# Support Vector Machine生醫光電所 吴育德 

## Hard-Margin Support Vector Machines

- Let $N d$-dimensional training inputs $\boldsymbol{x}_{i}(i=1, \ldots, N)$ belong to Class 1 or 2 and the labels be $y_{i}=1$ for Class 1 and -1 for Class 2 .
- If data are linearly separable, we can determine the decision function:

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

where $\mathbf{w}$ is an $d$-dimensional vector, $b$ is a bias term, $i=1, \ldots, N$

$$
\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\left\{\begin{array}{l}
>0 \text { for } y_{i}=1,  \tag{1}\\
<0 \text { for } y_{i}=-1
\end{array}\right.
$$

- Because the training data are linearly separable, no training data satisfy $\mathbf{w}^{T} \boldsymbol{x}+b=0$
- To control separability, instead of (1), we consider

$$
\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b \begin{cases}>1 & \text { for } y_{i}=1,  \tag{2}\\ <-1 & \text { for } y_{i}=-1\end{cases}
$$

Here, 1 and -1 can be replaced by a constant $a(>0)$ and $-a$.

- (2) is equivalent to

$$
y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1, i=1, \ldots, N
$$

- The hyperplane $D(x)=\mathbf{w}^{T} \boldsymbol{x}+b=\mathrm{c}$ for $-1<c<1$ forms a separating hyperplane that separates $x_{i}(i=1, \ldots, N)$.
- When $c=0$, the separating hyperplane is in the middle of the two hyperplanes with $c=1$ and -1 .
- The distance between the separating hyperplane and the training datum nearest to the hyperplane is called the margin
- The hyperplane with the maximum margin is called the optimal separating hyperplane
- The margin is a function of $\mathbf{w}$. Training the SVM consists of learning a $\mathbf{w}$ that maximizes the margin. So, margin is important.


## Optimal separating hyperplane in a two-dimensional space



## Normal distance between $\boldsymbol{x}$ and the hyperplane

- $x_{\text {proj }}$ : projection of $x$ onto the hyperplane $D(x)=0$.
- $\boldsymbol{d}$ : the normal distance between $x$ and $x_{p r o j}$.
- $\boldsymbol{x}=\boldsymbol{x}_{\text {proj }}+\boldsymbol{d} \frac{\mathbf{w}}{\|\mathbf{w}\|}$

$$
\begin{aligned}
D(x) & =\mathbf{w}^{T} \boldsymbol{x}+b \\
& =\mathbf{w}^{T}\left(x_{\text {proj }}+\boldsymbol{d} \frac{\mathbf{w}}{\|\mathbf{w}\|}\right)+b \\
& =\mathbf{w}^{T} x_{\text {proj }}+b+\boldsymbol{d} \frac{\mathbf{w}^{T} \mathbf{w}}{\|\mathbf{w}\|}=0+\boldsymbol{d}\|\mathbf{w}\| \\
\Rightarrow \boldsymbol{d} & =\frac{D(x)}{\|\mathbf{w}\|}
\end{aligned}
$$



## Cost function for obtaining the optimal separating hyperplane

$\cdot d_{+}=\left|\frac{D\left(x_{+}\right)}{\|\mathbf{w}\|}\right|=\frac{+1}{\|\mathbf{w}\|}, d_{-}=\left|\frac{D\left(x_{-}\right)}{\|\mathbf{w}\|}\right|=\left|\frac{-1}{| | \mathbf{w} \|}\right|=\frac{1}{\|\mathbf{w}\|}$

- $\operatorname{Margin}=d_{+}+d_{-}=\frac{2}{\|\mathbf{w}\|}$
- The optimal separating hyperplane can be obtained by minimizing

$$
\begin{equation*}
Q(\mathbf{w})=\frac{1}{2}\|\mathbf{w}\|^{2} \tag{3}
\end{equation*}
$$

with respect to $\mathbf{w}$ and $b$ subject to the constraints

$$
\begin{equation*}
y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1, i=1, \ldots, N \tag{4}
\end{equation*}
$$



## Optimization with $m$ inequality constraints

- Find $\boldsymbol{x}=\left[x_{1}, \cdots, x_{n}\right]^{T}$ that Minimize $F(\boldsymbol{x})$
subject to $g_{i}(\boldsymbol{x}) \leq 0, i=1, \cdots, m$
- If $x$ satisfies the inequality constraints (2), it is said to be feasible. Otherwise it is called infeasible
- The $i$ th constraint $g_{i}(\boldsymbol{x}) \leq 0$ is said to be active at a point $\boldsymbol{x}$ if $g_{i}(\boldsymbol{x})=0$.
- The constraints (2) can be converted to equality constraints by adding positive slack variables to get:

$$
\begin{align*}
& \text { Minimize } F(\boldsymbol{x})  \tag{1}\\
& \text { subject to } g_{i}(\boldsymbol{x})+y_{i}^{2}=0, i=1, \cdots, m
\end{align*}
$$

## Optimization with $m$ inequality constraints

- (1) (3) is an optimization problem with only $m$ equality constraints
- Let $\boldsymbol{y}=\left[y_{1}, \cdots, y_{m}\right]^{T}, \boldsymbol{\lambda}=\left[\lambda_{1}, \cdots, \lambda_{m}\right]^{T}$, the Lagrangian has the form:

$$
L(\boldsymbol{x}, \boldsymbol{y}, \lambda)=F(\boldsymbol{x})+\sum_{i=1}^{m} \lambda_{i}\left(g_{i}(\boldsymbol{x})+y_{i}^{2}\right)
$$

which has $\mathrm{n}+2 \mathrm{~m}$ unknown $\boldsymbol{x}^{*}, \boldsymbol{y}^{*}$ and $\boldsymbol{\lambda}^{*}$

- The optimal conditions are

$$
\begin{array}{ll}
\frac{\partial L}{\partial \boldsymbol{x}}=0 \Rightarrow \frac{\partial F(\boldsymbol{x})}{\partial \boldsymbol{x}}+\sum_{i=1}^{m} \lambda_{i} \frac{\partial g_{i}(\boldsymbol{x})}{\partial \boldsymbol{x}}=0, & \\
\frac{\partial L}{\partial y_{i}}=0 \Rightarrow 2 \lambda_{i} y_{i}=0, & i=1, \cdots, m \\
\frac{\partial L}{\partial \lambda_{i}}=0 \Rightarrow g_{i}(\boldsymbol{x})+y_{i}^{2}=0, & i=1, \cdots, m \tag{6}
\end{array}
$$

