Support Vector Machine Tutorial

Wu, Shih-Hung (Ph.D)

Dept. of CSIE, CYUT

References

- Book
  - Duda etal. “pattern classification”, Ch5
- Slides
  - Moore, Andrew (CMU)
    - http://www.cs.cmu.edu/~awm/tutorials
  - Lin, Chih-Jen (NTU)
    - http://www.csie.ntu.edu.tw/~cjlin/talks.html

5.11 Support Vector Machines

- Popular, easy-to-use, available

- Support Vector
- Data is mapped to a high dimension
- SVM training

- Example 2
  - SVM for the XOR Problem

Optimal hyperplane

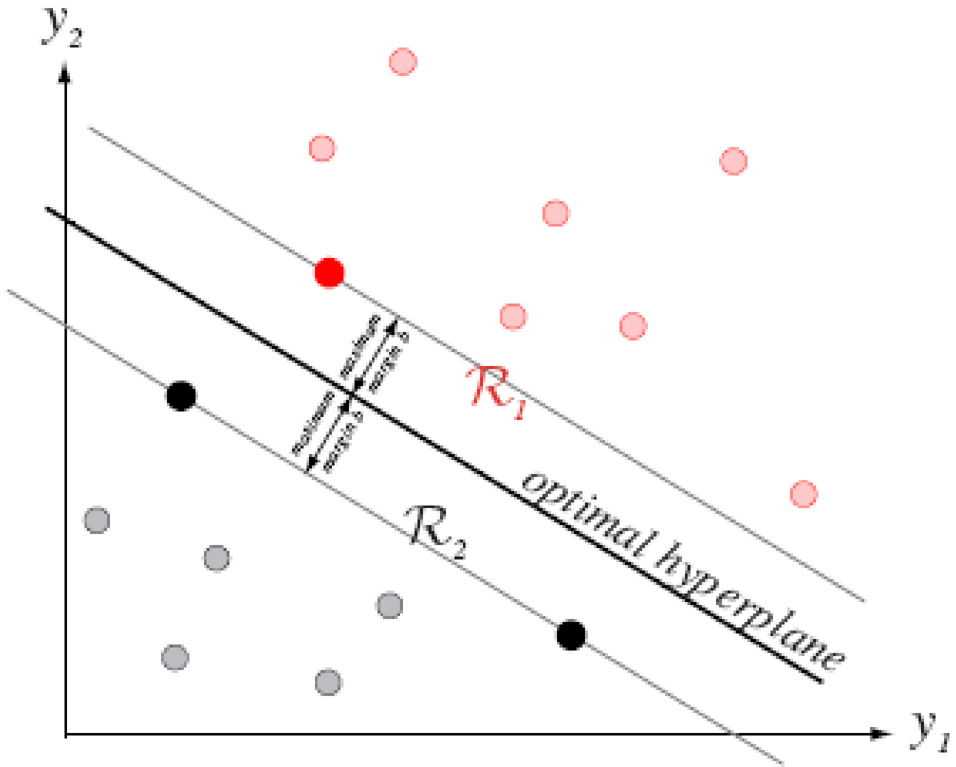
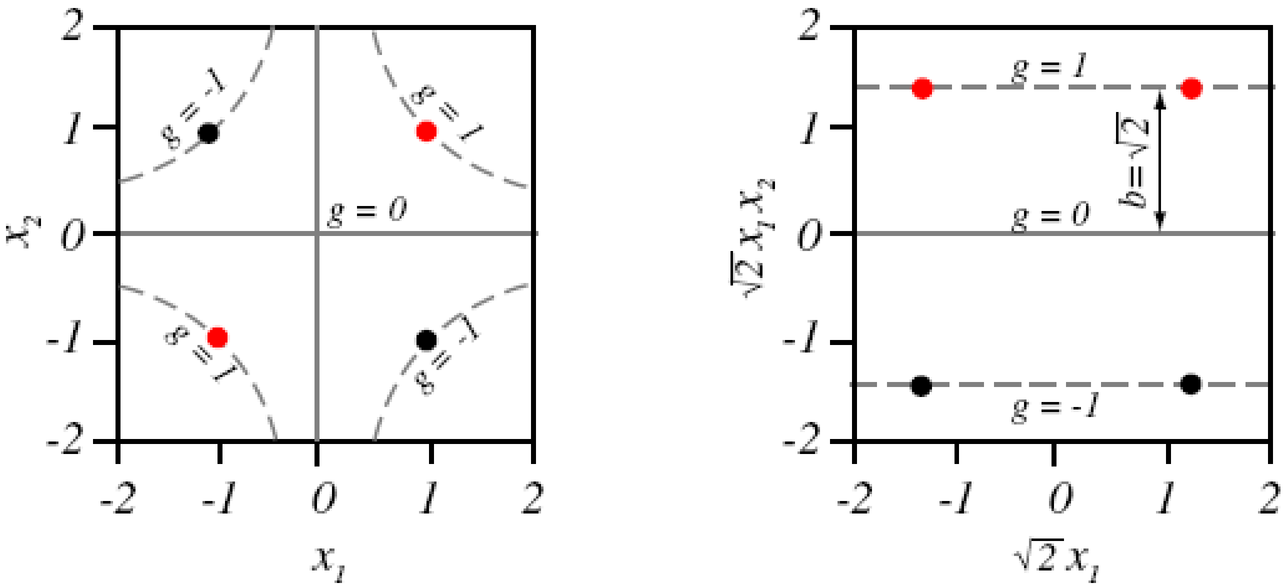


FIGURE 5.19. Training a support vector machine consists of finding the optimal hyperplane, that is, the one with the maximum distance from the nearest training patterns. The support vectors are those (nearest) patterns, a distance b from the hyperplane. The three support vectors are shown as solid dots. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Mapping to higher dimensional space

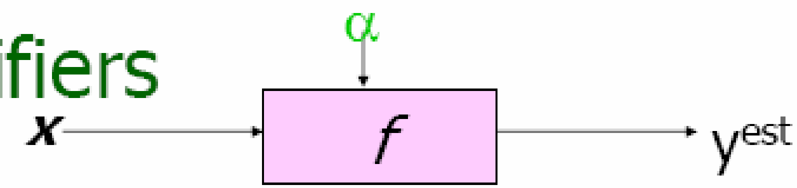


The XOR problem in the original $x_1 - x_2$ feature space is shown at the left; the two red patterns are in category ω_1 and the two black ones in ω_2. These four training patterns $\mathbf{x}$ are mapped to a six-dimensional space by 1, $\sqrt{2}x_1$, $\sqrt{2}x_2$, $\sqrt{2}x_1x_2$, x_1^2 and x_2^2. In this space, the optimal hyperplane is found to be $g(x_1, x_2) = x_1x_2 = 0$ and the margin is $b = \sqrt{2}$. A two-dimensional projection of this space is shown at the right. The hyperplanes through the support vectors are $\sqrt{2}x_1x_2 = \pm 1$, and correspond to the hyperbolas $x_1x_2 = \pm 1$ in the original feature space, as shown.

SVM introduction

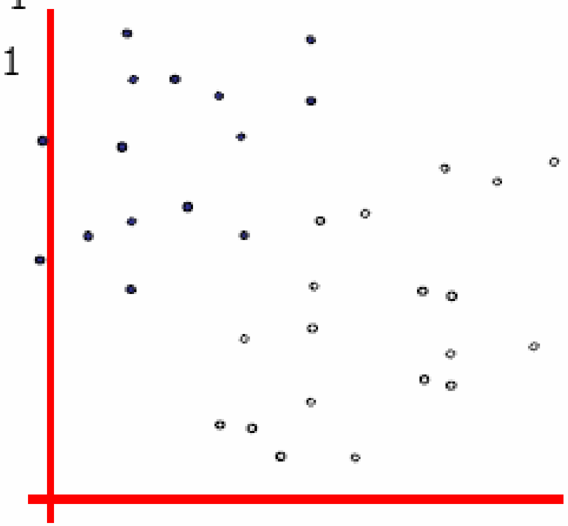
Example from Andrew Moor's slides

Linear Classifiers



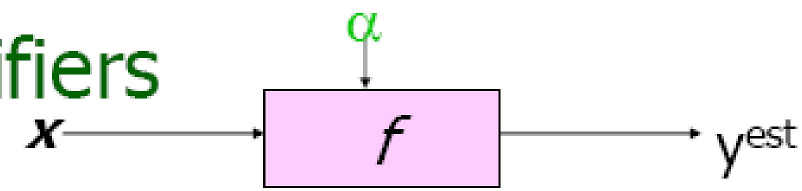
$$f(\mathbf{x}, \mathbf{w}, b) = sign(\mathbf{w} \cdot \mathbf{x} - b)$$

- denotes +1
- denotes -1



How would you classify this data?

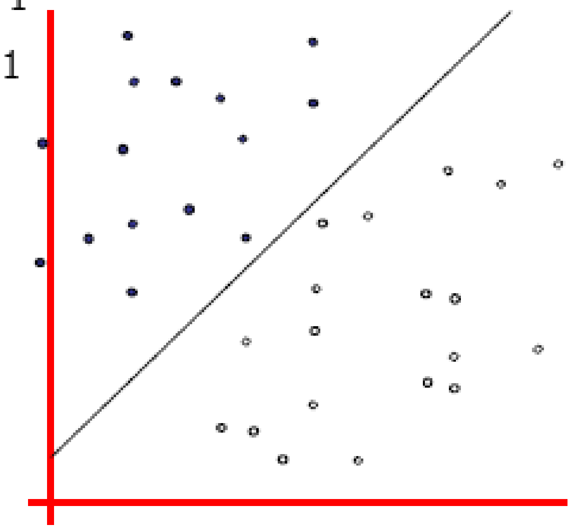
Linear Classifiers



$f(\boldsymbol{x}, \boldsymbol{w}, b) = sign(\boldsymbol{w}.\ \boldsymbol{x} - b)$

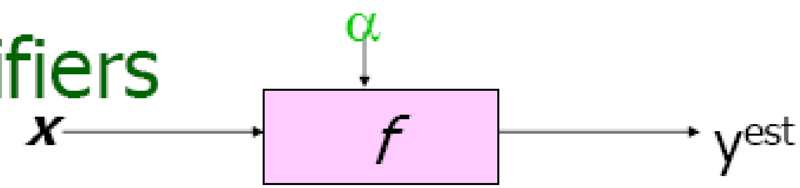
• denotes +1

° denotes -1



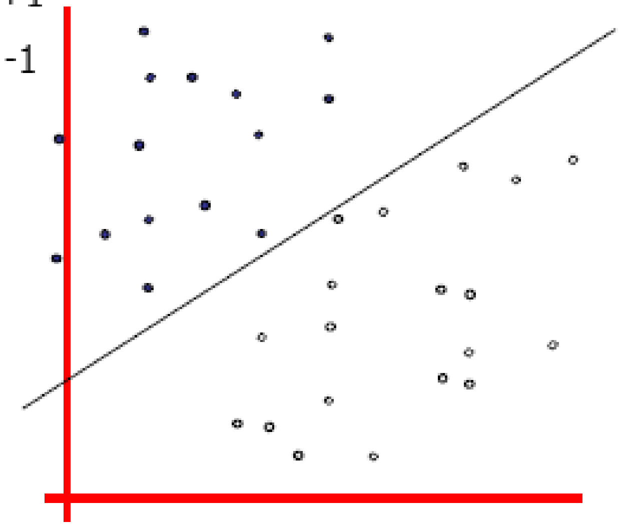
How would you classify this data?

