



Support Vector Machines

MEDINFO 2004,
T02: Machine Learning Methods for Decision Support and Discovery
Constantin F. Aliferis & Ioannis Tsamardinos
Discovery Systems Laboratory
Department of Biomedical Informatics
Vanderbilt University

Support Vector Machines

- Decision surface is a hyperplane (line in 2D) in **feature** space (similar to the Perceptron)
- Arguably, the most important recent discovery in machine learning
- In a nutshell:
 - map the data to a predetermined very high-dimensional space via a kernel function
 - Find the hyperplane that maximizes the margin between the two classes
 - If data are not separable find the hyperplane that maximizes the margin and minimizes the (a weighted average of the) misclassifications

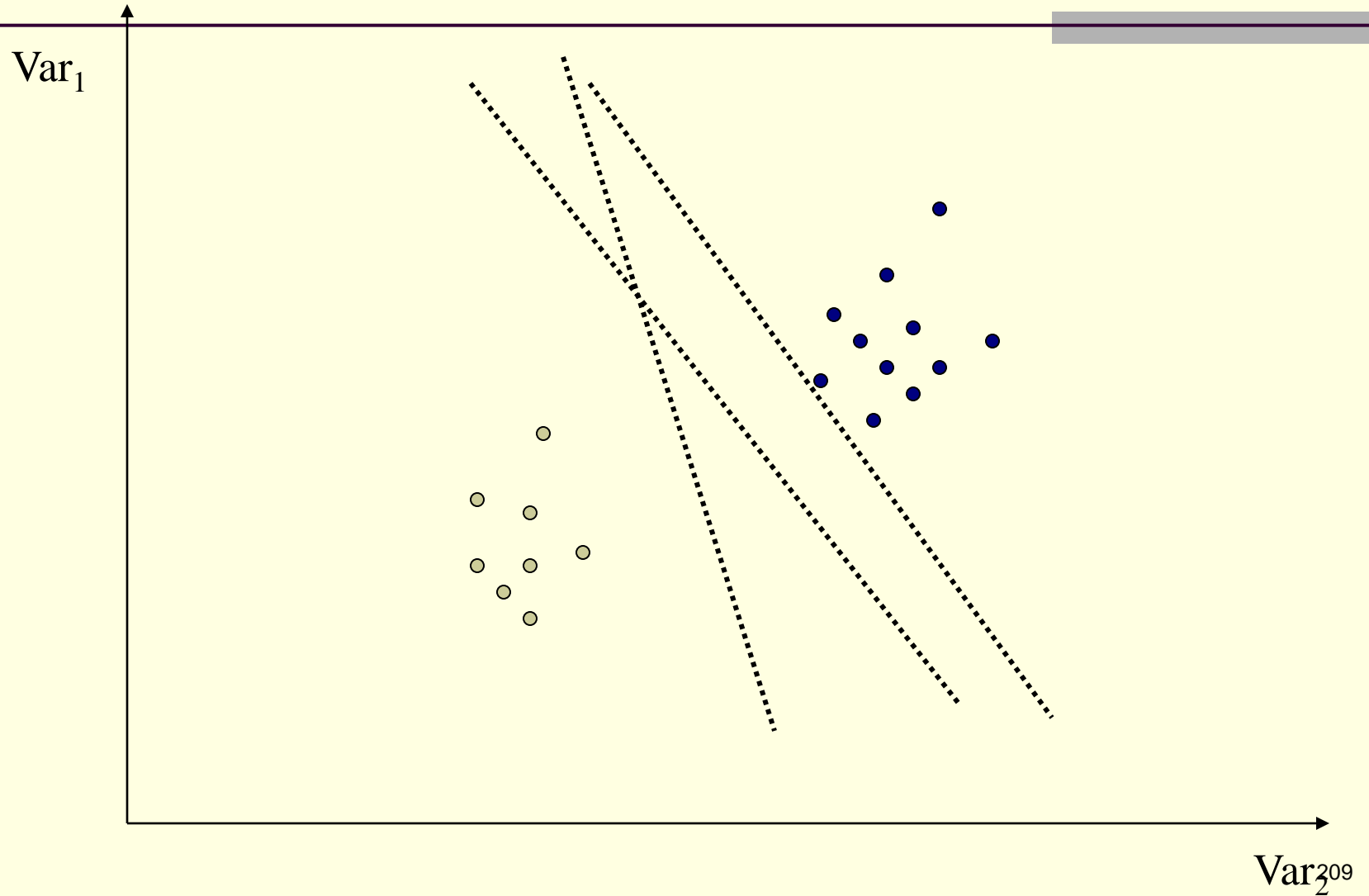
Support Vector Machines

- Three main ideas:
 1. Define what an optimal hyperplane is (in way that can be identified in a computationally efficient way): maximize margin
 2. Extend the above definition for non-linearly separable problems: have a penalty term for misclassifications
 3. Map data to high dimensional space where it is easier to classify with linear decision surfaces: reformulate problem so that data is mapped implicitly to this space

