## CS840a

## Learning and Computer Vision Prof. Olga Veksler

## Lecture 8 <br> SVM

Some pictures from C. Burges

- 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 15-20 years


## Linear Discriminant Functions

$$
\begin{aligned}
& \mathbf{g}(\mathbf{x})=\mathbf{w}^{\mathbf{t}} \mathbf{x}+\mathbf{w}_{\mathbf{0}} \\
& \mathbf{g}(\mathbf{x})>0 \quad \Rightarrow \mathbf{x} \in \text { class } 1 \\
& \mathbf{g}(\mathbf{x})<0 \quad \Rightarrow \mathbf{x} \in \text { class } 2
\end{aligned}
$$



- which separating hyperplane should we choose?


## Margin Intuition

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

- Poor generalization


## Margin Intuition

- Hyperplane as far as possible from any sample

- More likely that new samples close to old samples 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 $\boldsymbol{b}$ of the closest example to the separating hyperplane
- Better generalization
- 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, intuitively
- optimal hyperplane is completely defined by support vectors
- do not know which samples are support vectors beforehand


## SVM: Formula for the Margin

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

$$
\frac{\left|w^{t} x+w_{0}\right|}{\|w\|}
$$



- distance is unchanged for hyperplane $\mathbf{g}_{1}(\mathbf{x})=\alpha \mathbf{g}(\mathbf{x})$

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

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

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

- Now the largest margin hyperplane is unique


## SVM: Formula for the Margin

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

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

- Thus the margin is

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



## SVM: Optimal Hyperplane

- Maximize margin

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

- subject to constraints

$$
\begin{cases}\mathbf{w}^{t} \mathbf{x}_{1}+w_{0} \geq 1 & \text { if } \boldsymbol{x}_{1} \text { is positive example } \\ \mathbf{w}^{\mathrm{t}} \mathbf{x}_{1}+\mathbf{w}_{0} \leq-1 & \text { if } \boldsymbol{x}_{i} \text { is negative example }\end{cases}
$$

- Let $\begin{cases}\mathbf{z}_{i}=1 & \text { if } \mathbf{x}_{i} \text { is positive example } \\ \mathbf{z}_{i}=-1 & \text { if } \mathbf{x}_{i} \text { is negative example }\end{cases}$
- Convert our problem to

| minimize | $J(\mathbf{w})=\frac{1}{2}\\|\mathbf{w}\\|^{2}$ |
| :---: | :---: |
| constrained to | $\mathbf{z}^{\prime}\left(\mathbf{w}^{+} \mathbf{x}_{1}+\mathbf{w}_{0}\right) \geq 1 \quad \forall \mathbf{i}$ |

- $\mathbf{J}(\mathbf{w})$ is a convex function, thus it has a single global minimum


## SVM: Optimal Hyperplane

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

$$
\begin{array}{ll}
\text { maximize } & \mathbf{L}_{\mathrm{D}}(\alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} \mathbf{z}_{i} \mathbf{z}_{j} \mathbf{x}_{\mathrm{i}}^{\mathrm{t}} \mathbf{x}_{\mathrm{j}} \\
\text { ained to } & \alpha_{i} \geq 0 \quad \forall \mathbf{i} \text { and } \sum_{i=1}^{n} \alpha_{i} \mathbf{z}_{i}=0
\end{array}
$$

- $\alpha=\left\{\alpha_{1}, \ldots, \alpha_{n}\right\}$ are new variables, one for each sample
- Rewrite $L_{D}(\alpha)$ using $n$ by $n$ matrix $H$ :

$$
L_{D}(\alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2}\left[\begin{array}{c}
\alpha_{1} \\
\vdots \\
\alpha_{n}
\end{array}\right]^{t} H\left[\begin{array}{c}
\alpha_{1} \\
\vdots \\
\alpha_{n}
\end{array}\right]
$$

- where the value in the $\boldsymbol{i}$ th row and $\boldsymbol{j}$ th column of $\boldsymbol{H}$ is

$$
\mathbf{H}_{\mathrm{ij}}=\mathbf{z}_{\mathrm{i}} \mathbf{z}_{\mathrm{j}} \mathbf{x}_{\mathrm{i}}^{\mathrm{t}} \mathbf{x}_{\mathbf{j}}
$$

