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

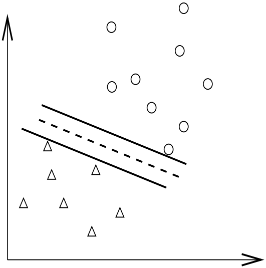
  Regression, density estimation, kernel PCA, etc.

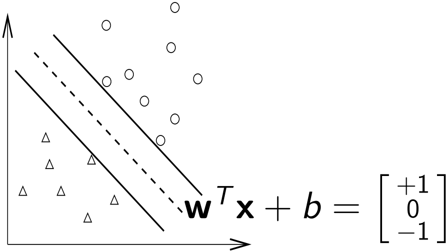
Support Vector Classification

- Training vectors : $\mathbf{x}_i, i = 1, \ldots, l$
- Feature vectors. For example,
  A patient $=$ [height, weight, $\ldots$]
- 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:

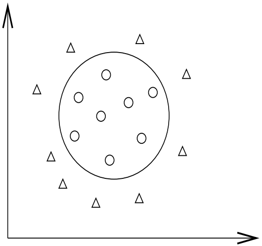
$$2/\|\mathbf{w}\| = 2/\sqrt{\mathbf{w}^T\mathbf{w}}$$

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

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

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]

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

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

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

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

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

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

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

  Then $\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$.
- 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 $\gamma > 0$.

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

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

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

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

where

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

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

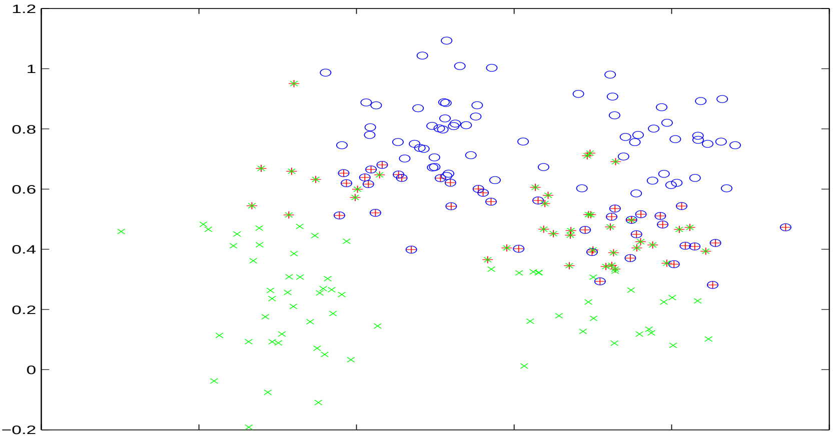
$$\boxed{\mathbf{w} = \textstyle\sum_{i=1}^{l} \alpha_i y_i \phi(\mathbf{x}_i)}$$

- 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

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

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)

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

- 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

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

- 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:

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

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

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