Support Vector Machines (Formal : Version 1)

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 (penalty associated with) misclassifications

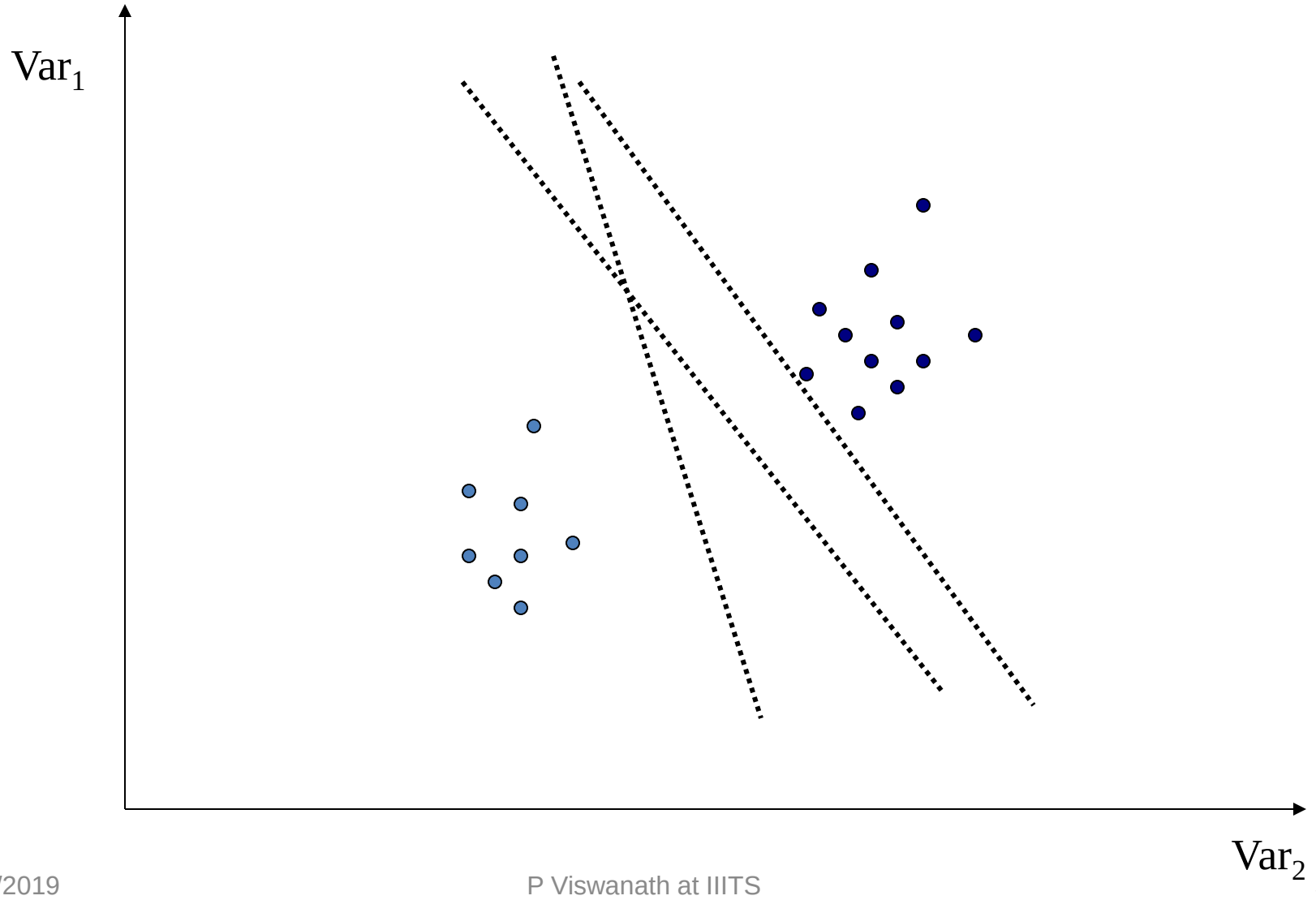
Support Vector Machines

