Support Vector Machines

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Outline

- Basic concepts
- SVM primal/dual problems
- Training linear and nonlinear SVMs
- Parameter/kernel selection and practical issues
- Multi-class classification
- Discussion and conclusions

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Why SVM and Kernel Methods

- SVM: in many cases competitive with existing classification methods

  Relatively easy to use
- Kernel techniques: many extensions

  Regression, density estimation, kernel PCA, etc.

Support Vector Classification

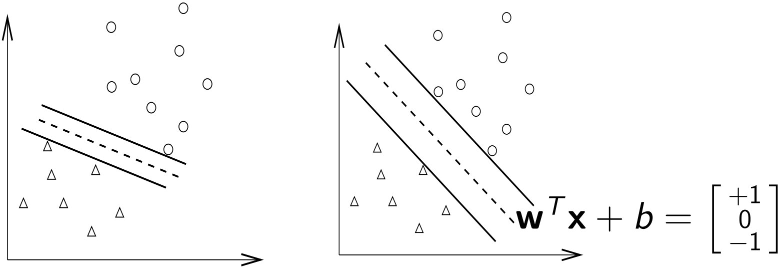
- Training vectors : $\mathbf{x}_i, i = 1, \ldots, l$
- Feature vectors. For example,

  A patient = [height, weight, ...]
- Consider a simple case with two classes:

  Define an indicator 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



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

$$\begin{array}{ll} (\mathbf{w}^T\mathbf{x}_i) + b > 0 & \text{if } y_i = 1 \\ (\mathbf{w}^T\mathbf{x}_i) + b < 0 & \text{if } y_i = -1 \end{array}$$

- Decision function $f(\mathbf{x}) = \text{sgn}(\mathbf{w}^T\mathbf{x} + b)$, $\mathbf{x}$: test data

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

Maximal Margin

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

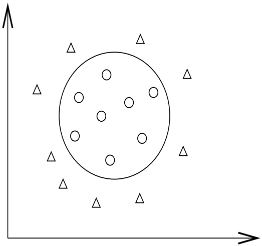
$$2/\|\mathbf{w}\| = 2/\sqrt{\mathbf{w}^T\mathbf{w}}$$

- A quadratic programming problem [Boser et al., 1992]

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

Data May Not Be Linearly Separable

- An example:



- Allow training errors
- Higher dimensional (maybe infinite) feature space

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

- Standard SVM [Cortes and Vapnik, 1995]

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

$$\text{subject to} \quad y_i(\mathbf{w}^T\phi(\mathbf{x}_i)+b) \geq 1-\xi_i,$$

$$\xi_i \geq 0,\ i=1,\ldots,l.$$

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

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

Finding the Decision Function

- $\mathbf{w}$: 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 $\mathbf{e} = [1, \ldots, 1]^T$

- At optimum

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

- A finite problem: #variables = #training data

Kernel Tricks

- $Q_{ij} = y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ needs a closed form
- 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 $\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$.

- Kernel: $K(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$; common kernels:

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

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

Can be inner product in infinite dimensional space

Assume $x \in R^1$ and $\gamma > 0$.

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

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

$$=e^{-\gamma x_i^2-\gamma x_j^2}\Big(1\cdot 1+\sqrt{\frac{2\gamma}{1!}}x_i\cdot\sqrt{\frac{2\gamma}{1!}}x_j+\sqrt{\frac{(2\gamma)^2}{2!}}x_i^2\cdot\sqrt{\frac{(2\gamma)^2}{2!}}x_j^2$$

$$+\sqrt{\frac{(2\gamma)^3}{3!}}x_i^3\cdot\sqrt{\frac{(2\gamma)^3}{3!}}x_j^3+\cdots\Big)=\phi(x_i)^T\phi(x_j),$$

where

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

More about Kernels

- How do we know kernels help to separate data?
- In R^l, any l independent vectors

  $\Rightarrow$ linearly separable

$$\begin{bmatrix} (\mathbf{x}^1)^T \\ \vdots \\ (\mathbf{x}^l)^T \end{bmatrix} \mathbf{w} = \begin{bmatrix} +\mathbf{e} \\ -\mathbf{e} \end{bmatrix}$$

- If K positive definite $\Rightarrow$ data linearly separable

  $K = LL^T$.

