MACHINE LEARNING

Support Vector Machines

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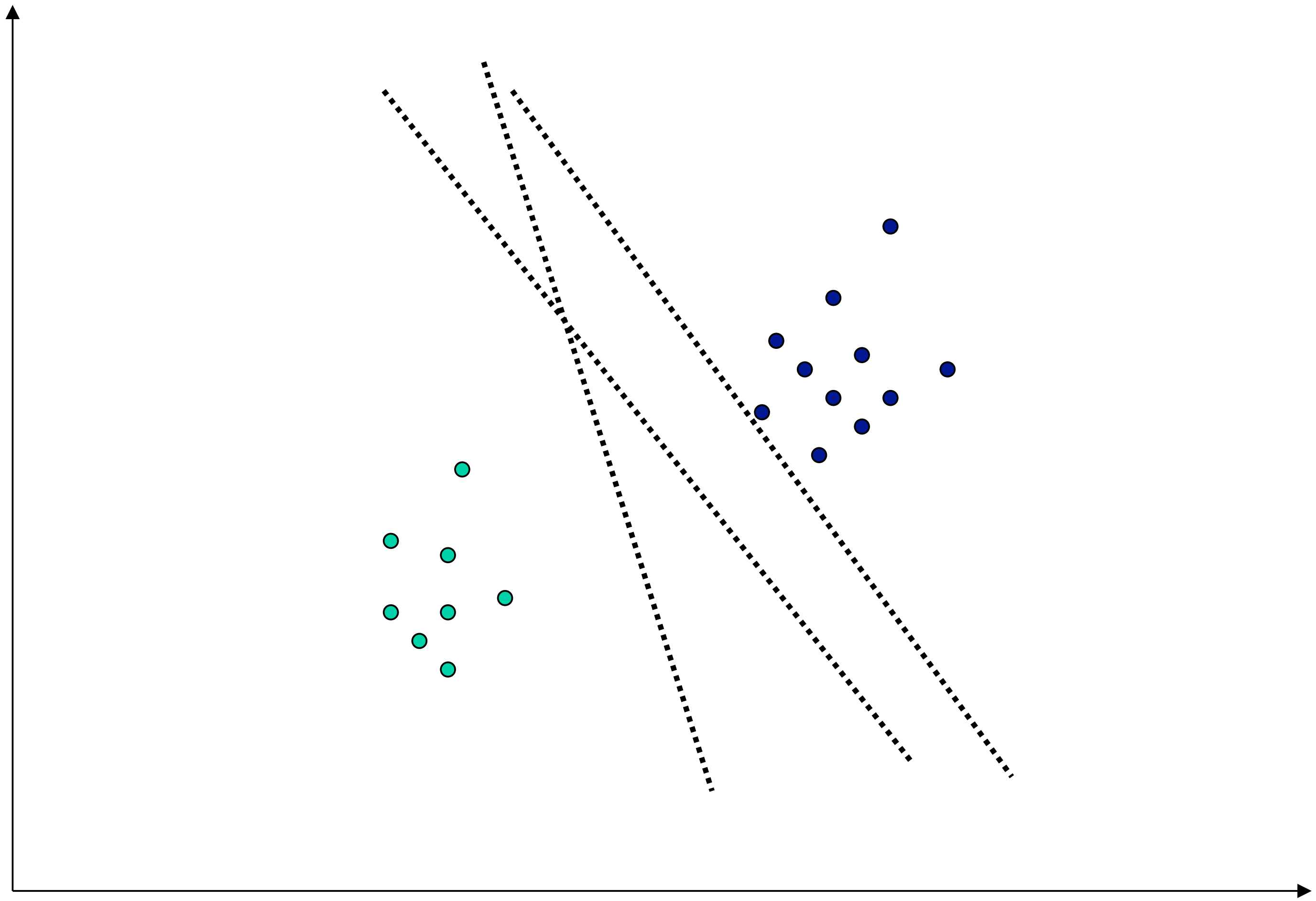
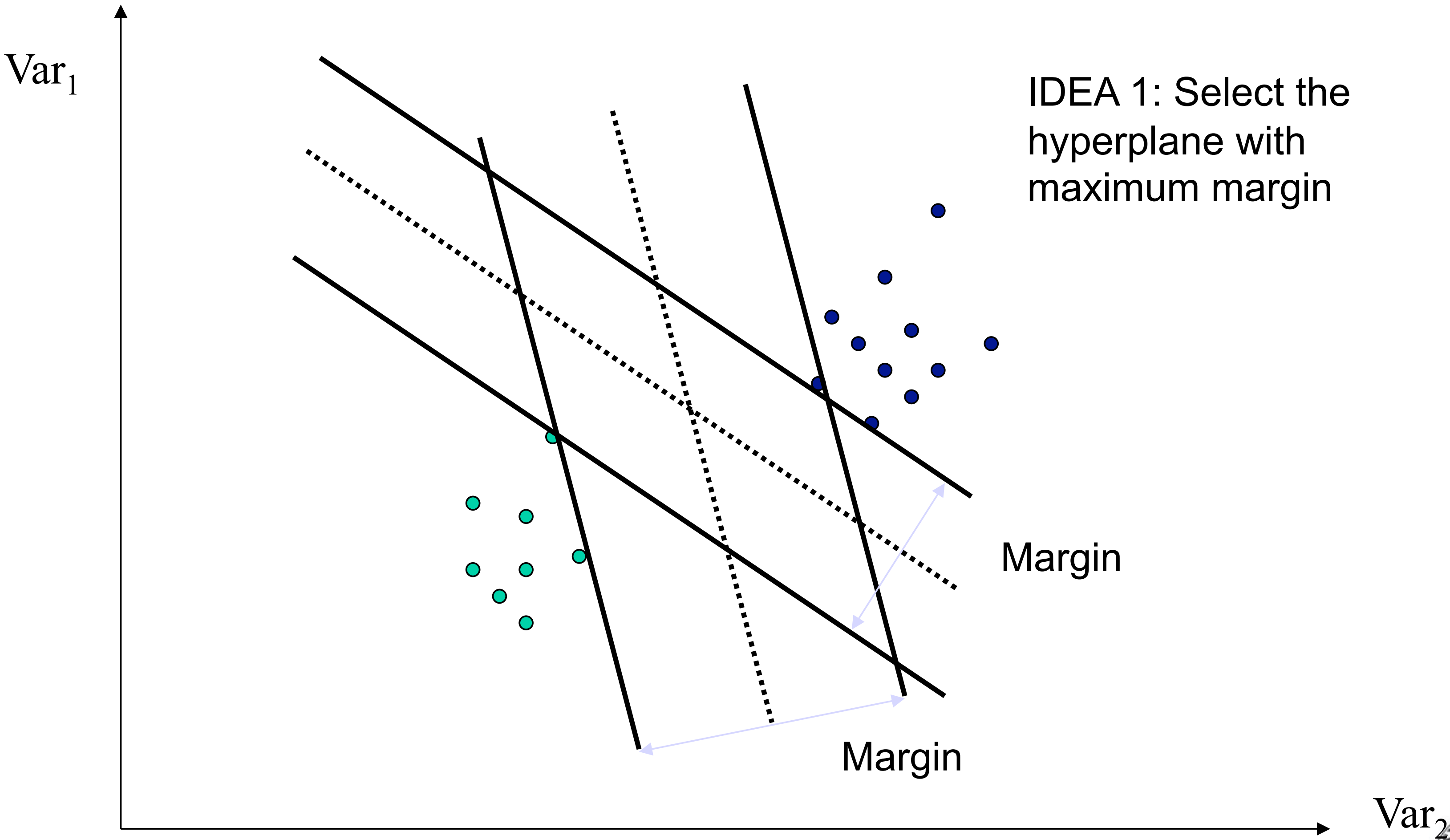
Summary

