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Xi'an Jiaotong-Liverpool University

Pattern Recognition

Lecture 15. Support Vector Machine

Dr. Shanshan ZHAO

School of AI and Advanced Computing
Xi'an Jiaotong-Liverpool University

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Introduction

- In the general case, the problem of finding linear discriminant functions can be formulated as a problem of **optimizing a criterion function**.
- Among all hyperplanes separating the data, there exists **a unique one yielding the maximum margin** of separation between the classes.

Binary Classification

Given training data (x_i, y_i) for $i = 1...N$, with $x_i \in \mathcal{R}^d$ and $y_i \in \{-1, 1\}$, learn a classifier $f(x)$ such that

$$f(x_i) \begin{cases} \geq 0 & y_i = +1 \\ < 0 & y_i = -1 \end{cases}$$

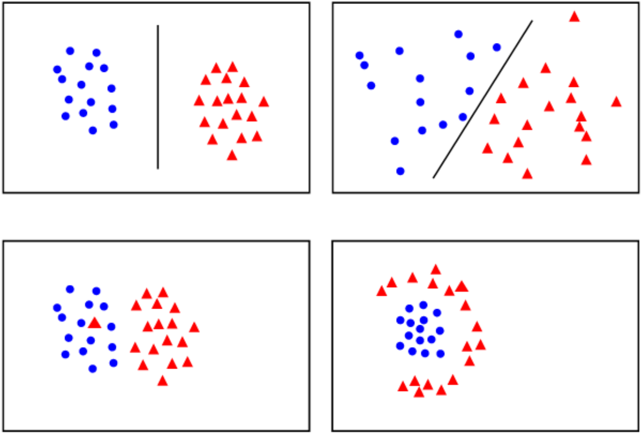
i.e.

$y_i f(x_i) > 0 \rightarrow$ a correction classification

Linear separability

linearly separable

not linearly separable

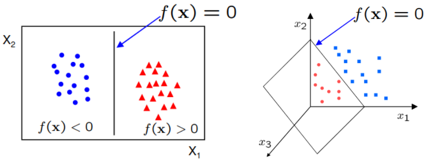


Linear Classifiers

A linear classifier has the form

$$f(x) = w^T x + b$$

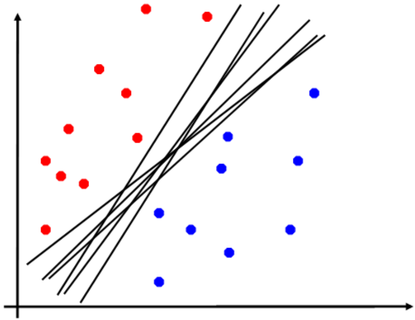
- w is **normal**(vertical) to the line, and the b is the bias/intercept
  - *whether the positive of f(x) is on the right or left of the line depends on the sign of the first parameter in vector* w.
- w is known as the weight vector.



(a) a line in 2D (b) a plane in 3D

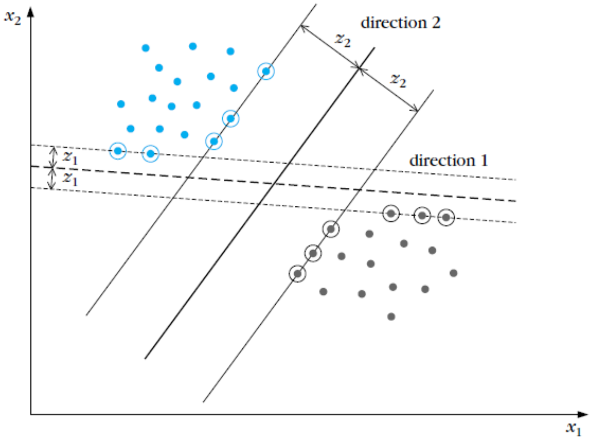
Linear Classifiers

- If training data is linearly separable, perceptron is guaranteed to find some linear separator/decision hyperplane.
- Which of these is optimal?



SVM Intuition

a very sensible choice for the hyperplane classifier would be the one that leaves the maximum margin from both classes.