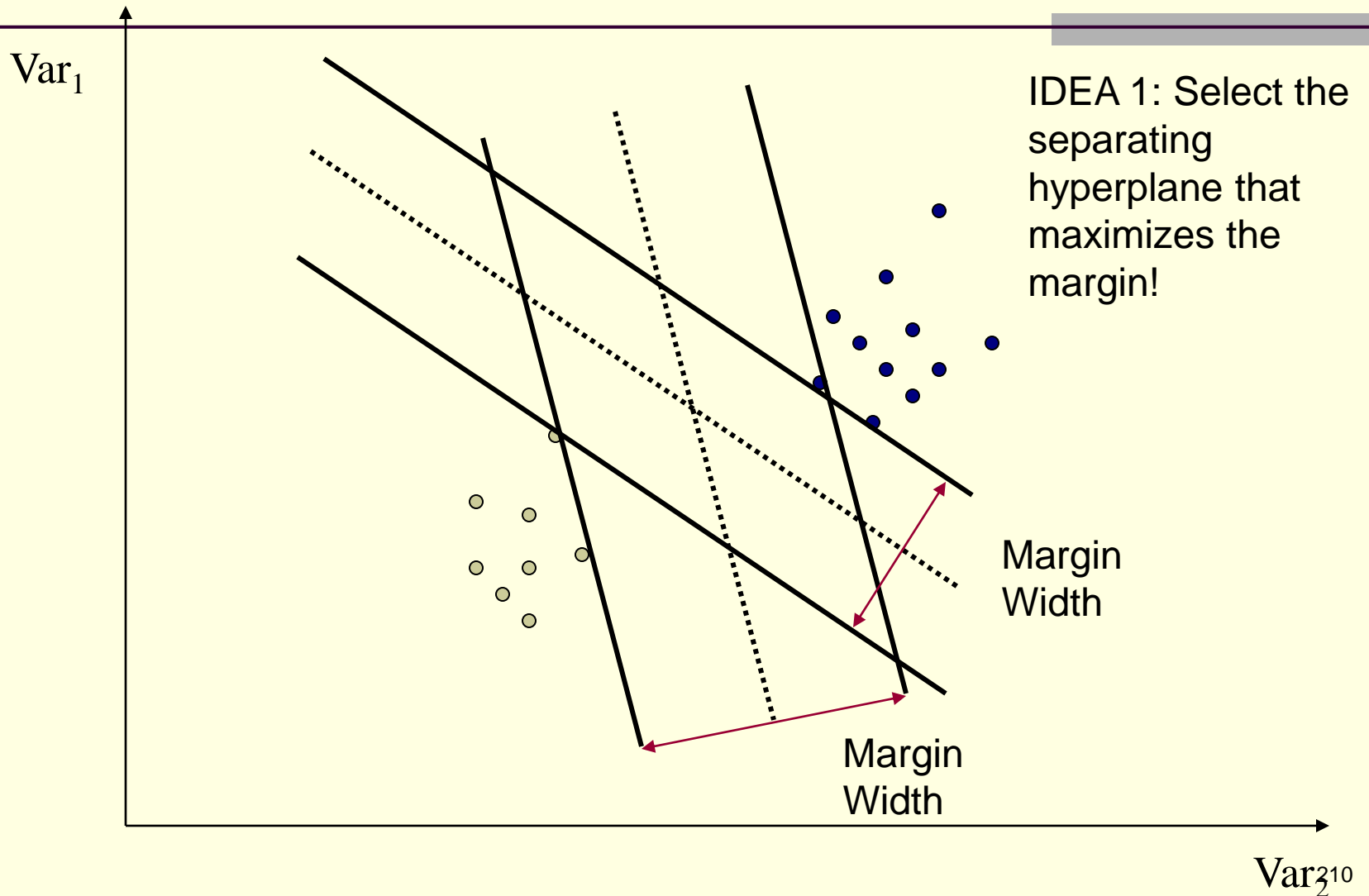
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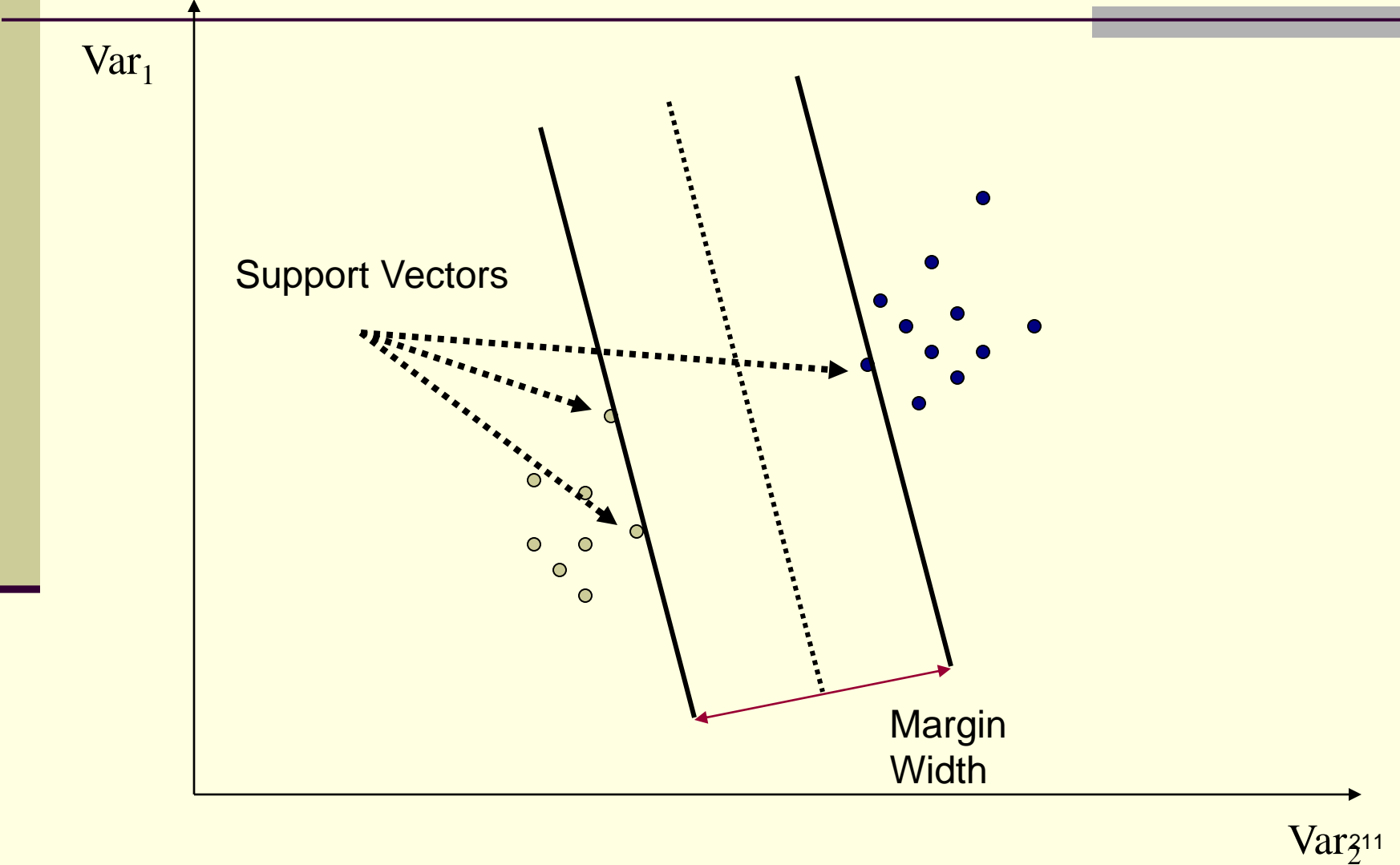
Which Separating Hyperplane to Use?