- 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

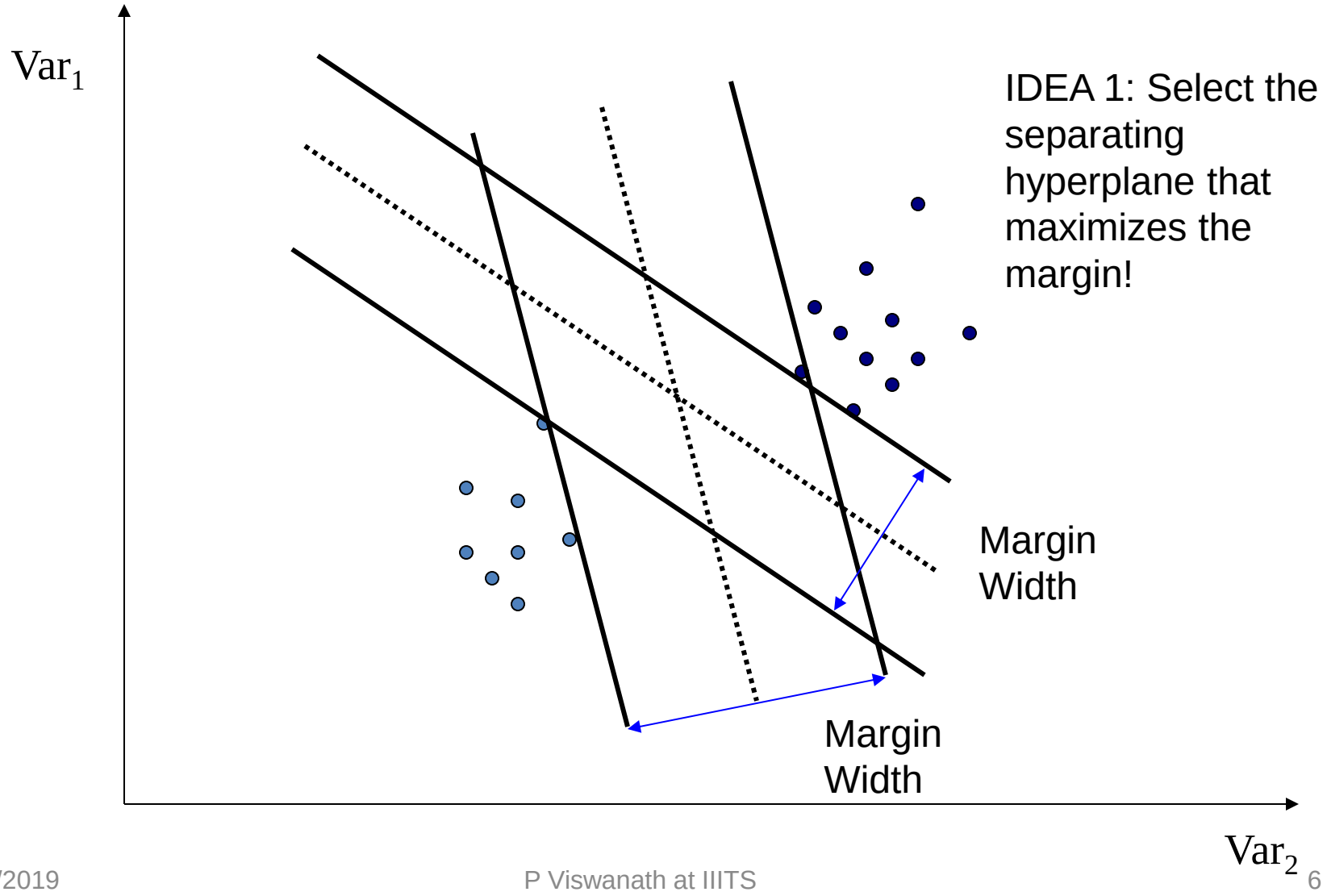
Support Vector Machines

- 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

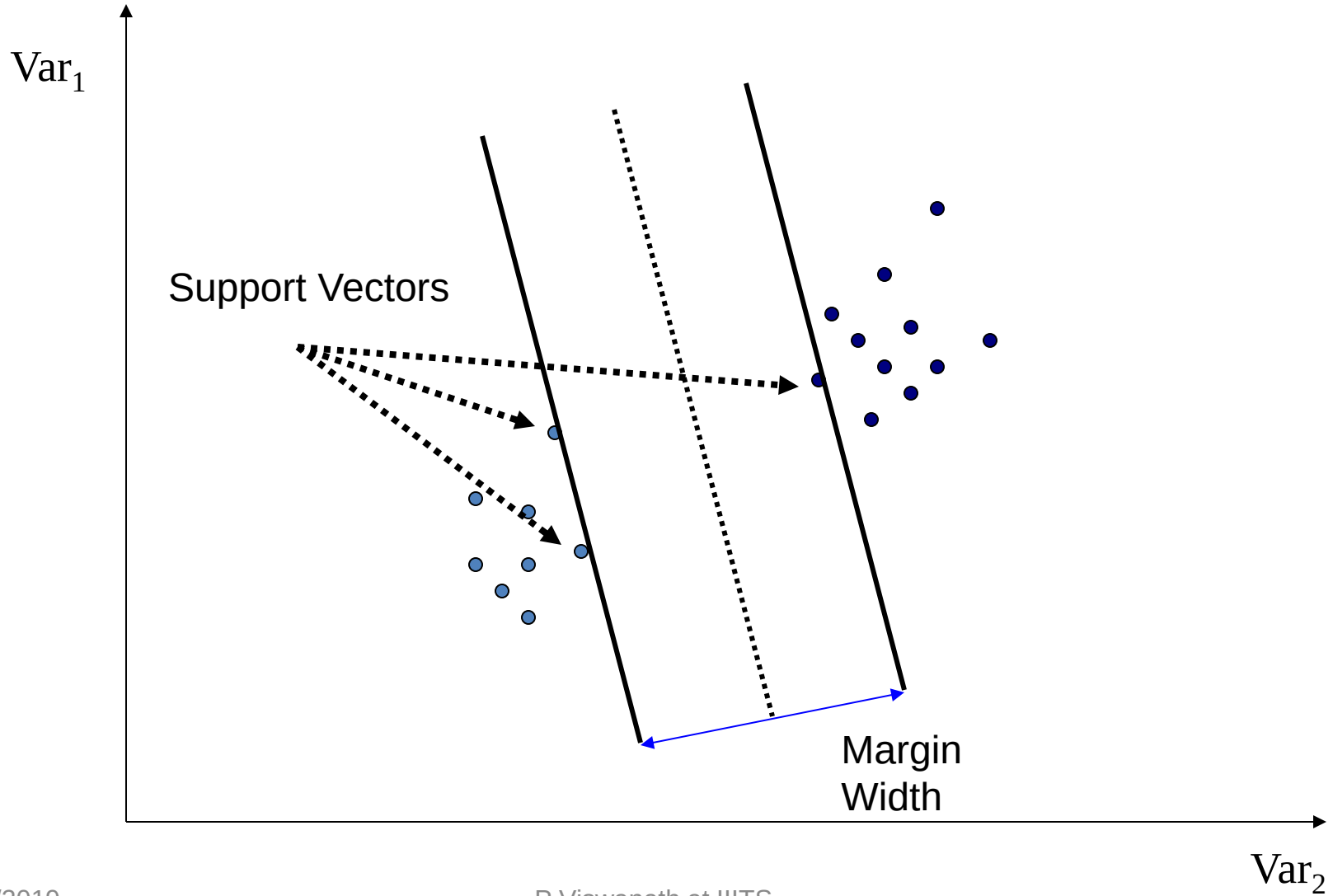
Which Separating Hyperplane to Use?



