

Slide09

Haykin Chapter 6: Support-Vector Machines

CPSC 636-600

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

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Optimal Hyperplane

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

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

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

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

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

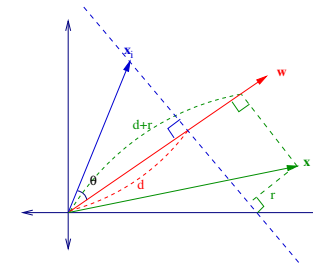
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Introduction

- 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).

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Distance to the Optimal Hyperplane

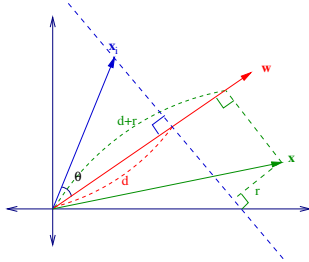


- From $\mathbf{w}_o^T \mathbf{x} = -b_o$, the distance from the origin to the hyperplane is calculated as

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

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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:

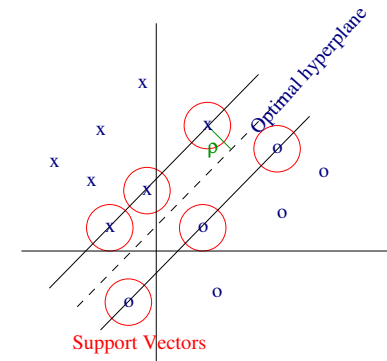
$$r = \|x\| \cos(\mathbf{x}, \mathbf{w}_o) - d = \frac{\mathbf{x}^T \mathbf{w}_o}{\|\mathbf{w}_o\|} + \frac{b_o}{\|\mathbf{w}_o\|} = \frac{\mathbf{x}^T \mathbf{w}_o + b_o}{\|\mathbf{w}_o\|}.$$

- When the point is in the negative area:

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

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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.

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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:

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

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

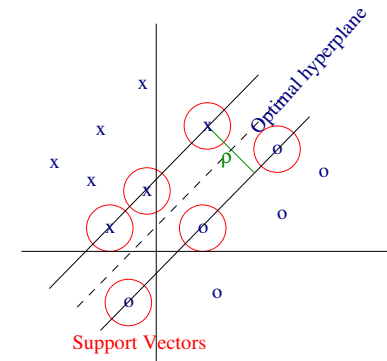
Note: $\geq +1$ and ≤ -1 , and support vectors are those $\mathbf{x}^{(s)}$ where equality holds (i.e., $\mathbf{w}_o^T \mathbf{x}^{(s)} + b_o = +1$ or -1).

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

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

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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 !

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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 $i = 1, 2, \dots, N$.
 - 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).

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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

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

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

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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 :

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

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Primal Problem: Constrained Optimization (cont'd)

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

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

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

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

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Primal Problem: Constrained Optimization (cont'd)

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

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

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

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

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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 $i = 1, 2, \dots, N$.
- 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.

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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**.

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

- So, $J(\mathbf{w}, b, \alpha) = Q(\alpha)$ ($\alpha_i \geq 0$).
- This results in the **dual problem** (next slide).

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Solution to the Optimization Problem

Once all the optimal Lagrange multipliers $\alpha_{o,i}$ 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!

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

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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 !

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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:

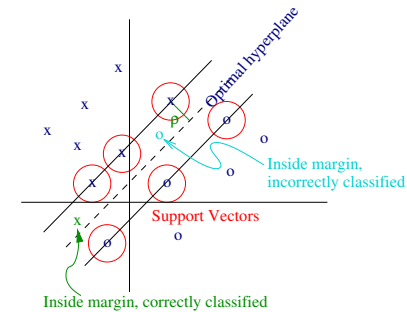
$$\Phi(\xi) = \sum_{i=1}^N \xi_i$$

- Furthermore, the weight vector can be factored in:

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

with a control parameter C . 19

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*.

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Soft-Margin Classification: Solution

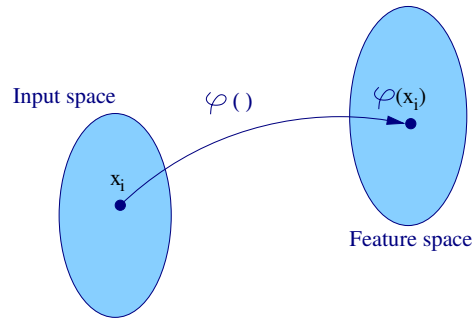
- Following a similar route involving Lagrange multipliers, and a more restrictive condition of $0 \leq \alpha_i \leq C$, we get the solution:

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

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

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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.

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Inner-Product Kernel (cont'd)

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

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

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:

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

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Inner-Product Kernel

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

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

- Using the steps in linear SVM, we get

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

- Combining the above two, we get the decision surface

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

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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 $\varphi^T(\mathbf{x})\varphi(\mathbf{x}_i)$ in the mapped feature space without any explicit calculation of the mapping function $\varphi(\cdot)$.

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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: $K(\mathbf{x}, \mathbf{x}_i) = \tanh(\beta_0 \mathbf{x}^T \mathbf{x}_i + \beta_1)$
(for some β_0 and β_1).

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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 additional constraint that $\alpha \leq C$ is added.

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

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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.

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