

CS145: INTRODUCTION TO DATA MINING

5: Vector Data: Support Vector Machine

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Methods to Learn: Last Lecture

	Vector Data	Set Data	Sequence Data	Text Data
Classification	Logistic Regression; Decision Tree; KNN SVM; NN			Naïve Bayes for Text
Clustering	K-means; hierarchical clustering; DBSCAN; Mixture Models			PLSA
Prediction	Linear Regression GLM*			
Frequent Pattern Mining		Apriori; FP growth	GSP; PrefixSpan	
Similarity Search			DTW	

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Support Vector Machine

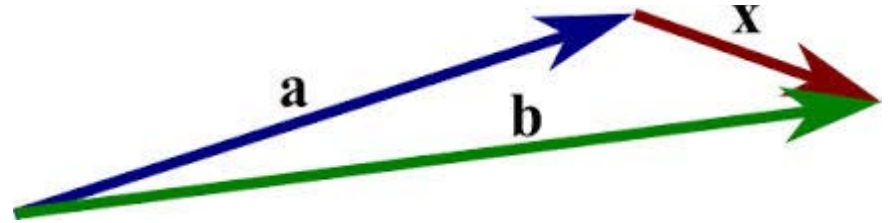
- Introduction 
- Linear SVM
- Non-linear SVM
- Scalability Issues*
- Summary

Math Review

- Vector

- $\mathbf{x} = (x_1, x_2, \dots, x_n)$

- Subtracting two vectors: $\mathbf{x} = \mathbf{b} - \mathbf{a}$

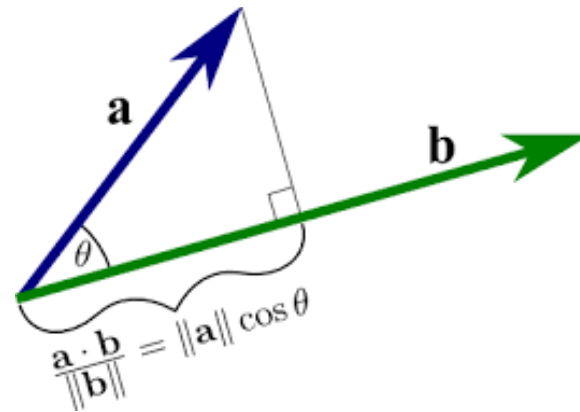


- Dot product

- $\mathbf{a} \cdot \mathbf{b} = \sum a_i b_i$

- Geometric interpretation: projection

- If \mathbf{a} and \mathbf{b} are orthogonal, $\mathbf{a} \cdot \mathbf{b} = 0$



Math Review (Cont.)

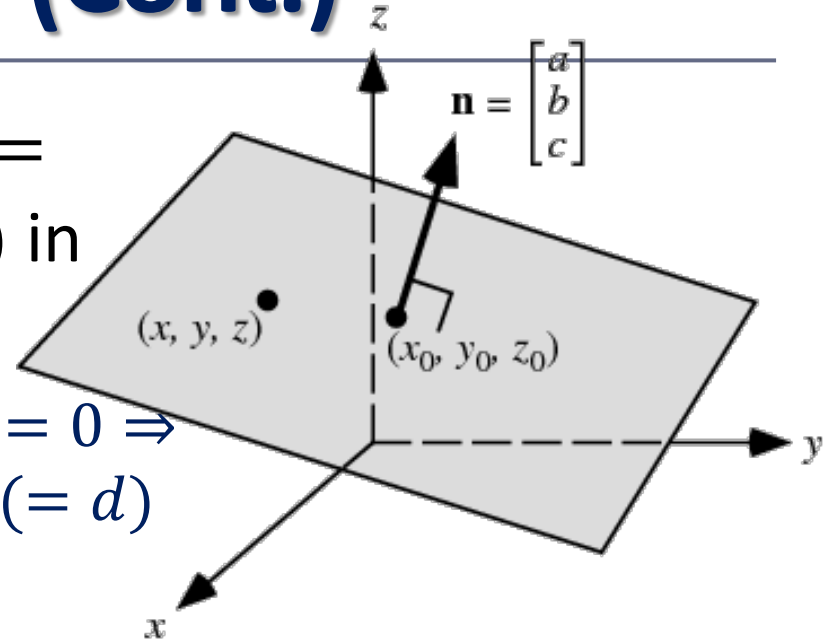
- Plane/Hyperplane
 - $a_1x_1 + a_2x_2 + \cdots + a_nx_n = c$
 - Line (n=2), plane (n=3), hyperplane (higher dimensions)
- Normal of a plane
 - $\mathbf{n} = (a_1, a_2, \dots, a_n)$
 - a vector which is perpendicular to the surface

Math Review (Cont.)