  Transforming training points to independent vectors in R^l

- So what kind of kernel should I use?
- What kind of functions are valid kernels?
- How to decide kernel parameters?
- Will be discussed later

Decision function

- At optimum

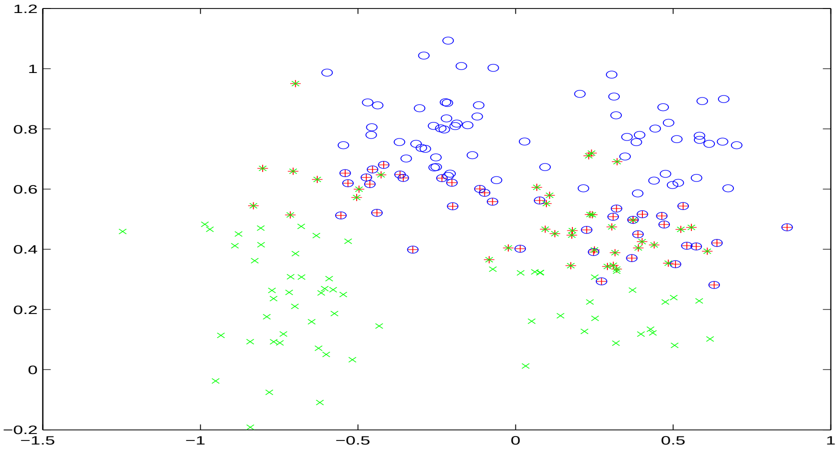
$$\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \phi(\mathbf{x}_i)$$

- Decision function

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

- Only $\phi(\mathbf{x}_i)$ of $\alpha_i > 0$ used $\Rightarrow$ support vectors

Support Vectors: More Important Data



- So we have roughly shown basic ideas of SVM
- A 3-D demonstration
  www.csie.ntu.edu.tw/~cjlin/libsvmtools/svmtoy3d
- Further references, for example,
  [Cristianini and Shawe-Taylor, 2000,
  Schölkopf and Smola, 2002]
- Also see discussion on kernel machines blackboard
  www.kernel-machines.org/phpbb/

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Deriving the Dual

- Consider the problem without ξ_i

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

- Its dual

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

Lagrangian Dual

$$\max_{\alpha \geq 0} \left(\min_{\mathbf{w}, b} L(\mathbf{w}, b, \boldsymbol{\alpha}) \right),$$

where

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^{l} \alpha_i \left(y_i (\mathbf{w}^T \phi(\mathbf{x}_i) + b) - 1 \right)$$

Strong duality (be careful about this)

$$\min \text{ Primal} = \max_{\alpha \geq 0} \left(\min_{\mathbf{w}, b} L(\mathbf{w}, b, \boldsymbol{\alpha}) \right)$$

- Simplify the dual. When $\boldsymbol{\alpha}$ is fixed,

$$\min_{\mathbf{w},b} L(\mathbf{w}, b, \boldsymbol{\alpha}) =$$

$$\begin{cases} -\infty & \text{if } \sum_{i=1}^{l} \alpha_i y_i \neq 0 \\ \min_{\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{l} \alpha_i [y_i(\mathbf{w}^T\phi(\mathbf{x}_i) - 1] & \text{if } \sum_{i=1}^{l} \alpha_i y_i = 0 \end{cases}$$

- If $\sum_{i=1}^{l} \alpha_i y_i \neq 0$,
  decrease

$$-b\sum_{i=1}^{l} \alpha_i y_i$$

in $L(\mathbf{w}, b, \boldsymbol{\alpha})$ to $-\infty$

- If $\sum_{i=1}^{l} \alpha_i y_i = 0$, optimum of the strictly convex $\frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{l} \alpha_i [y_i(\mathbf{w}^T \phi(\mathbf{x}_i) - 1]$ happens when

