Slide09

Haykin Chapter 6: Support-Vector Machines

CPSC 636-600
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Spring 2015

Note: Part of this lecture drew material from Ricardo Gutierrez-Osuna's Pattern Analysis lectures.

Introduction

- Support vector machine is a *linear machine* with some very nice properties.
- The basic idea of SVM is to construct a separating hyperplane where the *margin of separation* between positive and negative examples are maximized.
- Principled derivation: structural risk minimization
  - error rate is bounded by: (1) training error-rate and (2) VC-dimension of the model.
  - SVM makes (1) become zero and minimizes (2).

Optimal Hyperplane

For linearly separable patterns $\{(\mathbf{x}_i, d_i)\}_{i=1}^{N}$ (with $d_i \in \{+1, -1\}$):

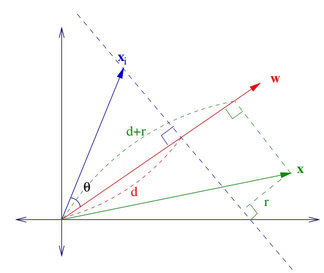
- The separating hyperplane is $\mathbf{w}^T\mathbf{x} + b = 0$:

$$\mathbf{w}^T\mathbf{x} + b \geq 0 \quad \text{for } d_i = +1$$

$$\mathbf{w}^T\mathbf{x} + b < 0 \quad \text{for } d_i = -1$$

- Let $\mathbf{w}_o$ be the optimal hyperplane and b_o the optimal bias.

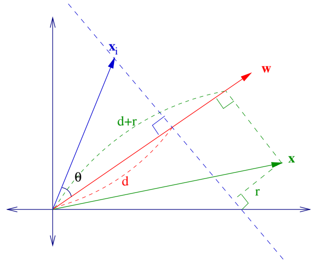
Distance to the Optimal Hyperplane



- From $\mathbf{w}_o^T\mathbf{x} = -b_o$, the distance from the origin to the hyperplane is calculated as

$$d = \|\mathbf{x}_i\| \cos(\mathbf{x}_i, \mathbf{w}_o) = \frac{-b_o}{\|\mathbf{w}_o\|}$$

Distance to the Optimal Hyperplane (cont'd)



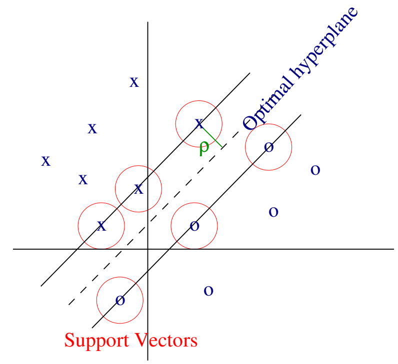
- The distance from an arbitrary point to the hyperplane can be calculated as:
  - When the point is in the positive area:

$$r = \|x\| \cos(\mathbf{x}, \mathbf{w}_o) - d = \frac{\mathbf{x}^T \mathbf{w}_o}{\|\mathbf{w}_o\|} + \frac{b_o}{\|\mathbf{w}_o\|} = \frac{\mathbf{x}^T \mathbf{w}_o + b_o}{\|\mathbf{w}_o\|}.$$

  - When the point is in the negative area:

$$r = d - \|x\| \cos(\mathbf{x}, \mathbf{w}_o) = -\frac{\mathbf{x}^T \mathbf{w}_o}{\|\mathbf{w}_o\|} - \frac{b_o}{\|\mathbf{w}_o\|} = -\frac{\mathbf{x}^T \mathbf{w}_o + b_o}{\|\mathbf{w}_o\|}.$$

Optimal Hyperplane and Support Vectors



- **Support vectors**: input points closest to the separating hyperplane.
- **Margin of separation** ρ: distance between the separating hyperplane and the closest input point.