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

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

- $\boldsymbol{\alpha}=\left\{\alpha_{1}, \ldots, \alpha_{n}\right\}$ are new variables, one for each sample
- $\mathrm{L}_{\boldsymbol{D}}(\boldsymbol{\alpha})$ can be optimized by quadratic programming
- $L_{D}(\boldsymbol{\alpha})$ formulated in terms of $\boldsymbol{\alpha}$
- depends on $\mathbf{w}$ and $\mathbf{w}_{\mathbf{0}}$


## SVM: Optimal Hyperplane

- After finding the optimal $\alpha=\left\{\alpha_{1}, \ldots, \alpha_{n}\right\}$
- for every sample $\mathbf{i}$, one of the following must hold
- $\boldsymbol{\alpha}_{\mathrm{i}}=0$ (sample $\boldsymbol{i}$ is not a support vector)
- $\alpha_{i} \neq 0$ and $z_{i}\left(w^{t} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}-1\right)=0$ (sample $\mathbf{i}$ is support vector)
- compute $w=\sum_{i=1}^{n} \alpha_{i} \mathbf{z}_{i} \mathbf{x}_{i}$
- solve for $\mathbf{w}_{0}$ using any $\alpha_{i}>0$ and $\alpha_{i}\left[z_{i}\left(\mathbf{w}^{t} \mathbf{x}_{i}+\mathbf{w}_{0}\right)-1\right]=0$

$$
\mathbf{w}_{0}=\frac{1}{\mathbf{z}_{\mathbf{i}}}-\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}
$$

- Final discriminant function:

$$
\mathbf{g}(\mathbf{x})=\left(\sum_{\mathbf{x}_{i} \in S} \alpha_{i} \mathbf{z}_{\mathbf{i}} \mathbf{x}_{\mathbf{i}}\right)^{\mathbf{t}} \mathbf{x}+\mathbf{w}_{0}
$$

- where $\boldsymbol{S}$ is the set of support vectors

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

## SVM: Optimal Hyperplane

$$
\begin{aligned}
\text { maximize } & L_{0}(\alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} z_{i} z_{j} \mathbf{j}_{i}^{t} x_{j} \\
\text { constrained to } & \alpha_{i} \geq 0 \quad \forall i \text { and } \sum_{i=1}^{n} \alpha_{i} \mathbf{z}_{i}=0
\end{aligned}
$$

- $\mathrm{L}_{\mathrm{D}}(\alpha)$ depends on the number of samples, not on dimension of samples
- samples appear only through the dot products $\mathbf{x}_{\mathbf{i}}^{\mathrm{t}} \mathbf{x}_{\mathbf{j}}$
- Will become important when looking for a nonlinear discriminant function


## SVM: Non Separable Case

- Linear classifier still be appropriate when data is not linearly separable, but almost linearly separable

- Can adapt SVM to almost linearly separable case


## SVM: Non Separable Case

- Introduce non-negative slack variables $\xi_{1}, \ldots, \xi_{n}$
- one for each sample
- Change constraints from $\mathbf{z}_{\mathbf{i}}\left(\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}\right) \geq 1 \quad \forall \mathbf{i}$ to

$$
\mathbf{z}_{\mathbf{i}}\left(\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}\right) \geq 1-\xi_{\mathbf{i}} \quad \forall \mathbf{i}
$$

- $\xi_{i}$ measures deviation from the ideal position for sample $\mathbf{x}_{\mathbf{i}}$
- $\xi_{i}>1$ : $\mathbf{x}_{\mathrm{i}}$ is on the wrong side of the hyperplane
- $0<\xi_{i}<1$ : $x_{i}$ is on the right side of the hyperplane but within the region of maximum margin



## SVM: Non Separable Case

- Wish to minimize

$$
\mathbf{J}\left(\mathbf{w}, \xi_{1}, \ldots, \xi_{\mathrm{n}}\right)=\frac{1}{2}\|\mathbf{w}\|^{2}+\beta \sum_{\mathrm{i}=1}^{\mathrm{n}} \mathbf{l}\left(\xi_{\mathbf{i}}>0\right) \quad \begin{gathered}
\text { \# of samples } \\
\text { not in ideal location }
\end{gathered}
$$

