CS840a
Learning and Computer Vision
Prof. Olga Veksler

Lecture 4

SVM

Some pictures from C. Burges

SVM

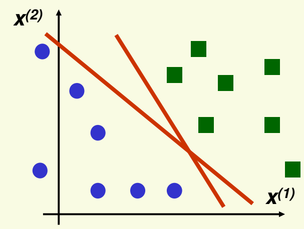
- Said to start in 1979 with Vladimir Vapnik's paper
- Major developments throughout 1990's
- Elegant theory
  - Has good generalization properties
- Have been applied to diverse problems very successfully in the last 10-15 years
- One of the most important developments in pattern recognition in the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

Linear Discriminant Functions

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

$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0$$

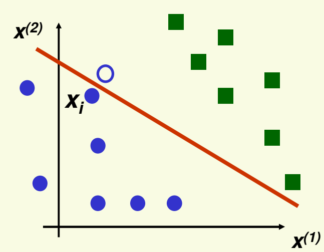
$$\begin{array}{l} g(x) > 0 \ \Rightarrow x \in \textit{class } 1 \\ g(x) < 0 \ \Rightarrow x \in \textit{class } 2 \end{array}$$



- which separating hyperplane should we choose?

Linear Discriminant Functions

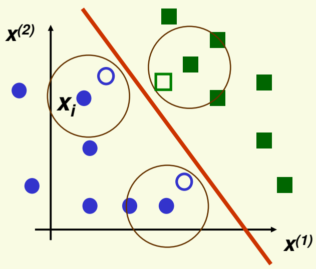
- Training data is just a subset of of all possible data
- Suppose hyperplane is close to sample $\mathbf{x}_i$
- If we see new sample close to sample $\boldsymbol{i}$, it is likely to be on the wrong side of the hyperplane



- Poor generalization (performance on unseen data)

Linear Discriminant Functions

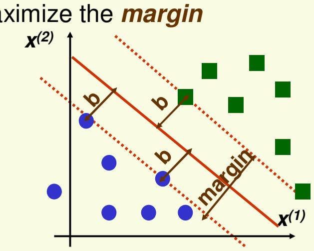
- Hyperplane as far as possible from any sample



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

SVM: Linearly Separable Case

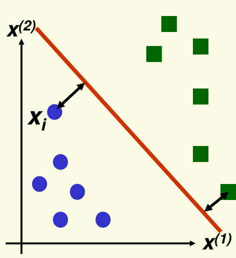
- SVM: maximize the ***margin***



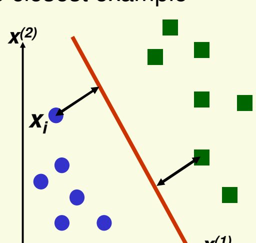
- ***margin*** is twice the absolute value of distance ***b*** of the closest example to the separating hyperplane
- Better generalization (performance on test data)
  - in practice
  - and in theory

SVM

- Idea: maximize distance to the closest example



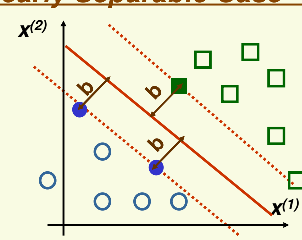
smaller distance



larger distance

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

SVM: Linearly Separable Case

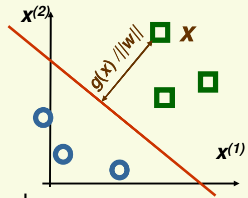


- ***Support vectors*** are the samples closest to the separating hyperplane
  - they are the most difficalt patterns to classify
  - Optimal hyperplane is completely defined by support vectors
    - of course, we do not know which samples are support vectors without finding the optimal hyperplane

SVM: Formula for the Margin

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

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



- distance is unchanged for hyperplane $g_1(\mathbf{x}) = \alpha g(\mathbf{x})$

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

- Let $\mathbf{x}_i$ be an example closest to the boundary. Set

$$|\mathbf{w}^t\mathbf{x}_i + w_0| = 1$$

- Now the largest margin hyperplane is unique

SVM: Optimal Hyperplane

- Maximize margin $m = \frac{2}{\|\mathbf{w}\|}$
  - subject to constraints

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

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

$$\text{minimize } J(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2$$
$$\text{constrained to } z_i(\mathbf{w}^t\mathbf{x}_i + w_0) \geq 1 \quad \forall i$$