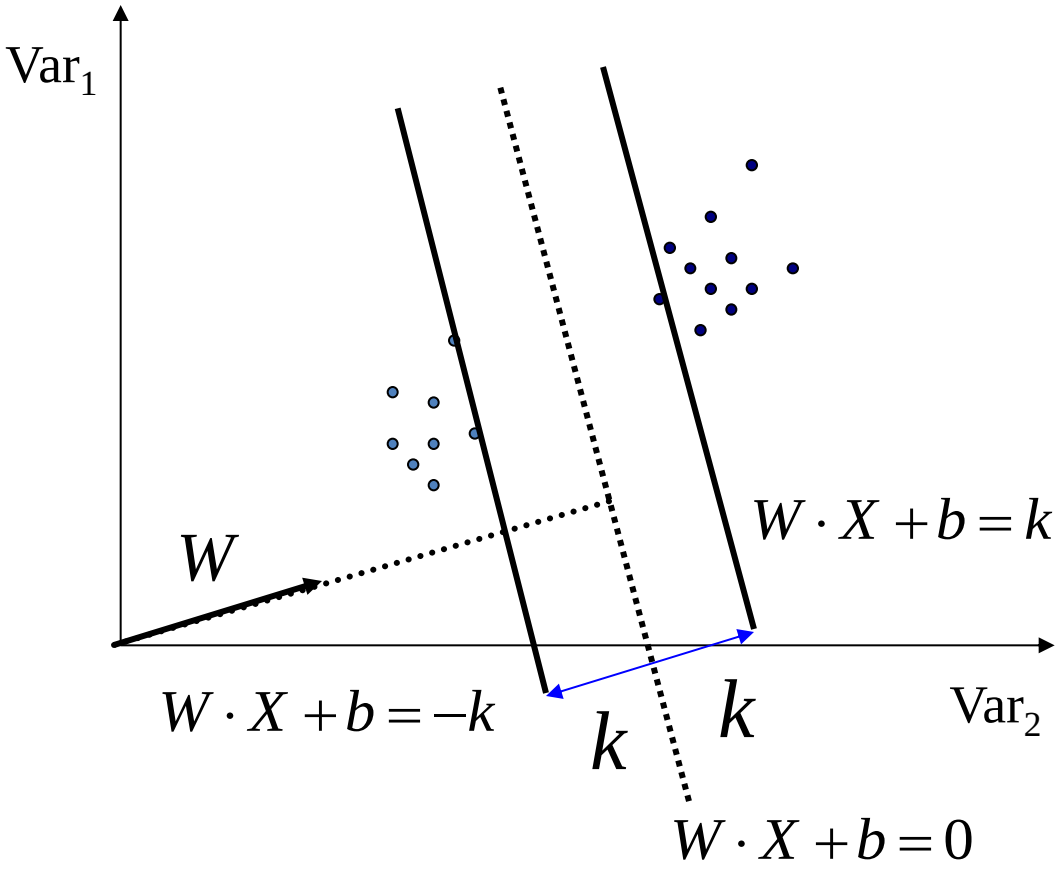
Maximizing the Margin



Support Vectors



Setting Up the Optimization Problem



The width of the margin is:

$$\frac{2|k|}{\|W\|}$$

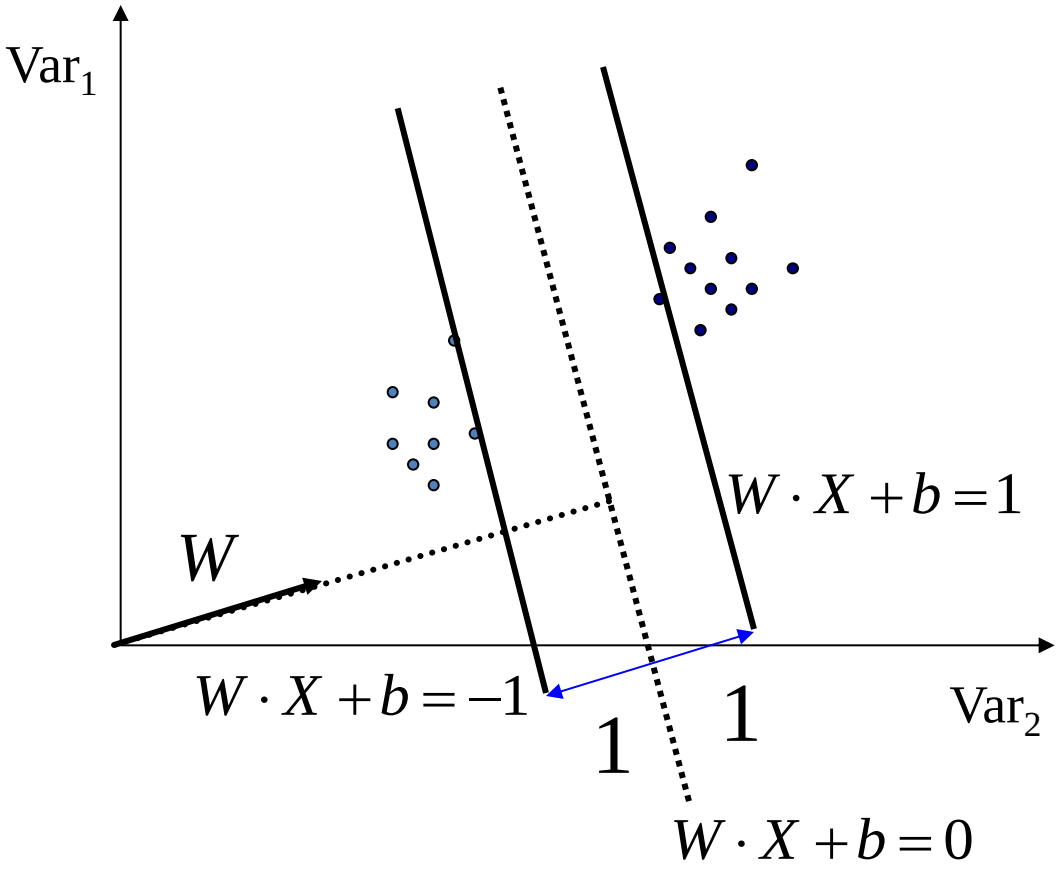
So, the problem is:

Maximize $\frac{2|k|}{\|W\|}$

s.t. $W \cdot X + b \geq k, \forall\ X\ in\ Class\ 1$

$W.X + b \leq -k, \forall\ X\ in\ Class\ 2$

Setting Up the Optimization Problem



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

So, the problem is:

Maximize $\frac{2}{\|W\|}$

s.t. $W \cdot X + b \geq 1, \forall\, X \; in \; Class\; 1$

$W.X + b \leq -1, \forall\, X \; in \; Class\; 2$

Setting Up the Optimization Problem

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

$$W \cdot X_i + b \geq 1, \forall\, X_i \; with \; y_i = 1$$
$$W.X_i + b \leq -1, \forall\, X_i \; with \; y_i = -1$$

- as

$$y_i(W \cdot X_i + b) \geq 1, \forall\, X_i$$

- So the problem becomes:

Maximize $\frac{2}{\|W\|}$
s.t. $y_i(W \cdot X_i + b) \geq 1, \forall\, X_i$

or

Minimize $\frac{1}{2}\|W\|^2$
s.t. $y_i(W \cdot X_i + b) \geq 1, \forall\, X_i$

Linear, Hard-Margin SVM Formulation

- Find *W, b* that solves

Minimize $\frac{1}{2}\|W\|^2$

s.t. $y_i(W \cdot X_i + b) \geq 1, \forall X_i$

- Problem is convex so, there is a unique global minimum value (when feasible)
- Non-solvable if the data is not linearly separable
- Quadratic Programming
  - Very efficient computationally with modern constraint optimization engines (handles thousands of constraints).

