CS559 Machine Learning
Support Vector Machine

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Week 14

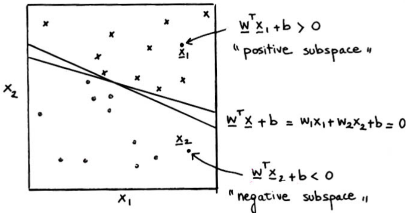
Outline

- Linear classifier, large margin, SVM
- Non-separable case, slack variable
- Non-linearity, kernels

Linear classifier, large margin, SVM

Linear Classifier

- Linear classifiers construct
  linear decision boundaries(hyperplanes) that try to separate the data into different classes as well as possible.



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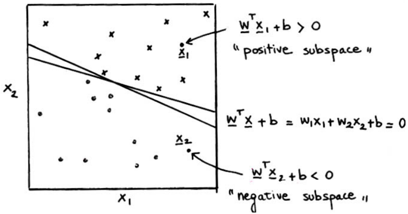

- Classification Rule (**the Perceptron model**):

$$\text{Input: } \mathbf{x} \in \mathbb{R}^d$$

$$\text{Output: } \operatorname{sign}(\mathbf{w}^\top \mathbf{x} + b)$$

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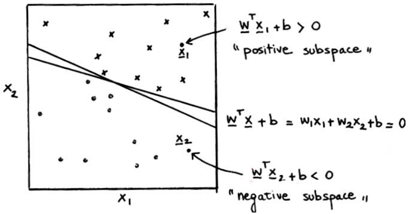

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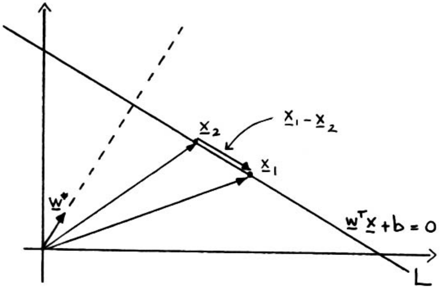
- The classifier computes a linear combination of the input features, and return the sign.

Some Vector Algebra

- Hyperplane L: $f(\mathbf{x}) = (\mathbf{w}^\top \mathbf{x} + b) = 0$, when $\mathbf{x} \in \mathbb{R}^2$, $f(\mathbf{x})$ is a line.



Property 1

- Consider any two points x_1, x_2, lying on hyperplane L:

$$\begin{matrix} \mathbf{w}^T\mathbf{x}_1 + b = 0 \\ \mathbf{w}^T\mathbf{x}_2 + b = 0 \end{matrix} \rightarrow \mathbf{w}^\top(\mathbf{x}_1 - \mathbf{x}_2) = 0$$

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- Note 1: All vectors here are column vectors.
- Note 2: Dot product (inner product) of two vectors $\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^\top\mathbf{b} = ||\mathbf{a}|| \times ||\mathbf{b}|| \times \cos\alpha$ where α is the angle between a and b.

Property 2

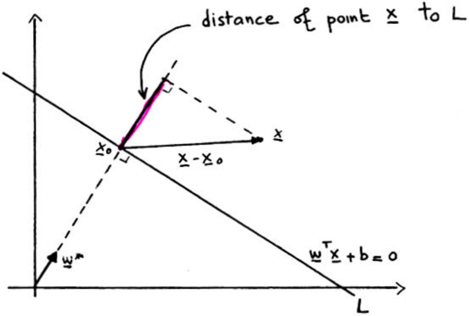
- For any point $\mathbf{x}_0$ on L:

$$\mathbf{w}^\top \mathbf{x}_0 + b = 0$$

Thus:

$$\mathbf{w}^\top \mathbf{x}_0 = -b$$

Property 3



The signed distance of any point $\mathbf{x}$ to L is:

$$(\mathbf{w}^*)^\top(\mathbf{x}-\mathbf{x}_0) = \frac{\mathbf{w}^\top}{||\mathbf{w}||}(\mathbf{x}-\mathbf{x}_0) =$$

$$\frac{1}{||\mathbf{w}||}(\mathbf{w}^\top\mathbf{x}-\mathbf{w}^\top\mathbf{x}_0) = \frac{1}{||\mathbf{w}||}(\mathbf{w}^\top\mathbf{x}+b)$$

Recall: perceptron classifier

Objective: Find a separating hyperplane that correctly classifies all input patterns.

