Support Vector Machines

Outline

- 1. Separating hyperplane
- 2. Optimal hyperplane for linearly separable patterns
- 3. Optimal hyperplane for linearly nonseparable patterns
- 4. Building SVM (support vector machine) for pattern recognition
- 5. SVM for nonlinear regression
- 6. SVM for handling imbalanced data

Linearly separable patterns can be separated by a hyperplane: Generator dataset.

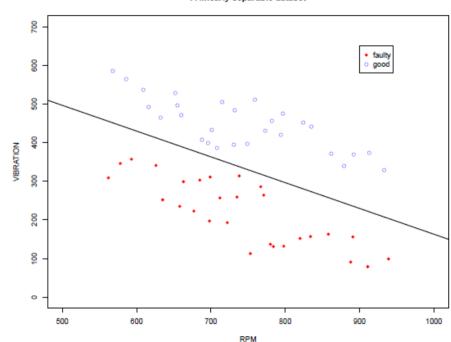
ID	RPM	Vibration	Status	
1	568	585	Good	
2	586	565	Good	
3	609	536	Good	
26	892	370	Good	
27	913	373	Good	
28	933	330	Good	

ID	RPM	Vibration	Status	
29	562	309	Faulty	
30	578	346	Faulty	
31	593	357	Faulty	
54	891	156	Faulty	
55	911	79	Faulty	
56	939	99	Faulty	

A linearly separable dataset

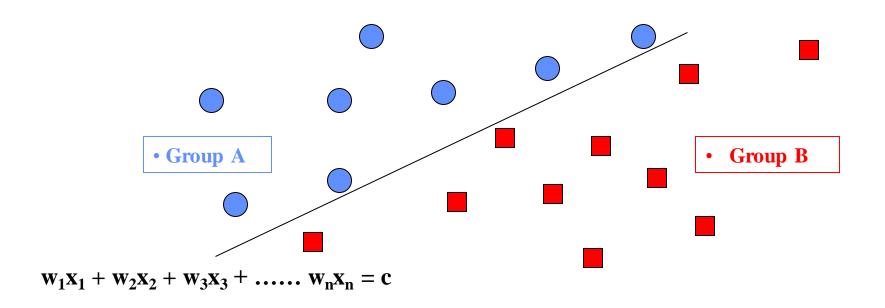
Scatter plot and <u>regression line</u>:

Vibration =
$$830 - 0.667 \times RPM$$



Linear programming for classification

Consider 2 groups of data samples, group A and group B. They are <u>linearly separable</u> if there exists a <u>hyperplane</u> that separates these two groups such that all group A samples are on one side of the plane, and all group B samples are on the other side of the plane.



Linear programming for classification

LP can be used to minimize the <u>maximum deviation</u>:

minimize a

subject to

$$w_1x_1 + w_2x_2 + \dots + w_nx_n \ge c - a,$$

 $w_1x_1 + w_2x_2 + \dots + w_nx_n \le c + a,$
 $a \ge 0$

What is the role of "deviation"?

- n_{gA} = number of samples in Group A
- n_{gB} = number of samples in Group B
- a is the <u>deviation</u>
- c is a parameter, use fixed cut-off c but experiment with both negative and positive c

Linearly separable patterns can be separated by a hyperplane: Generator dataset

ID	RPM	Vibration	Status
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31	593	357	Faulty
54	891	156	Faulty
55	911	79	Faulty
56	939	99	Faulty

minimize a subject to

$$568 \text{ w}_1 + 585 \text{ w}_2 \ge c - a$$
 $586 \text{ w}_1 + 565 \text{ w}_2 \ge c - a$... **Group A** $933 \text{ w}_1 + 339 \text{ w}_2 \ge c - a$

$$562 w_1 + 309 w_2 \le c + a$$
 $578 w_1 + 346 w_2 \le c + a$ **Group B** $939 w_1 + 99 w_2 \le c + a$

 $a \ge 0$

deviation

LP solution for the linearly separable Generator dataset

minimize a subject to

$$568 w_1 + 585 w_2 \ge c - a$$

 $586 w_1 + 565 w_2 \ge c - a$

...

$$933 w_1 + 339 w_2 \ge c - a$$

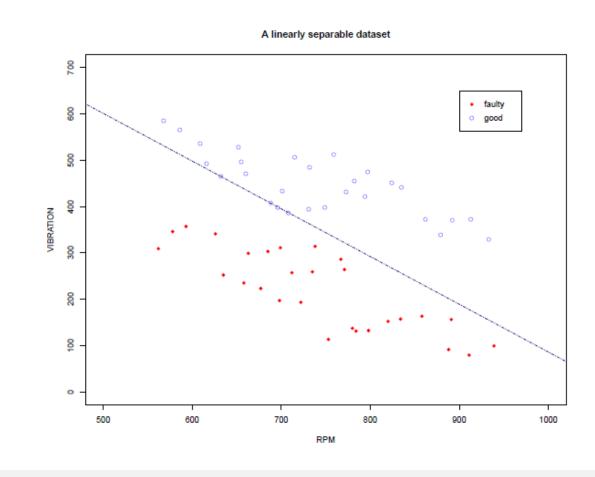
$$562 w_1 + 309 w_2 \le c + a$$

$$578 w_1 + 346 w_2 \le c + a$$

. . . .

$$939 w_1 + 99 w_2 \le c + a$$

 $a > 0$



- With c = 1000, the solution is $w_1 = 0.923439$, $w_2 = 0.895456$, $\mathbf{a} = \mathbf{0} \Leftarrow$ linearly separable data
- Two 'good' data points determine the solution: (632,465) and (696,399)

Finding a separating hyperplane by solving a **Quadratic programming problem**

minimize $\frac{1}{2} (w_1^2 + w_2^2) = \frac{1}{2} \|w\|^2$ subject to

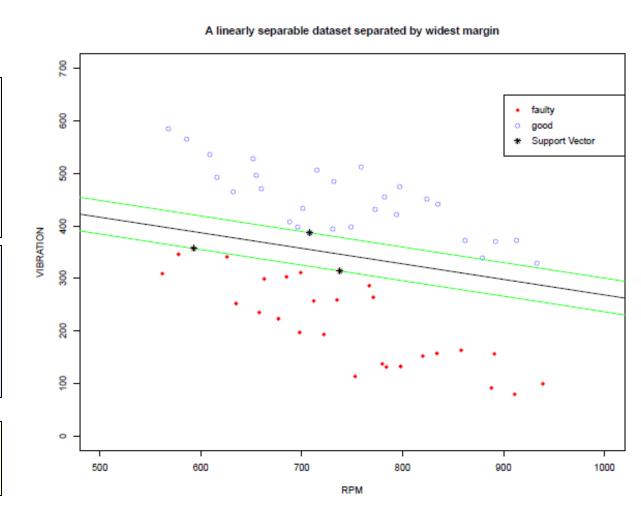
$$|w_0 + 568 w_1 + 585 w_2| \ge +1$$

 $|w_0 + 586 w_1| + 565 w_2| \ge +1$
...
 $|w_0 + 933 w_1| + 339 w_2| \ge +1$

$$w_0 + 562 w_1 + 309 w_2 \le -1$$

 $w_0 + 578 w_1 + 346 w_2 \le -1$
.....
 $w_0 + 939 w_1 + 99 w_2 \le -1$

This approach is Support Vector Machines (SVM)



Finding a separating hyperplane by solving a **Quadratic programming** problem

Solution:

$$w_0 = -17.6249$$

$$w_1 = 0.00925$$

$$w_2 = 0.03120$$

Three data points are found to be support vectors:

$$w_0 + 593 \times w_1 + 357 \times w_2 = -1$$

(738,314):

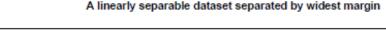
$$w_0 + 738 \times w_1 + 314 \times w_2 = -1$$