Optimal Hyperplane and Support Vectors (cont'd)

- The optimal hyperplane is supposed to maximize the margin of separation ρ.
- With that requirement, we can write the conditions that $\mathbf{w}_o$ and b_o must meet:

$$\mathbf{w}_o^T \mathbf{x} + b_o \geq +1 \quad \text{for } d_i = +1$$

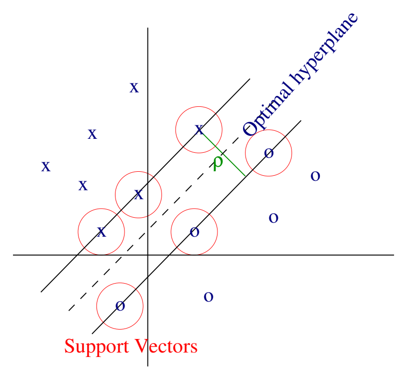
$$\mathbf{w}_o^T \mathbf{x} + b_o \leq -1 \quad \text{for } d_i = -1$$

  Note: $\geq +1$ and ≤ -1, and support vectors are those $\mathbf{x}^{(s)}$ where equality holds (i.e., $\mathbf{w}_o^T \mathbf{x}^{(s)} + b_o = +1$ or -1).

- Since $r = (\mathbf{w}_o^T \mathbf{x} + b_o)/\|\mathbf{w}_o\|$,

$$r = \begin{cases} 1/\|\mathbf{w}_o\| & \text{if } d = +1 \\ -1/\|\mathbf{w}_o\| & \text{if } d = -1 \end{cases}$$

Optimal Hyperplane and Support Vectors (cont'd)



- Margin of separation *between two classes* is

$$\rho = 2r = \frac{2}{\|\mathbf{w}_o\|}.$$

- Thus, maximizing the margin of separation *between two classes* is equivalent to minimizing the Euclidean norm of the weight $\mathbf{w}_o$!

Primal Problem: Constrained Optimization

For the training set $\mathcal{T} = \{(\mathbf{x}_i, d_i)\}_{i=1}^{N}$ find $\mathbf{w}$ and b such that

- they minimize a certain value ($1/\rho$) while satisfying a constraint (all examples are correctly classified):
  - Constraint: $d_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$ for $i = 1, 2, ..., N$.
  - Cost function: $\Phi(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w}$.

This problem can be solved using the *method of Lagrange multipliers* (see next two slides).

Mathematical Aside: Lagrange Multipliers

Turn a constrained optimization problem into an unconstrained optimization problem by absorbing the constraints into the cost function, weighted by the *Lagrange multipliers*.

Example: Find closest point on the circle $x^2 + y^2 = 1$ to the point $(2, 3)$ (adapted from Ballard, *An Introduction to Natural Computation*, 1997, pp. 119–120).

- Minimize $F(x, y) = (x-2)^2 + (y-3)^2$ subject to the constraint $x^2 + y^2 - 1 = 0$.
- Absorb the constraint into the cost function, after multiplying the *Lagrange multiplier* α:

$$F(x, y, \alpha) = (x-2)^2 + (y-3)^2 + \alpha(x^2 + y^2 - 1).$$

Lagrange Multipliers (cont'd)

Must find x, y, α that minimizes $F(x, y, \alpha) = (x-2)^2 + (y-2)^2 + \alpha(x^2 + y^2 - 1)$. Set the partial derivatives to 0, and solve the system of equations.

$$\frac{\partial F}{\partial x} = 2(x-2) + 2\alpha x = 0$$

$$\frac{\partial F}{\partial y} = 2(y-2) + 2\alpha y = 0$$

$$\frac{\partial F}{\partial \alpha} = x^2 + y^2 - 1 = 0$$

Solve for x and y in the 1st and 2nd, and plug in those to the 3rd equation

$$x = y = \frac{2}{1+\alpha}, \quad \text{so} \quad \left(\frac{2}{1+\alpha}\right)^2 + \left(\frac{2}{1+\alpha}\right)^2 = 1$$

from which we get $\alpha = 2\sqrt{2} - 1$. Thus, $(x, y) = (1/\sqrt{2}, 1/\sqrt{2})$.