- There are two types of error:

$$y_i = 1 \text{ and } \mathbf{w}^\top \mathbf{x}_i + b < 0$$

$$y_i = -1 \text{ and } \mathbf{w}^\top \mathbf{x}_i + b > 0$$

- Thus, for all misclassified points:

$$y_i(\mathbf{w}^\top \mathbf{x}_i + b) < 0$$

- To reduce the number of misclassified points, the goal is to minimize:

$$D(\mathbf{w}, b) = -\sum_{i \in M} y_i(\mathbf{w}^\top \mathbf{x}_i + b)$$

where M indexes the set of misclassified points.

Problems with perceptron classifier

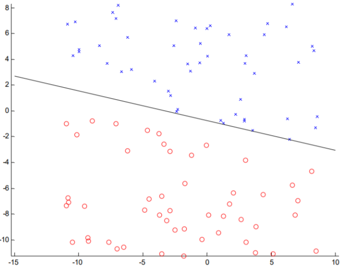


Figure: [A. Zisserman, C19, 2015]

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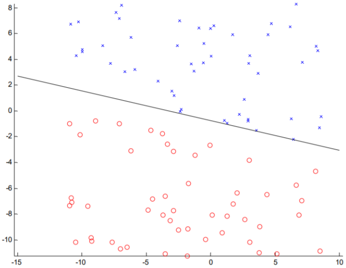

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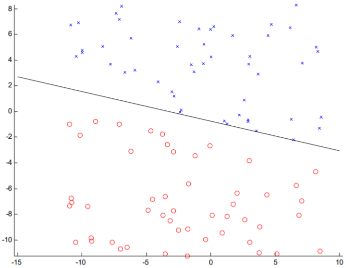

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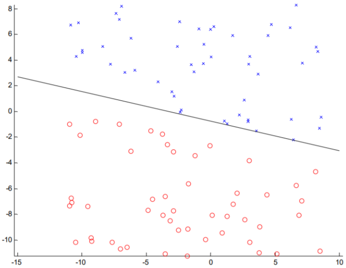

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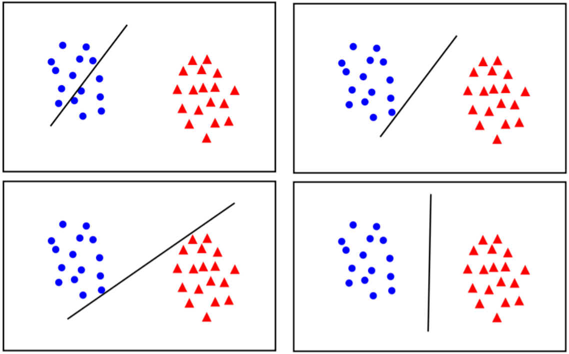
- If the data is linearly separable, then the algorithm will converge.
- Convergence can be slow.
- Separating line close to training data.
- Prefer a larger margin for better generalization.

What's the best $\mathbf{w}$



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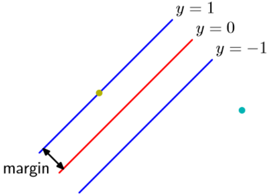
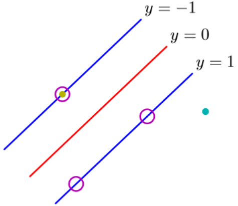
Maximum margin solution: most stable under perturbations of the inputs.

Largest Margin Hyperplanes

Goal: Find the hyperplane that separates the two classes and maximizes the distance to the closest points from either class.

- Such distance is called margin.





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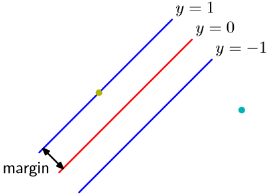

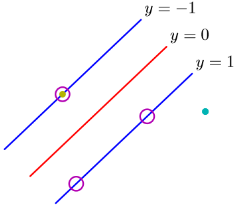

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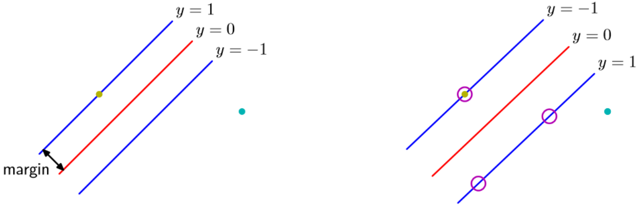

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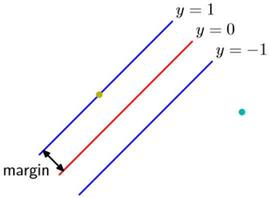

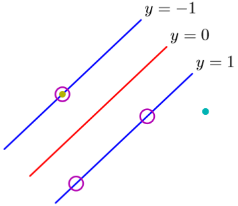

- The added constraint:
  - Provide a unique solution to the separating hyperplane problem;
  - Maximizing the margin between the two classes on the training data gives better classification performance on test data.

