# Support Vector Machine

生醫光電所 吳育德

#### Credit:

Chap2, Support Vector Machines for Pattern Classification, Shigeo Abe, 2005

Chap5. A First Course in Machine Learning, 2ed, Simon Rogers and Mark Girolami, 2017

### **Hard-Margin Support Vector Machines**

• Let N d-dimensional training inputs  $x_i$  (i = 1, ..., 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:  $D(x) = \mathbf{w}^T x + b$ 

where w is an d-dimensional vector, b is a bias term, i = 1, ..., N

$$\mathbf{w}^{T} \mathbf{x}_{i} + b \begin{cases} > 0 & \text{for } y_{i} = 1, \\ < 0 & \text{for } y_{i} = -1 \end{cases}$$

• Because the training data are linearly separable, no training data satisfy  $\mathbf{w}^T \mathbf{x} + b = 0$ 

• To control separability, instead of ①, we consider

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

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

• ② is equivalent to

$$y_i(\mathbf{w}^T x_i + b) \ge 1, i = 1, ..., N$$

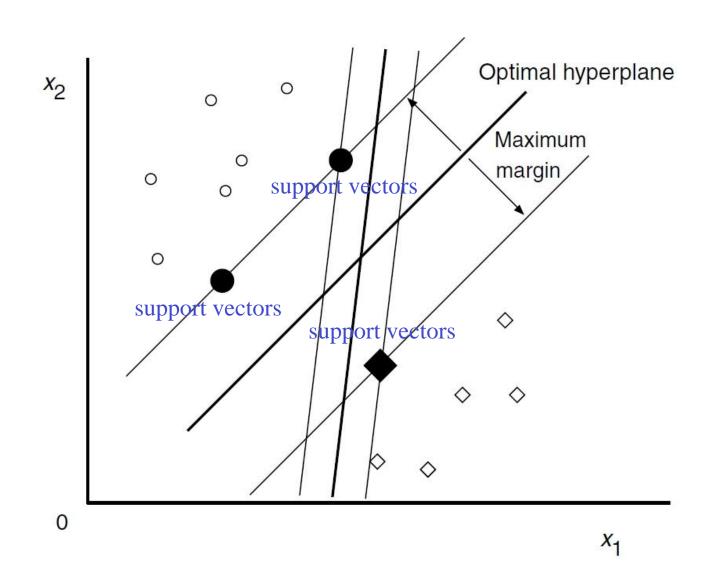
- The hyperplane  $D(x) = \mathbf{w}^T x + b = c$  for -1 < c < 1 forms a separating hyperplane that separates  $x_i$  (i = 1, ..., N).
- When c = 0, the separating hyperplane is in the middle of the two hyperplanes with c = 1 and -1.

• 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 w. Training the SVM consists of learning a w that maximizes the margin. So, margin is important.

#### Optimal separating hyperplane in a two-dimensional space



#### Normal distance between x and the hyperplane

- $x_{proj}$ : projection of x onto the hyperplane D(x) = 0.
- d: the normal distance between x and  $x_{proj}$ .

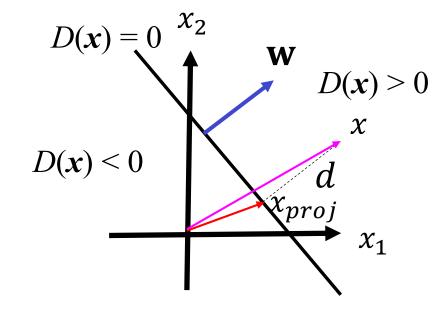
• 
$$x = x_{proj} + d \frac{\mathbf{w}}{||\mathbf{w}||}$$

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

$$= \mathbf{w}^{T} (x_{proj} + d \frac{\mathbf{w}}{||\mathbf{w}||}) + b$$

$$= \mathbf{w}^{T} x_{proj} + b + d \frac{\mathbf{w}^{T} \mathbf{w}}{||\mathbf{w}||} = 0 + d||\mathbf{w}||$$

$$\Rightarrow d = \frac{D(x)}{||\mathbf{w}||}$$



# Cost function for obtaining the optimal separating hyperplane

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

• Margin = 
$$d_+ + d_- = \frac{2}{||\mathbf{w}||}$$

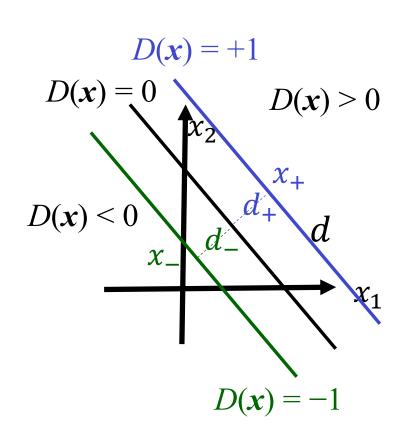
• The optimal separating hyperplane can be obtained by minimizing

$$Q(\mathbf{w}) = \frac{1}{2} ||\mathbf{w}||^2$$

with respect to w and b subject to the constraints

$$y_i(\mathbf{w}^T x_i + b) \ge 1, i = 1, ..., N$$

(4)



- Find  $\mathbf{x} = [x_1, \dots, x_n]^T$  that

  Minimize  $F(\mathbf{x})$  ①

  subject to  $g_i(\mathbf{x}) \leq 0, i = 1, \dots, m$  ②
- If x satisfies the inequality constraints 2, it is said to be *feasible*. Otherwise it is called *infeasible*
- The *i*th constraint  $g_i(x) \le 0$  is said to be active at a point x if  $g_i(x) = 0$ .
- The constraints ② can be converted to equality constraints by adding positive slack variables to get:

