Support Vector Machines (SVM)

Master MLDS - 2017/2018

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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



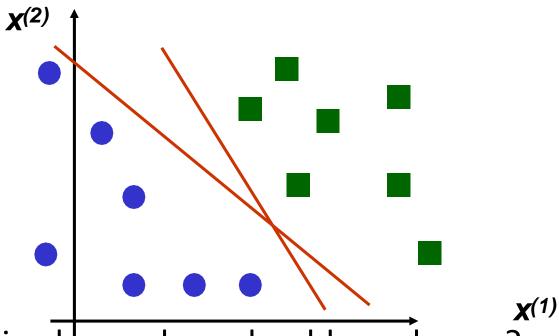
Linear Discriminant Functions

A discriminant function is linear if it can be written as

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

$$g(x) > 0 \Rightarrow x \in class 1$$

 $g(x) < 0 \Rightarrow x \in class 2$

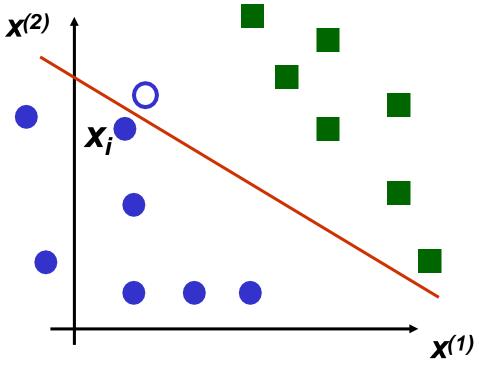


which separating hyperplane should we choose?

Linear Discriminant Functions

- Training data is just a subset of of all possible data
- Suppose hyperplane is close to sample x_i
- If we see new sample close to sample *i*, it is likely to be on the wrong side of the

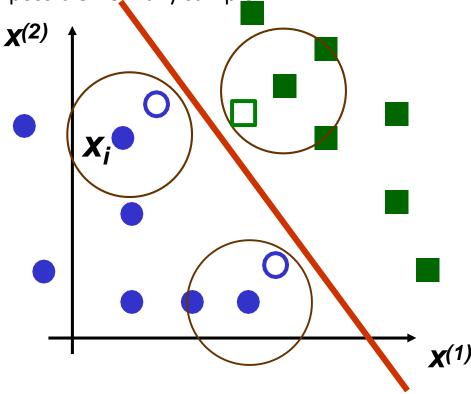
hyperplane



Poor generalization (performance on unseen data)

Linear Discriminant Functions

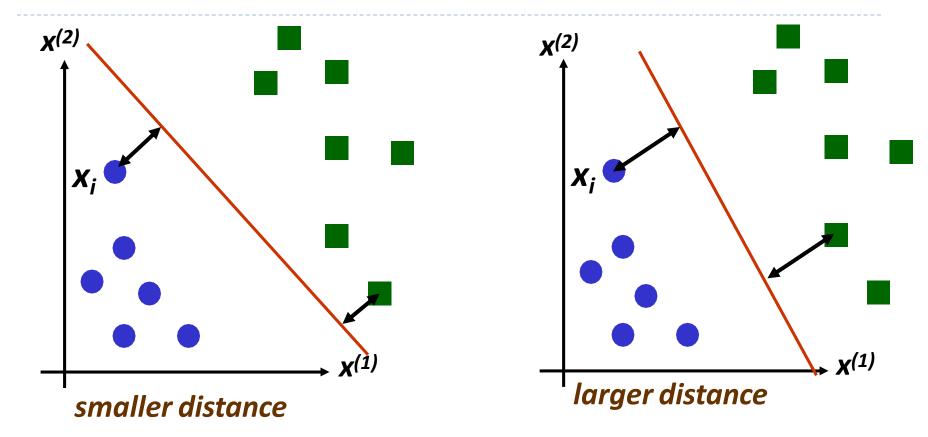
Hyperplane as far as possible from any sample