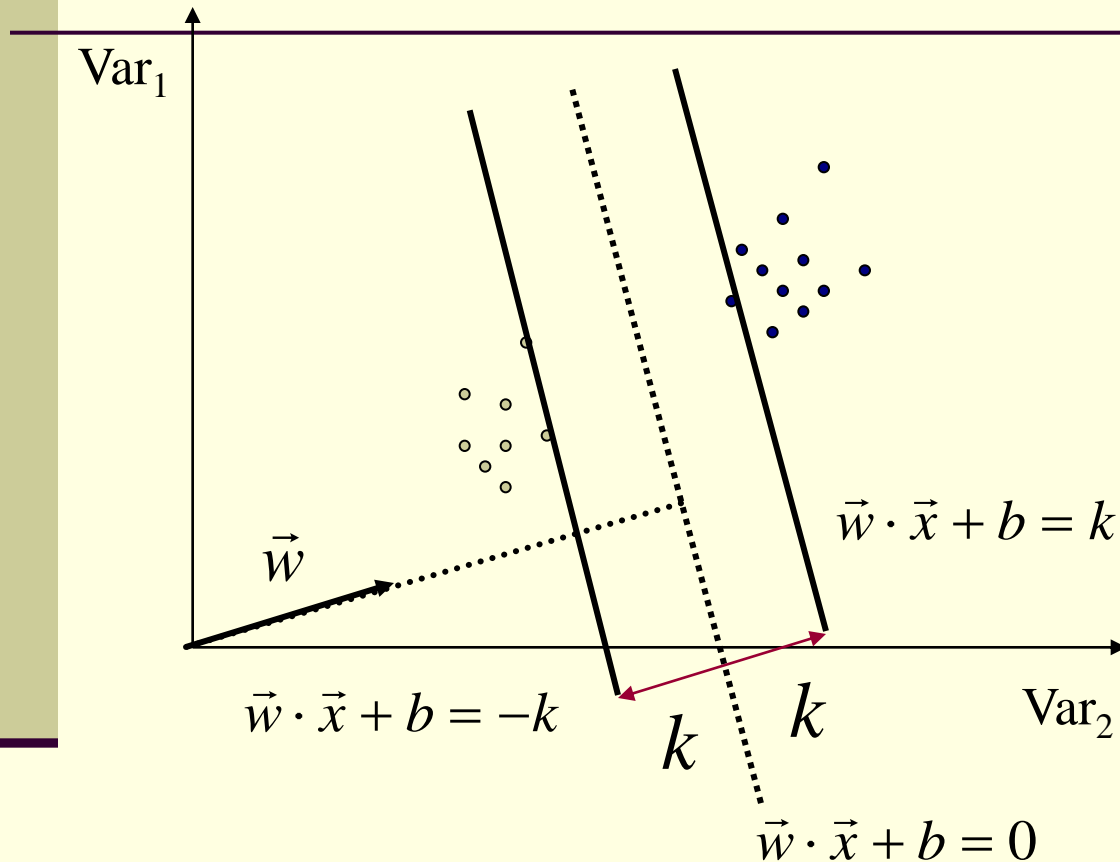
Maximizing the Margin



Support Vectors



Setting Up the Optimization Problem



The width of the margin is:

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

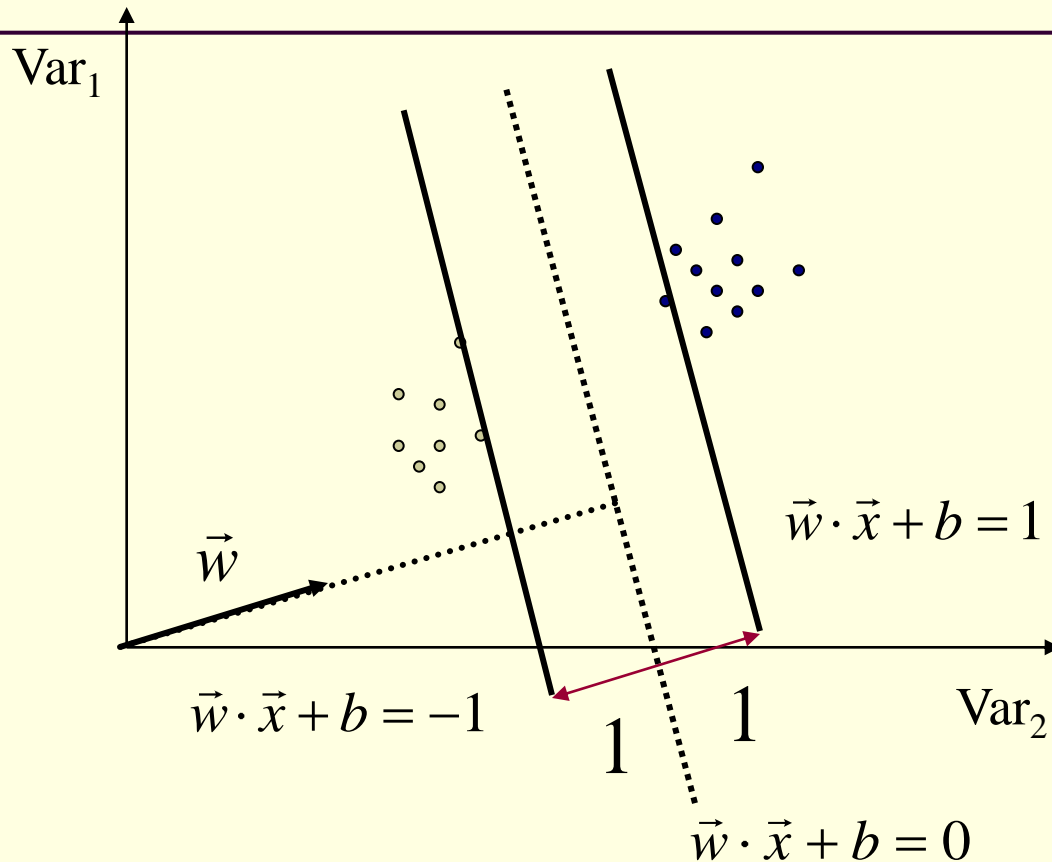
So, the problem is:

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

s.t. $(\vec{w} \cdot \vec{x} + b) \geq k, \forall x$ of class 1

$(\vec{w} \cdot \vec{x} + b) \leq -k, \forall x$ of class 2

Setting Up the Optimization Problem



There is a scale and unit for data so that $k=1$. Then problem becomes:

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

s.t. $(\vec{w} \cdot \vec{x} + b) \geq 1, \forall x$ of class 1
 $(\vec{w} \cdot \vec{x} + b) \leq -1, \forall x$ of class 2

Setting Up the Optimization Problem

- If class 1 corresponds to 1 and class 2 corresponds to -1, we can rewrite

$$(w \cdot x_i + b) \geq 1, \quad \forall x_i \text{ with } y_i = 1$$

$$(w \cdot x_i + b) \leq -1, \quad \forall x_i \text{ with } y_i = -1$$

- as

$$y_i (w \cdot x_i + b) \geq 1, \quad \forall x_i$$

- So the problem becomes:

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

$$s.t. \ y_i (w \cdot x_i + b) \geq 1, \quad \forall x_i$$

or

$$\min \frac{1}{2} \|w\|^2$$

$$s.t. \ y_i (w \cdot x_i + b) \geq 1, \quad \forall x_i$$

Linear, Hard-Margin SVM Formulation

- Find w, b that solves

$$\min \frac{1}{2} \|w\|^2$$

$$s.t. y_i (w \cdot x_i + b) \geq 1, \quad \forall x_i$$

- Problem is convex so, there is a unique global minimum value (when feasible)
- There is also a unique minimizer, i.e. weight and b value that provides the minimum
- Non-solvable if the data is not linearly separable
- Quadratic Programming
 - Very efficient computationally with modern constraint optimization engines (handles thousands of constraints and training instances).

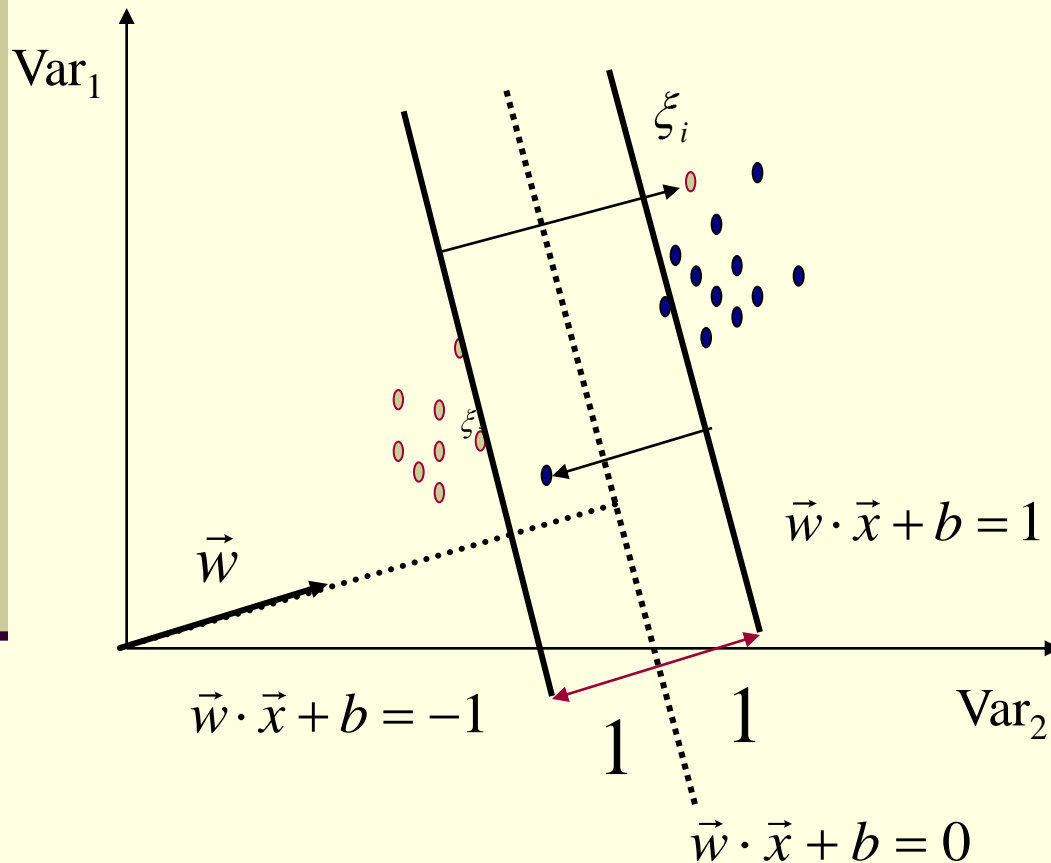
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Non-Linearly Separable Data



Introduce slack variables ξ_i

Allow some instances to fall within the margin, but penalize them

Formulating the Optimization Problem

Constraint becomes :

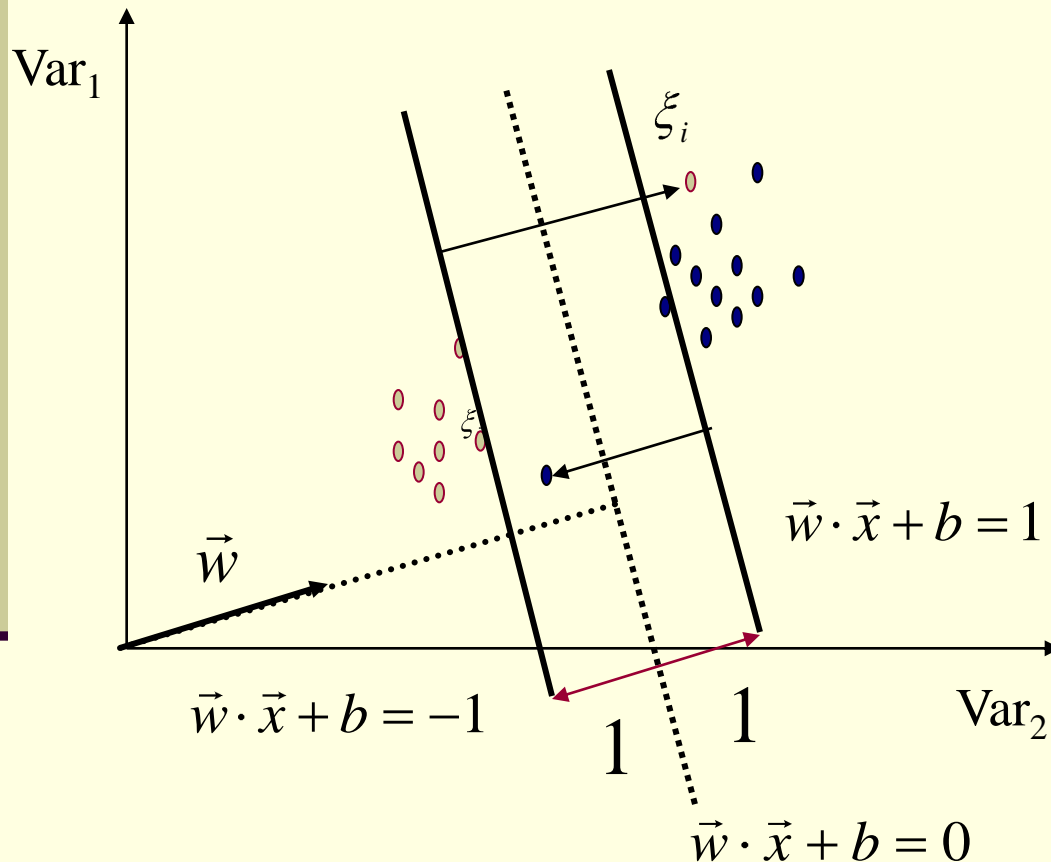
$$y_i(w \cdot x_i + b) \geq 1 - \xi_i, \quad \forall x_i$$