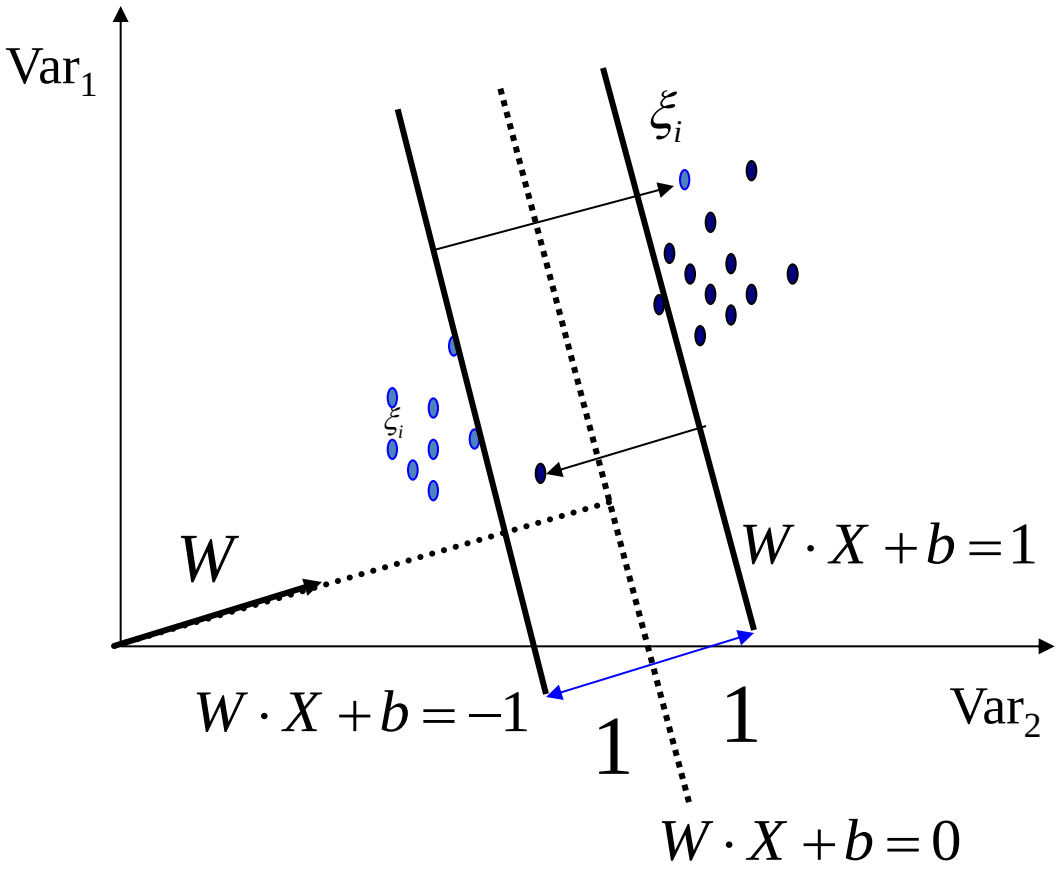
Support Vector Machines

- 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

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

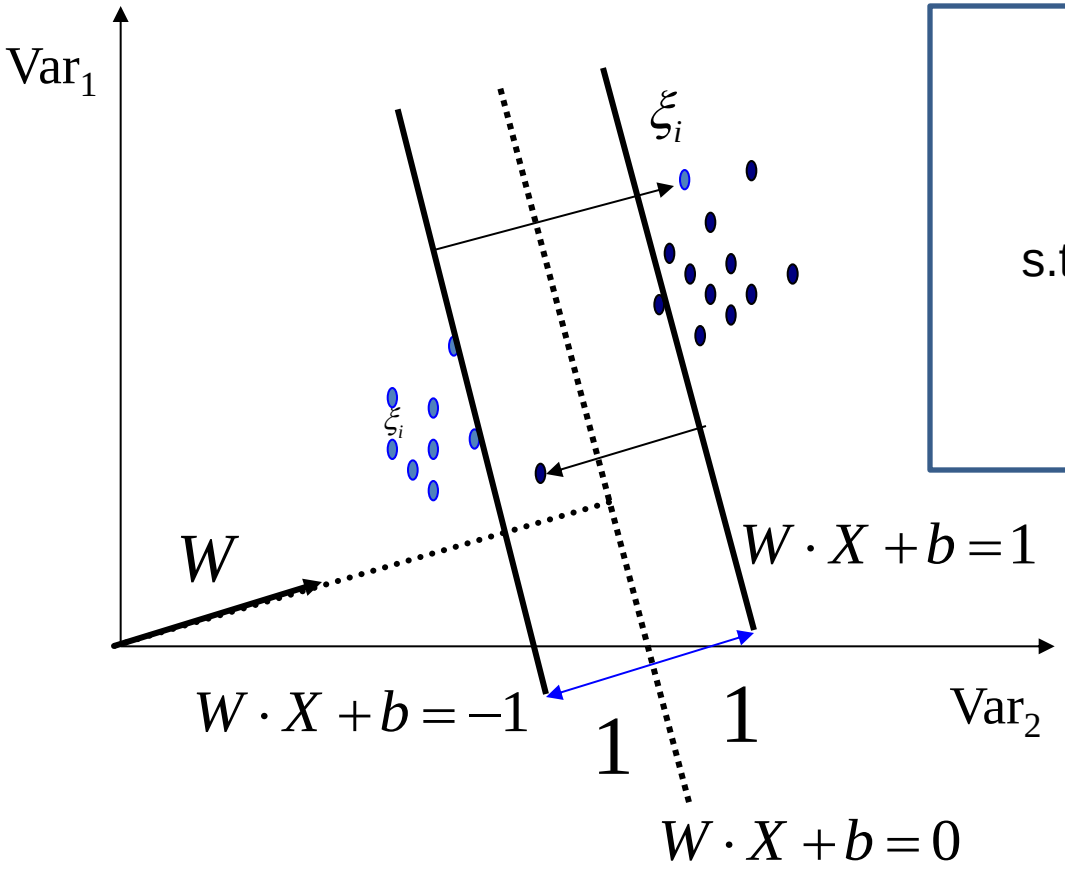
Non-Linearly Separable Data



Introduce slack variables ξ_i

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

Non-Linearly Separable Data



$$\text{Min } \frac{1}{2}\|W\|^2 + C\sum_i \xi_i$$

$$\text{s.t. } y_i(W \cdot X_i + b) \geq 1 - \xi_i, \forall X_i$$

$$\text{and} \quad \xi_i \geq 0$$

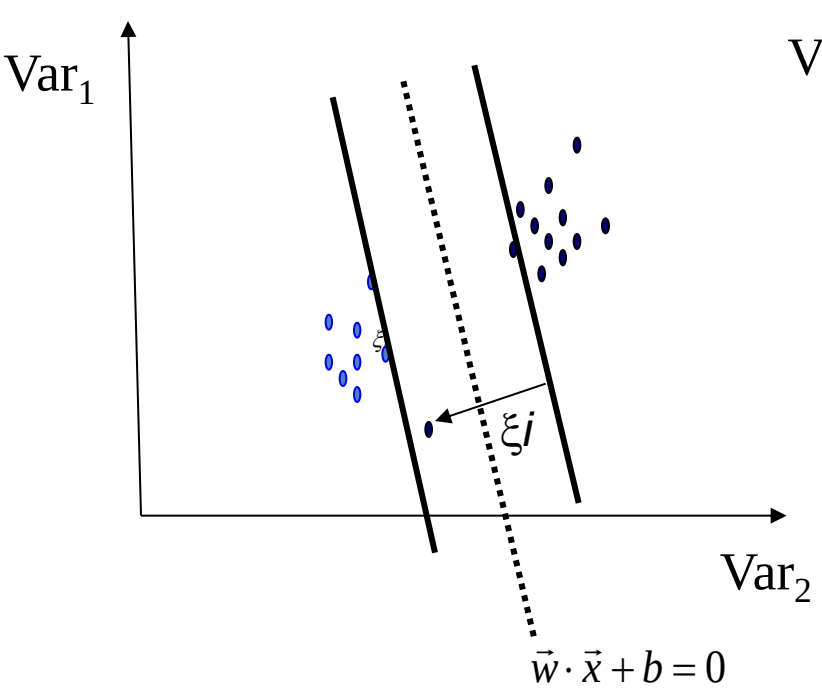
C trades-off margin width and misclassifications