The Training Data

For two classes:

$$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ..., (\mathbf{x}_N, y_N)$$

$$\mathbf{x}_i \in \mathbf{R}^d$$
$$y_i = \{-1, +1\}$$

We need to formalize the largest margin criterion.

Formulation

Consider the following optimization problem:

$$\max_{\mathbf{w},b} 2C$$

$$\text{subject to } \frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq C \quad i = 1, ..., N$$

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- This is a quadratic (convex) optimization problem subject to linear constraints and there is a unique minimum

Lagrange Multipliers

- Lagrange multiplier allows to take the constraints within the function to be minimized (Recall we briefly introduced Lagrange multipliers in PCA and FLD). Two reasons for doing this:
    1. The constraints will be replaced by constraints on the Lagrange multipliers themselves, which are easier to handle.
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- We introduce the Lagrange multipliers $\alpha_i \geq 0,\ i = 1, ..., N$, one for each of the inequality constraints.
- Recall the rule: for constraints of the form $C_i \geq 0$, the constraint equations are multiplied by Lagrange multipliers and subtracted from the objective function, to form the Lagrangian.

Lagrange Multipliers

- We then obtain the Lagrangian: (also called "primal form"):

$$L_p = \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{N} \alpha_i [y_i(\mathbf{w}^\top \mathbf{x}_i + b) - 1]$$

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- Setting the derivatives to zero gives:

$$\frac{\partial L_p}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i \qquad (1)$$

$$\frac{\partial L_p}{\partial b} = -\sum_{i=1}^{N} \alpha_i y_i = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i y_i = 0 \qquad (2)$$

Primal Form

- This is the primal form of the optimization problem.
- We could also solve the optimization problem by solving for the dual of the original problem
- What is the dual form?

Dual Form

Substituting eq. 1 and 2 in L_p gives:

$$
\begin{aligned}
L_D &= \frac{1}{2}\Big(\sum_{i=1}^{N}\alpha_i y_i \mathbf{x}_i\Big)\Big(\sum_{k=1}^{N}\alpha_k y_k \mathbf{x}_k\Big) - \sum_{i=1}^{N}\alpha_i\Big[y_i\Big(\mathbf{x}_i^\top\big(\sum_{k=1}^{N}\alpha_k y_k \mathbf{x}_k\big) + b\Big) - 1\Big] \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k y_i y_k \mathbf{x}_i^\top \mathbf{x}_k - \sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k y_i y_k \mathbf{x}_i^\top \mathbf{x}_k - b\underbrace{\sum_{i=1}^{N}\alpha_i y_i}_{=0} + \sum_{i=1}^{N}\alpha_i \\
&= \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k y_i y_k \mathbf{x}_i^\top \mathbf{x}_k
\end{aligned}
$$

subject to $\alpha_i \geq 0, \sum_{i=1}^{N}\alpha_i y_i = 0$

The Lagrangian Dual Form

- The solution is obtained by maximizing L_D with respect to the α_i, i.e., $\max_\alpha \min_{\mathbf{w},b} L_p$.

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- The solution is obtained by maximizing L_D with respect to the α_i, i.e., $\max_\alpha \min_{\mathbf{w},b} L_p$.
- It can be shown that the solution must satisfy the conditions:

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$
$$\sum_{i=1}^{N} \alpha_i y_i = 0 \tag{3}$$

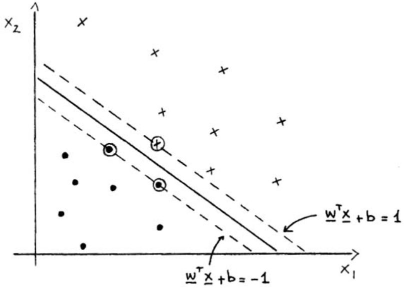
And the Karush-Kuhn-Tucker (KKT) conditions:

$$\begin{aligned} \alpha_i &\geq 0 \\ y_i(\mathbf{w}^\top \mathbf{x}_i + b) - 1 &\geq 0 \\ \alpha_i \left[y_i(\mathbf{w}^\top \mathbf{x}_i + b) - 1 \right] &= 0 \quad \forall i = 1, ..., N \end{aligned}$$