- where $I\left(\xi_{\mathrm{i}}>0\right)= \begin{cases}1 & \text { if } \xi_{\mathrm{i}}>0 \\ 0 & \text { if } \xi_{\mathrm{i}} \leq 0\end{cases}$
- constrained to $\mathbf{z}_{\mathbf{i}}\left(\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}\right) \geq 1-\xi_{\mathbf{i}}$ and $\xi_{\mathrm{i}} \geq 0 \quad \forall \mathbf{i}$
- $\boldsymbol{\beta}$ measures relative weight of first and second terms
- if $\beta$ is small, we allow a lot of samples not in ideal position
- if $\beta$ is large, we allow very few samples not in ideal position
- choosing $\beta$ appropriately is important


## SVM: Non Separable Case

$$
\mathbf{J}\left(\mathbf{w}, \xi_{1}, \ldots, \xi_{n}\right)=\frac{1}{2}\|\mathbf{w}\|^{2}+\beta \sum_{i=1}^{n} \mathbf{l}\left(\xi_{i}>0\right)
$$

\# of samples not in ideal location

large $\beta$, few samples not in ideal position
small $\beta$, many samples not in ideal position

## SVM: Non Separable Case

- Minimization problem is NP-hard due to discontinuity of $\mathbf{I}\left(\xi_{\mathrm{i}}\right)$

$$
\mathbf{J}\left(\mathbf{w}, \xi_{1}, \ldots, \xi_{n}\right)=\frac{1}{2}\|\mathbf{w}\|^{2}+\beta \sum_{i=1}^{n} \mathbf{I}\left(\xi_{i}>0\right) \quad \begin{gathered}
\text { \# of samples } \\
\text { not in ideal location }
\end{gathered}
$$

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


## SVM: Non Separable Case

- Instead we minimize

$$
\begin{aligned}
& \qquad \mathbf{J}\left(\mathbf{w}, \xi_{1}, \ldots, \xi_{\mathbf{n}}\right)=\frac{1}{2}\|\mathbf{w}\|^{2}+\beta \sum_{\mathbf{i}=1}^{\mathrm{n}} \xi_{\mathbf{i}} \quad \begin{array}{r}
\text { a measure of misclassified } \\
\text { examples }
\end{array} \\
& \text { - constrained to } \begin{cases}\mathbf{z}_{\mathbf{i}}\left(\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}\right) \geq 1-\xi_{\mathbf{i}} & \forall \mathbf{i} \\
\xi_{\mathbf{i}} \geq 0 & \forall \mathbf{i}\end{cases}
\end{aligned}
$$

- Use Kuhn-Tucker theorem to converted to

$$
\begin{aligned}
\text { maximize } & \mathbf{L}_{D}(\alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{i} z_{i} z_{j} x_{i}^{t} \mathbf{x}_{j} \\
\text { constrained to } & 0 \leq \alpha_{i} \leq \beta \quad \forall i \text { and } \sum_{i=1}^{n} \alpha_{i} z_{i}=0
\end{aligned}
$$

- find w using

$$
\mathbf{w}=\sum_{i=1}^{n} \alpha_{i} \mathbf{z}_{i} \mathbf{x}_{\mathrm{i}}
$$

- solve for $\mathbf{w}_{0}$ using any $0<\alpha_{i}<\boldsymbol{\beta}$ and $\alpha_{i}\left[z_{i}\left(\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}\right)-1\right]=0$


## 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 low-dimensional space"
- Not linearly separable in 1D
- Lift to 2 D space with $\mathbf{h ( x )}=\left(\mathbf{x}, \mathbf{x}^{\mathbf{2}}\right)$



## Non Linear Mapping

- To solve a non linear problem with a linear classifier

1. Project data $\boldsymbol{x}$ to high dimension using function $\varphi(\mathbf{x})$
2. Find a linear discriminant function for transformed data $\varphi(\mathbf{x})$
3. Final nonlinear discriminant function is $\mathbf{g}(\mathbf{x})=\mathbf{w}^{\mathbf{t}} \varphi(\mathbf{x})+\mathbf{w}_{0}$


