An Introduction of Support Vector Machine

In part from of Jinwei Gu

Support Vector Machine (SVM)

- A classifier derived from statistical learning theory by Vapnik, et al. in 1992
- SVM became famous when, using images as input, it gave accuracy comparable to neural networks in a handwriting recognition task
- Currently, SVM is widely used in object detection & recognition, content-based image retrieval, text recognition, biometrics, speech recognition, etc.
- Still one of the best non-deep methods in many tasks, comparable performance

Classification Functions learned by SVM

It can be an arbitrary function of y=f(x), such as:



Linear Function (Linear separator)

• f(x) is a linear function in R^n :

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

- Written in matrix/vector notation (T → traspose)
- f(x) is a hyper-plane in the ndimensional feature space, w and x are vectors (the coefficients w_i and variables x_i of the hyper-plane)
- (Unit-length) normal vector of the hyper-plane:

$$\mathbf{n} = \frac{\mathbf{w}}{\|\mathbf{w}\|}$$



If you divide a vector by its norm, you obtain a unit vector (=with norm =1)

Vector representation (just to recall..)





Linear Function

How would you classify these points using a linear function?

Infinite number of answers!



Linear Discriminant Function

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!



Linear Discriminant Function



Linear Discriminant Function

- How would you classify these points using a linear discriminant function in order to minimize the error rate?
- Infinite number of answers!
- Which one is the best?



• denotes +1



Large Margin Linear Classifier

- The linear discriminant function (classifier) with the maximum margin is the best!
- Margin is defined as the width that the boundary could be increased by before hitting a data point in the learning set
- Why it is the best?
 - Robust to outliers and thus stronger generalization ability



So our target is to learn a linear separator that maximizes margins

- Target of the ML task:
- Learn w, b

 (where w is a vector of coefficients and b is a constant)
 such that margins are maximized



• denotes +1

Maximizing the margin

We want a classifier with as big margin as possible.

Recall the distance from a point $x (x_1, x_2)$ to a line w1x+w2y+b = 0 is:

$$\frac{|w_1x_1 + w_2x_2 + b|}{\sqrt{w_1^2 + w_2^2}} = \frac{|\mathbf{w} \cdot \mathbf{x} + b|}{||w||}$$

The distance between H and H1 is then: |w•x+b|/||w||=1/||w||

The distance (margin) between H1 and H2 is then: 2/||w||



In order to maximize the margin, we need to minimize ||w||. With the

condition that there must be <u>no data points between H1 and H2</u>, e.g., for any x_i in D: $x_i \cdot w + b \ge +1$ when $y_i = +1$ $x_i \cdot w + b \le -1$ when $y_i = -1$ Can be combined into $y_i(x_i \cdot w) \ge 1$

Large Margin Linear Classifier • denotes +1 \odot denotes -1 Equivalent formulation: **X**₂ Margin minimize $\frac{1}{2} \|\mathbf{w}\|^2$ WTX+b=1 X⁺ $\frac{W^{T} X * b = 0}{W^{T} X * b} = .1$ **X**⁺ such that $y_i(\mathbf{w}^T\mathbf{x}_i + b) \ge 1$ n Q X-Ο \bigcirc \bigcirc \bigcirc **X**₁

Solving the Optimization Problem

Quadratic programming with linear constraints

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2$$

s.t. $y_i(\mathbf{w}^T \mathbf{x}_i + b) \ge 1$

Lagrangian Method:



minimize
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left(y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$

s.t. $\alpha_i \ge 0$

Lagrangian

Given a function f(x) and a set of constraints $c_{1..}c_n$, a Lagrangian is a function L(f,c1,..cn, $\alpha_{1,..} \alpha_n$) that "incorporates" constraints in the optimization problem

$$L(x,\alpha) = f(x) - \sum \alpha_i c_i(x)$$

The optimum is at a point where (Karush-Kuhn-Tucker (KKT) conditions):

$$1)\nabla f(x) - \sum \alpha_i \nabla c_i(x) = 0$$

2) $\alpha_i \ge 0$
3) $\alpha_i c_i(x) = 0 \quad \forall i$

The third condition is known as complementarity condition

Solving the Optimization Problem

$$\begin{array}{l} \text{minimize } L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left(y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right) \\ \text{Note: our variables here are} \\ \mathbf{w}, \text{ b and the } \alpha_i \end{array} \quad \text{s.t.} \quad \alpha_i \ge 0 \\ c_i(x) = (y_i(w^T x_i + b) - 1) \end{array}$$

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \qquad \longrightarrow \qquad \frac{2}{2} \mathbf{w} - \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i = 0 \quad \Rightarrow \mathbf{w} = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i$$
$$\frac{\partial L_p}{\partial b} = 0 \qquad \longrightarrow \qquad \sum_{i=1}^n \alpha_i y_i = 0$$
$$2)\alpha_i \ge 0$$
$$3)\alpha_i (y_i (w^T x_i + b) - 1)) = 0 \quad \forall i$$

To minimize *L* we need to maximize the red box

Dual Problem Formulation (2)



All the steps



Each non-zero α_i indicates that corresponding \mathbf{x}_i is a support vector SV.