The complementary slackness

$$\alpha_i \big[y_i(\mathbf{w}^\top \mathbf{x}_i + b) - 1 \big] = 0 \quad \forall i = 1, ..., N$$

- If $\alpha_i > 0$, then $y_i(\mathbf{w}^\top \mathbf{x}_i + b) = 1$, that is $\mathbf{x}_i$ is on the boundary of the margin.
- If $y_i(\mathbf{w}^\top \mathbf{x}_i + b) > 1$, $\mathbf{x}_i$ is not on the boundary of the margin, and $\alpha_i = 0$



Dual Form

- The solution vector $\mathbf{w}$ is: $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$. Thus: The solution is defined as a linear combination of those $\mathbf{x}_i$ for which $\alpha_i > 0$. Such $\mathbf{x}_i$ are the points on the boundary of the margin. They are called **SUPPORT VECTORS**. We have three support vectors in the above example.
- To obtain the value of b: solve $\alpha_i \left[y_i(\mathbf{w}^\top \mathbf{x}_i + b) - 1 \right] = 0$ for any of the support vectors.
- The largest margin hyperplane gives a function:
  $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$ for classifying new observations
  $\hat{y} = \text{sign}(f(\mathbf{x}))$

Observations

- The support vectors are the critical elements of the training set. They lie closest to the decision boundary.
- Only the support vectors affect the prediction.
- However, the identification of the support vectors requires the use of all the training data.
- Although none of the training observations fall within the margin (by construction), this will not necessarily be the case of test data. (The intuition is that a large margin on the training data indicates a good separation of the two classes and therefore a good separation on the test data as well)

Non-separable case

Summary for linear separable case

- Training data: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ..., (\mathbf{x}_N, y_N)$, $\mathbf{x}_i \in \mathbb{R}^d, y_i \in \{-1, +1\}$
- When the two classes are linearly separable, we can find a function $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$ with $y_i f(\mathbf{x}_i) > 0 \ \forall i$
- In particular, we can find the hyperplane that creates the largest margin between the training points.
- The optimization problem captures this concept

$$\max_{\mathbf{w}, b} 2C$$

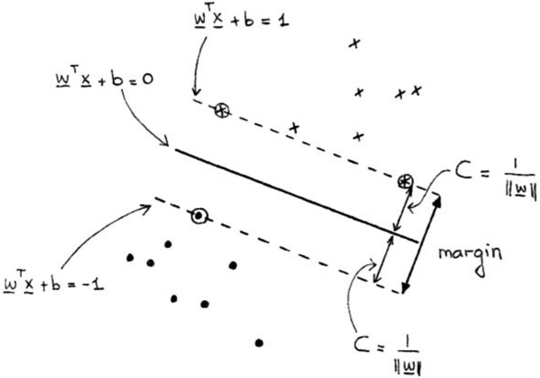
$$\text{subject to } \frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq C \quad i = 1, ..., N$$

- It can be more conveniently rewritten as below

$$\min_{\mathbf{w}, b} \frac{1}{2} ||\mathbf{w}||^2$$

$$\text{subject to } y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad i = 1, ..., N$$

Geometric perspective



The Non-separable Case

- Suppose now the classes overlap. We can still maximize C, but allow for some points to be on the wrong side of the margin.
- We need to modify the constraints we had for the separable case: $\frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq C \quad i = 1, ..., N$.
- To achieve this goal, we define N slack variables:

$$\xi_1, \xi_2, ..., \xi_N$$

- Then a natural way to modify the constraints above is:

$$\frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq C(1 - \xi_i) \quad i = 1, ..., N$$

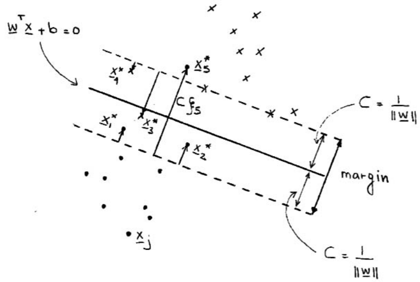
with $\xi_i \geq 0 \quad \forall i$

The Non-separable Case

- Idea of the formulation: ξ_i is the proportional amount by which the prediction $f(\mathbf{x}_i)$ is on the wrong side of the margin.
- Note: $C(1-\xi_i) = C - C\xi_i$