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Margin

margin: a hyperplane leaves from both classes.
Our goal is to search for the direction that gives the maximum possible margin.
Recall that the distance of a point from a hyperplane is given by

$$z = \frac{|g(x)|}{||w||}$$

We can scale w, b so that the value of $g(x)$, at the nearest points in c_1, c_2 (circled in figure).

SVM objective

We can scale w, w_0 so that the value of $g(x)$, at the nearest points in c_1, c_2 (circled in figure1), is equal to 1 for class c_1 and equal to -1 for class c_2, which is equivalent with

- 1. Having a margin of $\frac{1}{||w||} + \frac{1}{||w||} = \frac{2}{||w||}$
- 2. Requiring that

$$\begin{cases} w^T x + b \geq 1, & \forall x \in c_1 \\ w^T x + b \leq -1, & \forall x \in c_2 \end{cases}$$

- The support vectors lie on either of the two hyperplanes, that is

$$w^T x + b = \pm 1$$

Objective: Maximizing the margins

Maximize the margin (I) –Primal form(*)

- Optimization (Quadratic Programming) (known as a **Primal problem**.

$$\begin{cases} \text{minimize} \quad J(w,b) = \frac{1}{2}||w||^2 \\ \text{subject to} \quad y_i(w^T x_i + b) \geq 1, \quad i = 1, 2, ..., N \end{cases} \tag{1}$$

- Minimizing the norm makes the margin maximum

It belongs to the convex programming family of problems, since the cost function is convex and the constraints are linear and define a convex set of feasible solutions. Such problems can be solved by considering the socalled Lagrangian duality.

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Maximize the margin (II) –Dual form(*)

- The objective in Eq. (1) is a standard quadratic programming problem.
- Let $\boldsymbol{\lambda} \in \mathscr{R}^N$ be the dual variables, corresponding to Lagrange multipliers that enforce the N inequality constraints.

The generalized Lagrangian is given below

$$\mathscr{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} - \sum_{i=1}^{N} \lambda_i[y_i(\boldsymbol{w}^T\boldsymbol{x}_i + b) - 1] \qquad (2)$$

- where $\boldsymbol{\lambda}$ is the Lagrange multiplier, $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \cdots, \lambda_N)^T$.
- we are **minimizing** with respect to $\boldsymbol{w}$ and b, and **maximizing** with respect to $\boldsymbol{\lambda}$.

Dual problem *

We are **minimizing** with respect to $\boldsymbol{w}$ and b, and **maximizing** with respect to $\boldsymbol{\lambda}$.

The dual problem is

$$\max_{\boldsymbol{\lambda} \geq 0} \min_{\boldsymbol{w}, b} \mathscr{L}(\boldsymbol{w}, b, \boldsymbol{\lambda})$$

Explaination:

- Appendix C.4 from *Pattern Recognition by Segios*
- cs229-notes3 by *Andrew Ng*, page 7-9.

`https://core.xjtlu.edu.cn/mod/folder/view.php?id=69950`

Maximize the margin (II) –Dual form(*)

Lets find the dual form of the problem. To do so, we need to first minimize $L(\boldsymbol{w}, b, \boldsymbol{\lambda})$ with respect to w and b (for fixed λ), which we'll do by setting the derivatives of L with respect to $\boldsymbol{w}$ and b to zero. We obtain the following two conditions

$$\frac{\partial}{\partial \boldsymbol{w}} \mathscr{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) = 0 \tag{3}$$

$$\frac{\partial}{\partial b} \mathscr{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) = 0 \tag{4}$$

$$\tag{5}$$

Combining (3) (4) and (2), results in

$$\boldsymbol{w} = \sum_{i=1}^{N} \lambda_i y_i \boldsymbol{x}_i \tag{6}$$

$$\sum_{i=1}^{N} \lambda_i y_i = 0 \tag{7}$$

Support Vectors

The Lagrange multipliers can be either zero or positive (Appendix C).Thus,the vector parameter $\boldsymbol{w}$ of the optimal solution is a linear combination of $N_s \leq N$ feature vectors that are associated with $\lambda_i \neq 0$. That is,

$$\boldsymbol{w} = \sum_{i=1}^{N_s} \lambda_i y_i \boldsymbol{x}_i$$

These are known as **support vectors** and the optimum hyperplane classifier as a support vector machine (SVM). As it is pointed out in Appendix C, a nonzero Lagrange multiplier corresponds to a so called active constraint.