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

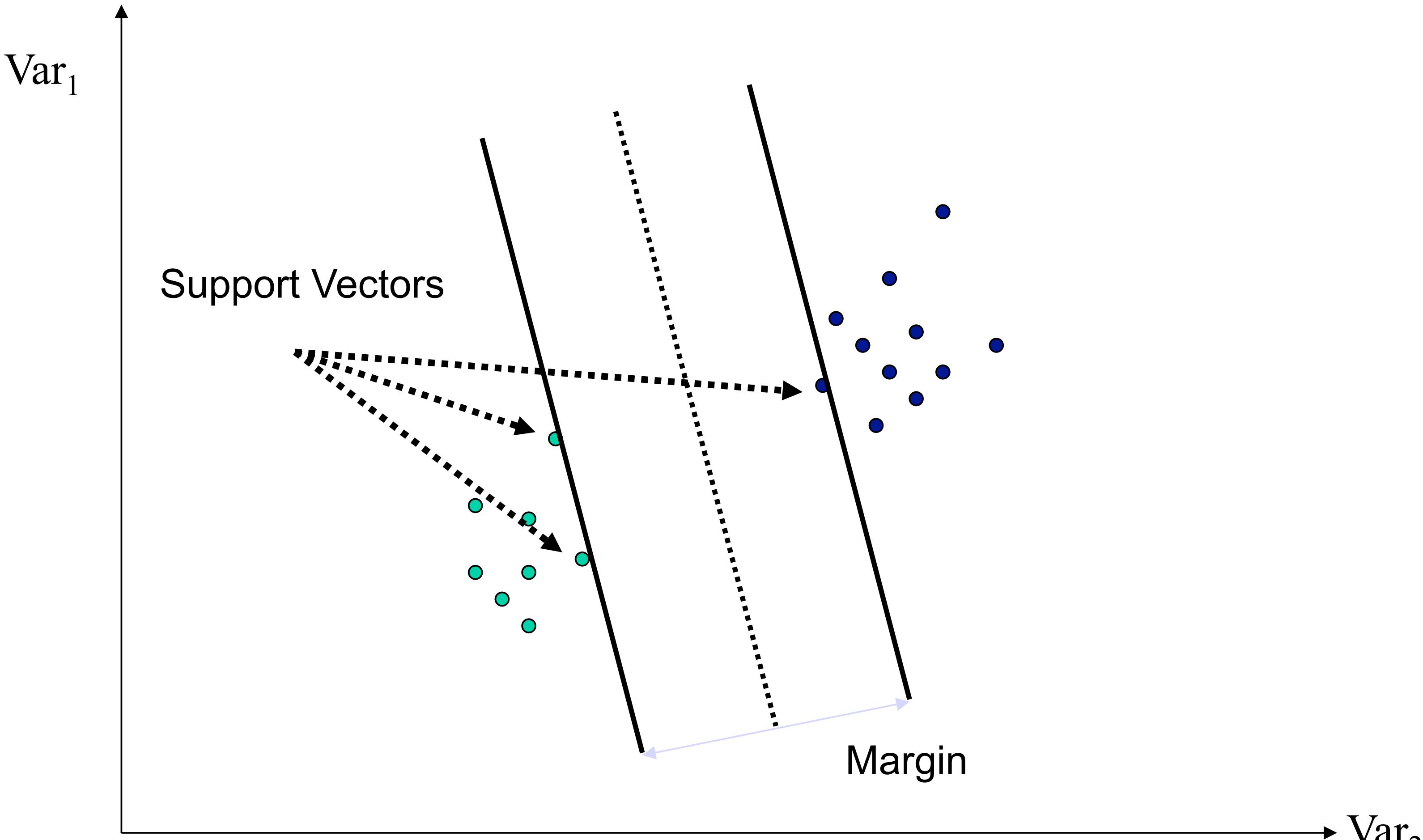
Which hyperplane choose?