$$\xi_i \geq 0$$

Objective function penalizes for misclassified instances and those within the margin

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

C trades-off margin width and misclassifications ²¹⁹

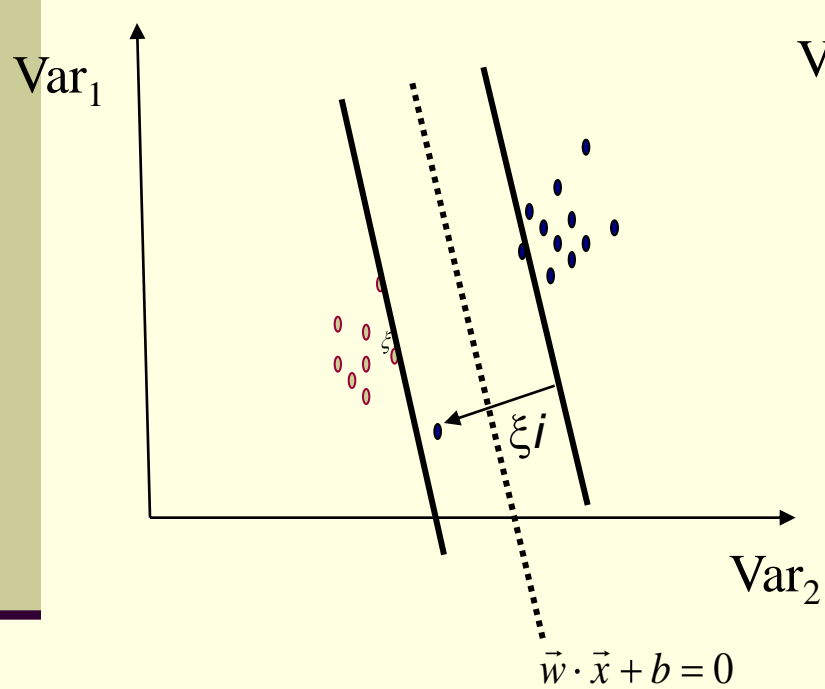


Linear, Soft-Margin SVMs

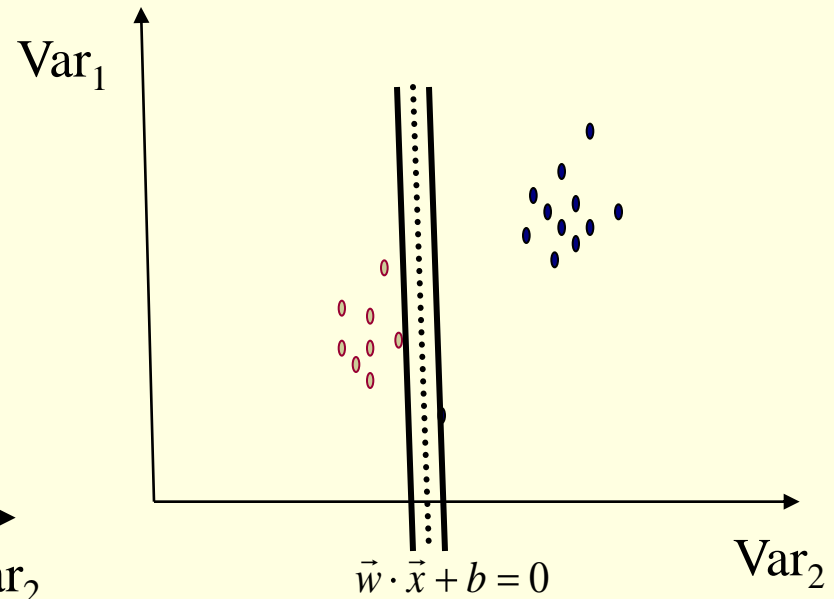
$$\min \frac{1}{2} \|w\|^2 + C \sum_i \xi_i \quad \begin{array}{l} y_i(w \cdot x_i + b) \geq 1 - \xi_i, \quad \forall x_i \\ \xi_i \geq 0 \end{array}$$

- Algorithm tries to maintain ξ_j to zero while maximizing margin
- Notice: algorithm does not minimize the *number* of misclassifications (NP-complete problem) but the sum of distances from the margin hyperplanes
- Other formulations use ξ_j^2 instead
- As $C \rightarrow \infty$, we get closer to the hard-margin solution

Robustness of Soft vs Hard Margin SVMs



Soft Margin SVN



Hard Margin SVN

Soft vs Hard Margin SVM

- Soft-Margin always have a solution
- Soft-Margin is more robust to outliers
 - Smoother surfaces (in the non-linear case)
- Hard-Margin does not require to guess the cost parameter (requires no parameters at all)