- $J(\mathbf{w})$ is a quadratic function, thus there is a single global minimum

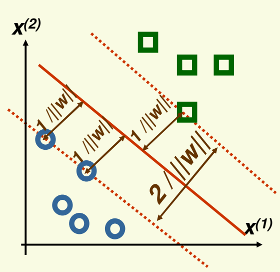
SVM: Formula for the Margin

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

$$\frac{|\mathbf{w}^t\mathbf{x}_i + w_0|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$$

- Thus the margin is

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



SVM: Optimal Hyperplane

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

$$\text{maximize } L_D(\alpha) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j z_i z_j \mathbf{x}_i^t \mathbf{x}_j$$
$$\text{constrained to } \alpha_i \geq 0 \quad \forall i \quad \text{and} \quad \sum_{i=1}^{n}\alpha_i z_i = 0$$

- $\alpha = \{\alpha_1, \ldots, \alpha_n\}$ 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

$$H_{ij} = z_i z_j \mathbf{x}_i^t \mathbf{x}_j$$

SVM: Optimal Hyperplane

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

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

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

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

SVM: Optimal Hyperplane

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

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

- $L_D(\alpha)$ 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

SVM: Optimal Hyperplane

- After finding the optimal $\alpha = \{\alpha_1, \dots, \alpha_n\}$
  - 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 $\alpha_i [z_i (w^t x_i + w_0) - 1] = 0$

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

- Final discriminant function:

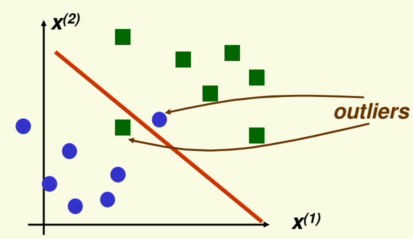
$$g(x) = \left(\sum_{x_i \in S} \alpha_i z_i x_i \right)^t x + w_0$$

  - where S is the set of support vectors

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

SVM: Non Separable Case

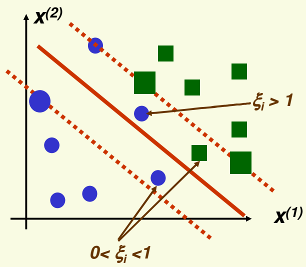
- Data is most likely to be not linearly separable, but linear classifier may still be appropriate



- Can apply SVM in non linearly separable case
  - data should be "almost" linearly separable for good performance

SVM: Non Separable Case

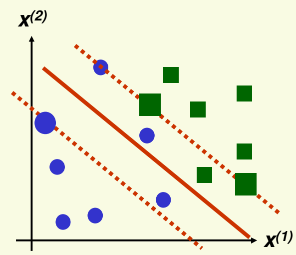
- Use non-negative slack variables $\xi_1, \ldots, \xi_n$ (one for each sample)
- Change constraints from $z_i(w^t x_i + w_0) \geq 1 \quad \forall i$ to
  $z_i(w^t x_i + w_0) \geq 1 - \xi_i \quad \forall i$
- ξ_i is a measure of deviation from the ideal for sample i
  - $\xi_i > 1$ sample i is on the wrong side of the separating hyperplane
  - $0 < \xi_i < 1$ sample i is on the right side of separating hyperplane but within the region of maximum margin



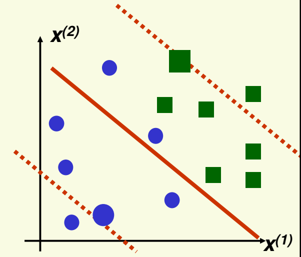
SVM: Non Separable Case

$$J(w, \xi_1, \ldots, \xi_n) = \frac{1}{2}\|w\|^2 + \beta \sum_{i=1}^{n} I(\xi_i > 0)$$

# of examples not in ideal location



large β, few samples not in ideal position



small β, a lot of samples not in ideal position

SVM: Non Separable Case

- Would like to minimize

$$J(w, \xi_1, \ldots, \xi_n) = \frac{1}{2}\|w\|^2 + \beta \sum_{i=1}^{n} I(\xi_i > 0)$$