Hence, as the set of constraints in equation (7) suggests for $\lambda_i \neq 0$, the support vectors lie on either of the two hyperplanes, that is,

$$w^T x + b = \pm 1$$

Maximize the margin (II) –Dual form(*)

Plugging equation (6) and (7) into Lagrangian Equation (2) yields the following

$$\begin{aligned}
\mathscr{L}(w,b,\lambda) &= \frac{1}{2}w^Tw - \sum_{i=1}^{N}\lambda_i y_i w^T x_i - \sum_{i=1}^{N}\lambda_i y_i b + \sum_{i=1}^{N}\lambda_i \\
&= \frac{1}{2}w^Tw - w^Tw - 0 + \sum_{i=1}^{N}\lambda_i \\
&= -\frac{1}{2}w^Tw + \sum_{i=1}^{N}\lambda_i \\
&= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j y_i y_j x_i^T x_j + \sum_{n=1}^{N}\lambda_i
\end{aligned}$$

Recall that we got to the equation above by minimizing L with respect to $\boldsymbol{w}$ and b. Putting this together with the constraints $\lambda_i \geq 0$ and the constraint $\sum_{i=1}^{N} \lambda_i y_i = 0$, we obtain the following dual optimization problem:

$$\max_{\boldsymbol{\lambda}} W(\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda}} \left(\sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j y_i y_j \boldsymbol{x}_i^T \boldsymbol{x}_j \right) \tag{8}$$

$$\text{subject to} \quad \sum_{i=1}^{N} \lambda_i y_i = 0 \tag{9}$$

$$\boldsymbol{\lambda} \geq 0 \tag{10}$$

We should be able to verify that the Karush-Kuhn-Tucker (KKT) conditions to hold are indeed satisfied in our optimization problem.

- Hence, we can solve the dual in lieu of solving the primal problem. Specifically, in the dual problem above, we have a maximization problem in which the parameters are the λ_i.
- the specific algorithm that we're going to use to solve the dual problem is : **SMO**.
- Most materials leave this part (how to find λ) to the end, but turns to introduce the kernels. *Don't get lost.*
- Details of *SMO* algorighm: cs229-notes3 by *Andrew Ng*, page 20-25.
- Let's leave it alone, as well :)

- If we are indeed able to solve it (i.e., find the λ_i that maximize $W(\boldsymbol{\lambda})$ subject to the constraints)
- then we can use Equation (6) $\boldsymbol{w} = \sum_{i=1}^{N} \lambda_i y_i \boldsymbol{x}_i$ to go back and find the optimal $\boldsymbol{w}$ as a function of the $\boldsymbol{\lambda}$.
- Having found $\boldsymbol{w}^*$, by considering the primal problem, it is also straightforward to find the optimal value for the intercept term b.
- In practice, b is computed as an average value obtained using all conditions of this type.

