Support Vector Machines (SVM)

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SVM

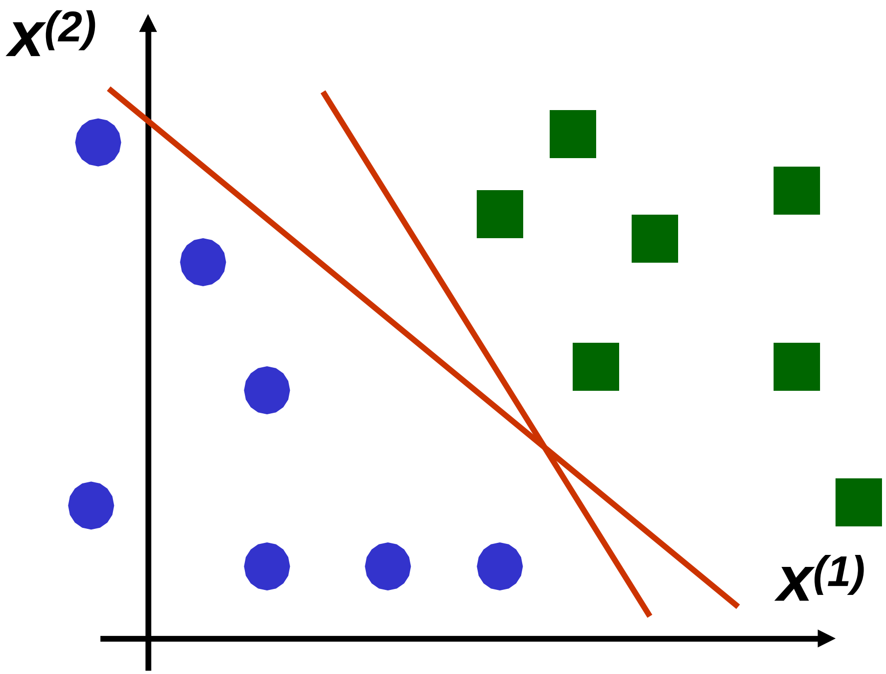
- Said to start in 1979 with Vladimir Vapnik's paper
- Major developments throughout 1990's
- Elegant theory
  - Has good generalization properties
- Have been applied to diverse problems very successfully in the last 10-15 years
- One of the most important developments in pattern recognition in the last 15 years

Linear Discriminant Functions

- A discriminant function is linear if it can be written as

$$g(x) = w^t x + w_0$$

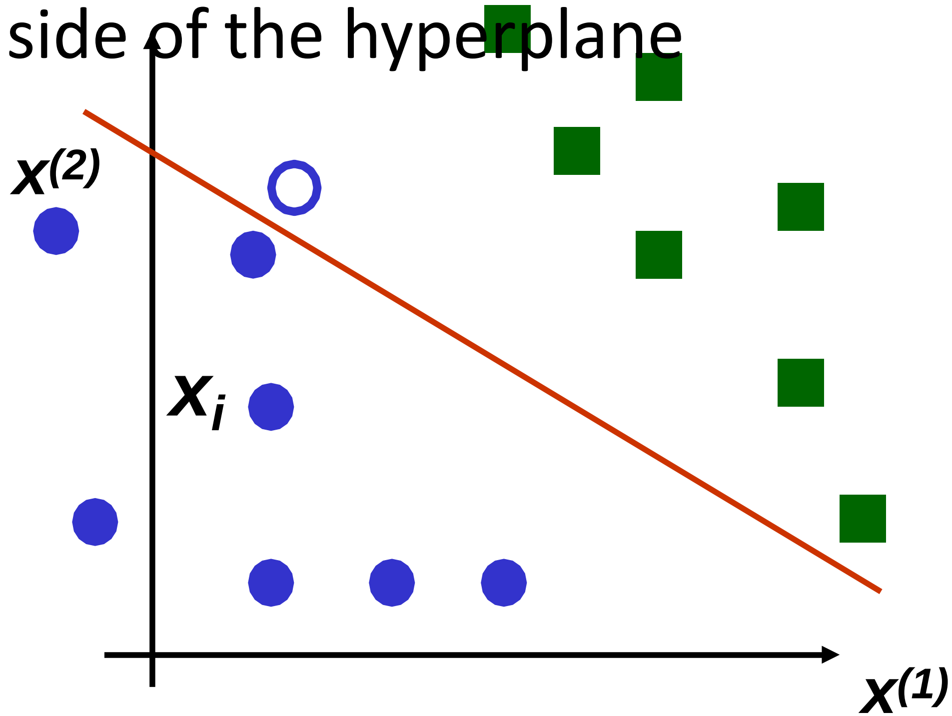
$$\boxed{\begin{array}{ll} g(x) > 0 & \Rightarrow x \in class\ 1 \\ g(x) < 0 & \Rightarrow x \in class\ 2 \end{array}}$$



- which separating hyperplane should we choose?