- Define a plane using normal $\mathbf{n} = (a, b, c)$ and a point (x_0, y_0, z_0) in the plane:

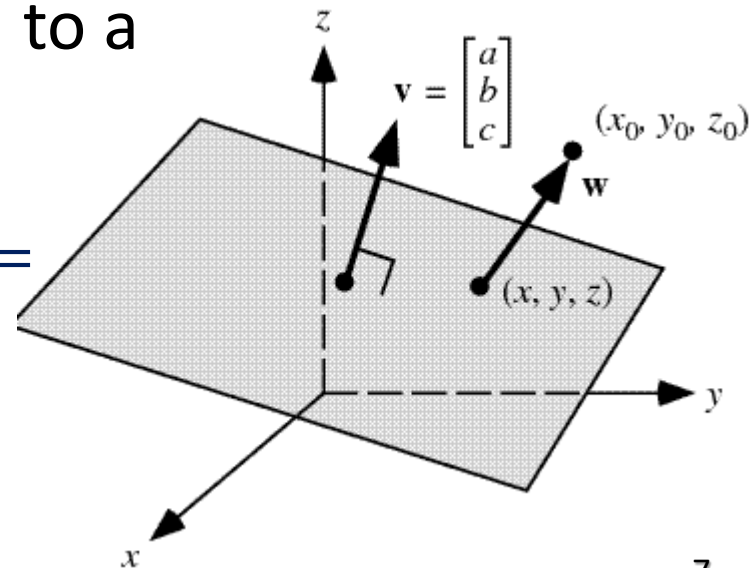
- $$(a, b, c) \cdot (x_0 - x, y_0 - y, z_0 - z) = 0 \Rightarrow$$

$$ax + by + cz = ax_0 + by_0 + cz_0 (= d)$$



- Distance from a point (x_0, y_0, z_0) to a plane $ax + by + cz = d$

- $$\frac{\left| (x_0 - x, y_0 - y, z_0 - z) \cdot \frac{(a, b, c)}{\|(a, b, c)\|} \right|}{\frac{|ax_0 + by_0 + cz_0 - d|}{\sqrt{a^2 + b^2 + c^2}}} =$$



Linear Classifier

- Given a training dataset $\{\mathbf{x}_i, y_i\}_{i=1}^N$
 - A separating hyperplane can be written as a linear combination of attributes

$$\mathbf{W} \bullet \mathbf{X} + b = 0$$

where $\mathbf{W} = \{w_1, w_2, \dots, w_n\}$ is a weight vector and b a scalar (bias)

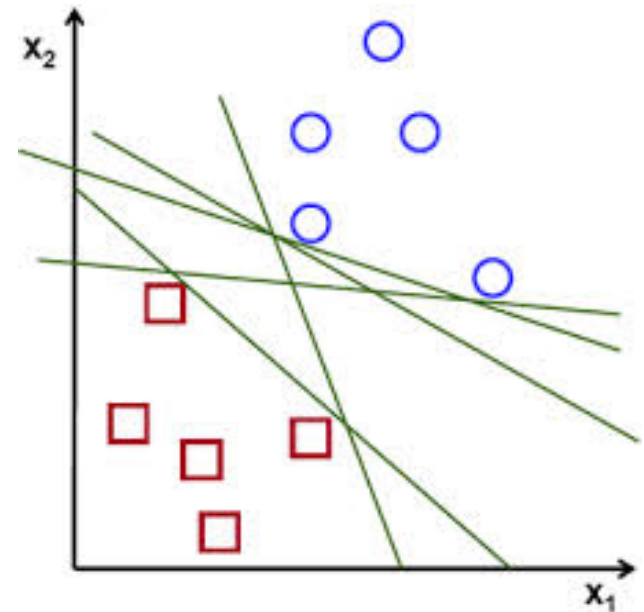
- For 2-D it can be written as

$$w_0 + w_1 x_1 + w_2 x_2 = 0$$

- Classification:

$$w_0 + w_1 x_1 + w_2 x_2 > 0 \Rightarrow y_i = +1$$

$$w_0 + w_1 x_1 + w_2 x_2 \leq 0 \Rightarrow y_i = -1$$



Recall

- Is the decision boundary for logistic regression linear?
- Is the decision boundary for decision tree linear?

Simple Linear Classifier: Perceptron

$$\mathbf{x} = (\mathbf{1}, x_1, x_2, \dots, x_d)^T \quad \mathbf{w} = (\omega_0, \omega_1, \omega_2, \dots, \omega_d)^T$$
$$y = \{1, -1\} \quad \alpha \in (0, 1] \text{ (learning rate)}$$

Initialize $\mathbf{w} = \mathbf{0}$ (can be any vector)

Repeat:

- For each training example (\mathbf{x}_i, y_i) :
 - Compute $\hat{y}_i = \text{sign}(\mathbf{w}^T \mathbf{x}_i)$
 - if $(y_i \neq \hat{y}_i)$ $\mathbf{w} = \mathbf{w} + \alpha(y_i \mathbf{x}_i)$