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

- Thus,

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

- Note that

$$\begin{aligned}\mathbf{w}^T\mathbf{w} &= \Big(\sum_{i=1}^{l}\alpha_i y_i \phi(\mathbf{x}_i)\Big)^T\Big(\sum_{j=1}^{l}\alpha_j y_j \phi(\mathbf{x}_j)\Big)\\ &= \sum_{i,j}\alpha_i\alpha_j y_i y_j \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)\end{aligned}$$

- The dual is

$$\max_{\boldsymbol{\alpha}\geq 0}\begin{cases}\sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y_i y_j \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j) & \text{if } \sum_{i=1}^{l}\alpha_i y_i = 0,\\ -\infty & \text{if } \sum_{i=1}^{l}\alpha_i y_i \neq 0.\end{cases}$$

- Lagrangian dual: $\max_{\boldsymbol{\alpha} \geq 0} \left(\min_{\mathbf{w}, b} L(\mathbf{w}, b, \boldsymbol{\alpha}) \right)$
- $-\infty$ definitely not maximum of the dual

  Dual optimal solution not happen when

$$\sum_{i=1}^{l} \alpha_i y_i \neq 0$$

  .
- Dual simplified to

$$\begin{aligned} \max_{\boldsymbol{\alpha} \in R^l} \quad & \sum_{i=1}^{l} \alpha_i - \frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) \\ \text{subject to} \quad & \mathbf{y}^T \boldsymbol{\alpha} = 0, \\ & \alpha_i \geq 0, i = 1, \ldots, l. \end{aligned}$$

More about Dual Problems

- After SVM is popular

  Quite a few people think that for any optimization problem

  $\Rightarrow$ Lagrangian dual exists and strong duality holds
- Wrong! We usually need

  Convex programming; Constraint qualification
- We have them

  SVM primal is convex; Linear constraints

- Our problems may be infinite dimensional
- Can still use Lagrangian duality

  See a rigorous discussion in [Lin, 2001]

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Training Nonlinear SVMs

- If using kernels, we solve the dual

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

- Large dense quadratic programming
- $Q_{ij} \neq 0$, Q : an l by l fully dense matrix
- 30,000 training points: 30,000 variables:
  $(30,000^2 \times 8/2)$ bytes $=$ 3GB RAM to store Q:
- Traditional methods:
  Newton, Quasi Newton cannot be directly applied

Decomposition Methods

- Working on some variables each time (e.g., [Osuna et al., 1997, Joachims, 1998, Platt, 1998])
- Similar to coordinate-wise minimization
- Working set B, $N = \{1, \ldots, l\} \backslash B$ fixed
- Sub-problem at each iteration:

$$\min_{\boldsymbol{\alpha}_B} \quad \frac{1}{2} \begin{bmatrix} \boldsymbol{\alpha}_B^T & (\boldsymbol{\alpha}_N^k)^T \end{bmatrix} \begin{bmatrix} Q_{BB} & Q_{BN} \\ Q_{NB} & Q_{NN} \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha}_B \\ \boldsymbol{\alpha}_N^k \end{bmatrix} - \begin{bmatrix} \mathbf{e}_B^T & (\mathbf{e}_N^k)^T \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha}_B \\ \boldsymbol{\alpha}_N^k \end{bmatrix}$$

$$\text{subject to} \quad 0 \leq \alpha_t \leq C, t \in B, \ \mathbf{y}_B^T \boldsymbol{\alpha}_B = -\mathbf{y}_N^T \boldsymbol{\alpha}_N^k$$

Avoid Memory Problems

- The new objective function

$$\frac{1}{2}\boldsymbol{\alpha}_B^T Q_{BB}\boldsymbol{\alpha}_B + (-\mathbf{e}_B + Q_{BN}\boldsymbol{\alpha}_N^k)^T\boldsymbol{\alpha}_B + \text{ constant}$$

- B columns of Q needed
- Calculated when used

  Trade time for space

Does it Really Work?