Primal Problem: Constrained Optimization (cont'd)

Putting the constrained optimization problem into the Lagrangian form, we get (utilizing the Kunh-Tucker theorem)

$$J(\mathbf{w}, b, \alpha) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{N}\alpha_i\left[d_i(\mathbf{w}^T\mathbf{x}_i + b) - 1\right].$$

- From $\frac{\partial J(\mathbf{w},b,\alpha)}{\partial \mathbf{w}} = 0$:

$$\mathbf{w} = \sum_{i=1}^{N}\alpha_i d_i \mathbf{x}_i.$$

- From $\frac{\partial J(\mathbf{w},b,\alpha)}{\partial b} = 0$:

$$\sum_{i=1}^{N}\alpha_i d_i = 0$$

Primal Problem: Constrained Optimization (cont'd)

- Note that when the optimal solution is reached, the following condition must hold (Karush-Kuhn-Tucker complementary condition)

  $$\alpha_i \left[d_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right] = 0$$

  for all $i = 1, 2, ..., N$.

- Thus, *non-zero* α_is can be attained only when $\left[d_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right] = 0$, i.e., when the α_i is associated with a support vector $\mathbf{x}^{(s)}$!

- Other conditions include $\alpha_i \geq 0$.

Primal Problem: Constrained Optimization (cont'd)

- Plugging in $\mathbf{w} = \sum_{i=1}^N \alpha_i d_i \mathbf{x}_i$ and $\sum_{i=1}^N \alpha_i d_i = 0$ back into $J(\mathbf{w}, b, \alpha)$, we get the **dual problem**.

$$\begin{aligned}
J(\mathbf{w}, b, \alpha) &= \tfrac{1}{2}\mathbf{w}^T\mathbf{w} - \textstyle\sum_{i=1}^N \alpha_i \left[d_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right] \\
&= \tfrac{1}{2}\mathbf{w}^T\mathbf{w} - \textstyle\sum_{i=1}^N \alpha_i d_i \mathbf{w}^T \mathbf{x}_i \\
&\quad - b \textstyle\sum_{i=1}^N \alpha_i d_i + \sum_{i=1}^N \alpha_i \\
&\quad \Big\{ \text{noting } \mathbf{w}^T\mathbf{w} = \textstyle\sum_{i=1}^N \alpha_i d_i \mathbf{w}^T \mathbf{x}_i \\
&\quad \text{and from } \textstyle\sum_{i=1}^N \alpha_i d_i = 0 \Big\} \\
&= -\tfrac{1}{2} \textstyle\sum_{i=1}^N \alpha_i d_i \mathbf{w}^T \mathbf{x}_i + \sum_{i=1}^N \alpha_i \\
&= -\tfrac{1}{2} \textstyle\sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^N \alpha_i \\
&= Q(\alpha).
\end{aligned}$$

- So, $J(\mathbf{w}, b, \alpha) = Q(\alpha)$ ($\alpha_i \geq 0$).

- This results in the **dual problem** (next slide).

Dual Problem

- Given the training sample $\{(\mathbf{x}_i, d_i)\}_{i=1}^N$, find the Lagrange multipliers $\{\alpha_i\}_{i=1}^N$ that maximize the objective function:

  $$Q(\alpha) = -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^N \alpha_i$$

  subject to the constraints

  - $\sum_{i=1}^N \alpha_i d_i = 0$
  - $\alpha_i \geq 0$ for all $i = 1, 2, ..., N$.

- The problem is stated entirely in terms of the training data $(\mathbf{x}_i, d_i)$, and the dot products $\mathbf{x}_i^T \mathbf{x}_j$ play a key role.

Solution to the Optimization Problem

Once all the optimal Lagrange mulitpliers $\alpha_{o,i}$ are found, $\mathbf{w}_o$ and b_o can be found as follows:

$$\mathbf{w}_o = \sum_{i=1}^N \alpha_{o,i} d_i \mathbf{x}_i$$

and from $\mathbf{w}_o^T \mathbf{x}_i + b_o = d_i$ when $\mathbf{x}_i$ is a support vector:

$$b_o = d^{(s)} - \mathbf{w}_o^T \mathbf{x}^{(s)}$$

Note: calculation of final estimated function does not need any explicit calculation of $\mathbf{w}_o$ since they can be calculated from the dot product between the input vectors!

$$\mathbf{w}_o^T \mathbf{x} = \sum_{i=1}^N \alpha_{o,i} d_i \mathbf{x}_i^T \mathbf{x}$$

Margin of Separation in SVM and VC Dimension

Statistical learning theory shows that it is desirable to reduce both the error (empirical risk) and the VC dimension of the classifier.