- (4)(5) (6) are usually called the Karush-Kuhn-Tucker (KKT) conditions


## Optimization with $m$ inequality constraints

- (4) $\Rightarrow \frac{\partial F(x)}{\partial x}$ is a linear combination of $\frac{\partial g_{i}(x)}{\partial x}$ with $\lambda_{i} \neq 0$
- $\lambda_{i} y_{i}=0$ (5) $\Rightarrow$ either $\lambda_{i}=0 \Rightarrow y_{i} \neq 0$ and $g_{i}(\boldsymbol{x})+y_{i}^{2}=0 \Rightarrow g_{i}(\boldsymbol{x})<0$ (inactive) or $\quad \lambda_{i} \neq 0 \Rightarrow y_{i}=0$ and $g_{i}(\boldsymbol{x})+y_{i}^{2}=0 \Rightarrow g_{i}(x)=0$ (active).

$$
\Rightarrow \lambda_{i} g_{i}(\boldsymbol{x})=0\left(\text { we will show } \lambda_{i}>0 \text { when } g_{i}(\boldsymbol{x})=0\right)
$$

- Combining (4)\& (5), one concludes that at the optimal solution, $\frac{\partial F(x)}{\partial x}$ is a linear combination of the gradients of active constraints.

An illustration of the optimality conditions for inequality constraints; the feasible region is defined by 3 constraints and at the optimal point, $g_{1}(\boldsymbol{x})$ and $g_{2}(\boldsymbol{x})$ are active. At this point, $\nabla F(\boldsymbol{x})$ is a linear function of the gradients of the active constraints $\nabla g_{1}(x), \nabla g_{2}(x)$


## Optimization with $m$ inequality constraints

- The necessary KKT condition for inequality constraints can thus be cast in the standard form

$$
\begin{array}{ll}
\frac{\partial F(\boldsymbol{x})}{\partial x_{i}}+\sum_{j=1}^{m} \lambda_{j} \frac{\partial g_{j}(\boldsymbol{x})}{\partial x_{i}}=0, & i=1, \cdots, n \\
\lambda_{j} g_{j}(\boldsymbol{x})=0, & \text { complementarity condition } j=1, \cdots, m \\
g_{j}(\boldsymbol{x}) \leq 0, & j=1, \cdots, m \\
\lambda_{j} \geq 0, & j=1, \cdots, m
\end{array}
$$

- Condition $\lambda_{j} \geq 0$ (10) for the inequality constraints $g_{j}(\boldsymbol{x}) \leq 0$ ensures $F$ will not be reduced by a move off any of the active constraints at $\boldsymbol{x}^{*}$ to the interior of the feasible region.


## Convert constrained into unconstrained optimization

- The square of the Euclidean norm w in (3) is to make the optimization problem quadratic programming.
- The assumption of linear separability means that there exist $\mathbf{w}$ and $b$ that satisfy (4). We call the solutions that satisfy (4) feasible solutions.
- We first convert the constrained problem given by (3) and (4) into the unconstrained problem

$$
\begin{equation*}
Q(\mathbf{w}, b, \boldsymbol{\alpha})=\frac{1}{2} \mathbf{w}^{T} \mathbf{w}+\sum_{i=1}^{N} \alpha_{i}\left\{1-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\} \tag{5}
\end{equation*}
$$

where $\boldsymbol{\alpha}=\left(\alpha_{1}, \ldots, \alpha_{N}\right)^{T}$ and $\alpha_{i}$ are the nonnegative Lagrange multipliers.

## Karush-Kuhn-Tucker (KKT) conditions

- The optimal solution of (5) is given by minimizing w.r.t $\mathbf{w}$ and $b$ and maximizing w.r.t $\alpha_{i}(\geq 0)$ satisfying the following KKT conditions

$$
\begin{equation*}
\frac{\partial Q(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial \mathbf{w}}=\mathbf{w}-\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{\boldsymbol{i}}=0 \Rightarrow \mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{i} \tag{*}
\end{equation*}
$$

$$
\begin{aligned}
& \frac{\partial Q(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial b}=-\sum_{i=1}^{N} \alpha_{i} y_{i}=0 \\
& \alpha_{i}\left\{1-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\}=0, \quad i=1, \ldots, N \\
& \alpha_{i} \geq 0, i=1, \ldots, N
\end{aligned}
$$

- (6) are called KKT complementarity conditions: $\alpha_{i}=0$, or $\alpha_{i}>0$ and $y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)=1$ must be satisfied.
- The training data $\boldsymbol{x}_{\boldsymbol{i}}$ with $\alpha_{i}>0$ are called support vectors
- Substituting (*) and $(* *)$ into (5), we obtain the dual problem. Maximize

$$
\begin{aligned}
& Q(\mathbf{w}, b, \boldsymbol{\alpha})=\frac{\mathbf{1}}{\mathbf{2}} \mathbf{w}^{T} \mathbf{w}+\sum_{i=1}^{N} \alpha_{i}\left\{1-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\} \\
& =\frac{1}{2} \sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{i}^{T} \sum_{j=1}^{N} \alpha_{j} y_{j} \boldsymbol{x}_{\boldsymbol{j}}+\sum_{i=1}^{N} \alpha_{i}\left\{1-y_{i}\left(\sum_{j=1}^{N} \alpha_{j} y_{j} \boldsymbol{x}_{j}^{T} \boldsymbol{x}_{i}+b\right)\right\} \\
& =\sum_{i=1}^{N} \alpha_{i}-\frac{\mathbf{1}}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j}-b \sum_{i=1}^{N} \alpha_{i} y_{i} \\
& =\sum_{i=1}^{N} \alpha_{i}-\frac{\mathbf{1}}{\mathbf{2}} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j}-b \times 0
\end{aligned}
$$

w.r.t. $\alpha_{i}$ subject to

$$
\sum_{i=1}^{N} \alpha_{i} y_{i}=0, \quad \alpha_{i} \geq 0, \quad i=1, \ldots, N
$$

