Support Vector Machine & Its Applications

A portion (1/3) of the slides are taken from Prof. Andrew Moore's SVM tutorial at

http://www.cs.cmu.edu/~awm/tutorials

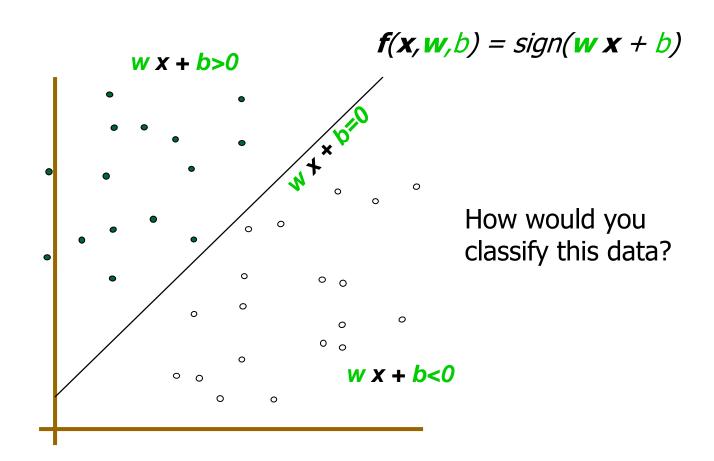
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Overview

- Intro. to Support Vector Machines (SVM)
- Properties of SVM
- Applications
 - Gene Expression Data Classification
 - Text Categorization if time permits
- Discussion

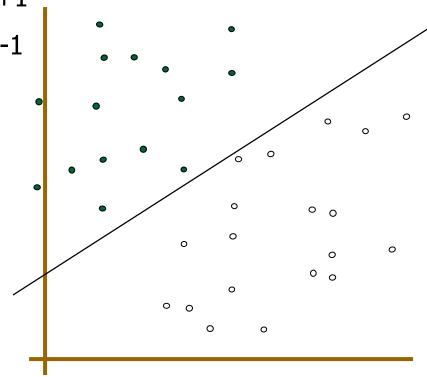
- denotes +1
- denotes -1



$$f(x, w, b) = sign(w x + b)$$

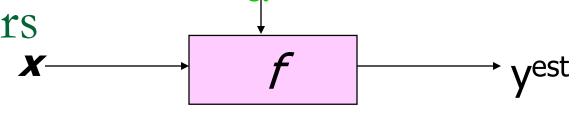
• denotes +1

° denotes -1

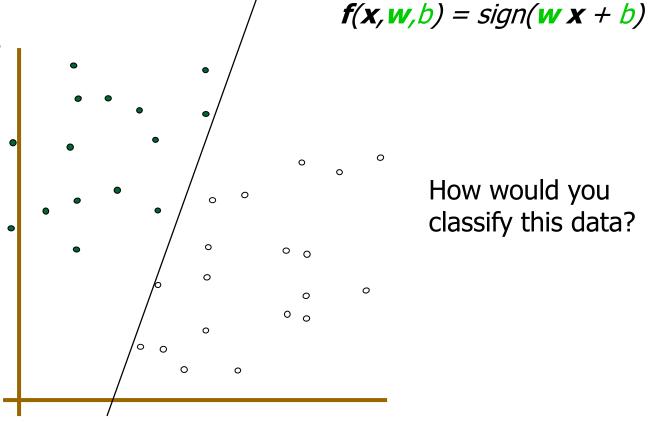


How would you classify this data?

Linear Classifiers



- denotes +1
- denotes -1



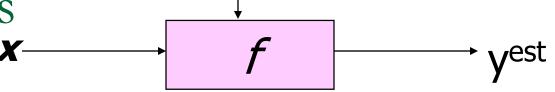
How would you classify this data?

Linear Classifiers f(x, w, b) = sign(w x + b)denotes +1 denotes -1 Any of these would be fine..

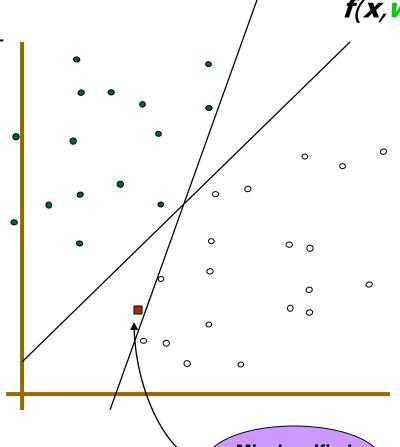
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..but which is best?