- Compared to Newton, Quasi-Newton
  Slow convergence
- However, no need to have very accurate $\boldsymbol{\alpha}$

$$\operatorname{sgn}\left(\sum_{i=1}^{l} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b\right)$$

  Prediction not affected much
- In some situations, # support vectors $\ll$ # training points
  Initial $\boldsymbol{\alpha}^1 = 0$, some elements never used
- Machine learning knowledge affects optimization

- An example of training 50,000 instances using LIBSVM

```
$ ./svm-train -m 200 -c 16 -g 4 22features
optimization finished, #iter = 24981
Total nSV = 3370
time     5m1.456s
```

- On a Pentium M 1.4 GHz Laptop
- Calculating Q may have taken more than 5 minutes
- $\#\text{SVs} = 3{,}370 \ll 50{,}000$

  A good case where some remain at zero all the time

Issues of Decomposition Methods

- Working set size/selection
- Asymptotic convergence
- Finite termination & stopping conditions
- Convergence rate
- Numerical issues

Optimization researchers are now also interested in these issues

If interested in them, check my talk to optimization researchers in Rome last year:

http://www.csie.ntu.edu.tw/~cjlin/talks/rome.pdf

Caching and Shrinking

- Speed up decomposition methods
- Caching [Joachims, 1998]

  Store recently used kernel columns in computer memory
- 100K Cache

  ```
  $ time ./libsvm-2.81/svm-train -m 0.01 a4a
  11.463s
  ```
- 40M Cache

  ```
  $ time ./libsvm-2.81/svm-train -m 40 a4a
  7.817s
  ```

- Shrinking [Joachims, 1998]

  Some bounded elements remain until the end

  Heuristically resized to a smaller problem
- After certain iterations, most bounded elements identified and not changed [Lin, 2002]

  So caching and shrinking are useful

Caching: Issues

- A simple way:
  Store recently used columns
- What if in working set selection,
  deliberately select some indices in cache
- Goal: minimize the total number of columns calculated
- Difficult to connect algorithm and this goal

SVM doesn't Scale Up

Yes, if you use kernels

- Training millions of data is time consuming
- But other nonlinear methods face the same problem
  e.g., kernel logistic regression

Two possibilities

1. Linear SVMs: in some situations, can solve much larger problems
2. Approximation

Training Linear SVMs

- Linear kernel:

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

$$\text{subject to} \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \qquad \xi_i \geq 0.$$

- At optimum:

$$\xi_i = \max\bigl(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\bigr)$$

- Remaining variables: $\mathbf{w}, b$

$$\min_{\mathbf{w},b} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l} \max\big(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\big)$$

- #variables = #features + 1
- If #features small, easier to solve

- Traditional optimization methods can be applied
- Training time similar to methods such as logistic regression
- What if #features and #instances both large?
  Very challenging
- Some language/document problems are of this type

Decomposition Methods for Linear SVMs

- Could we still solve the dual by decomposition methods?
- Even if #features small
  Slow convergence when C is large

```
$bsvm-train -b 500 -c 500 -t 0 australian_scale
optimization finished, #iter = 260092
obj = -99310.588975, rho = 0.000000
```

- $K_{ij} = \mathbf{x}_i^T \mathbf{x}_j$, rank $\leq$ #features
  positive semi-definite only
- Still a research topic in understanding this

Decomposition Methods for Linear SVMs

- But no need to use large C
- C large enough, $\mathbf{w}$ the same [Keerthi and Lin, 2003]

  decision function the same
- Remember

$$\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \mathbf{x}_i \in R^n, \quad b \in R^1$$

  $|\# \text{ of } 0 < \alpha_i < C| \leq n + 1$
- As C changes, optimal $\boldsymbol{\alpha}$ share many elements at 0 and C

Decomposition Methods for Linear SVMs (Cont'd)

- Warm start very effective [Kao et al., 2004]

  Starting from small C, faster convergence
- Using $C = 1, 2, 4, 8, \ldots$

  ```
  $bsvm-train -c 500 -t 0 australian_scale
  optimization finished, #iter = 10087
  ```
- So decomposition methods can still handle large linear SVMs

Approximations

- #instances large and using nonlinear kernels
  Difficult to solve the dual
- Subsampling
  Simple and often effective
- From this many more advanced techniques
- E.g., stratified subsampling

Approximations (Cont'd)