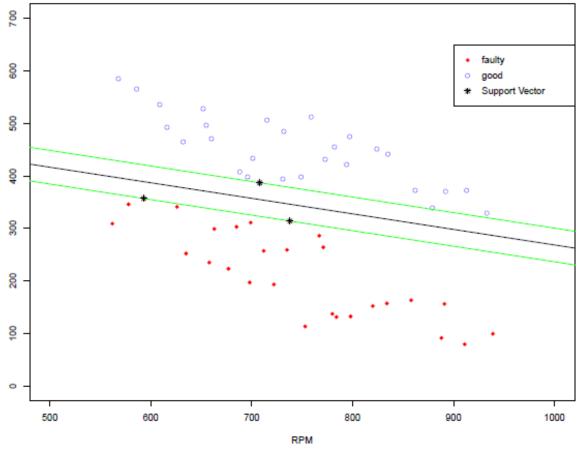
 $(\bigcirc 708,387)$:

$$w_0 + 708 \times w_1 + 387 \times w_2 = +1$$

Decision boundary:

$$w_0 + w_1 \times RPM + w_2 \times Vibration = 0$$



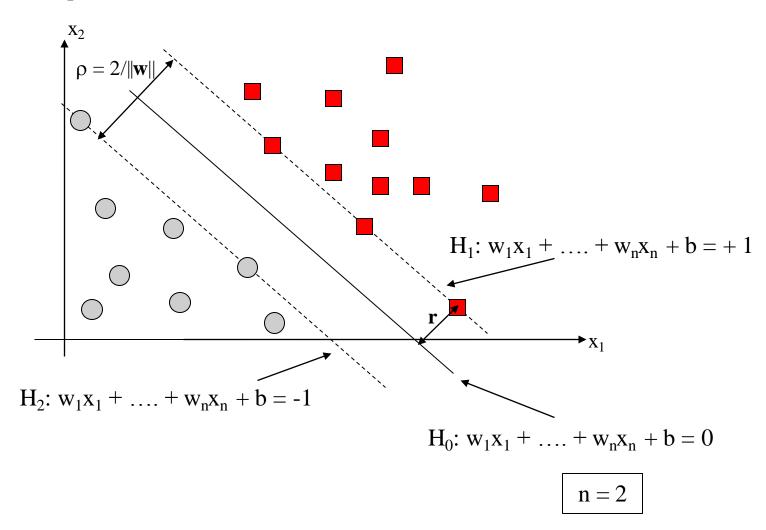


- Let the training samples be x_i , i = 1, 2, ..., N, where x_i is n-dimensional.
- Associated with each $\mathbf{x_i}$ is a target value d_i with value of -1 or 1.
- The class represented by the subset with $d_i = -1$ and the class represented by the subset with $d_i = +1$ are linearly separable if there exists (w,b) such that

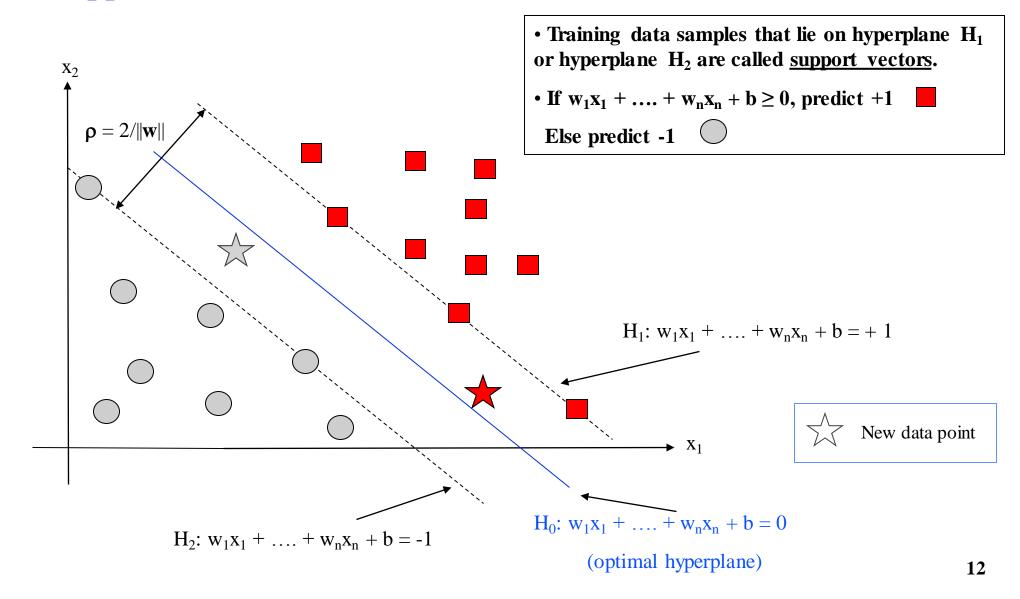
$$\begin{aligned} \mathbf{w}^T \, \mathbf{x_i} + \mathbf{b} &\geq 0 & \text{for } \mathbf{d_i} = +1 \\ \mathbf{w}^T \, \mathbf{x_i} + \mathbf{b} &< 0 & \text{for } \mathbf{d_i} = -1 \end{aligned} \qquad \boxed{b = \mathbf{w_0}}$$

- The margin of separation \mathbf{r} is the separation between the hyperplane $\mathbf{w}^T\mathbf{x} + \mathbf{b} = 0$ and the closest data point.
- The goal of a support vector machine is to find the optimal hyperplane with the maximum margin of separation.

Consider the hyperplane that maximizes the margin of separation



Support Vector Machine (SVM):



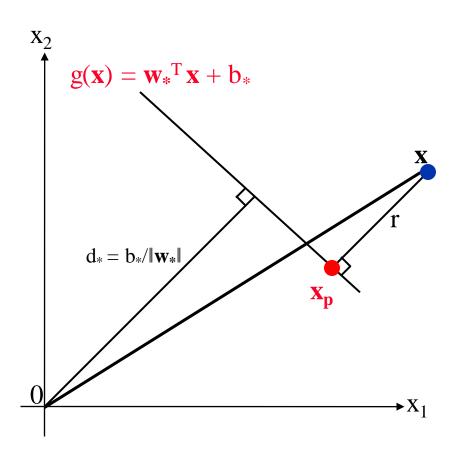
- How to compute the margin of separation?
- Define discriminant function

$$g(\mathbf{x}) = \mathbf{w}_*^T \mathbf{x} + \mathbf{b}_*$$
 and let
$$\mathbf{x} = \mathbf{x}_p + r |\mathbf{w}_*/||\mathbf{w}_*||$$

where $\mathbf{x}_{\mathbf{p}}$ is the normal projection of \mathbf{x} onto the optimal hyperplane.

- r is the distance, r is positive if **x** is on the positive side of the optimal hyperplane, negative otherwise.
- Since $g(\mathbf{x_p}) = 0$, it follows that $g(\mathbf{x}) = \mathbf{w_*}^T \mathbf{x} + \mathbf{b_*} = r ||\mathbf{w_*}|| \quad \text{or}$ $r = g(\mathbf{x})/||\mathbf{w_*}||$

Details on next slide



Note:

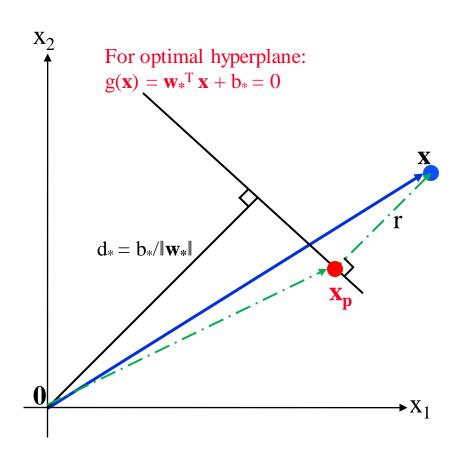
- $\mathbf{x} = \mathbf{x_p} + \mathbf{r} \ \mathbf{w_*} / ||\mathbf{w_*}||$
- $\bullet \quad g(\mathbf{x}) = \mathbf{w}_*^{\mathsf{T}} \mathbf{x} + \mathbf{b}_*$
- $\mathbf{w}_*^T (\mathbf{x} \mathbf{x}_p) = r \mathbf{w}_*^T \mathbf{w}_* / ||\mathbf{w}_*||$
- $\mathbf{w}_*^T \mathbf{x} \mathbf{w}_*^T \mathbf{x}_{\mathbf{p}} = r \|\mathbf{w}_*\|$
- $\mathbf{w}_*^T \mathbf{x} + \mathbf{b}_* = \mathbf{r} \|\mathbf{w}_*\|$

