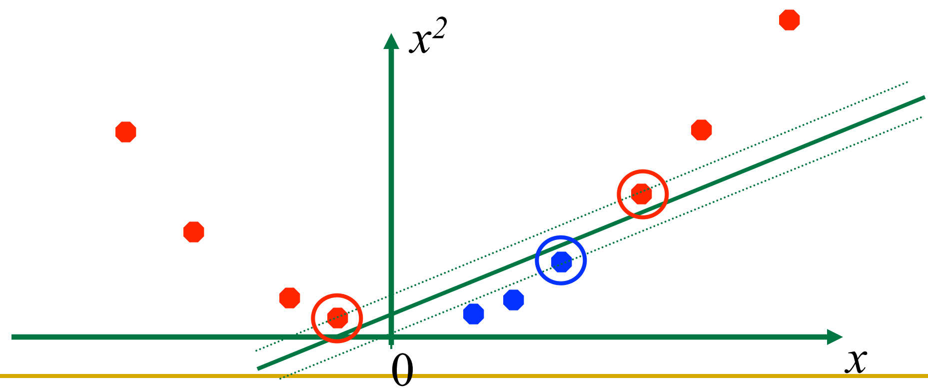
- Datasets that are linearly separable with noise work out great:



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

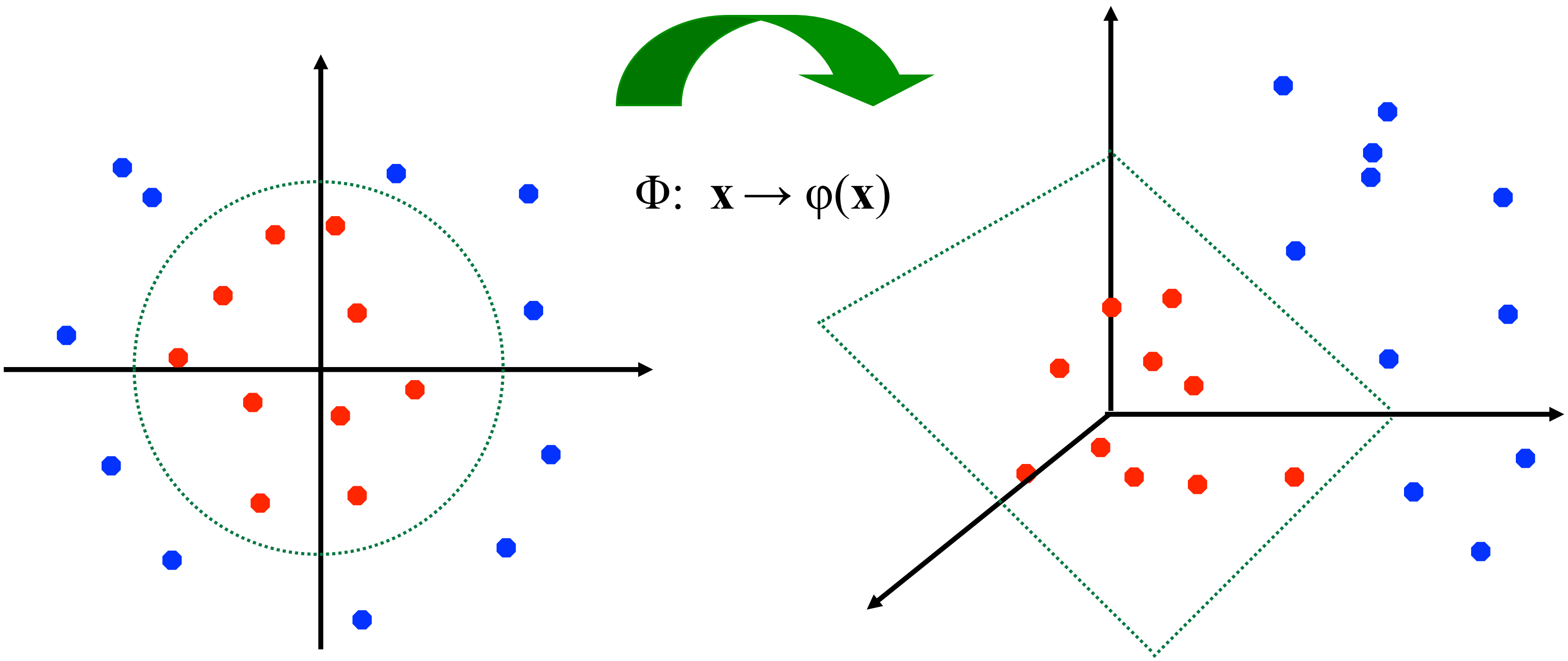


- How about… mapping data to a higher-dimensional space:



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:

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

- 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:

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

Mercer's theorem: ***Every semi-positive definite symmetric function is a kernel.***

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

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

- 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.

Demo of LibSVM

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

References on SVM and Stock Prediction

http://www.svms.org/finance/HuangNakamoriWang2005.pdf

http://cs229.stanford.edu/proj2012/ShenJiangZhang-StockMarketForecastingusingMachineLearningAlgorithms.pdf

http://research.ijcaonline.org/volume41/number3/pxc3877555.pdf

and other references online …