Linear Classifiers



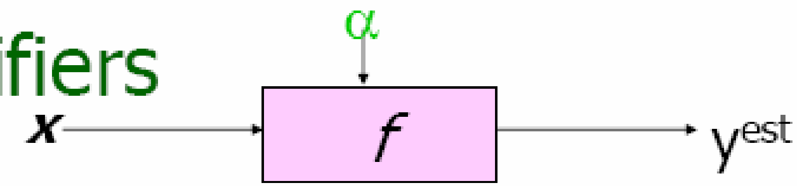
$$f(\boldsymbol{x},\boldsymbol{w},b) = sign(\boldsymbol{w}.\ \boldsymbol{x} - b)$$

- denotes +1
- denotes -1



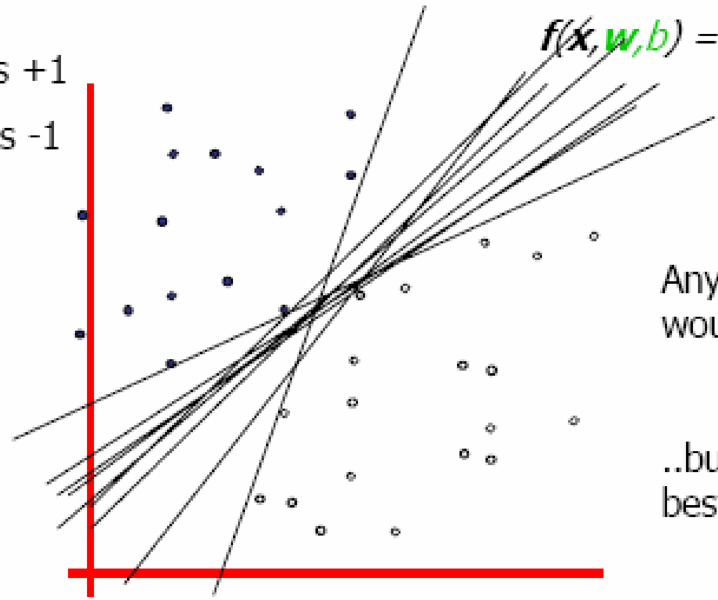
How would you classify this data?

Linear Classifiers



$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}.\ \mathbf{x} - b)$

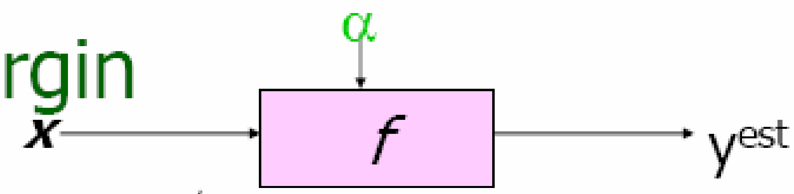
- • denotes +1
- ◦ denotes -1



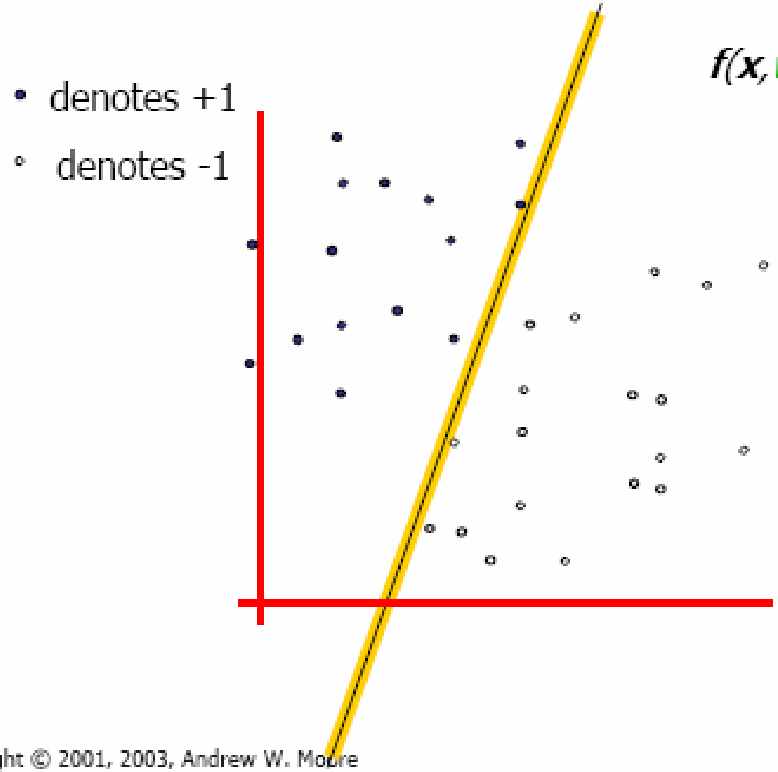
Any of these would be fine..

..but which is best?

Classifier Margin

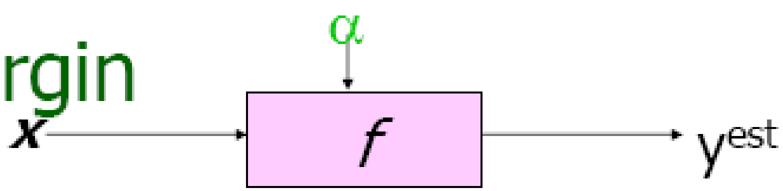


$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}.\ \mathbf{x} - b)$

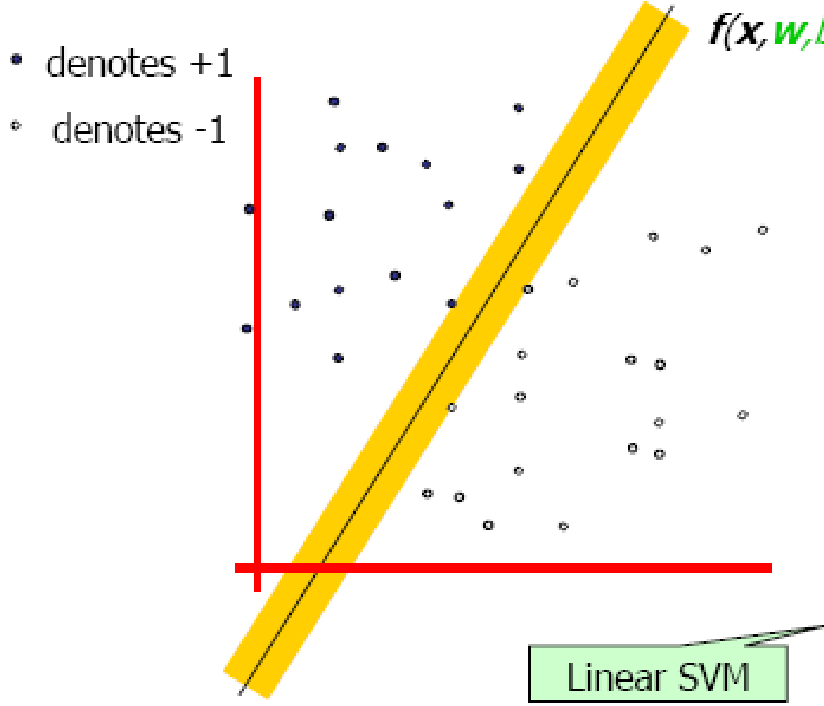


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Maximum Margin



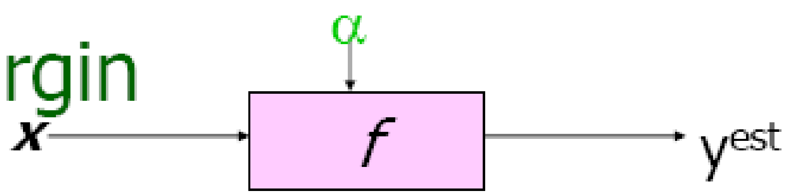
$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}.\ \mathbf{x} - b)$



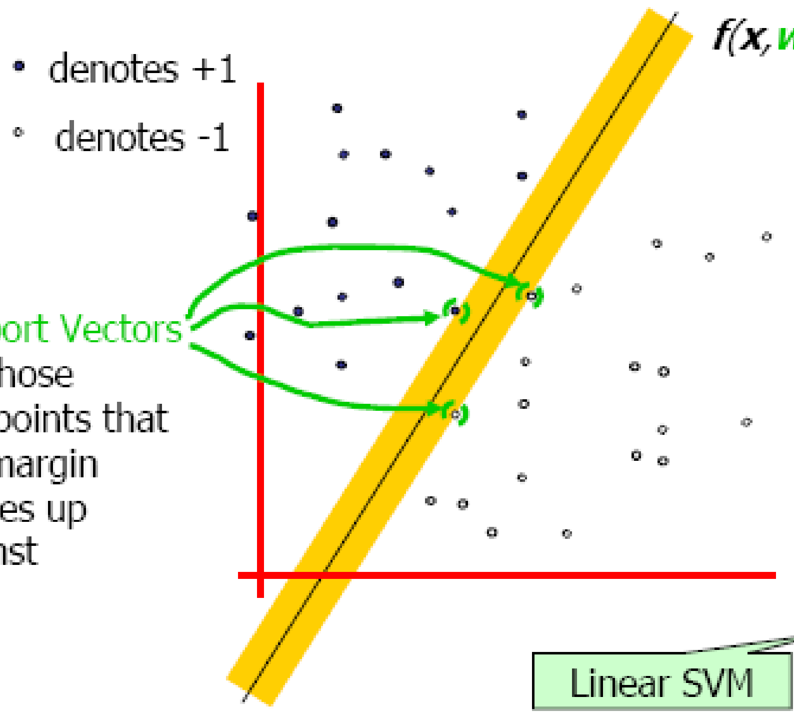
The maximum margin linear classifier is the linear classifier with the, um, maximum margin.