Slack Variables

- A geometric perspective:



- The points $(\mathbf{x}_1^*, \mathbf{x}_2^*, \mathbf{x}_3^*, \mathbf{x}_4^*, \mathbf{x}_5^*)$ are on the wrong side of their margin.
- Point $\mathbf{x}_i^*$ is on the wrong side of its margin by an amount $C\xi_i$
- $0 < \xi_i \leq 1$: inside the margin, correct side of hyperplane. $C\xi_i \leq C$, Margin Violation
- $\xi_i > 1$: $C\xi_i > C$, misclassification

Slack Variables–soft margin

- We normalize $\mathbf{w}$ and consider soft-margin version:

$$\min_{\mathbf{w},b} \frac{||\mathbf{w}||^2}{2} + \gamma \sum_{i=1}^{N} \xi_i$$

subject to: $y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \quad i = 1, ..., N$

with $\xi_i \geq 0 \quad \forall i$

- Goal: maximize the margin while softly penalizing points that lie on the wrong side of margin boundary.

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- γ is a parameter to be chosen by the user. A larger γ corresponds to assigning a higher penalty to errors.
- We have obtained a quadratic optimization problem with linear constraints. We will solve it using Lagrange multipliers.

Lagrange Multipliers for Slack Variables

$$\min_{\mathbf{w},b} \frac{||\mathbf{w}||^2}{2} + \gamma \sum_{i=1}^{N} \xi_i$$

subject to: $y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \quad i = 1, ..., N$

with $\xi_i \geq 0 \quad \forall i$

- Introducing the Lagrange multipliers α_i and μ_i (one for each constraint), gives the following Lagrange (primal) function:

$$L_p = \frac{1}{2}||\mathbf{w}||^2 + \gamma \sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i \left[y_i(\mathbf{w}^\top \mathbf{x}_i + b) - (1 - \xi_i) \right] - \sum_{i=1}^{N} \mu_i \xi_i$$

- Our objective is:

$$\min_{\mathbf{w},b,\xi_i} L_p$$

Lagrange Multipliers Solution

- Setting the respective derivatives to zero gives:

$$\frac{\partial L_p}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i \tag{4}$$

$$\frac{\partial L_p}{\partial b} = -\sum_{i=1}^{N} \alpha_i y_i = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i y_i = 0 \tag{5}$$

$$\frac{\partial L_p}{\partial \xi_i} = \gamma - \alpha_i - \mu_i \quad \forall i \Rightarrow \alpha_i = \gamma - \mu_i \quad \forall i \tag{6}$$

along with the positivity constraints $\alpha_i, \mu_i, \xi_i \geq 0 \quad \forall i$

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- Substituting eq. 4, 5, 6 in L_p, we obtain the so called dual objective function:

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^{\top} \mathbf{x}_j$$

Lagrange Multipliers Solution

The solution is obtained by maximizing L_D w.r.t the α_i, subject to:(similar to the separable case, but the constraints are different)

$$\sum_i^N \alpha_i y_i = 0, \quad 0 \leq \alpha_i \leq \gamma$$

Lagrange Multiplier Solution

It can be shown that the solution must satisfy the conditions:

$$\mathbf{w} = \sum_{i}^{N} \alpha_i y_i \mathbf{x}_i \tag{7}$$

$$\sum_{i}^{N} \alpha_i y_i = 0 \tag{8}$$

$$\alpha_i = \gamma - \mu_i, \quad \forall i \tag{9}$$

$$\tag{10}$$

Also the KKT conditions: (complementary slackness)

$$\alpha_i \left[y_i(\mathbf{w}^\top \mathbf{x}_i + b) - (1 - \xi_i) \right] = 0, \quad \forall i \tag{11}$$

$$\mu_i \xi_i = 0 \ \ \forall i \tag{12}$$

$$y_i(\mathbf{w}^\top \mathbf{x}_i + b) - (1 - \xi_i) \geq 0 \ \ \forall i \tag{13}$$

along with the positivity constraints $\alpha_i, \mu_i, \xi_i \geq 0 \ \ \forall i$

Lagrange Multipliers Solution

- From 7, the solution is $\mathbf{w} = \sum_i^N \alpha_i y_i \mathbf{x}_i$. From 11, $\alpha_i > 0$ when constraint 13 are exactly met, i.e., $y_i(\mathbf{w}^\top \mathbf{x}_i + b) - (1 - \xi_i) = 0$

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- We have two kinds of support vectors:
  - If $\alpha_i < \gamma$, then $\mu_i > 0$, implies $\xi_i = 0$, such point $\mathbf{x}_i$ lie on the margin.
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$$\hat{y} = \text{sign}(f(\mathbf{x})) = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$$

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- Need to tune γ.