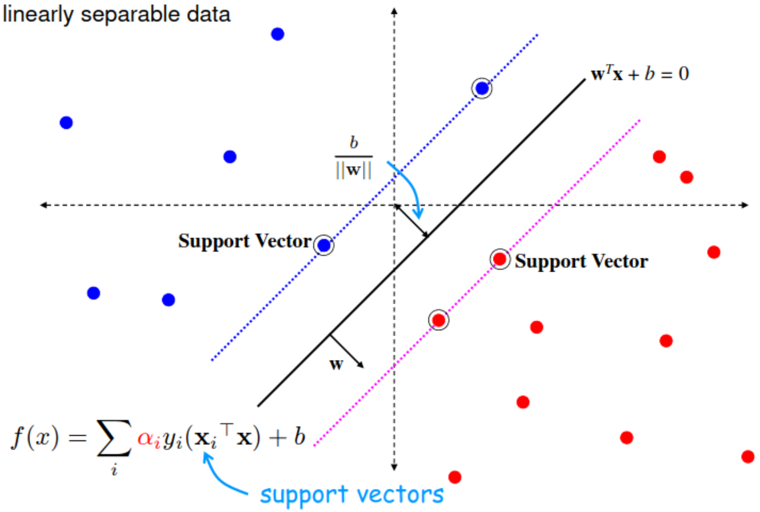
SVM

In practice, b is computed as an average value obtained using all conditions of this type.

$$
\begin{aligned}
b &= \frac{1}{|\mathcal{S}|}\sum_{i\in\mathcal{S}}(y_i - \boldsymbol{w}^T\boldsymbol{x}_i) \\
&= \frac{1}{|\mathcal{S}|}\sum_{i\in\mathcal{S}}(y_i - \sum_{j\in\mathcal{S}}\lambda_j y_j \boldsymbol{x}_j^T\boldsymbol{x}_i) \\
&= \frac{1}{|\mathcal{S}|}\sum_{i\in\mathcal{S}}(y_i - \sum_{j\in\mathcal{S}}\lambda_j y_j \langle\boldsymbol{x}_j, \boldsymbol{x}_i\rangle)
\end{aligned}
$$

where $\mathcal{S}$ is the set of support vectors. We end up with the equivalent optimization task.

SVM


linearly separable data
$\mathbf{w}^T\mathbf{x} + b = 0$
$\frac{b}{||\mathbf{w}||}$
Support Vector
Support Vector
$\mathbf{w}$
$f(x) = \sum_i \alpha_i y_i(\mathbf{x}_i{}^\top \mathbf{x}) + b$
support vectors

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- Suppose we've fit our model's parameters to a training set, and now wish to **make a prediction at a new point input** x.
- We would then calculate $w^T x + b$, and predict $y = 1$ if and only if this quantity is bigger than zero. With equation (6), this quantity can also be written:

$$\boldsymbol{w}^T \boldsymbol{x} + b = (\sum_{i=1}^{N_s} \lambda_i y_i \boldsymbol{x}_i)^T \boldsymbol{x} + b \tag{11}$$

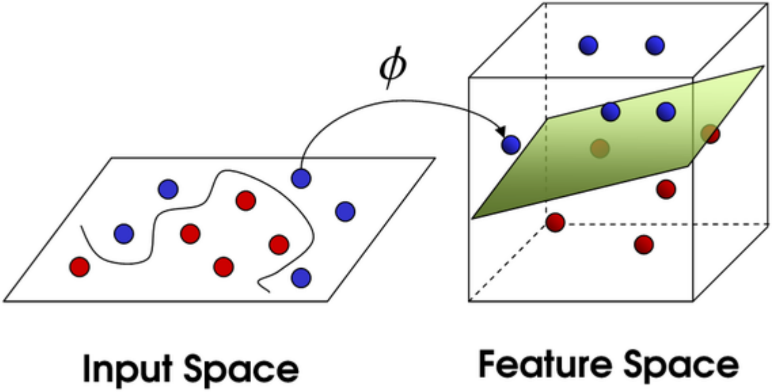
$$= \sum_{i=1}^{N_s} \lambda_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle + b \tag{12}$$

Hence, if we've found the λ_i, in order to make a prediction, we have to calculate a quantity that depends only on the **inner product** between x and the points in the training set.

- Moreover, we saw earlier that the λ_i will all be zero except for the support vectors.
- Thus, many of the terms in the sum above will be zero, and we really need to find only the inner products between x and the support vectors (of which there is often only a small number) in order calculate equation (12) and make our prediction.
- What if we have non-linear cases in the original space?
  - We discussed that we can map x into higher space where exists a linear hyperplane.

Kernel trick : Feature mapping

- Rather than applying SVMs using the original input attributes x, we may instead want to learn using some features $\phi(x)$.