- Incremental way: (e.g., [Syed et al., 1999])
  Data $\Rightarrow$ 10 parts
  train 1st part $\Rightarrow$ SVs, train SVs + 2nd part, ...
- Select good points first: KNN or heuristics
  e.g., [Bakır et al., 2005]
- Hierarchical settings (e.g., [Yu et al., 2003])
  Clustering training data to several groups
  SVM models built for each group

Approximations (Cont'd)

- Using only a subset to construct **w**

$$\mathbf{w} = \sum_{i \in B} \alpha_i y_i \phi(\mathbf{x}_i).$$

- Put this into the primal

$$\begin{aligned} \min_{\boldsymbol{\alpha}_B, b, \boldsymbol{\xi}} \quad & \frac{1}{2} \boldsymbol{\alpha}_B^T Q_{BB} \boldsymbol{\alpha}_B + C \sum_{i=1}^{l} \xi_i \\ \text{subject to} \quad & Q_{:,B} \boldsymbol{\alpha}_B + b\mathbf{y} \geq \mathbf{e} - \boldsymbol{\xi} \end{aligned}$$

- Without considering ξ_i, $\#\text{variables} = |B| + 1$

Approximations (Cont'd)

- Selecting B:
  random [Lee and Mangasarian, 2001],
  incremental [Keerthi et al., 2006],
  and many other ways

Approximations (Cont'd)

- All these approaches

  some simple but some sophisticated
- In machine learning, very often

  balance between simplification and performance

Outline

Let's Try a Practical Example

A problem from astroparticle physics

```
1 1:2.6173e+01 2:5.88670e+01 3:-1.89469e-01 4:1.25122e+02
1 1:5.7073e+01 2:2.21404e+02 3:8.60795e-02  4:1.22911e+02
1 1:1.7259e+01 2:1.73436e+02 3:-1.29805e-01 4:1.25031e+02
1 1:2.1779e+01 2:1.24953e+02 3:1.53885e-01  4:1.52715e+02
1 1:9.1339e+01 2:2.93569e+02 3:1.42391e-01  4:1.60540e+02
1 1:5.5375e+01 2:1.79222e+02 3:1.65495e-01  4:1.11227e+02
1 1:2.9562e+01 2:1.91357e+02 3:9.90143e-02  4:1.03407e+02
```

Training and testing sets available: 3,089 and 4,000

The Story Behind this Data Set

- User:

  `I am using libsvm in a astroparticle physics application .. First, let me congratulate you to a really easy to use and nice package. Unfortunately, it gives me astonishingly bad results...`
- OK. Please send us your data
- I am able to get 97% test accuracy. Is that good enough for you ?
- User:

  `You earned a copy of my PhD thesis`

Training and Testing

Training

```
$./svm-train train.1
optimization finished, #iter = 6131
nSV = 3053, nBSV = 724
Total nSV = 3053
```

Testing

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

nSV and nBSV: number of SVs and bounded SVs ($\alpha_i = C$).

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:

$$K_{ij} = e^{-\|\mathbf{x}_i - \mathbf{x}_j\|^2/4} \begin{cases} = 1 & \text{if } i = j, \\ \to 0 & \text{if } i \neq j. \end{cases}$$

- Some features in rather large ranges

Data Scaling

- Without scaling

  Attributes in greater numeric ranges may dominate

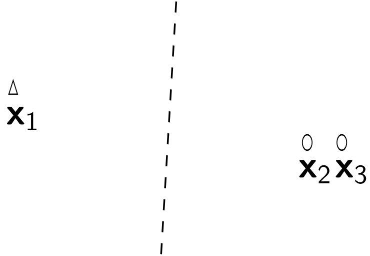
- Example:

	height	gender
$\mathbf{x}_1$	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 almost vertical



- Strongly depends on the first attribute; but second may be also important
- Linearly scale the first to $[0, 1]$ by:

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

- Scaling generally helps, but not always

- Other ways for scaling
- Needed for k Nearest Neighbor, Neural networks as well

  unless the method is scale-invariant

Data Scaling: Same Factors

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.scale
$./svm-scale -r range1 test.1 > test.1.scale
```

After Data Scaling

Train scaled data and then prediction

