MACHINE LEARNING

Support Vector Machines

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UNIVERSITAS ATHESINA STUDIORUM

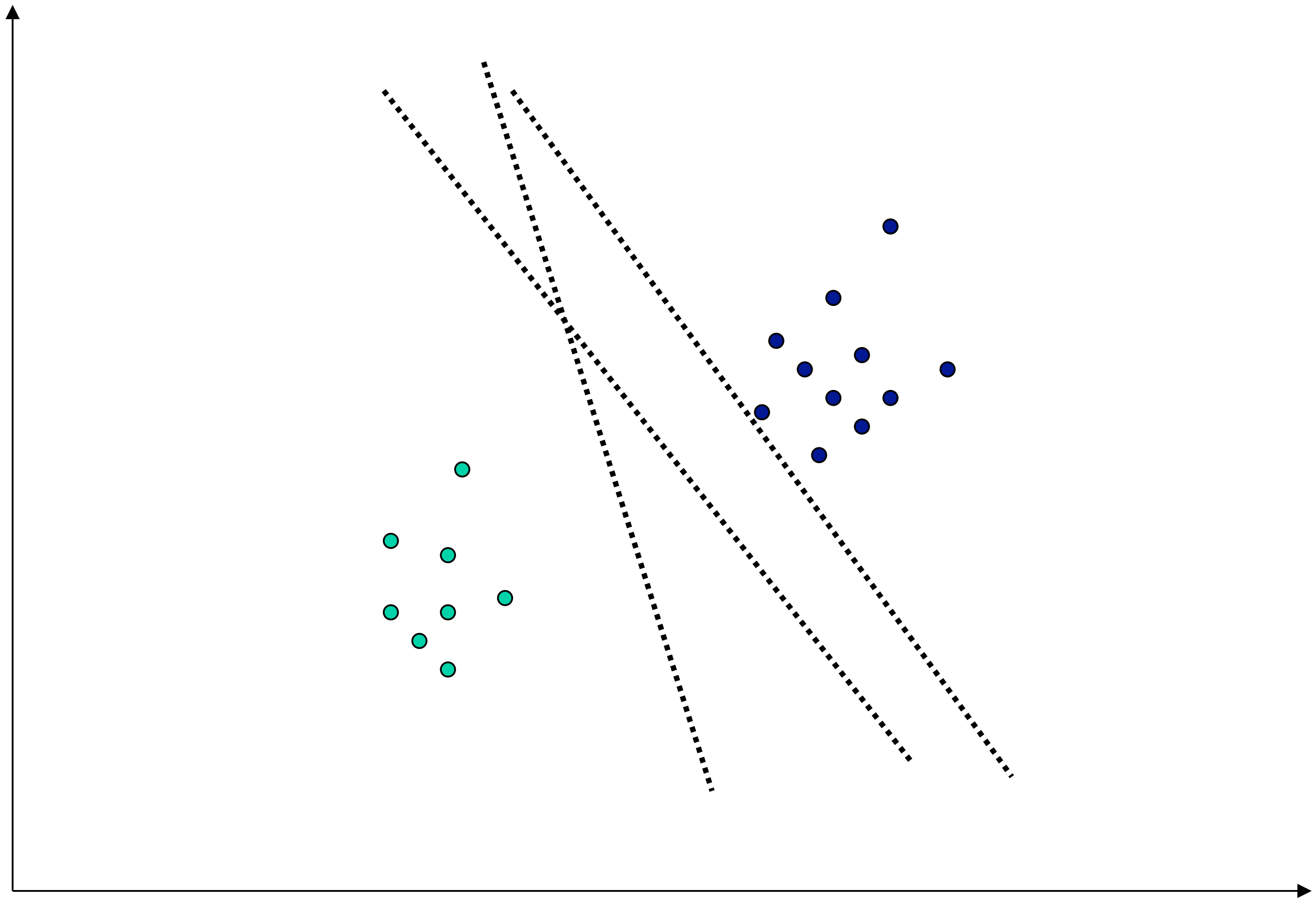
Summary

- Support Vector Machines
  - *Hard-margin SVMs*
  - *Soft-margin SVMs*

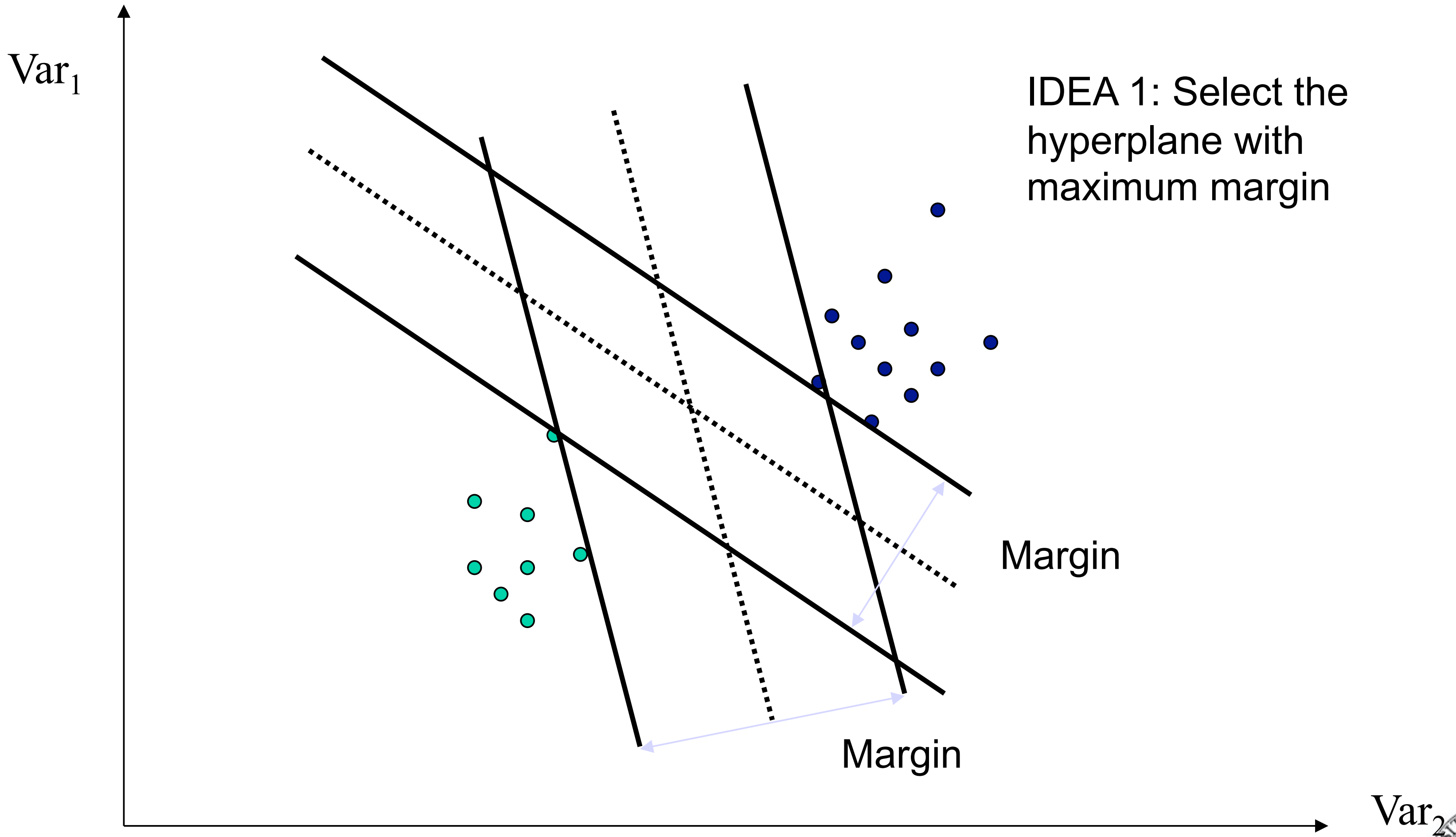
Communications