This is the simplest kind of SVM (Called an LSVM)

Maximum Margin



$f(\mathbf{x},\mathbf{w},b) = \mathrm{sign}(\mathbf{w}.\ \mathbf{x} - b)$

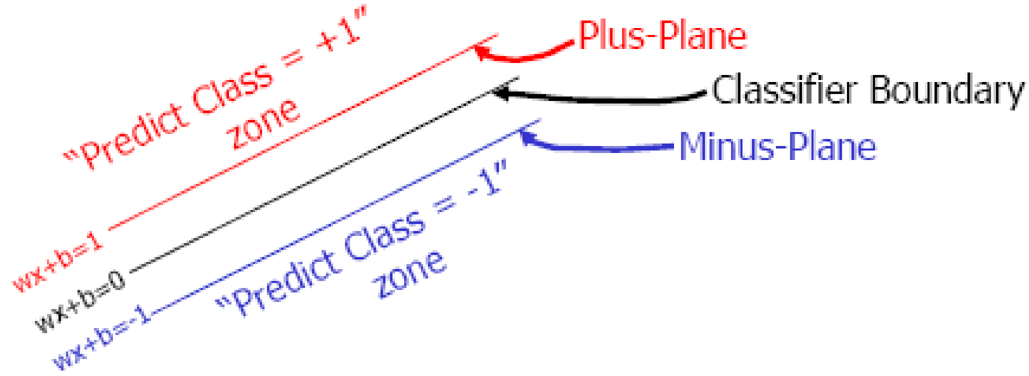


Support Vectors are those datapoints that the margin pushes up against

The maximum margin linear classifier is the linear classifier with the, um, maximum margin.

This is the simplest kind of SVM (Called an LSVM)

Specifying a line and margin

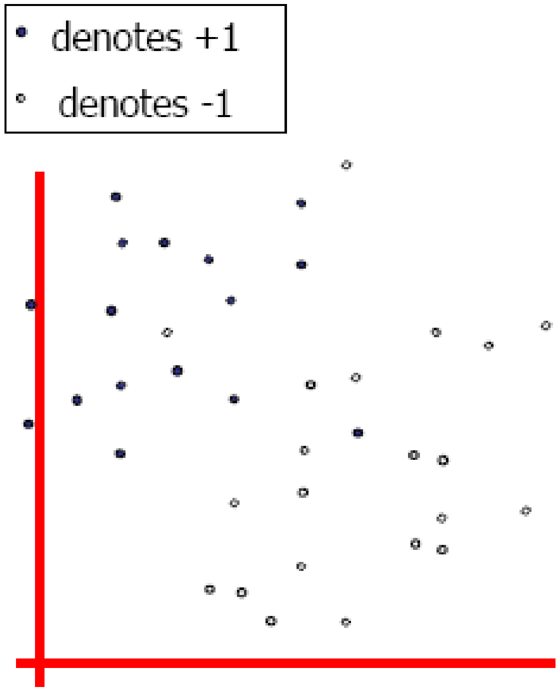


- Plus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \}$
- Minus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = -1 \}$

Classify as..	+1	if	$\mathbf{w} \cdot \mathbf{x} + b >= 1$
	-1	if	$\mathbf{w} \cdot \mathbf{x} + b <= -1$
	Universe explodes	if	$-1 < \mathbf{w} \cdot \mathbf{x} + b < 1$

How to deal with Noisy Data?

Uh-oh!



This is going to be a problem!

What should we do?

Idea 1.1:

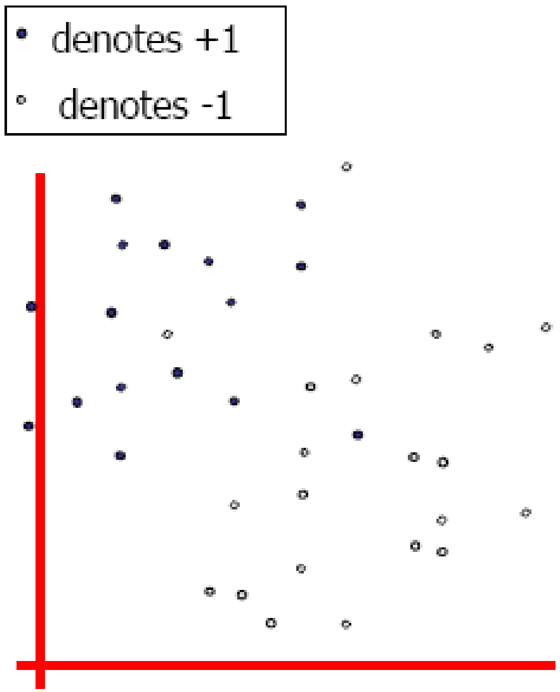
Minimize

$\boldsymbol{w}.\boldsymbol{w}$ + *C (#train errors)*

Tradeoff parameter

There's a serious practical problem that's about to make us reject this approach. Can you guess what it is?

Uh-oh!



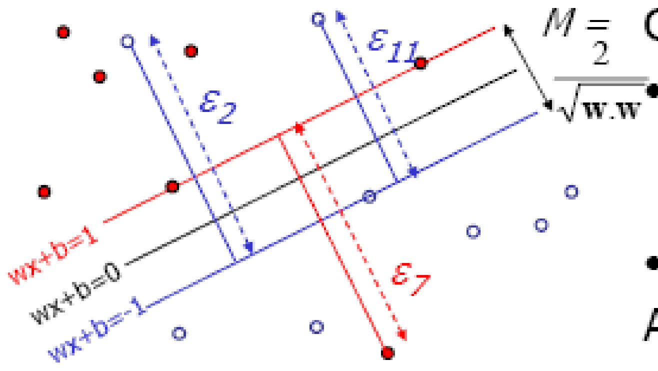
This is going to be a problem!

What should we do?

Idea 2.0:

Minimize
w.w *+ C (distance of error points to their correct place)*

Learning Maximum Margin with Noise



Given guess of ***w*** , *b* we can

- Compute sum of distances of points to their correct zones
- Compute the margin width

Assume *R* datapoints, each $(\mathbf{x}_k, y_k)$ where $y_k = +/- 1$

What should our quadratic optimization criterion be?

Minimize

$$\frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$$

How many constraints will we have? *R*

What should they be?

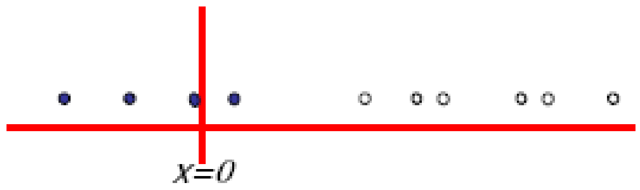
$\mathbf{w} \,.\, \mathbf{x}_k + b >= 1\text{-}\varepsilon_k$ *if* $y_k = 1$

$\mathbf{w} \,.\, \mathbf{x}_k + b <= -1+\varepsilon_k$ *if* $y_k = -1$

Mapping to a higher Dimensional space

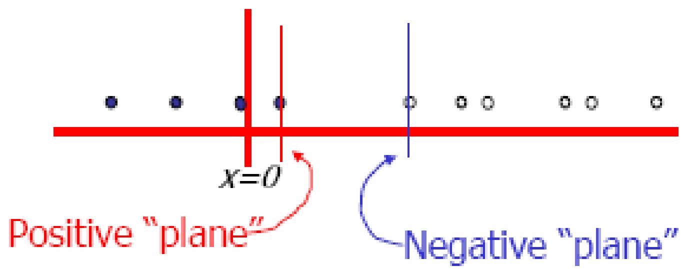
Suppose we're in 1-dimension

What would SVMs do with this data?

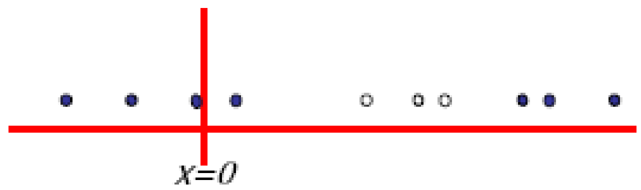


Suppose we're in 1-dimension

Not a big surprise



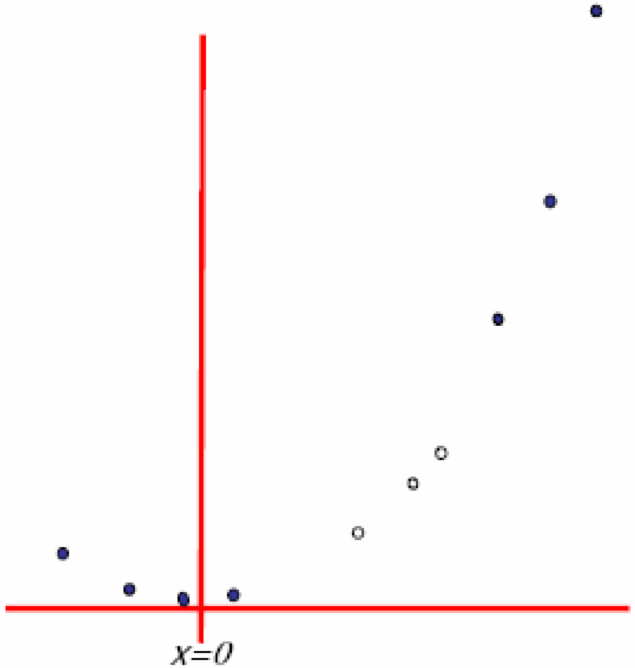
Harder 1-dimensional dataset



That's wiped the smirk off SVM's face.

What can be done about this?