- This is the dual problem and it is in terms of $\alpha_{i}$ 's only $\Rightarrow \alpha_{i}$ 's are used to get optimal $\mathbf{w}$ and $b$
- This is a convex optimization problem. It is possible to obtain $\boldsymbol{\alpha}$ vector corresponding to the global optimum. $\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{i}$.
- Many of the $\alpha_{i}$ are 0 . Support Vectors (SVs) are the $\boldsymbol{x}_{\boldsymbol{i}}{ }^{\prime}$ s corresponding to the nonzero $\alpha_{i}{ }^{\prime}$ s. Let $S=\left\{x_{i} \mid \alpha_{i}>0\right\}$ be the set of SVs.
a. By complementary slackness condition,
$\boldsymbol{x}_{i} \in S \Rightarrow \alpha_{i}>0 \Rightarrow y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{i}+b\right)=1 \Rightarrow x_{i}$ is the closest to the decision boundary.
b. Optimal $\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{i}=\sum_{x_{i} \in S} \alpha_{i} y_{i} \boldsymbol{x}_{i}$ is a linear combination of SVs.
c. $y_{i} \times y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{i}+b\right)=y_{i} \Rightarrow b=y_{i}-\mathbf{w}^{T} \boldsymbol{x}_{i}$ where $i$ is such that $\alpha_{i}>0$.
d. It is better to average the SVs : $b=\frac{1}{\#\left(\boldsymbol{x}_{i} \in S\right)} \sum_{x_{i} \in S}\left(y_{i}-\mathbf{w}^{T} \boldsymbol{x}_{i}\right)$


## Making Prediction

- Data associated with $\alpha_{i}$ 's $>0$ are support vectors for Classes 1 and 2.
- $\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} x_{i}(*)$, the decision function is (do not need to use $\mathbf{w}$ and $b$ explicitly, use $\alpha_{i}>0, y_{i}$ and $\boldsymbol{x}_{i}$ only )

$$
D(x)=\mathbf{w}^{T} x+b=\sum_{x_{i} \in S} \alpha_{i} y_{i} \boldsymbol{x}_{i}^{T} x+\left(y_{i}-\sum_{x_{i} \in S} \alpha_{i} y_{i} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{i}\right)
$$

- Then unknown datum $x$ is classified into:

$$
\left\{\begin{array}{l}
\text { Class } 1, \text { if } D(x)>0 \\
\text { Class } 2, \text { if } D(x)<0
\end{array}\right.
$$

If $D(x)=0, x$ is on the boundary and thus is unclassifiable

## Example

- Consider a linearly separable case shown in Fig. 2.2, $\left(x_{1}, y_{1}\right)=(-1,1)$, $\left(x_{2}, y_{2}\right)=(0,-1),\left(x_{3}, y_{3}\right)=(1,-1)$, The inequality constraints given by $y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1, i=1, \ldots, 3$ are

$$
-w+b \geq 1,-b \geq 1,-(w+b) \geq 1
$$

- The region of $(w, b)$ that satisfies $(* * *)$ are given by the shaded region in Fig. 2.3. Thus the solution that minimizes $\|w\|^{2}$ is given by
$b=-1, w=-2$.
- The decision function is $D(x)=-2 x-1$
- The class boundary is $x=-1 / 2$
- $x=0$ and -1 are support vectors


Fig. 2.2. Linearly separable one-dimensional case


Fig. 2.3. Region that satisfies constraints

- The dual problem is to maximize

$$
\begin{gathered}
Q(\boldsymbol{\alpha})=\sum_{i=1}^{3} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j},\left(x_{1}, y_{1}\right)=(-1,1),\left(x_{2}, y_{2}\right)=(0,-1),\left(x_{3}, y_{3}\right)=(1,-1) \\
=\alpha_{1}+\alpha_{2}+\alpha_{3}-\frac{1}{2}\left\{\alpha_{1}^{2} 1^{2}(-1)^{2}+\alpha_{1} \alpha_{2}(-1) 0+\alpha_{1} \alpha_{3}(-1)(-1)+\right. \\
\alpha_{2} \alpha_{1}(-1) 0+\alpha_{2}^{2}(-1)^{2}(0)^{2}+\alpha_{2} \alpha_{3}(-1)(-1) 0+ \\
\left.\alpha_{3} \alpha_{1}(-1)(-1)+\alpha_{3} \alpha_{2}(-1)^{2} 0+\alpha_{3}^{2}(-1)^{2} 1\right\} \\
=\alpha_{1}+\alpha_{2}+\alpha_{3}-\frac{1}{2}\left(\alpha_{1}+\alpha_{3}\right)^{2} \quad(* * * *)
\end{gathered}
$$

subject to

$$
\sum_{i=1}^{3} \alpha_{i} y_{i}=\alpha_{1}-\alpha_{2}-\alpha_{3}=0, \alpha_{i} \geq 0, i=1, \ldots, 3
$$

- Substituting $\alpha_{2}=\alpha_{1}-\alpha_{3}$ into ( $* * * *$ ), we obtain
$Q(\boldsymbol{\alpha})=2 \alpha_{1}-\frac{1}{2}\left(\alpha_{1}+\alpha_{3}\right)^{2}$ subject to $\alpha_{i} \geq 0, i=1, \ldots, 3$
which is maximized when $\alpha_{3}=0$, since $\alpha_{3} \geq 0$
- Now $Q(\alpha)=2 \alpha_{1}-\frac{1}{2} \alpha_{1}{ }^{2}=-\frac{1}{2}\left(\alpha_{1}-2\right)^{2}+2, \alpha_{1} \geq 0$
which is maximized for $\alpha_{1}=2$.
- The optimal solution for $(* * * *)$ is $\alpha_{1}=2, \alpha_{3}=0, \alpha_{2}=\alpha_{1}-\alpha_{3}=2$
- Therefore $x=-1\left(\alpha_{1}=2>0\right)$ and $0\left(\alpha_{2}=2>0\right)$ are support vectors and $w=\sum_{i=1}^{3} \alpha_{i} y_{i} x_{i}=2(1)(-1)+2(-1) 0+0(-1)(1)=-2$ and $b=y_{i}-w^{T} x_{i}=y_{1}-(-2) x_{1}=1-(-2)(-1)=-1\left(\alpha_{1}=2>0, x_{1}\right.$ is a support vector $\left.\Rightarrow y_{1}\left(w^{T} x_{1}+b\right)=1\right)$, which are the same as the solution obtained by solving the primary problem.
- Consider changing the label of $x_{3}$ into that of the opposite class, i.e., $y_{3}=$ 1. Then the problem becomes inseparable and last inequality in ( $* * *$ ) becomes $w+b \geq 1$. Thus, from Fig 2.3 there is no feasible solution.

