An Introduction to Support Vector Machine

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-network with hand-designed features in a handwriting recognition task
- Currently, SVM is widely used in object detection & recognition, content-based image retrieval, text recognition, biometrics, speech recognition, etc.
- Also used for regression

Outline

- Linear Discriminant Function
- Large Margin Linear Classifier
- Nonlinear SVM: The Kernel Trick

g(x) is a linear function:

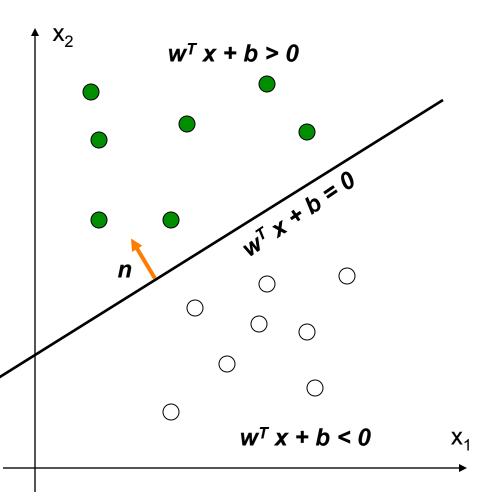
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$

A hyper-plane in the feature space

$$\mathbf{w}^{\mathsf{T}} \mathbf{x} + b = 0$$

(Unit-length) normal vector of the hyper-plane:

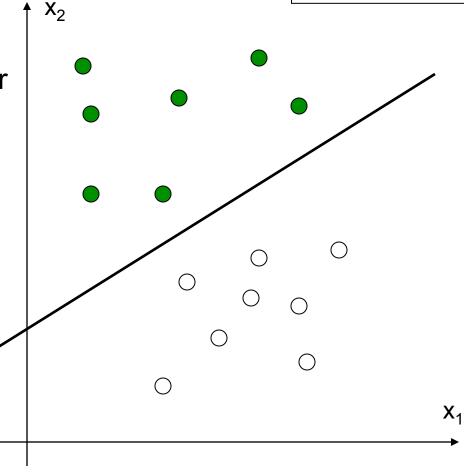
$$\mathbf{n} = \frac{\mathbf{w}}{\|\mathbf{w}\|}$$



- denotes +1
 - denotes -1

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

Infinite number of answers!

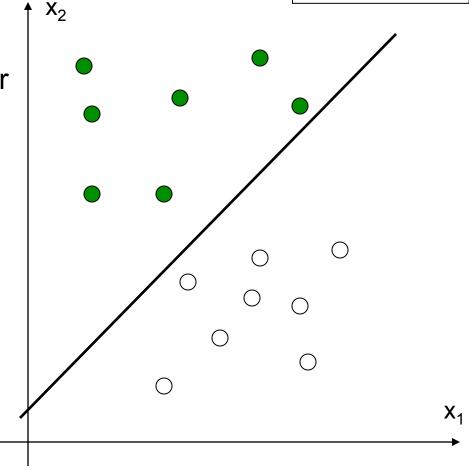


denotes +1

denotes -1

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

Infinite number of answers!

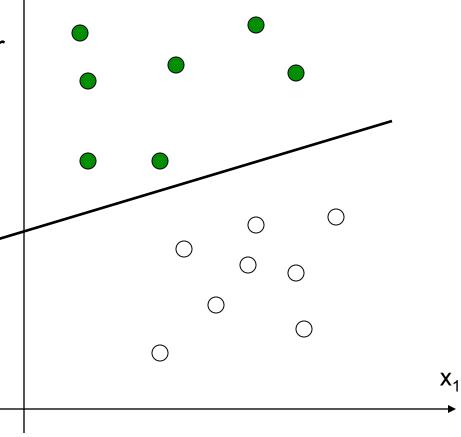


 X_2

- denotes +1
 - denotes -1

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

Infinite number of answers!



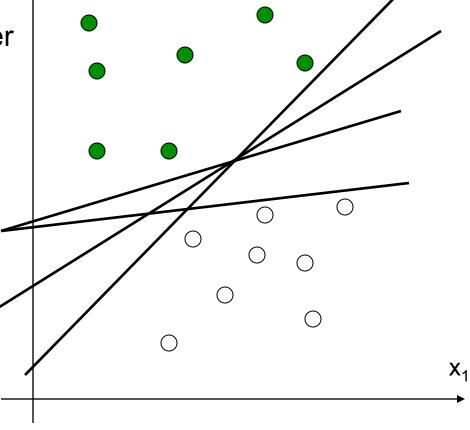
 X_2

- denotes +1
 - denotes -1

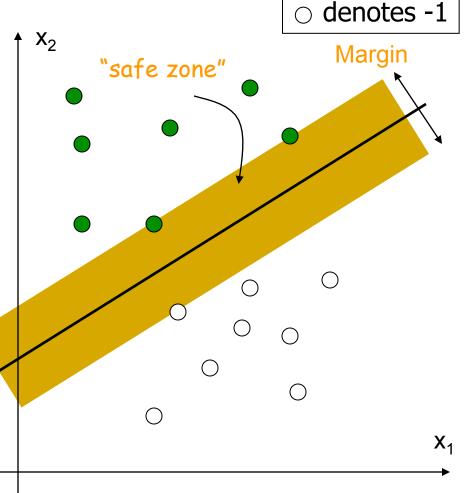
How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!