Minimize F(x) ①

subject to  $g_i(x) + y_i^2 = 0, i = 1, \dots, m$  3

- 1 3 is an optimization problem with only m equality constraints
- Let  $\mathbf{y} = [y_1, \dots, y_m]^T$ ,  $\lambda = [\lambda_1, \dots, \lambda_m]^T$ , the Lagrangian has the form:

$$L(\mathbf{x}, \mathbf{y}, \lambda) = F(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i (g_i(\mathbf{x}) + y_i^2),$$

which has n+2m unknown  $x^*$ ,  $y^*$  and  $\lambda^*$ 

• The optimal conditions are

$$\frac{\partial L}{\partial x} = 0 \implies \frac{\partial F(x)}{\partial x} + \sum_{i=1}^{m} \lambda_i \frac{\partial g_i(x)}{\partial x} = 0,$$

$$\frac{\partial L}{\partial y_i} = 0 \implies 2\lambda_i y_i = 0,$$

$$\frac{\partial L}{\partial \lambda_i} = 0 \implies g_i(x) + y_i^2 = 0,$$

$$i = 1, \dots, m$$

$$\vdots$$

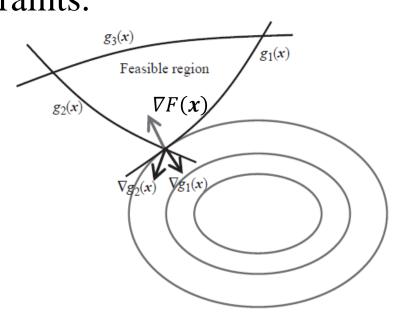
$$i = 1, \dots, m$$

$$\vdots$$

• 456 are usually called the Karush–Kuhn–Tucker (KKT) conditions

- $4 \Rightarrow \frac{\partial F(x)}{\partial x}$  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  $g_i(x) + y_i^2 = 0 \Rightarrow g_i(x) < 0$  (inactive) or  $\lambda_i \neq 0 \Rightarrow y_i = 0$  and  $g_i(x) + y_i^2 = 0 \Rightarrow g_i(x) = 0$  (active).  $\Rightarrow \lambda_i g_i(x) = 0$  (we will show  $\lambda_i > 0$  when  $g_i(x) = 0$ )
- 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,  $g_1(\mathbf{x})$  and  $g_2(\mathbf{x})$  are active. At this point,  $\nabla F(\mathbf{x})$  is a linear function of the gradients of the active constraints  $\nabla g_1(\mathbf{x})$ ,  $\nabla g_2(\mathbf{x})$ 



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

$$\frac{\partial F(\mathbf{x})}{\partial x_i} + \sum_{j=1}^m \lambda_j \frac{\partial g_j(\mathbf{x})}{\partial x_i} = 0, \qquad i = 1, \dots, n$$

$$\lambda_j g_j(\mathbf{x}) = 0, \quad complementarity \ condition \quad j = 1, \dots, m$$

$$g_j(\mathbf{x}) \leq 0, \qquad \qquad j = 1, \dots, m$$

$$\lambda_i \geq 0, \qquad \qquad j = 1, \dots, m$$

$$0$$

$$j = 1, \dots, m$$

$$0$$

• Condition  $\lambda_j \geq 0$  (10) for the inequality constraints  $g_j(x) \leq 0$  ensures F will not be reduced by a move off any of the active constraints at  $x^*$  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  $\mathbf{b}$  that satisfy  $\mathbf{\hat{4}}$ . We call the solutions that satisfy  $\mathbf{\hat{4}}$  feasible solutions.

• We first convert the constrained problem given by 3 and 4 into the unconstrained problem

$$Q(\mathbf{w}, b, \alpha) = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} + \sum_{i=1}^{N} \alpha_{i} \{1 - y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b)\}$$
 5

where  $\alpha = (\alpha_1, \ldots, \alpha_N)^T$  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  $\mathbf{b}$  and maximizing w.r.t  $\alpha_i$  ( $\geq 0$ ) satisfying the following KKT conditions

$$\frac{\partial Q(\mathbf{w}, b, \alpha)}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{N} \alpha_i y_i x_i = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i x_i \quad (*)$$

$$\frac{\partial Q(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial b} = -\sum_{i=1}^{N} \alpha_i \, y_i = 0 \tag{**}$$

$$\alpha_i \{1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)\} = 0, i = 1, ..., N$$

$$\alpha_i \geq 0$$
,  $i = 1, \ldots, N$ 

- 6 are called KKT complementarity conditions:  $\alpha_i = 0$ , or  $\alpha_i > 0$  and  $y_i(\mathbf{w}^T \mathbf{x}_i + b) = 1$  must be satisfied.
- The training data  $x_i$  with  $\alpha_i > 0$  are called support vectors

• Substituting (\*) and (\*\*) into ⑤, we obtain the dual problem. Maximize

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

$$= \frac{1}{2} \sum_{i=1}^{N} \alpha_{i} y_{i} \mathbf{x}_{i}^{T} \sum_{j=1}^{N} \alpha_{j} y_{j} \mathbf{x}_{j} + \sum_{i=1}^{N} \alpha_{i} \{1 - y_{i} (\sum_{j=1}^{N} \alpha_{j} y_{j} \mathbf{x}_{j}^{T} \mathbf{x}_{i} + b)\}$$

$$= \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j} - b \sum_{i=1}^{N} \alpha_{i} y_{i}$$

$$= \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j} - b \times 0$$

w.r.t.  $\alpha_i$  subject to

$$\sum_{i=1}^{N} \alpha_i y_i = 0, \quad \alpha_i \ge 0, \quad i = 1, ..., N$$

• This is the *dual problem* and it is in terms of  $\alpha_i$ 's only  $\Rightarrow \alpha_i$ 's are used to get optimal **w** and *b* 

- This is a *convex optimization problem*. It is possible to obtain  $\alpha$  vector corresponding to the *global optimum*.  $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$ .
- Many of the  $\alpha_i$  are 0. Support Vectors (SVs) are the  $x_i$ 's corresponding to the nonzero  $\alpha_i$ 's. Let  $S = \{x_i | \alpha_i > 0\}$  be the set of SVs.
- a. By complementary slackness condition,

$$x_i \in S \Rightarrow \alpha_i > 0 \Rightarrow y_i(\mathbf{w}^T x_i + b) = 1 \Rightarrow x_i$$
 is the closest to the decision boundary.