Decision boundary and support vectors for a linear SVM (svmhard.m)


```
%% svmhard.m
% From A First Course in Machine Learning, Chapter 5.
% Simon Rogers, 01/11/11 [simon.rogers@glasgow.ac.uk]
% Hard margin SVM
clear all;close all;
%% Generate the data
x = [randn (20, 2); randn (20, 2) +4];
t = [repmat (-1,20,1);repmat (1, 20,1)];
%% Plot the data
ma = {'ko','ks'};
fc = {[0 0 0],[[1 1 1]}};
tv = unique(t);
figure(1); hold off
for i = 1:length(tv)
    pos = find(t==tv(i));
    plot(x(pos,1),x(pos,2),ma{i},'markerfacecolor',fc{i});
    hold on
end
```

\%\% Setup the optimisation problem
$\mathrm{N}=\operatorname{size}(\mathrm{x}, 1)$;
$\mathrm{K}=\mathrm{x}^{*} \mathrm{X}^{\prime}$;
H = (t*t').*K + 1e-5*eye (N);
f = repmat(1,N,1);

$$
Q(\mathbf{w}, b, \boldsymbol{\alpha})=\sum_{i=1}^{N} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j}
$$

$$
\sum_{i=1}^{N} \alpha_{i} y_{i}=0, \quad \alpha_{i} \geq 0, \quad i=1, \ldots, N
$$

$\mathrm{A}=[] ; \mathrm{b}=[] ;$
$\mathrm{LB}=\operatorname{repmat}(0, \mathrm{~N}, 1) ; \mathrm{UB}=\operatorname{repmat}(\mathrm{inf}, \mathrm{N}, 1)$;
Aeq = t';beq = 0;
\% Following line runs the SVM
alpha = quadprog(H,-f,A,b,Aeq,beq, LB, UB);
\% Compute the bias
fout $=\operatorname{sum}(r e p m a t(a l p h a . * t, 1, N) . * K, 1) ' ;$ pos $=$ find (alpha>1e-6); $\quad \alpha_{i}$ 's $>0$ are support vectors

$$
\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{\boldsymbol{i}}
$$

bias $=$ mean(t(pos)-fout(pos));

$$
b=\frac{1}{\#\left(\boldsymbol{x}_{i} \in S\right)} \sum_{x_{i} \in S}\left(y_{i}-\mathbf{w}^{T} \boldsymbol{x}_{i}\right)
$$

$S=\left\{x_{i} \mid \alpha_{i}>0\right\}$ be the set of SVs

```
%% Plot the data, decision boundary and Support vectors
figure(1);hold off
pos = find(alpha>1e-6); 和's>0 are support vectors for Classes 1 and 2
plot(x(pos,1),x(pos,2),'ko','markersize',15,'markerfacecolor',[0.6 0.6 0.6],...
    'markeredgecolor',[0.6 0.6 0.6]);
hold on
for i = 1:length(tv)
    pos = find(t==tv(i));
    plot(x(pos,1),x(pos,2),ma{i},'markerfacecolor',fc{i});
end
xp = xlim;
% Because this is a linear SVM, we can compute w and plot the decision
% boundary exactly.
w = sum(repmat(alpha.*t,1,2).*x,1)';
yp = -(bias + w(1)*xp)/w(2);
plot(xp,yp,'k','linewidth',2)
\[
\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} x_{i}
\]
```


## Soft-Margin Support Vector Machines

- When linearly inseparable, there is no feasible solution, and the hard-margin support vector machine is unsolvable.
- The SVM is extended to inseparable case.
- Introduce slack variables $\xi_{i} \geq 0$ into $y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1$.
$\Rightarrow y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1-\xi_{i}, i=1, \ldots, N$

If $\xi_{i}<1$, this data is correctly classified.
If $\xi_{i} \geq 1$, this data is misclassified.


- Minimize $Q(\mathbf{w})=\frac{\mathbf{1}}{\mathbf{2}}\|\mathbf{w}\|^{2}+\sum_{i=1}^{N} \theta\left(\xi_{i}\right), \theta\left(\xi_{i}\right)=\left\{\begin{array}{l}1, \text { for } \xi_{i}>0 \\ 0, \text { for } \xi_{i}=0\end{array}\right.$ subject to $y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1-\xi_{i}, i=1, \ldots, N$
- This is a combinatorial optimization and difficult to solve
- Instead, we minimize $Q(\mathbf{w}, \mathbf{b}, \boldsymbol{\xi})=\frac{1}{2}\|\mathbf{w}\|^{2}+\mathrm{C} \sum_{i=1}^{N} \xi_{i}{ }^{p}, \xi_{i} \geq 0$

$$
\text { subject to } \quad y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right) \geq 1-\xi_{i}, i=1, \ldots, N
$$

where $\xi=\left(\xi_{1}, \ldots, \xi_{N}\right)^{\mathbf{T}}, C$ determines the trade-off between the maximization of margin and minimization of classification error, and $p=1\left(l_{1}\right.$ soft-margin SVM), or 2( $l_{2}$ soft-margin SVM)

- We call the obtained hyperplane the soft-margin hyperplane.
- Introduce the nonnegative Lagrange multipliers $\alpha_{i}$ and $\beta_{i}$, we obtain ( $\mathrm{p}=1$ ) $Q(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})=\frac{\mathbf{1}}{\mathbf{2}} \mathbf{w}^{T} \mathbf{w}+\mathrm{C} \sum_{i=1}^{N} \xi_{i}+\sum_{i=1}^{N} \alpha_{i}\left\{1-\xi_{i}-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\}$

$$
\begin{equation*}
+\sum_{i=1}^{N} \beta_{i}\left(-\xi_{i}\right), i=1, \ldots, N \tag{1}
\end{equation*}
$$

- For the optimal solution, the following KKT conditions are satisfied

$$
\begin{align*}
& \frac{\partial Q(\mathbf{w}, b, \xi, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \mathbf{W}}=\mathbf{w}-\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{\boldsymbol{i}}  \tag{*}\\
& \frac{\partial Q(\mathbf{w}, b, \xi, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial b}=-\sum_{i=1}^{N} \alpha_{i} y_{i}=0
\end{align*}
$$

$$
\frac{\partial Q(\mathbf{w}, b, \xi, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \xi_{i}}=\mathrm{C}-\alpha_{i}-\beta_{i}=0 \quad \Rightarrow \alpha_{i}+\beta_{i}=\mathrm{C}, i=1, \ldots, N(* * *)
$$

$$
\begin{equation*}
\alpha_{i}\left\{1-\xi_{i}-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\}=0, \quad i=1, \ldots, N \tag{2}
\end{equation*}
$$

$$
\begin{equation*}
\beta_{i} \xi_{i}=0, \quad i=1, \ldots, N \tag{3}
\end{equation*}
$$

$$
\alpha_{i} \geq 0, \beta_{i} \geq 0, \xi_{i} \geq 0, \quad i=1, \ldots, N
$$

- Substituting $(*),(* *),(* * *)$ into (1), we obtain the dual problem.