Optimization

- A constrained optimization problem over $\mathbf{w}$ and ξ

$$\min_{\mathbf{w},b} \frac{||\mathbf{w}||^2}{2} + \gamma \sum_{i=1}^{N} \xi_i$$

subject to: $y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \quad i = 1, ..., N$

- The constraint can be written more concisely as $y_i f(\mathbf{x}_i) \geq 1 - \xi_i$, together with $\xi_i > 0$ is equivalent to

$$\xi = \max(0, 1 - y_i f(\mathbf{x}_i))$$

- Hence the learning problem is equivalent to the unconstrained optimization problem over $\mathbf{w}$:

$$\min_{\mathbf{w},b} \frac{||\mathbf{w}||^2}{2} + \gamma \sum_{i=1}^{N} \max(0, 1 - y_i f(\mathbf{x}_i))$$

Loss function

$$\min_{\mathbf{w},b} \frac{||\mathbf{w}||^2}{2} + \gamma \sum_{i=1}^{N} \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{Hinge loss}}$$

- $y_i f(\mathbf{x}_i) > 1$: points outside margin. No contribution to loss
- $y_i f(\mathbf{x}_i) = 1$: points on margin. No contribution to loss (hard margin case)
- $y_i f(\mathbf{x}_i) < 1$: points violates margin constraints. Contribute to loss.

Hinge Loss

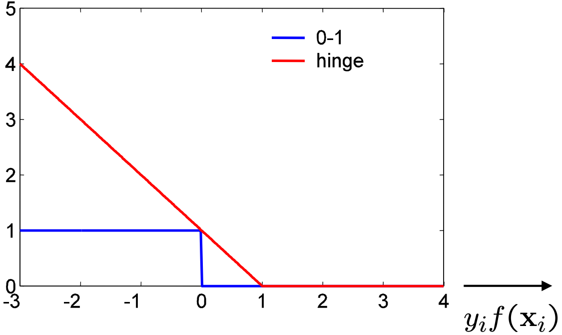

Figure: Hinge loss vs 0-1 loss

An approximation to the 0-1 loss.

Implementation

- Solving the Quadratic Programming Problems (slow)
- Use an interior point method that uses Newton-like iterations to find a solution of the Karush–Kuhn–Tucker conditions of the primal and dual problems
- Platt's sequential minimal optimization (SMO) algorithm
- Stochastic sub-gradient descent algorithms.

Primal vs dual formulation

- Primal problem: $\mathbf{w} \in R^{M-1}, b \in R$

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- Dual form only involve $\mathbf{x}_i^T \mathbf{x}_j$.

Primal vs dual formulation

- Primal version of classifier:

$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

- Dual version of classifier:

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- At first sight, dual form requires all training data points $\mathbf{x}_i$, however, many of α_i are zero, only **support vectors** matters.

Non-linearity, kernels

Non-linear SVM

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- One major observation (look at the dual objective function obtained earlier):

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- The only way in which the data appear in the training problem is in the form of dot products.

Non-linear SVM

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Non-linear SVM

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- From $\mathbf{w} = \sum_i^N \alpha_i y_i \mathbf{x}_i$, the solution function can be written as:

$$
\begin{aligned}
f(\mathbf{x}) &= \mathbf{w}^\top \mathbf{x} + b \\
&= \sum_{i=1}^{N_s} \alpha_i y_i \mathbf{x}_i^\top \mathbf{x} + b \\
&= \sum_{i=1}^{N_s} \alpha_i y_i < \mathbf{x}_i, \mathbf{x} > +b
\end{aligned}
$$

where N_s is the number of support vectors.
$\Rightarrow$Also in the prediction function, the data appear in the form of dot products where the $(\mathbf{x}_i)$s are the support vectors.