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

SVM

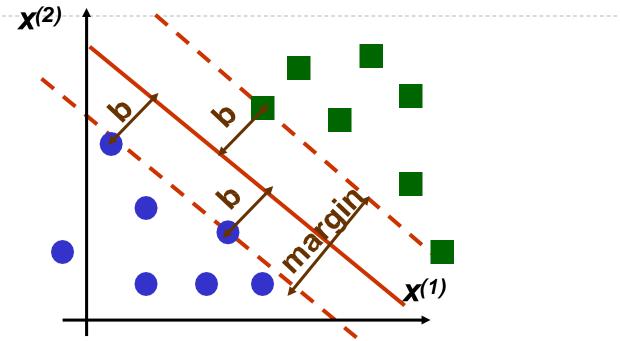
• Idea: maximize distance to the closest example



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

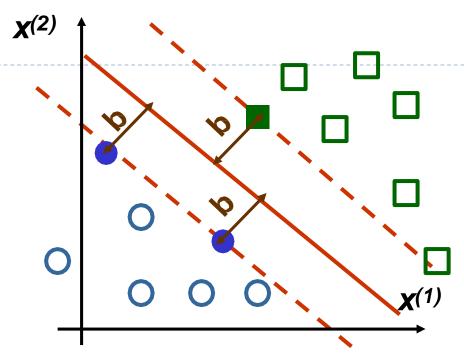
SVM: Linearly Separable Case

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

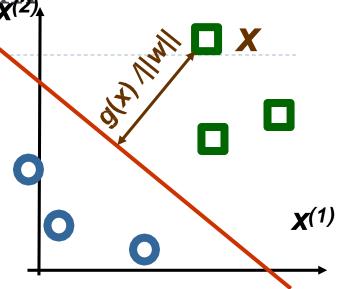


- Support vectors are samples closest to separating hyperplane
 - they are the most difficult patterns to classify
 - Optimal hyperplane is completely defined by support vectors
 - of course, we do not know which samples are support vectors without finding the optimal hyperplane

SVM: Formula for the Margin

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

$$\frac{\left| \boldsymbol{W}^{t} \boldsymbol{X} + \boldsymbol{W}_{0} \right|}{\left\| \boldsymbol{W} \right\|}$$



distance is unchanged for hyperplane

$$g_1(x) = \alpha g(x)$$

$$\frac{\left|\alpha \mathbf{w}^{t} \mathbf{X} + \alpha \mathbf{w}_{0}\right|}{\|\alpha \mathbf{w}\|} = \frac{\left|\mathbf{w}^{t} \mathbf{X} + \mathbf{w}_{0}\right|}{\|\mathbf{w}\|}$$

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

$$\left| \mathbf{W}^t \mathbf{X}_i + \mathbf{W}_0 \right| = \mathbf{1}$$

Now the largest margin hyperplane is unique

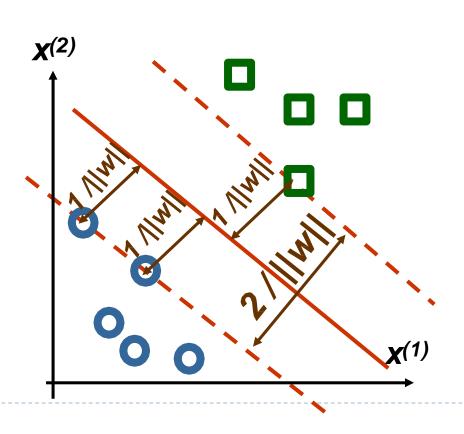
SVM: Formula for the Margin

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

$$\frac{\left|\mathbf{w}^{t}\mathbf{X}_{i}+\mathbf{w}_{0}\right|}{\left\|\mathbf{w}\right\|} = \frac{1}{\left\|\mathbf{w}\right\|}$$