Maximize

$$
\begin{aligned}
Q(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})= & \frac{1}{2} \mathbf{w}^{T} \mathbf{w}+\sum_{i=1}^{N} \xi_{i}\left(\alpha_{i}+\beta_{i}\right)+\sum_{i=1}^{N} \alpha_{i}\left\{1-\xi_{i}-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\} \\
& \quad+\sum_{i=1}^{N} \beta_{i}\left(-\xi_{i}\right), \\
= & \frac{\mathbf{1}}{2} \mathbf{w}^{T} \mathbf{w}+\sum_{i=1}^{N} \alpha_{i}\left\{1-y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)\right\} \\
= & \sum_{i=1}^{N} \alpha_{i}-\frac{\mathbf{1}}{\mathbf{2}} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j}
\end{aligned}
$$

with respect to $\alpha_{i}$ subject to the constraints

$$
\sum_{i=1}^{N} \alpha_{i} y_{i}=0, \mathrm{C} \geq \alpha_{i} \geq 0, i=1, \ldots, N
$$

- The only difference between $l_{1}$ soft-margin SVM and hard margin SVM is that $\alpha_{i}$ cannot exceed $C$ (since $\alpha_{i}+\beta_{i}=\mathrm{C}, \beta_{i} \geq 0$ ).
- Especially, (2) and (3) are called KKT (complementarity) conditions
- From $\alpha_{i}+\beta_{i}=\mathrm{C}, \beta_{i} \xi_{i}=0$ and (2) there are three cases for $\alpha_{i}$ :

1. $\alpha_{i}=0$. Then $\beta_{i}=\mathrm{C}, \xi_{i}=0$. Thus $\boldsymbol{x}_{\boldsymbol{i}}$ is correctly classified
2. $0<\alpha_{i}<C$. Then (2) $\Rightarrow y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)-1+\xi_{i}=0$, and $\beta_{i} \neq 0, \Rightarrow \xi_{i}=0$. Therefore, $y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)=1$ and $\boldsymbol{x}_{\boldsymbol{i}}$ is a support vector. We call the support vector with $C>\alpha_{i}>0$ a good (unbounded) SV.
3. $\alpha_{i}=C$. Then (2) $\Rightarrow y_{i}\left(\mathbf{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}+b\right)-1+\xi_{i}=0$ and $\xi_{i} \geq 0$. Thus $\boldsymbol{x}_{\boldsymbol{i}}$ is a support vector. We call the support vector with $\alpha_{i}=C$ a bad (bounded) SV.
If $0 \leq \xi_{i}<1, \boldsymbol{x}_{\boldsymbol{i}}$ is correctly classified.
If $\xi_{i} \geq 1, \boldsymbol{x}_{\boldsymbol{i}}$ is misclassified

- Data associated with $S=\left\{\boldsymbol{x}_{i} \mid C \geq \alpha_{i}>0\right\}$ are SVs for Classes 1 and 2. Then from $\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} \boldsymbol{x}_{i} \quad(*)$, the decision function is

$$
D(x)=\mathbf{w}^{T} x+b=\sum_{x_{i} \in S} \alpha_{i} y_{i} x_{i}^{T} x+b
$$

- For the unbounded $\alpha_{i}, b=y_{i}-\mathbf{w}^{T} \boldsymbol{x}_{i}$ is satisfied.
- To ensure the precision of calculations, we take the average of $b$ that is calculated for unbounded support vectors, $b=\frac{1}{\#\left(\boldsymbol{x}_{i} \in G\right)} \sum_{x_{i} \in G}\left(y_{i}-\mathbf{w}^{T} \boldsymbol{x}_{i}\right)$ where $G$ is the set of good support vector
- Then unknown datum $x$ is classified into:

$$
\left\{\begin{array}{l}
\text { Class } 1, \text { if } D(x)>0 \\
\text { Class } 2, \text { if } D(x)<0
\end{array}\right.
$$

If $D(x)=0, x$ is on the boundary and thus is unclassifiable

```
% From A First Course in Machine Learning, Chapter 5.
% Simon Rogers, 01/11/11 [simon.rogers@glasgow.ac.uk]
% Soft margin SVM
clear all;close all;
%% Generate the data
x = [randn (20, 2); randn (20, 2) +4];
t = [repmat (-1,20,1);repmat(1, 20,1)];
% Add a bad point
x = [x;2 1];
t = [t;1];
%% Plot the data
ma = {'ko','ks'};
fc}={[0000]\mp@code{,[[1 1 1 1]};
tv = unique(t);
figure(1); hold off
for i = 1:length(tv)
    pos = find(t==tv(i));
    plot(x(pos,1),x(pos,2),ma{i},'markerfacecolor',fc{i});
    hold on
end
```

```
%% Setup the optimisation problem
N = size(x,1);
K = X* X';
H=(t*t').*K + 1e-5*eye(N);
f = repmat(1,N,1);
A = [];b = [];
LB = repmat (0,N,1);
UB = repmat(inf,N,1);
Aeq = t';beq = 0;
```

\% Loop over various values of the margin parameter
Cvals $=\left[\begin{array}{llllllll}10 & 5 & 2 & 0.5 & 0.1 & 0.05 & 0.01] ;\end{array}\right.$
for $C V=1: l e n g t h(C v a l s) ;$
$\%$
$\mathrm{UB}=$ repmat (Cvals (Cv), $\mathrm{N}, 1)$;
\% Following line runs the SVM
alpha $=$ quadprog $(H,-f, A, b, A e q, b e q, L B, U B)$;
\% Compute the bias
fout $=$ sum(repmat (alpha.*t, 1,N).*K, 1)';
pos $=$ find (alpha>1e-6); $\alpha_{i} ’ s>0$ are support vectors
bias $=$ mean (t (pos) -fout (pos));

$$
\begin{array}{r}
Q(\mathbf{w}, b, \boldsymbol{\alpha})=\sum_{i=1}^{N} \alpha_{i}-\frac{\mathbf{1}}{\mathbf{2}} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j} \\
\sum_{i=1}^{N} \alpha_{i} y_{i}=0, \quad \mathrm{C} \geq \alpha_{i} \geq 0, \quad i=1, \ldots, N
\end{array}
$$

$$
\begin{aligned}
\mathbf{w} & =\sum_{i=1}^{N} \alpha_{i} y_{i} x_{i} \\
b & =\frac{1}{\#\left(\boldsymbol{x}_{i} \in G\right)} \sum_{x_{i} \in G}\left(y_{i}-\mathbf{w}^{T} \boldsymbol{x}_{i}\right) \\
G & =\left\{x_{i} \mid \mathrm{C}>\alpha_{i}>0\right\}
\end{aligned}
$$