(since $g(\mathbf{x_p}) = 0$ by definition, $0 = \mathbf{w_*}^T \mathbf{x_p} + b_*$)

• Hence,

$$r = (\mathbf{w}_*^T \mathbf{x} + \mathbf{b}_*) / \|\mathbf{w}_*\| = g(\mathbf{x}) / \|\mathbf{w}_*\|$$

• Setting $\mathbf{x} = \mathbf{0}$ for the origin, we have the distance from the origin to the optimal hyperplane $\mathbf{d}_* = \mathbf{b}_* / \|\mathbf{w}_*\|$



Note (on the note):

• Suppose w is an n-dimensional vector

$$\mathbf{w} = (\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_n)^{\mathrm{T}}$$

- Then $\|\mathbf{w}\| = \operatorname{sqrt}(w_1^2 + w_2^2 + \dots + w_n^2)$ and $\|\mathbf{w}\|^2 = (w_1^2 + w_2^2 + \dots + w_n^2) = \mathbf{w}^T \mathbf{w}$
- If $\mathbf{v} = \mathbf{w}/||\mathbf{w}||$

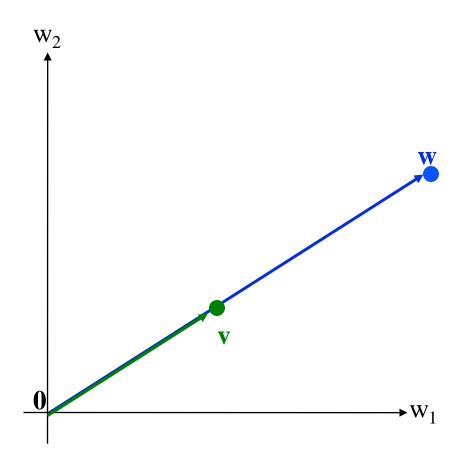
then
$$\|\mathbf{v}\| = \operatorname{sqrt}(v_1^2 + v_2^2 + \dots + v_n^2)$$

$$= \operatorname{sqrt}[(w_1^2 + w_2^2 + \dots + w_n^2)/\|\mathbf{w}\|^2]$$

$$= \operatorname{sqrt}(w_1^2 + w_2^2 + \dots + w_n^2)/\|\mathbf{w}\|$$

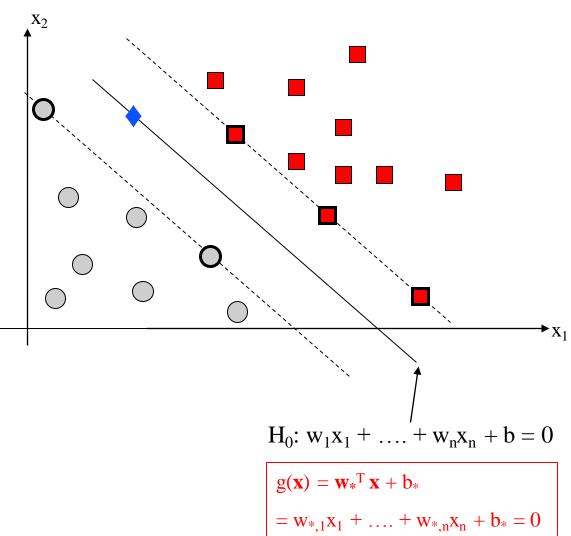
$$= 1$$

that is, v is a <u>unit vector</u>.



Another note (on the note):

- w* is the optimal weight vector
 and b* is its corresponding bias/threshold
- Given the values of $\mathbf{x} = (x_1, x_2 \dots, x_n)$:
 - \circ for $\mathbf{g}(\mathbf{x}) = +1$
 - \circ for $\mathbf{g}(\mathbf{x}) > +1$
 - \circ for \mathbf{O} $g(\mathbf{x}) = -1$
 - \circ for \bigcirc $g(\mathbf{x}) < -1$
 - $\circ \text{ for } \bullet g(\mathbf{x}) = 0$



• The algebraic distance from the support vector $\mathbf{x}^{(s)}$ to the optimal hyperplane is

$$r = g(\mathbf{x}^{(s)}) / \|\mathbf{w}_*\| = 1 / \|\mathbf{w}_0\| \text{ if } d^{(s)} = +1 \quad (\mathbf{w}_*^T \mathbf{x}^{(s)} + \mathbf{b}_* = 1) \text{ and}$$

$$r = g(\mathbf{x}^{(s)}) / \|\mathbf{w}_*\| = -1 / \|\mathbf{w}_0\| \text{ if } d^{(s)} = -1 \quad (\mathbf{w}_*^T \mathbf{x}^{(s)} + b_* = -1)$$

where the plus sign indicates $\mathbf{x}^{(s)}$ lies on the positive side of the hyperplane, and the minus sign indicates $\mathbf{x}^{(s)}$ lies on the negative side.

• Let ρ denote the optimum value of the margin of separation between the two classes of patterns, then

$$\rho = 2 r = 2 / \|\mathbf{w}_*\|$$

• Maximising the margin of separation is equivalent to minimizing the Euclidean norm of the weight vector **w**.

Given the training sample {(x_i,d_i)}, i = 1,, N, the quadratic programming
 (QP) problem is:

minimise
$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

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

The characteristics of the above QP are:

convex quadratic objective function and linear constraints in w.

• The Lagrangian of the QP is

$$J(\mathbf{w}, \mathbf{b}, \boldsymbol{\alpha}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} - \sum_{i=1}^{N} \alpha_{i} [d_{i}(\mathbf{w}^{\mathrm{T}} \mathbf{x}_{i} + \mathbf{b}) - 1]$$

- $\alpha_i \ge 0$, i = 1, ..., N is the Lagrange multiplier for constraint i.
- Optimality conditions:

$$\partial J(\mathbf{w}, \mathbf{b}, \alpha) / \partial \mathbf{w} = 0 \quad \text{and} \quad \partial J(\mathbf{w}, \mathbf{b}, \alpha) / \partial \mathbf{b} = 0$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \, \mathbf{d}_i \, \mathbf{x_i} \qquad \sum_{i=1}^{N} \alpha_i \, \mathbf{d}_i = 0$$

The two optimality conditions yield the following:

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \, \mathbf{d_i} \, \mathbf{x_i} \qquad \text{and}$$

$$\sum_{i=1}^{N} \alpha_i \, \mathbf{d_i} \, = \, 0$$

- Note that the solution vector **w** is defined in terms of a sum that involves the N training samples.
- The <u>Kuhn-Tucker optimality conditions</u> also require that

$$\alpha_i \left[d_i(\mathbf{w}^T \mathbf{x_i} + b) - 1 \right] = 0 \text{ for } i = 1, \dots, N.$$
• If $\alpha_i > 0$, then $d_i(\mathbf{w}^T \mathbf{x_i} + b) = 1$.
this is called the complementarity condition.
• If $d_i(\mathbf{w}^T \mathbf{x_i} + b) \neq 1$, then $\alpha_i = 0$

• Instead of solving QP, we could also solve its dual problem and obtain the same optimal value.