```
$./svm-train train.1.scale
$./svm-predict test.1.scale train.1.scale.model
  test.1.predict
Accuracy = 96.15%
```

Training accuracy now is

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

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.m
Accuracy = 100% (3089/3089)
```

- 100% training accuracy but

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

- Very bad test accuracy
- Overfitting happens

Overfitting

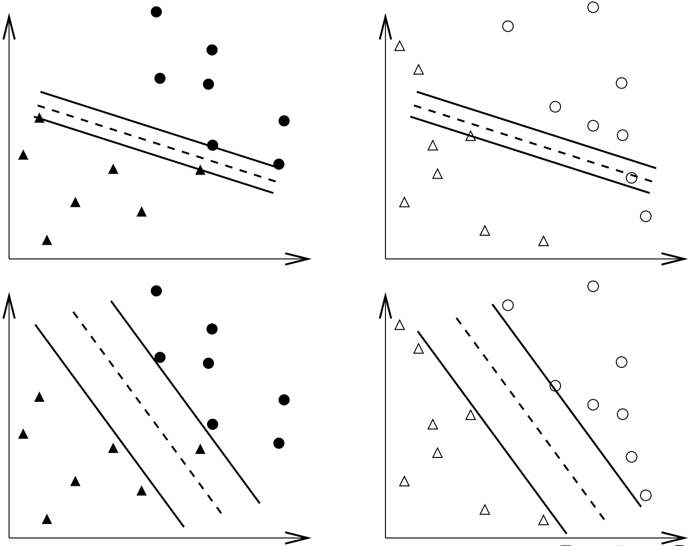
- In theory

  You can easily achieve 100% training accuracy
- This is useless
- When training and predicting a data, we should

  Avoid underfitting: small training error

  Avoid overfitting: small testing error

● and ▲: training; ○ and △: testing



Parameter Selection

- Is 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?

Parameter Selection (Cont'd)

- Also how to select kernels?

  e.g., RBF or polynomial
- Moreover, how to select methods?

  e.g., SVM or decision trees?

Performance Evaluation

- l training data, $\mathbf{x}_i \in R^n, y_i \in \{+1, -1\}, i = 1, \ldots, l$, a learning machine:

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

  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):

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

- Training errors not important; only test errors count
- $\frac{1}{2}|y_i - f(\mathbf{x}_i, \alpha)|$: loss, choose $0 \leq \eta \leq 1$, with probability at least $1 - \eta$:

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

- A good classification method:

  minimize both terms at the same time

- But $R_{emp}(\alpha) \rightarrow 0$; another term $\rightarrow$ large
- SVM:

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

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

- $\sum_{i=1}^{l}\xi_i$ related to training error
- $\mathbf{w}^T\mathbf{w}/2$ relate to another term: called regularization term
- C: balance between the two

Performance Evaluation (Cont'd)

- 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

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

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
- Available data with class labels

  $\Rightarrow$ training, validation, testing

Selecting Kernels

- RBF, polynomial, or others?
  or even combinations
- Two situations:
  Too many kernels complicates the selection
  Design kernels suitable for target applications

Selecting Kernels (Cont'd)

Contradicting but practically ok

- We have few general kernels
  RBF, polynomial, etc. somewhat related
  Beginners' don't have many choices
- On the other hand
  researchers design many special ones
  e.g., string kernels

Selecting Kernels (Cont'd)

- For beginners, use RBF first
- Linear kernel: special case of RBF

  Performance of linear the same as RBF under certain parameters [Keerthi and Lin, 2003]
- Polynomial: numerical difficulties