Why only SV have $\alpha > 0$?

$$\begin{array}{rcl} \alpha_i &\geq & 0\\ y_i(w^\top x_i + b) - 1 &\geq & 0\\ \alpha_i(y_i(w^\top x_i + b) - 1) &= & 0. \end{array}$$

The complementarity condition (the **third one of KKT**, see previous definition of Lagrangians) implies that one of the 2 multiplicands is zero. However, $y_i(w^T x_i + b) > 1$ for non-SV **x**i.

Therefore **only data points on the margin (=SV)** will have a non-zero α (because they are the only ones for wich **y**i (**w**^T**x**i + **b**) = 1)

Final Formulation

To summarize:

Find $\alpha_1 \dots \alpha_n$ such that $\mathbf{Q}(\mathbf{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_j$ is maximized and (1) $\sum \alpha_i y_i = 0$ (2) $\alpha_i \ge 0$ for all α_i

- Again, remember that the constraint (2) can be verified with a non-equality to zero only for the SV!!
- Q(α) can be computed since we know the y_iy_jx_i^Tx_j (they are the pairs <x_i,y_i> of the training set D!!)
- So, in this final formulation the only variables to be computed are the α_i of the support vectors. Wrt the original formulation, b and w_i have disappeared!

The Optimization Problem Solution

Given a solution to the dual problem Q(α) (i.e. computing the α₁...α_n), solution to the primal (i.e. computing w and b) is:

w =
$$\Sigma \alpha_i y_i \mathbf{x}_i$$
 $b = y_k - \Sigma \alpha_i y_i \mathbf{x}_i$ for any $\alpha_k > 0$

- Each non-zero α_i indicates that corresponding \mathbf{x}_i is a support vector.
- Then the classifying function for a new point x is (note that we don' t need to compute w explicitly):

 $\Phi(\mathbf{x}) = \Sigma \alpha_i y_i \mathbf{x}_i^{\mathsf{T}} \mathbf{x} + b \quad (x) \text{ are } SV)$

- Notice to predict the class of x we perform an *inner (dot)* product x_i^Tx between the test point x and the support vectors x_i. Only SV are useful for classification of new instances!! (since the other α values are zero).
- Also keep in mind that solving the optimization problem involved computing the inner (dot) products x_i^Tx_j between all training points.

Inner or dot product between two vectors (example)

a: (a_1, a_2, a_3) **b**: (b_1, b_2, b_3)

Dot product: Σa_ib_i

 $\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3,$

Example:

Let a=(1,2,3) and b=(4,-5,6)

a · **b**=1(4)+2(-5)+3(6)=4-10+18=12.

Example

• Suppose we have the dataset: $\left\{ \begin{pmatrix} 3\\1 \end{pmatrix}, \begin{pmatrix} 3\\-1 \end{pmatrix}, \begin{pmatrix} 6\\1 \end{pmatrix}, \begin{pmatrix} 6\\-1 \end{pmatrix} \right\} \quad \left\{ \begin{pmatrix} 1\\0 \end{pmatrix}, \begin{pmatrix} 0\\1 \end{pmatrix}, \begin{pmatrix} 0\\-1 \end{pmatrix}, \begin{pmatrix} -1\\0 \end{pmatrix} \right\}$



negative



By simple inspection, we can identify 3 SVs



$$\left\{s_1 = \left(\begin{array}{c}1\\0\end{array}\right), s_2 = \left(\begin{array}{c}3\\1\end{array}\right), s_3 = \left(\begin{array}{c}3\\-1\end{array}\right)\right\}$$

First step is to write system of equations to find the "alfas"