Harder 1-dimensional dataset

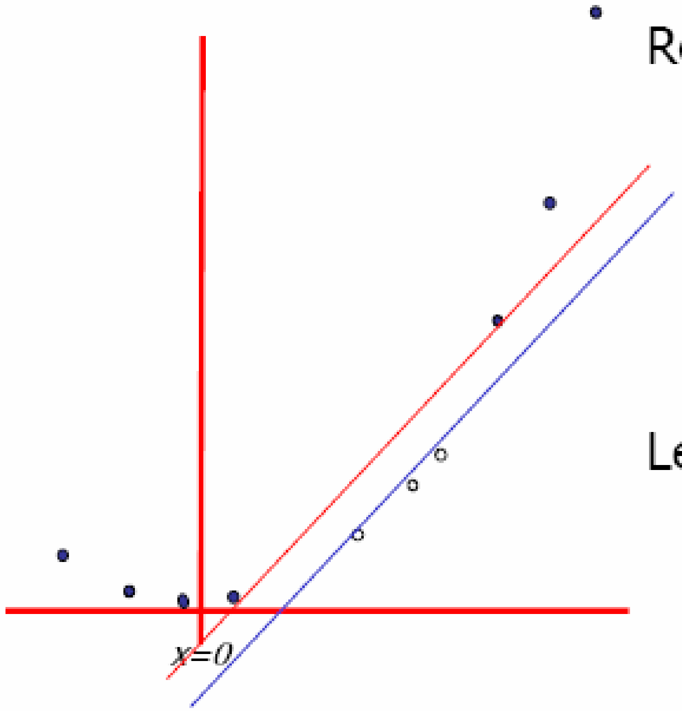


Remember how permitting non-linear basis functions made linear regression so much nicer?

Let's permit them here too

$$\mathbf{z}_k = (x_k, x_k^2)$$

Harder 1-dimensional dataset



Remember how permitting non-linear basis functions made linear regression so much nicer?

Let's permit them here too

$$\mathbf{z}_k = (x_k, x_k^2)$$

Common SVM basis functions

$\boldsymbol{z}_k$ = (polynomial terms of $\boldsymbol{x}_k$ of degree 1 to q)

$\boldsymbol{z}_k$ = (radial basis functions of $\boldsymbol{x}_k$)

$$\mathbf{z}_k[j] = \varphi_j(\mathbf{x}_k) = \mathrm{KernelFn}\left(\frac{|\mathbf{x}_k - \mathbf{c}_j|}{\mathrm{KW}}\right)$$

$\boldsymbol{z}_k$ = (sigmoid functions of $\boldsymbol{x}_k$)

This is sensible.

Is that the end of the story?

No…there's one more trick!

Quadratic Basis Functions

$$
\Phi(\mathbf{x}) = \begin{pmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \vdots \\ \sqrt{2}x_m \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_m^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \sqrt{2}x_2x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \vdots \\ \sqrt{2}x_{m-1}x_m \end{pmatrix}
\begin{matrix} \}\ \text{Constant Term} \\ \}\ \text{Linear Terms} \\ \}\ \text{Pure Quadratic Terms} \\ \}\ \text{Quadratic Cross-Terms} \end{matrix}
$$

Number of terms (assuming m input dimensions) = (m+2)-choose-2

= (m+2)(m+1)/2

= (as near as makes no difference) $m^2/2$

You may be wondering what those $\sqrt{2}$'s are doing.

- You should be happy that they do no harm
- You'll find out why they're there soon.

SVM tool

Example from Lin, Chih-Jen's slides

Outline

- Support vector classification
- Two practical example
- Support vector regression
- Discussion and conclusions

Data Classification

- Given training data in different classes (labels known)
  Predict test data (labels unknown)
- Examples
  - Handwritten digits recognition
  - Spam filtering
  - Text classification
  - Prediction of signal peptide in human secretory proteins
- Training and testing

- Methods:
  - Nearest Neighbor
  - Neural Networks
  - Decision Tree
- Support vector machines: a new method
- Becoming more and more popular

Why Support Vector Machines

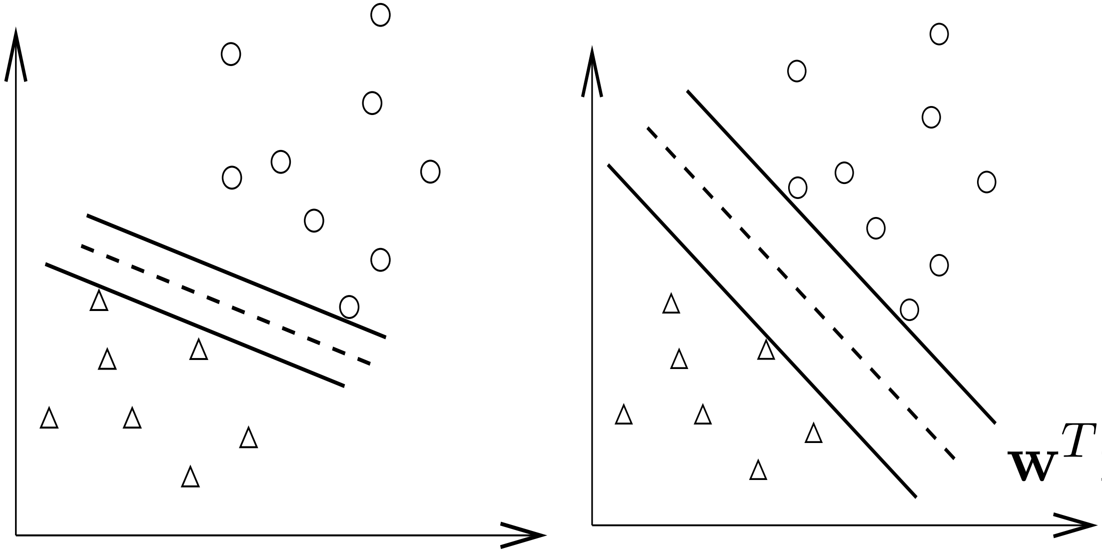
- Existing methods:
  Nearest neighbor, Neural networks, decision trees.
- SVM: a new one
- In my opinion, after careful data pre-processing
  Appropriately use NN or SVM $\Rightarrow$ similar accuracy
- But, users may not use them properly
- The chance of SVM
  - Easier for users to appropriately use it
  - The ambition: replacing NN on some applications

Support Vector Classification

- Training vectors : $\mathbf{x}_i, i = 1, \ldots, l$
- Consider a simple case with two classes:
  Define a vector $\mathbf{y}$

$$y_i = \begin{cases} 1 & \text{if } \mathbf{x}_i \text{ in class 1} \\ -1 & \text{if } \mathbf{x}_i \text{ in class 2,} \end{cases}$$

- A hyperplane which separates all data



$$\mathbf{w}^T\mathbf{x} + b = \begin{bmatrix} +1 \\ 0 \\ -1 \end{bmatrix}$$

- A separating hyperplane: $\mathbf{w}^T\mathbf{x} + b = 0$

$$(\mathbf{w}^T\mathbf{x}_i) + b > 0 \quad \text{if } y_i = 1$$
$$(\mathbf{w}^T\mathbf{x}_i) + b < 0 \quad \text{if } y_i = -1$$

- Decision function $f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$, $\mathbf{x}$: test data
  Variables: $\mathbf{w}$ and b : Need to know coefficients of a plane

  Many possible choices of $\mathbf{w}$ and b

- Select $\mathbf{w}, b$ with the maximal margin.
  Maximal distance between $\mathbf{w}^T\mathbf{x} + b = \pm 1$

$$
\begin{aligned}
(\mathbf{w}^T\mathbf{x}_i) + b &\geq 1 \quad \text{if } y_i = 1 \\
(\mathbf{w}^T\mathbf{x}_i) + b &\leq -1 \quad \text{if } y_i = -1
\end{aligned}
$$

- Distance between $\mathbf{w}^T\mathbf{x} + b = 1$ and -1:

$$2/\|\mathbf{w}\| = 2/\sqrt{\mathbf{w}^T\mathbf{w}}$$

- $\max 2/\|\mathbf{w}\| \equiv \min \mathbf{w}^T\mathbf{w}/2$

$$\begin{aligned} \min_{\mathbf{w},b} \quad & \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ \text{subject to} \quad & y_i((\mathbf{w}^T\mathbf{x}_i) + b) \geq 1, \\ & i = 1, \ldots, l. \end{aligned}$$

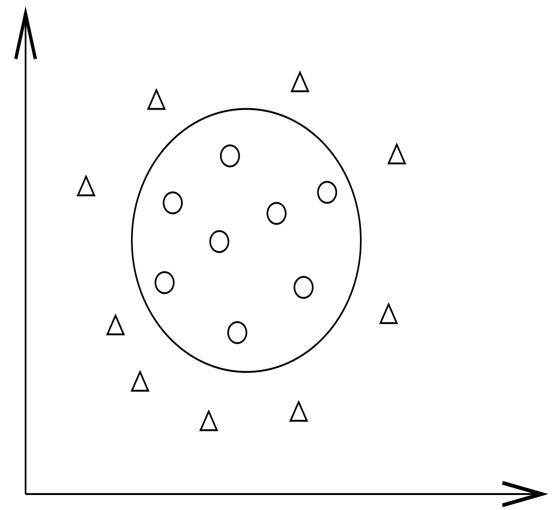
Higher Dimensional Feature Spaces

- Earlier we tried to find a linear separating hyperplane
  Data may not be linear separable
- Non-separable case: allow training errors

$$
\begin{aligned}
\min_{\mathbf{w},b,\boldsymbol{\xi}} \quad & \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l}\xi_i \\
& y_i((\mathbf{w}^T\mathbf{x}_i) + b) \geq 1 - \xi_i, \\
& \xi_i \geq 0, \ i = 1, \ldots, l
\end{aligned}
$$

- $\xi_i > 1$, $\mathbf{x}_i$ not on the correct side of the separating plane
- C: large penalty parameter, most ξ_i are zero

- Nonlinear case: linear separable in other spaces ?