# of samples not in ideal location

  - where $I(\xi_i > 0) = \begin{cases} 1 & \text{if } \xi_i > 0 \\ 0 & \text{if } \xi_i \leq 0 \end{cases}$
  - constrained to $z_i(w^t x_i + w_0) \geq 1 - \xi_i$ and $\xi_i \geq 0 \quad \forall i$
  - β is a constant which measures relative weight of the first and second terms
    - if β is small, we allow a lot of samples not in ideal position
    - if β is large, we want to have very few samples not in ideal positon

SVM: Non Separable Case

- Unfortunately this minimization problem is NP-hard due to discontinuity of functions $I(\xi_i)$

$$J(w, \xi_1, \ldots, \xi_n) = \frac{1}{2}\|w\|^2 + \beta \sum_{i=1}^{n} I(\xi_i > 0)$$

# of examples not in ideal location

  - where $I(\xi_i > 0) = \begin{cases} 1 & \text{if } \xi_i > 0 \\ 0 & \text{if } \xi_i \leq 0 \end{cases}$
  - constrained to $z_i(w^t x_i + w_0) \geq 1 - \xi_i$ and $\xi_i \geq 0 \quad \forall i$

SVM: Non Separable Case

- Instead we minimize

$$J(w,\xi_1,\ldots,\xi_n)=\frac{1}{2}\|w\|^2+\beta\sum_{i=1}^{n}\xi_i$$

a measure of # of misclassified examples

- constrained to $\begin{cases} z_i(w^t x_i + w_0) \ge 1-\xi_i & \forall i \\ \xi_i \ge 0 & \forall i \end{cases}$

- Can use Kuhn-Tucker theorem to converted to

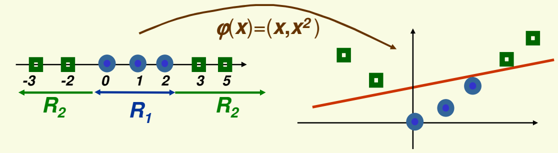
maximize $L_D(\alpha)=\sum_{i=1}^{n}\alpha_i-\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j z_i z_j x_i^t x_j$

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

- find w using $w=\sum_{i=1}^{n}\alpha_i z_i x_i$
- solve for w_0 using any $0<\alpha_i<\beta$ and $\alpha_i\left[z_i\left(w^t x_i+w_0\right)-1\right]=0$

Non Linear Mapping

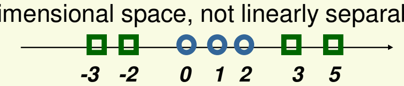
- To solve a non linear classification problem with a linear classifier
  1. Project data x to high dimension using function $\varphi(x)$
  2. Find a linear discriminant function for transformed data $\varphi(x)$
  3. Final nonlinear discriminant function is $g(x) = w^t \varphi(x) + w_0$



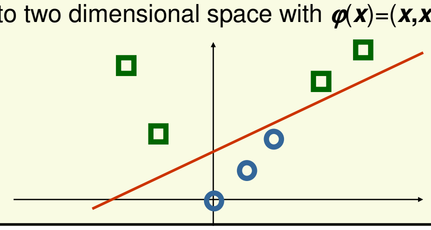
- In 2D, discriminant function is linear
$$g\left(\begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix}\right)=\begin{bmatrix} w_1 & w_2 \end{bmatrix}\begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix}+w_0$$
- In 1D, discriminant function is not linear $g(x)=w_1x+w_2x^2+w_0$

Non Linear Mapping

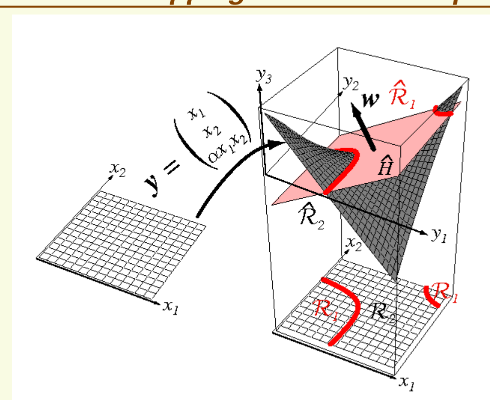
- Cover's theorem:
  - "*pattern-classification problem cast in a high dimensional space non-linearly is more likely to be linearly separable than in a low-dimensional space*"
- One dimensional space, not linearly separable



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



Non Linear Mapping: Another Example



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

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

- Recall SVM optimization

  maximize $L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j z_i z_j x_i^t x_j$
- Note this optimization depends on samples x_i only through the dot product $x_i^t x_j$
- If we lift x_i to high dimension using $\varphi(x)$, need to compute high dimensional product $\varphi(x_i)^t\varphi(x_j)$

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

  $K(x_i, x_j)$
- Idea: find ***kernel*** function $K(x_i, x_j)$ s.t.