Linear, Soft-Margin SVMs

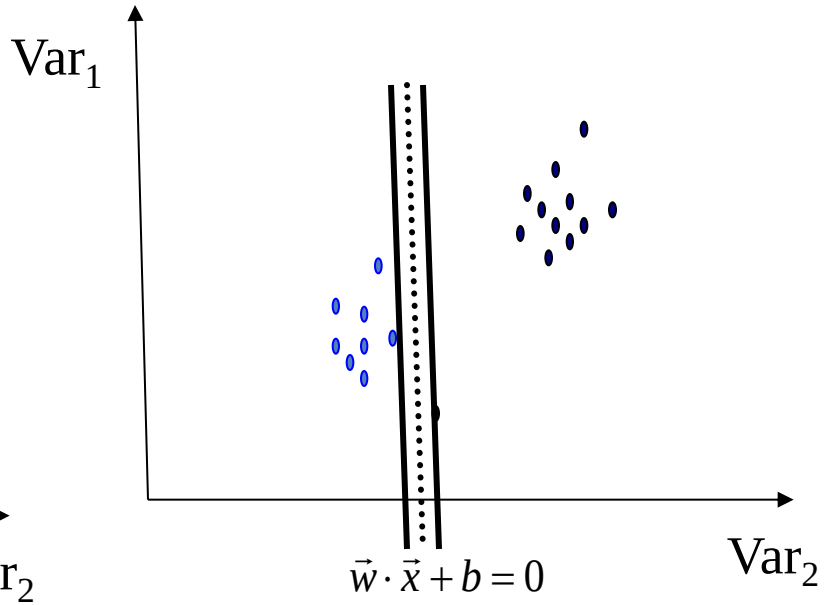
$$\min \frac{1}{2}\|w\|^2 + C\sum_i \xi_i \qquad y_i(w \cdot x_i + b) \geq 1 - \xi_i, \ \forall x_i$$
$$\xi_i \geq 0$$

- Algorithm tries to maintain ξ_i 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_i^2 instead
- As $C \to \infty$, we get closer to the hard-margin solution

Robustness of Soft vs Hard Margin SVMs



Soft Margin SVM



Hard Margin SVM

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)