Linear Discriminant Functions

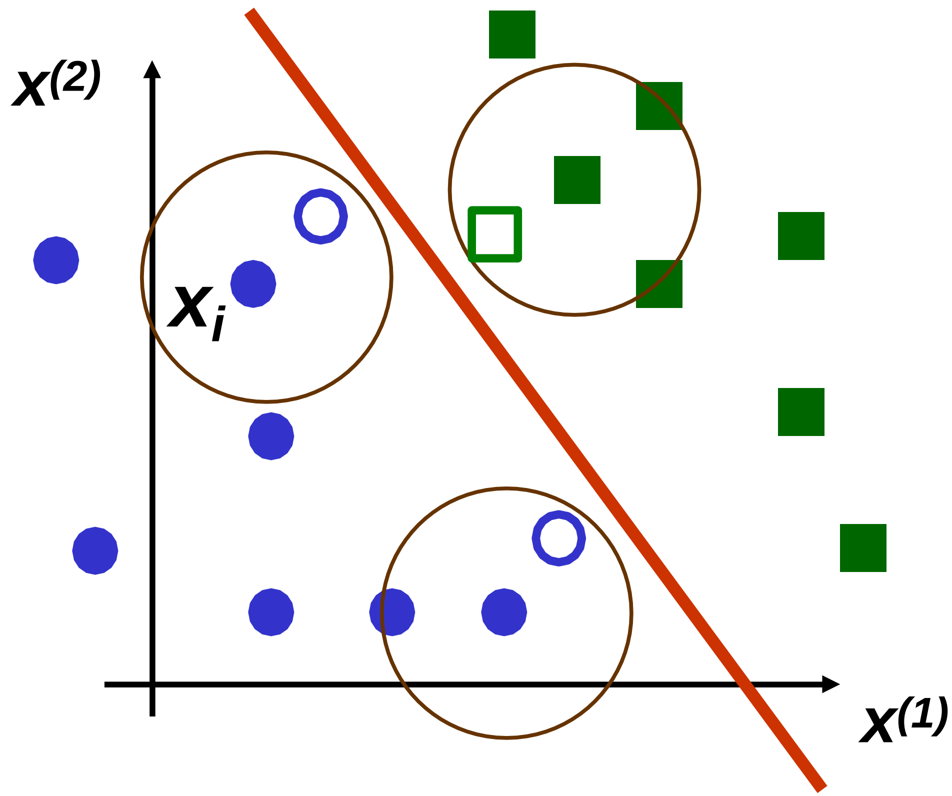
- Training data is just a subset of of all possible data
- Suppose hyperplane is close to sample $\boldsymbol{x}_i$
- If we see new sample close to sample $\boldsymbol{i}$, it is likely to be on the wrong side of the hyperplane



- Poor generalization (performance on unseen data)

Linear Discriminant Functions

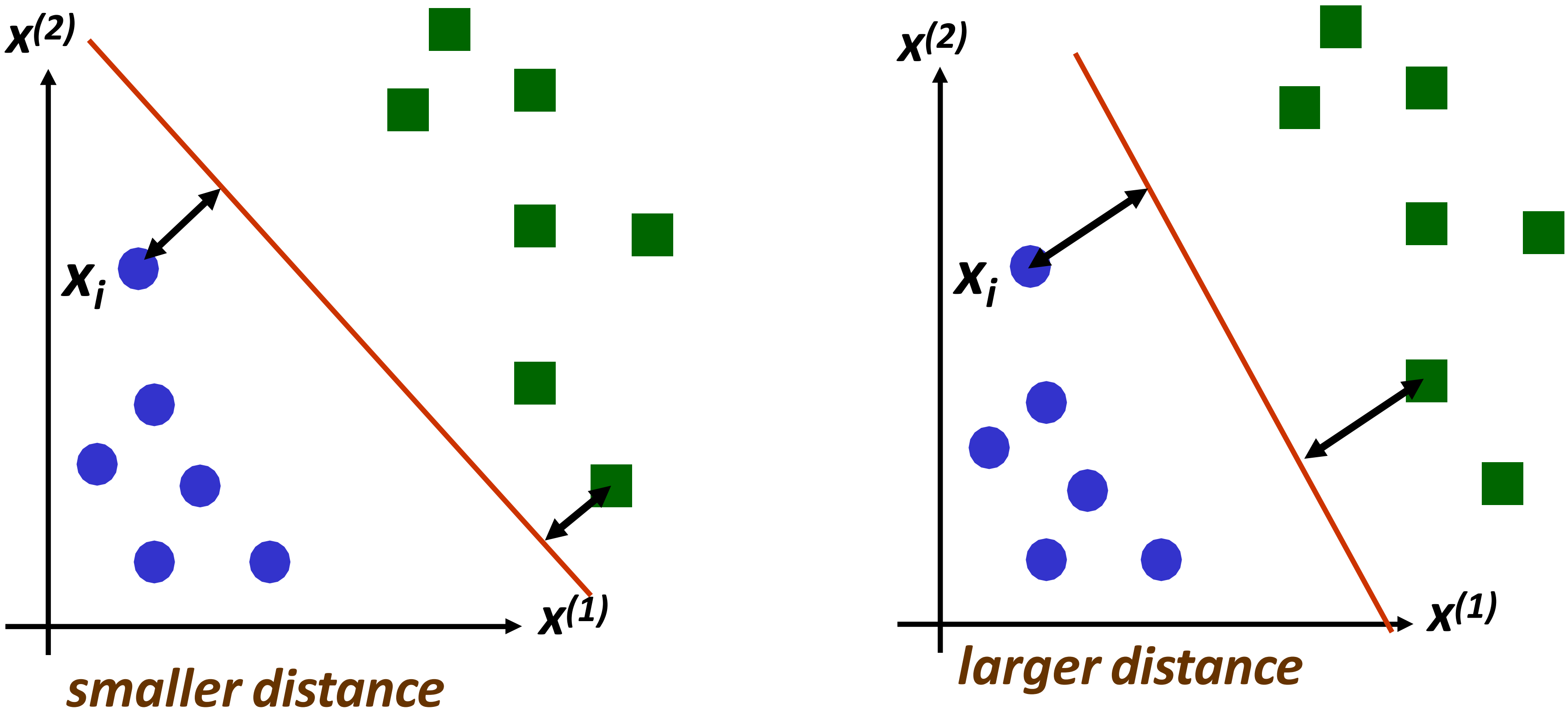
- Hyperplane as far as possible from any sample



- New samples close to old samples will be classified correctly
- Good generalization