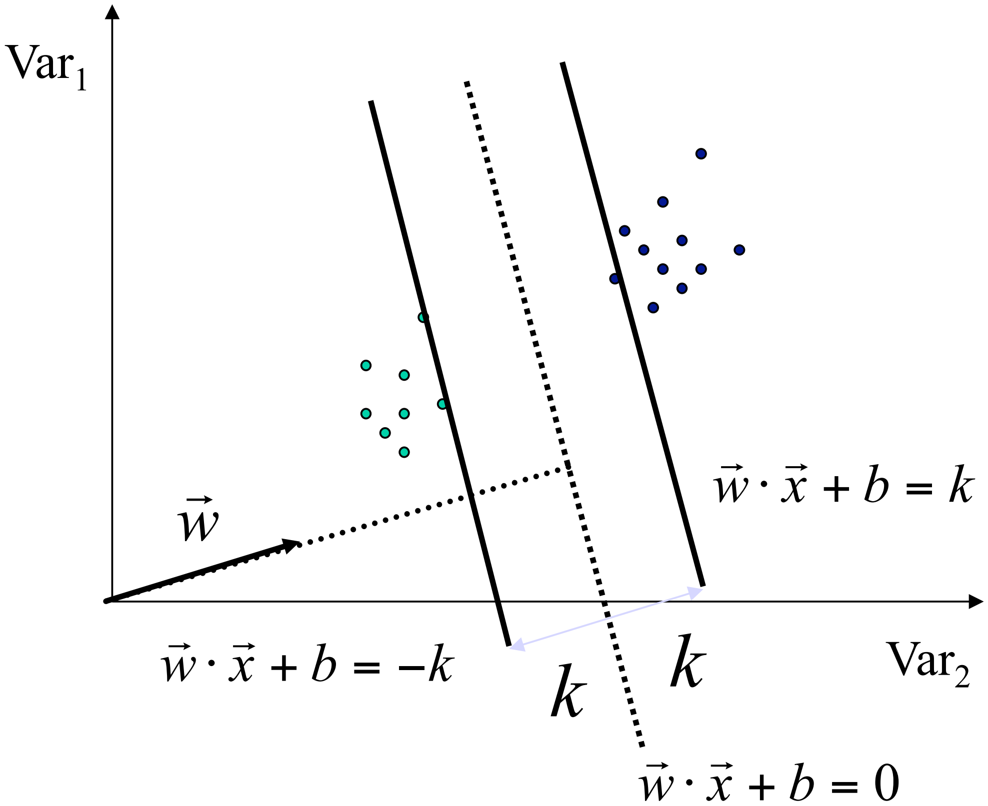
Classifier with a Maximum Margin



Support Vector

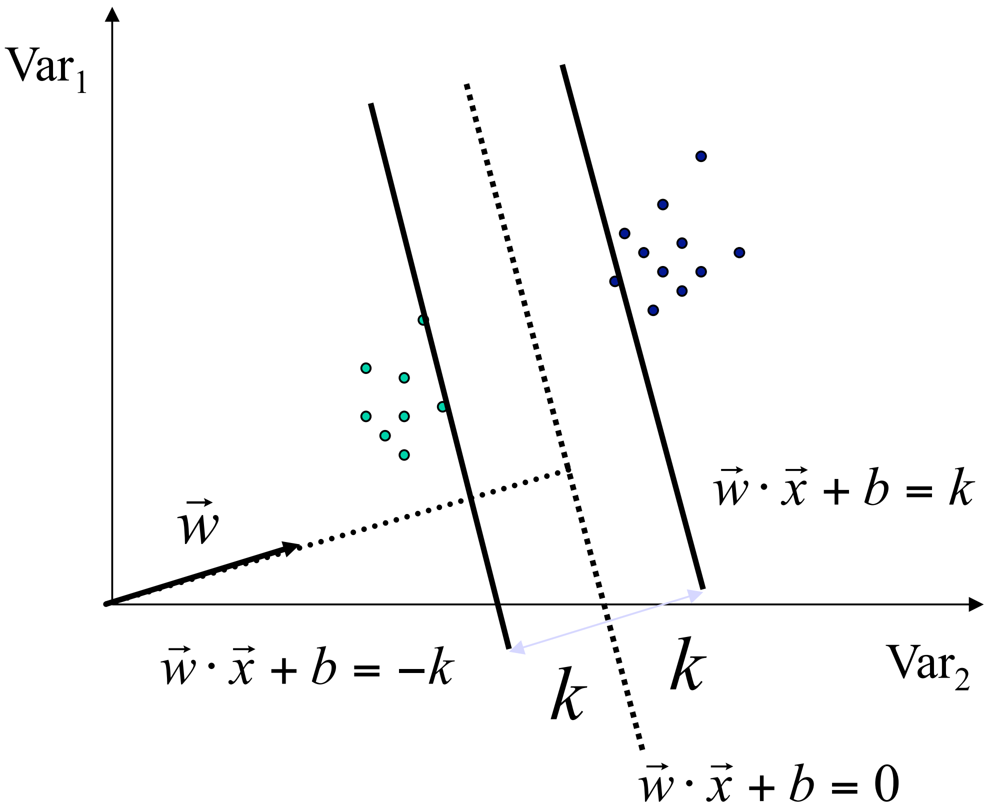


Support Vector Machine Classifiers



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

Support Vector Machines



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

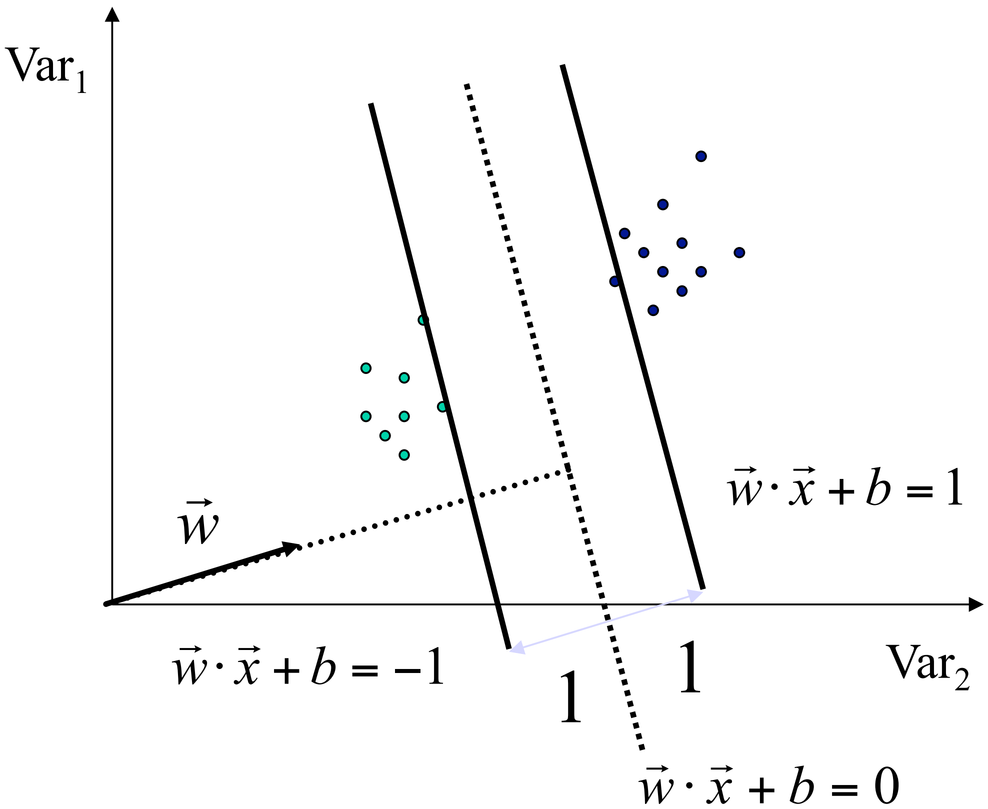
We need to solve

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

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

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

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

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

$$\vec{w} \cdot \vec{x}_i + b \geq +1, \quad y_i = 1$$

$$\vec{w} \cdot \vec{x}_i + b \leq -1, \quad y_i = -1$$

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

$$y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