- No lecture tomorrow (neither Dec. 8)
- ML Exams
  - 12 January 2011 at 9:00,
  - 26 January 2011 at 9:00
- Exercise in Lab
  - A201 (Polo scientifico e tecnologico)
  - Wednesday 15 and 22 December, 2011
  - Time: 8.30-10.30

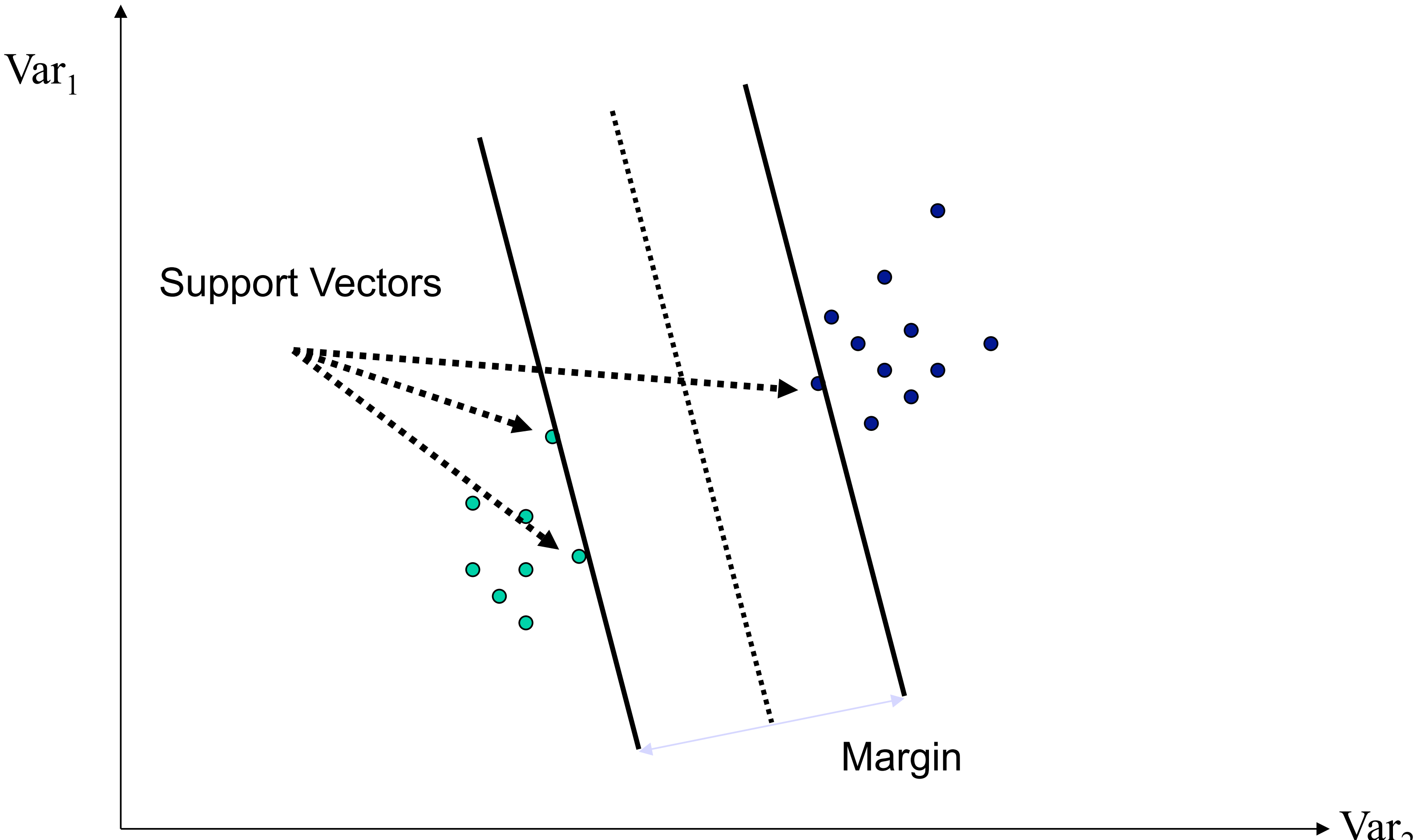
Which hyperplane choose?