Which one is the best?



- 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
- Why it is the best?
 - Robust to outliners and thus strong generalization ability
 - Good according to PAC (Probably Approximately Correct) theory.



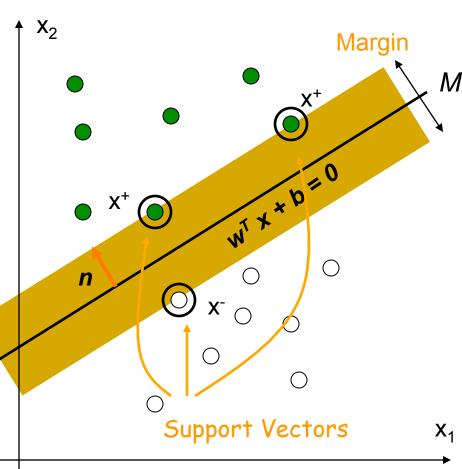
denotes +1

Maximum Margin Classification

Distance from point x_i to the hyperplane is:

$$r = \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|}$$

- Examples closest to the hyperplane are support vectors.
- Margin M of the classifier is the distance between support vectors on both sides.
- Only support vectors matter;
 other training points are ignorable.



- denotes +1
 - denotes -1

Given a set of data points:

$$\{(\mathbf{x}_i, y_i)\}, i = 1, 2, L, n, \text{ where}$$

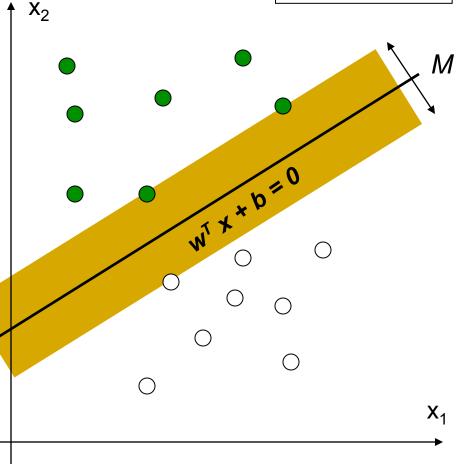
$$\mathbf{w}^\mathsf{T}\mathbf{x}_i + b \ge M/2$$
 if $y_i = +1$

$$\mathbf{w}^{\mathsf{T}}\mathbf{x}_{i} + b \le -M/2$$
 if $y_{i} = -1$

With a scale transformation on both w and b, the above is equivalent to

For
$$y_i = +1$$
, $\mathbf{w}^T \mathbf{x}_i + b \ge 1$

For
$$y_i = -1$$
, $\mathbf{w}^T \mathbf{x}_i + b \le -1$



- denotes +1
 - denotes -1

We know that

$$\mathbf{w}^T \mathbf{x}^+ + b = 1$$

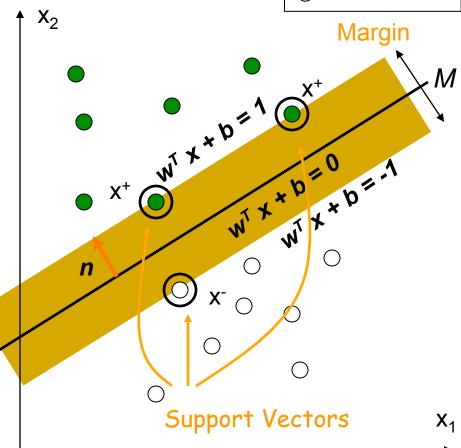
$$\mathbf{w}^T \mathbf{x}^- + b = -1$$

Thus
$$w^T (x^+-x^-) = 2$$

The margin width is:

$$M = (\mathbf{x}^+ - \mathbf{x}^-)^{\top} \mathbf{n}$$

$$= (\mathbf{x}^+ - \mathbf{x}^-) \cdot \frac{\mathbf{w}}{\|\mathbf{w}\|} = \frac{2}{\|\mathbf{w}\|}$$