SVM : Kernel trick

- Rather than applying SVMs using the original input attributes x, we may instead want to learn using some features $\phi(x)$.
- To do so, we simply need to go over our previous algorithm, and replace x everywhere in it with $\phi(x)$.
- Since the algorithm can be written entirely in terms of the inner products $\langle x, z\rangle$, this means that we would replace all those inner products with $\langle\phi(x), \phi(z)\rangle$.

SVM : Kernel trick

- Both the quadratic programming problem and the final decision function

$$g(x) = \text{sign}(\sum_{i=1}^{n} \lambda_i y_i \langle x \cdot x_i \rangle + b) \tag{13}$$

depend only on the dot procucts.

- We can generalize this result to the non-linear case by mapping the original input space into some other space $\mathscr{F}$ using a non-linear map $\phi : \mathscr{R}^d \to \mathscr{F}$ and perform the linear algorithm in the $\mathscr{F}$ space which only requires the inner products.

$$k(x, y) = \phi(x)^T \phi(y)$$

SVM : Kernel trick

- This results in the non-linear decision function of the form

$$g(x) = \text{sign}\left(\sum_{i=1}^{n} \lambda_i y_i k(x, x_i) + b\right) \tag{14}$$

  where the parameters λ_i are computed as the solution of the quadratic programming problem.
- In the original input space, the hyperplane corresponds to a non-linear decision function whose form is determined by the kernel.
- **We can use $k(x, x')$ directly for computation without transforming x and x', as long as ϕ exists.**

Example 1:

Suppose $x, z \in \mathscr{R}^2$, i.e., $x = [x_1, x_2]^T$, $z = [z_1, z_2]^T$, consider

$$k(x, z) = (x^T z)^2$$

$k(x, z)$ would be a valid kernel if we can find a projection function $\phi(x)$ that satisfy $k(x, z) = \phi(x)^T \phi(z)$

We may check $\phi(x) = [x_1^2, \sqrt{2}x_1x_2, x_2^2]^T$ *(yes, this is kind of cheating, but we just want to understand how kernel function works for now.)*

$$\begin{aligned} \phi(a)^T\phi(b) &= [a_1^2, \sqrt{2}a_1a_2, a_2^2]^T[b_1^2, \sqrt{2}b_1b_2, b_2^2] \\ &= a_1^2b_2^2 + 2a_1a_2b_1b_2 + a_2^2b_2^2 \end{aligned}$$

$$\begin{aligned} k(a,b) &= (a^Tb)^2 \\ &= ([a_1,a_2]^T[b_1,b_2])^2 \\ &= (a_1b_1 + a_2b_2)^2 \\ &= a_1^2b_2^2 + 2a_1a_2b_1b_2 + a_2^2b_2^2 \end{aligned}$$

So,

$$k(a,b) = \phi(a)^T\phi(b)$$

Example 2.

what if $x, z \in \mathscr{R}^n$?
page 14 on *cs229-notes3 by Andrew Ng*

Kernel : inner product

Polynomial kernels

$\forall x, x' \in \mathscr{R}^2$,

$$k(x, x') = (1 + x^T x')^2 = (1 + x_1 x_1' + x_2 x_2')^2$$
$$= 1 + x_1^2 x_1'^2 + x_2^2 x_2'^2 + 2x_1 x_1' + 2x_2 x_2' + 2x_1 x_1' x_2 x_2'$$

$\Downarrow$ above is an inner product of two vectors

$$= \begin{bmatrix} 1 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \sqrt{2}x_1 x_2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ x_1'^2 \\ x_2'^2 \\ \sqrt{2}x_1' \\ \sqrt{2}x_2' \\ \sqrt{2}x_1' x_2' \end{bmatrix}$$
$$= z^T z'$$

with $z = \phi(x) = [1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2]$

Example

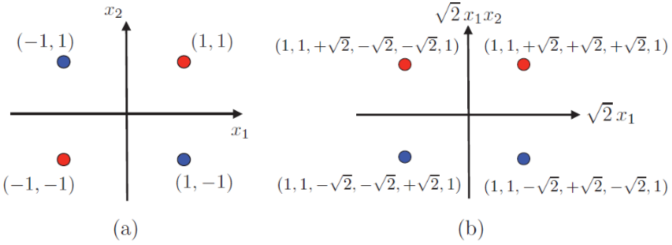


Figure 5.2 Illustration of the XOR classification problem and the use of polynomial kernels. (a) XOR problem linearly non-separable in the input space. (b) Linearly separable using second-degree polynomial kernel.