Thus the margin is

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



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

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

- 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

minimize
$$J(w) = \frac{1}{2} ||w||^2$$

constrained to $z_i (w^t x_i + w_0) \ge 1 \quad \forall i$

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

Use Kuhn-Tucker theorem to convert our problem to:

maximize
$$L_{D}(\alpha) = \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} \mathbf{z}_{i} \mathbf{z}_{j} \mathbf{x}_{i}^{t} \mathbf{x}_{j}$$
 constrained to $\alpha_{i} \geq 0 \quad \forall i \quad and \quad \sum_{i=1}^{n} \alpha_{i} \mathbf{z}_{i} = 0$

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

$$L_{D}(\alpha) = \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \begin{bmatrix} \alpha_{1} \\ \vdots \\ \alpha_{n} \end{bmatrix}^{t} H^{t} \begin{bmatrix} \alpha_{1} \\ \vdots \\ \alpha_{n} \end{bmatrix}$$

where the value in the *i*th row and *j*th column of *H* is

$$H_{ij} = Z_i Z_j X_i^t X_j$$

Use Kuhn-Tucker theorem to convert our problem 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 $\alpha_{i} \ge 0 \quad \forall i \quad and \quad \sum_{i=1}^{n} \alpha_{i} z_{i} = 0$

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

- After finding the optimal $\alpha = \{\alpha_1, ..., \alpha_n\}$
 - 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 \mathbf{w} using $\mathbf{w} = \sum_{i} \alpha_i \mathbf{z}_i \mathbf{x}_i$
 - can solve for \mathbf{w}_0 using any $\alpha_i > 0$ and $\alpha_i \left[\mathbf{z} \left(\mathbf{w}^t \mathbf{x}_i + \mathbf{w}_0 \right) 1 \right] = 0$ $\mathbf{w}_0 = \frac{1}{7} \mathbf{w}^t \mathbf{x}_i$
 - 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

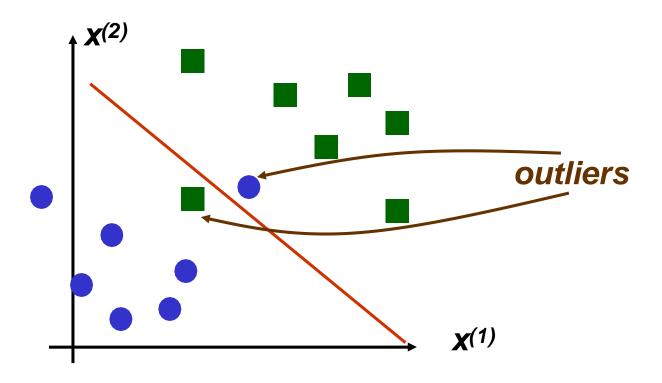
$$S = \left\{ x_{i} \mid \alpha_{i} \neq \mathbf{0} \right\}$$



maximize
$$L_{D}(\alpha) = \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha z_{i} z_{j} x_{i}^{t} x$$
constrained to $\alpha_{i} \ge 0 \quad \forall i \quad and \quad \sum_{i=1}^{n} \alpha_{i} z_{i} = 0$

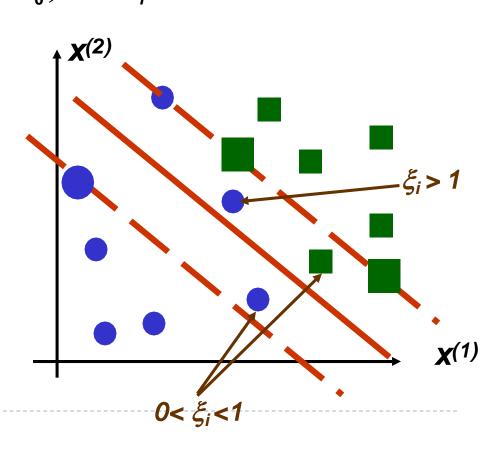
- $L_D(\alpha)$ depends on the number of samples, not on dimension of samples
- samples appear only through the dot products $\mathbf{x}_{i}^{t}\mathbf{x}_{j}$
- This will become important when looking for a *nonlinear* discriminant function, as we will see soon
- Code available on the web to optimize