The dual of QP can be obtained as follows:

•
$$J(\mathbf{w}, \mathbf{b}, \alpha) = \frac{1}{2} \ \mathbf{w}^T \mathbf{w} - \sum_{i=1}^{N} \alpha_i [d_i(\mathbf{w}^T \mathbf{x_i} + \mathbf{b}) - 1]$$

$$= \frac{1}{2} \ \mathbf{w}^T \mathbf{w} - \sum_{i=1}^{N} \alpha_i \ d_i \ \mathbf{w}^T \mathbf{x_i} - \mathbf{b} \sum_{i=1}^{N} \alpha_i \ d_i + \sum_{i=1}^{N} \alpha_i$$

$$\text{but } \mathbf{w}^T \mathbf{w} = \sum_{i=1}^{N} \alpha_i \ d_i \ \mathbf{w}^T \mathbf{x_i} = \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \ d_i \ d_j \mathbf{x_i}^T \mathbf{x_j}$$
and
$$\sum_{i=1}^{N} \alpha_i \ d_i = 0 \text{ (the two optimality conditions on previous slide)}$$

• Hence, we <u>maximise</u> the dual quadratic programming

$$Q(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j d_i d_j \mathbf{x_i}^T \mathbf{x_j}$$
subject to:
$$\sum_{i=1}^{N} \alpha_i d_i = 0 \text{ and } \alpha_i \ge 0 \text{ for } i = 1, 2, \dots, N.$$

- Note that the dual problem is given in terms of x_i and that the unknown variables are α_i , i = 1, ..., N.
- Once the <u>optimal value variables</u> of dual QP, $\alpha_{*,i}$ have been computed, the optimum weight vector \mathbf{w}_0 is equal to

$$\mathbf{w}_* = \sum_{i=1}^N \alpha_{*,i} \mathbf{d}_i \ \mathbf{x}_i$$

and the optimum bias b* is

$$b_* = 1 - \mathbf{w_*}^T \mathbf{x^{(s)}} \text{ for } \mathbf{d^{(s)}} = +1$$

 $\mathbf{b}_* = 1 - \mathbf{w}_*^T \mathbf{x}^{(s)}$ for $\mathbf{d}^{(s)} = +1$ where $\mathbf{x}^{(s)}$ is a support vector

Notation used:

- for n-dimensional vectors \mathbf{x} and \mathbf{y} , $\mathbf{x}^T\mathbf{y} = \sum_{i=1}^{n} (\mathbf{x}_i \times \mathbf{y}_i)$
- $\|\mathbf{x}\|$ = the Euclidean distance of \mathbf{x} from the origin

= sqrt[
$$\sum_{i=1}^{n} x_i^2$$
] = sqrt ($x_1^2 + x_2^2 + \dots + x_n^2$)

• Example.

i	\mathbf{x}_1	$\mathbf{X_2}$	Class	$\mathbf{d_i}$
1	0	2	Bad	-1
2	2	2.4	Bad	-1
3	2	5	Good	+1
4	3	4	Good	+1
5	1	4.5	Good	+1
6	1	4	Good	+1
7	1	2	Bad	-1
8	0	1.2	Bad	-1

minimize subject to

$$\frac{1}{2} (w_1^2 + w_2^2) = \frac{1}{2} \|w\|^2$$

i=1:
$$0 w_1 + 2 w_2 + b \le -1$$

i=2: $2 w_1 + 2.4 w_2 + b \le -1$
i=7: $1 w_1 + 2 w_2 + b \le -1$
i=8: $0 w_1 + 1.2 w_2 + b \le -1$

i=3:
$$2 w_1 + 5 w_2 + b \ge +1$$

i=4: $3 w_1 + 4 w_2 + b \ge +1$
i=5: $1 w_1 + 4.5 w_2 + b \ge +1$
i=6: $1 w_1 + 4 w_2 + b \ge +1$

Example.

QP: minimize $\frac{1}{2}(w_1^2 + w_2^2) = \frac{1}{2} \|w\|^2$

subject to

$$0 \ w_1 + 2 \ w_2 + b \le -1$$

$$2 w_1 + 2.4 w_2 + b \le -1$$

$$1 w_1 + 2 w_2 + b \le -1$$

$$0 w_1 + 1.2 w_2 + b \le -1$$

$$2 w_1 + 5 w_2 + b \ge +1$$

$$3 w_1 + 4 w_2 + b \ge +1$$

$$1 w_1 + 4.5 w_2 + b \ge +1$$

$$1 w_1 + 4 w_2 + b \ge +1$$

Target = +1 Target = -1 Is this the widest margin separating the 2 groups? g e Equations of separating hyperplanes

Maximum margin separation by SVM

Check if $w_1 = 0$, $w_2 = 5/4$ and b = -4satisfy all the optimality conditions (page 22)

minimize subject to

$$\frac{1}{2} (w_1^2 + w_2^2) = \frac{1}{2} \|w\|^2$$

$$0 \ w_1 + 2 \ w_2 + b \le -1$$

$$2 w_1 + 2.4 w_2 + b \le -1$$

$$1 w_1 + 2 w_2 + b \le -1$$

$$0 w_1 + 1.2 w_2 + b \le -1$$

$$2 w_1 + 5 w_2 + b \ge +1$$

$$3 w_1 + 4 w_2 + b \ge +1$$

$$1 w_1 + 4.5 w_2 + b \ge +1$$

$$1 w_1 + 4 w_2 + b \ge +1$$

Check if $w_1 = 0$, $w_2 = 5/4$ and b = -4 satisfy all the optimality conditions (page 22)

• First check feasibility:

$$0 w_1 + 2 w_2 + b = 0 + 2(5/4) - 4 < -1$$

$$2 w_1 + 2.4 w_2 + b = 0 + 2.4(5/4) - 4 = -1$$

$$1 w_1 + 2 w_2 + b = 0 + 2(5/4) - 4 < -1$$

$$0 w_1 + 1.2 w_2 + b = 0 + 1.2(5/4) - 4 < -1$$

$$2 w_1 + 5 w_2 + b = 0 + 5(5/4) - 4 > +1$$

$$3 w_1 + 4 w_2 + b = 0 + 4(5/4) - 4 = +1$$

1
$$w_1 + 4.5 w_2 + b = 0 + 4.5(5/4) - 4 > +1$$

$$1 w_1 + 4 w_2 + b = 0 + 4(5/4) - 4 = +1$$

$$0 w_1 + 2 w_2 + b = 0 + 2(5/4) - 4 < -1$$

$$2 w_1 + 2.4 w_2 + b = 0 + 2.4(5/4) - 4 = -1$$

$$1 w_1 + 2 w_2 + b = 0 + 2(5/4) - 4 < -1$$

$$0 w_1 + 1.2 w_2 + b = 0 + 1.2(5/4) - 4 < -1$$

2
$$w_1 + 5 w_2 + b = 0 + 5(5/4) - 4 > +1$$

3 $w_1 + 4 w_2 + b = 0 + 4(5/4) - 4 = +1$
1 $w_1 + 4.5 w_2 + b = 0 + 4.5(5/4) - 4 > +1$
1 $w_1 + 4 w_2 + b = 0 + 4(5/4) - 4 = +1$

Then check complementarity conditions:

$$\alpha_i \left[d_i(w^Tx_i + b) - 1 \right] = 0$$
 for $i = 1, \, \dots, \, N.$

For samples with $d_{i} = -1$:

$$0 w_1 + 2 w_2 + b < -1 \rightarrow \text{let } \alpha_1 = 0$$

$$2 w_1 + 2.4 w_2 + b = -1 \rightarrow \alpha_2 = ?$$

$$1 w_1 + 2 w_2 + b < -1 \rightarrow \text{let } \alpha_7 = 0$$

$$0 w_1 + 1.2 w_2 + b < -1 \rightarrow \text{let } \alpha_8 = 0$$

For samples with $d_{i} = +1$:

2
$$w_1 + 5 w_2 + b > +1 \rightarrow let \alpha_3 = 0$$

$$3 w_1 + 4 w_2 + b = +1 \rightarrow let \alpha_4 = ?$$

1
$$w_1 + 4.5 w_2 + b > +1 \rightarrow let \alpha_5 = 0$$

$$1 w_1 + 4 w_2 + b = +1 \rightarrow let \alpha_6 = ?$$

For samples with $d_i = -1$:

$$0 \ w_1 + 2 \ w_2 + b < -1 \rightarrow let \ \alpha_1 = 0$$

$$2 w_1 + 2.4 w_2 + b = -1 \rightarrow \alpha_2 = ?$$

1
$$w_1 + 2 w_2 + b < -1 \rightarrow let \alpha_7 = 0$$

$$0 w_1 + 1.2 w_2 + b < -1 \rightarrow let \alpha_8 = 0$$

For samples with $d_i = +1$:

$$2 w_1 + 5 w_2 + b > +1 \rightarrow let \alpha_3 = 0$$

$$3 w_1 + 4 w_2 + b = +1 \rightarrow let \alpha_4 = ?$$

1
$$w_1 + 4.5 w_2 + b > +1 \rightarrow let \alpha_5 = 0$$

$$1 w_1 + 4 w_2 + b = +1 \rightarrow let \alpha_6 = ?$$

• Are there values of α_2 , α_4 , $\alpha_6 \ge 0$ such that:

$$\mathbf{w} = \sum_{i=1}^{8} \alpha_i \, \mathbf{d}_i \, \mathbf{x}_i$$
 and $\sum_{i=1}^{8} \alpha_i \, \mathbf{d}_i = 0$

$$\binom{w_1}{w_2} = \binom{0}{5/4} = -\alpha_2 \binom{2}{2.4} + \alpha_4 \binom{3}{4} + \alpha_6 \binom{1}{4}$$

$$-\alpha_2 + \alpha_4 + \alpha_6 = 0$$
?