- b. Optimal  $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \ \mathbf{x}_i = \sum_{\mathbf{x}_i \in S} \alpha_i y_i \mathbf{x}_i$  is a linear combination of SVs.
- c.  $y_i \times y_i(\mathbf{w}^T \mathbf{x}_i + b) = y_i \Rightarrow b = y_i \mathbf{w}^T \mathbf{x}_i$  where i is such that  $\alpha_i > 0$ .
- d. It is better to average the SVs :  $b = \frac{1}{\#(x_i \in S)} \sum_{x_i \in S} (y_i \mathbf{w}^T \mathbf{x}_i)$

#### **Making Prediction**

• Data associated with  $\alpha_i$ 's > 0 are support vectors for Classes 1 and 2.

•  $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$  (\*), the decision function is (do not need to use  $\mathbf{w}$  and b explicitly, use  $\alpha_i > 0$ ,  $y_i$  and  $\mathbf{x}_i$  only)

$$D(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{x_i \in S} \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + (y_i - \sum_{x_i \in S} \alpha_i y_i \mathbf{x}_i^T \mathbf{x}_i)$$

• Then unknown datum x is classified into:

$$\begin{cases} \text{Class 1, if } D(\mathbf{x}) > 0 \\ \text{Class 2, if } D(\mathbf{x}) < 0 \end{cases}$$

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

# **Example**

• Consider a linearly separable case shown in Fig. 2.2,  $(x_1, y_1) = (-1,1)$ ,  $(x_2, y_2) = (0,-1)$ ,  $(x_3, y_3) = (1,-1)$ , The inequality constraints given by  $y_i(\mathbf{w}^T \mathbf{x}_i + b) \ge 1$ ,  $i = 1, \ldots, 3$  are

$$-w + b \ge 1$$
,  $-b \ge 1$ ,  $-(w + b) \ge 1$  (\*\*\*)

• 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) = -2x 1
- The class boundary is x = -1/2
- x = 0 and -1 are support vectors

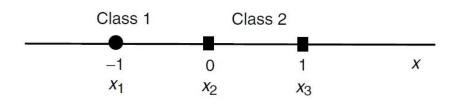


Fig. 2.2. Linearly separable one-dimensional case

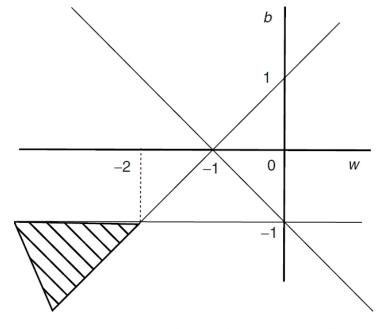


Fig. 2.3. Region that satisfies constraints

• The dual problem is to maximize

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

subject to

$$\sum_{i=1}^{3} \alpha_i y_i = \alpha_1 - \alpha_2 - \alpha_3 = 0, \, \alpha_i \ge 0, \, i = 1, \dots, 3$$

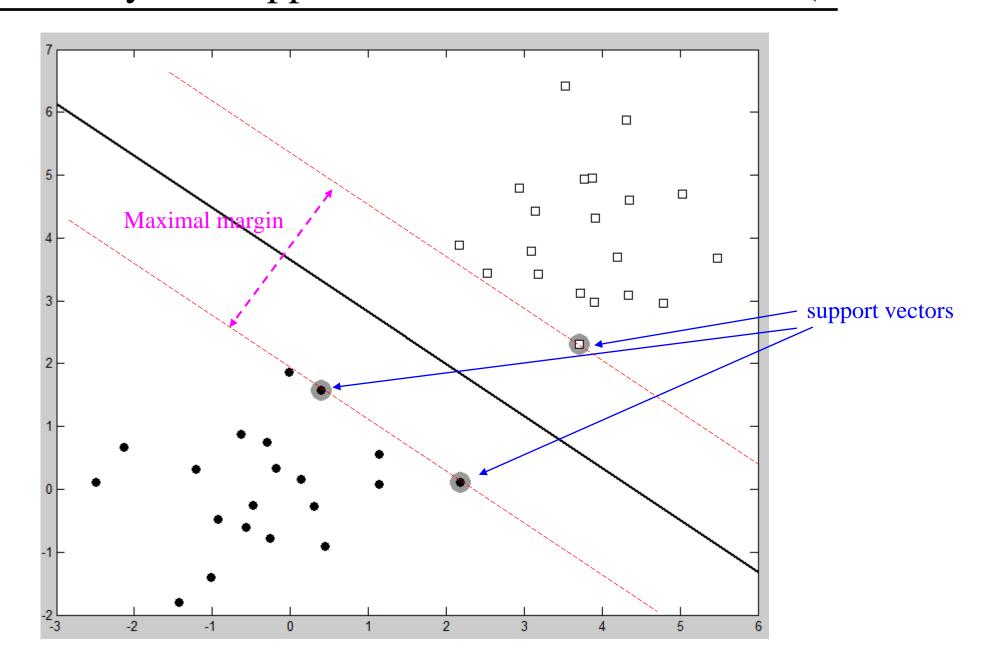
• Substituting  $\alpha_2 = \alpha_1 - \alpha_3$  into (\*\*\*\*), we obtain

$$Q(\alpha) = 2\alpha_1 - \frac{1}{2}(\alpha_1 + \alpha_3)^2$$
 subject to  $\alpha_i \ge 0, i = 1, ..., 3$  which is maximized when  $\alpha_3 = 0$ , since  $\alpha_3 \ge 0$ 

- Now  $Q(\alpha) = 2\alpha_1 \frac{1}{2}\alpha_1^2 = -\frac{1}{2}(\alpha_1 2)^2 + 2$ ,  $\alpha_1 \ge 0$  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 ( $\alpha_1 = 2 > 0$ ) and 0 ( $\alpha_2 = 2 > 0$ ) 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  $b = y_i w^T x_i = y_1 (-2)x_1 = 1 (-2)(-1) = -1$  ( $\alpha_1 = 2 > 0$ ,  $\alpha_1$  is a support vector  $\Rightarrow y_1(w^T x_1 + b) = 1$ ), 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  $w + b \ge 1$ . Thus, from Fig 2.3 there is no feasible solution.