- Higher dimensional (maybe infinite) feature space

$$\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots).$$

- Example: $\mathbf{x} \in R^3, \phi(\mathbf{x}) \in R^{10}$

$$\begin{aligned}\phi(\mathbf{x}) \;=\; & (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_3, x_1^2, \\ & x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3)\end{aligned}$$

- A standard problem [Cortes and Vapnik, 1995]:

$$\min_{\mathbf{w},b,\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l}\xi_i$$

subject to $\quad y_i(\mathbf{w}^T\phi(\mathbf{x}_i) + b) \geq 1 - \xi_i, \;\; \xi_i \geq 0, \; i = 1, \ldots, l.$

Finding the Decision Function

- $\mathbf{w}$: a vector in a high dimensional space $\Rightarrow$ maybe infinite variables
- The dual problem

$$
\begin{aligned}
\min_{\boldsymbol{\alpha}} \quad & \frac{1}{2}\boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha} \\
\text{subject to} \quad & 0 \le \alpha_i \le C, i = 1, \ldots, l \\
& \mathbf{y}^T \boldsymbol{\alpha} = 0,
\end{aligned}
$$

where $Q_{ij} = y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ and $\mathbf{e} = [1, \ldots, 1]^T$

$$\boxed{\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \phi(\mathbf{x}_i)}$$

- Primal and dual: optimization theory. Not trivial.
  Infinite dimensional programming.
- A finite problem:
  #variables = #training data
- $Q_{ij} = y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ needs a closed form
  Efficient calculation of high dimensional inner products
  Kernel trick, $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

- Example: $\mathbf{x}_i \in R^3, \phi(\mathbf{x}_i) \in R^{10}$

$$\begin{aligned}\phi(\mathbf{x}_i) &= (1, \sqrt{2}(x_i)_1, \sqrt{2}(x_i)_2, \sqrt{2}(x_i)_3, (x_i)_1^2,\\ &\quad (x_i)_2^2, (x_i)_3^2, \sqrt{2}(x_i)_1(x_i)_2, \sqrt{2}(x_i)_1(x_i)_3, \sqrt{2}(x_i)_2(x_i)_3\end{aligned}$$

  Then $\phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j) = (1 + \mathbf{x}_i^T\mathbf{x}_j)^2$.
- Popular methods: $K(\mathbf{x}_i, \mathbf{x}_j) =$

$$e^{-\gamma\|\mathbf{x}_i - \mathbf{x}_j\|^2},\ \text{(Radial Basis Function)}$$

$$(\mathbf{x}_i^T\mathbf{x}_j/a + b)^d\ \text{(Polynomial kernel)}$$

Kernel Tricks

- Kernel: $K(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$
- No need to explicitly know $\phi(\mathbf{x})$
- Common kernels $K(\mathbf{x}_i, \mathbf{x}_j) =$

$$e^{-\gamma\|\mathbf{x}_i - \mathbf{x}_j\|^2}, \text{ (Radial Basis Function)}$$

$$(\mathbf{x}_i^T \mathbf{x}_j / a + b)^d \text{ (Polynomial kernel)}$$

- They can be inner product in infinite dimensional space
- Assume $x \in R^1$ and $\gamma > 0$.

$$
\begin{aligned}
& e^{-\gamma\|x_i-x_j\|^2} = e^{-\gamma(x_i-x_j)^2} = e^{-\gamma x_i^2+2\gamma x_i x_j-\gamma x_j^2} \\
= \;& e^{-\gamma x_i^2-\gamma x_j^2}\left(1+\frac{2\gamma x_i x_j}{1!}+\frac{(2\gamma x_i x_j)^2}{2!}+\frac{(2\gamma x_i x_j)^3}{3!}+\cdots\right) \\
= \;& e^{-\gamma x_i^2-\gamma x_j^2}\Big(1\cdot 1+\sqrt{\frac{2\gamma}{1!}}x_i\cdot\sqrt{\frac{2\gamma}{1!}}x_j+\sqrt{\frac{(2\gamma)^2}{2!}}x_i^2\cdot\sqrt{\frac{(2\gamma)^2}{2!}}x_j^2 \\
& \qquad +\sqrt{\frac{(2\gamma)^3}{3!}}x_i^3\cdot\sqrt{\frac{(2\gamma)^3}{3!}}x_j^3+\cdots\Big) \\
= \;& \phi(x_i)^T\phi(x_j),
\end{aligned}
$$

where

$$
\phi(x) = e^{-\gamma x^2}\left[1,\sqrt{\frac{2\gamma}{1!}}x,\sqrt{\frac{(2\gamma)^2}{2!}}x^2,\sqrt{\frac{(2\gamma)^3}{3!}}x^3,\cdots\right]^T.
$$

Decision function

- $\mathbf{w}$: maybe an infinite vector
- At optimum

$$\boxed{\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \phi(\mathbf{x}_i)}$$

- Decision function

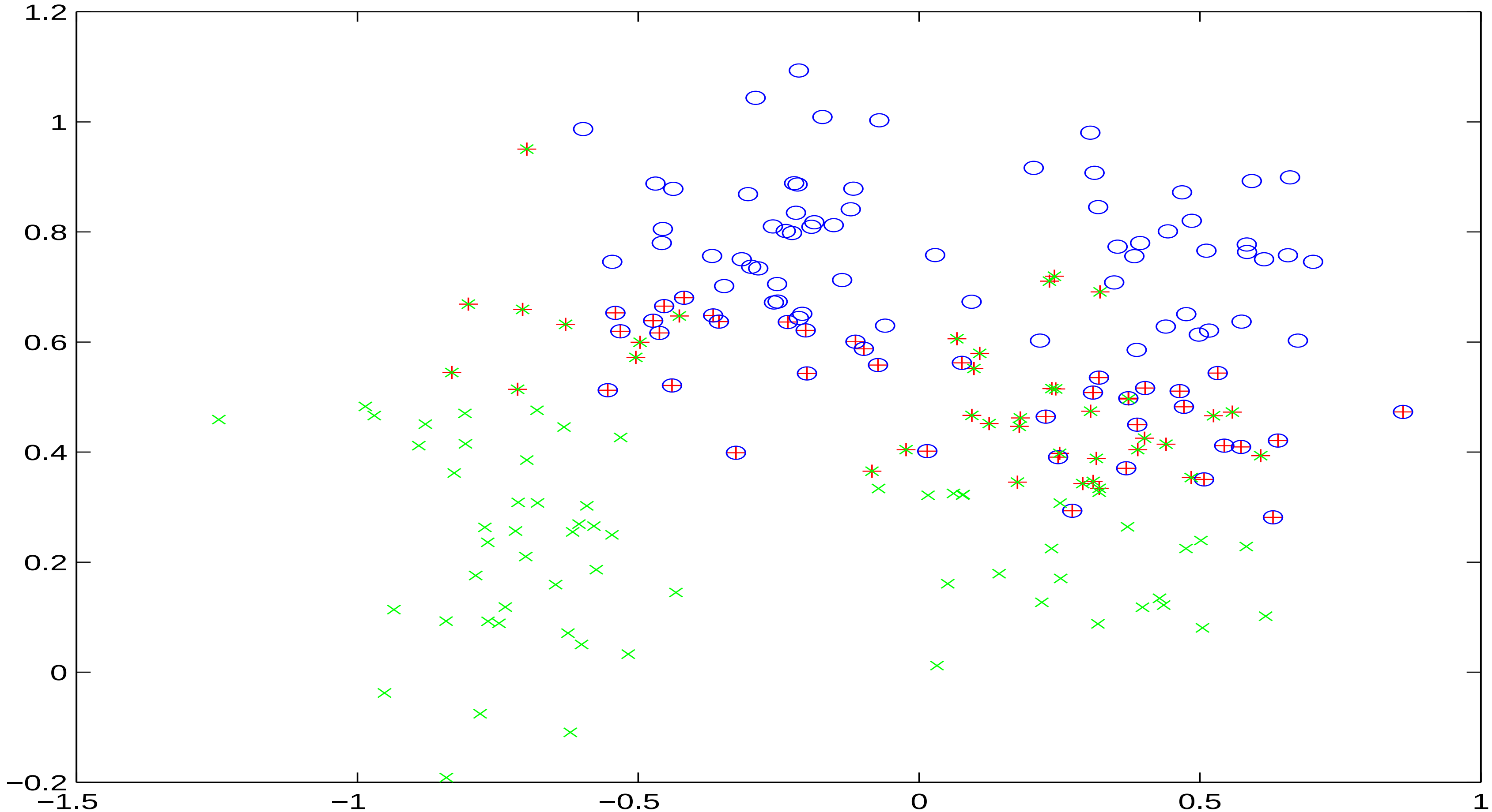
$$\begin{aligned}
& \mathbf{w}^T \phi(\mathbf{x}) + b \\
= & \sum_{i=1}^{l} \alpha_i y_i \phi(\mathbf{x}_i)^T \phi(\mathbf{x}) + b \\
= & \sum_{i=1}^{l} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b
\end{aligned}$$

No need to have $\mathbf{w}$

- > 0: 1st class, < 0: 2nd class
- Only $\phi(\mathbf{x}_i)$ of $\alpha_i > 0$ used

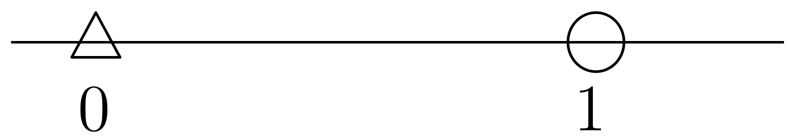
$\alpha_i > 0 \Rightarrow$ support vectors

Support Vectors: More Important Data



A Toy Example

- Two training data in R^1:



- What is the separating hyperplane ?

Primal Problem

- $\mathbf{x}_1 = 0, \mathbf{x}_2 = 1$ with $\mathbf{y} = [-1, 1]^T$.
- Primal problem

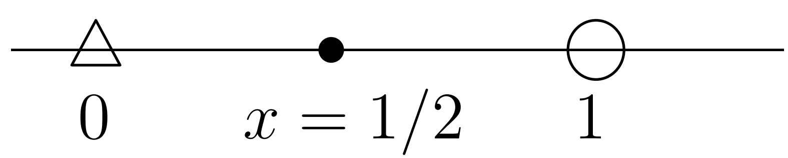
$$
\begin{aligned}
\min_{w,b} \quad & \frac{1}{2}w^2 \\
\text{subject to} \quad & w \cdot 1 + b \geq 1, && (1) \\
& -1(w \cdot 0 + b) \geq 1. && (2)
\end{aligned}
$$

- $-b \geq 1$ and $w \geq 1 - b \geq 2$.
- For any (w, b) satisfying two inequality constraints

$$w \geq 2$$

- We are minimizing $\frac{1}{2}w^2$

  The smallest possibility is $w = 2$.
- $(w, b) = (2, -1)$ is the optimal solution.
- The separating hyperplane $2x - 1 = 0$
  In the middle of the two training data:



Dual Problem

- Formula derived before

$$\min_{\boldsymbol{\alpha}\in R^l} \quad \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j) - \sum_{i=1}^{l}\alpha_i$$

subject to $\alpha_i \geq 0, i = 1,\ldots,l,$ and $\sum_{i=1}^{l}\alpha_i y_i = 0.$

- Get the objective function

$$\mathbf{x}_1^T\mathbf{x}_1 = 0, \mathbf{x}_1^T\mathbf{x}_2 = 0$$
$$\mathbf{x}_2^T\mathbf{x}_1 = 0, \mathbf{x}_2^T\mathbf{x}_2 = 1$$

- Objective function

$$
\begin{aligned}
& \frac{1}{2}\alpha_1^2 - (\alpha_1 + \alpha_2) \\
= \quad & \frac{1}{2}\begin{bmatrix}\alpha_1 & \alpha_2\end{bmatrix}\begin{bmatrix}0 & 0 \\ 0 & 1\end{bmatrix}\begin{bmatrix}\alpha_1 \\ \alpha_2\end{bmatrix} - \begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}\alpha_1 \\ \alpha_2\end{bmatrix}.
\end{aligned}
$$

- Constraints

$$
\alpha_1 - \alpha_2 = 0, 0 \leq \alpha_1, 0 \leq \alpha_2.
$$

- $\alpha_2 = \alpha_1$ to the objective function,

$$\frac{1}{2}\alpha_1^2 - 2\alpha_2$$

- Smallest value at $\alpha_1 = 2$.