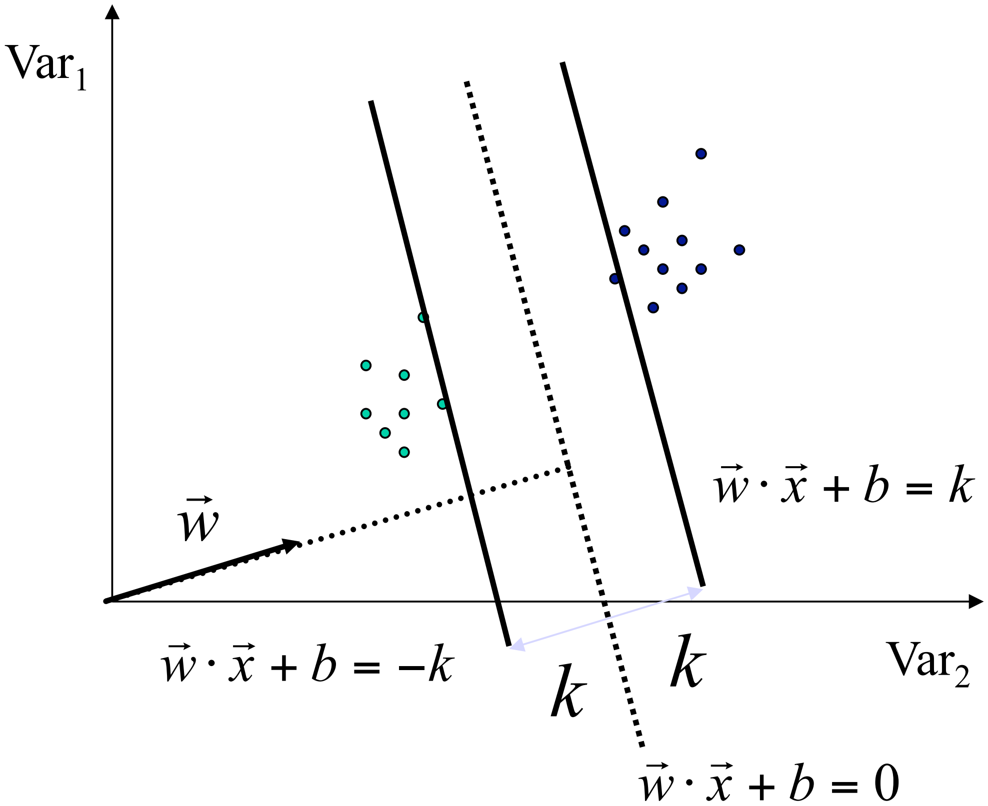
Classifier with a Maximum Margin



Support Vector

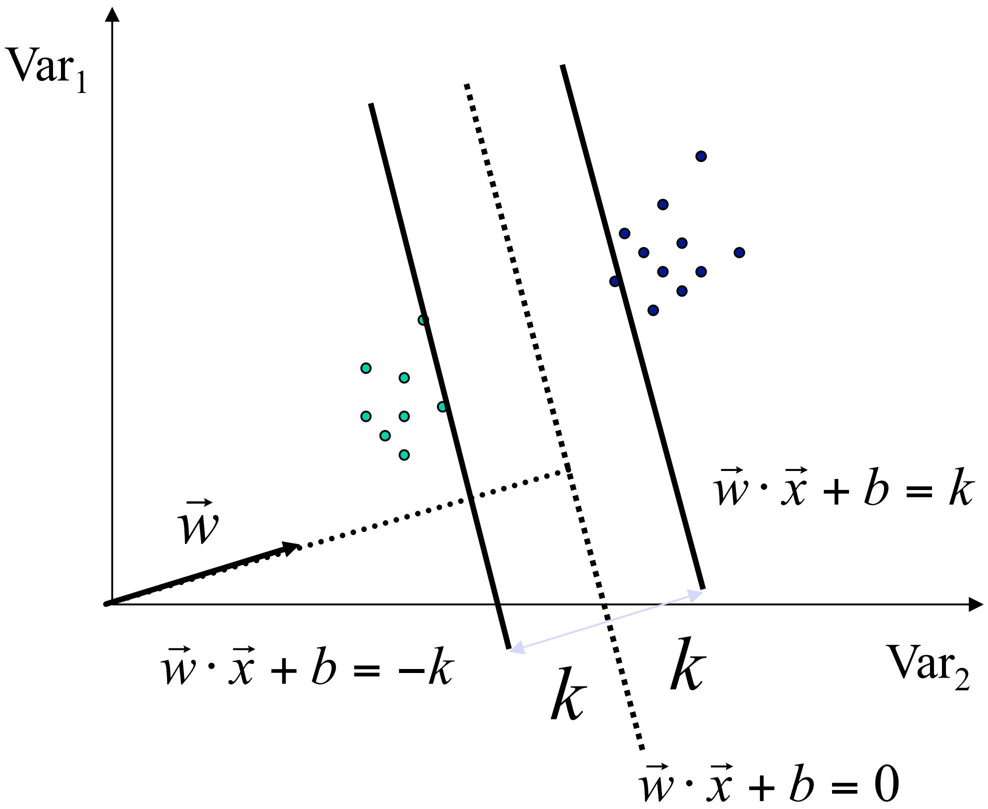


Support Vector Machine Classifiers



The margin is equal to $\dfrac{2|k|}{\|w\|}$

Support Vector Machines



The margin is equal to $\dfrac{2|k|}{\|w\|}$

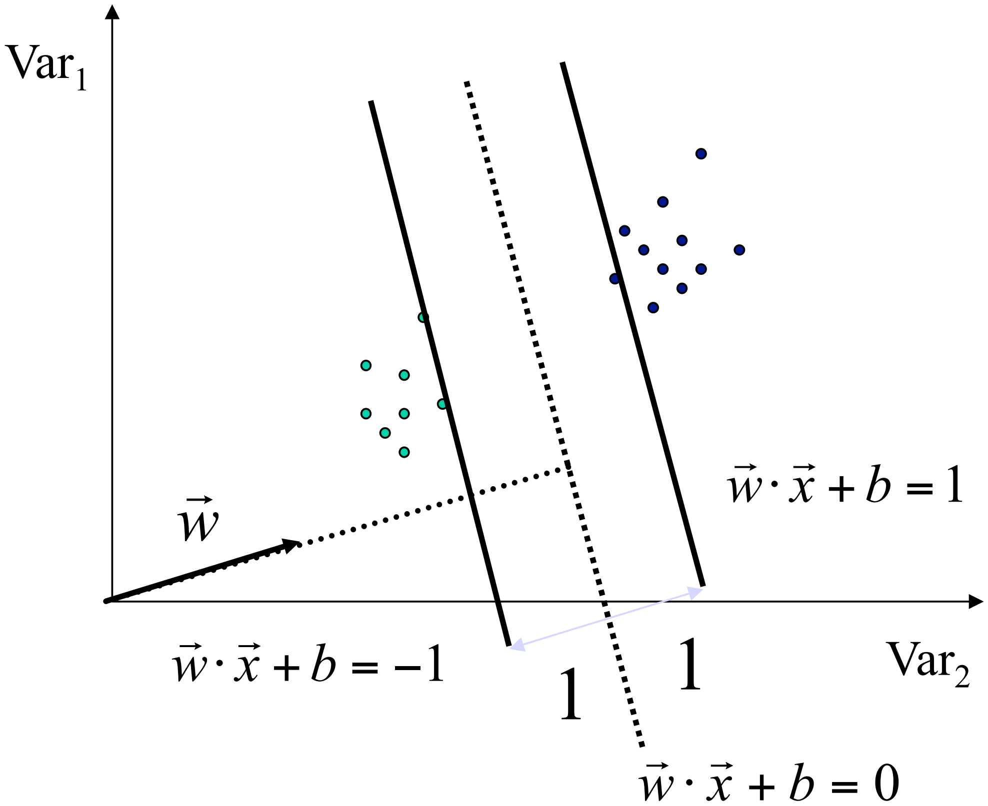
We need to solve

$$\max \frac{2|k|}{\|\vec{w}\|}$$

$$\vec{w}\cdot\vec{x}+b \geq +k, \ \text{ if } \vec{x} \text{ is positive}$$

$$\vec{w}\cdot\vec{x}+b \leq -k, \ \text{ if } \vec{x} \text{ is negative}$$

Support Vector Machines



There is a scale for which *k=1*.