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



```
%% symhard.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
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;
% Following line runs the SVM
alpha = quadprog(H, -f, A, b, Aeq, beq, LB, UB);
% 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));
```

$$Q(\mathbf{w}, b, \boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$
$$\sum_{i=1}^{N} \alpha_i y_i = 0, \quad \alpha_i \ge 0, \quad i = 1, \dots, N$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i x_i$$

$$b = \frac{1}{\#(x_i \in S)} \sum_{x_i \in S} (y_i - \mathbf{w}^T x_i)$$

$$S = \{x_i | \alpha_i > 0\} \text{ be the set of SVs}$$

```
%% Plot the data, decision boundary and Support vectors
figure (1); hold off
                              \alpha_i's > 0 are support vectors for Classes 1 and 2
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: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)
```

# **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  $\xi_i \ge 0$  into  $y_i(\mathbf{w}^T \mathbf{x_i} + b) \ge 1$ .

$$\Rightarrow y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i, i = 1, \dots, N$$

If  $\xi_i < 1$ , this data is correctly classified.

If  $\xi_i \ge 1$ , this data is misclassified.

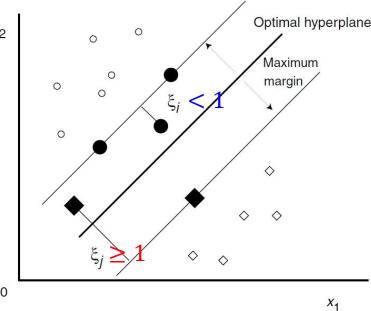


Fig. 2.4. Inseparable case in a two-dimensional space

• Minimize 
$$Q(\mathbf{w}) = \frac{1}{2} ||\mathbf{w}||^2 + \sum_{i=1}^{N} \theta(\xi_i), \theta(\xi_i) = \begin{cases} 1, \text{ for } \xi_i > 0 \\ 0, \text{ for } \xi_i = 0 \end{cases}$$
 subject to  $y_i(\mathbf{w}^T \mathbf{x}_i + b) \ge 1 - \xi_i, i = 1, \dots, N$ 

- This is a combinatorial optimization and difficult to solve
- Instead, we minimize  $Q(\mathbf{w}, \mathbf{b}, \boldsymbol{\xi}) = \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^N \xi_i^p$ ,  $\xi_i \ge 0$  subject to  $y_i(\mathbf{w}^T x_i + b) \ge 1 \xi_i$ ,  $i = 1, \ldots, N$  where  $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)^T$ , C determines the trade-off between the maximization of margin and minimization of classification error, and p = 1 ( $l_1$  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 (p=1)

$$Q(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} + C \sum_{i=1}^{N} \xi_{i} + \sum_{i=1}^{N} \alpha_{i} \{1 - \xi_{i} - y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b)\} + \sum_{i=1}^{N} \beta_{i} (-\xi_{i}), i = 1, ..., N$$
(1)

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

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

$$\frac{\partial Q(\mathbf{w}, b, \xi, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial b} = -\sum_{i=1}^{N} \alpha_{i} y_{i} = 0 \quad (**)$$

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

$$\alpha_{i} \{1 - \xi_{i} - y_{i} (\mathbf{w}^{T} \boldsymbol{x}_{i} + b)\} = 0, i = 1, \dots, N \quad (2)$$

 $\beta_i \xi_i = 0, \qquad i = 1, \dots, N$ 

$$\alpha_i \geq 0, \beta_i \geq 0, \xi_i \geq 0, \qquad i = 1, \ldots, N$$

• Substituting (\*), (\*\*), (\*\*\*) into ①, we obtain the dual problem.

Maximize

$$Q(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} + \sum_{i=1}^{N} \xi_{i} (\alpha_{i} + \beta_{i}) + \sum_{i=1}^{N} \alpha_{i} \{1 - \xi_{i} - y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b)\} + \sum_{i=1}^{N} \beta_{i} (-\xi_{i}),$$

$$= \frac{1}{2} \mathbf{w}^{T} \mathbf{w} + \sum_{i=1}^{N} \alpha_{i} \{1 - y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b)\}$$

$$= \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j}$$

with respect to  $\alpha_i$  subject to the constraints

$$\sum_{i=1}^{N} \alpha_i y_i = 0, C \ge \alpha_i \ge 0, i = 1, ..., N$$

• The only difference between  $l_1$  soft-margin SVM and hard margin SVM is that  $\alpha_i$  cannot exceed C (since  $\alpha_i + \beta_i = C$ ,  $\beta_i \ge 0$ ).

- Especially, ② and ③ are called KKT (complementarity) conditions
- From  $\alpha_i + \beta_i = \mathbb{C}$ ,  $\beta_i \xi_i = 0$  and ② there are three cases for  $\alpha_i$ :
- 1.  $\alpha_i = 0$ . Then  $\beta_i = C$ ,  $\xi_i = 0$ . Thus  $x_i$  is correctly classified
- 2.  $0 < \alpha_i < C$ . Then  $\textcircled{2} \Rightarrow y_i(\mathbf{w}^T \mathbf{x}_i + b) 1 + \xi_i = 0$ , and  $\beta_i \neq 0, \Rightarrow \xi_i = 0$ . Therefore,  $y_i(\mathbf{w}^T \mathbf{x}_i + b) = 1$  and  $\mathbf{x}_i$  is a support vector. We call the support vector with  $C > \alpha_i > 0$  a good (unbounded) SV.
- 3.  $\alpha_i = C$ . Then  $\textcircled{2} \Rightarrow y_i(\mathbf{w}^T \mathbf{x}_i + b) 1 + \xi_i = 0$  and  $\xi_i \ge 0$ . Thus  $\mathbf{x}_i$  is a support vector. We call the support vector with  $\alpha_i = C$  a bad (bounded) SV. If  $0 \le \xi_i < 1$ ,  $\mathbf{x}_i$  is correctly classified.
- If  $\xi_i \geq 1$ ,  $x_i$  is misclassified

• Data associated with  $S = \{x_i | C \ge \alpha_i > 0\}$  are SVs for Classes 1 and 2.

