Outline

- Basic concepts: SVM and kernels
- SVM primal/dual problems

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Data Classification

- Given training data in different classes (labels known)

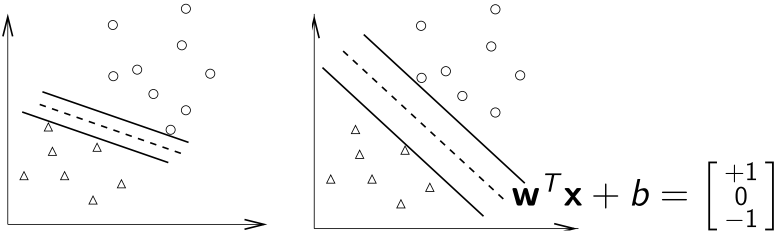
  Predict test data (labels unknown)
- Training and testing

Support Vector Classification

- Training vectors : $\mathbf{x}_i, i = 1, \ldots, l$
- Feature vectors. For example,
  A patient $=$ [height, weight, $\ldots$]^T
- 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: $\mathbf{w}^T\mathbf{x} + b = 0$

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

- 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:

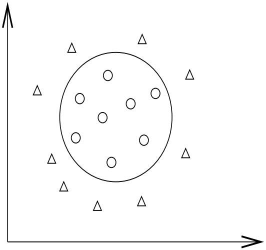
$$2/\|\mathbf{w}\| = 2/\sqrt{\mathbf{w}^T\mathbf{w}}$$

- 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

$$\phi(\mathbf{x}) = [\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots]^T.$$

- Standard SVM (Boser et al., 1992; 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: $\mathbf{x} \in R^3, \phi(\mathbf{x}) \in R^{10}$

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

Finding the Decision Function

- **w**: maybe infinite variables
- The dual problem: finite number of variables

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

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

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

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 $\gamma > 0$.

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

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

- At optimum

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

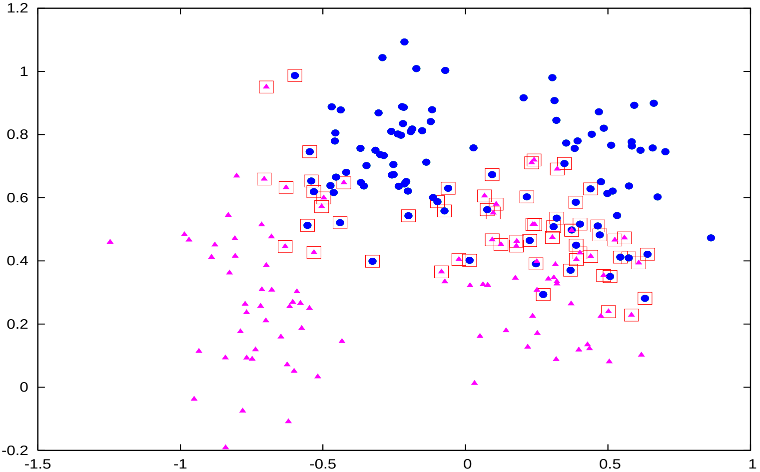
- Decision function

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

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

Support Vectors: More Important Data

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



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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

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

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

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

- 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

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

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

  See a rigorous discussion in Lin (2001)

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