The problem transforms in:

$$\max \frac{2}{\|\vec{w}\|}$$

$$\vec{w}\cdot\vec{x}+b\geq +1,\ \text{ if } \vec{x} \text{ is positive}$$

$$\vec{w}\cdot\vec{x}+b\leq -1,\ \text{ if } \vec{x} \text{ is negative}$$

Final Formulation

$$\max \frac{2}{\|\vec{w}\|}$$
$$\vec{w} \cdot \vec{x}_i + b \geq +1, \quad y_i = 1$$
$$\vec{w} \cdot \vec{x}_i + b \leq -1, \quad y_i = -1$$

$$\Rightarrow \quad \max \frac{2}{\|\vec{w}\|} \quad y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1 \quad \Rightarrow$$

$$\Rightarrow \quad \min \frac{\|\vec{w}\|}{2} \quad y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

$$\Rightarrow \quad \min \frac{\|\vec{w}\|^2}{2} \quad y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

Optimization Problem

- Optimal Hyperplane:
  - Minimize $\tau(\vec{w}) = \frac{1}{2}\|\vec{w}\|^2$
  - Subject to $y_i((\vec{w} \cdot \vec{x}_i) + b) \geq 1, i = 1, \ldots, m$
- The dual problem is simpler

Lagrangian Definition

Def. 2.24 *Let* $f(\vec{w})$, $h_i(\vec{w})$ *and* $g_i(\vec{w})$ *be the objective function, the equality constraints and the inequality constraints (i.e.* ≤*) of an optimization problem, and let* $L(\vec{w}, \vec{\alpha}, \vec{\beta})$ *be its Lagrangian, defined as follows:*

$$L(\vec{w}, \vec{\alpha}, \vec{\beta}) = f(\vec{w}) + \sum_{i=1}^{m} \alpha_i g_i(\vec{w}) + \sum_{i=1}^{l} \beta_i h_i(\vec{w})$$

Dual Optimization Problem

The **Lagrangian dual problem** *of the above primal problem is*

$$maximize \quad \theta(\vec{\alpha}, \vec{\beta})$$

$$subject\ \ to \quad \vec{\alpha} \geq \vec{0}$$

where $\theta(\vec{\alpha}, \vec{\beta}) = inf_{w \in W} \quad L(\vec{w}, \vec{\alpha}, \vec{\beta})$

Dual Transformation

- Given the Lagrangian associated with our problem

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}\vec{w} \cdot \vec{w} - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x}_i + b) - 1]$$

- To solve the dual problem we need to evaluate:

$$\theta(\vec{\alpha}, \vec{\beta}) = inf_{w \in W} \; L(\vec{w}, \vec{\alpha}, \vec{\beta})$$

- Let us impose the derivatives to 0, with respect to $\vec{w}$

$$\frac{\partial L(\vec{w}, b, \vec{\alpha})}{\partial \vec{w}} = \vec{w} - \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i = \vec{0} \quad \Rightarrow \quad \vec{w} = \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i$$

Dual Transformation (cont'd)

- and wrt *b*

$$\frac{\partial L(\vec{w}, b, \vec{\alpha})}{\partial b} = \sum_{i=1}^{m} y_i \alpha_i = 0$$

- Then we substituted them in the Lagrange function

$$\begin{aligned} L(\vec{w}, b, \vec{\alpha}) &= \frac{1}{2}\vec{w} \cdot \vec{w} - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1] = \\ &= \frac{1}{2}\sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} - \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} + \sum_{i=1}^{m} \alpha_i \\ &= \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} \end{aligned}$$

Final Dual Problem

$$\begin{aligned} &maximize && \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} \\ &subject\ \ to && \alpha_i \geq 0, \quad i = 1, .., m \\ & && \sum_{i=1}^{m} y_i \alpha_i = 0 \end{aligned}$$

Khun-Tucker Theorem

- Necessary and sufficient conditions to optimality

$$
\begin{aligned}
\frac{\partial L(\vec{w}^*, \vec{\alpha}^*, \vec{\beta}^*)}{\partial \vec{w}} &= \vec{0} \\
\frac{\partial L(\vec{w}^*, \vec{\alpha}^*, \vec{\beta}^*)}{\partial b} &= \vec{0} \\
\alpha_i^* g_i(\vec{w}^*) &= 0, \qquad i = 1, .., m \\
g_i(\vec{w}^*) &\leq 0, \qquad i = 1, .., m \\
\alpha_i^* &\geq 0, \qquad i = 1, .., m
\end{aligned}
$$

Properties coming from constraints

- Lagrange constraints: $\sum_{i=1}^{m} a_i y_i = 0 \qquad \vec{w} = \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i$
- Karush-Kuhn-Tucker constraints

$$\alpha_i \cdot [y_i(\vec{x}_i \cdot \vec{w} + b) - 1] = 0, \quad i = 1,\ldots,m$$

- Support Vectors have α_i not null
- To evaluate *b,* we can apply the following equation

$$b^* = -\frac{\vec{w}^* \cdot \vec{x}^+ + \vec{w}^* \cdot \vec{x}^-}{2}$$

Warning!

- On the graphical examples, we always consider normalized hyperplane (hyperplanes with normalized gradient)
- b in this case is exactly the distance of the hyperplane from the origin
- So if we have an equation not normalized we may have

  $\vec{x} \cdot \vec{w}' + b = 0$ with $\vec{x} = (x, y)$ and $\vec{w}' = (1,1)$
- and b is not the distance

Warning!

- Let us consider a normalized gradient

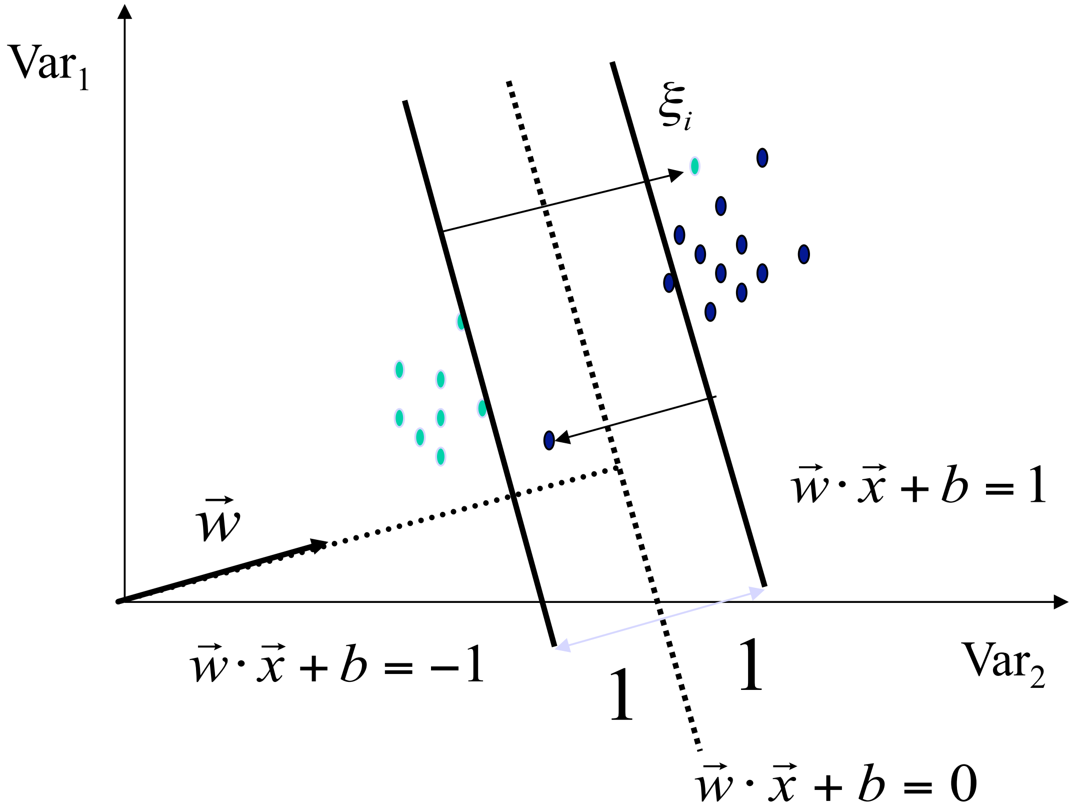
$$\vec{w} = \left(1/\sqrt{2}, 1/\sqrt{2}\right)$$