  $(< 1)^d \rightarrow 0, (> 1)^d \rightarrow \infty$

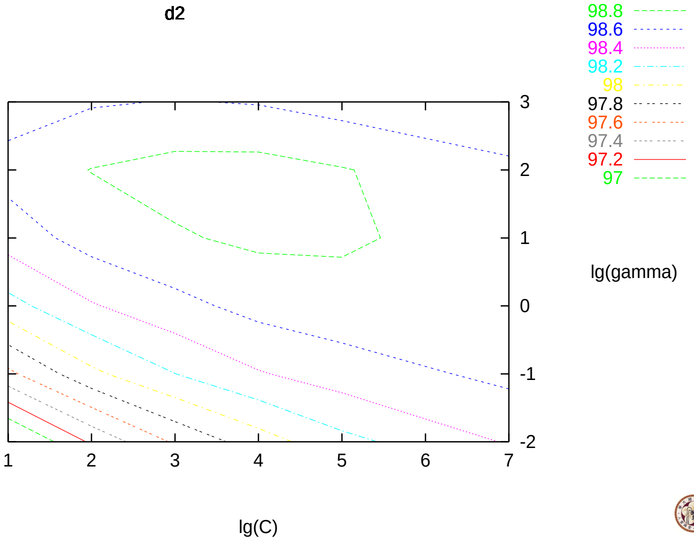
  More parameters than RBF

A Simple Procedure

1. Conduct simple scaling on the data
2. Consider RBF kernel $K(\mathbf{x}, \mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|^2}$
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

For beginners only, you can do a lot more

Contour of Parameter Selection



- The good region of parameters is quite large
- SVM is sensitive to parameters, but not that sensitive
- Sometimes default parameters work

  but it's good to select them if time is allowed

Efficient Parameter Selection

- CV on grid points may be time consuming
  OK if one or two parameters
- But if more than two?
  E.g., feature scaling:

$$K(\mathbf{x}, \mathbf{y}) = e^{-\sum_{i=1}^{n} \gamma_i (x_i - y_i)^2}$$

  Some features more important
- Still a challenging research issue

- Remember given parameters C and γ, we solve SVM to obtain optimal $\mathbf{w}$ or $\boldsymbol{\alpha}$
- Model a function of parameters

$$\min_{C,\gamma_1,\ldots,\gamma_n} f(\boldsymbol{\alpha}(C,\gamma_1,\ldots,\gamma_n), C,\gamma_1,\ldots,\gamma_n)$$

  But usually non-convex
- The function

  from Bayesian frameworks (e.g., [Chu et al., 2003])

  or

  smoothing CV bound

$$\mathrm{CV}(C,\gamma_1,\ldots,\gamma_n) \le f(\boldsymbol{\alpha}(C,\gamma_1,\ldots,\gamma_n), C,\gamma_1,\ldots,\gamma_n)$$

- The minimization:
  Gradient-type methods
  or
  global optimization (e.g., genetic algorithms)
- The difficulty:
  Certainly more efforts than one single γ
  But performance may be just similar?

Kernel Combination

- How about using

$$t_1 K_1 + t_2 K_2 + \cdots + t_r K_r,$$

  where

$$t_1 + \cdots + t_r = 1$$

  as the kernel
- Related to parameter selection

$$t_1 e^{-\gamma_1 \|\mathbf{x}-\mathbf{y}\|} + \cdots + t_r e^{-\gamma_r \|\mathbf{x}-\mathbf{y}\|}$$

  If γ_1 good $\Rightarrow$ t_1 close to 1, others close to 0

- [Lanckriet et al., 2004] form a convex

$$f(\boldsymbol{\alpha}(t_1, \ldots, t_r), t_1, \ldots, t_r)$$

  when C is fixed
- Semi-definite programming problem
- But computational cost is also high
- Need more empirical studies

Design Kernels

- Still a research issue

  e.g., in bioinformatics and vision, many new kernels
- But, should be careful if the function is a valid one

$$K(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$$

- For example, any two strings s_1, s_2 we can define edit distance

$$e^{-\gamma \text{edit}(s_1, s_2)}$$

  It's not a valid kernel [Cortes et al., 2003]

Mercer condition

- What kind of K_{ij} can be represented as $\phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$?
- $K(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x})^T\phi(\mathbf{y})$ if and only if $\forall g$ s.t.

$$\int g(\mathbf{x})^2 d\mathbf{x} \text{ finite}$$
$$\Rightarrow \int K(\mathbf{x},\mathbf{y})g(\mathbf{x})g(\mathbf{y})d\mathbf{x}d\mathbf{y} \geq 0$$