Then from  $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$  (\*), the decision function is

$$D(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{x_i \in S} \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

- For the unbounded  $\alpha_i$ ,  $b = y_i \mathbf{w}^T \mathbf{x}_i$  is satisfied.
- To ensure the precision of calculations, we take the average of b that is calculated for unbounded support vectors,  $b = \frac{1}{\#(x_i \in G)} \sum_{x_i \in G} (y_i \mathbf{w}^T \mathbf{x}_i)$

where G is the set of good support vector

• Then unknown datum x is classified into:

$$\begin{cases} \text{Class 1, if } D(\mathbf{x}) > 0 \\ \text{Class 2, if } D(\mathbf{x}) < 0 \end{cases}$$

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 = \{[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
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 = [10 5 2 1 0.5 0.1 0.05 0.01];
for cv = 1:length(Cvals);
    응응
    UB = repmat(Cvals(cv), N, 1);
    % Following line runs the SVM
    alpha = quadprog(H, -f, A, b, Aeq, beq, LB, UB);
    % 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));
```

$$Q(\mathbf{w}, b, \alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$
$$\sum_{i=1}^{N} \alpha_i y_i = 0, \quad \mathbf{C} \ge \alpha_i \ge 0, \quad i = 1, \dots, N$$

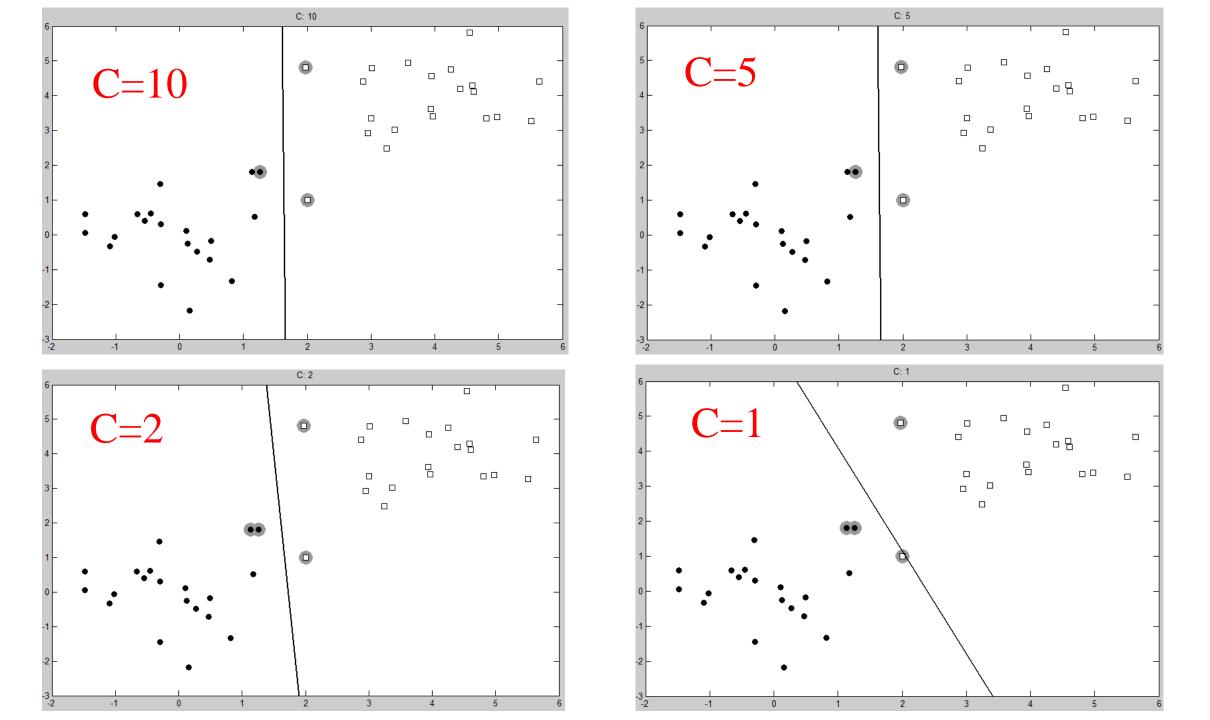
$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i x_i$$

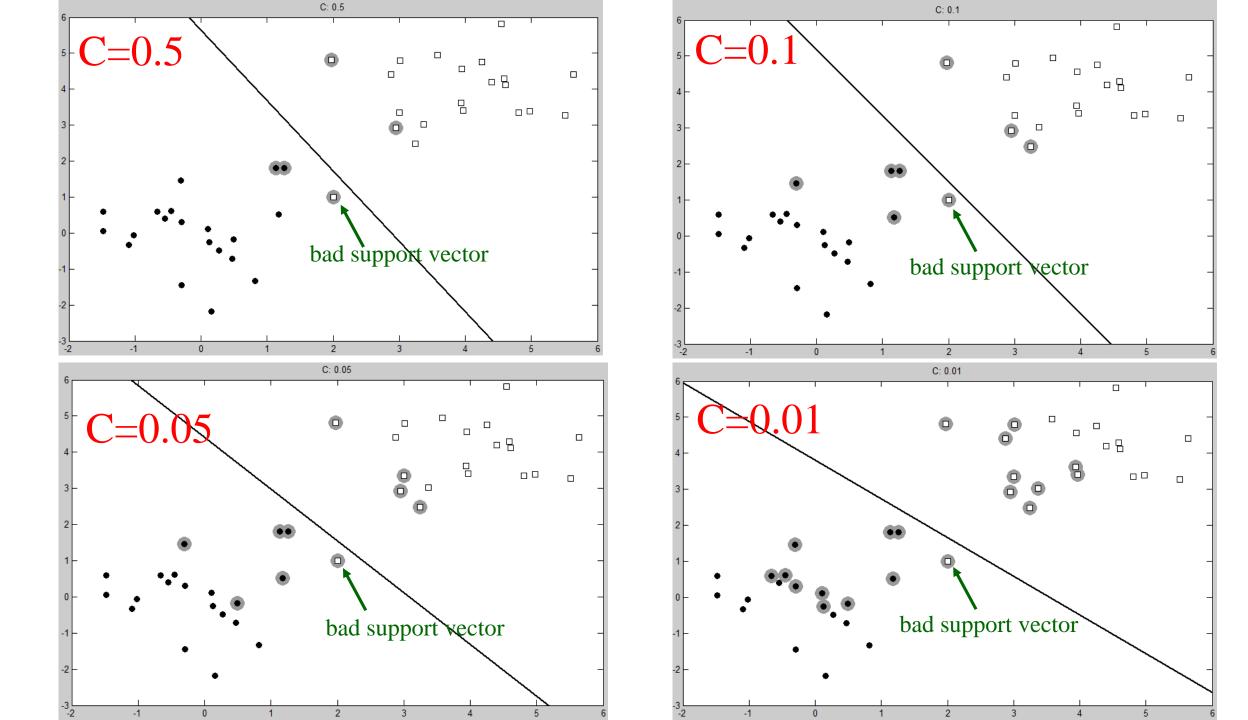
$$b = \frac{1}{\#(x_i \in G)} \sum_{x_i \in G} (y_i - \mathbf{w}^T x_i)$$

$$G = \{x_i | \mathbf{C} > \alpha_i > 0\}$$