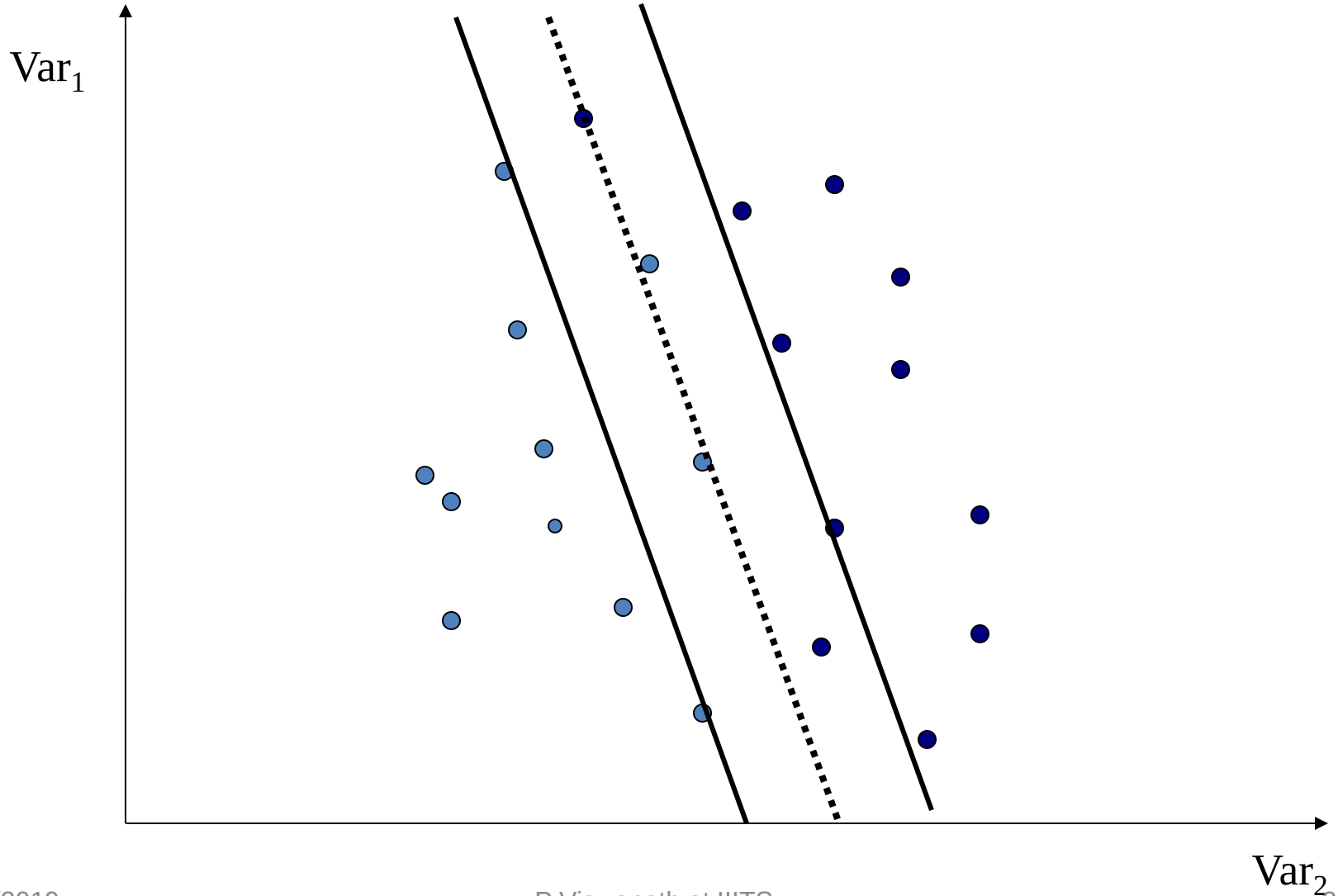
Support Vector Machines

- 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

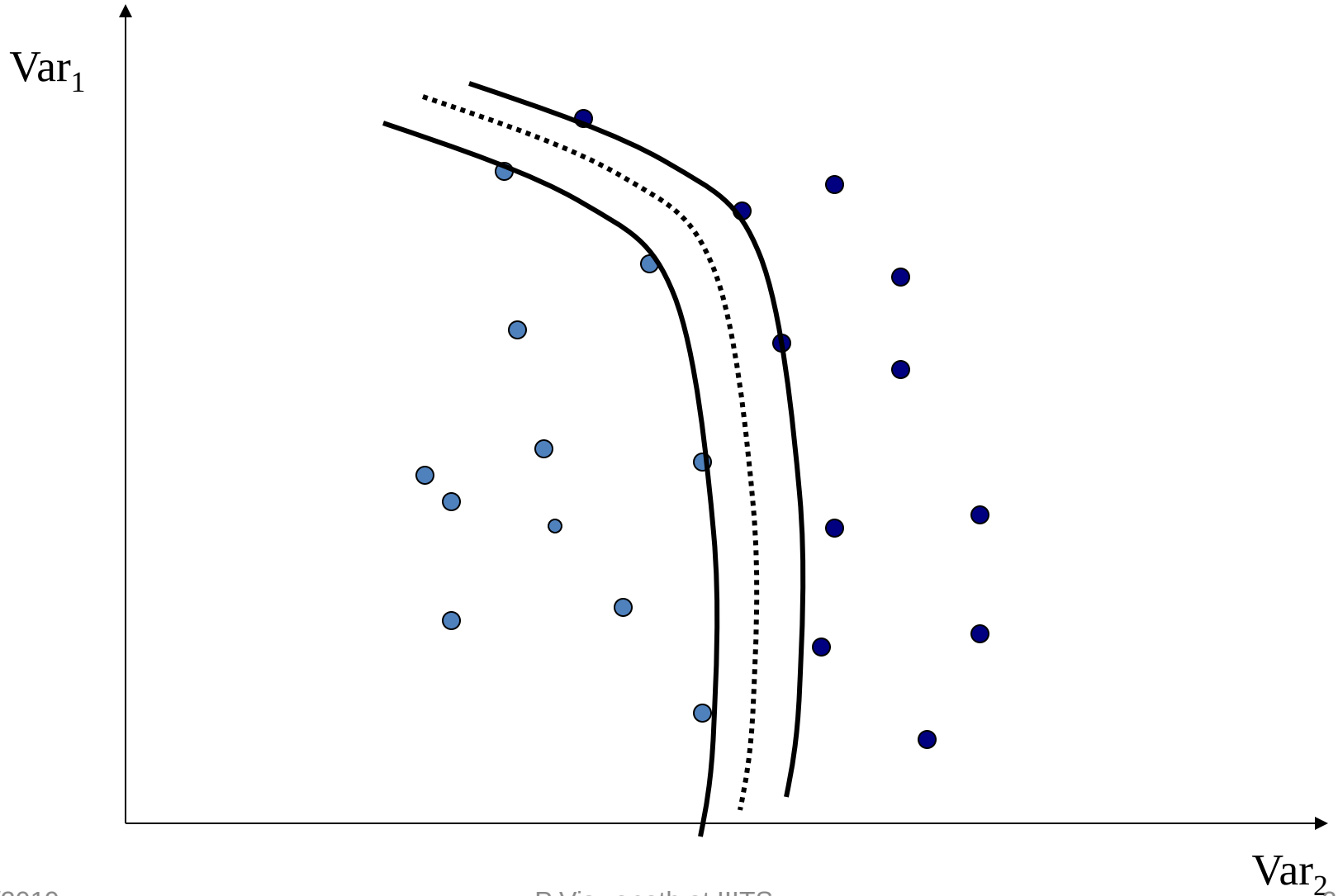
Support Vector Machines

- 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

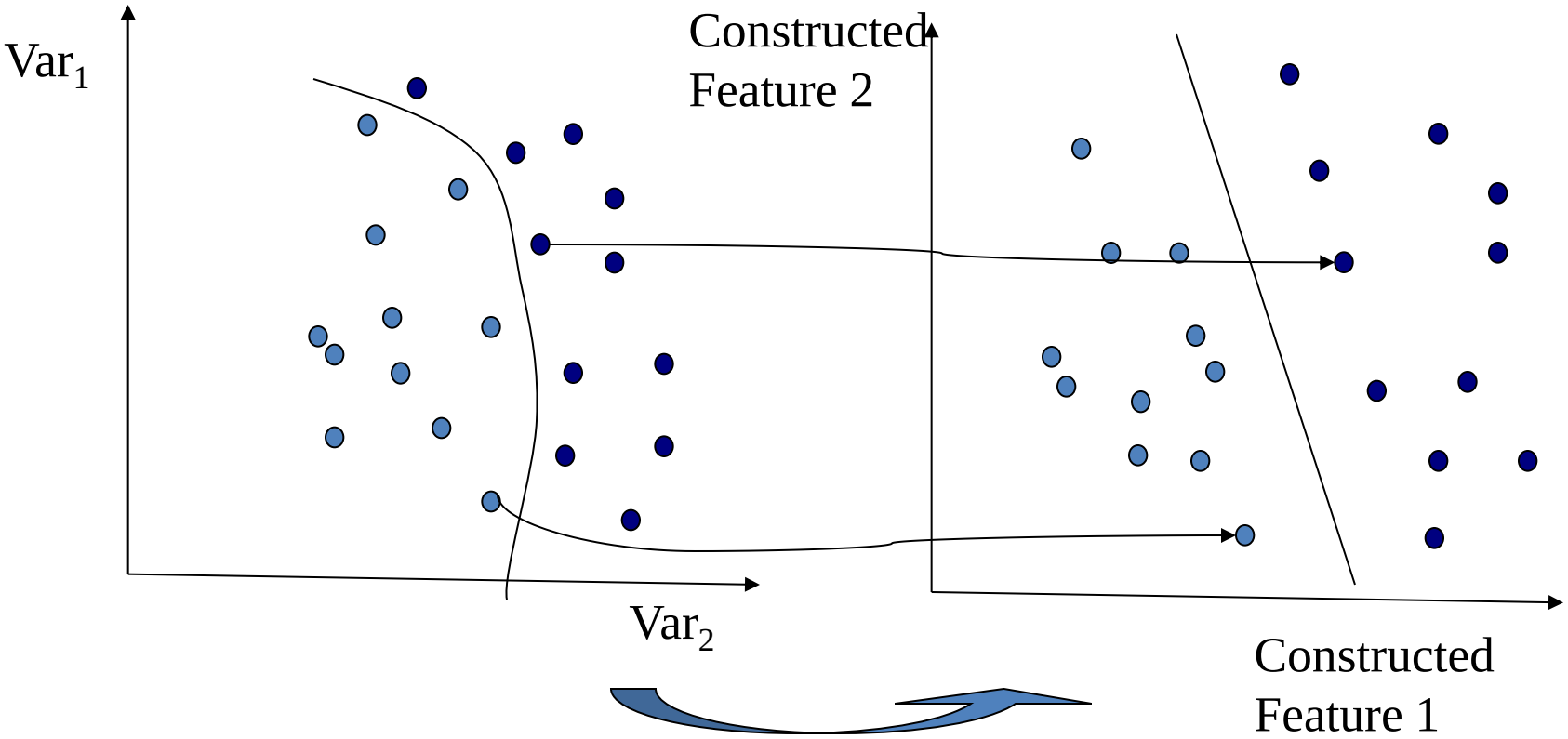
Disadvantages of Linear Decision Surfaces



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:

- $\min \frac{1}{2}\left|\left|W\right|\right|^2 + C\sum_i \xi_i$ $\quad s.t.\ \ y_i(W\cdot\Phi(X)+b) \geq 1-\xi_i, \forall X_i$ $\quad \xi_i \geq 0$

- 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

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

$$s.t.\ \ y_i(W \cdot \Phi(X) + b) \geq 1 - \xi_i, \forall X_i$$

$$\xi_i \geq 0$$

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

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

$$s.t.\ \ \mathrm{C} \geq \alpha_\mathrm{i} \geq 0, \forall X_i$$

$$\sum_i \alpha_i y_i = 0$$

- 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: $K(X_i, X_j) = \Phi(X_l) \cdot \Phi(X_j)$, 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

$$\text{sgn}(W \cdot X + b) = \text{sgn}(\sum_i \alpha_i y_i K(X_i, X) + b)$$

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

$$\text{for any } j \text{ with } \alpha_j \neq 0$$

Examples of Kernels

- Assume we measure two quantities

- Consider the function:

$$\Phi : (x_1, x_2) \rightarrow (x_1^2, x_2^2, \sqrt{2}x_1x_2, x_1, x_2, 1)$$