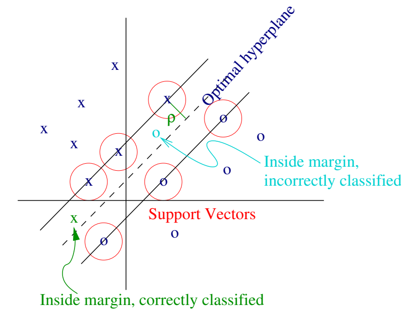
- Vapnik (1995, 1998) showed: Let D be the diameter of the smallest ball containing all input vectors $\mathbf{x}_i$. The set of optimal hyperplanes defined by $\mathbf{w}_o^T\mathbf{x} + b_o = 0$ has a VC dimension h bounded from above as

  $$h \leq min\left\{ \left\lceil \frac{D^2}{\rho^2} \right\rceil, m_0 \right\} + 1$$

  where $\lceil \cdot \rceil$ is the ceiling, ρ the margin of separation equal to $2/\|\mathbf{w}_o\|$, and m_0 the dimensionality of the input space.

- The implication is that the VC dimension can be controlled independently of m_0, by choosing an appropriate (large) ρ!

Soft-Margin Classification



- Some problems can violate the condition:

  $$d_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$$

- We can introduce a new set of variables $\{\xi_i\}_{i=1}^N$:

  $$d_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i$$

  where ξ_i is called the *slack variable*.

Soft-Margin Classification (cont'd)

- We want to find a separating hyperplane that minimizes:

  $$\Phi(\xi) = \sum_{i=1}^{N} I(\xi_i - 1)$$

  where $I(\xi) = 0$ if $\xi \leq 0$ and 1 otherwise.

- Solving the above is NP-complete, so we instead solve an approximation:

  $$\Phi(\xi) = \sum_{i=1}^{N} \xi_i$$

- Furthermore, the weight vector can be factored in:

  $$\Phi(\mathbf{x}, \xi) = \underbrace{\frac{1}{2}\mathbf{w}^T\mathbf{w}}_{\text{Controls VC dim}} + \underbrace{C\sum_{i=1}^{N}\xi_i}_{\text{Controls error}}$$

  with a control parameter C.

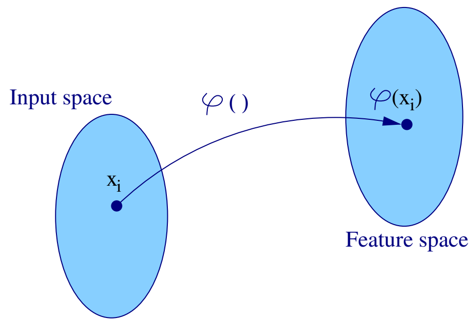
Soft-Margin Classification: Solution

- Following a similar route involving Lagrange multipliers, and a more restrictive condition of $0 \leq \alpha_i \leq C$, we get the solution:

  $$\mathbf{w}_o = \sum_{i=1}^{N_s} \alpha_{o,i} d_i \mathbf{x}_i$$

  $$b_o = d_i(1 - \xi_i) - \mathbf{w}_o^T\mathbf{x}_i$$

Nonlinear SVM



- Nonlinear mapping of an input vector to a high-dimensional *feature space* (exploit Cover's theorem)
- Construction of an optimal hyperplane for separating the features identified in the above step.

Inner-Product Kernel

- Input $\mathbf{x}$ is mapped to $\boldsymbol{\varphi}(\mathbf{x})$.
- With the weight $\mathbf{w}$ (including the bias b), the decision surface in the feature space becomes (assume $\varphi_0(\mathbf{x}) = 1$):

$$\mathbf{w}^T \boldsymbol{\varphi}(\mathbf{x}) = 0$$

- Using the steps in linear SVM, we get

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i d_i \boldsymbol{\varphi}(\mathbf{x}_i)$$

- Combining the above two, we get the decision surface

$$\sum_{i=1}^{N} \alpha_i d_i \boldsymbol{\varphi}^T(\mathbf{x}_i)\boldsymbol{\varphi}(\mathbf{x}) = 0.$$

Inner-Product Kernel (cont'd)