- In 2D, discriminant function is linear

$$
\mathbf{g}\left(\left[\begin{array}{l}
\mathbf{x}^{(1)} \\
\mathbf{x}^{(2)}
\end{array}\right]\right)=\left[\begin{array}{ll}
\mathbf{w}_{1} & \mathbf{w}_{2}
\end{array}\right]\left[\begin{array}{l}
\mathbf{x}^{(1)} \\
\mathbf{x}^{(2)}
\end{array}\right]+\mathbf{w}_{0}
$$

- In 1D, discriminant function is not linear

$$
\mathbf{g}(\mathbf{x})=\mathbf{w}_{1} \mathbf{x}+\mathbf{w}_{2} \mathbf{x}^{2}+\mathbf{w}_{0}
$$

## Non Linear Mapping: Another Example



- 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" by
- enforcing largest margin permits good generalization
- computation in the higher dimensional case is performed only implicitly through the use of kernel functions


## Non Linear SVM: Kernels

- Recall SVM optimization
maximize

$$
L_{D}(\alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{i} z_{i} z_{i} \mathbf{z}_{i}^{t} \mathbf{x}_{j}
$$

- Optimization depends on samples $\boldsymbol{x}_{\boldsymbol{i}}$ only through the dot product $\boldsymbol{x}_{i}^{\boldsymbol{t}_{j}}$
- If we lift $\boldsymbol{x}_{\boldsymbol{i}}$ to high dimension using $\boldsymbol{\varphi}(\mathbf{x})$, need to compute high dimensional product $\boldsymbol{\varphi}\left(x_{i}\right)^{t} \boldsymbol{\varphi}\left(x_{j}\right)$

$$
\begin{array}{r}
\operatorname{maximize} \quad \mathbf{L}_{\mathrm{D}}(\alpha)=\sum_{\mathrm{i}=1}^{n} \alpha_{\mathrm{i}}-\frac{1}{2} \sum_{\mathrm{i}=1}^{n} \sum_{\mathrm{j}=1}^{n} \alpha_{\mathrm{i}} \alpha_{i} \mathbf{z}_{\mathrm{i}} \mathbf{z}_{\mathbf{j}} \varphi\left(\mathbf{x}_{\mathrm{i}}\right)^{\mathrm{t}} \varphi\left(\mathbf{x}_{\mathbf{j}}\right) \\
K\left(\mathbf{x}_{\mathrm{i}}, \mathbf{x}_{\mathrm{j}}\right)
\end{array}
$$

- Idea: find kernel function $K\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathrm{j}}\right)$ s.t. $\mathrm{K}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right)=\boldsymbol{\varphi}\left(\mathbf{x}_{\mathbf{i}}\right)^{\mathbf{t}} \boldsymbol{\varphi}\left(\mathbf{x}_{\mathrm{j}}\right)$


## Non Linear SVM: Kernels

maximize

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

- Kernel trick
- only need to compute $\mathbf{K}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right)$ instead of $\boldsymbol{\varphi}\left(\mathbf{x}_{\mathrm{i}}\right)^{\mathbf{t}} \boldsymbol{\varphi}\left(\mathbf{x}_{\mathrm{j}}\right)$
- no need to lift data in high dimension explicitely, computation is performed in the original dimension


## Non Linear SVM: Kernels

- $\quad$ Suppose we have 2 features and $\mathbf{K}(\mathbf{x}, \mathbf{y})=\left(\mathbf{x}^{\mathbf{t}} \mathbf{y}\right)^{\mathbf{2}}$
- Which mapping $\boldsymbol{\varphi}(\mathbf{x})$ does it correspond to?