Linear Classifiers



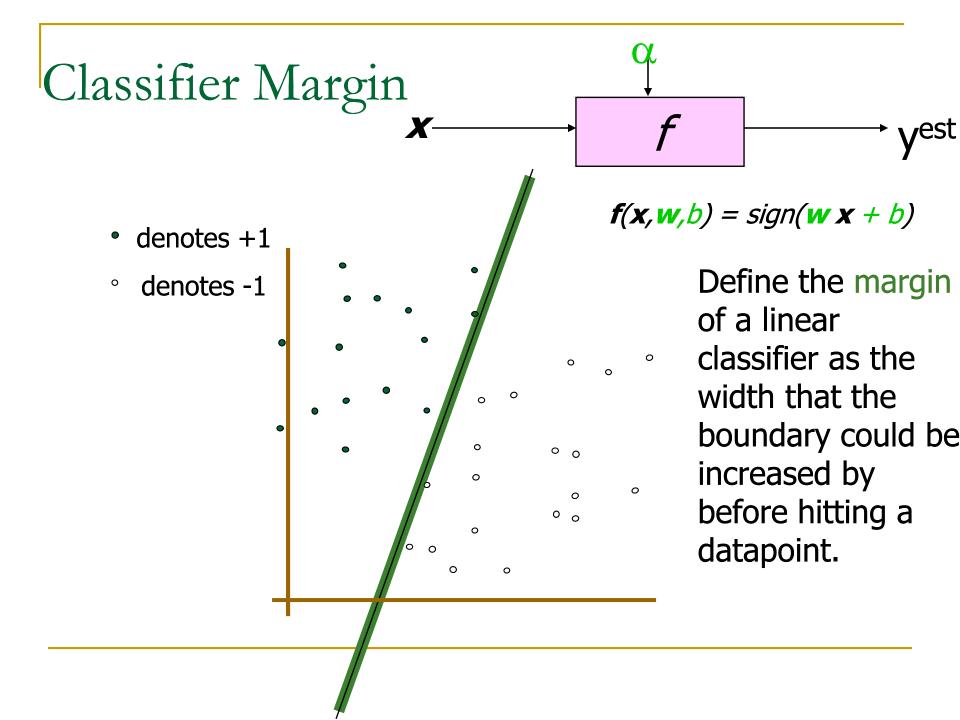
- denotes +1
- ° denotes -1

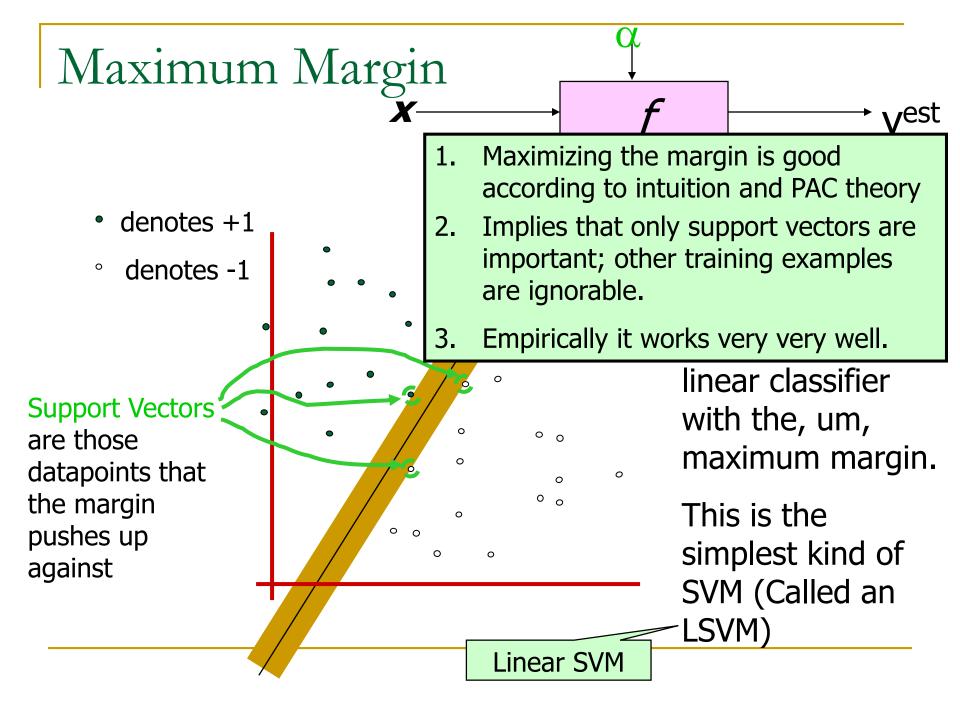


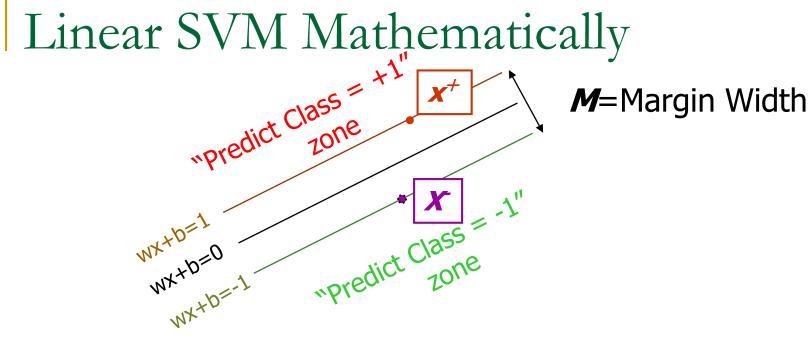
f(x, w, b) = sign(w x + b)

How would you classify this data?

Misclassified to +1 class







What we know:

•
$$\mathbf{W} \cdot \mathbf{X}^+ + b = +1$$

•
$$w \cdot x + b = -1$$

$$w \cdot (x^+-x^-)=2$$

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

Linear SVM Mathematically

Goal: 1) Correctly classify all training data

$$wx_i + b \ge 1 \qquad \text{if } y_i = +1 \\ wx_i + b \le 1 \qquad \text{if } y_i = -1 \\ y_i(wx_i + b) \ge 1 \qquad \text{for all i } 2$$
2) Maximize the Margin
$$M = \frac{2}{|w|}$$
 same as minimize
$$\frac{1}{2}w^t w$$

- We can formulate a Quadratic Optimization Problem and solve for w and b
- Minimize $\Phi(w) = \frac{1}{2} w^t w$ subject to $y_i(wx_i + b) \ge 1$ $\forall i$

Solving the Optimization Problem

```
Find w and b such that \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} is minimized; and for all \{(\mathbf{x_i}, y_i)\}: y_i(\mathbf{w}^{\mathrm{T}} \mathbf{x_i} + b) \ge 1
```

- Need to optimize a quadratic function subject to linear constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems, and many (rather intricate) algorithms exist for solving them.