$$(x,y)\cdot\left(1/\sqrt{2}, 1/\sqrt{2}\right) + b = 0 \Rightarrow x/\sqrt{2} + y/\sqrt{2} = -b$$

$$\Rightarrow y = -x - b\sqrt{2}$$

- Now we see that *-b* is exactly the distance.
- For $x = 0$, we have the intersection with $-b\sqrt{2}$. This distance projected on $\vec{w}$ is *-b*

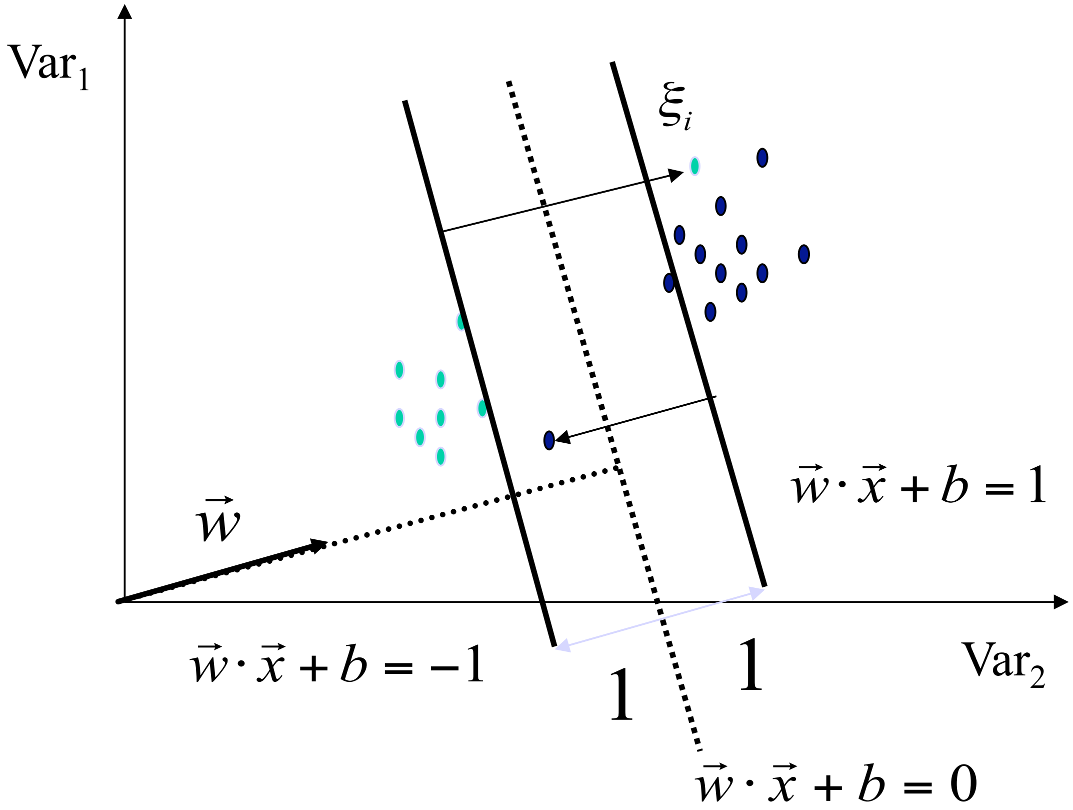
Soft Margin SVMs



ξ_i slack variables are added

Some errors are allowed but they should penalize the objective function

Soft Margin SVMs



The new constraints are

$$y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1 - \xi_i$$
$$\forall \vec{x}_i \quad \text{where} \quad \xi_i \geq 0$$

The objective function penalizes the incorrect classified examples

$$\min \frac{1}{2} \| \vec{w} \|^2 + C \sum_i \xi_i$$

C is the trade-off between margin and the error

Dual formulation

$$\begin{cases} min \quad \frac{1}{2}||\vec{w}|| + C\sum_{i=1}^{m} \xi_i^2 \\ y_i(\vec{w} \cdot \vec{x_i} + b) \geq 1 - \xi_i, \quad \forall i = 1,..,m \\ \xi_i \geq 0, \quad i = 1,..,m \end{cases}$$

$$L(\vec{w}, b, \vec{\xi}, \vec{\alpha}) = \frac{1}{2}\vec{w} \cdot \vec{w} + \frac{C}{2}\sum_{i=1}^{m} \xi_i^2 - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1 + \xi_i],$$

- By deriving wrt $\vec{w}$,$\vec{\xi}$ and b

Partial Derivatives

$$\frac{\partial L(\vec{w}, b, \vec{\xi}, \vec{\alpha})}{\partial \vec{w}} = \vec{w} - \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i = \vec{0} \quad \Rightarrow \quad \vec{w} = \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i$$

$$\frac{\partial L(\vec{w}, b, \vec{\xi}, \vec{\alpha})}{\partial \vec{\xi}} = C\vec{\xi} - \vec{\alpha} = \vec{0}$$

$$\frac{\partial L(\vec{w}, b, \vec{\xi}, \vec{\alpha})}{\partial b} = \sum_{i=1}^{m} y_i \alpha_i = 0$$

Substitution in the objective function

$$
\begin{aligned}
&= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} + \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} - \frac{1}{C} \vec{\alpha} \cdot \vec{\alpha} = \\
&= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} - \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} = \\
&= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left(\vec{x_i} \cdot \vec{x_j} + \frac{1}{C} \delta_{ij} \right),
\end{aligned}
$$

- δ_{ij} of Kronecker

Final dual optimization problem

$$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left(\vec{x_i} \cdot \vec{x_j} + \frac{1}{C}\delta_{ij}\right)$$