- The inner product $\boldsymbol{\varphi}^T(\mathbf{x})\boldsymbol{\varphi}(\mathbf{x}_i)$ is between two vectors in the feature space.
- The calculation of this inner product can be simpified by use of a *inner-product kernel* $K(\mathbf{x}, \mathbf{x}_i)$:

$$K(\mathbf{x}, \mathbf{x}_i) = \boldsymbol{\varphi}^T(\mathbf{x})\boldsymbol{\varphi}(\mathbf{x}_i) = \sum_{j=0}^{m_1} \varphi_j(\mathbf{x})\varphi_j(\mathbf{x}_i)$$

  where m_1 is the dimension of the feature space. (Note: $K(\mathbf{x}, \mathbf{x}_i) = K(\mathbf{x}_i, \mathbf{x})$.)
- So, the optimal hyperplane becomes:

$$\sum_{i=1}^{N} \alpha_i d_i K(\mathbf{x}, \mathbf{x}_i) = 0$$

Inner-Product Kernel (cont'd)

- **Mercer's theorem** states that $K(\mathbf{x}, \mathbf{x}_i)$ that follow certain conditions (continuous, symmetric, positive semi-definite) can be expressed in terms of an inner-product in a nonlinearly mapped feature space.
- Kernel function $K(\mathbf{x}, \mathbf{x}_i)$ allows us to calculate the inner product $\boldsymbol{\varphi}^T(\mathbf{x})\boldsymbol{\varphi}(\mathbf{x}_i)$ in the mapped feature space without any explicit calculation of the mapping function $\boldsymbol{\varphi}(\cdot)$.

Examples of Kernel Functions

- Linear: $K(\mathbf{x}, \mathbf{x}_i) = \mathbf{x}^T \mathbf{x}_i$.
- Polynomial: $K(\mathbf{x}, \mathbf{x}_i) = (\mathbf{x}^T \mathbf{x}_i + 1)^p$.
- RBF: $K(\mathbf{x}, \mathbf{x}_i) = \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{x} - \mathbf{x}_i\|^2\right)$.
- Two-layer perceptron: $K(\mathbf{x}, \mathbf{x}_i) = \tanh\left(\beta_0 \mathbf{x}^T \mathbf{x}_i + \beta_1\right)$ (for some β_0 and β_1).

Kernel Example

- Expanding

$$K(\mathbf{x}, \mathbf{x}_i) = (1 + \mathbf{x}^T \mathbf{x}_i)^2$$

with $\mathbf{x} = [x_1, x_2]^T, \mathbf{x}_i = [x_{i1}, x_{i2}]^T$,

$$\begin{aligned} K(\mathbf{x}, \mathbf{x}_i) &= 1 + x_1^2 x_{i1}^2 + 2x_1 x_2 x_{i1} x_{i2} \\ &\quad + x_2^2 x_{i2}^2 + 2x_1 x_{i1} + 2x_2 x_{i2} \\ &= [1, x_1^2, \sqrt{2}x_1 x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2] \\ &\quad [1, x_{i1}^2, \sqrt{2}x_{i1} x_{i2}, x_{i2}^2, \sqrt{2}x_{i1}, \sqrt{2}x_{i2}]^T \\ &= \boldsymbol{\varphi}(\mathbf{x})^T \boldsymbol{\varphi}(\mathbf{x}_i), \end{aligned}$$

where $\boldsymbol{\varphi}(\mathbf{x}) = [1, x_1^2, \sqrt{2}x_1 x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2]^T$.

Nonlinear SVM: Solution

- The solution is basically the same as the linear case, where $\mathbf{x}^T \mathbf{x}_i$ is replaced with $K(\mathbf{x}, \mathbf{x}_i)$, and an additinoal constraint that $\alpha \leq C$ is added.

Nonlinear SVM Summary

Project input to high-dimensional space to turn the problem into a linearly separable problem.

Issues with a projection to higher dimensional feature space:

- **Statistical problem**: Danger of invoking curse of dimensionality and higher chance of overfitting
  - Use large margins to reduce VC dimension
- **Computational problem**: computational overhead for calculating the mapping $\boldsymbol{\varphi}(\cdot)$:
  - Solve by using the kernel trick.