SVM

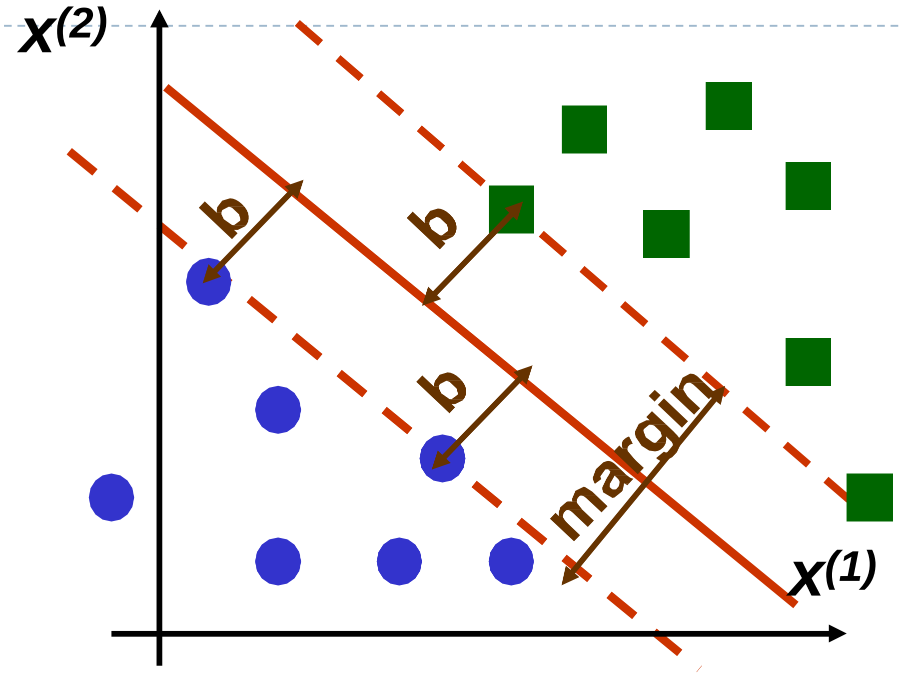
- Idea: maximize distance to the closest example



- For the optimal hyperplane
  - distance to the closest negative example = distance to the closest positive example

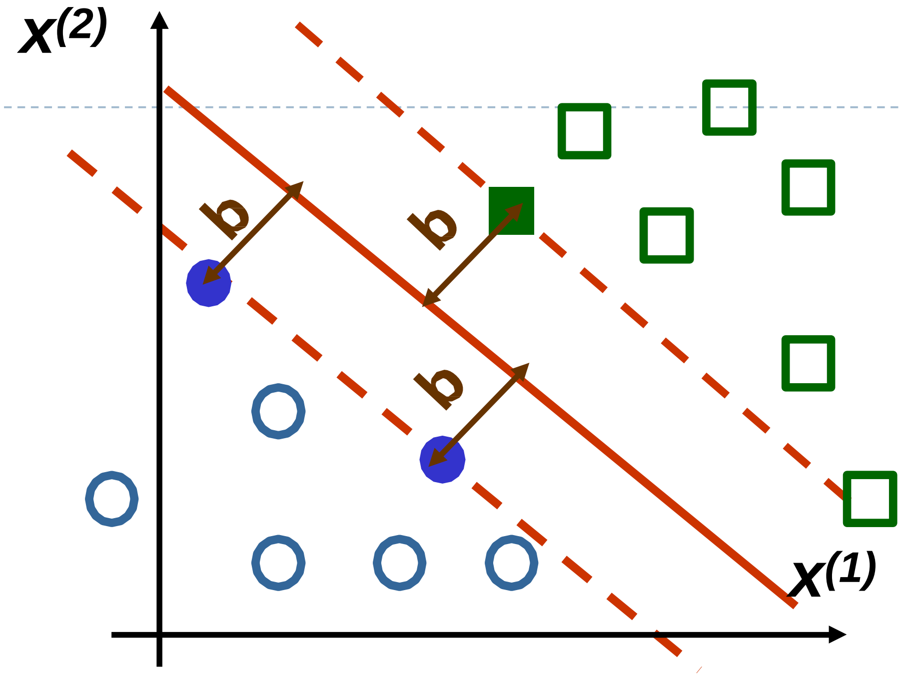
SVM: Linearly Separable Case

- SVM: maximize the ***margin***



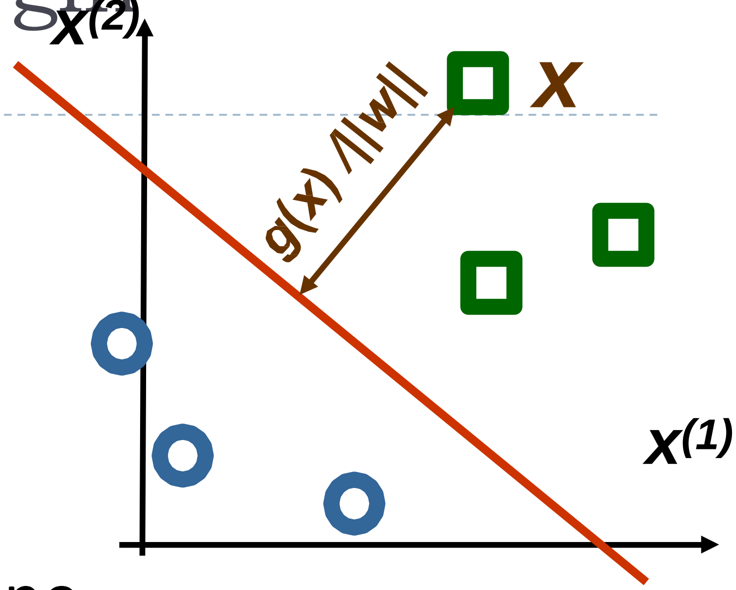
- ***margin*** is twice the absolute value of distance ***b*** of the closest example to the separating hyperplane
- Better generalization (performance on test data)
  - in practice
  - and in theory

SVM: Linearly Separable Case



- ***Support vectors*** are samples closest to separating hyperplane
  - they are the most difficult patterns to classify
  - Optimal hyperplane is completely defined by support vectors
    - of course, we do not know which samples are support vectors without finding the optimal hyperplane

SVM: Formula for the Margin



- $g(x) = w^t x + w_0$
- absolute distance between x and the boundary $g(x) = 0$

$$\frac{|w^t x + w_0|}{\|w\|}$$

- distance is unchanged for hyperplane $g_1(x) = \alpha\, g(x)$

$$\frac{|\alpha w^t x + \alpha w_0|}{\|\alpha w\|} = \frac{|w^t x + w_0|}{\|w\|}$$