$$\Rightarrow \quad \min \frac{\|\vec{w}\|}{2}$$

$$y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

$$\Rightarrow \quad \min \frac{\|\vec{w}\|^2}{2}$$

$$y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

Definition of Training Set error

- Training Data

$$f : R^N \to \{\pm 1\} \qquad (\vec{x}_1, y_1), \ldots, (\vec{x}_l, y_l) \in R^N \times \{\pm 1\}$$

- Empirical Risk (error)

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

- 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***):

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

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

where d is theVC-dimension, l 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* $\vec{d}_i$

$$|\vec{w} \cdot \vec{d}_i + b| \geq 1, \text{ with } ||\vec{w}|| = A \qquad (5)$$

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

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

Optimization Problem

- Optimal Hyperplane:
  - Minimize $\tau(\vec{w}) = \frac{1}{2}\|\vec{w}\|^2$
  - Subject to $y_i\,((\vec{w}\cdot\vec{x}_i) + b) \geq 1, i = 1,\ldots,l$
- 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.* $\geq$*) 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 objective 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

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

Khun-Tucker Theorem

- Necessary and sufficient conditions to optimality

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

Properties coming from constraints

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

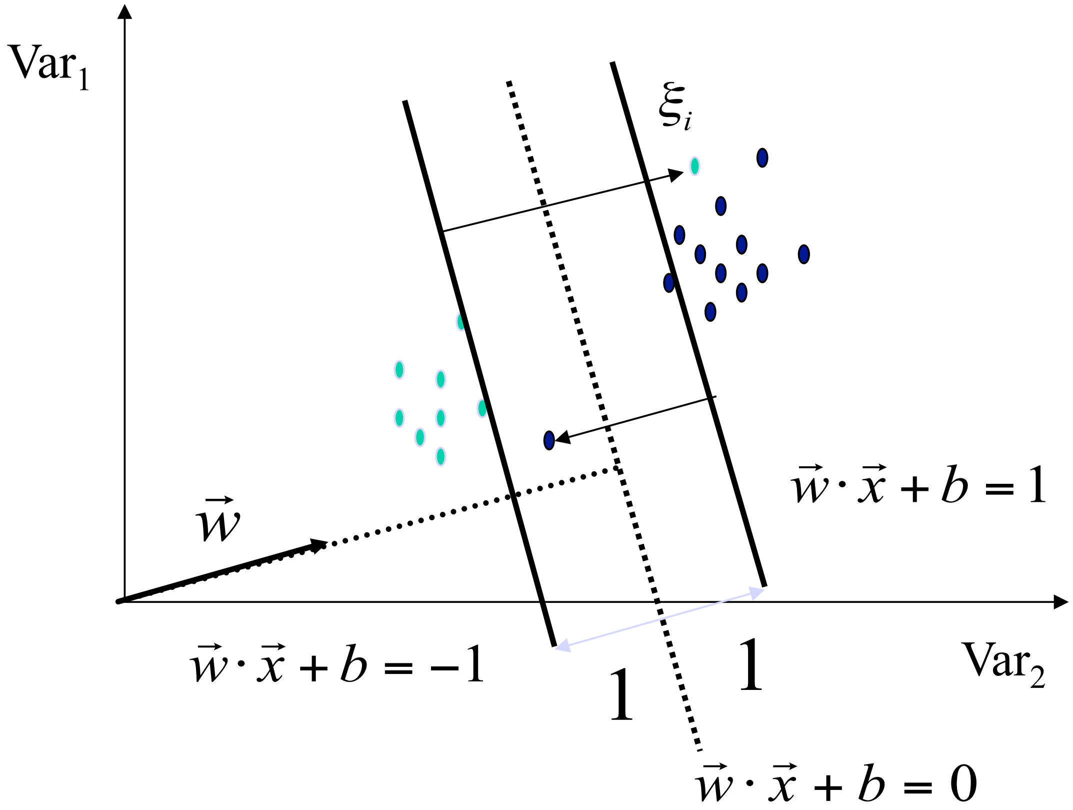
$$\alpha_i \cdot [y_i(\vec{x}_i \cdot \vec{w} + b) - 1] = 0, \quad i = 1,\ldots,l$$

