MLEA : Machine Learning

Linear Support Vector Machines

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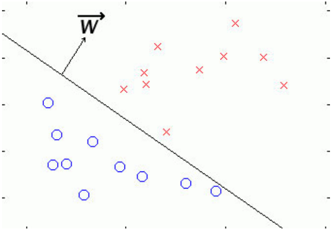
1. Linear Support Vector Machines
2. Linear Learning Machines
    - Perceptron
3. Soft Margin Linear SVM
4. Multiclass SVM
5. Bibliography

History

- Classifier derived from statistical Learning theory by Vapnick and Chervonenkis.
- Introduced in COLT[1]-1992 by Boser, Guyon and Vapnik
- Kernel Machines: Large class of learning algorithms, SVMs a particular instance
- Centralized website: www.kernel-machines.org
- Successful applications in many fields (text, image recognition, bioinformatics, ...)
- An important and active field of all Machine Learning research: A large and diverse community, machine learning, optimization, statistics, neural networks, functional analysis, etc.

[1] Annual Conference on Learning Theory

Linear Algebra



- Inner product between vectors :

$$< x, z >= x^T z = \sum_i x_i z_i$$

- Hyperplane:

$$< w, x > +b = 0$$

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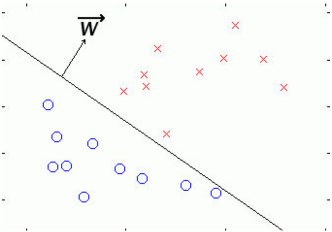
Linear Learning Machines

- Classification : Decision Function is a hyperplane in input space
- The Perceptron algorithm (Rosenblatt, 57)
- Useful to analyse the Perceptron algorithm, before looking at SVMs and Kernel Methods in general

Perceptron

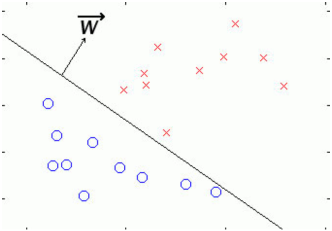


Linear Separation of the input space

$$f(x) = < w, x > +b$$

$$h(x) = \text{sign}\left(f\left(x\right)\right)$$

Perceptron Algorithm



Optimisation criteria:

$$\arg\min_{w,b} \|f(x) - y\|^2$$

Update rule :

if $y_i\,(< w_k, x_i > + b_k) \leq 0$ **then**

$$w_{k+1} \leftarrow w_k + \eta y_i x_i$$

Observations

- Solution is a linear combination of training points

$$w = \sum_i \alpha_i y_i x_i$$

$$\alpha_i \geq 0$$

- Only used informative points (mistake driven)
- The coefficient of a point in combination reflects its difficulty

Dual representation

- The decision function can be re-written as follows

$$f(x) =< w, x > +b = \sum_i \alpha_i y_i < x_i, x > +b$$

avec $w = \sum_i \alpha_i y_i x_i$

- and the update rule

$$\textbf{if } y_i \left(\sum_i \alpha_i y_i < x_i, x > +b \right) \leq 0 \textbf{ then } \alpha_i \longrightarrow \alpha_i + \eta$$