- Let x_i be an example closest to the boundary. Set

$$|w^t x_i + w_0| = 1$$

- Now the largest margin hyperplane is unique

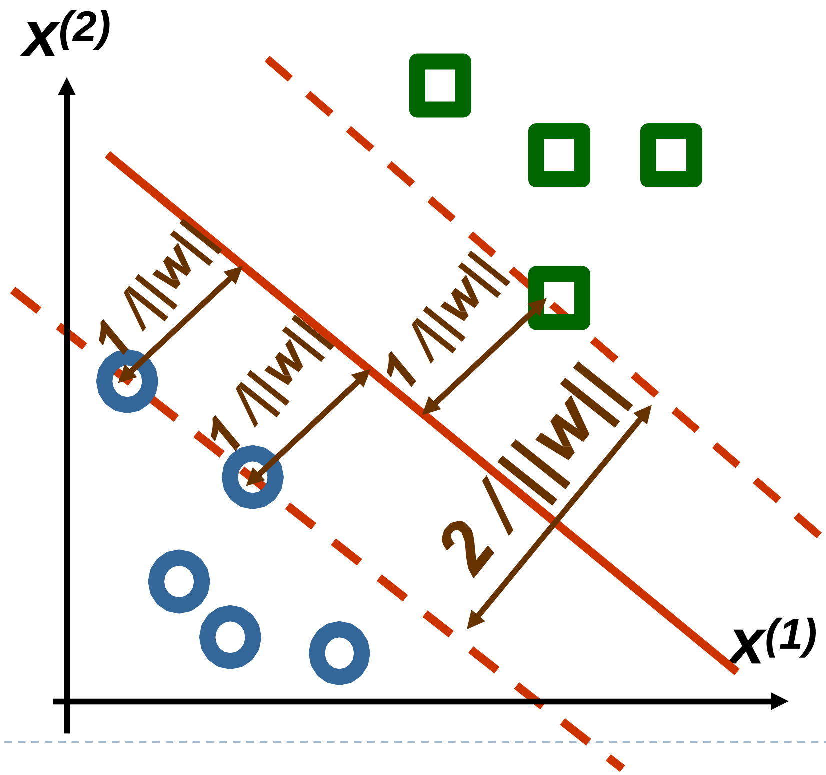
SVM: Formula for the Margin

- For uniqueness, set $\left|w^t x_i + w_0\right| = 1$ for any example x_i closest to the boundary
- now distance from closest sample x_i to $g(x) = 0$ is

$$\frac{\left|w^t x_i + w_0\right|}{\|w\|} = \frac{1}{\|w\|}$$

- Thus the margin is

$$\boxed{m = \frac{2}{\|w\|}}$$



SVM: Optimal Hyperplane

- Maximize margin $\quad m = \dfrac{2}{\|w\|}$
  - subject to constraints

$$\begin{cases} w^t x_i + w_0 \geq 1 & \text{if } x_i \text{ is positive example} \\ w^t x_i + w_0 \leq -1 & \text{if } x_i \text{ is negative example} \end{cases}$$

- Let $\begin{cases} z_i = 1 & \text{if } x_i \text{ is positive example} \\ z_i = -1 & \text{if } x_i \text{ is negative example} \end{cases}$
- Can convert our problem to

$$\boxed{\begin{array}{ll} \text{minimize} & J(w) = \frac{1}{2}\|w\|^2 \\ \text{constrained to} & z_i\left(w^t x_i + w_0\right) \geq 1 \quad \forall i \end{array}}$$

- ***J***(***w***) is a quadratic function, thus there is a single global minimum

SVM: Optimal Hyperplane

- Use Kuhn-Tucker theorem to convert our problem to:

$$\boxed{\begin{array}{ll} \text{maximize} & L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j x_i^t x_j \\ \text{constrained to} & \alpha_i \geq 0 \quad \forall i \quad \text{and} \quad \sum_{i=1}^{n} \alpha_i z_i = 0 \end{array}}$$

- $\alpha = \{\alpha_1, \ldots, \alpha_n\}$ are new variables, one for each sample
- Can rewrite $L_D(\alpha)$ using n by n matrix H:

$$L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix}^t H \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix}$$

  - where the value in the ith row and jth column of H is
$$H_{ij} = z_i z_j x_i^t x_j$$

SVM: Optimal Hyperplane

- Use Kuhn-Tucker theorem to convert our problem to:

$$\text{maximize} \quad L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j x_i^t x_j$$

$$\text{constrained to} \quad \alpha_i \geq 0 \quad \forall i \quad \textbf{and} \quad \sum_{i=1}^{n} \alpha_i z_i = 0$$

- $\alpha = \{\alpha_1, \ldots, \alpha_n\}$ are new variables, one for each sample
- $L_D(\alpha)$ can be optimized by quadratic programming
- $L_D(\alpha)$ formulated in terms of α
  - depends on w and w_0

SVM: Optimal Hyperplane

- After finding the optimal $\alpha = \{\alpha_1, \ldots, \alpha_n\}$
  - For every sample i, one of the following must hold
    - $\alpha_i = 0$ (sample i is not a support vector)
    - $\alpha_i \neq 0$ and $z_i(w^t x_i + w_0 - 1) = 0$ (sample i is support vector)
  - can find w using $w = \sum_{i=1}^{n} \alpha_i z_i x_i$
  - can solve for w_0 using any $\alpha_i > 0$ and $\alpha_i \left[z_i \left(w^t x_i + w_0 \right) - 1 \right] = 0$

$$w_0 = \frac{1}{z_i} - w^t x_i$$

- Final discriminant function:

$$g(x) = \left(\sum_{x_i \in S} \alpha_i z_i x_i \right)^t x + w_0$$

  - where S is the set of support vectors

$$S = \{ x_i \mid \alpha_i \neq 0 \}$$

SVM: Optimal Hyperplane

$$\text{maximize} \quad L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j x_i^t x_j$$