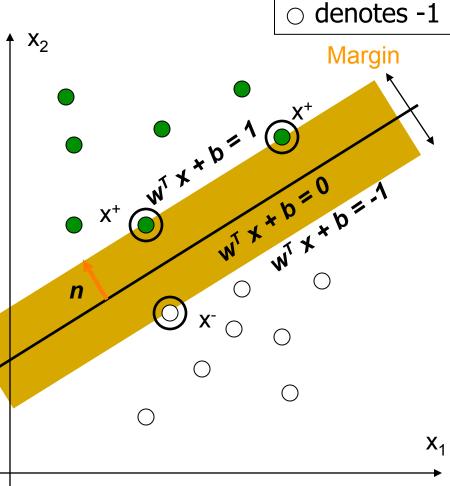
- denotes +1

Formulation:

maximize
$$\frac{2}{\|\mathbf{w}\|}$$

For
$$y_i = +1$$
, $\mathbf{w}^T \mathbf{x}_i + b \ge 1$

For
$$y_i = -1$$
, $\mathbf{w}^T \mathbf{x}_i + b \le -1$



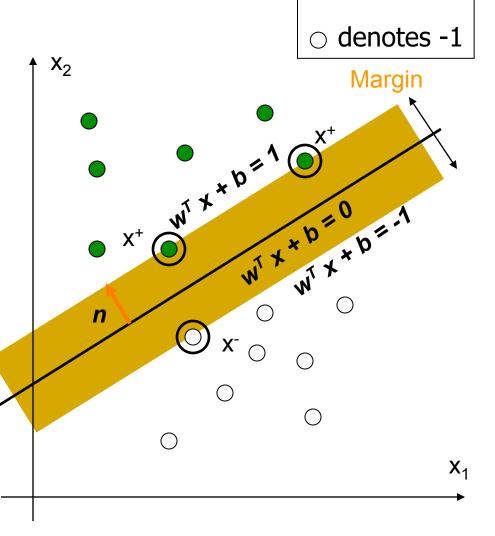
denotes +1

Formulation:

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

For
$$y_i = +1$$
, $\mathbf{w}^T \mathbf{x}_i + b \ge 1$

For
$$y_i = -1$$
, $\mathbf{w}^T \mathbf{x}_i + b \le -1$

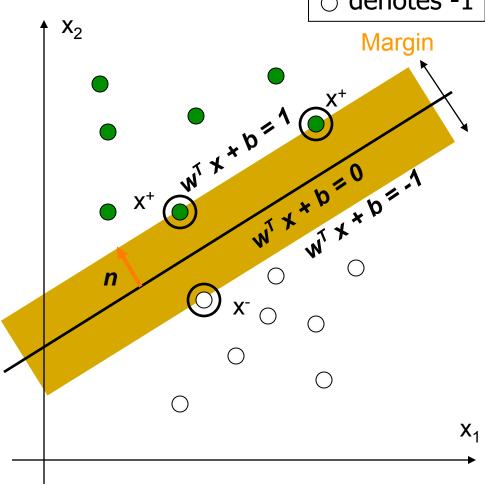


- denotes +1
- denotes -1

Formulation:

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

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



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 Function



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.
$$\alpha_i \ge 0$$

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. $\alpha_i \ge 0$

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \qquad \mathbf{w} = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i$$

$$\frac{\partial L_p}{\partial b} = 0 \qquad \sum_{i=1}^n \alpha_i y_i = 0$$

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 Dual Problem



maximize
$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

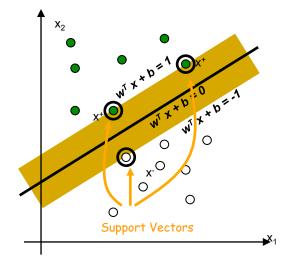
s.t.
$$\alpha_i \ge 0$$
, and $\sum_{i=1}^n \alpha_i y_i = 0$

From KKT (Karush–Kuhn–Tucker) condition, we know:

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

- Thus, only support vectors have $\alpha_i \neq 0$
- The solution has the form:

$$\mathbf{W} = \sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{X}_{i} = \sum_{i \in \mathbb{N}} \alpha_{i} y_{i} \mathbf{X}_{i}$$



get *b* from $y_k(\mathbf{w}^T\mathbf{x}_k + b) - 1 = 0$, where \mathbf{x}_k is any support vector

Thus, $b = y_i - \Sigma \alpha_i y_i \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_k$ for any $\alpha_k > 0$

The linear discriminant function is:

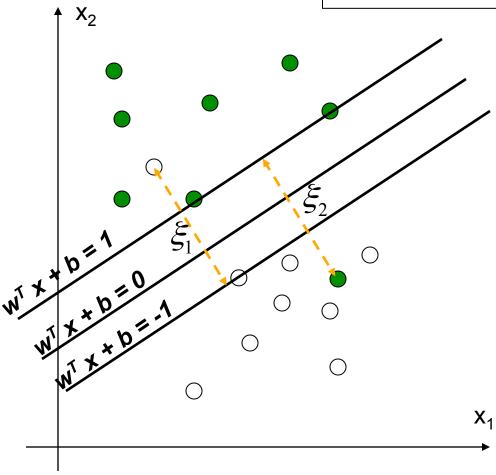
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{i \in SV} \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

That is, no need to compute w explicitly for classification.