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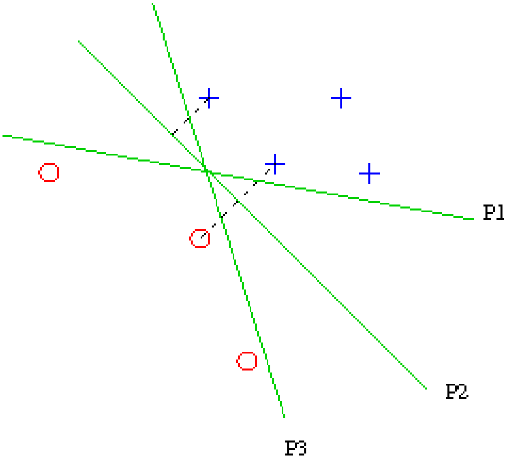
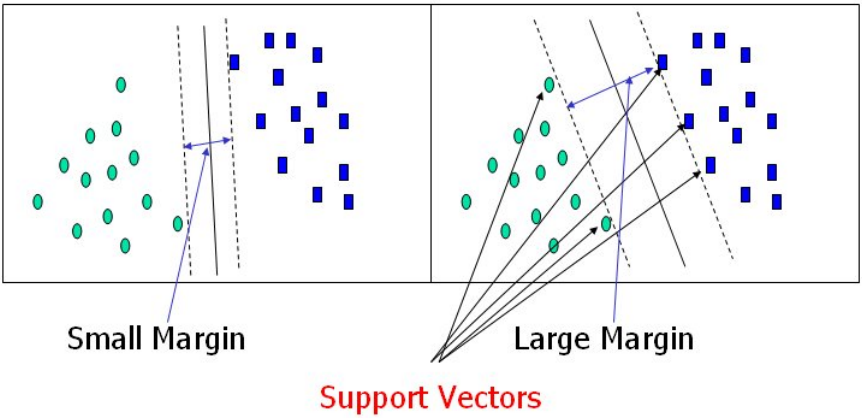
Note:

In dual representation, data appears only inside dot products

Separating Hyperplane

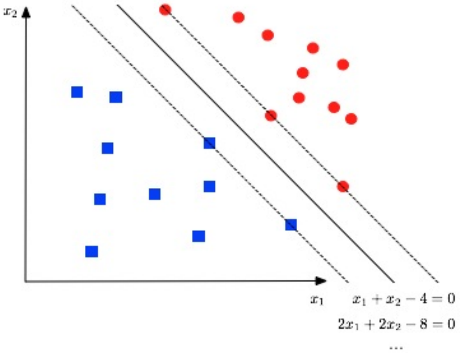


Margin and Support Vectors



Margin should be large

The decision boundary should be as far from the data as possible
$\Rightarrow$ the margin m should be maximized



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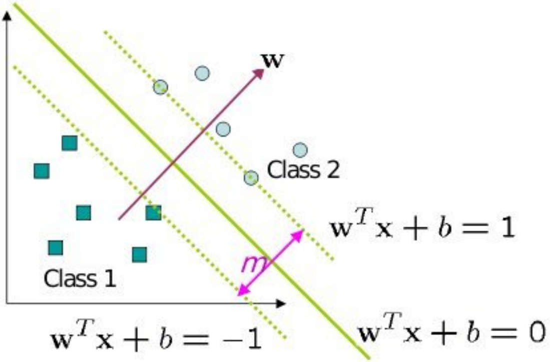
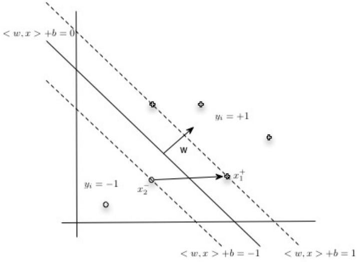


Margin as a function of the weight vector

Let's consider two support vectors x_1^+ et x_2^-:

$$
\begin{aligned}
< w, x_1^+ > +b &= 1 \qquad (1)\\
< w, x_2^- > +b &= -1 \qquad (2)
\end{aligned}
$$



$$
\begin{aligned}
Then \;\; < w, x_1^+ > - < w, x_2^- > &= 2\\
< w, x_1^+ - x_2^- > &= 2\\
\|w\| \|x_1^+ - x_2^-\| \cos\left(\vec{w}, \overrightarrow{x_2^- x_1^+}\right) &= 2\\
\|x_1^+ - x_2^-\| \cos\left(\vec{w}, \overrightarrow{x_2^- x_1^+}\right) &= \frac{2}{\|w\|}
\end{aligned}
$$

$$m = \frac{2}{||w||}$$

Hard Margin SVM Problem

- Let $x_1, \ldots, x_n$ be our dataset, and $y_i \in \{-1, 1\}$ the class label of x_i
- $\forall i, y_i(w^T x_i + b) \geq 1$
- Resolve the optimization problem:
  - **Maximize margin** $m = \frac{2}{||w||} \Rightarrow$ **Minimize norm** of the separating hyperplane $\frac{1}{2}||w||^2$
  - **Subject to** $y_i(w^T x_i + b) \geq 1$