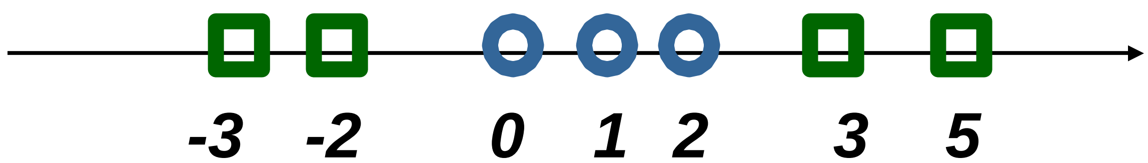
$$\text{constrained to} \quad \alpha_i \geq 0 \quad \forall i \quad \textit{and} \quad \sum_{i=1}^{n} \alpha_i z_i = 0$$

- $L_D(\alpha)$ depends on the number of samples, not on dimension of samples
- samples appear only through the dot products $x_i^t x_j$
- This will become important when looking for a ***nonlinear*** discriminant function, as we will see soon
- Code available on the web to optimize

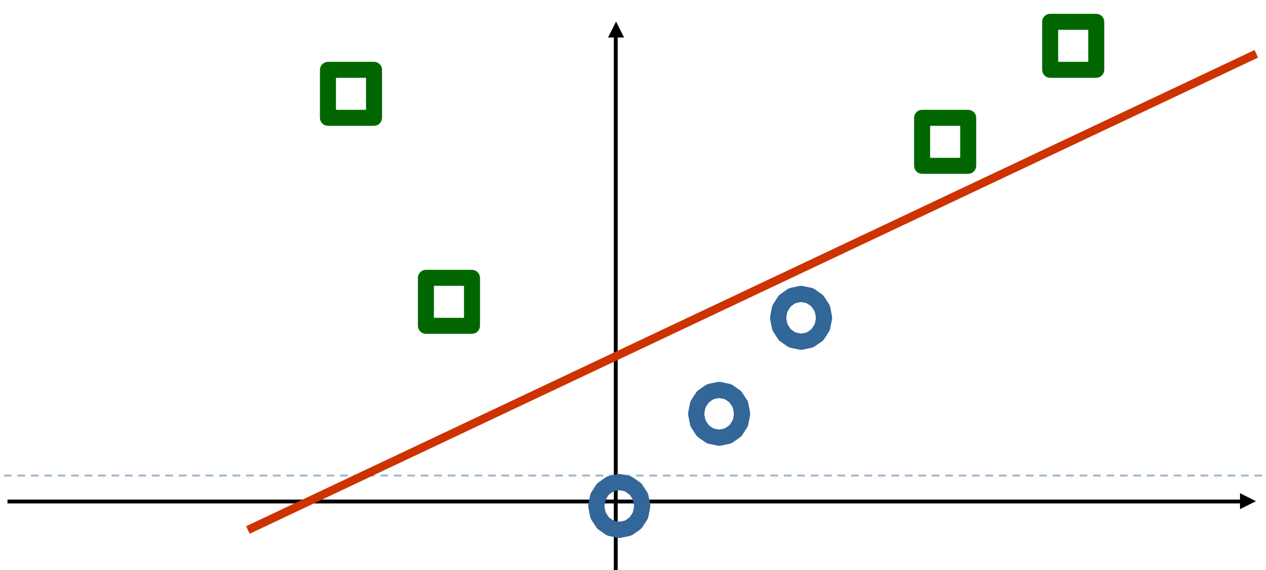
Non Linear Mapping

- Cover's theorem:
  - *"pattern-classification problem cast in a high dimensional space non-linearly is more likely to be linearly separable than in a low-dimensional space"*

- One dimensional space, not linearly separable

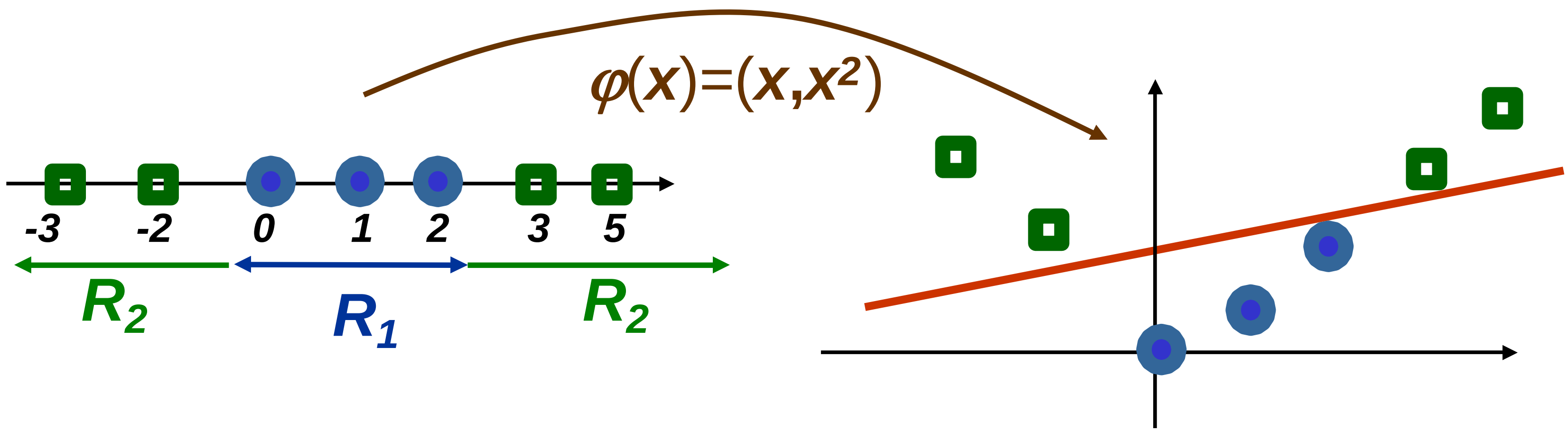


- Lift to two dimensional space with $\varphi(x)=(x,x^2)$



Non Linear Mapping

- To solve a non linear problem with a linear classifier
  1. Project data $\boldsymbol{x}$ to high dimension using function $\varphi(\boldsymbol{x})$
  2. Find a linear discriminant function for transformed data $\varphi(\boldsymbol{x})$
  3. Final nonlinear discriminant function is $g(\boldsymbol{x}) = \boldsymbol{w}^t \varphi(\boldsymbol{x}) + w_0$