  A condition developed early last century
- However, still not easy to check

Outline

- Basic concepts
- SVM primal/dual problems
- Training linear and nonlinear SVMs
- Parameter/kernel selection and practical issues
- Multi-class classification
- Discussion and conclusions

Multi-class Classification

- k classes
- One-against-the rest: Train k binary SVMs:

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

- k decision functions

$$\begin{gathered} (\mathbf{w}^1)^T\phi(\mathbf{x}) + b_1 \\ \vdots \\ (\mathbf{w}^k)^T\phi(\mathbf{x}) + b_k \end{gathered}$$

- Prediction:

$$\arg\max_{j} \ (\mathbf{w}^j)^T\phi(\mathbf{x}) + b_j$$

- Reason: If the 1st class, then we should have

$$\begin{aligned}
(\mathbf{w}^1)^T\phi(\mathbf{x}) + b_1 &\geq +1 \\
(\mathbf{w}^2)^T\phi(\mathbf{x}) + b_2 &\leq -1 \\
&\vdots \\
(\mathbf{w}^k)^T\phi(\mathbf{x}) + b_k &\leq -1
\end{aligned}$$

Multi-class Classification (Cont'd)

- One-against-one: train $k(k-1)/2$ binary SVMs $(1,2),(1,3),\ldots,(1,k),(2,3),(2,4),\ldots,(k-1,k)$
- If 4 classes $\Rightarrow$ 6 binary SVMs

$y_i = 1$	$y_i = -1$	Decision functions
class 1	class 2	$f^{12}(\mathbf{x}) = (\mathbf{w}^{12})^T\mathbf{x} + b^{12}$
class 1	class 3	$f^{13}(\mathbf{x}) = (\mathbf{w}^{13})^T\mathbf{x} + b^{13}$
class 1	class 4	$f^{14}(\mathbf{x}) = (\mathbf{w}^{14})^T\mathbf{x} + b^{14}$
class 2	class 3	$f^{23}(\mathbf{x}) = (\mathbf{w}^{23})^T\mathbf{x} + b^{23}$
class 2	class 4	$f^{24}(\mathbf{x}) = (\mathbf{w}^{24})^T\mathbf{x} + b^{24}$
class 3	class 4	$f^{34}(\mathbf{x}) = (\mathbf{w}^{34})^T\mathbf{x} + b^{34}$

- For a testing data, predicting all binary SVMs

Classes		winner
1	2	1
1	3	1
1	4	1
2	3	2
2	4	4
3	4	3

- Select the one with the largest vote

class	1	2	3	4
# votes	3	1	1	1

- May use decision values as well

More Complicated Forms

- For example,
  [Vapnik, 1998, Weston and Watkins, 1999]:

$$\min_{\mathbf{w},b,\xi} \quad \frac{1}{2}\sum_{m=1}^{k}\mathbf{w}_m^T\mathbf{w}_m + C\sum_{i=1}^{l}\sum_{m\neq y_i}\xi_i^m$$

$$\mathbf{w}_{y_i}^T\phi(\mathbf{x}_i) + b_{y_i} \geq \mathbf{w}_m^T\phi(\mathbf{x}_i) + b_m + 2 - \xi_i^m,$$

$$\xi_i^m \geq 0, i = 1,\ldots,l, \ m \in \{1,\ldots,k\}\backslash y_i.$$

  y_i: class of $\mathbf{x}_i$
- kl constraints
- Dual: kl variables; very large

- There are many other methods
- A comparison in [Hsu and Lin, 2002]
- Accuracy similar for many problems
  But 1-against-1 fastest for training

Why 1vs1 Faster in Training

- 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

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

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Future Directions

I mentioned quite a few. Here are others.

- Better ways to handle unbalanced data

  i.e., some classes few data, some classes a lot
- Multi-label classification

  An instance associated with ≥ 2 labels

  e.g., a document in both politics, sports
- Structural data sets

  An instance may not be a vector

  e.g., a tree from a sentence

Conclusions

- Dealing with data is interesting
  especially if you get good accuracy
- Some basic understandings are essential when applying classification methods
- SVM is a rather mature topic
  but still quite a few interesting research issues

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