  α_2 as well
- If smallest value < 0

  clipped to 0

Let Us Try A Practical Example

- A problem from astroparticle physics

```
1.0 1:2.617300e+01 2:5.886700e+01 3:-1.894697e-01 4:1.251225e+02
1.0 1:5.707397e+01 2:2.214040e+02 3:8.607959e-02 4:1.229114e+02
1.0 1:1.725900e+01 2:1.734360e+02 3:-1.298053e-01 4:1.250318e+02
1.0 1:2.177940e+01 2:1.249531e+02 3:1.538853e-01 4:1.527150e+02
1.0 1:9.133997e+01 2:2.935699e+02 3:1.423918e-01 4:1.605402e+02
1.0 1:5.537500e+01 2:1.792220e+02 3:1.654953e-01 4:1.112273e+02
1.0 1:2.956200e+01 2:1.913570e+02 3:9.901439e-02 4:1.034076e+02
```

- Training and testing sets available: 3,089 and 4,000
- Data format is an issue

SVM software: LIBSVM

- `http://www.csie.ntu.edu.tw/~cjlin/libsvm`
- Now one of the most used SVM software
- Installation
- On Unix:
  Download zip file and make
- On Windows:
  - Download zip file and make
  - `c:nmake -f Makefile.win`
  - Windows binaries included in the package

Usage of LIBSVM

- Training

```
Usage: svm-train [options] training_set_file
options:
-s svm_type : set type of SVM (default 0)
        0 -- C-SVC
        1 -- nu-SVC
        2 -- one-class SVM
        3 -- epsilon-SVR
        4 -- nu-SVR
-t kernel_type : set type of kernel function
```

- Testing

```
Usage: svm-predict test_file model_file outp
```

Training and Testing

- Training

```
$./svm-train train.1
......*
optimization finished, #iter = 6131
nu = 0.606144
obj = -1061.528899, rho = -0.495258
nSV = 3053, nBSV = 724
Total nSV = 3053
```

- Testing

```
$./svm-predict test.1 train.1.model
  test.1.predict
Accuracy = 66.925% (2677/4000)
```

What does this Output Mean

- obj: the optimal objective value of the dual SVM
- rho: $-b$ in the decision function
- nSV and nBSV: number of support vectors and bounded support vectors

  (i.e., $\alpha_i = C$).
- nu-svm is a somewhat equivalent form of C-SVM where C is replaced by ν.

Why this Fails

- After training, nearly 100% support vectors
- Training and testing accuracy different

```
$./svm-predict train.1 train.1.model o
Accuracy = 99.7734% (3082/3089)
```

- Most kernel elements:

$$K_{ij} \begin{cases} = 1 & \text{if } i = j, \\ \to 0 & \text{if } i \neq j. \end{cases}$$

Data Scaling

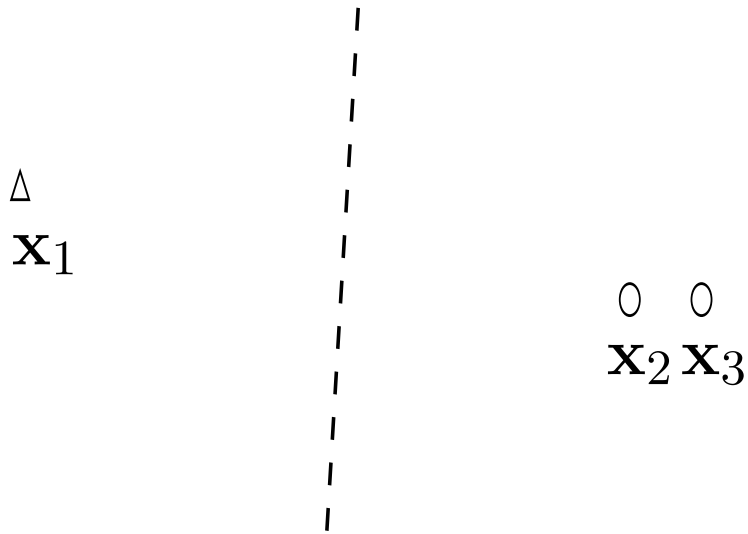
- Without scaling
  Attributes in greater numeric ranges may dominate
- Example:

	height	sex
$\mathbf{x}_1$	150	F
$\mathbf{x}_2$	180	M
$\mathbf{x}_3$	185	M

and

$$y_1 = 0, y_2 = 1, y_3 = 1.$$

- The separating hyperplane

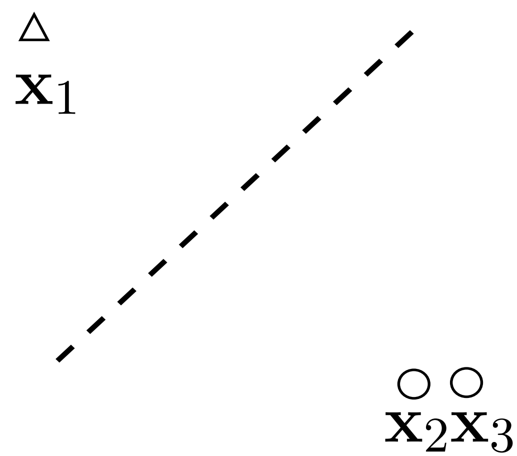


- Decision strongly depends on the first attribute
- What if the second is more important

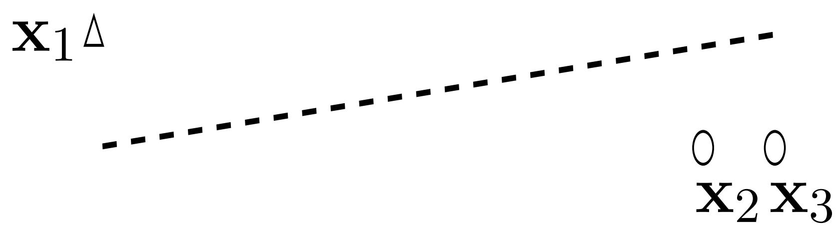
- Linearly scale the first to $[0,1]$ by:

$$\frac{\text{1st attribute} - 150}{185 - 150},$$

- New points and separating hyperplane



- Transformed to the original space,



- The second attribute plays a role

After Data Scaling

- A common mistake

```
$./svm-scale -l -1 -u 1 train.1 > train.1.scale
$./svm-scale -l -1 -u 1 test.1 > test.1.scale
```

- Same factor on training and testing

```
$./svm-scale -s range1 train.1 > train.1.sca
$./svm-scale -r range1 test.1 > test.1.scale
$./svm-train train.1.scale
$./svm-predict test.1.scale train.1.scale.mod
  test.1.predict
```

$\rightarrow$ Accuracy = 96.15%

- We store the scaling factor used in training and apply them for testing set

More on Training

- Train scaled data and then prediction

```
$./svm-train train.1.scale
$./svm-predict test.1.scale train.1.scale.mod
  test.1.predict
```

$\rightarrow$ `Accuracy = 96.15%`

- Training accuracy now is

```
$./svm-predict train.1.scale train.1.scale.mo
Accuracy = 96.439% (2979/3089) (classificati
```

- Default parameter
- $C = 1, \gamma = 0.25$

Different Parameters

- If we use $C = 20, \gamma = 400$

```
$./svm-train -c 20 -g 400 train.1.scale
./svm-predict train.1.scale train.1.scale.mo
Accuracy = 100% (3089/3089) (classification)
```