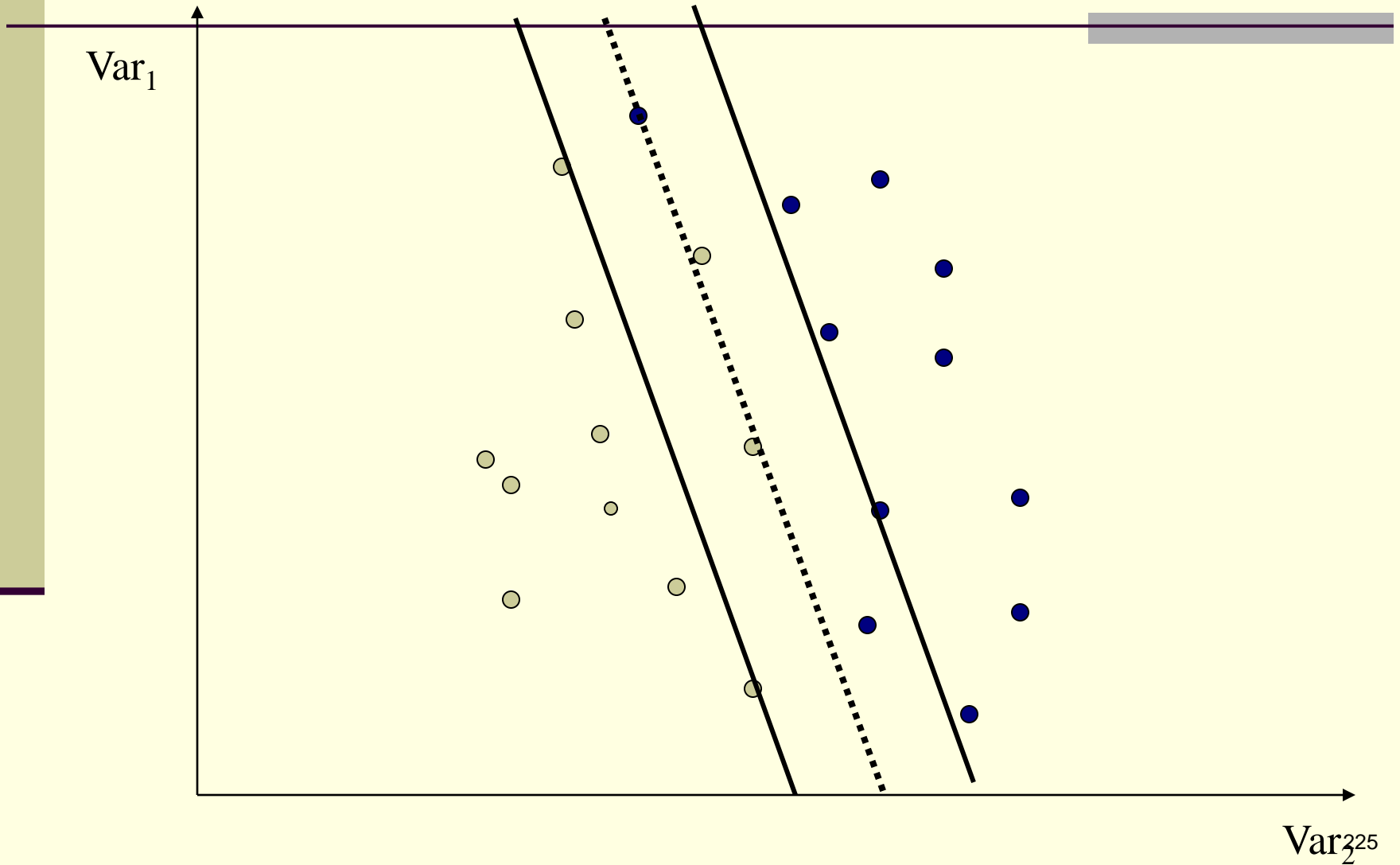
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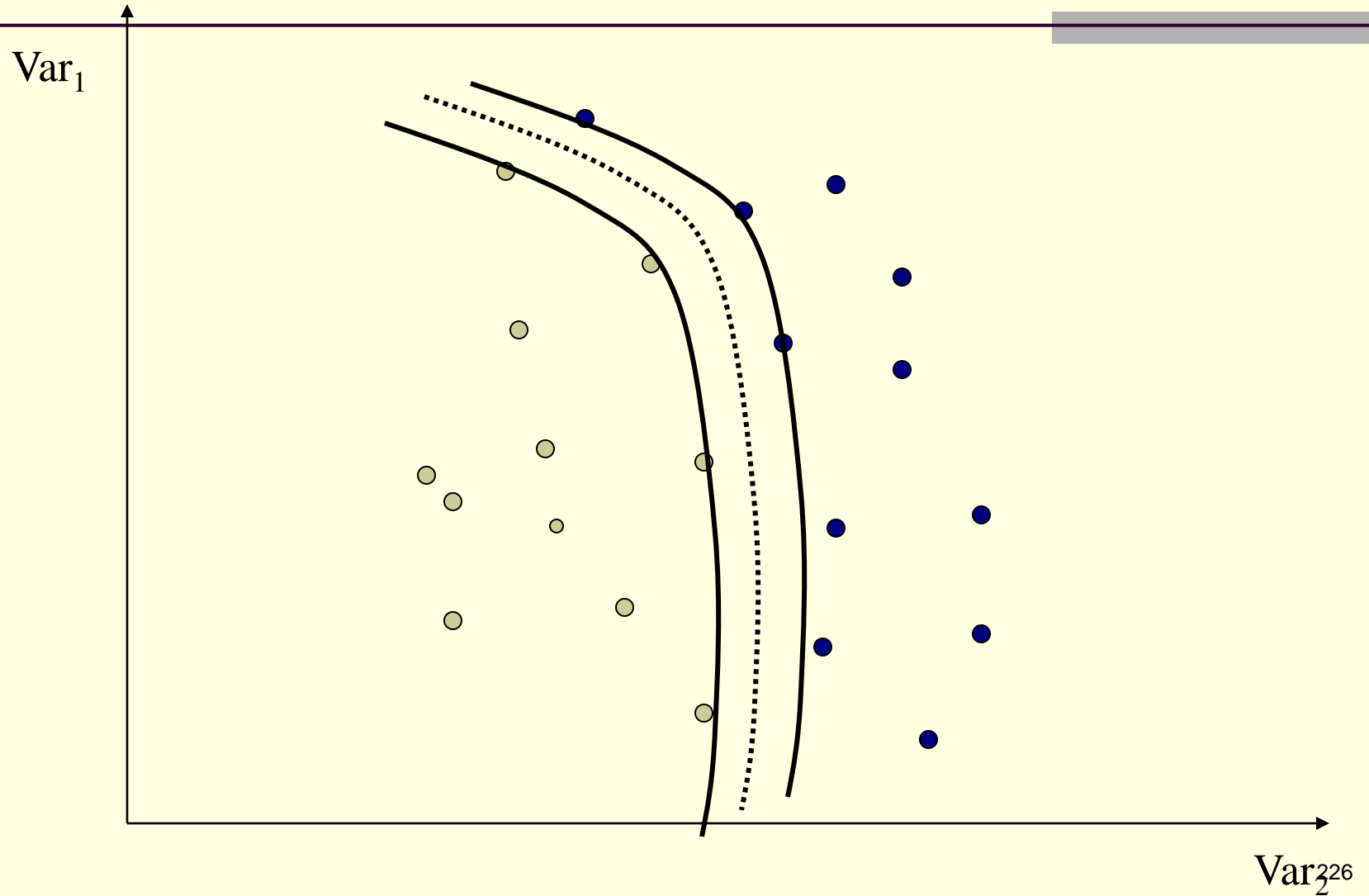