```
%% 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:length(tv)
       pos = find(t==tv(i));
       plot(x(pos,1),x(pos,2),ma{i},'markerfacecolor',fc{i});
   end
   xp = xlim;
   yl = ylim;
   % 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);
   ylim(yl);
  ti = sprintf('C: %g', Cvals(cv));
   title(ti);
   pause
```

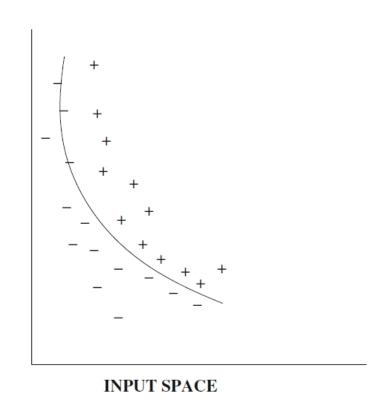
end

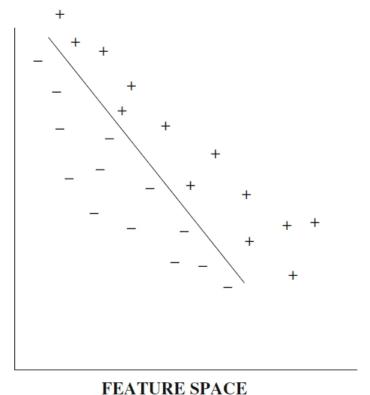




# Mapping to a High-Dimensional Space: Kernel Tricks

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





Nonlinear decision boundary

• Using a nonlinear  $g(x) = (g_1(x), ..., g_l(x))^T$ , that maps the *d*-dimensional input vector x into the *l*-dimensional feature space

• The linear decision function

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

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

• According to the Hilbert-Schmidt theory, if a symmetric H(x, x') satisfies

$$\sum_{i,j=1}^{N} h_i h_j H(\boldsymbol{x_i}, \boldsymbol{x_j}) \ge 0$$

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

$$H(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\mathbf{x})^T \mathbf{g}(\mathbf{x}')$$
 (2)

• If ② is satisfied,

$$\sum_{i,j=1}^{N} h_i h_j H(\mathbf{x}_i, \mathbf{x}_j) = \left( \sum_{i=1}^{N} \mathbf{g}(\mathbf{x}_i)^T h_i \right) \left( \sum_{j=1}^{N} \mathbf{g}(\mathbf{x}_j) h_j \right) \ge 0$$
 3

- 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 
$$Q(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j H(\boldsymbol{x_i}, \boldsymbol{x_j})$$
  
subject to  $\sum_{i=1}^{N} \alpha_i y_i = 0$ ,  $C \ge \alpha_i \ge 0$ ,  $i = 1, ..., N$ 

• Because H(x, x') is a positive semidefinite kernel, the optimization problem is a convex quadratic programming problem.

Decision function is

$$D(\mathbf{x}) = \mathbf{w}^T \mathbf{g}(\mathbf{x}) + b = \sum_{x_i \in S} \alpha_i y_i H(\mathbf{x}_i, \mathbf{x}) + b$$
  
$$b = y_j - \sum_{x_i \in S} \alpha_i y_i H(\mathbf{x}_i, \mathbf{x}_j), \mathbf{x}_j \text{ is an unbounded support vector}$$

• To ensure stability of calculations, we take the average:

$$b = \frac{1}{\#(x_i \in G)} \sum_{x_j \in G} (y_j - \sum_{x_i \in S} \alpha_i y_i H(x_i, x_j))$$

• Then unknown datum *x* is classified into:

$$\begin{cases} \text{Class 1, if } D(\mathbf{x}) > 0 \\ \text{Class 2, if } D(\mathbf{x}) < 0 \end{cases}$$

If D(x) = 0, x is unclassifiable

#### Kernels used in SVM

#### • Linear Kernels:

If the problem is linearly separable, we use linear kernels:  $H(x, x') = x^T x'$ 

### • Polynomial Kernels:

The polynomial kernel with degree  $m \ge 1$  is  $H(x, x') = (x^T x' + 1)^m$ When m = 1, the kernel is the linear kernel by adjusting 1 into bWhen m = 2, d = 2,  $H(x, x') = 1 + 2x_1x_1' + 2x_2x_2' + 2x_1x_1'x_2x_2' + x_1^2x_1'^2 + x_2^2x_2'^2$  $= g(x)^T g(x') \ge 0$  satisfy Mercer's condition where  $g(x) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2)^T$ 

• In general, polynomial kernels satisfy Mercer's condition

#### • Radial Basis Function (RBF) Kernels:

$$H(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma ||\boldsymbol{x} - \boldsymbol{x}'||^2), \gamma > 0 \text{ controlling the radius}$$
$$= \exp(-\gamma ||\boldsymbol{x}||^2) \exp(-\gamma ||\boldsymbol{x}'||^2) \exp(2\gamma \boldsymbol{x}^T \boldsymbol{x}') \tag{*}$$

Because  $\exp(2\gamma x^T x') = 1 + 2\gamma x^T x' + 2\gamma^2 (x^T x')^2 + \frac{2\gamma^3}{3!} (x^T x')^3 + \cdots$ 

is an infinite summation of polynomials  $\Rightarrow$  it is a kernel.

 $\exp(-\gamma ||x||^2)$  and  $\exp(-\gamma ||x'||^2)$  are proved to be kernels and the product of kernels is also a kernel. Thus (\*) is a kernel.

• The decision function is

$$D(\mathbf{x}) = \sum_{x_i \in S} \alpha_i y_i H(\mathbf{x}_i, \mathbf{x}) + b = \sum_{x_i \in S} \alpha_i y_i \exp(-\gamma ||\mathbf{x}_i - \mathbf{x}||^2) + b$$

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