- Notice it relies on a dot product between the test point x and the support vectors x_i
- Also keep in mind that solving the optimization problem involved computing the dot products x_i^Tx_j between all pairs of training points

Slack variables ξ_i can be added to allow mis-classification of difficult or noisy data points

outliers, etc.)



denotes +1

denotes -1

Formulation: minimize $\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i$ such that $y_i(\mathbf{w}^T \mathbf{x}_i + b) \ge 1 - \xi_i$ $\xi_i \ge 0$

- Parameter C can be viewed as a way to control over-fitting: it "trades off" the relative importance of maximizing the margin and fitting the training data.
 - For large values of C, the optimization will choose a smaller-margin hyperplane if that hyperplane does a better job of getting all the training points classified correctly. Conversely, a very small value of C will cause the optimizer to look for a larger-margin separating hyperplane, even if that hyperplane misclassifies more points.

Formulation: (Lagrangian Dual Problem)

maximize
$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$0 \le \alpha_i \le C$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

- Again, \mathbf{x}_i with non-zero α_i will be support vectors.
- Solution to the dual problem is:

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i} = \sum_{i \in SV} \alpha_{i} y_{i} \mathbf{x}_{i}$$

$$b = y_{k} (1 - \xi_{k}) - \Sigma \alpha_{i} y_{i} \mathbf{x}_{i}^{\mathsf{T}} \mathbf{x}_{k} \quad \text{for any } k \text{ s.t. } \alpha_{k} > 0$$

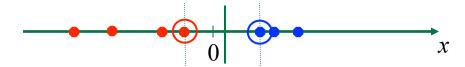
$$b = y_k (1 - \xi_k) - \Sigma \alpha_i y_i \mathbf{x}_i^\mathsf{T} \mathbf{x}_k$$
 for any k s.t. $\alpha_k > 0$

Again, we don't need to compute w explicitly for classification:

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{i \in SV} \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

Non-linear SVMs

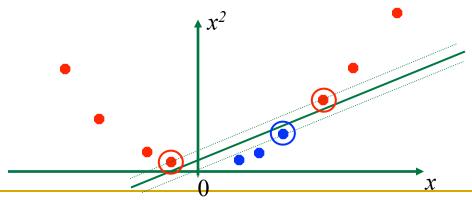
Datasets that are linearly separable with noise work out great:



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

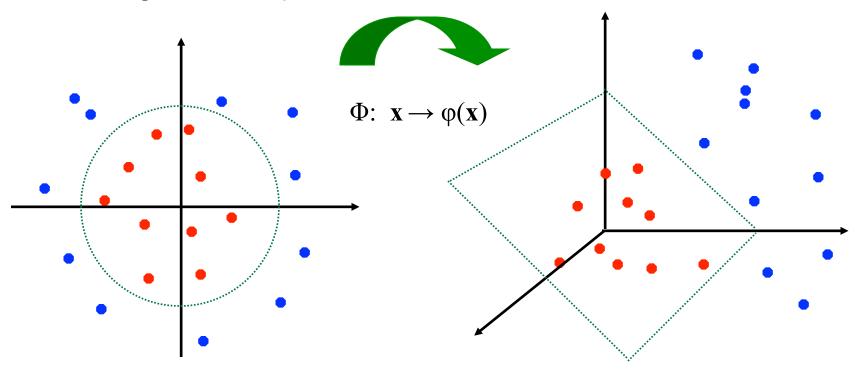


How about... mapping data to a higher-dimensional space:



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:



Nonlinear SVMs: The Kernel Trick

With this mapping, our discriminant function is now:

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

- No need to know this mapping 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:

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

Nonlinear SVMs: The Kernel Trick

An example:

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

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

Need to show that $K(x_i,x_i) = \varphi(x_i)^T \varphi(x_i)$:

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:

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

Mercer's theorem: *Every semi-positive definite* symmetric function is a kernel.

Nonlinear SVM: Optimization

Formulation: (Lagrangian Dual Problem)

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

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

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

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.

Demo of LibSVM

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

References on SVM and Stock Prediction

http://www.svms.org/finance/HuangNakamoriWang2005.pdf

http://cs229.stanford.edu/proj2012/ShenJiangZhang-StockMarketForecastingusingMachineLearningAlgorithms.pdf

http://research.ijcaonline.org/volume41/number3/pxc3877555.pdf

and other references online ...