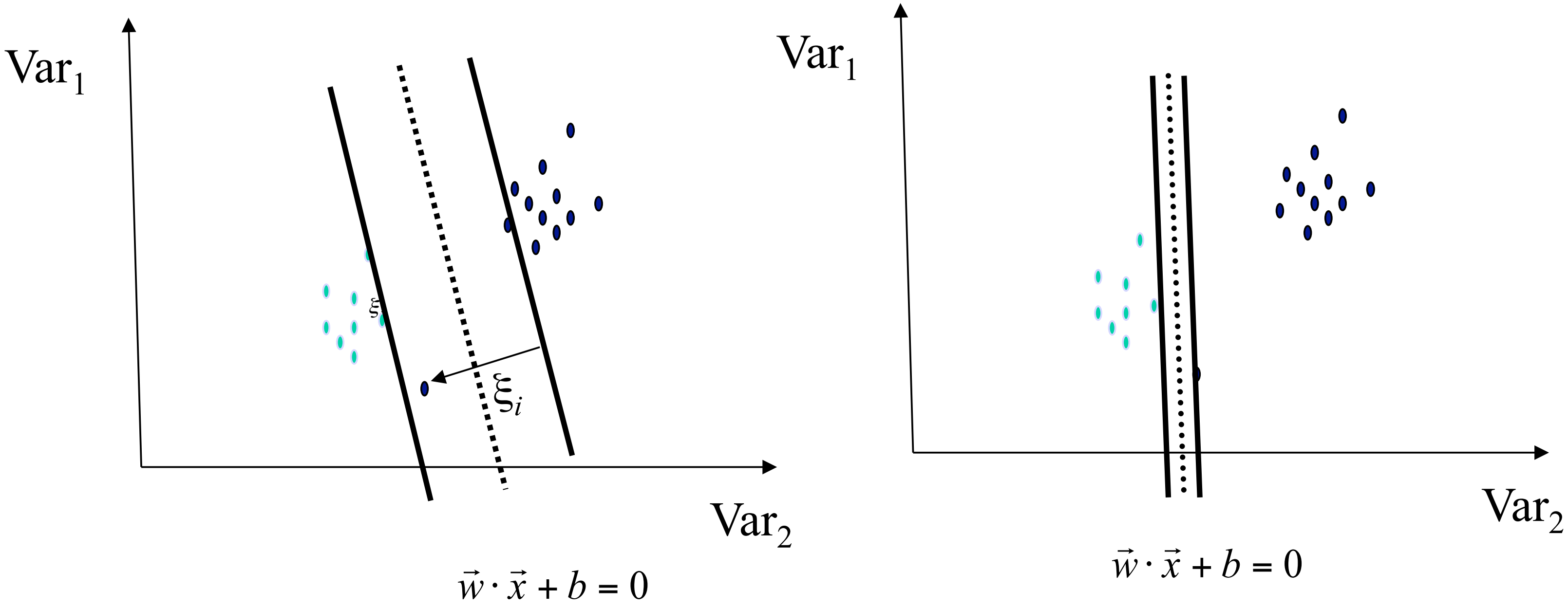
$$\alpha_i \geq 0, \quad \forall i = 1, .., m$$
$$\sum_{i=1}^{m} y_i \alpha_i = 0$$

Soft Margin Support Vector Machines

$$\min \frac{1}{2} \| \vec{w} \|^2 + C \sum_i \xi_i \qquad \begin{array}{l} y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1 - \xi_i \quad \forall \vec{x}_i \\ \xi_i \geq 0 \end{array}$$

- The algorithm tries to keep ξ_i low and maximize the margin
- NB: The number of error is not directly minimized (NP-complete problem); the distances from the hyperplane are minimized
- If $C \to \infty$, the solution tends to the one of the *hard-margin* algorithm
- *Attention !!!:* if $C = 0$ we get $\| \vec{w} \| = 0$, since $y_i b \geq 1 - \xi_i \quad \forall \vec{x}_i$
- If C increases the number of error decreases. When C tends to infinite the number of errors must be 0, i.e. the *hard-margin* formulation

Robusteness of *Soft* vs. *Hard Margin* SVMs



Soft Margin SVM

Hard Margin SVM

Soft vs Hard Margin SVMs

- *Soft-Margin* has ever a solution
- Soft-Margin is more robust to odd examples
- *Hard-Margin* does not require parameters

Parameters

$$\min \frac{1}{2} \|\vec{w}\|^2 + C \sum_i \xi_i = \min \frac{1}{2} \|\vec{w}\|^2 + C^+ \sum_i \xi_i^+ + C^- \sum_i \xi_i^-$$

$$= \min \frac{1}{2} \|\vec{w}\|^2 + C \left(J \sum_i \xi_i^+ + \sum_i \xi_i^- \right)$$

- C: trade-off parameter
- J: cost factor

Theoretical Justification

Definition of Training Set error

- Training Data

$$f : R^N \rightarrow \{\pm 1\} \qquad (\vec{x}_1, y_1), \ldots, (\vec{x}_m, y_m) \in R^N \times \{\pm 1\}$$

- Empirical Risk (error)

$$R_{emp}[f] = \tfrac{1}{m} \sum_{i=1}^{m} \tfrac{1}{2} \left| f(\vec{x}_i) - y_i \right|$$

- Risk (error)

$$R[f] = \int \frac{1}{2} \left| f(\vec{x}) - y \right| dP(\vec{x}, y)$$

Error Characterization (part 1)

- From PAC-learning Theory (***Vapnik***):

$$R(\alpha) \leq R_{emp}(\alpha) + \varphi(\tfrac{d}{m}, \tfrac{\log(\delta)}{m})$$

$$\varphi(\tfrac{d}{m}, \tfrac{\log(\delta)}{m}) = \sqrt{\frac{d(\log\frac{2m}{d}+1)-\log(\frac{\delta}{4})}{m}}$$

where d is theVC-dimension, m is the number of examples, δ is a bound on the probability to get such error and α is a classifier parameter.

There are many versions for different bounds

Theorem 2.11 *(Vapnik and Chervonenkis, [Vapnik, 1995])*
Let H be a hypothesis space having VC dimension d. For any probability distribution D on $X \times \{-1, 1\}$, with probability $1-\delta$ over m random examples S, any hypothesis $h \in H$ that is consistent with S has error no more than

$$error(h) \leq \epsilon(m, H, \delta) = \frac{2}{m}\left(d \times ln\frac{2e \times m}{d} + ln\frac{2}{\delta}\right),$$

provided that $d \leq m$ and $m \geq 2/\epsilon$.

Error Characterization (part 2)

Lemma 1. [Vapnik, 1982] *Consider hyperplanes* $h(\vec{d}) = sign\{\vec{w} \cdot \vec{d} + b\}$ *as hypotheses. If all example vectors* $\vec{d}_i$ *are contained in a ball of radius* R *and it is required that for all examples* $\vec{d}_i$

$$|\vec{w} \cdot \vec{d}_i + b| \geq 1, \ with \ ||\vec{w}|| = A \tag{5}$$

then this set of hyperplane has a VCdim d *bounded by*

$$d \leq min([R^2 A^2], n) + 1 \tag{6}$$

Ranking, Regression and Multiclassification

The Ranking SVM
[Herbrich et al. 1999, 2000; Joachims et al. 2002]

- The aim is to classify instance pairs as correctly ranked or incorrectly ranked
  - This turns an ordinal regression problem back into a binary classification problem
- We want a ranking function *f* such that