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- Suppose we map the data to some high dimension Euclidean space using a mapping Φ:

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  usually $h > d$

- The idea is to enlarge the input space to achieve better training class separation.
- In general, linear boundaries in the enlarged space translate to nonliear boundaries in the original space (true for any nonlinear mapping Φ)

Mapping

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- The training algorithm would only depend on the data through dot products in $\mathbb{R}^h$, i.e., $< \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) >$ where $\Phi(\mathbf{x}_i) \in \mathbb{R}^h$.
- Suppose we have a function (called **kernel function**) K that computes such dot products in the transformed space:

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- Replace $< \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) >$ with $K(\mathbf{x}_i, \mathbf{x}_j)$ everywhere in the training algorithm.
- Example of K: $K(\mathbf{x}_i, \mathbf{x}_j) = e^{\frac{-||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma^2}}$ (Gaussian kernel)

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- It achieves this objective in roughly the same amount of time it would take to train on the un-mapped data.
- In testing phase, given the test points $\mathbf{x}$:

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\begin{aligned}
f(x) &= \sum_{i=1}^{N_s} \alpha_i y_i < \mathbf{x}_i, \mathbf{x} > + b \\
&= \sum_{i=1}^{N_s} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b
\end{aligned}
$$

where $\mathbf{x}_i$ are the support vectors and N_s is the number of support vectors.

Mapping

- The algorithm constructs a linear support vector machine in $\mathbb{R}^h$.
- It achieves this objective in roughly the same amount of time it would take to train on the un-mapped data.
- In testing phase, given the test points $\mathbf{x}$:

$$f(x) = \sum_{i=1}^{N_s} \alpha_i y_i < \mathbf{x}_i, \mathbf{x} > + b$$
$$= \sum_{i=1}^{N_s} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b$$

  where $\mathbf{x}_i$ are the support vectors and N_s is the number of support vectors.
- The fact that, through the kernel function K, we can work with vectors in input space, without even knowing the mapping function Φ is known as the "**kernel trick**".

Example - kernel functions

Example: an allowed kernel for which we can construct the mapping Φ

- Training data are vectors in $\mathbb{R}^2$.

Example - kernel functions

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Example - kernel functions

Example: an allowed kernel for which we can construct the mapping Φ

- Training data are vectors in $\mathbb{R}^2$.
- Suppose we choose $K(\mathbf{x}_i, \mathbf{x}_j) = (<\mathbf{x}_i, \mathbf{x}_j>)^2$.
- We can find a mapping

$$\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^h$$

such that $(<\mathbf{x}_i, \mathbf{x}_j>)^2 = <\Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j)>$

- One such mapping is:

$$\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

defined as

$$\Phi(\mathbf{x}) = \begin{pmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{pmatrix}$$

where $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

Example - kernel functions

- We can verify that this is indeed the case:

$$
\begin{aligned}
K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}, \mathbf{y})^2 &= (x_1 y_1 + x_2 y_2)^2 \\
&= x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 y_1 x_2 y_2
\end{aligned}
$$

$$
\begin{aligned}
< \Phi(\mathbf{x}), \Phi(\mathbf{y}) > &= \Phi(\mathbf{x})^\top \Phi(\mathbf{y}) \\
&= (x_1^2, \sqrt{2} x_1 x_2, x_2^2) \begin{pmatrix} y_1^2 \\ \sqrt{2} y_1 y_2 \\ y_2^2 \end{pmatrix} \\
&= x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 y_1 x_2 y_2
\end{aligned}
$$

- Note: in general neither the mapping Φ nor the space $\mathbb{R}^h$ are unique for a given kernel.

Which functions are allowable as kernels?

- As long as kernel K is positive definite, then there always exists the mapping Φ. (Mercer theorem)

Which functions are allowable as kernels?

- As long as kernel K is positive definite, then there always exists the mapping Φ. (Mercer theorem)
- Two popular choices for K are:
  - d^{th} degree polynomial: $K(\mathbf{x}, \mathbf{y}) = (1 + <\mathbf{x}, \mathbf{y}>)^d$
  - Radial basis: $K(\mathbf{x}, \mathbf{y}) = e^{\frac{-||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma^2}}$

Acknowledgement and Further Reading

Slides are adapted from Dr. Y. Ning's Spring 19 offering of CS-559.

Part of the materials are taken from A. Zisserman's C19 Machine Learning course.

Further Reading:
Chapter 7.1.1 of *Pattern Recognition and Machine Learning* by C. Bishop.