- The solution involves constructing a *dual problem* where a Lagrange multiplier α_i is associated with every constraint in the primary problem:

```
Find \alpha_1...\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}^T \mathbf{x_j} \text{ is maximized and}
(1) \sum \alpha_i y_i = 0
(2) \alpha_i \ge 0 for all \alpha_i
```

The Optimization Problem Solution

The solution has the form:

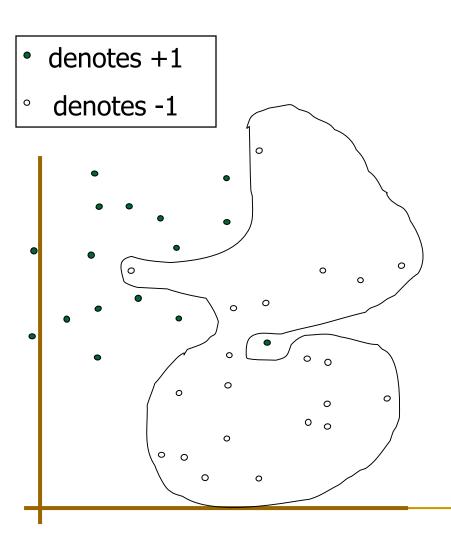
$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x_i}$$
 $b = y_k - \mathbf{w^T} \mathbf{x_k}$ for any $\mathbf{x_k}$ such that $\alpha_k \neq 0$

- Each non-zero $α_i$ indicates that corresponding $\mathbf{x_i}$ is a support vector.
- Then the classifying function will have the form:

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x_i}^{\mathsf{T}} \mathbf{x} + b$$

- Notice that it relies on an inner product between the test point x and the support vectors x_i – we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products x_i^Tx_j between all pairs of training points.

Dataset with noise

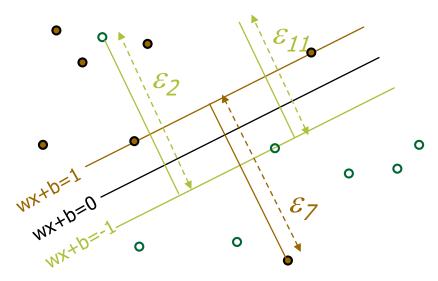


- Hard Margin: So far we require all data points be classified correctly
 - No training error
- What if the training set is noisy?
 - Solution 1: use very powerful kernels

OVERFITTING!