 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

- Use non-negative slack variables $\xi_1,...,\xi_n$
 - one for each sample
- Change constraints from $z_i(w x_i + w_0) \ge 1$ to $z_i(w x_i + w_0) \ge 1 \xi_i$ $\forall i$
- 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



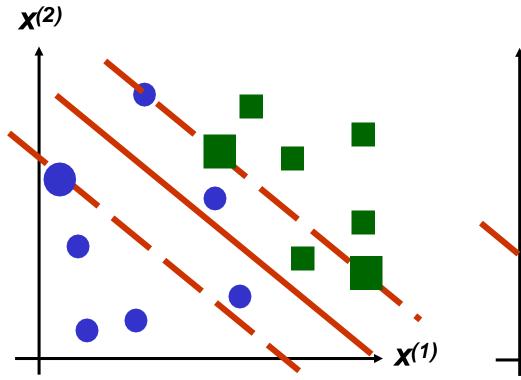
Would like to minimize

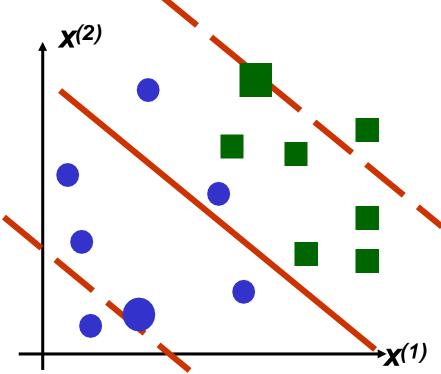
$$J(w,\xi_1,...,\xi_n) = \frac{1}{2} ||w||^2 + \beta \sum_{i=1}^n I(\xi_i > 0)$$
 # of samples not in ideal location

- where $I(\xi_i > 0) = \begin{cases} 1 & \text{if } \xi_i > 0 \\ 0 & \text{if } \xi_i \le 0 \end{cases}$
- constrained to $z_i(w^t x_i + w_0) \ge 1 \xi_i$ and $\xi_i \ge 0 \ \forall i$
- β measures relative weight of 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 position
 - choosing βappropriately is important

$$J(\mathbf{W},\xi_{1},...,\xi_{n}) = \frac{1}{2} \|\mathbf{W}\|^{2} + \beta \sum_{i=1}^{n} I(\xi_{i} > 0)$$

of examples not in ideal location





large β , few samples not in ideal position

small β , a lot of samples not in ideal position

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

$$J(w,\xi_1,...,\xi_n) = \frac{1}{2} ||w||^2 + \beta \sum_{i=1}^n I(\xi_i > 0)$$
 # of examples not in ideal location

- where $I(\xi_i > 0) = \begin{cases} 1 & \text{if } \xi_i > 0 \\ 0 & \text{if } \xi_i \le 0 \end{cases}$
- constrained to $\mathbf{z}_{i}(\mathbf{w}^{t}\mathbf{x}_{i} + \mathbf{w}_{0}) \ge 1 \xi_{i}$ and $\xi_{i} \ge \mathbf{0} \ \forall i$

Instead we minimize

$$J(w,\xi_1,...,\xi_n) = \frac{1}{2} \|w\|^{2} + \beta \sum_{i=1}^n \xi_i$$
 # of misclassified examples

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

Use Kuhn-Tucker theorem to converted to

maximize
$$L_D(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \mathbf{z}_j \mathbf{z}_j^t \mathbf{x}_i^t \mathbf{x}$$