- We know that $\mathbf{w}^T \mathbf{x} + b = \Sigma \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b = -1$ for negative SVs (s₁) and $\mathbf{w}^T \mathbf{x} + b = \Sigma \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b =$ 1 for positive SVs (s₂,s₃)
- Furthermore, $\mathbf{w} = \sum_{i \in \mathbf{a}} \alpha_i y_i \mathbf{x}_i$ (first contraint from derivative) and $\boldsymbol{\alpha}_i \bar{\mathbf{a}}_i^{\mathrm{tr}}$ non-zero only for SVs.
- we can write a system of equations for each of the 3 $|\alpha_1 k(s_1, s_1) + \alpha_2 k(s_2, s_1) + \alpha_3 k(s_3, s_1) = -1$ $\alpha_1 k(s_1, s_2) + \alpha_2 k(s_2, s_2) + \alpha_3 k(s_3, s_2) = 1$ $\alpha_1 k(s_1, s_3) + \alpha_2 k(s_2, s_3) + \alpha_3 k(s_3, s_3) = 1$

Where k(x,y) is the dot product x^Ty

Then we compute the dot products

$$k(s_1, s_1) = (1 \ 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1$$
$$k(s_1, s_2) = (1 \ 0) \begin{pmatrix} 3 \\ 1 \end{pmatrix} = 3$$
$$k(s_2, s_3) = (3 \ 1) \begin{pmatrix} 3 \\ -1 \end{pmatrix} = 9 - 1 = 8$$

Etc. (do it yourself)

Finally, we obtain the system of equations

$$\alpha_1 + 3\alpha_2 + 3\alpha_3 = -1 3\alpha_1 + 10\alpha_2 + 8\alpha_3 = 1 3\alpha_1 + 8\alpha_2 + 10\alpha_3 = 1$$

From the optimization conditions, we also know that:

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$-\alpha_{1} + \alpha_{2} + \alpha_{3} = 0$$

$$\alpha_{2} = \alpha_{3} = \frac{1}{8}; \ \alpha_{1} = \frac{1}{4}; b = -2$$

The solution (graphically)



The w_i are computed using **w** = $\Sigma \alpha_i y_i \mathbf{x}_i$

$$w_1 = 1, w_2 = 0, b = -2$$

The solution (graphically)



The w_i are computed using **w** = $\Sigma \alpha_i y_i \mathbf{x}_i$

$$w_1 = 1, w_2 = 0, b = -2$$

Dataset with noise



- Hard Margin: So far we require all data points be classified correctly
 - No training error
- What if the training set is noisy?
- Solution 1: use more complex separator

OVERFITTING!

Soft Margin Classification

- A better solution: slack variables
- Slack variables ξ_i can be added to <u>allow misclassification</u> of outliers or noisy examples, resulting margins are



x_i are the misclassified examples

Large Margin Linear Classifier

• New Formulation:

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i$$

such that

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \ge 1 - \xi_i$$
$$\xi_i \ge 0$$

Slack variables allow an example in the margin $0 \le \xi_i \le 1$. to be misclassified, while if $\xi_i > 1$ it is an error

Parameter C can be viewed as a way to control over-fitting.
 For large C a large penalty is assigned to errors.

Hard Margin v.s. Soft Margin

The old formulation:

Find w and b such that

 $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \text{ is minimized and for all } \{(\mathbf{x}_{\mathbf{i}}, y_{i})\}$ $y_{i} (\mathbf{w}^{\mathrm{T}} \mathbf{x}_{\mathbf{i}} + \mathbf{b}) \ge 1$

The new formulation incorporating slack variables:

Find w and b such that $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} + C \Sigma \xi_{i} \text{ is minimized and for all } \{(\mathbf{x}_{\mathbf{i}}, y_{i})\}$ $y_{i} (\mathbf{w}^{\mathrm{T}} \mathbf{x}_{\mathbf{i}} + b) \ge 1 - \xi_{i} \text{ and } \xi_{i} \ge 0 \text{ for all } i$

Parameter C can be viewed as a way to control overfitting.

Effect of soft-margin constant C



Non-linear SVMs

 Datasets that are linearly separable (possibly with noise) work out great:



But what are we going to do if the dataset is just too hard?



• How about... mapping data to a higher-dimensional space:



This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm_tutorial.ppt

Non-linear SVMs: Feature Space

 General idea: the original input space can be mapped to some higher-dimensional feature space where the training set is separable:



This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm_tutorial.ppt

The original points (left side of the schematic) are mapped, i.e., rearranged, using a set of mathematical functions, known as **kernels**.