$$
\left.\left.\begin{array}{rl}
\boldsymbol{K}(\mathbf{x}, \mathbf{y}) & =\left(\mathbf{x}^{\mathbf{t}} \mathbf{y}\right)^{2}=\left(\left[\begin{array}{ll}
\mathbf{x}^{(1)} & \mathbf{x}^{(2)}
\end{array}\right]\left[\begin{array}{l}
\mathbf{y}^{(1)} \\
\mathbf{y}^{(2)}
\end{array}\right]\right)^{2}=\left(\mathbf{x}^{(1)} \mathbf{y}^{(1)}+\mathbf{x}^{(2)} \mathbf{y}^{(2)}\right)^{2} \\
& =\left(\mathbf{x}^{(1)} \mathbf{y}^{(1)}\right)^{2}+2\left(\mathbf{x}^{(1)} \mathbf{y}^{(1)}\right)\left(\mathbf{x}^{(2)} \mathbf{y}^{(2)}\right)+\left(\mathbf{x}^{(2)} \mathbf{y}^{(2)}\right)^{2} \\
& =\left[\begin{array}{llll}
\left(\mathbf{x}^{(1)}\right)^{2} & \sqrt{2} \mathbf{x}^{(1)} \mathbf{x}^{(1)} \mathbf{x}^{(2)} & \left(\mathbf{x}^{(2)}\right)^{2}
\end{array}\right]\left[\left(\mathbf{y}^{(1)}\right)^{2}\right. \\
\sqrt{2} \mathbf{y}^{(1)} \mathbf{y}^{(1)} \mathbf{y}^{(2)} & \left(\mathbf{y}^{(2)}\right)^{2}
\end{array}\right]^{\mathbf{t}}\right]
$$

Thus

$$
\varphi(\mathbf{x})=\left[\begin{array}{lll}
\left(\mathbf{x}^{(1)}\right) & \sqrt{2} \mathbf{x}^{(1)} \mathbf{x}^{(2)} & \left(\mathbf{x}^{(2)}\right)
\end{array}\right]
$$



## Non Linear SVM: Kernels

- How to choose kernel $K\left(\mathbf{x}_{\mathrm{i}}, \mathbf{x}_{\mathrm{j}}\right)$ ?
- $\quad \mathbf{K}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathrm{j}}\right)$ should correspond to product $\boldsymbol{\varphi}\left(\boldsymbol{x}_{i}\right)^{\boldsymbol{t}} \boldsymbol{\varphi}\left(\boldsymbol{x}_{j}\right)$ in a higher dimensional space
- Mercer's condition states 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
- Common choices satisfying Mercer's condition
- Polynomial kernel $\mathbf{K}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right)=\left(\mathbf{x}_{\mathbf{i}}^{\mathbf{t}} \mathbf{x}_{\mathbf{j}}+1\right)^{\mathbf{p}}$
- Gaussian radial Basis kernel (data is lifted in infinite dimensions)

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

## Non Linear SVM

- search for separating hyperplane in high dimension

$$
\mathbf{w} \varphi(\mathbf{x})+\mathbf{w}_{0}=0
$$

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

$$
\varphi(\mathbf{x})=\left[\begin{array}{llll}
1 & \mathbf{x}^{(1)} & \mathbf{x}^{(2)} & \mathbf{x}^{(1)} \mathbf{x}^{(2)}
\end{array}\right]^{\mathrm{t}}
$$

- Threshold $\mathbf{w}_{0}$ gets folded into vector $\mathbf{w}$

$$
\begin{gathered}
{\left[\begin{array}{ll}
\mathbf{w}_{0} & \mathbf{w}
\end{array}\right]\left[\begin{array}{l}
1 \\
*
\end{array}\right]=0} \\
\varphi(\mathbf{x})
\end{gathered}
$$

## Non Linear SVM

## Thus seeking hyperplane

$$
\mathbf{w} \varphi(\mathbf{x})=0
$$

Or, equivalently, a hyperplane that goes through the origin in high dimensions

- removes only one degree of freedom
- but we introduced many new degrees when lifted the data in high dimension


## Non Linear SVM Recepie

- Start with $\mathbf{x}_{1}, \ldots, \mathbf{x}_{\mathbf{n}}$ in original feature space of dimension $\mathbf{d}$
- Choose kernel $\mathbf{K}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right)$
- implicitly chooses function $\boldsymbol{\varphi}\left(\mathbf{x}_{\mathbf{i}}\right)$ that takes $\mathbf{x}_{\mathbf{i}}$ to a higher dimensional space
- gives dot product in the high dimensional space