- In 2D, discriminant function is linear

$$g\left(\begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix}\right) = \begin{bmatrix} w_1 & w_2 \end{bmatrix} \begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix} + w_0$$

- In 1D, discriminant function is not linear $g(x) = w_1 x + w_2 x^2 + w_0$

Non Linear SVM

- Can use any linear classifier after lifting data into a higher dimensional space. However we will have to deal with the "curse of dimensionality"
  1. poor generalization to test data
  2. computationally expensive

- SVM avoids the "curse of dimensionality" problems by
  - enforcing largest margin permits good generalization
    - It can be shown that generalization in SVM is a function of the margin, independent of the dimensionality
  - computation in the higher dimensional case is performed only implicitly through the use of ***kernel*** functions

Non Linear SVM: Kernels

- Recall SVM optimization

$$\text{maximize} \quad L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j x_i^t x_j$$

- Note this optimization depends on samples $\boldsymbol{x}_i$ only through the dot product $\boldsymbol{x}_i^t \boldsymbol{x}_j$
- If we lift $\boldsymbol{x}_i$ to high dimension using $\boldsymbol{\varphi}(\boldsymbol{x})$, need to compute high dimensional product $\boldsymbol{\varphi}(\boldsymbol{x}_i)^t \boldsymbol{\varphi}(\boldsymbol{x}_j)$

$$\text{maximize} \quad L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j \varphi(x_i)^t \varphi(x_j)$$

$K(x_i,x_j)$

- Idea: find ***kernel*** function $\boldsymbol{K}(\boldsymbol{x}_i,\boldsymbol{x}_j)$ s.t.

$$\boldsymbol{K}(\boldsymbol{x}_i,\boldsymbol{x}_j) = \boldsymbol{\varphi}(\boldsymbol{x}_i)^t \boldsymbol{\varphi}(\boldsymbol{x}_j)$$

Non Linear SVM: Kernels

maximize $L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j \varphi(x_i)^t \varphi(x_j)$

$K(x_i, x_j)$

- Then we only need to compute $K(x_i, x_j)$ instead of $\varphi(x_i)^t \varphi(x_j)$
  - "kernel trick": do not need to perform operations in high dimensional space explicitly

Non Linear SVM: Kernels

- Suppose we have 2 features and $\boldsymbol{K}(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x}^t\boldsymbol{y})^2$

- Which mapping $\boldsymbol{\varphi}(\boldsymbol{x})$ does it correspond to?

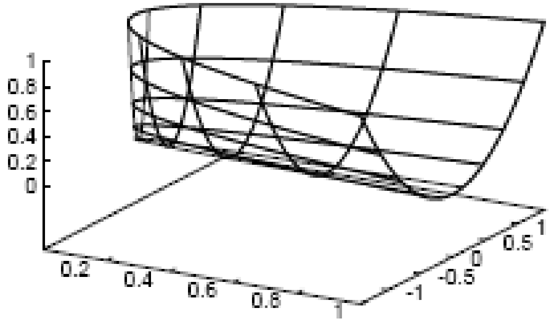
$$K(x,y) = (x^t y)^2 = \left(\begin{bmatrix} x^{(1)} & x^{(2)} \end{bmatrix} \begin{bmatrix} y^{(1)} \\ y^{(2)} \end{bmatrix} \right)^2 = \left(x^{(1)}y^{(1)} + x^{(2)}y^{(2)}\right)^2$$

$$= \left(x^{(1)}y^{(1)}\right)^2 + 2\left(x^{(1)}y^{(1)}\right)\left(x^{(2)}y^{(2)}\right) + \left(x^{(2)}y^{(2)}\right)^2$$

$$= \begin{bmatrix} \left(x^{(1)}\right)^2 & \sqrt{2}x^{(1)}x^{(2)} & \left(x^{(2)}\right)^2 \end{bmatrix} \begin{bmatrix} \left(y^{(1)}\right)^2 & \sqrt{2}y^{(1)}y^{(2)} & \left(y^{(2)}\right)^2 \end{bmatrix}^t$$

- Thus

$$\varphi(x) = \begin{bmatrix} \left(x^{(1)}\right)^2 & \sqrt{2}x^{(1)}x^{(2)} & \left(x^{(2)}\right)^2 \end{bmatrix}$$



Non Linear SVM: Kernels

- How to choose kernel function $\boldsymbol{K}(\boldsymbol{x}_i,\boldsymbol{x}_j)$?
  - $\boldsymbol{K}(\boldsymbol{x}_i,\boldsymbol{x}_j)$ should correspond to product $\boldsymbol{\varphi}(\boldsymbol{x}_i)^t\boldsymbol{\varphi}(\boldsymbol{x}_j)$ in a higher dimensional space
  - Mercer's condition tells us which kernel function can be expressed as dot product of two vectors
  - Kernel's not satisfying Mercer's condition can be sometimes used, but no geometrical interpretation
- Some common choices (satisfying Mercer's condition):
  - Polynomial kernel

$$K(x_i, x_j) = (x_i^t x_j + 1)^p$$

  - Gaussian radial Basis kernel (data is lifted in infinite dimensions)

$$K(x_i, x_j) = \exp\left(-\frac{1}{2\sigma^2}\|x_i - x_j\|^2\right)$$

Non Linear SVM

- search for separating hyperplane in high dimension

$$w\varphi(x) + w_0 = 0$$

- Choose $\varphi(\boldsymbol{x})$ so that the first ("0"th) dimension is the augmented dimension with feature value fixed to 1

$$\varphi(x) = \begin{bmatrix} 1 & x^{(1)} & x^{(2)} & x^{(1)}x^{(2)} \end{bmatrix}^t$$

- Threshold parameter $\boldsymbol{w_0}$ gets folded into the weight vector $\boldsymbol{w}$

$$\begin{bmatrix} w_0 & w \end{bmatrix} \underbrace{\begin{bmatrix} 1 \\ * \end{bmatrix}}_{\varphi(x)} = 0$$