SVM with a polynomial Kernel visualization

Created by: Udi Aharoni

Nonlinear SVMs: The Kernel Trick

• With this mapping, our discriminant function is now:

$$g(\mathbf{x}) = \mathbf{w}^{T} \phi(\mathbf{x}) + b = \sum_{i \in SV} \alpha_{i} \phi(\mathbf{x}_{i})^{T} \phi(\mathbf{x}) + b$$

Original formulation was $f(\mathbf{x}) = \mathbf{w}^{T} \mathbf{x} + b = \Sigma \alpha_{i} y_{i} \mathbf{x}_{i}^{T} \mathbf{x} + b$

- No need to know this mapping function explicitly, because we only use the dot product of feature vectors in both the training and test.
- A *kernel function* is defined as a function that corresponds to a dot product of two feature vectors **in some expanded feature space**: $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

• Note that, obviously, the dot product $\mathbf{x}_i^T \mathbf{x} = \mathbf{x}_i \cdot \mathbf{x}$ IS a kernel function!

Nonlinear SVMs: The Kernel Trick

• An example:

2-dimensional vectors $\mathbf{x} = [x_1 \ x_2];$

let $K(x_i, x_j) = (1 + x_i^T x_j)^2$,

Need to show that $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$, e.g., that it is a kernel function:

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

$$= 1 + x_{iI}^{2}x_{jI}^{2} + 2 x_{iI}x_{jI} x_{i2}x_{j2} + x_{i2}^{2}x_{j2}^{2} + 2x_{iI}x_{jI} + 2x_{i2}x_{j2}$$

$$= [1 \ x_{iI}^{2} \sqrt{2} x_{iI}x_{i2} \ x_{i2}^{2} \sqrt{2x_{iI}} \sqrt{2x_{i2}}]^{T} [1 \ x_{jI}^{2} \sqrt{2} x_{jI}x_{j2} \ x_{j2}^{2} \sqrt{2x_{jI}} \sqrt{2x_{j2}}]$$

$$= \varphi(\mathbf{x}_{i})^{T}\varphi(\mathbf{x}_{j}), \text{ where } \varphi(\mathbf{x}) = [1 \ x_{I}^{2} \sqrt{2} x_{I}x_{2} \ x_{2}^{2} \sqrt{2x_{I}} \sqrt{2x_{2}}]$$

$$Ex: x: (1,2) \Rightarrow \varphi(\mathbf{x}) = (1,1^{2}, \sqrt{2}(1 \times 2), 2^{2}, \sqrt{2} \times 1, \sqrt{2} \times 2) = (1,1,2,4, \sqrt{2},2)$$

This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm_tutorial.ppt

Nonlinear SVMs: The Kernel Trick

- Examples of commonly-used kernel functions:
 - Linear kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$

• Polynomial kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$

• Gaussian (Radial-Basis Function (RBF)) kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2})$

• Sigmoid:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$$

 In general, functions that satisfy *Mercer's condition* can be kernel functions.

Nonlinear SVM: Optimization

Formulation: (Lagrangian Dual Problem) find α1, α2,... $α_n$ such that:

maximize
$$\sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$
such that
$$0 \le \alpha_{i} \le C$$
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

The solution of the discriminant function is

$$g(\mathbf{x}) = \sum_{i \in SV} \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b$$

The optimization technique is the same.

Support Vector Machine: Algorithm

- 1. Choose a kernel function
- 2. Choose a value for C
- 3. Solve the quadratic programming problem (many software packages available)
- 4. Construct the discriminant function from the support vectors

Some Issues

- Choice of kernel
 - Gaussian or polynomial kernel is default
 - if ineffective, more elaborate kernels are needed
 - domain experts can give assistance in formulating appropriate similarity measures
- Choice of kernel parameters
 - e.g. σ in Gaussian kernel
 - σ is the distance between closest points with different classifications
 - In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.
- Optimization criterion Hard margin v.s. Soft margin
 - a lengthy series of experiments in which various parameters are tested

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Issues

- Large margin classifiers are known to be sensitive to the way features are scaled. Therefore it is essential to **normalize** the data.
- Also sensible to unbalanced data
- Hyper-parameter tuning (C, kernel): read

A User's Guide to Support Vector Machines

Asa Ben-Hur Department of Computer Science Colorado State University Jason Weston NEC Labs America Princeton, NJ 08540 USA Summary: Support Vector Machine

1. Large Margin Classifier

Better generalization ability & less over-fitting

2. The Kernel Trick

- Map data points to higher dimensional space in order to make them linearly separable.
- Since only dot product is used, we do not need to represent the mapping explicitly.

Additional Resource

http://www.kernel-machines.org/

LibSVM (best implementation for SVM)

http://www.csie.ntu.edu.tw/~cjlin/libsvm/