Find largest margin linear classifier in the higher dimensional space by using quadratic programming package to solve
maximize $\quad \mathbf{L}_{\mathbf{D}}(\alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{i} \mathbf{i}_{i}, \mathbf{j} \mathbf{k}\left(\mathbf{x}_{i}, \mathbf{x}_{\mathrm{j}}\right)$
constrained to

$$
0 \leq \alpha_{i} \leq \beta \quad \forall i \text { and } \sum_{i=1}^{n} \alpha_{i} \mathbf{z}_{i}=0
$$

## Non Linear SVM Recipe

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

$$
\mathbf{w}=\sum_{\mathbf{x}_{\mathrm{i}} \in S} \alpha_{\mathrm{i}} \mathbf{z}_{\mathrm{i}} \varphi\left(\mathbf{x}_{\mathrm{i}}\right)
$$

- where $\boldsymbol{S}$ is the set of support vectors

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

- Linear discriminant function in the high dimensional space

$$
\mathbf{g}(\varphi(\mathbf{x}))=\mathbf{w}^{\mathbf{t}} \varphi(\mathbf{x})=\left(\sum_{\mathbf{x}_{\mathbf{i}} \in \mathbf{S}} \alpha_{\mathbf{i}} \mathbf{z}_{\mathrm{i}} \varphi\left(\mathbf{x}_{\mathbf{i}}\right)\right)^{\mathbf{t}} \varphi(\mathbf{x})
$$

- Non linear discriminant function in the original space:

$$
\mathbf{g}(\mathbf{x})=\left(\sum_{x_{i} \in S} \alpha_{i} \mathbf{z}_{i} \varphi\left(\mathbf{x}_{i}\right)\right)^{t} \varphi(\mathbf{x})=\sum_{x_{i} \in S} \alpha_{i} \mathbf{z}_{i} \varphi^{t}\left(x_{i}\right) \varphi(\mathbf{x})=\sum_{x_{i} \in S} \alpha_{i} \mathbf{z}_{i} \mathbf{K}\left(x_{i}, \mathbf{x}\right)
$$

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


## Non Linear SVM

- Nonlinear discriminant function

$$
g(x)=\sum_{v=\mathbf{q}} \alpha_{i} z_{i} K\left(x_{i}, x\right)
$$

$$
\mathbf{g ( \mathbf { x } ) = \sum _ { \begin{array} { c } 
{ \text { most important } } \\
{ \text { training samples, } } \\
{ \text { i.e. support vectors } }
\end{array} } ^ { \begin{array} { c } 
{ \text { weight of support } } \\
{ \text { vector } \mathbf { x } _ { \mathbf { i } } }
\end{array} }} \begin{array}{|c|c|}
\boldsymbol{\mp 1} & \begin{array}{c}
\text { similarity } \\
\text { between } \boldsymbol{x} \text { and } \\
\text { support vector } \mathbf{x}_{\mathbf{i}}
\end{array} \\
\hline \mathbf{K}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}\right)=\exp \left(-\frac{1}{2 \sigma^{2}}\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{x}\right\|^{2}\right)
\end{array}
$$

## 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

- $K\left(x_{i}, x_{j}\right)=\left(\mathbf{x}_{\mathrm{i}}{ }^{t} \mathbf{x}_{\mathrm{j}}+\mathbf{1}\right)^{\mathbf{2}}$
- Kernel corresponds to mapping

$$
(\mathbf{x})=\left[\begin{array}{lllll}
1 & \sqrt{2} x^{(1)} & \sqrt{2} \mathbf{x}^{(2)} & \sqrt{2} \mathbf{x}^{(1)} \mathbf{x}^{(2)} & \left(\mathbf{x}^{(1)}\right)^{2}
\end{array} \quad\left(\mathbf{x}^{(2)}\right)^{2}\right]^{\mathbf{t}}
$$

- Need to maximize $L_{D}(\alpha)=\sum_{i=1}^{4} \alpha_{i} \frac{1}{2} \sum_{i=1}^{4} \sum_{j=1}^{4} \alpha_{i} \alpha_{i} \mathbf{z}_{i} \mathbf{z}_{\mathbf{j}}\left(\mathbf{x}_{\mathbf{i}}^{\mathrm{t}} \mathbf{x}_{\mathrm{j}}+1\right)^{2}$
constrained to

$$
0 \leq \alpha_{i} \forall \mathbf{i} \text { and } \alpha_{1}+\alpha_{2}-\alpha_{3}-\alpha_{4}=0
$$