Soft Margin Classification

Slack variables ξi can be added to allow misclassification of difficult or noisy examples.



What should our quadratic optimization criterion be?

Minimize

$$\frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_{k=1}^{R} \varepsilon_k$$

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} is minimized and for all \{(\mathbf{x_i}, y_i)\} y_i (\mathbf{w}^{\mathrm{T}} \mathbf{x_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 \sum_{i} \xi_{i}  is minimized and for all \{(\mathbf{x_{i}}, y_{i})\}  y_{i} (\mathbf{w}^{\mathrm{T}} \mathbf{x_{i}} + b) \ge 1 - \xi_{i}  and \xi_{i} \ge 0 for all i
```

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

Linear SVMs: Overview

- The classifier is a separating hyperplane.
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points x_i are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation of the problem and in the solution training points appear only inside dot products:

Find $\alpha_1 ... \alpha_N$ such that

 $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_i y_i y_j x_i^T x_j$ is maximized and

- (1) $\sum \alpha_i y_i = 0$
- (2) $0 \le \alpha_i \le C$ for all α_i

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x_i}^{\mathsf{T}} \mathbf{x} + \mathbf{b}$$

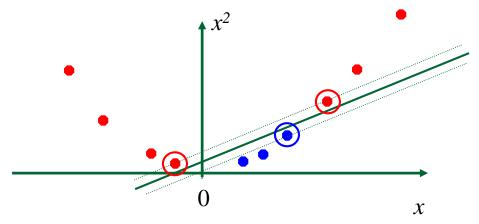
Non-linear SVMs

Datasets that are linearly separable with some noise work out great:

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

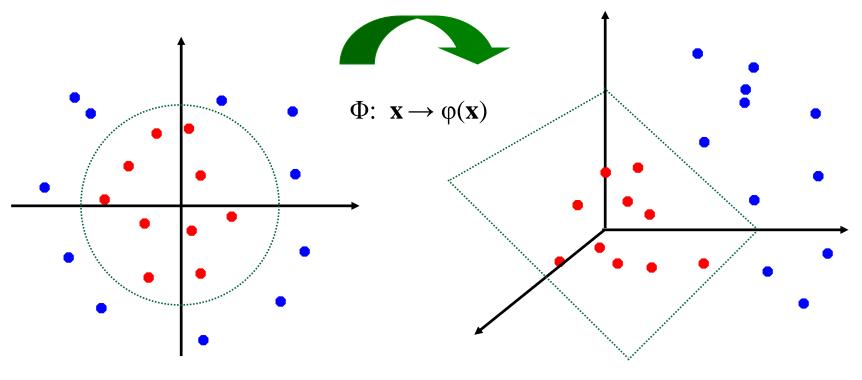


How about... mapping data to a higher-dimensional space:



Non-linear SVMs: Feature spaces

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



The "Kernel Trick"

- The linear classifier relies on dot product between vectors $K(x_i,x_j)=x_i^Tx_j$
- If every data point is mapped into high-dimensional space via some transformation Φ : $x \to \phi(x)$, the dot product becomes:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$$

- **A** *kernel function* is some function that corresponds to an inner product in some expanded feature space.
- Example:

2-dimensional vectors $\mathbf{x} = [x_1 \ x_2]$; let $K(\mathbf{x_i}, \mathbf{x_j}) = (1 + \mathbf{x_i}^T \mathbf{x_j})^2$, Need to show that $K(\mathbf{x_i}, \mathbf{x_j}) = \phi(\mathbf{x_i})^T \phi(\mathbf{x_j})$:

What Functions are Kernels?

- For some functions $K(\mathbf{x_i, x_j})$ checking that $K(\mathbf{x_i, x_j}) = \phi(\mathbf{x_i})^{\mathrm{T}} \phi(\mathbf{x_j}) \text{ can be cumbersome.}$
- Mercer's theorem:

Every semi-positive definite symmetric function is a kernel

Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

	$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x_1},\mathbf{x_2})$	$K(\mathbf{x}_1,\mathbf{x}_3)$	• • •	$K(\mathbf{x_1},\mathbf{x_N})$
K=		$K(\mathbf{x_2},\mathbf{x_2})$			$K(\mathbf{x_2},\mathbf{x_N})$
	• • •	• • •	•••	• • •	• • •
	$K(\mathbf{x_N},\mathbf{x_1})$	$K(\mathbf{x_N},\mathbf{x_2})$	$K(\mathbf{x_N},\mathbf{x_3})$	• • •	$K(\mathbf{x_N},\mathbf{x_N})$

Examples of Kernel Functions

- Linear: $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
- Polynomial of power p: K(x_i,x_j)= (1+ x_i ^Tx_j)^p
- Gaussian (radial-basis function network):

$$K(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\frac{\|\mathbf{x_i} - \mathbf{x_j}\|^2}{2\sigma^2})$$

• Sigmoid: $K(\mathbf{x_i}, \mathbf{x_i}) = \tanh(\beta_0 \mathbf{x_i}^T \mathbf{x_i} + \beta_1)$

Non-linear SVMs Mathematically

Dual problem formulation:

Find $\alpha_1...\alpha_N$ such that

$$Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$
 is maximized and

- (1) $\Sigma \alpha_i y_i = 0$
- (2) $\alpha_i \ge 0$ for all α_i

The solution is:

$$f(\mathbf{x}) = \sum \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j) + b$$