Non Linear SVM

- Will not use notation $\boldsymbol{a} = [\boldsymbol{w_0} \;\; \boldsymbol{w}]$, we'll use old
  - notation $\boldsymbol{w}$ and seek hyperplane through the origin

$$w\varphi(x) = 0$$

- If the first component of $\varphi(x)$ is not 1, the above is equivalent to saying that the hyperplane has to go through the origin in high dimension
  - removes only one degree of freedom
  - But we have introduced many new degrees when we lifted the data in high dimension

Non Linear SVM Recepie

- Start with data $\boldsymbol{x_1},\ldots,\boldsymbol{x_n}$ which lives in feature space of dimension $\boldsymbol{d}$
- Choose kernel $\boldsymbol{K}(\boldsymbol{x_i},\boldsymbol{x_j})$ or function $\boldsymbol{\varphi}(\boldsymbol{x_i})$ which takes sample $\boldsymbol{x_i}$ to a higher dimensional space
- Find the largest margin linear discriminant function in the higher dimensional space by using quadratic programming package to solve:

$$\text{maximize} \quad L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j K(x_i, x_j)$$

$$\text{constrained to} \quad 0 \le \alpha_i \le \beta \quad \forall i \quad \text{and} \quad \sum_{i=1}^{n} \alpha_i z_i = 0$$

Non Linear SVM Recipe

- Weight vector $\boldsymbol{w}$ in the high dimensional space:

$$w = \sum_{x_i \in S} \alpha_i z_i \varphi(x_i)$$

  - where $\boldsymbol{S}$ is the set of support vectors $\quad S = \{x_i \mid \alpha_i \neq 0\}$

- Linear discriminant function of largest margin in the high dimensional space:

$$g(\varphi(x)) = w^t \varphi(x) = \left(\sum_{x_i \in S} \alpha_i z_i \varphi(x_i) \right)^t \varphi(x)$$

- Non linear discriminant function in the original space:

$$g(x) = \left(\sum_{x_i \in S} \alpha_i z_i \varphi(x_i) \right)^t \varphi(x) = \sum_{x_i \in S} \alpha_i z_i \varphi^t(x_i) \varphi(x) = \sum_{x_i \in S} \alpha_i z_i K(x_i, x)$$

- decide class 1 if $\boldsymbol{g}(\boldsymbol{x}) > 0$, otherwise decide class 2

Non Linear SVM

- Nonlinear discriminant function

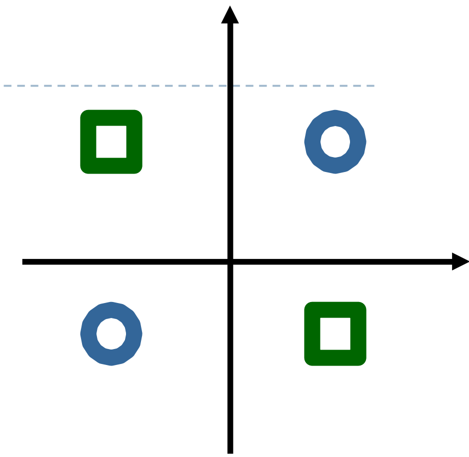
$$g(x) = \sum_{x_i \in S} \boxed{\alpha_i} \boxed{z_i} \boxed{K(x_i, x)}$$

$g(x) = \sum$ weight of support vector x_i ∓ 1 similarity between x and support vector x_i

most important training samples, i.e. support vectors

$$K(x_i, x) = \exp\left(-\frac{1}{2\sigma^2}\|x_i - x\|^2\right)$$

SVM Example: XOR Problem



- Class 1: $\mathbf{x_1} = [1,-1]$, $\mathbf{x_2} = [-1,1]$
- Class 2: $\mathbf{x_3} = [1,1]$, $\mathbf{x_4} = [-1,-1]$
- Use polynomial kernel of degree 2:
  - $K(x_i,x_j) = (x_i{}^t x_j + 1)^2$
  - This kernel corresponds to mapping

$$(\mathbf{x}) = \left[1 \quad \sqrt{2}\mathbf{x}^{(1)} \quad \sqrt{2}\mathbf{x}^{(2)} \quad \sqrt{2}\mathbf{x}^{(1)}\mathbf{x}^{(2)} \quad \left(\mathbf{x}^{(1)}\right)^2 \quad \left(\mathbf{x}^{(2)}\right)^2 \right]$$

- Need to maximize

$$L_D(\alpha) = \sum_{i=1}^{4} \alpha_i \quad \frac{1}{2} \sum_{i=1}^{4} \sum_{j=1}^{4} \alpha_i \alpha_j \mathbf{z}_i \mathbf{z}_j \left(\mathbf{x}_i^t \mathbf{x}_j + 1\right)^2$$

constrained to $\quad 0 \le \alpha_i \quad \forall i \quad \textit{and} \quad \alpha_1 + \alpha_2 - \alpha_3 - \alpha_4 = 0$

SVM Example: XOR Problem

- Can rewrite $L_D(\alpha) = \sum_{i=1}^{4} \alpha_i - \frac{1}{2}\alpha^t H \alpha$
  - where $\alpha = [\alpha_1 \quad \alpha_2 \quad \alpha_3 \quad \alpha_4]^t$ and $H = \begin{bmatrix} 9 & 1 & -1 & -1 \\ 1 & 9 & -1 & -1 \\ -1 & -1 & 9 & 1 \\ -1 & -1 & 1 & 9 \end{bmatrix}$
- Take derivative with respect to α and set it to 0

$$\frac{d}{da} L_D(\alpha) = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 9 & 1 & -1 & -1 \\ 1 & 9 & -1 & -1 \\ -1 & -1 & 9 & 1 \\ -1 & -1 & 1 & 9 \end{bmatrix} \alpha = 0$$

- Solution to the above is $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0.25$
  - satisfies the constraints $\forall i,\ 0 \le \alpha_i \text{ and } \alpha_1 + \alpha_2 - \alpha_3 - \alpha_4 = 0$
  - all samples are support vectors