Reformulation

- The problem could be reformulated using Lagrange Multiplier method as find $w, b, and \alpha = (\alpha_1, ..., \alpha_n) \neq 0$ and ≥ 0 minimizing:

$$L(\alpha, w, b) = \frac{1}{2}||w||^2 - \sum_i \alpha_i(y_i(w^T x_i + b) - 1)$$

- The maximum margin classifier will be found for $\frac{\partial L}{\partial w} = 0$ and $\frac{\partial L}{\partial b} = 0$
- Reformulate the problem

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- $\frac{\partial L}{\partial w} = 0 \Rightarrow w = \sum \alpha_i y_i x_i$
- $\frac{\partial L}{\partial b} = 0 \Rightarrow \sum y_i \alpha_i = 0$

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- Reformulate the problem
- $\frac{\partial L}{\partial w} = 0 \Rightarrow w = \sum \alpha_i y_i x_i$
- $\frac{\partial L}{\partial b} = 0 \Rightarrow \sum y_i \alpha_i = 0$
- $L(\alpha, w, b) = Q(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j < x_i, x_j >$

Proof

$$\begin{aligned} L(\alpha, w, b) &= \frac{1}{2}||w||^2 - \sum_i \alpha_i (y_i (w^T x_i + b) - 1) \\ &= \frac{1}{2}||w||^2 - w^T \sum_i \alpha_i y_i x_i - \sum_i \alpha_i y_i b + \sum_i \alpha_i \\ &= \frac{1}{2}||w||^2 - ||w||^2 - b * 0 + \sum_i \alpha_i \\ &= \sum_i \alpha_i - \frac{1}{2}||w||^2 \end{aligned}$$

Since

$$(\sum_{i=1}^{N} x_i)^2 = \sum_i \sum_j x_i x_j$$

then

$$L(\alpha, w, b) = Q(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j < x_i, x_j >$$

Support Vector

- Only the data near the hyperplane is usefull to train the classifier
- We don't need to take into account the data far from the hyperplane
- the elements that we will consider to build the hyperplane are called the support vectors
- We want to maximize

$$Q(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j < x_i, x_j >$$

with constraints

$$\alpha_i \geq 0$$

and

$$\sum_i \alpha_i y_i = 0$$

Support Vector

- this is a recurrent mathematical optimisation problem, many specialized heuristics have been designed to resolve it (SMO[2])
- the resulting decision function will be

$$f(x) = w^T x + b = \sum_i \alpha_i y_i < x_i, x > + b$$

[2] SMO: Sequential Minimal Optimization

Finding b

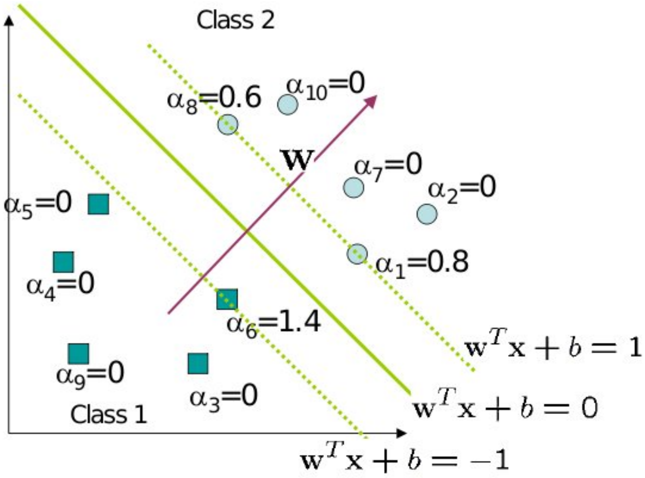
Once the α_i are computed, you know which elements are the support vectors.
For all support vector x_{SV}, $y_{SV} = w^T x_{SV} + b \Rightarrow b = y_{SV} - w^T x_{SV}$