• Answer: $\alpha_2 = 50/64$, $\alpha_4 = 25/64$, $\alpha_6 = 25/64$

Conclusion:

- $w_1 = 0$, $w_2 = 5/4$ and b = -4 is the optimal solution to QP.
- $5/4 x_2 4 = 0$ is the optimal separating hyperplane.
- Samples i = 2,4,6 are support vectors.
- $\|\mathbf{w}\| = \operatorname{sqrt}(0^2 + (5/4)^2) = 5/4$
- $g(\binom{1}{4}) = 1$, distance to optimal hyperplane = $g(x)/\|w\| = 4/5$.

- We consider now the case of nonseparable patterns where it is <u>not</u> possible to construct a hyperplane without encountering classification errors.
- The margin of separation between classes is <u>soft</u> if a data point $(\mathbf{x_i}, d_i)$ violates the condition $d_i(\mathbf{w}^T\mathbf{x_i} + b) \ge 1$ for i = 1, ..., N
- We introduce a set of nonnegative scalars ξ_i , i=1,...,N and have the new condition

$$d_{i}(\mathbf{w}^{T}\mathbf{x}_{i} + \mathbf{b}) \geq 1 - \xi_{i}, i = 1,...,N$$

- ξ_i is also called a <u>slack variable</u>.
- For $0 \le \xi_i \le 1$, the data point falls inside the region of separation, but on the right side of the decision surface (optimal hyperplane).
- For $\xi_i > 1$, it falls on the wrong side of the separating hyperplane.

For this case, the support vectors are data points that satisfy

$$d_{i}(\mathbf{w}^{T}\mathbf{x}_{i} + \mathbf{b}) = 1 - \xi_{i}, i = 1,..., N$$

- ξ_i is a slack variable.
- The goal now is to find a separating hyperplane that minimises the classification errors, for example:

minimise
$$\Phi(\xi) = \sum_{i=1}^{N} I(\xi_i - 1)$$

where $I(\xi)$ is an <u>indicator function</u> and $I(\xi) = 0$ if $\xi \le 0$, and 1 otherwise.

• The minimisation problem becomes non-convex and it is NP-complete.

- NP = "Nondeterministic Polynomial"
- NP complete problem: no polynomial time algorithms are known to solve this problem

• We approximate the misclassification counts by

$$\Phi(\boldsymbol{\xi}) = \sum_{i=1}^{N} \xi_{i}$$

The primal quadratic programming problem for nonseparable case is

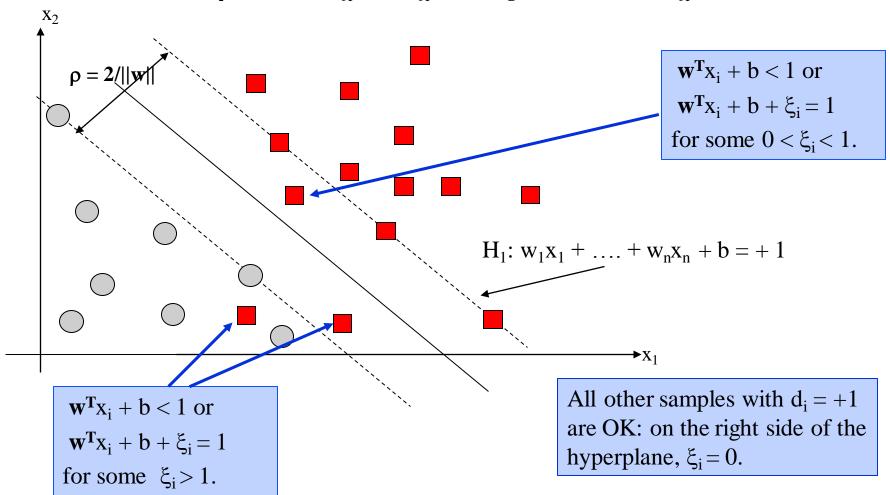
minimise
$$\Phi(\mathbf{w}, \boldsymbol{\xi}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^{N} \boldsymbol{\xi}_i$$

subject to $d_i(\mathbf{w}^T \mathbf{x}_i + \mathbf{b}) \ge 1 - \boldsymbol{\xi}_i$
and $\boldsymbol{\xi}_i \ge 0$ for $i = 1, ..., N$

where C is a user-specified parameter that can be determined experimentally.

• Consider samples with $d_i = +1$

we want $(\mathbf{w}^T\mathbf{x_i} + \mathbf{b}) \ge 1 - \xi_i$ with $\xi_i = 0$ if possible, if not $\xi_i > 0$



• The dual of the above QP is <u>maximize</u>

$$Q(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j d_i d_j \mathbf{x_i}^T \mathbf{x_j}$$

subject to the constraints:

$$\sum_{i=1}^{N} \alpha_i d_i = 0 \text{ and } 0 \le \alpha_i \le C \text{ for } i = 1, 2, \dots, N.$$

• The optimum solution for the weight vector w is given by

$$\mathbf{w}_* = \sum_{i=1}^{N_S} \alpha_{*,i} d_i \mathbf{x_i}$$
 where N_s is the number of support vectors.

The complementarity conditions are

$$\alpha_{i} \left[d_{i}(\mathbf{w}^{T}\mathbf{x_{i}} + \mathbf{b}) - 1 + \xi_{i} \right] = 0, \qquad i = 1, 2, \dots, N$$

$$\mu_{i} \xi_{i} = 0$$

$$\xi_{i} (C - \alpha_{i}) = 0$$

$$\alpha_{i} > 0$$

 $(\mu_i \text{ is Lagrange multiplier associated with the constraint } \xi_i \geq 0 \text{ in the primal problem})$

• To determine the optimal bias b_* , take the points with $0 < \alpha_{*,i} < C$. For these points, $\xi_i = 0$, and compute b from the first complementarity condition above:

$$d_i(\mathbf{w}^T\mathbf{x_i} + \mathbf{b}) = 1$$

and take the mean value of b resulting from all such data points in the training sample.

- The construction of svm for a pattern recognition task hinges on two important ideas:
 - 1. Nonlinear mapping of an input vector into a high dimensional feature space that is hidden from both the input and the output.
 - 2. Construction of an optimal hyperplane for separating the features discovered in Step 1.
- Cover's theorem on the separability of patterns:
 - A complex pattern-classification problem cast in a high dimensional space nonlinearly is more likely to be linearly separable than in a low dimensional space.
- The separating hyperplane is to be defined as a linear function of vectors drawn from the feature space rather than in the original space. How is this hyperplane to be constructed?

Inner-product kernel

- Let \mathbf{x} denote a vector drawn from the \mathbf{m}_0 dimensional input space.
- Let $\phi_j(\mathbf{x})$, $j = 1,..., m_1$ denote a set of nonlinear transformation from the input space to the m_1 dimensional feature space.
- It is assumed that $\phi_i(\mathbf{x})$ is defined a priori for all $j = 1, ..., m_1$.
- Let $\varphi_0(\mathbf{x}) = 1$ for all \mathbf{x} .
- Define a decision hyperplane in the feature space as follows

$$\sum_{j=0}^{m_1} \mathbf{w}_j \, \mathbf{\phi}_j(\mathbf{x}) = 0$$

(note that w_0 denotes the <u>bias</u> of the hyperplane).