SVM : Kernel trick

- Even though $\mathscr{F}$ may be high-dimensional, a simple kernel $k(x, y)$ such as the following can be computed efficiently.

Polynomial	$k(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y})^p$
Sigmoidal	$k(\mathbf{x}, \mathbf{y}) = \tanh(\kappa(\mathbf{x} \cdot \mathbf{y}) + \theta)$
Radial basis function	$k(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|^2/(2\sigma^2))$

Figure 2: Common kernel functions

- Once a kernel function is chosen, we can substitute $\phi(x_i)$ for each training example x_i, and perform the optimal hyperplane algorithm in $\mathscr{F}$.

Kernel Matrix

consider some finite set of m points (not necessarily the training set) $\{x(1), \cdots, x(m)\}$, and let a square, m-by-m matrix K be defined so that its (i, j)-entry is given by $K_{ij} = K(x(i), x(j))$. This matrix is called the **Kernel matrix**.

- K must be symmetric
- K is positive semi-definite.

> It turns out to be a necessary and a sufficient condition for k to be a valid kernel (also called a Mercer kernel) if its correspoinding Kernel Matrix is symmetric positive semidefinite.

- proof also in the Andrew Ng's note.

Theorem(Mercer)

Let $k : \mathscr{R}^n \times \mathscr{R}^n \mapsto \mathscr{R}$ be given. Then for k to be a valid (Mercer) kernel, it is necessary and sufficient that for any $\{x(1), \cdots, x(m)\}$, $(m < \infty)$, the corresponding kernel matrix is symmetric positive semi-definite.

Given a function k, apart from trying to find a feature mapping ϕ that corresponds to it, this theorem therefore gives another way of testing if it is a valid kernel.

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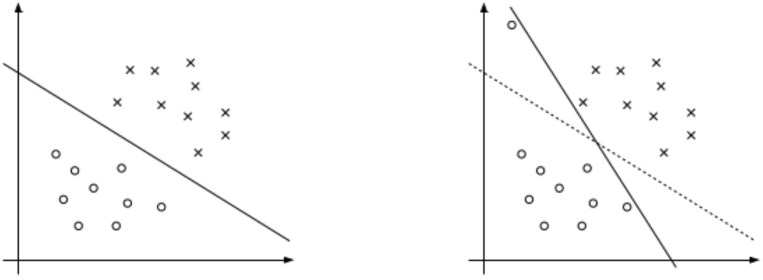
Regularization and the non-separable case

- The derivation of the SVM as presented so far assumed that the data is linearly separable. While mapping data to a high dimensional feature space via ϕ does generally increase the likelihood that the data is separable, we can't guarantee that it always will be so.
- Also, in some cases it is not clear that finding a separating hyperplane is exactly what we'd want to do, since that might be susceptible to outliers.

Regularization and the non-separable case



the left figure below shows an optimal margin classifier, and when a single outlier is added in the upper-left region (right figure), it causes the decision boundary to make a dramatic swing, and the resulting classifier has a much smaller margin.