```
%% svmqauss.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 qv = 1:length(gamvals)
     응응
     qam = qamvals(qv);
                               \boldsymbol{H}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp(-\gamma ||\boldsymbol{x}_i - \boldsymbol{x}_j||^2)
     for n = 1:N
          for n2 = 1:N
              K(n,n2) = \exp(-\text{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
   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';
```

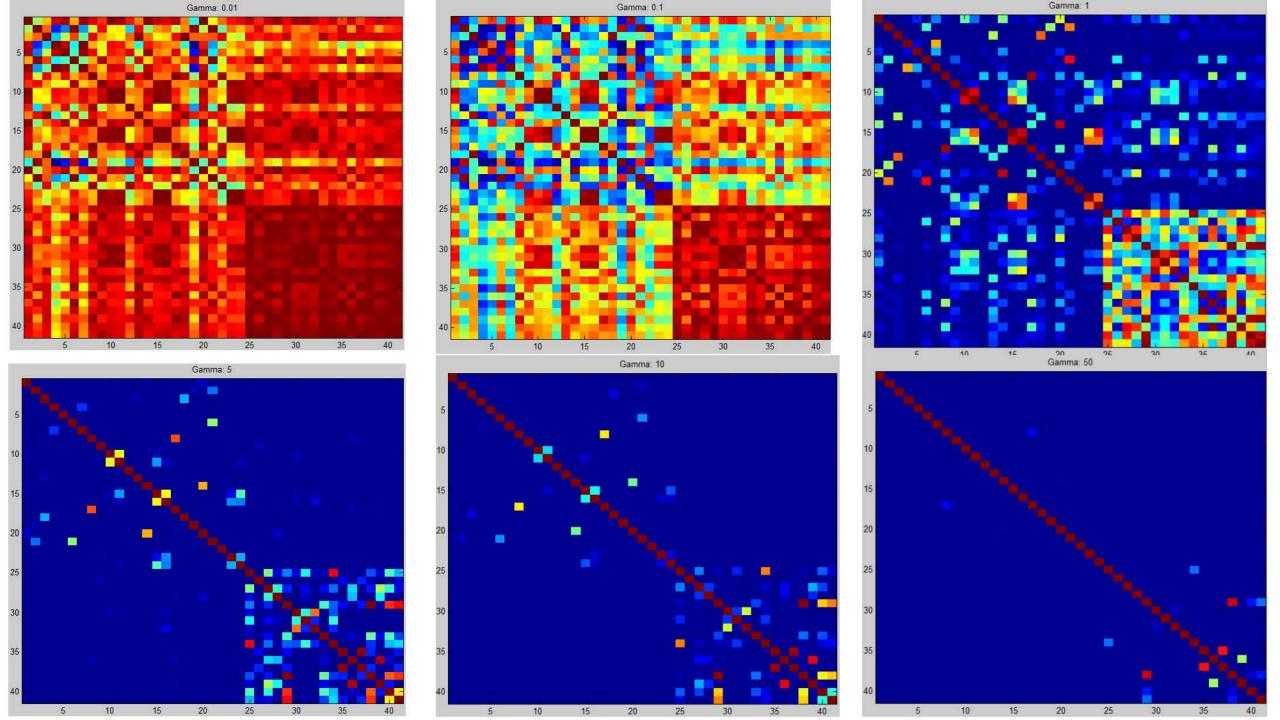
$$Q(\mathbf{w}, b, \alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{H}(\mathbf{x}_i, \mathbf{x}_j)$$
$$\sum_{i=1}^{N} \alpha_i y_i = 0, \quad \mathbf{C} \ge \alpha_i \ge 0, \quad i = 1, \dots, N$$

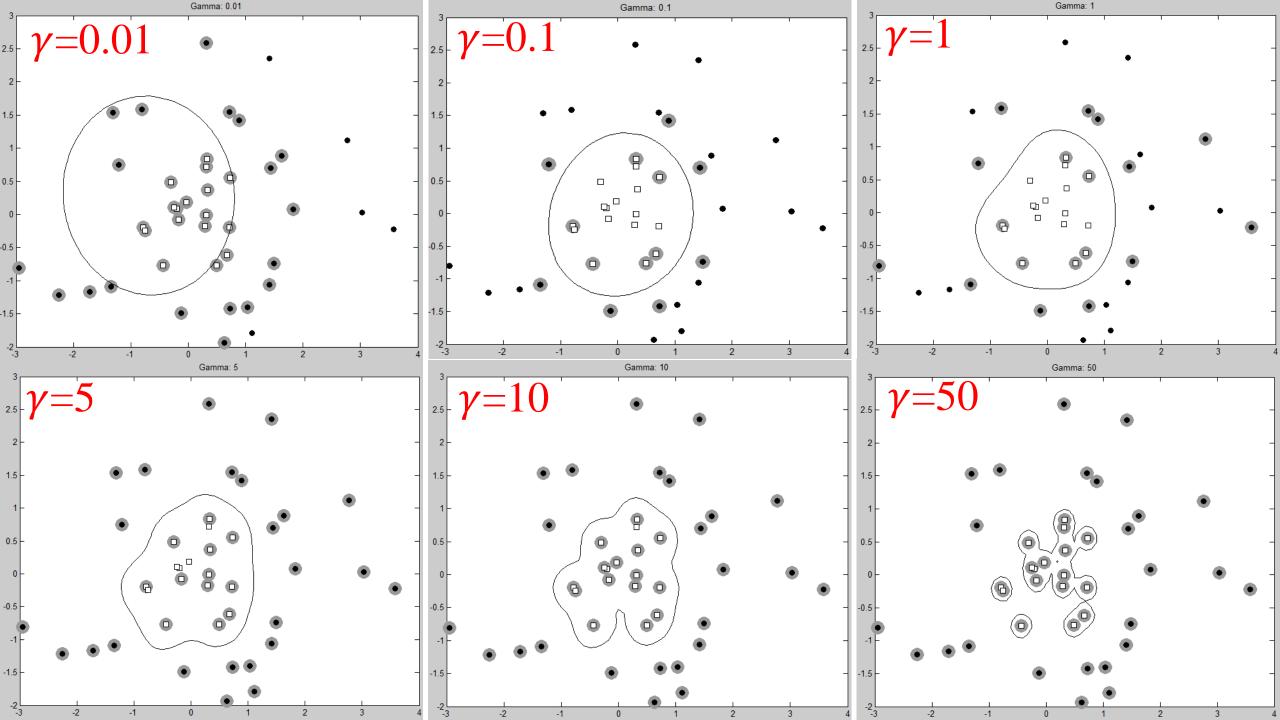
 $\alpha_i$ 's > 0 are support vectors

$$\sum_{x_i \in S} \alpha_i y_i \exp(-\gamma ||\mathbf{x}_i - \mathbf{x}||^2) + b$$