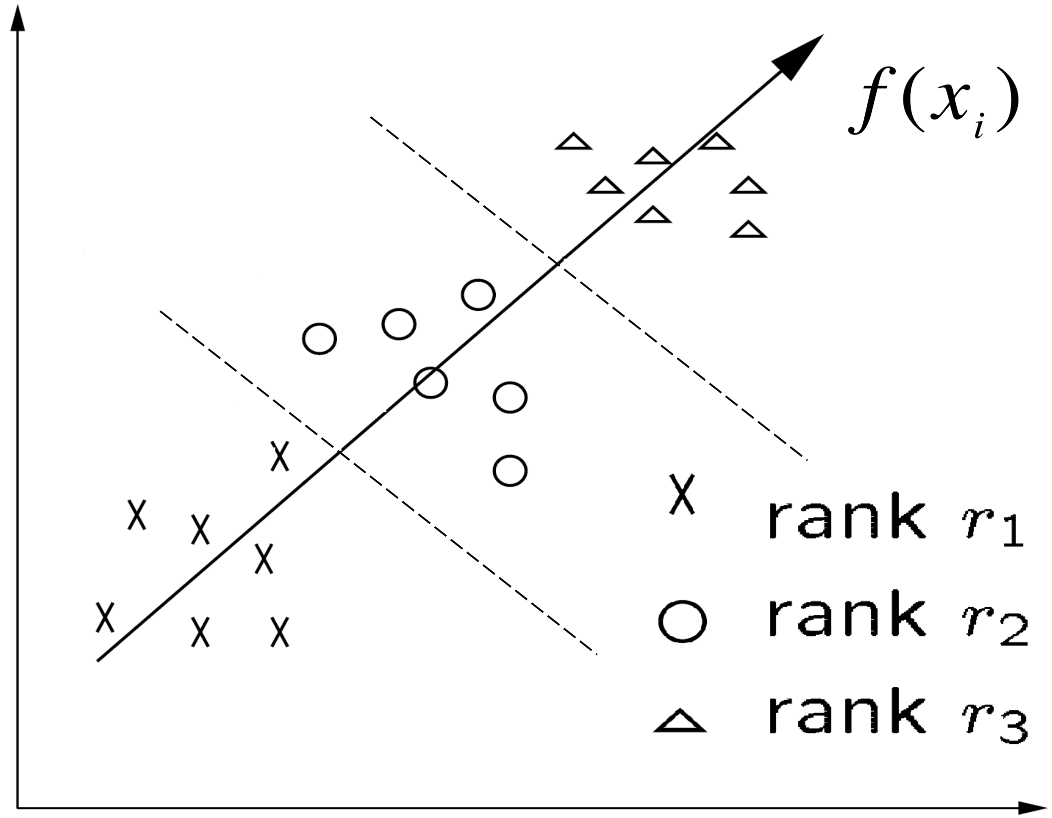
$$\boldsymbol{x}_i > \boldsymbol{x}_j \text{ iff } f(\boldsymbol{x}_i) > f(\boldsymbol{x}_j)$$

- … or at least one that tries to do this with minimal error
- Suppose that *f* is a linear function

$$f(\boldsymbol{x}_i) = \mathbf{w} \bullet \boldsymbol{x}_i$$

The Ranking SVM

- Ranking Model: $f(\boldsymbol{x}_i)$



The Ranking SVM

- Then (combining the two equations on the last slide):

$$\boldsymbol{x}_i > \boldsymbol{x}_j \text{ iff } \mathbf{w}\bullet\boldsymbol{x}_i - \mathbf{w}\bullet\ \boldsymbol{x}_j > 0$$

$$\boldsymbol{x}_i > \boldsymbol{x}_j \text{ iff } \mathbf{w}\bullet(\boldsymbol{x}_i - \boldsymbol{x}_j) > 0$$

- Let us then create a new instance space from such pairs: $z_k = x_i - x_k$

$$y_k = +1, -1 \text{ as } \boldsymbol{x}_i \geq , < \boldsymbol{x}_k$$

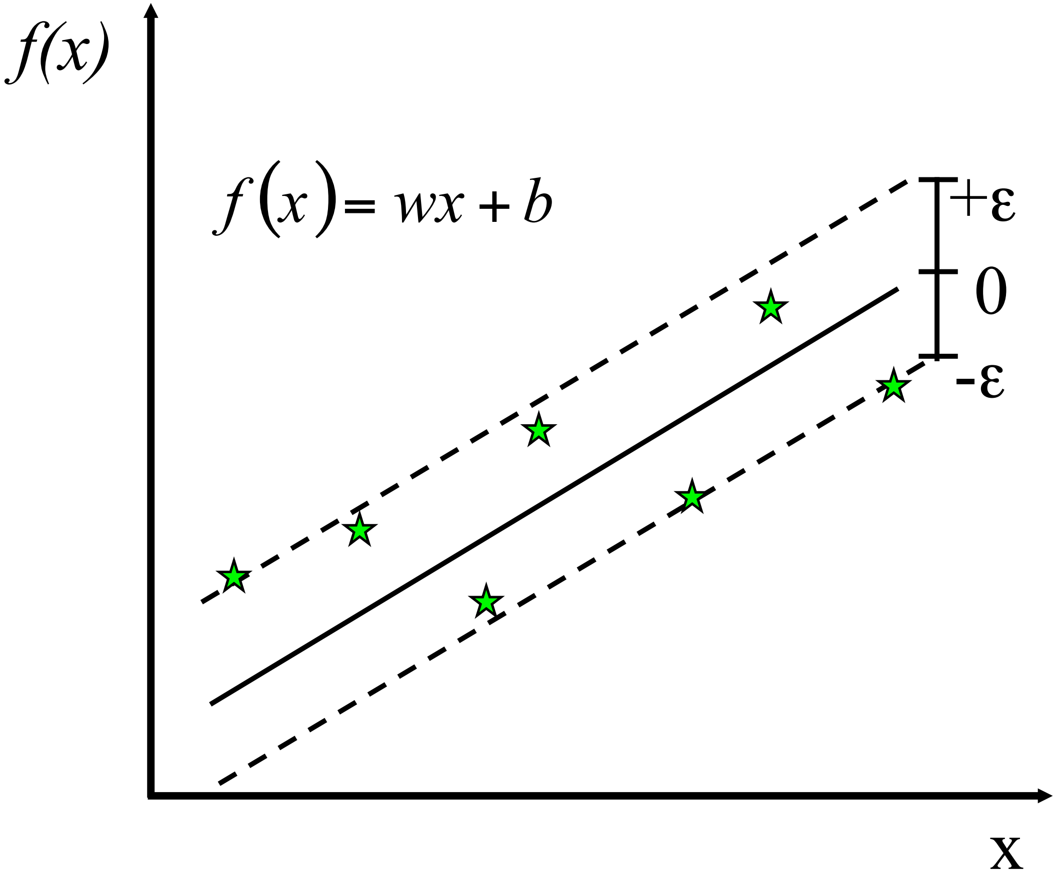
Support Vector Ranking

$$\begin{cases} min \quad \frac{1}{2}||\vec{w}|| + C\sum_{i=1}^{m}\xi_i^2 \\ y_k(\vec{w}\cdot(\vec{x_i}-\vec{x_j})+b) \geq 1-\xi_k, \quad \forall i,j=1,..,m \\ \xi_k \geq 0, \quad k=1,..,m^2 \end{cases}$$

y_k = 1 if $rank(\vec{x_i}) > rank(\vec{x_j})$,–1otherwise, where $k = i \times m + j$