- We can verify that:

$$K(X_1, X_2) = (X_1 \cdot X_2 + 1)^2$$

- These type of kernels are called Polynomial kernels.

Polynomial and Gaussian Kernels

$$K(X \cdot Z) = (X \cdot Z + 1)^p$$

- is called the polynomial kernel of degree *p*.
- Another commonly used Kernel is the Gaussian (maps to an infinite dimensional space):

$$K(X \cdot Z) = \exp(-\|X - Z\| / 2\sigma^2)$$

The Mercer Condition

- Is there a mapping $\Phi(x)$ for any given symmetric function $K(x,z)$? No.
- The SVM dual formulation requires calculation $K(x_i, x_j)$ for each pair of training instances. The matrix $G_{ij} = K(x_i, x_j)$ 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)

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

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
- Kernel-PCA, Kernel-SVD

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

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

Conclusions, before going in to the solution

- 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.
- N. Cristianini. ICML'01 tutorial, 2001.
- K.-R. Müller, S. Mika, G. Rätsch, K. Tsuda, and B. Schölkopf. An introduction to kernel-based learning algorithms. *IEEE Neural Networks*, 12(2):181-201, May 2001.
- B. Schölkopf. SVM and kernel methods, 2001. Tutorial given at the NIPS Conference.
- Hastie, Tibshirani, Friedman, The Elements of Statistical Learning, Springel 2001