\%\% Plot the data, decision boundary and Support vectors
figure (1);hold off
pos $=$ find (alpha>1e-6);
plot(x (pos,1),x(pos,2),'ko','markersize',15,'markerfacecolor', [0.6 0.6 0.6],...
'markeredgecolor', [0.6 0.6 0.6]);
hold on
for $i=1: l e n g t h(t v)$
pos $=$ find (t==tv(i));
plot (x (pos, 1) , x (pos, 2) , ma\{i\},'markerfacecolor',fc\{i\});
end
$\mathrm{xp}=\mathrm{xlim} ;$
$y l=y l i m ;$
\% Because this is a linear SVM, we can compute w and plot the decision
\% boundary exactly.
$\mathrm{w}=\operatorname{sum}($ repmat (alpha.*t,1,2) .*x,1)';
$\mathrm{yp}=-(\mathrm{bias}+\mathrm{w}(1) * \mathrm{xp}) / \mathrm{w}(2) ;$
plot(xp,yp,'k','linewidth', 2);
ylim(yl);
$\mathbf{w}=\sum_{i=1}^{N} \alpha_{i} y_{i} x_{i}$
ti $=$ sprintf('C: \%g',Cvals(cv));
title(ti);
pause
end



## Mapping to a High-Dimensional Space: Kernel Tricks

- If the training data are not linearly separable, to enhance linear separability, the original input space is mapped into a highdimensional dot-product space called the feature space.



Nonlinear decision boundary

- Using a nonlinear $\boldsymbol{g}(\boldsymbol{x})=\left(g_{1}(\boldsymbol{x}), \ldots, g_{l}(\boldsymbol{x})\right)^{\mathbf{T}}$, that maps the $d$-dimensional input vector $\boldsymbol{x}$ into the $l$-dimensional feature space
- The linear decision function

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

where $\mathbf{w} \in \mathbb{R}^{l}$ and $b$ is a bias term.

- According to the Hilbert-Schmidt theory, if a symmetric $H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)$ satisfies

$$
\begin{equation*}
\sum_{i, j=1}^{N} h_{i} h_{j} H\left(\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{x}_{\boldsymbol{j}}\right) \geq 0 \tag{1}
\end{equation*}
$$

for all $N, \boldsymbol{x}_{\boldsymbol{i}}$, and $h_{i}$, where $h_{i} \in \mathbb{R}, \exists$ a $\boldsymbol{g}(\boldsymbol{x})$ that maps $\mathbf{x}$ into the dot-product feature space

$$
\begin{equation*}
H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)=\boldsymbol{g}(\boldsymbol{x})^{T} \boldsymbol{g}\left(\boldsymbol{x}^{\prime}\right) \tag{2}
\end{equation*}
$$

- If (2) is satisfied,

$$
\begin{equation*}
\sum_{i, j=1}^{N} h_{i} h_{j} H\left(\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{x}_{\boldsymbol{j}}\right)=\left(\sum_{i=1}^{N} \boldsymbol{g}\left(\boldsymbol{x}_{\boldsymbol{i}}\right)^{T} h_{i}\right)\left(\sum_{j=1}^{N} \boldsymbol{g}\left(\boldsymbol{x}_{\boldsymbol{j}}\right) h_{j}\right) \geq 0 \tag{3}
\end{equation*}
$$

- (1) or (3) is called Mercer's condition, and function satisfies (1) or (3) is called positive semidefinite kernel or the Mercer kernel or simply the kernel.
- Using the kernel, the dual problem in the feature space is

Maximize $Q(\boldsymbol{\alpha})=\sum_{i=1}^{N} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} H\left(\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{x}_{\boldsymbol{j}}\right)$
subject to $\sum_{i=1}^{N} \alpha_{i} y_{i}=0, \mathrm{C} \geq \alpha_{i} \geq 0, i=1, \ldots, N$

- Because $H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)$ is a positive semidefinite kernel, the optimization problem is a convex quadratic programming problem.
- Decision function is
$D(x)=\mathbf{w}^{T} \boldsymbol{g}(\boldsymbol{x})+b=\sum_{x_{i} \in S} \alpha_{i} y_{i} H\left(\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{x}\right)+b$
$b=y_{j}-\sum_{x_{i} \in S} \alpha_{i} y_{i} H\left(\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{x}_{\boldsymbol{j}}\right), \boldsymbol{x}_{\boldsymbol{j}}$ is an unbounded support vector
- To ensure stability of calculations, we take the average:
$b=\frac{1}{\#\left(\boldsymbol{x}_{\boldsymbol{j}} \in G\right)} \sum_{x_{j} \in G}\left(y_{j}-\sum_{x_{i} \in S} \alpha_{i} y_{i} H\left(\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{x}_{\boldsymbol{j}}\right)\right)$
- Then unknown datum $x$ is classified into:
$\left\{\begin{array}{l}\text { Class } 1, \text { if } D(x)>0 \\ \text { Class } 2, \text { if } D(x)<0\end{array}\right.$
If $D(x)=0, x$ is unclassifiable


## Kernels used in SVM

- Linear Kernels:

If the problem is linearly separable, we use linear kernels: $H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)=\boldsymbol{x}^{\boldsymbol{T}} \boldsymbol{x}^{\prime}$

- Polynomial Kernels:

The polynomial kernel with degree $m \geq 1$ is $H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)=\left(\boldsymbol{x}^{\boldsymbol{T}} \boldsymbol{x}^{\prime}+1\right)^{\boldsymbol{m}}$
When $m=1$, the kernel is the linear kernel by adjusting 1 into $b$
When $m=2, d=2$,

$$
\begin{aligned}
& \qquad \begin{array}{l}
H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)=1+2 x_{1} x_{1}^{\prime}+2 x_{2} x_{2}^{\prime}+2 x_{1} x_{1}^{\prime} x_{2} x_{2}^{\prime}+x_{1}^{2} x_{1}^{\prime 2}+x_{2}^{2} x_{2}^{\prime 2} \\
=\boldsymbol{g}(\boldsymbol{x})^{T} \boldsymbol{g}\left(\boldsymbol{x}^{\prime}\right) \geq 0 \quad \text { satisfy Mercer's condition }
\end{array} \\
& \text { where } \boldsymbol{g}(\boldsymbol{x})=\left(1, \sqrt{2} x_{1}, \sqrt{2} x_{2}, \sqrt{2} x_{1} x_{2}, x_{1}^{2}, x_{2}^{2}\right)^{\boldsymbol{T}}
\end{aligned}
$$

- In general, polynomial kernels satisfy Mercer's condition
- Radial Basis Function (RBF) Kernels:

$$
\begin{align*}
H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right) & =\exp \left(-\gamma\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\|^{2}\right), \gamma>0 \text { controlling the radius } \\
& =\exp \left(-\gamma\|\boldsymbol{x}\|^{2}\right) \exp \left(-\gamma\left\|\boldsymbol{x}^{\prime}\right\|^{2}\right) \exp \left(2 \gamma \boldsymbol{x}^{T} \boldsymbol{x}^{\prime}\right) \tag{*}
\end{align*}
$$

Because $\exp \left(2 \gamma \boldsymbol{x}^{T} \boldsymbol{x}^{\prime}\right)=1+2 \gamma \boldsymbol{x}^{T} \boldsymbol{x}^{\prime}+2 \gamma^{2}\left(\boldsymbol{x}^{T} \boldsymbol{x}^{\prime}\right)^{2}+\frac{2 \gamma^{3}}{3!}\left(\boldsymbol{x}^{T} \boldsymbol{x}^{\prime}\right)^{3}+\cdots$ is an infinite summation of polynomials $\Rightarrow$ it is a kernel.
$\exp \left(-\gamma| | x \|^{2}\right)$ and $\exp \left(-\gamma\left\|x^{\prime}\right\|^{2}\right)$ are proved to be kernels and the product of kernels is also a kernel. Thus (*) is a kernel.

- The decision function is

$$
D(x)=\sum_{x_{i} \in S} \alpha_{i} y_{i} H\left(\boldsymbol{x}_{i}, x\right)+b=\sum_{x_{i} \in S} \alpha_{i} y_{i} \exp \left(-\gamma\left\|x_{i}-\boldsymbol{x}\right\|^{2}\right)+b
$$

Here, the support vectors are the centers of the radial basis functions.

```
%% svmgauss.m
% From A First Course in Machine Learning, Chapter 5.
% Simon Rogers, 01/11/11 [simon.rogers@glasgow.ac.uk]
% SVM with Gaussian kernel
clear all;close all;
%% Load the data
load t.csv
load X.cSV
% Put in class order for visualising the kernel
[t I] = sort(t);
X = X(I,:);
%% Plot the data
ma = {'ko','ks'};
fc = {[0 0 0],[[1 1 1]};
tv = unique(t);
figure(1); hold off
for i = 1:length(tv)
    pos = find(t==tv(i));
    plot(X(pos,1),X(pos,2),ma{i},'markerfacecolor',fc{i});
    hold on
    pause
end
```

```
%% Compute Kernel and test Kernel
[Xv Yv] = meshgrid(-3:0.1:3,-3:0.1:3);
testX = [Xv(:) Yv(:)];
N = size(X,1);
Nt = size(testX,1);
K = zeros(N);
testK = zeros(N,Nt);
% Set kernel parameter
gamvals = [0.01 0.1 1 5 10 50];
for gv = 1:length(gamvals)
    %%
    gam = gamvals(gv);
    for n = 1:N
    H}(\mp@subsup{\boldsymbol{x}}{i}{},\mp@subsup{\boldsymbol{x}}{j}{})=\operatorname{exp}(-\gamma||\mp@subsup{\boldsymbol{x}}{i}{}-\mp@subsup{\boldsymbol{x}}{\boldsymbol{j}}{|}\mp@subsup{|}{}{2}
        for n2 = 1:N
            K(n,n2) = exp(-gam*sum((X(n,:)-X(n2,:)).^2));
        end
        for n2 = 1:Nt
                testK(n,n2) = exp(-gam*sum((X(n,:)-testX(n2,:)).^2));
        end
    end
    figure(1);hold off
    imagesc(K);
    ti = sprintf('Gamma: %g',gam);
    title(ti);
```

\% Construct the optimisation
$\mathrm{H}=$ (t*t').*K + 1e-5*eye (N) ;
$\mathrm{f}=$ repmat $(1, \mathrm{~N}, 1)$;
$\mathrm{A}=$ [];b $=$ [];
$\mathrm{LB}=\operatorname{repmat}(0, \mathrm{~N}, 1)$;
$\mathrm{UB}=\operatorname{repmat}(\mathrm{inf}, \mathrm{N}, 1)$;
Aeq $=t^{\prime} ;$ beq $=0$;

$$
\begin{array}{r}
Q(\mathbf{w}, b, \boldsymbol{\alpha})=\sum_{i=1}^{N} \alpha_{i}-\frac{\mathbf{1}}{\mathbf{2}} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \boldsymbol{H}\left(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}\right) \\
\sum_{i=1}^{N} \alpha_{i} y_{i}=0, \quad \mathrm{C} \geq \alpha_{i} \geq 0, \quad i=1, \ldots, N
\end{array}
$$

\% Fix C
$C=10$;
$\mathrm{UB}=\operatorname{repmat}(\mathrm{C}, \mathrm{N}, 1)$;
\% Following line runs the SVM
alpha $=$ quadprog ( $\mathrm{H},-\mathrm{f}, \mathrm{A}, \mathrm{b}, \mathrm{Aeq}, \mathrm{beq}, \mathrm{LB}, \mathrm{UB})$;
fout $=$ sum(repmat (alpha.*t, $1, N$ ). ${ }^{*} \mathrm{~K}, 1$ )';
pos $=$ find (alpha>1e-6);
$\alpha_{i}$ 's $>0$ are support vectors
\% Compute the test predictions
testpred $=(\mathrm{alpha} . * t) ' * t e s t K ~+~ b i a s ; ~$
testpred $=$ testpred';

$$
\sum_{x_{i} \in S} \alpha_{i} y_{i} \exp \left(-\gamma\left\|x_{i}-x\right\|^{2}\right)+b
$$