• Let $\Psi(\mathbf{x}) = [\phi_0(\mathbf{x}), \phi_1(\mathbf{x}),, \phi_{m1}(\mathbf{x})]^T$ then the decision surface can be written as

$$\mathbf{W}^{\mathrm{T}} \mathbf{\Psi}(\mathbf{x}) = 0$$

• Example:

$$b + w^{T} x = 5 + 2x_{1} - 7x_{2} = 0$$

 $b = 5, w_{1} = 2, w_{2} = -7$

• Or similarly

$$\mathbf{w}^{T} \mathbf{y} = 0$$
, where $\mathbf{w} = [5 \ 2 \ -7]^{t}$ $\mathbf{y} = [1 \ x_{1} \ x_{2}]^{t}$

Inner-product kernel (continued)

• In the new space, we search for linear separability of the features, that is we want a weight vector **w** such that

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \, \mathbf{d_i} \, \Psi(\mathbf{x_i})$$
 Compare to the original equation for w on page 19

where $\Psi(\mathbf{x_i})$ is the feature vector which corresponds to the input pattern $\mathbf{x_i}$.

• The decision surface computed in the feature space is

$$\sum_{i=1}^{N} \alpha_i d_i \Psi^T(\mathbf{x_i}) \Psi(\mathbf{x}) = 0$$
 This is just w^Tx = 0 in the original space

• The term $\Psi^T(\mathbf{x_i}) \Psi(\mathbf{x})$ represents the <u>inner product</u> of two vectors induced in the feature space by the input vector \mathbf{x} and the i-th input vector $\mathbf{x_i}$.

Inner-product kernel (continued)

Define the inner-product kernel $K(\mathbf{x}, \mathbf{x}_i)$ as follows:

$$K(\mathbf{x}, \mathbf{x_i}) = \Psi^{T}(\mathbf{x}) \Psi(\mathbf{x_i})$$

$$= \sum_{j=0}^{m_1} \varphi_j(\mathbf{x}) \varphi_j(\mathbf{x_i}) \qquad \text{for } i = 1, 2, ..., N$$

The inner-product kernel is a symmetric function:

$$K(\mathbf{x}, \mathbf{x_i}) = K(\mathbf{x_i}, \mathbf{x})$$
 for all i.

Using the inner-product kernel $K(\mathbf{x}, \mathbf{x}_i)$, we may construct the optimal hyperplane in the feature space without having to consider the feature space itself in explicit

form. The optimal hyperplane is
$$\sum_{i=1}^{N} \alpha_i \ d_i \ K(\mathbf{x}, \mathbf{x_i}) = 0$$
• $\mathbf{x_i}$ is the i-th "training" data sample
• \mathbf{x} is a new point with "unknown" target value.

Optimum design of SVM

- Given the training sample $\{(\mathbf{x_i}, d_i)\}$, i = 1, 2, ..., N, find the Lagrange multipliers $\{\alpha_i\}$, i = 1, 2, ..., N that maximise the objective function
- $Q(\alpha) = \sum_{i=1}^{N} \alpha_i \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j d_i d_j K(\mathbf{x_i}^T, \mathbf{x_j})$ Compare with dual QP on pg 31

subject to the constraints:

$$\sum_{i=1}^{N} \alpha_{i} d_{i} = 0 \text{ and } 0 \leq \alpha_{i} \leq C \text{ for } i = 1, 2,, N$$

where C is a user-specified positive parameter.

• We may view $K(\mathbf{x_i}^T, \mathbf{x_j})$ as the ij-th element of a symmetric N-by-N matrix as shown by $K = \{K(\mathbf{x_i}^T, \mathbf{x_i})\}$ for i, j = 1, 2, ..., N

Inner product kernel for 3 common types of SVM:

• Type: polynomial learning machine

Inner product kernel: $K(\mathbf{x}, \mathbf{x_i}) = (\mathbf{x}^T \mathbf{x_i} + 1)^p$

Comment: p is specified a priori by the user.

• Type: Radial basis function network.

Inner product kernel: $K(\mathbf{x}, \mathbf{x}_i) = \exp(-1/(\sigma^2) || \mathbf{x} - \mathbf{x}_i ||^2)$

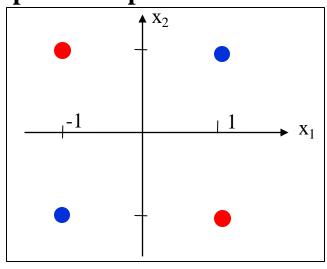
Comment: the width σ^2 is specified a priori by the user.

• Type: two-layer perceptron

Inner product kernel: $tanh(\beta_0 \mathbf{x}^T \mathbf{x_i} + \beta_1)$

Comment: only for some values of β_0 and β_1 .

Example: XOR problem



XOR problem:				
i	Input vector $\mathbf{x_i}$	Desired response d _i		
1	(-1,-1)	- 1		
2	(-1,+1)	+1		
3	(+1,-1)	+1		
4	(+1,+1)	-1		

• Let $K(\mathbf{x}, \mathbf{x_i}) = (\mathbf{x}^T \mathbf{x_i} + 1)^2$ = $(x_1 x_{i1} + x_2 x_{i2} + 1)^2$

2D samples mapped into 5D feature space

$$= 1 + x_1^2 x_{i1}^2 + 2x_1 x_2 x_{i1} x_{i2} + x_2^2 x_{i2}^2 + 2x_1 x_{i1} + 2x_2 x_{i2}$$

- Hence, $\Psi(\mathbf{x}) = [1, x_1^2, \sqrt{2} x_1 x_2, x_2^2, \sqrt{2} x_1, \sqrt{2} x_2]^T$ and $\Psi(\mathbf{x_i}) = [1, x_{i1}^2, \sqrt{2} x_{i1} x_{i2}, x_{i2}^2, \sqrt{2} x_{i1}, \sqrt{2} x_{i2}]^T$
- We also find $K(1,1) = [(-1,-1)^T(-1,-1) + 1)]^2 = 3^2 = 9$.

Example: XOR problem

XOR problem:				
i	Input vector $\mathbf{x_i}$	Desired response d _i		
1	(-1,-1)	-1		
2	(-1,+1)	+1		
3	(+1,-1)	+1		
4	(+1,+1)	-1		

•
$$\Psi(\mathbf{x}) = [1, x_1^2, \sqrt{2} x_1 x_2, x_2^2, \sqrt{2} x_1, \sqrt{2} x_2]^T$$

and
$$\Psi(\mathbf{x_i}) = [1, x_{i1}^2, \sqrt{2} x_{i1}^2 x_{i2}, x_{i2}^2, \sqrt{2} x_{i1}, \sqrt{2} x_{i2}]^T$$

$$\Psi(\mathbf{x_4}) = [1, 1, \sqrt{2}, 1, \sqrt{2}, \sqrt{2}]^T$$

Example:

$$\Psi(\mathbf{x_1})^{\mathrm{T}} \Psi(\mathbf{x_1}) =$$

$$1 + 1 + 2 + 1 + 2 + 2 = 9$$

$$\Psi(\mathbf{x_1})^{\mathrm{T}} \Psi(\mathbf{x_3}) =$$

$$1 + 1 - 2 + 1 - 2 + 2 = 1$$

Example: XOR problem (continued)

The matrix **K** is then

$$\mathbf{K} = \begin{bmatrix} 9 & 1 & \mathbf{1} & 1 \\ 1 & 9 & 1 & 1 \\ 1 & 1 & 9 & 1 \\ 1 & 1 & 1 & 9 \end{bmatrix}$$

Example:

$$\mathbf{K} = \begin{bmatrix} 9 & 1 & 1 & 1 \\ 1 & 9 & 1 & 1 \\ 1 & 1 & 9 & 1 \\ 1 & 1 & 1 & 9 \end{bmatrix}$$
$$\mathbf{K}(1,3) = [\mathbf{x}_1 \ \mathbf{x}_3 + 1]^2$$
$$= [(-1,-1)^{\mathrm{T}}(+1,-1) + 1)]^2$$
$$= (0+1)^2 = 1$$

The dual objective function $Q(\alpha)$ is

$$Q(\alpha) = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 - \frac{1}{2} (9\alpha_1^2 - 2\alpha_1\alpha_2 - 2\alpha_1\alpha_3 + 2\alpha_1\alpha_4 + 9\alpha_2^2 + 2\alpha_2\alpha_3 - 2\alpha_2\alpha_4 + 9\alpha_3^2 - 2\alpha_3\alpha_4 + 9\alpha_4^2)$$

See Equation on page 37.