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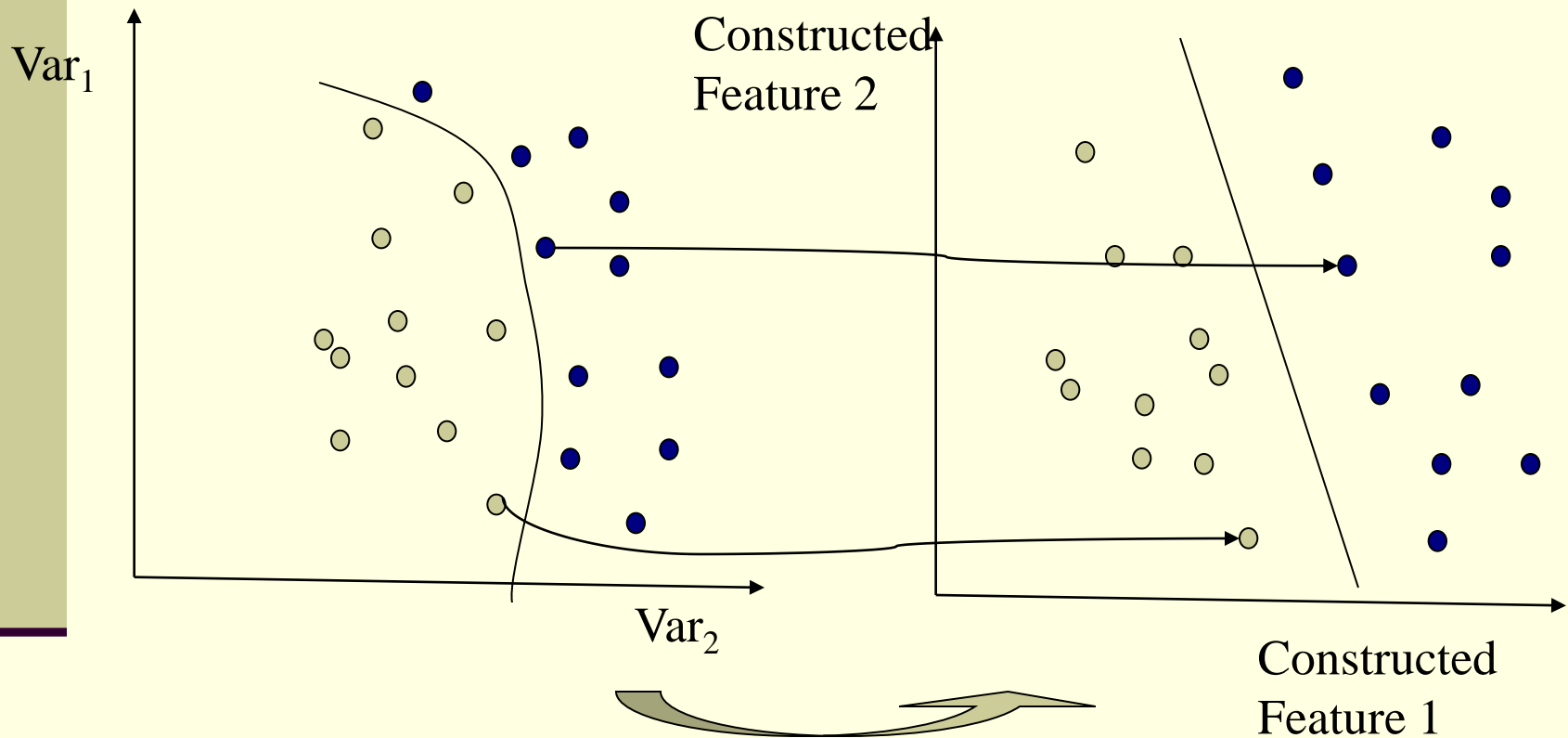
Disadvantages of Linear Decision Surfaces