SVM Example: XOR Problem

$$(\mathbf{x}) = \begin{bmatrix} 1 & \sqrt{2}\mathbf{x}^{(1)} & \sqrt{2}\mathbf{x}^{(2)} & \sqrt{2}\mathbf{x}^{(1)}\mathbf{x}^{(2)} & \left(\mathbf{x}^{(1)}\right)^2 & \left(\mathbf{x}^{(2)}\right)^2 \end{bmatrix}^T$$

- Weight vector ***w*** is:

$$\boldsymbol{w} = \sum_{i=1}^{4} \alpha_i z_i \varphi(x_i) = 0.25\left(\varphi(x_1) + \varphi(x_2) - \varphi(x_3) - \varphi(x_4)\right)$$

$$= \begin{bmatrix} 0 & 0 & 0 & \sqrt{2} & 0 & 0 \end{bmatrix}$$

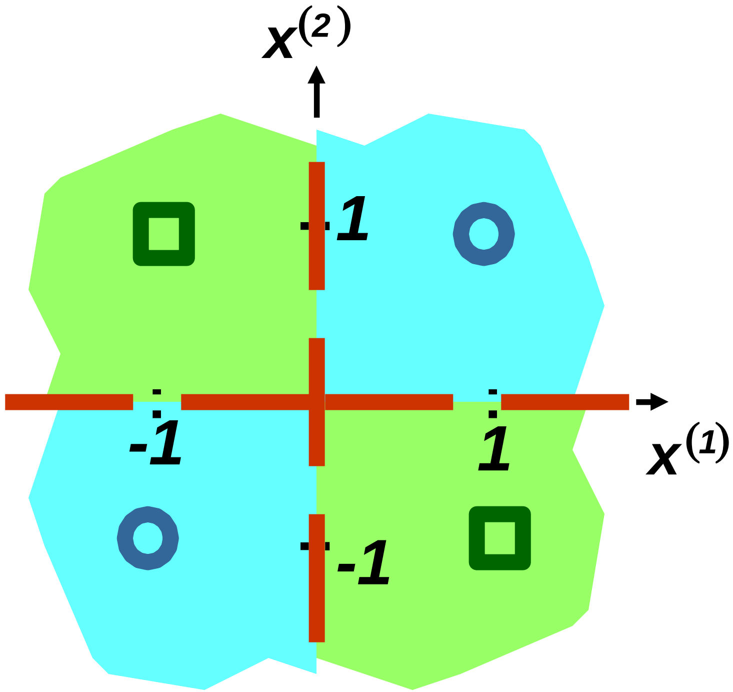
  - by plugging in $\mathbf{x}_1 = [1,-1]$, $\mathbf{x}_2 = [-1,1]$, $\mathbf{x}_3 = [1,1]$, $\mathbf{x}_4 = [-1,-1]$

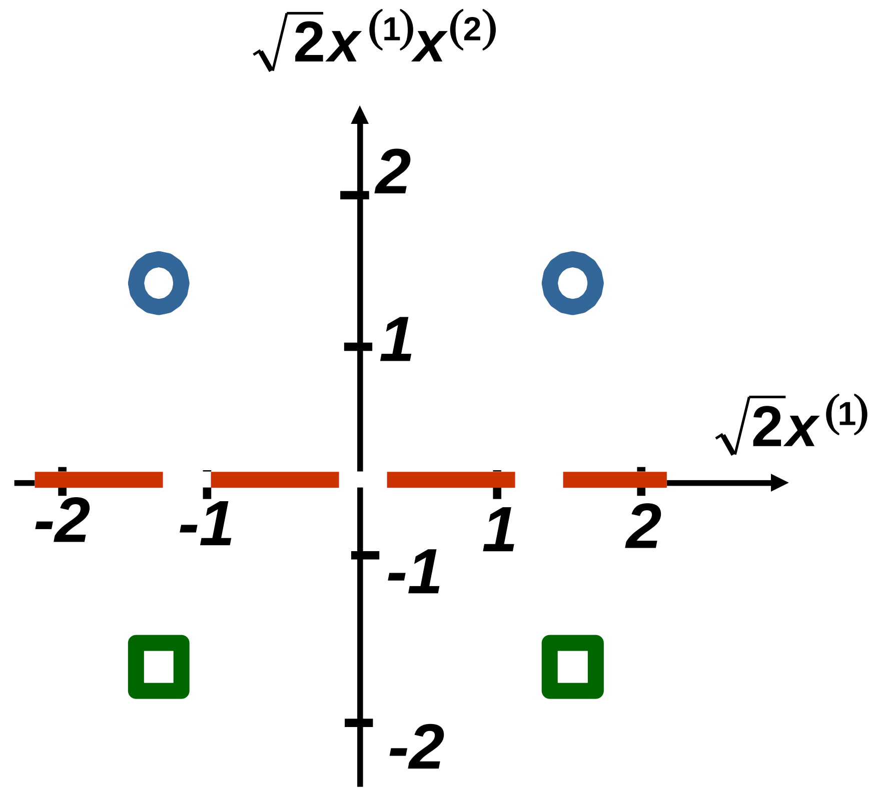
- Thus the nonlinear discriminant function is:

$$g(x) = w\varphi(x) = \sum_{i=1}^{6} w_i \varphi_i(x) = \sqrt{2}\left(\sqrt{2}\mathbf{x}^{(1)}\mathbf{x}^{(2)}\right) = 2\mathbf{x}^{(1)}\mathbf{x}^{(2)}$$

SVM Example: XOR Problem

$$g(x) = -2x^{(1)}x^{(2)}$$





decision boundaries nonlinear

decision boundary is linear

SVM Summary

- Advantages:
  - Based on nice theory
  - excellent generalization properties
  - objective function has no local minima
  - can be used to find non linear discriminant functions
  - Complexity of the classifier is characterized by the number of support vectors rather than the dimensionality of the transformed space

- Disadvantages:
  - tends to be slower than other methods
  - quadratic programming is computationally expensive
  - Not clear how to choose the Kernel