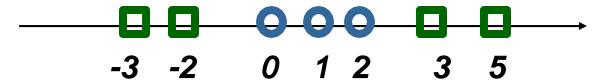
constrained to $0 \le \alpha_i \le \beta \quad \forall i \quad and \quad \sum_{i=1}^n \alpha_i \mathbf{z}_i = 0$

• find
$$\mathbf{w}$$
 using $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \mathbf{z}_i \mathbf{x}_i$

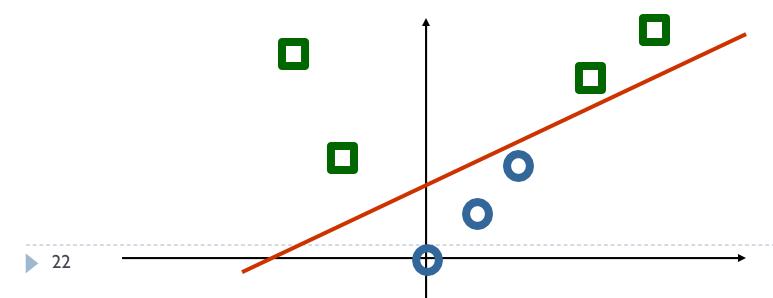
• solve for \mathbf{w}_0 using any $0 < \alpha_i < \beta$ and $\alpha_i \left[\mathbf{z}_i (\mathbf{w}^t \mathbf{x}_i + \mathbf{w}_0) - 1 \right] = 0$

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 lowdimensional space"
- One dimensional space, not linearly separable

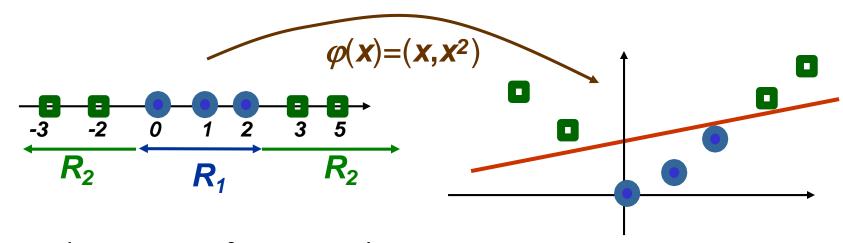


• Lift to two dimensional space with $\varphi(x) = (x, x^2)$



Non Linear Mapping

- To solve a non linear problem with a linear classifier
 - 1. Project data 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

$$g\left(\begin{bmatrix} \mathbf{X}^{(1)} \\ \mathbf{X}^{(2)} \end{bmatrix}\right) = \begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_2 \end{bmatrix} \begin{bmatrix} \mathbf{X}^{(1)} \\ \mathbf{X}^{(2)} \end{bmatrix} + \mathbf{W}_0$$

• 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

Recall SVM optimization

maximize
$$L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \mathbf{z}_j \mathbf{z}_j \mathbf{x}_i^t \mathbf{x}_j$$

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

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

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

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

maximize
$$L_D(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_i \mathbf{z}_i \mathbf{z}_j \varphi(\mathbf{x}_i)^{\dagger} \varphi(\mathbf{x}_j)$$

$$K(\mathbf{x}_i, \mathbf{x}_j)$$

- 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

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

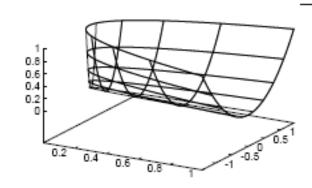
$$K(x,y) = (x^{t}y)^{2} = \left[\left[x^{(1)} \quad x^{(2)} \right] \left[y^{(1)} \right] \right]^{2} = \left(x^{(1)}y^{(1)} + x^{(2)}y^{(2)} \right)^{2}$$

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

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

Thus

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



- How to choose kernel function $K(x_i,x_i)$?
 - $K(x_i,x_j)$ 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 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

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

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

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

• Threshold parameter \mathbf{w}_{o} gets folded into the weight vector \mathbf{w}