\% Plot the data, support vectors and decision boundary

## figure (2) ;hold off

pos $=$ find (alpha>1e-6) ;
$\alpha_{i}$ 's $>0$ are support vectors
plot (X (pos, 1) , X(pos, 2) ,'ko','markersize', 15,'markerfacecolor', [0.6 0.6 0.6],...
'markeredgecolor', [0.6 0.6 0.6]);
hold on
for $i=1: l e n g t h(t v)$
pos $=$ find (t==tv(i));
plot (X(pos,1), X(pos,2),ma\{i\},'markerfacecolor',fc\{i\});
end
contour (Xv, Yv, reshape (testpred, size (Xv)), [0 0], 'k');
ti $=$ sprintf('Gamma: \% '',gam);
title(ti);
pause
end



## Summary of Kernel Trick

- A kernel function, $H: \mathbb{R}^{l} \times \mathbb{R}^{l} \rightarrow \mathbb{R}$ where $H\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)=\boldsymbol{g}(\boldsymbol{x})^{T} \boldsymbol{g}\left(\boldsymbol{x}^{\prime}\right)$
- $\mathbf{w}=\sum_{x_{i} \in S} \alpha_{i} y_{i} \boldsymbol{g}\left(\boldsymbol{x}_{i}\right)$, where $S$ is the set of support vectors.
- Given a test pattern $\boldsymbol{x}$, we can classify it based on $D(\boldsymbol{x})=\mathbf{w}^{T} \boldsymbol{g}(\boldsymbol{x})+b$ by $\sum_{x_{i} \in S} \alpha_{i} y_{i} \boldsymbol{g}\left(\boldsymbol{x}_{i}\right)^{T} \boldsymbol{g}(\boldsymbol{x})+b$
- $b$ is obtained by
$b=y_{j}-\sum_{x_{i} \in S} \alpha_{i} y_{i} \boldsymbol{g}\left(\boldsymbol{x}_{\boldsymbol{i}}\right)^{T} \boldsymbol{g}\left(\boldsymbol{x}_{\boldsymbol{j}}\right), \boldsymbol{x}_{\boldsymbol{j}}$ is a good support vector

|  |  | True Status |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | Yes | No |  |
| Predicted <br> status | Yes | True Positive (TP) | False Positive <br> (FP) <br> Type I error | Positive False <br> Predictive Rate, Discovery Rate <br> Precision FP/(TP+FP) <br> TP/(TP+FP)  <br>   |
|  | No | False Negative (FN) <br> Type II error | True Negative (TN) | False Omission Negative <br> Rate Predictive Rate <br> FN/(FN+TN) TN/(FN+TN) |
| Total number |  | True positive Rate Sensitivity, Recall TP/(TP+FN) | False positive Rate $\mathrm{FP} /(\mathrm{FP}+\mathrm{TN})$ | F1 score $=2 *$ precision*Recall/ (precision+Recall) |
| Accuracy $(\mathbf{T P}+\mathbf{T N}) / 1$ |  | False Negative Rate $\mathrm{FN} /(\mathrm{TP}+\mathrm{FN})$ | True Negative Rate Specificity TN/(FP+TN) |  |

```
%% svmroc.m
% From A First Course in Machine Learning, Chapter 5.
% Simon Rogers, 01/11/11 [simon.rogers@glasgow.ac.uk]
% ROC analysis of SVM
clear all;close all;
%% Load the data
load t.csv
load X.csv
load testt.csv
load testX.csv
%% Compute the kernels
gam = 10; % Experiment with this value
N = size(X,1);
Nt = size(testX,1);
for n = 1:N
    for n2 = 1:N
        K(n,n2) = exp(-gam*sum((X(n,:)-X(n2,:)).^2));
    end
    for n2 = 1:Nt
        testK(n,n2) = exp(-gam*sum((X(n,:)-testX(n2,:)).^2));
    end
end
```

```
%% Train the SVM
H = (t*t').*K + 1e-5*eye(N);
f = repmat (1,N,1);
A = [];b = [];
LB = repmat (0,N,1); UB = repmat(inf,N,1);
Aeq = t';beq = 0;
% Fix C
C = 10;
UB = repmat (C,N,1);
% Following line runs the SVM
alpha = quadprog(H,-f,A,b,Aeq,beq,LB,UB);
fout = sum(repmat(alpha.*t,1,N).*K,1)';
pos = find(alpha>1e-6);
bias = mean(t(pos)-fout(pos));
%% Compute the test predictions
testpred = (alpha.*t)'*testK + bias;
testpred = testpred';
```

\%\% Do the ROC analysis
th_vals $=$ [min(testpred):0.01:max(testpred) +0.01$]$;
sens = []; spec = [];
for i = 1:length(th_vals)
b_pred = testpred>=th_vals(i);
\% Compute true positives, false positives, true negatives, true
\% positives
TP = sum(b_pred==1 \& testt == 1);
FP = sum (b_pred==1 \& testt == -1);
TN = sum (b_pred==0 \& testt == -1);
FN $=$ sum (b_pred==0 \& testt == 1);
\% Compute sensitivity and specificity
sens(i) = TP/(TP+FN);
spec(i) $=T N /(T N+F P)$;
end
\%\% Plot the ROC curve
figure(1);hold off
cspec = 1-spec;
cspec $=$ cspec (end:-1:1);
sens = sens(end:-1:1);
plot(cspec,sens,'k')
\%\% Compute the AUC
AUC $=\operatorname{sum}\left(0.5^{*}(\operatorname{sens}(2: e n d)+\operatorname{sens}(1: e n d-1)) . *(\operatorname{cspec}(2: e n d)-\operatorname{cspec}(1: e n d-1))\right) ;$
fprintf('\n AUC: \%g\n',AUC);

ROC curve (svmroc.m)


The ROC curve traces out two types of error as we vary the threshold value for the prediction values $\sum_{x_{i} \in S} \alpha_{i} y_{i} \exp \left(-\gamma\left\|x_{i}-\boldsymbol{x}\right\|^{2}\right)+b$. The actual thresholds are not shown. The true positive rate is the sensitivity: the fraction of test data (labeled 1) that are correctly identified, using a given threshold value. The false positive rate is 1specificity: the fraction of test data (labeled -1) that we classify incorrectly as 1 , using that same threshold value. The ideal ROC curve hugs the top left corner, indicating a high true positive rate and a low false positive rate.