## SVM Example: XOR Problem

- Rewrite

$$
\left.\begin{array}{l}
\mathbf{L}_{\mathrm{D}}(\alpha)=\sum_{\mathrm{i}=1}^{4} \alpha_{\mathrm{i}}-\frac{1}{2} \alpha^{\mathrm{t}} \mathrm{H} \alpha \\
\mathrm{l}_{1} \\
\alpha_{2}
\end{array} \alpha_{3} \alpha_{4}\right]^{\mathrm{t}} \text { and } \mathbf{H}=\left[\begin{array}{rrrr}
9 & 1 & -1 & -1 \\
1 & 9 & -1 & -1 \\
-1 & -1 & 9 & 1 \\
-1 & -1 & 1 & 9
\end{array}\right]
$$

- Take derivative with respect to $\boldsymbol{\alpha}$ and set it to $\mathbf{0}$

$$
\frac{d}{d a} L_{D}(\alpha)=\left[\begin{array}{l}
1 \\
1 \\
1 \\
1
\end{array}\right]-\left[\begin{array}{rrrr}
9 & 1 & -1 & -1 \\
1 & 9 & -1 & -1 \\
-1 & -1 & 9 & 1 \\
-1 & -1 & 1 & 9
\end{array}\right] \alpha=0
$$

- Solution to the above is $\alpha_{1}=\alpha_{2}=\alpha_{3}=\alpha_{4}=0.25$
- $\quad$ satisfies the constraints $\forall \mathbf{i}, 0 \leq \alpha_{i}$ and $\alpha_{1}+\alpha_{2}-\alpha_{3}-\alpha_{4}=0$
- all samples are support vectors


## SVM Example: XOR Problem

$$
(\mathbf{x})=\left[\begin{array}{llllll}
1 & \sqrt{2} \mathbf{x}^{(1)} & \sqrt{2} \mathbf{x}^{(2)} & \sqrt{2} \mathbf{x}^{(1)} \mathbf{x}^{(2)} & \left(\mathbf{x}^{(1)}\right)^{2} & \left(\mathbf{x}^{(2)}\right)^{2}
\end{array}\right]^{t}
$$

- Weight vector $\mathbf{w}$ is:

$$
\begin{aligned}
\mathbf{w}=\sum_{\mathbf{i}=1}^{4} \alpha_{\mathbf{i}} \mathbf{z}_{\mathbf{i}} \varphi\left(\mathbf{x}_{\mathbf{i}}\right) & =0.25\left(\varphi\left(\mathbf{x}_{1}\right)+\varphi\left(\mathbf{x}_{2}\right)-\varphi\left(\mathbf{x}_{3}\right)-\varphi\left(\mathbf{x}_{4}\right)\right) \\
& =\left[\begin{array}{llllll}
0 & 0 & 0 & \sqrt{2} & 0 & 0
\end{array}\right]
\end{aligned}
$$

- by plugging in $\mathbf{x}_{1}=[1,-1], \mathbf{x}_{2}=[-1,1], \mathbf{x}_{3}=[1,1], \mathbf{x}_{4}=[-1,-1]$
- Nonlinear discriminant function is

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

## SVM Example: XOR Problem


decision boundaries nonlinear
decision boundary is linear

## Degree 3 Polynomial Kernel



- Left: In linearly separable case, decision boundary is roughly linear, indicating that dimensionality is controlled
- Right: nonseparable case is handled by a polynomial of degree 3


## SVM as Unconstrained Minimization

- SVM formulated as constrained optimization, minimize

$$
\begin{aligned}
& \mathrm{s}\left(\mathbf{w}, \xi_{1}, \ldots, \xi_{n}\right)=\frac{1}{2}\|\mathbf{w}\|^{2}+\beta \sum_{i=1}^{n} \xi_{i} \\
& \text { - constrained to } \quad \begin{cases}\mathbf{z}_{\mathbf{i}}\left(\mathbf{w}^{+} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}\right) \geq 1-\xi_{\mathbf{i}} & \forall \mathbf{i} \\
\xi_{\mathbf{i}} \geq 0 & \forall \mathbf{i}\end{cases}
\end{aligned}
$$