  $K(x_i, x_j) = \varphi(x_i)^t\varphi(x_j)$

Non Linear SVM: Kernels

- Suppose we have 2 features and $K(x, y) = (x^t y)^2$
- Which mapping $\varphi(x)$ does it correspond to?

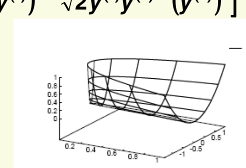
$$K(x,y) = (x^t y)^2 = \left(\begin{bmatrix} x^{(1)} & x^{(2)} \end{bmatrix}\begin{bmatrix} y^{(1)} \\ y^{(2)} \end{bmatrix}\right)^2 = \left(x^{(1)}y^{(1)} + x^{(2)}y^{(2)}\right)^2$$

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

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

- Thus

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



Non Linear SVM: Kernels

- How to choose kernel function $K(x_i,x_j)$?
  - $K(x_i,x_j)$ should correspond to product $\varphi(x_i)^t\varphi(x_j)$ 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 dimension)

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

Non Linear SVM

- Will not use notation $a = [w_0 \ \ w]$, we'll use old notation 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

- search for separating hyperplane in high dimension

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

- Choose $\varphi(x)$ 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 w_0 gets folded into the weight vector w

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

Non Linear SVM Recepie

- Start with data $x_1,\ldots,x_n$ which lives in feature space of dimension d
- Choose kernel $K(x_i,x_j)$ or function $\varphi(x_i)$ which takes sample 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:

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

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

Non Linear SVM Recipe

- Weight vector w in the high dimensional space:

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

  - where S is the set of support vectors $S = \{x_i \mid \alpha_i \neq 0\}$
- 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 $g(x) > 0$, 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] ["inverse distance" from x to support vector x_i]

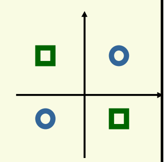
most important training samples, i.e. support vectors

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

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

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



- Need to maximize

$$L_D(\alpha) = \sum_{i=1}^{4} \alpha_i - \frac{1}{2} \sum_{i=1}^{4} \sum_{j=1}^{4} \alpha_i \alpha_j z_i z_j \left(x_i^t x_j + 1 \right)^2$$

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

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 $\forall i, \ 0 \leq \alpha_i \ \text{and} \ \alpha_1 + \alpha_2 - \alpha_3 - \alpha_4 = 0$
  - all samples are support vectors

SVM Example: XOR Problem

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

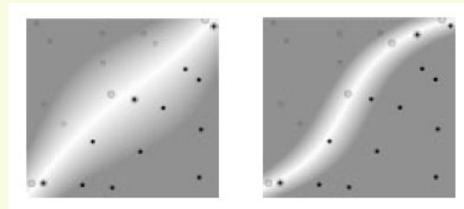
- Weight vector w is:

$$w = \sum_{i=1}^{4} \alpha_i z_i \varphi(x_i) = 0.25(\varphi(x_1) + \varphi(x_2) - \varphi(x_3) - \varphi(x_4))$$
$$= \begin{bmatrix} 0 & 0 & 0 & -\sqrt{2} & 0 & 0 \end{bmatrix}$$

- Thus the nonlinear discriminant function is:

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

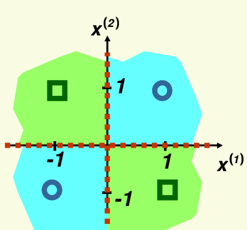
Degree 3 Polynomial Kernel



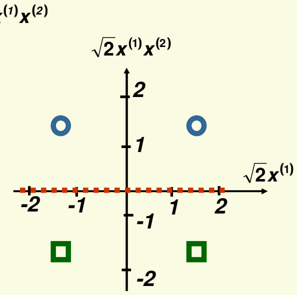
- In linearly separable case (on the left), decision boundary is roughly linear, indicating that dimensionality is controlled
- Nonseparable case (on the right) is handled by a polynomial of degree 3

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