Support Vector Machines for Data Classification

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Outline

- Support vector classification
- Practical use of SVM
- Support vector regression
- An Example
- 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 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



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

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

- Decision function f(x) = sign(w^Tx + b), x: test data
 Variables: w and b : Need to know coefficients of a plane
 Many possible choices of w and b
- Select w, b with the maximal margin.
 Maximal distance between w^Tx + b = ±1

$$(\mathbf{w}^T \mathbf{x}_i) + b \ge 1$$
 if $y_i = 1$
 $(\mathbf{w}^T \mathbf{x}_i) + b \le -1$ if $y_i = -1$

Distance between
$$\mathbf{w}^T \mathbf{x} + b = 1$$
 and -1 :
 $2/\|\mathbf{w}\| = 2/\sqrt{\mathbf{w}^T \mathbf{w}}$
 $\max 2/\|\mathbf{w}\| \equiv \min \mathbf{w}^T \mathbf{w}/2$
 $\min_{\mathbf{w}, b} \quad \frac{1}{2} \mathbf{w}^T \mathbf{w}$
subject to $y_i((\mathbf{w}^T \mathbf{x}_i) + b) \ge 1,$
 $i = 1, \dots, l.$

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

$$\min_{\mathbf{w},b,\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l} \xi_i$$
$$y_i((\mathbf{w}^T\mathbf{x}_i) + b) \ge 1 - \xi_i,$$
$$\xi_i \ge 0, \ i = 1, \dots, l$$

• $\xi_i > 1$, \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: $\mathbf{x} \in R^3, \phi(\mathbf{x}) \in R^{10}$

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

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
$$y_i(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b) \ge 1 - \xi_i, \quad \xi_i \ge 0, \quad i = 1, \dots, l.$$

Finding the Decision Function

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

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha}$$
subject to
$$0 \le \alpha_i \le C, i = 1, \dots, l$$

$$\mathbf{y}^T \boldsymbol{\alpha} = 0,$$

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

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

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

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

Then
$$\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$$
.

• Popular methods: $K(\mathbf{x}_i, \mathbf{x}_j) =$

 $e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$, (Radial Basis Function) $(\mathbf{x}_i^T \mathbf{x}_j / a + b)^d$ (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 $K(\mathbf{x}_i, \mathbf{x}_j) =$

 $e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$, (Radial Basis Function) $(\mathbf{x}_i^T \mathbf{x}_j / a + b)^d$ (Polynomial kernel)

They can be inner product in infinite dimensional space
 Assume x ∈ R¹ and γ > 0.

$$e^{-\gamma ||x_i - x_j||^2} = e^{-\gamma (x_i - x_j)^2} = e^{-\gamma x_i^2 + 2\gamma x_i x_j - \gamma x_j^2}$$

= $e^{-\gamma x_i^2 - \gamma x_j^2} \left(1 + \frac{2\gamma x_i x_j}{1!} + \frac{(2\gamma x_i x_j)^2}{2!} + \frac{(2\gamma x_i x_j)^3}{3!} + \cdots\right)$
= $e^{-\gamma x_i^2 - \gamma x_j^2} \left(1 \cdot 1 + \sqrt{\frac{2\gamma}{1!}} x_i \cdot \sqrt{\frac{2\gamma}{1!}} x_j + \sqrt{\frac{(2\gamma)^2}{2!}} x_i^2 \cdot \sqrt{\frac{(2\gamma)^2}{2!}} x_j^2 + \sqrt{\frac{(2\gamma)^3}{3!}} x_j^3 + \cdots\right)$
= $\phi(x_i)^T \phi(x_j),$

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

- w: maybe an infinite vector
- At optimum

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

Decision function

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

$$= \sum_{i=1}^{l} \alpha_{i} y_{i} \phi(\mathbf{x}_{i})^{T} \phi(\mathbf{x}) + b$$

$$= \sum_{i=1}^{l} \alpha_{i} y_{i} K(\mathbf{x}_{i}, \mathbf{x}) + b$$

No need to have $\ensuremath{\mathbf{w}}$

- \blacksquare > 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

x₁ = 0, **x**₂ = 1 with **y** = [-1, 1]^T.
 Primal problem

$$\min_{w,b} \quad \frac{1}{2}w^2$$
subject to
$$w \cdot 1 + b \ge 1, \qquad (1)$$

$$-1(w \cdot 0 + b) \ge 1. \qquad (2)$$

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

$$w \ge 2$$

- 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 = 0In the middle of the two training data:



Dual Problem

Formula derived before

$$\begin{split} \min_{\boldsymbol{\alpha}\in R^l} & \quad \frac{1}{2}\sum_{i=1}^l\sum_{j=1}^l\alpha_i\alpha_jy_iy_j\mathbf{x}_i^T\mathbf{x}_j - \sum_{i=1}^l\alpha_i\\ \text{subject to} & \quad \alpha_i\geq 0, i=1,\ldots,l, \text{ and } \sum_{i=1}^l\alpha_iy_i=0. \end{split}$$

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

$$\frac{1}{2}\alpha_1^2 - (\alpha_1 + \alpha_2)$$

$$= \frac{1}{2} \begin{bmatrix} \alpha_1 & \alpha_2 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} - \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}$$

Constraints

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

• $\alpha_2 = \alpha_1$ 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 < 0clipped 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 output

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	Μ
\mathbf{x}_3	185	Μ

and

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



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



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

New points and separating hyperplane







The second attribute plays a role

After Data Scaling

A common mistake

\$./svm-scale -l -l -u l train.l > train.l.scale \$./svm-scale -l -l -u l test.l > test.l.scale

Same factor on training and testing

\$./svm-scale -s range1 train.1 > train.1.scal

- \$./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) (classification)

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.mod 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 \blacktriangle : training; \bigcirc and \triangle : testing



. – p.42/64

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
- I training data, $x_i ∈ R^n, y_i ∈ \{+1, -1\}, i = 1, ..., l$, 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 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 $0 \le \eta \le 1$, 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
- $R_{emp}(\alpha) \to 0$ another term \to 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)

x₁(k): periodically nine 0s, one 1, nine 0s, one 1, and so on.

Example:

• $x_4(k)$ 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 *k*th 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



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.

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