- Given two examples we build one example (x_i , x_j)

Support Vector Regression (SVR)



Solution:

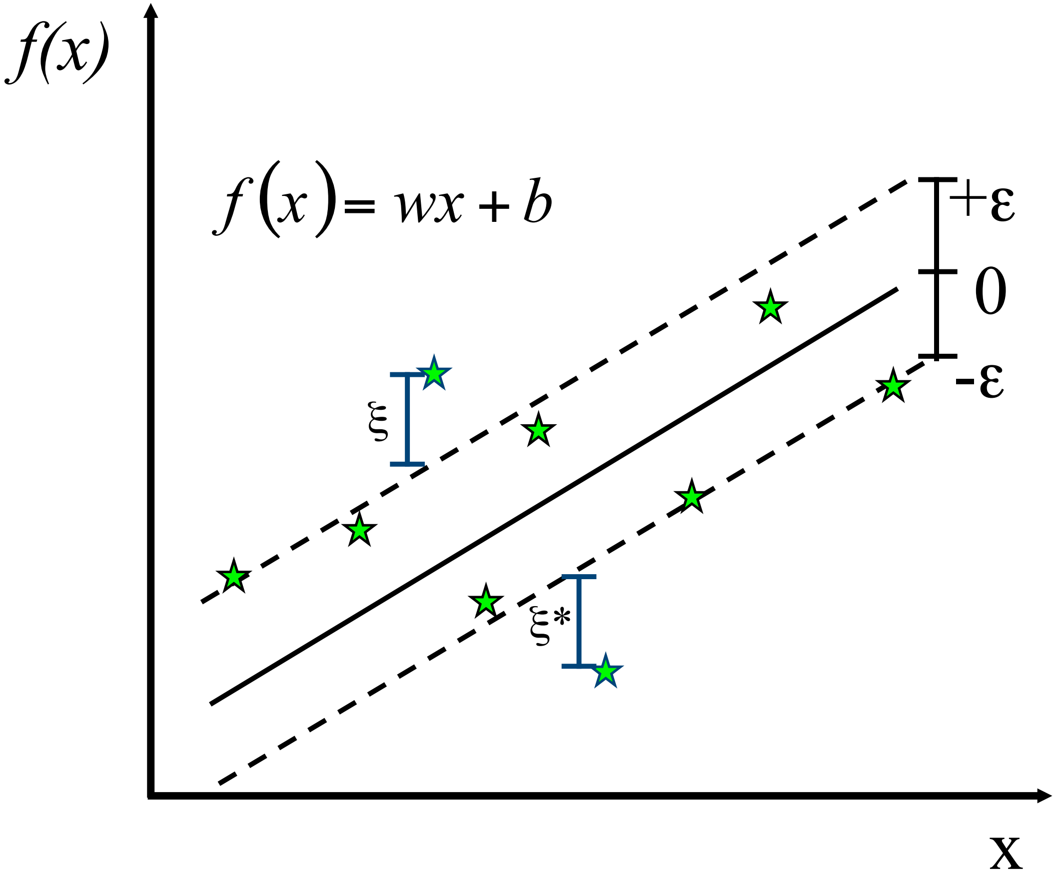
$$Min \frac{1}{2} w^T w$$

Constraints:

$$y_i - w^T x_i - b \leq \varepsilon$$

$$w^T x_i + b - y_i \leq \varepsilon$$

Support Vector Regression (SVR)



Minimise:

$$\frac{1}{2} w^T w + \boxed{C \sum_{i=1}^{N} \left(\xi_i + \xi_i^* \right)}$$

Constraints:

$$y_i - w^T x_i - b \le \varepsilon \boxed{+ \xi_i}$$

$$w^T x_i + b - y_i \le \varepsilon \boxed{+ \xi_i^*}$$

$$\boxed{\xi_i, \xi_i^* \ge 0}$$

Support Vector Regression

$$\min_{\mathbf{w},b,\xi,\xi^*} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i^*)$$

$$\begin{aligned} \text{s.t. } & y_i - \mathbf{w}^\top \mathbf{x}_i - b \leq \epsilon + \xi_i, \ \xi_i \geq 0 \quad \forall 1 \leq i \leq n; \\ & \mathbf{w}^\top \mathbf{x}_i + b - y_i \leq \epsilon + \xi_i^*, \ \xi_i^* \geq 0 \quad \forall 1 \leq i \leq n. \end{aligned}$$

- y_i is not -1 or 1 anymore, now it is a value
- ε is the tollerance of our function value

From Binary to Multiclass classifiers

- Three different approaches:
- **ONE-vs-ALL (OVA)**
  - Given the example sets, {E1, E2, E3, …} for the categories: {C1, C2, C3,…} the binary classifiers: {b1, b2, b3,…} are built.
  - For b1, E1 is the set of positives and E2∪E3 ∪… is the set of negatives, and so on
  - For testing: given a classification instance x, the category is the one associated with the maximum margin among all binary classifiers

From Binary to Multiclass classifiers

- **ALL-vs-ALL (AVA)**
  - Given the examples: {E1, E2, E3, …} for the categories {C1, C2, C3,…}
    - build the binary classifiers:

      {b1_2, b1_3,…, b1_n, b2_3, b2_4,…, b2_n,…,bn-1_n}
    - by learning on E1 (positives) and E2 (negatives), on E1 (positives) and E3 (negatives) and so on…
  - For testing: given an example x,
    - all the votes of all classifiers are collected
    - where $b_{E1E2} = 1$ means a vote for C1 and $b_{E1E2} = -1$ is a vote for C2
  - Select the category that gets more votes

From Binary to Multiclass classifiers

- **Error Correcting Output Codes** (ECOC)
  - The training set is partitioned according to binary sequences (codes) associated with category sets.
    - For example, 10101 indicates that the set of examples of C1,C3 and C5 are used to train the C_{10101} classifier.
    - The data of the other categories, i.e. C2 and C4 will be negative examples
  - In testing: the code-classifiers are used to decode one the original class, e.g.

    $C_{10101} = 1$ and $C_{11010} = 1$ indicates that the instance belongs to C1

  That is, the only one consistent with the codes

SVM-light: an implementation of SVMs

- Implements soft margin
- Contains the procedures for solving optimization problems
- Binary classifier
- Examples and descriptions in the web site:

  http://www.joachims.org/

  (http://svmlight.joachims.org/)

References

- *A tutorial on Support Vector Machines for Pattern Recognition*
  - **Downloadable article (Chriss Burges)**
- *The Vapnik-Chervonenkis Dimension and the Learning Capability of Neural Nets*
  - **Downloadable Presentation**
- Computational Learning Theory
  (Sally A Goldman Washington University St. Louis Missouri)
  - **Downloadable Article**
- *AN INTRODUCTION TO SUPPORT VECTOR MACHINES*
  (and other kernel-based learning methods)
  N. Cristianini and J. Shawe-Taylor Cambridge University Press
  - **Check our library**
- *The Nature of Statistical Learning Theory*
  Vladimir Naumovich Vapnik - Springer Verlag (December, 1999)
  - **Check our library**