Taking the derivative of $Q(\alpha)$ with respect to α_1 , α_2 , α_3 and α_4 :

$$9\alpha_{1} - \alpha_{2} - \alpha_{3} + \alpha_{4} = 1$$

$$-\alpha_{1} + 9\alpha_{2} + \alpha_{3} - \alpha_{4} = 1$$

$$-\alpha_{1} + \alpha_{2} + 9\alpha_{3} - \alpha_{4} = 1$$

$$\alpha_{1} - \alpha_{2} - \alpha_{3} + 9\alpha_{4} = 1$$

The XOR problem (continued)

- The solution: $\alpha_{*,1} = \alpha_{*,2} = \alpha_{*,3} = \alpha_{*,4} = \frac{1}{8}$
- The optimum value of $Q(\alpha)$ is $Q(\alpha_*) = \frac{1}{8} + \frac{1}{8} + \frac{1}{8} + \frac{1}{8} \frac{1}{2}(9/64 \dots + 9/64) = \frac{1}{4}$.
- This optimal value of the dual QP is equal to the optimal value of the primal QP, i.e.

$$Q(\alpha_*) = \frac{1}{4} = \frac{1}{2} \|\mathbf{w}_*\|^2$$
 hence $\|\mathbf{w}_*\| = \frac{1}{\sqrt{2}}$

• The optimum weight vector is

$$\mathbf{w}_* = \frac{1}{8} \left[-\Psi(\mathbf{x_1}) + \Psi(\mathbf{x_2}) + \Psi(\mathbf{x_3}) - \Psi(\mathbf{x_4}) \right]$$
 See Equation on page 35
$$= [0, 0, -1/\sqrt{2}, 0, 0, 0]^T$$

- The bias b is the first element of \mathbf{w}_* and it is equal to $\mathbf{0}$.
- The optimal hyperplane is $\mathbf{w}_*^T \Psi(\mathbf{x}) = 0$

The XOR problem (continued)

• The optimal hyperplane is $\mathbf{w_0}^T \Psi(\mathbf{x}) = 0$

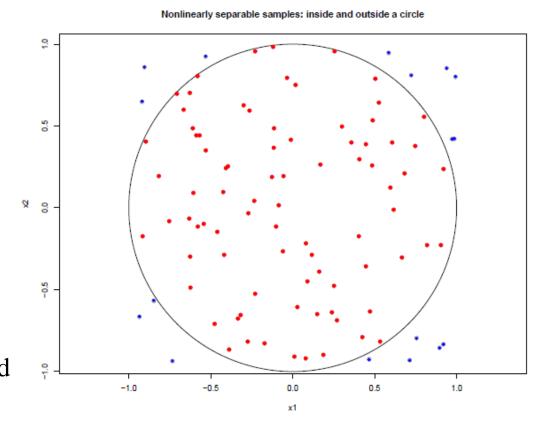
$$= [0, \ 0, \ -1/\sqrt{2}, 0, \ 0, \ 0]^T \ [1, \ x_1^2, \sqrt{2} \ x_1 x_2, \ x_2^2, \sqrt{2} \ x_1, \sqrt{2} \ x_2]$$
 which reduces to $-x_1 \ x_2 = 0$.

• Hence the outputs of the SVM can be summarised as follows:

XOR problem:					
Input vector x	Desired response d	Output $-x_1 x_2$			
(-1,-1)	-1	-1			
(-1,+1)	+1	+1			
(+1,-1)	+1	+1			
(+1,+1)	-1	-1			

Another example:

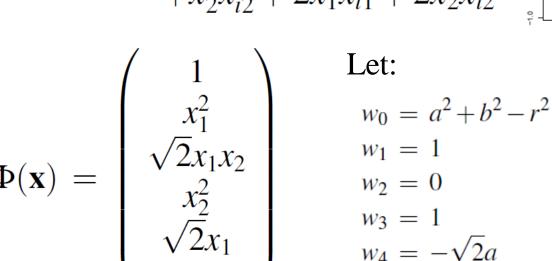
- Data in the original 2-dimensional space are not linearly separable.
- Suppose samples outside the circle are assigned Class A with $d_i = +1$, those on the circle or inside it Class B $d_i = -1$.
- Let the center of the circle be (a,b) and its radius be r
- Class A: $(x_1 a)^2 + (x_2 b)^2 > r^2$
- Class B: $(x_1 a)^2 + (x_2 b)^2 \le r^2$

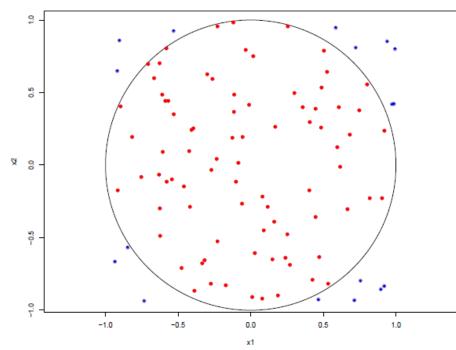


Another example (continued):

- Class A: $(x_1 a)^2 + (x_2 b)^2 > r^2$
- Class B: $(x_1 a)^2 + (x_2 b)^2 \le r^2$
- Apply polynomial kernel:

$$K(\mathbf{x}, \mathbf{x}_i) = 1 + x_1^2 x_{i1}^2 + 2x_1 x_2 x_{i1} x_{i2} + x_2^2 x_{i2}^2 + 2x_1 x_{i1} + 2x_2 x_{i2}$$





Nonlinearly separable samples: inside and outside a circle

Samples can be separated by the hyperplane

$$\mathbf{w}^{\mathrm{T}} \Phi(\mathbf{x}) = 0$$

Another example (continued):

- Class A: $(x_1 a)^2 + (x_2 b)^2 > r^2$
- Class B: $(x_1 a)^2 + (x_2 b)^2 \le r^2$

Samples can be separated by the hyperplane $\mathbf{w}^{\mathrm{T}} \Phi(\mathbf{x}) = 0$

$$a^2 + b^2 - r^2 + x_1^2 + 0 + x_2^2 - 2ax_1 - 2bx_2 = 0$$

$$x_1^2 - 2ax_1 + a^2 + x_2^2 - 2bx_2 + b^2 - r^2 = 0$$

$$(x_1 - a)^2 + (x_2 - b)^2 - r^2 = 0$$

Decision:

If $\mathbf{w}^{\mathrm{T}} \Phi(\mathbf{x}) > 0$, then class A, else class B

$$\begin{array}{c}
1\\
x_1^2\\
\sqrt{2}x_1x_2\\
x_2^2\\
\sqrt{2}x_1\\
\sqrt{2}x_2
\end{array}$$

$$\Phi(\mathbf{x}) = \begin{pmatrix} 1 \\ x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \\ \sqrt{2}x_1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \end{pmatrix} \text{ Let: } \\ w_0 = a^2 + b^2 - r^2 \\ w_1 = 1 \\ w_2 = 0 \\ w_3 = 1 \\ w_4 = -\sqrt{2}a \\ w_5 = -\sqrt{2}b \end{pmatrix}$$

Definition: ε-insensitive loss function

- Let d be the desired response and y its estimated value.
- The $\underline{\varepsilon}$ -insensitive loss function is defined as follows:

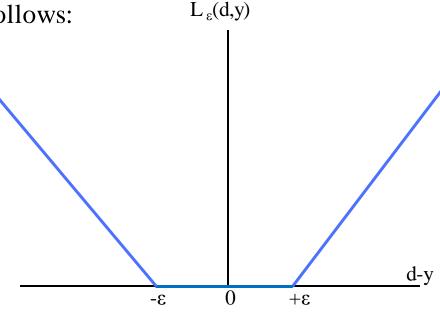
$$L_{\epsilon}(d,y) = |d-y| - \epsilon \ \ if \ \ |d-y| \geq \epsilon,$$

$$0 \ otherwise$$

Expressing $L_{\varepsilon}(d, y)$ as a linear program:

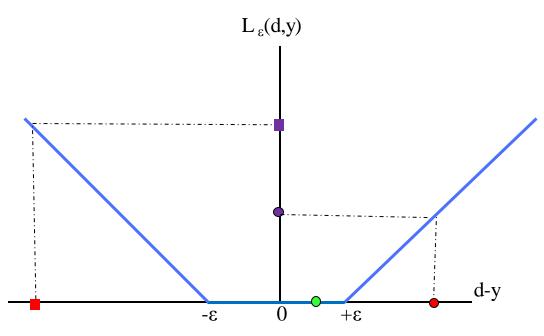
minimise
$$\xi + \xi'$$

subject to $d - y \le \varepsilon + \xi$
 $y - d \le \varepsilon + \xi'$
 $\xi', \xi \ge 0$



ε-insensitive loss function (continued)

• Note: if $d - y \ge \epsilon$, then let $\xi = d - y - \epsilon \ge 0$, $\xi' = 0$ and $y - d \le -\epsilon \le \epsilon$. if $d - y \le -\epsilon$, then let $\xi' = y - d - \epsilon \ge 0$ and $\xi = 0$.