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 Recepie

- Start with data $x_1,...,x_n$ 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
$$L_D(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_i z_i z_j K(x_i, x_j)$$

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

Non Linear SVM Recipe

Weight vector w in the high dimensional space:

$$\mathbf{w} = \sum_{\mathbf{x}_i \in S} \alpha_i \mathbf{z}_i \varphi(\mathbf{x}_i)$$

- 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

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

$$g(x) = \sum_{x \in \mathcal{X}} f(x)$$

weight of support vector **x**_i

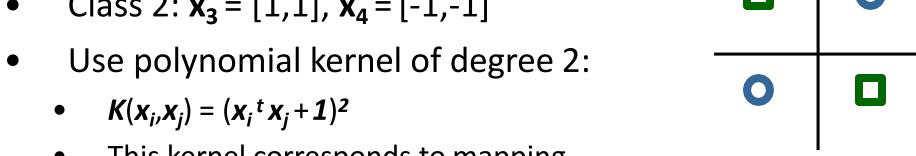
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similarity between **x** and support vector **x**_i

most important training samples, i.e. support vectors

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

- Class 1: $\mathbf{x_1} = [1,-1], \mathbf{x_2} = [-1,1]$
- Class 2: $\mathbf{x_3} = [1,1], \mathbf{x_4} = [-1,-1]$



This kernel corresponds to mapping

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

Need to maximize

$$\mathbf{L}_{D}(\alpha) = \sum_{i=1}^{4} \alpha_{i} \frac{1}{2} \sum_{i=1}^{4} \sum_{j=1}^{4} \alpha_{i} \alpha_{i} \mathbf{z}_{i} \mathbf{z}_{j} \left(\mathbf{x}_{i}^{t} \mathbf{x}_{j} + 1 \right)$$

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

• Can rewrite
$$L_D(\alpha) = \sum_{i=1}^4 \alpha_i - \frac{1}{2} \alpha^i H \alpha$$

• where $\alpha = \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \end{bmatrix}$ 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 $oldsymbol{lpha}$ and set it to $oldsymbol{0}$

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

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

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

Weight vector w is:

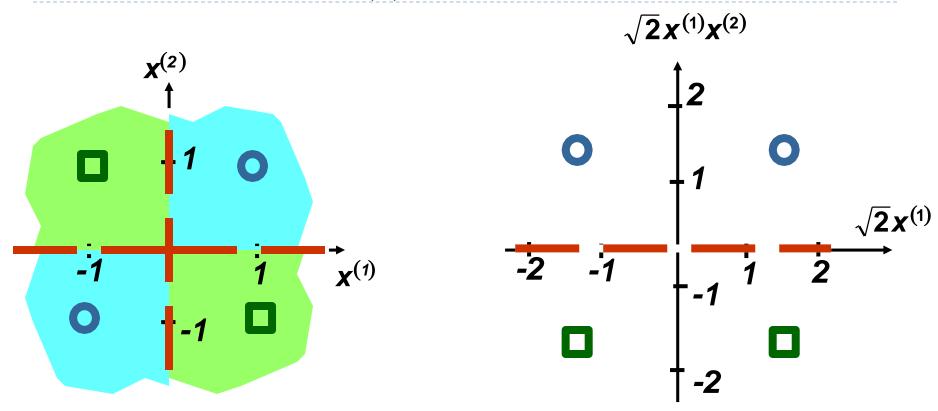
$$w = \sum_{i=1}^{4} \alpha_i \mathbf{z}_i \varphi(\mathbf{x}_i) = 0.25 (\varphi(\mathbf{x}_1) + \varphi(\mathbf{x}_2) - \varphi(\mathbf{x}_3) - \varphi(\mathbf{x}_4))$$
$$= \begin{bmatrix} 0 & 0 & 0 & \sqrt{2} & 0 & 0 \end{bmatrix}$$

- 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:

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

36

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



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