- Let us name $\mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)=\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}$
- The constraint can be rewritten as $\begin{cases}\mathbf{z}_{\mathbf{i}} f\left(\mathbf{x}_{\mathbf{i}}\right) \geq 1-\xi_{\mathrm{i}} & \forall \mathbf{i} \\ \xi_{i} \geq 0 & \forall \mathbf{i}\end{cases}$
- Which implies $\xi_{\mathrm{i}}=\max \left(0,1-\mathbf{z}_{\mathrm{i}} \mathbf{f}\left(\mathbf{x}_{\mathrm{i}}\right)\right)$
- SVM objective can be rewritten as unconstrained optimization

$$
\mathbf{J}\left(\mathbf{w}, \xi_{1}, \ldots, \xi_{\mathbf{n}}\right)=\underbrace{\frac{1}{2}\|\mathbf{w}\|^{2}}_{\begin{array}{c}
\text { weights } \\
\text { regularization }
\end{array}}+\beta \underbrace{\beta}_{\text {loss function }} \sum_{i=1}^{n} \max \left(0,1-\mathbf{z}_{\mathbf{i}} \mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)\right)
$$

## SVM as Unconstrained Minimization

- SVM objective can be rewritten as unconstrained optimization

$$
\mathbf{J}(\mathbf{w})=\underbrace{\frac{1}{2}\|\mathbf{w}\|^{2}+\beta}_{\begin{array}{c}
\text { weights } \\
\text { regularization }
\end{array}} \underbrace{}_{\text {loss function }} \sum_{i=1}^{\operatorname{n}} \max \left(0,1-\mathbf{z}_{\mathbf{i}} \mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)\right)
$$

- $\mathbf{z}_{\mathrm{i}} \mathrm{f}\left(\mathbf{x}_{\mathrm{i}}\right)>1$ : $\mathrm{x}_{\mathrm{i}}$ is on the right side of the hyperplane and outside margin, no loss
- $\mathrm{z}_{\mathrm{i}} \mathrm{f}\left(\mathrm{x}_{\mathrm{i}}\right)=1$ : $\mathrm{x}_{\mathrm{i}}$ on the margin, no loss
- $\mathbf{z}_{\mathrm{i}} \mathrm{f}\left(\mathrm{x}_{\mathrm{i}}\right)<1: \mathrm{x}_{\mathrm{i}}$ is inside margin, or on the wrong side of the hyperplane, contributes to loss



## SVM: Hinge Loss

- $\quad$ SVM uses Hinge loss per sample $\mathbf{x}_{\mathbf{i}}$

$$
\mathbf{L}_{\mathbf{i}}\left(\mathbf{x}_{\mathbf{i}}\right)=\max \left(0,1-\mathbf{z}_{\mathbf{i}} \mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)\right)
$$



- $\quad$ Hinge loss encourages classification with a margin of 1


## SVM: Hinge Loss

- Can optimize with gradient descent, convex function

$$
\begin{gathered}
\mathbf{J}(\mathbf{w})=\frac{1}{2}\|\mathbf{w}\|^{2}+\beta \sum_{\mathbf{i}=1}^{\mathbf{n}} \max \left(0,1-\mathbf{z}_{\mathbf{i}} \mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)\right) \\
\mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)=\mathbf{w}^{\mathbf{t}} \mathbf{x}_{\mathbf{i}}+\mathbf{w}_{0}
\end{gathered}
$$

- Gradient

- Gradient descent, single sample

$$
\mathbf{w}=\left\{\begin{array}{cc}
\mathbf{w}-\alpha\left(\mathbf{w}-\beta \mathbf{z}_{\mathbf{i}} \mathbf{x}_{\mathbf{i}}\right) & \text { if } \mathbf{z}_{\mathbf{i}} \mathbf{f}\left(\mathbf{x}_{\mathbf{i}}\right)<1 \\
\mathbf{w}-\alpha \mathbf{w} & \text { otherwise }
\end{array}\right.
$$

## SVM Summary

- Advantages:
- nice theory
- good generalization properties
- objective function has no local minima
- can be used to find non linear discriminant functions
- often works well in practice, even if not a lot of training data
- Disadvantages:
- tends to be slower than other methods
- quadratic programming is computationally expensive