- Support Vectors have α_i not null

- To evaluate *b,* we can apply the following equation

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

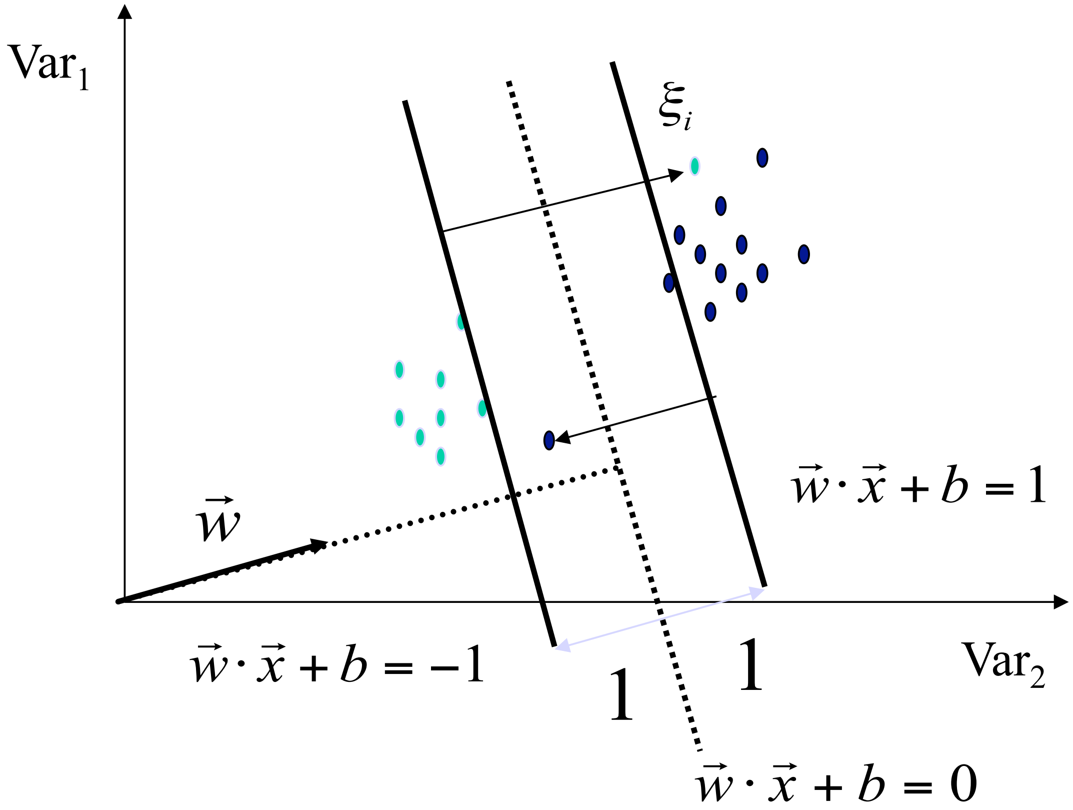
Soft Margin SVMs



ξ_i slack variables are added

Some errors are allowed but they should penalize the objective function

Soft Margin SVMs



The new constraints are

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

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

$$= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} + \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} - \frac{1}{C} \vec{\alpha} \cdot \vec{\alpha} =$$

$$= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} - \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} =$$