For a better numerical stability, b can be averaged as:

$$b = \frac{1}{N_{SV}} \sum_{i \in SupportVectors} y_i - w^T x_i$$

with N_{SV} the number of support vectors

Considerations



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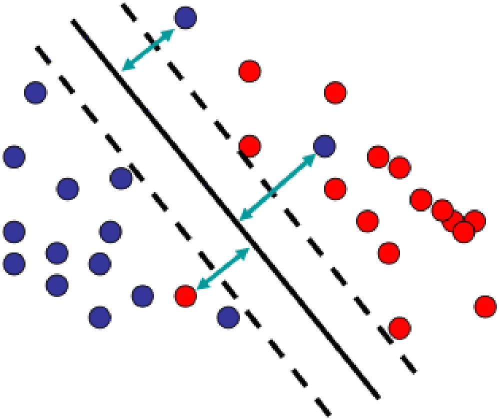
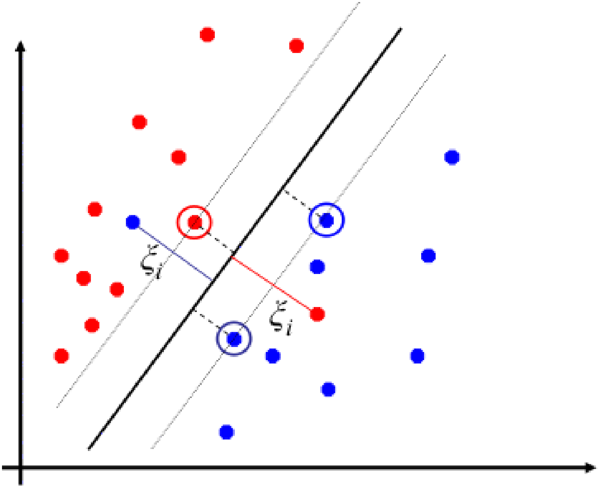
Dealing with noise



Minimizing Errors



Soft Margin SVM formulation

- Minimize $\frac{1}{2}||w||^2 + C\sum \xi_i$
- with $y_i(w^T x_i + b) \geq 1 - \xi_i$
- $\xi_i \geq 0$

Equivalent to maximizing

$$Q(\alpha) = \sum_i \alpha_i - \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j x_i^T x_j$$

with constraints

$$0 \leq \alpha_i \leq C$$

and

$$\sum_i \alpha_i y_i = 0$$

C intuitive meaning

- tradeoff parameter between error and margin

C intuitive meaning

- tradeoff parameter between error and margin
- http://www.svms.org/parameters/
- weighting data
- Deal with unbalanced dataset

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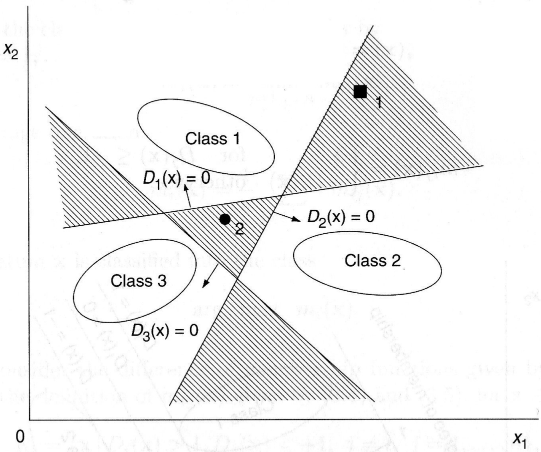
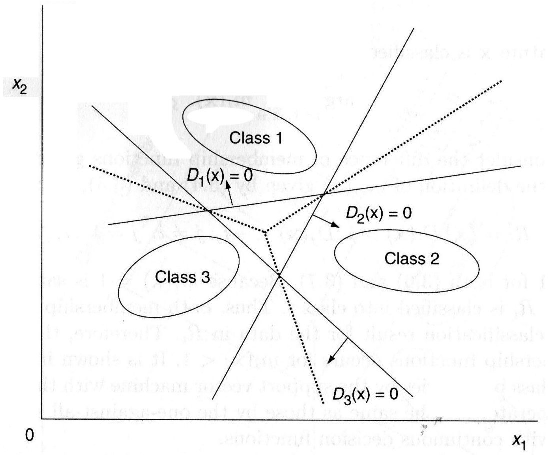
One Against Rest (OAR)