- 100% training accuracy but

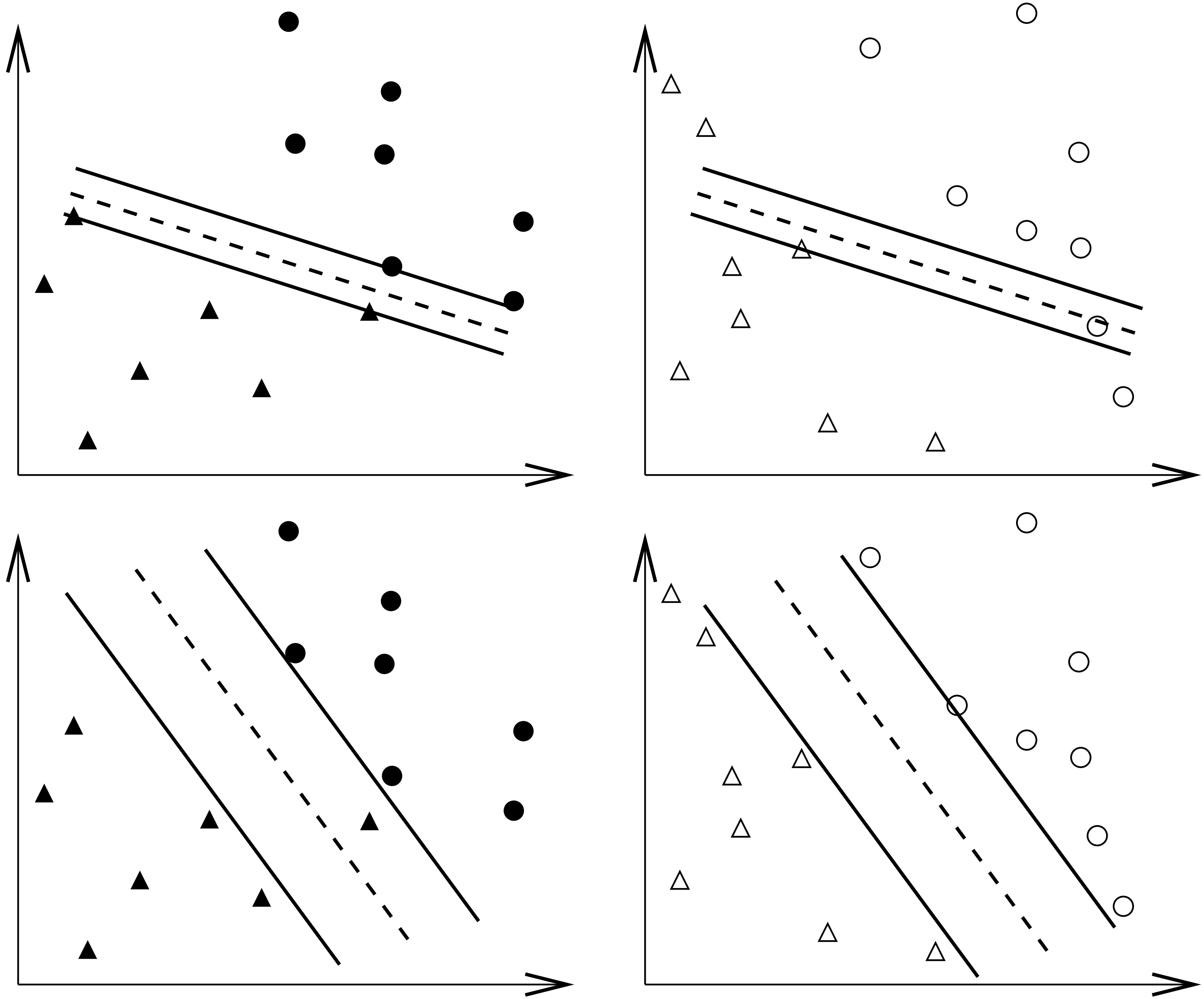
```
$./svm-predict test.1.scale train.1.scale.mo
Accuracy = 82.7% (3308/4000) (classification
```

- Very bad test accuracy
- Overfitting happens

Overfitting and Underfitting

- When training and predicting a data, we should
  - Avoid underfitting: small training error
  - Avoid overfitting: small testing error

● and ▲: training; ○ and △: testing



Overfitting

- In theory

  You can easily achieve 100% training accuracy
- This is useless
- Surprisingly

  Many application papers did this

Parameter Selection

- Is very important
- Now parameters are

  C, kernel parameters
- Example:

$$\gamma \text{ of } e^{-\gamma\|\mathbf{x}_i - \mathbf{x}_j\|^2}$$

$$a, b, d \text{ of } (\mathbf{x}_i^T \mathbf{x}_j / a + b)^d$$

- How to select them ?

  So performance better ?

Performance Evaluation

- Training errors not important; only test errors count
- l training data, $\mathbf{x}_i \in R^n, y_i \in \{+1, -1\}, i = 1, \ldots, l$, a learning machine:

$$x \to f(\mathbf{x}, \alpha), f(\mathbf{x}, \alpha) = 1 \text{ or } -1.$$

  Different α: different machines
- The expected test error (generalized error)

$$R(\alpha) = \int \frac{1}{2} |y - f(\mathbf{x}, \alpha)| dP(\mathbf{x}, y)$$

  y: class of $\mathbf{x}$ (i.e. 1 or -1)

- $P(\mathbf{x}, y)$ unknown, empirical risk (training error):

$$R_{emp}(\alpha) = \frac{1}{2l} \sum_{i=1}^{l} |y_i - f(\mathbf{x}_i, \alpha)|$$

- $\frac{1}{2}|y_i - f(\mathbf{x}_i, \alpha)|$: loss, choose $0 \leq \eta \leq 1$, with probability at least $1 - \eta$:

$$R(\alpha) \leq R_{emp}(\alpha) + \text{ another term}$$

  - A good pattern recognition method: minimize both terms at the same time
  - $R_{emp}(\alpha) \rightarrow 0$
    another term $\rightarrow$ large

Performance Evaluation (Cont.)

- In practice

  Available data $\Rightarrow$ training and validation
- Train the training
- Test the validation
- k-fold cross validation:
  - Data randomly separated to k groups.
  - Each time $k-1$ as training and one as testing

CV and Test Accuracy

- If we select parameters so that CV is the highest,
  - Does CV represent future test accuracy ?
  - Slightly different
- If we have enough parameters, we can achieve 100% CV as well
  - e.g. more parameters than # of training data
  - But test accuracy may be different
- So
  - Available data with class labels
  - $\Rightarrow$ training, validation, testing

- Using CV on training + validation
- Predict testing with the best parameters from CV

A Simple Procedure

1. Conduct simple scaling on the data
2. Consider RBF kernel $K(x, y) = e^{-\gamma\|x-y\|^2}$
3. Use cross-validation to find the best parameter C and γ
4. Use the best C and γ to train the whole training set
5. Test

- Best C and γ by training $k-1$ and the whole ?

  In theory, a minor difference

  No problem in practice

Parameter Selection Procedure in LIBSVM

- grid search + CV

```
$./grid.py train.1 train.1.scale
[local] -1 -7 85.1408  (best c=0.5, g=0.0078125, rate=85.1408)
[local] 5 -7 95.4354  (best c=32.0, g=0.0078125, rate=95.4354)
.
.
.
```

- grid.py: a python script in the python directory of LIBSVM

- Easy parallelization on a cluster

```
$./grid.py train.1 train.1.scale
[linux1] -1 -7 85.1408  (best c=0.5, g=0.0078125, rate=85.1408)
[linux7] 5 -7 95.4354  (best c=32.0, g=0.0078125, rate=95.4354)
.
.
.
```

Parallel Parameter Selection

- Specify machine names in grid.py

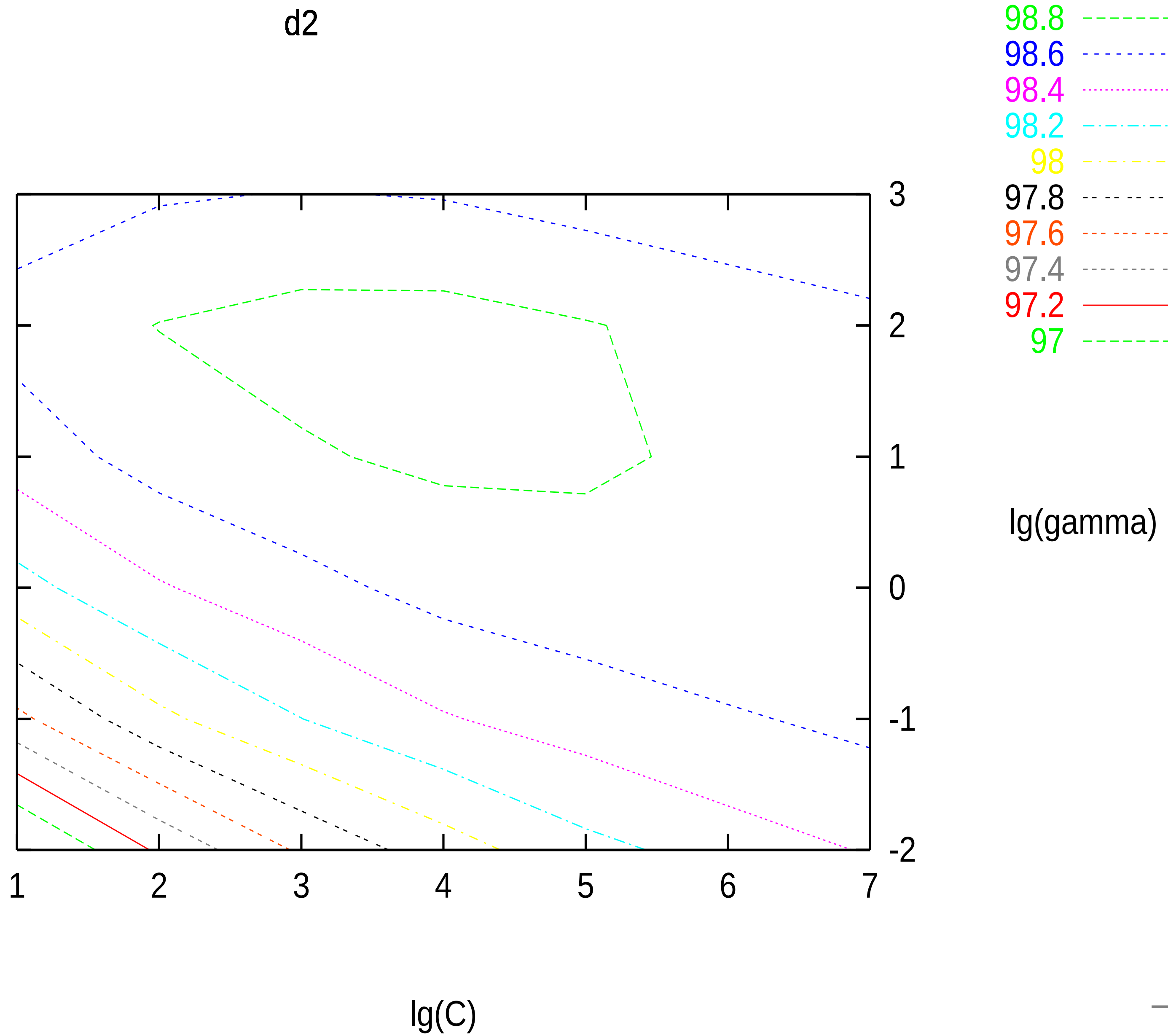
  ```
  telnet_workers = []
  ssh_workers = ['linux1','linux1','linux2',
  'linux3']
  nr_local_worker = 1
  ```

  linux1: more powerful or two CPUs
- A simple centralized control

  Load balancing not a problem
- We can use other tools

  Too simple so not consider them

Contour of Parameter Selection



Simple script in LIBSVM

- easy.py: a script for dummies

```
$python easy.py train.1 test.1
Scaling training data...
Cross validation...
Best c=2.0, g=2.0
Training...
Scaling testing data...
Testing...
Accuracy = 96.875% (3875/4000)
```