Advantages of Non-Linear Surfaces



Linear Classifiers in High-Dimensional Spaces



Find function $\Phi(x)$ to map to a different space

Mapping Data to a High-Dimensional Space

- Find function $\Phi(x)$ to map to a different space, then SVM formulation becomes:

$$\min \frac{1}{2} \|w\|^2 + C \sum_i \xi_i \quad \text{s.t. } y_i(w \cdot \Phi(x) + b) \geq 1 - \xi_i, \forall x_i$$
$$\xi_i \geq 0$$

- Data appear as $\Phi(x)$, weights w are now weights in the new space
- Explicit mapping expensive if $\Phi(x)$ is very high dimensional
- Solving the problem without explicitly mapping the data is desirable

The Dual of the SVM Formulation

- Original SVM formulation
 - n inequality constraints
 - n positivity constraints
 - n number of ξ variables

$$\min_{w,b} \frac{1}{2} \|w\|^2 + C \sum_i \xi_i$$

$$s.t. \quad y_i(w \cdot \Phi(x) + b) \geq 1 - \xi_i, \forall x_i$$
$$\xi_i \geq 0$$

- The (Wolfe) dual of this problem
 - one equality constraint
 - n positivity constraints
 - n number of α variables (Lagrange multipliers)
 - Objective function more complicated

$$\min_{\alpha_i} \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j (\Phi(x_i) \cdot \Phi(x_j)) - \sum_i \alpha_i$$

$$s.t. \quad C \geq \alpha_i \geq 0, \forall x_i$$

$$\sum_i \alpha_i y_i = 0$$

- NOTICE: Data only appear as $\Phi(x_i) \cdot \Phi(x_j)$

The Kernel Trick

- $\Phi(x_i) \cdot \Phi(x_j)$: means, map data into new space, then take the inner product of the new vectors
- We can find a function such that: $K(x_i \cdot x_j) = \Phi(x_i) \cdot \Phi(x_j)$, i.e., the image of the inner product of the data is the inner product of the images of the data
- Then, we do not need to explicitly map the data into the high-dimensional space to solve the optimization problem (for training)
- How do we classify without explicitly mapping the new instances? Turns out

$$\text{sgn}(wx + b) = \text{sgn}\left(\sum_i \alpha_i y_i K(x_i, x) + b\right)$$

$$\text{where } b \text{ solves } \alpha_j (y_j \sum_i \alpha_i y_i K(x_i, x_j) + b - 1) = 0,$$

for any j with $\alpha_j \neq 0$

Examples of Kernels

- Assume we measure two quantities, e.g. expression level of genes *TrkC* and *SonicHedghog* (*SH*) and we use the mapping:

$$\Phi : \langle x_{TrkC}, x_{SH} \rangle \rightarrow \{x_{TrkC}^2, x_{SH}^2, \sqrt{2}x_{TrkC}x_{SH}, x_{TrkC}, x_{SH}, 1\}$$

- Consider the function:

$$K(x \cdot z) = (x \cdot z + 1)^2$$

- We can verify that:

$$\Phi(x) \cdot \Phi(z) =$$

$$x_{TrkC}^2 z_{TrkC}^2 + x_{SH}^2 z_{SH}^2 + 2x_{TrkC}x_{SH}z_{TrkC}z_{SH} + x_{TrkC}z_{TrkC} + x_{SH}z_{SH} + 1 =$$

$$= (x_{TrkC}z_{TrkC} + x_{SH}z_{SH} + 1)^2 = (x \cdot z + 1)^2 = K(x \cdot z)$$

Polynomial and Gaussian Kernels

$$K(x \cdot z) = (x \cdot z + 1)^p$$

- is called the polynomial kernel of degree p .
- For $p=2$, if we measure 7,000 genes using the kernel once means calculating a summation product with 7,000 terms then taking the square of this number
- Mapping explicitly to the high-dimensional space means calculating approximately 50,000,000 new features for both training instances, then taking the inner product of that (another 50,000,000 terms to sum)
- In general, using the Kernel trick provides huge computational savings over explicit mapping!
- Another commonly used Kernel is the Gaussian (maps to a dimensional space with number of dimensions equal to the number of training cases):

$$K(x \cdot z) = \exp(-\|x - z\| / 2\sigma^2)$$

The Mercer Condition

- Is there a mapping $\Phi(x)$ for any symmetric function $K(x,z)$? No
- The SVM dual formulation requires calculation $K(x_i, x_j)$ for each pair of training instances. The array $G_{ij} = K(x_i, x_j)$ is called the Gram matrix
- There is a feature space $\Phi(x)$ when the Kernel is such that G is always semi-positive definite (Mercer condition)

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Other Types of Kernel Methods

- SVMs that perform regression
- SVMs that perform clustering
- ν -Support Vector Machines: maximize margin while bounding the number of margin errors
- Leave One Out Machines: minimize the bound of the leave-one-out error
- SVM formulations that take into consideration difference in cost of misclassification for the different classes
- Kernels suitable for sequences of strings, or other specialized kernels

Variable Selection with SVMs

- Recursive Feature Elimination
 - Train a linear SVM
 - Remove the variables with the lowest weights (those variables affect classification the least), e.g., remove the lowest 50% of variables
 - Retrain the SVM with remaining variables and repeat until classification is reduced
- Very successful
- Other formulations exist where minimizing the number of variables is folded into the optimization problem
- Similar algorithm exist for non-linear SVMs
- Some of the best and most efficient variable selection methods

Comparison with Neural Networks

Neural Networks

- Hidden Layers map to lower dimensional spaces
- Search space has multiple local minima
- Training is expensive
- Classification extremely efficient
- Requires number of hidden units and layers
- Very good accuracy in typical domains

SVMs

- Kernel maps to a very-high dimensional space
- Search space has a unique minimum
- Training is extremely efficient
- Classification extremely efficient
- Kernel and cost the two parameters to select
- Very good accuracy in typical domains
- Extremely robust

Why do SVMs Generalize?

- Even though they map to a very high-dimensional space
 - They have a very strong bias in that space
 - The solution has to be a linear combination of the training instances
- Large theory on Structural Risk Minimization providing bounds on the error of an SVM
 - Typically the error bounds too loose to be of practical use

MultiClass SVMs

- One-versus-all
 - Train n binary classifiers, one for each class against all other classes.
 - Predicted class is the class of the most confident classifier
- One-versus-one
 - Train $n(n-1)/2$ classifiers, each discriminating between a pair of classes
 - Several strategies for selecting the final classification based on the output of the binary SVMs
- Truly MultiClass SVMs
 - Generalize the SVM formulation to multiple categories
- More on that in the nominated for the student paper award: “Methods for Multi-Category Cancer Diagnosis from Gene Expression Data: A Comprehensive Evaluation to Inform Decision Support System Development”, Alexander Statnikov, Constantin F. Aliferis, Ioannis Tsamardinos

Conclusions

- SVMs express learning as a mathematical program taking advantage of the rich theory in optimization
- SVM uses the kernel trick to map indirectly to extremely high dimensional spaces
- SVMs extremely successful, robust, efficient, and versatile while there are good theoretical indications as to why they generalize well

Suggested Further Reading

- <http://www.kernel-machines.org/tutorial.html>
- C. J. C. Burges. A Tutorial on Support Vector Machines for Pattern Recognition. *Knowledge Discovery and Data Mining*, 2(2), 1998.
- P.H. Chen, C.-J. Lin, and B. Schölkopf. A tutorial on nu -support vector machines. 2003.
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- B. Schölkopf. SVM and kernel methods, 2001. Tutorial given at the NIPS Conference.
- Hastie, Tibshirani, Friedman, The Elements of Statistical Learning, Springel 2001