Example 1: \bullet d-y = 2 ϵ ξ = d - y - ϵ = 2 ϵ - ϵ = ϵ (this is the penalty) \bullet ξ '= 0

Example 2:
$$d - y = -3 \epsilon$$

$$\xi' = y - d - \epsilon = 2 \epsilon \text{ (this is the penalty)}$$

$$\xi = 0$$

Example 3:
$$0$$
d-y = $\frac{1}{2} \epsilon$
 $\xi = \xi' = 0$ (no penalty)

In all three examples, check that:

$$d - y \le \varepsilon + \xi$$

 $y - d \le \varepsilon + \xi'$

• For nonlinear regression problem, given the training data $\{(\mathbf{x_i}, d_i)\}\ i = 1, 2, ..., N$, where $\mathbf{x_i}$ is a sample value of the input vector \mathbf{x} and d_i is the corresponding value of the model output d, we minimise the following QP:

minimise
$$\Phi(\mathbf{w}, \boldsymbol{\xi}, \boldsymbol{\xi'}) = C(\sum_{i=1}^{N} (\xi_i + \xi_i')) + \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

subject to $d_i - \mathbf{w}^T \ \Psi(\mathbf{x_i}) \le \epsilon + \xi_i$

$$\mathbf{w}^T \ \Psi(\mathbf{x_i}) - d_i \le \epsilon + \xi_i'$$

$$\xi_i', \ \xi_i \ge 0, \ i = 1, 2,, N$$

• C is a positive parameter selected by the user.

The dual of the quadratic problem is

$$\begin{aligned} \text{maximise } Q(\pmb{\alpha_i},\pmb{\alpha_i'}) &= \sum_{i=1}^N \, d_i(\alpha_i \, - \alpha_i') \, - \epsilon \, \sum_{i=1}^N \, (\alpha_i \, + \alpha_i') \\ &- \frac{1}{2} \, \sum_{i=1}^N \, \sum_{i=1}^N \, (\alpha_i \, - \alpha_i')(\alpha_j \, - \alpha_j') \, K(\pmb{x_i}, \, \pmb{x_j}) \\ \text{subject to } \sum_{i=1}^N (\alpha_i \, - \alpha_i') &= 0 \\ &0 \leq \alpha_i \leq C, \quad i = 1, 2, \dots, N \\ &0 \leq \alpha_i' \leq C, \quad i = 1, 2, \dots, N \end{aligned}$$

- The parameter ε and C must be tuned simultaneously.
- Regression is intrinsically more difficult than pattern classification.

- The paper "A synthetic informative minority over-sampling (SIMO) algorithm leveraging support vector machine to enhance learning from imbalanced datasets", S. Piri, D. Delen, T. Liu, Decision Support Systems 106 (2018) 15-29 presents methods to oversample minority examples in the data by using SVM.
- Idea: pay more attention to minority examples that are close to the SVM decision boundary.
 - Calculate the Euclidean distance of minority data points form D_B

$$Euc_{D}(x^{k+}) = \frac{|\sum_{t=1}^{m} w_{t} x_{t}^{k+} + b|}{\sqrt{\sum_{t=1}^{m} w_{t}^{2}}}$$

- SIMO algorithm: informative minority examples close to the SVM decision boundary are over-sampled.
- W-SIMO: weighted SIMO, incorrectly classified informative minority examples are over-sampled with a higher-degree compared to the correctly classified informative minority examples.

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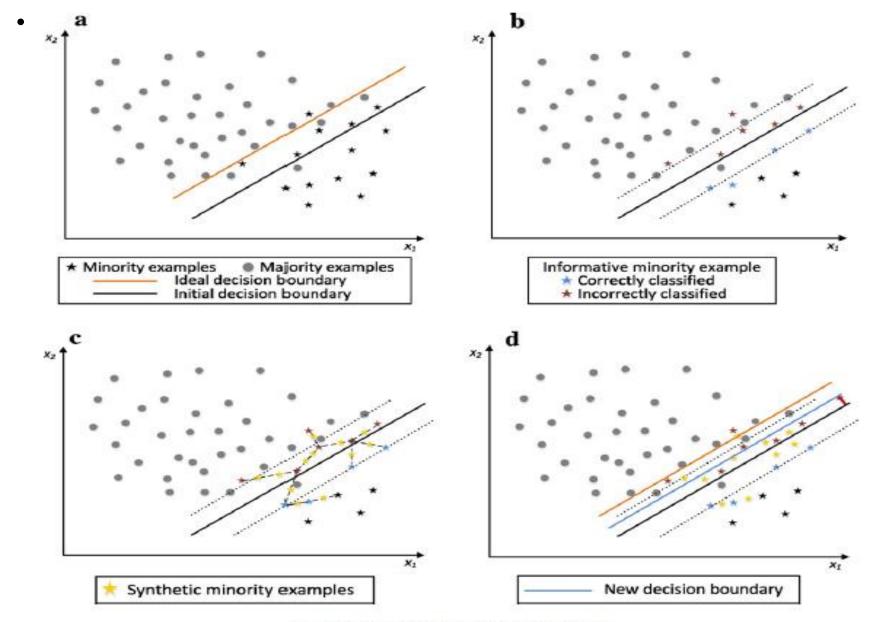


Fig. 2. W-SIMO algorithm mechanism (simplified).

• Experiments on 15 data sets:

Table 2
Benchmark datasets characteristics.

Dataset	Minority class	Majority class	# of variables	# of records	Imbalance ratio
Liver disorders (liver)	"1"	"2"	7	345	1:1.38
Ionosphere	Bad	Good	34	351	1;1,79
Pima Indians Diabetes (Pima)	"1"	"0"	8	768	1:1.87
Breast Cancer Wisconsin Original (BreastCO)	Malignant	Benign	10	699	1:1.91
Iris	Versicolor	All other	5	150	1:2
Yeast	NUC	All other	8	1484	1:2,6
Statlog Vehicle Silhouettes (vehicle)	Van	All other	18	846	1:3.25
Contraceptive Method Choice (CMC)	Long-term	All other	9	1473	1:3,42
Breast Cancer Wisconsin_20% (BreastC20)	Malignant	Benign	10	699	1:3.91
Connectionist Bench_Vowel Recognition (vowel)	"0" & "1"	All other	11	990	1:4.5
Ecoli	pp	All other	8	336	1:5.46
Libras Movement_12 (Libras 12)	"1" & "2"	All other	91	360	1:5.88
Libras Movement_34 (Libras34)	"3" & "4"	All other	91	360	1:6.34
Glass identification (glass)	-7 -	All other	9	214	1:6.38
Breast Cancer Wisconsin_10% (BreastC10)	Malignant	Benign	10	699	1:8.9

• Experiments on 15 data sets:

Table 6 Overall ranking on linear SVM.

Approach	G mean	AUC
W-SIMO	1,1	1.1
SIMO	1.9	1.9
SMOTE-IPF	4.6	4.5
Cluster SMOTE	5.3	5.0
Cost sensitive	5.7	6.1
SMOTE	6.3	6.4
Safe level SMOTE	6.3	6.7
Under sampling	7.3	7.1
BorSMOTE	8.1	8.1
Original data	8.6	8.1

• $G mean = sqrt(TPR \times TNR)$

Reference

- S. Haykin, Neural Networks A comprehensive foundation, second edition,
 1999, Prentice Hall.
- Slide 3 data set is from J.D. Kelleher et al, Fundamentals of Machine Learning for Predictive Data Analytics
- Also visit http://www.support-vector-machines.org Q325.5 Cri 2000 and http://www.csie.ntu.edu.tw/~cjlin/libsvm/index.html (a library for support vector machines).