- Train N binary SVM with the whole dataset
- each SVM should discriminate one class versus all other

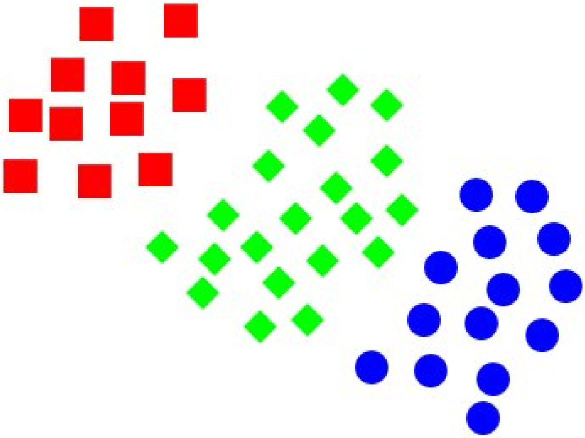
Unclassifiable Regions



Using Decision Function



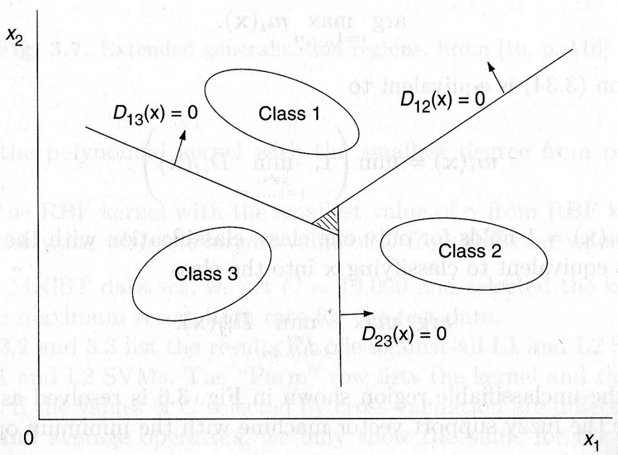
Unadapted Paradigm?



One Against One (OAO)

- build pairwise classifiers
- $\frac{N(N-1)}{2}$ binary classifiers
- decision done through a vote
- smaller training time (the observed speedup is between 3 and 9)
- bigger classification time

Draw...



Fuzzy OAO

Membership function

$m_{ij}(x) = 1$ for $D_{ij}(x) \geq 1$
$m_{ij}(x) = D_{ij}(x)$ otherwise

Minimum Operator

$m_i(x) = \min_{j \neq i} m_{ij}(x)$

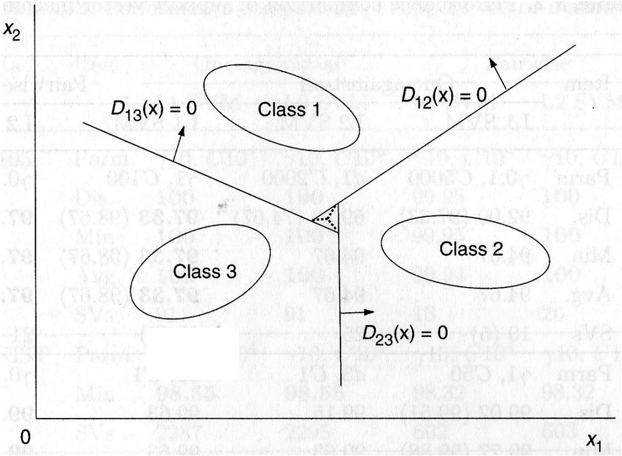
Average Operator

$m_i(x) = \frac{1}{n-1} \sum_{j \neq i} m_{ij}(x)$

Classification

$argmax(m_i(x))$

Resolution



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D. Tsujinishi, Y. Koshiba, and S. Abe.
Why pairwise is better than one-against-all or all-at-once.
Neural Networks, 2004. Proceedings. 2004 IEEE International Joint Conference on, 1, 2004.