• Optimization techniques for finding α_i 's remain the same!

Nonlinear SVM - Overview

- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.

Properties of SVM

- Flexibility in choosing a similarity function
- Sparseness of solution when dealing with large data sets
 - only support vectors are used to specify the separating hyperplane
- Ability to handle large feature spaces
 - complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Nice math property: a simple convex optimization problem which is guaranteed to converge to a single global solution
- Feature Selection

SVM Applications

- SVM has been used successfully in many real-world problems
 - text (and hypertext) categorization
 - image classification
 - bioinformatics (Protein classification, Cancer classification)
 - hand-written character recognition

Application 1: Cancer Classification

- High Dimensional
 - p>1000; n<100
- Imbalanced
 - less positive samples

$$K[x,x] = k(x,x) + \lambda \frac{n^+}{N}$$

- Many irrelevant features
- Noisy

Genes							
Patients	g-1	g-2	••••	д-р			
P-1							
p-2							
p-n							

FEATURE SELECTION

In the linear case, w_i² gives the ranking of dim i

SVM is sensitive to noisy (mis-labeled) data 🕾

Weakness of SVM

- It is sensitive to noise
 - A relatively small number of mislabeled examples can dramatically decrease the performance
- It only considers two classes
 - how to do multi-class classification with SVM?
 - Answer:
 - 1) with output arity m, learn m SVM's
 - SVM 1 learns "Output==1" vs "Output != 1"
 - SVM 2 learns "Output==2" vs "Output != 2"
 - **-**:
 - SVM m learns "Output==m" vs "Output != m"
 - 2)To predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

Application 2: Text Categorization

- Task: The classification of natural text (or hypertext) documents into a fixed number of predefined categories based on their content.
 - email filtering, web searching, sorting documents by topic, etc..
- A document can be assigned to more than one category, so this can be viewed as a series of binary classification problems, one for each category

Representation of Text

IR's vector space model (aka bag-of-words representation)

- A doc is represented by a vector indexed by a pre-fixed set or dictionary of terms
- Values of an entry can be binary or weights

$$\phi_i(x) = \frac{\mathrm{tf}_i \mathrm{log}(\mathrm{idf}_i)}{\kappa},$$

- Normalization, stop words, word stems
- Doc $x => \phi(x)$

Text Categorization using SVM

- The distance between two documents is $\varphi(x) \cdot \varphi(z)$
- $K(x,z) = \langle \varphi(x) \cdot \varphi(z) \rangle$ is a valid kernel, SVM can be used with K(x,z) for discrimination.
- Why SVM?
 - -High dimensional input space
 - -Few irrelevant features (dense concept)
 - -Sparse document vectors (sparse instances)
 - -Text categorization problems are linearly separable

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

Additional Resources

- An excellent tutorial on VC-dimension and Support Vector Machines:
 - C.J.C. Burges. A tutorial on support vector machines for pattern recognition. Data Mining and Knowledge Discovery, 2(2):955-974, 1998.
- The VC/SRM/SVM Bible:

Statistical Learning Theory by Vladimir Vapnik, Wiley-Interscience; 1998

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

Reference

- Support Vector Machine Classification of Microarray Gene Expression Data, Michael P. S. Brown William Noble Grundy, David Lin, Nello Cristianini, Charles Sugnet, Manuel Ares, Jr., David Haussler
- www.cs.utexas.edu/users/mooney/cs391L/svm.ppt
- Text categorization with Support Vector Machines: learning with many relevant features
 - T. Joachims, ECML 98