The training feature vectors now belong to one of the following three categories:

1. Vectors that fall outside the band and are correctly classified. These vectors comply with the constraints

$$y_i(w^T x_i + b) \geq 1, i = 1, 2, \cdots, N$$

2. Vectors falling inside the band and are correctly classified. These are the points placed in circles in Figure 3, and they satisfy the inequality

$$0 \leq y_i(w^T x_i + b) < 1$$

3. Vectors that are misclassified. They are enclosed by circles and obey the inequality

$$y_i(w^T x_i + b) < 0$$

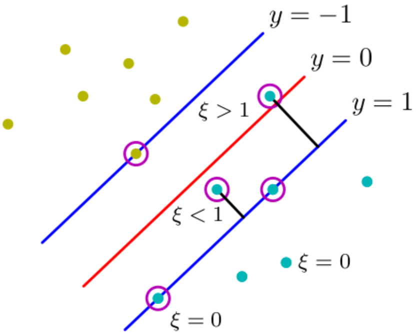
All three cases can be treated under a single type of constraints by introducing a new set of variables, namely,

$$y_i(w^T x_i + b) \geq 1 - \xi_i$$

slack variables

$$y_i(w^T x_i + b) \geq 1 - \xi_i$$

The first category of data corresponds to $\xi = 0$, the second to $0 < \xi_i \leq 1$, and the third to $\xi_i > 1$. The variables ξ_i are known as **slack variables**. The slack variables ξ_i are used to handle misclassified instances.



Regularization and the non-separable case

The goal now is to make the margin as large as possible but at the same time to keep the number of points with $\xi_i > 0$ as small as possible.

we reformulate our optimization

$$\begin{cases} \text{minimize} & J(w, b, \xi) = \frac{1}{2}||w||^2 + C\sum_{i=1}^{N} \xi_i \\ \text{subject to} & y_i(w^T x_i + b) \geq 1 - \xi_i, \quad i = 1, 2, ..., N \\ & \xi_i \geq 0, i = 1, \cdots, N \end{cases} \tag{15}$$

- This is still a quadratic optimization problem and there is a unique minimum.
- Thus, samples are now permitted to have (functional) margin less than 1, and if a sample whose functional margin is $1 - \xi_i$, we would pay a cost of the objective function being increased by $C\xi_i$.

Regularization parameter C

- The term $C\sum_{i=1}^{n}\xi_i$ can be thought of as measuring some amount of misclassification where lowering the value of C corresponds to a smaller penalty for misclassification.
- The parameter $C > 0$ controls the trade-off between the slack variable penalty and the margin.
- Because any point that is misclassified has $\xi_i > 1$, it follows that $\sum_i \xi_i$ is an upper bound on the number of misclassified points.
- The parameter C is therefore analogous to a regularization coefficient because it controls the trade-off between minimizing training errors and controlling model complexity.
- In the limit $C \to \infty$, we will recover the earlier support vector machine for separable data.

we can form the Lagrangian:

$$\mathscr{L}(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\lambda}, \gamma) =$$

$$\frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\lambda_i[y_i(\boldsymbol{w}^T\boldsymbol{x} + b) - 1 + \xi_i] - \sum_{i=1}^{N}\gamma_i\xi_i$$

the λ_i and γ_i are our Lagrange multipliers.(constrained to be ≥ 0).
We won't go through the derivation of the dual again in detail, but after setting the derivatives with respect to $\boldsymbol{w}$ and b to zero as before, substituting them back in, and simplifying,

we obtain the following dual form of the problem:

$$\max_{\boldsymbol{\lambda}} W(\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda}}\left(\sum_{i=1}^{N}\lambda_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j y_i y_j \boldsymbol{x}_i^T\boldsymbol{x}_j\right) \tag{16}$$

$$\text{subject to} \quad 0 \leq \lambda_i \leq C, i = 1, \cdots, N \tag{17}$$

$$\sum_{i=1}^{N}\lambda y_i = 0 \tag{18}$$

The corresponding set of KKT conditions can be given and used for testing for the convergence of the SMO algorithm.

SVM Training Methodology

- Training is formulated as an optimization problem
  - Dual problem - Makes use of Lagrange multipliers
  - Kernel trick
- Determination of the model parameters corresponds to a convex optimization problem
  - Solution is straightforward (local solution is a global optimum)
- Noisy labels – Soft Margin

Check the code.

Requirements

You should be able to describe

- the idea behind SVM.
- concept of the kernel trick, use examples.
- how the regularization parameter C works in SVM.

Thank You !

Q & A