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

- δ_{ij} of Kronecker

Final dual optimization problem

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

$$\alpha_i \geq 0, \quad \forall i = 1, .., m$$

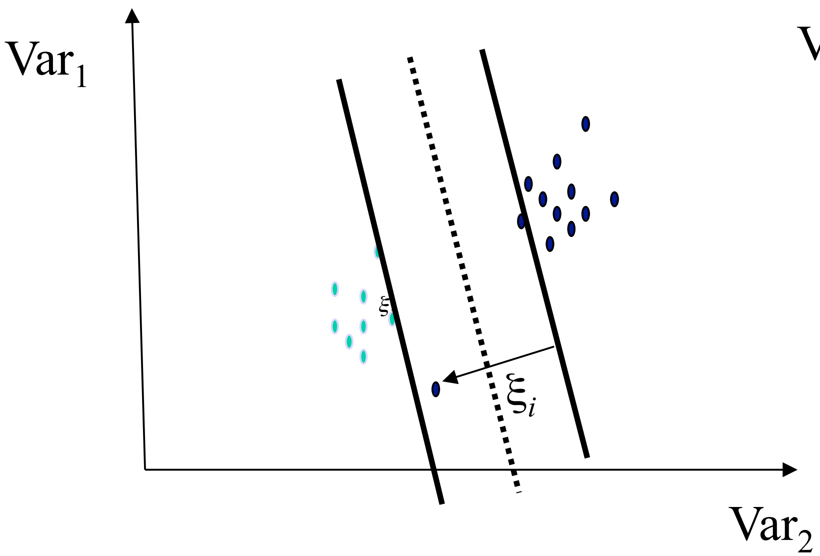
$$\textstyle\sum_{i=1}^{m} y_i \alpha_i = 0$$

Soft Margin Support Vector Machines

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

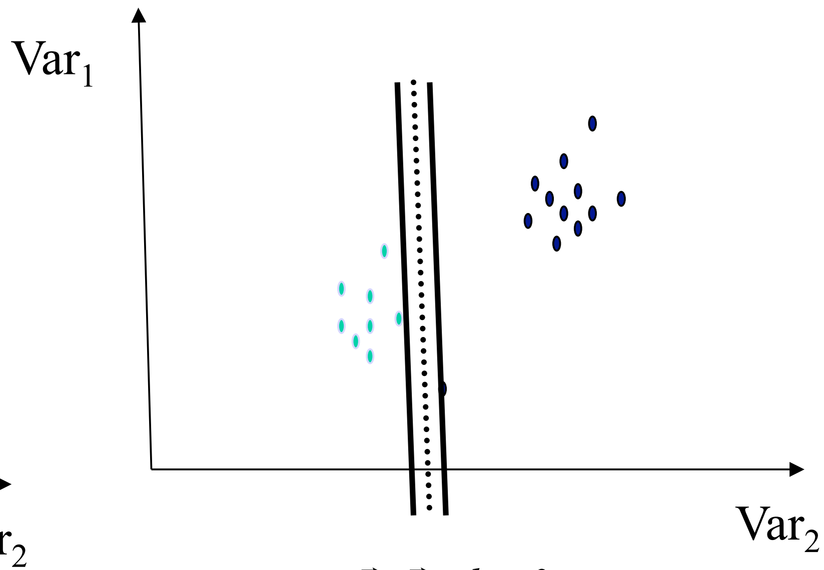
- The algorithm tries to keep ξ_i low and maximize the margin
- NB: The number of error is not directly minimized (NP-complete problem); the distances from the hyperplane are minimized
- If $C\to\infty$, the solution tends to the one of the *hard-margin* algorithm
- *Attention !!!:* if $C = 0$ we get $\|\vec{w}\| = 0$, 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



$\vec{w} \cdot \vec{x} + b = 0$

Soft Margin SVM



$\vec{w} \cdot \vec{x} + b = 0$

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

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 $rank(\vec{x_i}) > rank(\vec{x_j})$, 0 otherwise, where $k = i \times m + j$

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

Support Vector Regression

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

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

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

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**