```
% 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:length(tv)
       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: %q',qam);
   title(ti);
   pause
```

end





# **Summary of Kernel Trick**

- A kernel function,  $H: \mathbb{R}^l \times \mathbb{R}^l \to \mathbb{R}$  where  $H(x, x') = g(x)^T g(x')$
- $\mathbf{w} = \sum_{x_i \in S} \alpha_i y_i \, \mathbf{g}(\mathbf{x}_i)$ , where S is the set of support vectors.
- Given a test pattern  $\mathbf{x}$ , we can classify it based on  $D(\mathbf{x}) = \mathbf{w}^T \mathbf{g}(\mathbf{x}) + b$  by  $\sum_{x_i \in S} \alpha_i y_i \mathbf{g}(\mathbf{x}_i)^T \mathbf{g}(\mathbf{x}) + b$

• b is obtained by

$$b = y_j - \sum_{x_i \in S} \alpha_i y_i \, \boldsymbol{g}(\boldsymbol{x}_i)^T \boldsymbol{g}(\boldsymbol{x}_i), \, \boldsymbol{x}_i \text{ is a good support vector}$$

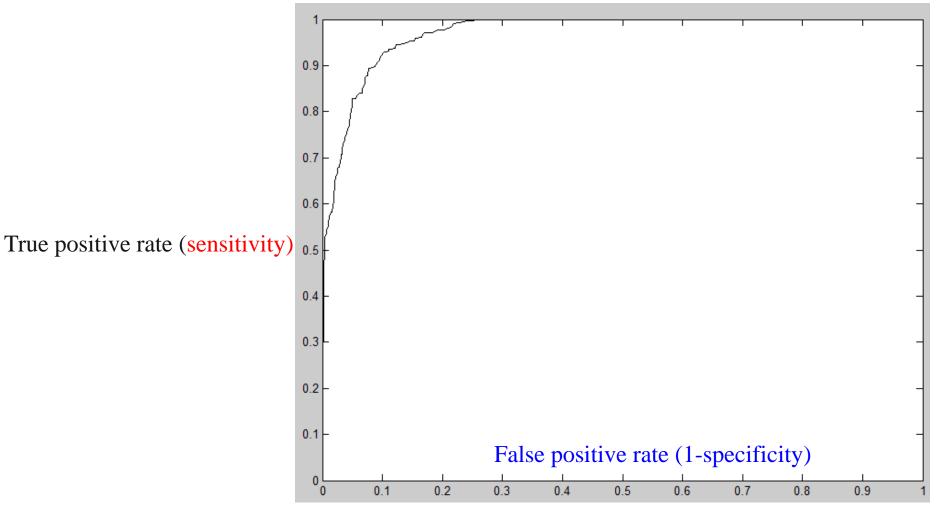
		True Status			
		Yes	No		
Predicted status	Yes	True Positive (TP)	False Positive (FP) Type I error	Positive Predictive Rate, Precision TP/(TP+FP)	False Discovery Rate FP/(TP+FP)
	No	False Negative (FN) Type II error	True Negative (TN)	False Omission Rate FN/(FN+TN)	Negative Predictive Rate TN/(FN+TN)
Total number		True positive Rate Sensitivity, Recall TP/(TP+FN)	False positive Rate  FP/(FP+TN)	F1 score =2*precision*Recall/ (precision+Recall)	
Accuracy (TP+TN)/T		False Negative Rate FN/(TP+FN)	True Negative Rate Specificity TN/(FP+TN)		

```
%% symroc.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(-\text{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) = TN/(TN+FP);
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 = sum(0.5*(sens(2:end)+sens(1:end-1)).*(cspec(2:end) - cspec(1:end-1)));
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  $\sum_{x_i \in S} \alpha_i y_i \exp(-\gamma ||x_i - x||^2) + b$ . 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 1-specificity: 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.