Example: Engine Misfire Detection

Problem Description

- First problem of IJCNN Challenge 2001, data from Ford
- Given time series length $T = 50,000$
- The kth data

$$x_1(k), x_2(k), x_3(k), x_4(k), x_5(k), y(k)$$

- $y(k) = \pm 1$: output, affected only by $x_1(k), \ldots, x_4(k)$
- $x_5(k) = 1$, kth data considered for evaluating accuracy
- 50,000 training data, 100,000 testing data (in two sets)

- Past and future information may affect $y(k)$
- $x_1(k)$: periodically nine 0s, one 1, nine 0s, one 1, and so on.
- Example:

```
0.000000 -0.999991 0.169769 0.000000 1.00000
0.000000 -0.659538 0.169769 0.000292 1.00000
0.000000 -0.660738 0.169128 -0.020372 1.0000
1.000000 -0.660307 0.169128 0.007305 1.00000
0.000000 -0.660159 0.169525 0.002519 1.00000
0.000000 -0.659091 0.169525 0.018198 1.00000
0.000000 -0.660532 0.169525 -0.024526 1.0000
0.000000 -0.659798 0.169525 0.012458 1.00000
```

- $x_4(k)$ more important

Background: Engine Misfire Detection

- How engine works

  Air-fuel mixture injected to cylinder

  intact, compression, combustion, exhaustion
- Engine misfire: a substantial fraction of a cylinder's air-fuel mixture fails to ignite
- Frequent misfires: pollutants and costly replacement
- On-board detection:

  Engine crankshaft rational dynamics with a position sensor
- Training data: from some expensive experimental environment

Encoding Schemes

- For SVM: each data is a vector
- $x_1(k)$: periodically nine 0s, one 1, nine 0s, one 1, ...
  - 10 binary attributes
    $x_1(k-5), \ldots, x_1(k+4)$ for the kth data
  - $x_1(k)$: an integer in 1 to 10
  - Which one is better
  - We think 10 binaries better for SVM
- $x_4(k)$ more important

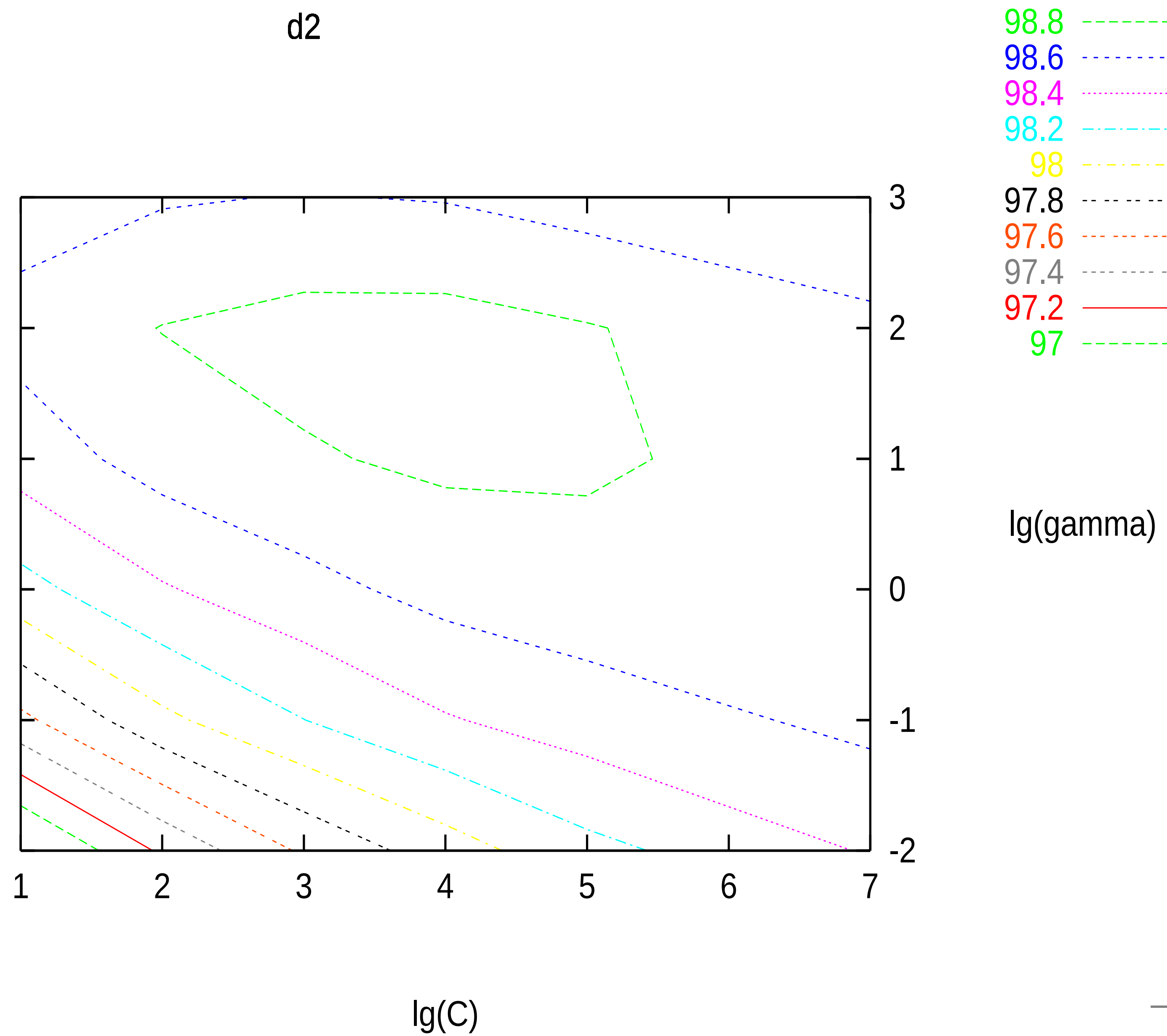
  Including $x_4(k-5), \ldots, x_4(k+4)$ for the kth data
- Each training data: 22 attributes

Training SVM

- Selecting parameters; generating a good model for prediction
- RBF kernel $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$
- Two parameters: γ and C
- Five-fold cross validation on 50,000 data

  Data randomly separated to five groups.

  Each time four as training and one as testing
- Use $C = 2^4, \gamma = 2^2$ and train 50,000 data for the final model



d2
98.8
98.6
98.4
98.2
98
97.8
97.6
97.4
97.2
97
3
2
1
0
-1
-2
lg(gamma)
1
2
3
4
5
6
7
lg(C)

- Test set 1: 656 errors, Test set 2: 637 errors
- About 3000 support vectors of 50,000 training data

  A good case for SVM
- This is just the outline. There are other details.
- It is essential to do model selection.

Dual Problems for Other Formulas

- So we think that for any optimization problem Lagrangian dual exists
- This is wrong
- Remember we calculate

$$\min \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{l} \alpha_i[y_i(\mathbf{w}^T\phi(\mathbf{x}_i) - 1]$$

by

$$\frac{\partial}{\partial \mathbf{w}} L(\mathbf{w}, b, \boldsymbol{\alpha}) = 0.$$

- Note that

$$f'(x) = 0 \Leftrightarrow x \text{ minimum}$$

  is wrong

- Example

$$f(x) = x^3, x = 0 \text{ not minimum}$$

- This function must satisfy certain conditions
- Some papers wrongly derived the dual of their new formulations without checking conditions

- $[2, 2]^T$ satisfies constraints $0 \leq \alpha_1$ and $0 \leq \alpha_2$

  It is optimal
- Primal-dual relation

$$
\begin{aligned}
w &= y_1 \alpha_1 x_1 + y_2 \alpha_2 x_2 \\
&= 1 \cdot 2 \cdot 1 + (-1) \cdot 2 \cdot 0 \\
&= 2
\end{aligned}
$$

- The same as solving the primal

Multi-class Classification

- k classes
- One-against-all: Train k binary SVMs:

$$\begin{array}{lll} 1\text{st class} & \text{vs.} & (2-k)\text{th class} \\ 2\text{nd class} & \text{vs.} & (1,3-k)\text{th class} \\ & \vdots & \end{array}$$

- k decision functions

$$(\mathbf{w}^1)^T\phi(\mathbf{x}) + b_1$$

$$\vdots$$

$$(\mathbf{w}^k)^T\phi(\mathbf{x}) + b_k$$

- Select the index with the largest $(\mathbf{w}^j)^T\phi(\mathbf{x}) + b_j$

Multi-class Classification (Cont.)

- One-against-one: train $k(k-1)/2$ binary SVMs
  $(1,2),(1,3),\ldots,(1,k),(2,3),(2,4),\ldots,(k-1,k)$
  Select the one with the largest vote
- This is the method used by LIBSVM
- Try a 4-class problem
  6 binary SVMs

```
$libsvm-2.5/svm-train bsvm-2.05/vehicle.scale
optimization finished, #iter = 173
obj = -142.552559, rho = 0.748453
nSV = 194, nBSV = 183
optimization finished, #iter = 330
obj = -149.912202, rho = -0.786410
nSV = 227, nBSV = 217
optimization finished, #iter = 169
obj = -139.655613, rho = 0.998277
nSV = 186, nBSV = 177
optimization finished, #iter = 268
obj = -185.161735, rho = -0.674739
nSV = 253, nBSV = 244
optimization finished, #iter = 477
obj = -378.264371, rho = 0.177314
nSV = 405, nBSV = 394
optimization finished, #iter = 337
obj = -186.182860, rho = 1.104943
nSV = 261, nBSV = 247
Total nSV = 739
```

- There are many other methods

  A comparison in [Hsu and Lin, 2002]

- For a software

  We select one which is generally good but not always the best

- Finally I chose 1 vs. 1

  Similar accuracy to others

  Shortest training

  A bit longer on testing than 1 vs. all

Why Shorter Training Time

- 1 vs. 1

  $k(k-1)/2$ problems, each $2l/k$ data on average
- 1 vs. all

  k problems, each l data
- If solving the optimization problem:

  polynomial of the size with degree d
- Their complexities

$$\frac{k(k-1)}{2}O\left(\left(\frac{2l}{k}\right)^d\right) \text{ vs. } kO(l^d)$$

Conclusions

- Dealing with data is interesting

  especially if you get good accuracy
- Some basic understandings are essential when applying methods

  e.g. the importance of validation
- No method is the best for all data

  Deep understanding of one or two methods very helpful