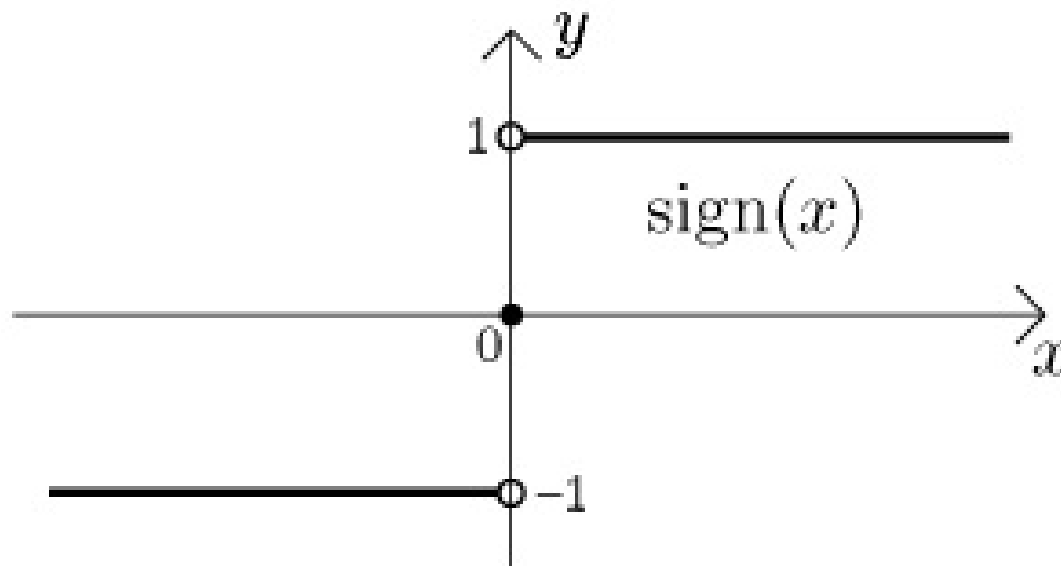
Until $(y_i = \hat{y}_i \quad \forall i = 1 \dots N)$

Return \mathbf{w}

Loss function: $\max\{0, -y_i * w^T x_i\}$

More on Sign Function


- $$\text{sign}(x) = \begin{cases} 1, & x > 0; \\ 0, & x = 0; \\ -1, & x < 0. \end{cases}$$



Example ($\alpha = 0.9$)

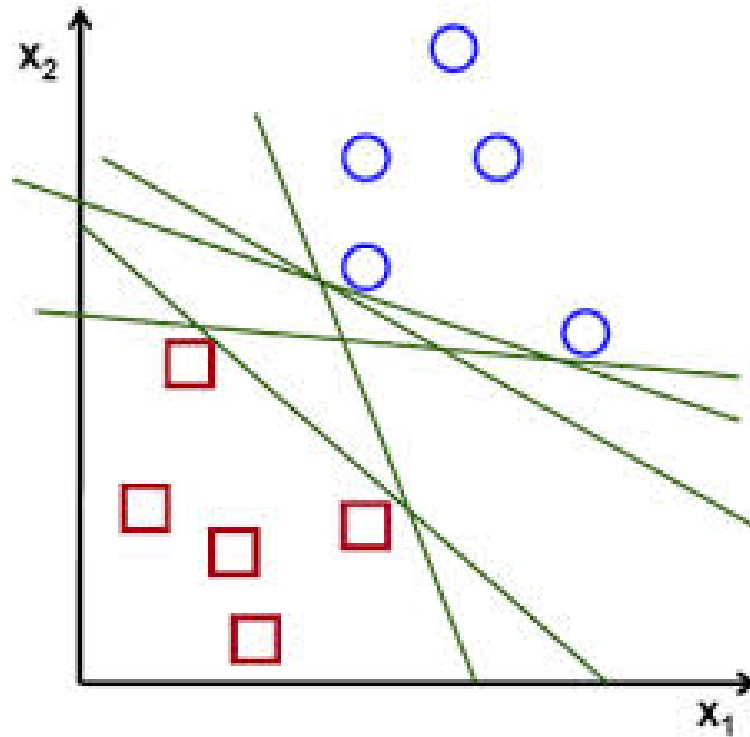
x0	x1	x2	true label	w before update	predicted label	w after update
1	0	1	Y	(0.0, 0.0, 0.0)	N	(0.9, 0.0, 0.9)
1	1	1	N	(0.9, 0.0, 0.9)	Y	(0.0, -0.9, 0.0)
1	0	0	Y	(0.0, -0.9, 0.0)	N	(0.9, -0.9, 0.0)
1	1	0	Y	(0.9, -0.9, 0.0)	N	(1.8, 0.0, 0.0)
1	0	1	Y	(1.8, 0.0, 0.0)	Y	(1.8, 0.0, 0.0)
1	1	1	N	(1.8, 0.0, 0.0)	Y	(0.9, -0.9, -0.9)
1	0	0	Y	(0.9, -0.9, -0.9)	Y	(0.9, -0.9, -0.9)
1	1	0	Y	(0.9, -0.9, -0.9)	N	(1.8, 0.0, -0.9)
1	0	1	Y	(1.8, 0.0, -0.9)	Y	(1.8, 0.0, -0.9)
1	1	1	N	(1.8, 0.0, -0.9)	Y	(0.9, -0.9, -1.8)
1	0	0	Y	(0.9, -0.9, -1.8)	Y	(0.9, -0.9, -1.8)
1	1	0	Y	(0.9, -0.9, -1.8)	N	(1.8, 0.0, -1.8)

Support Vector Machine

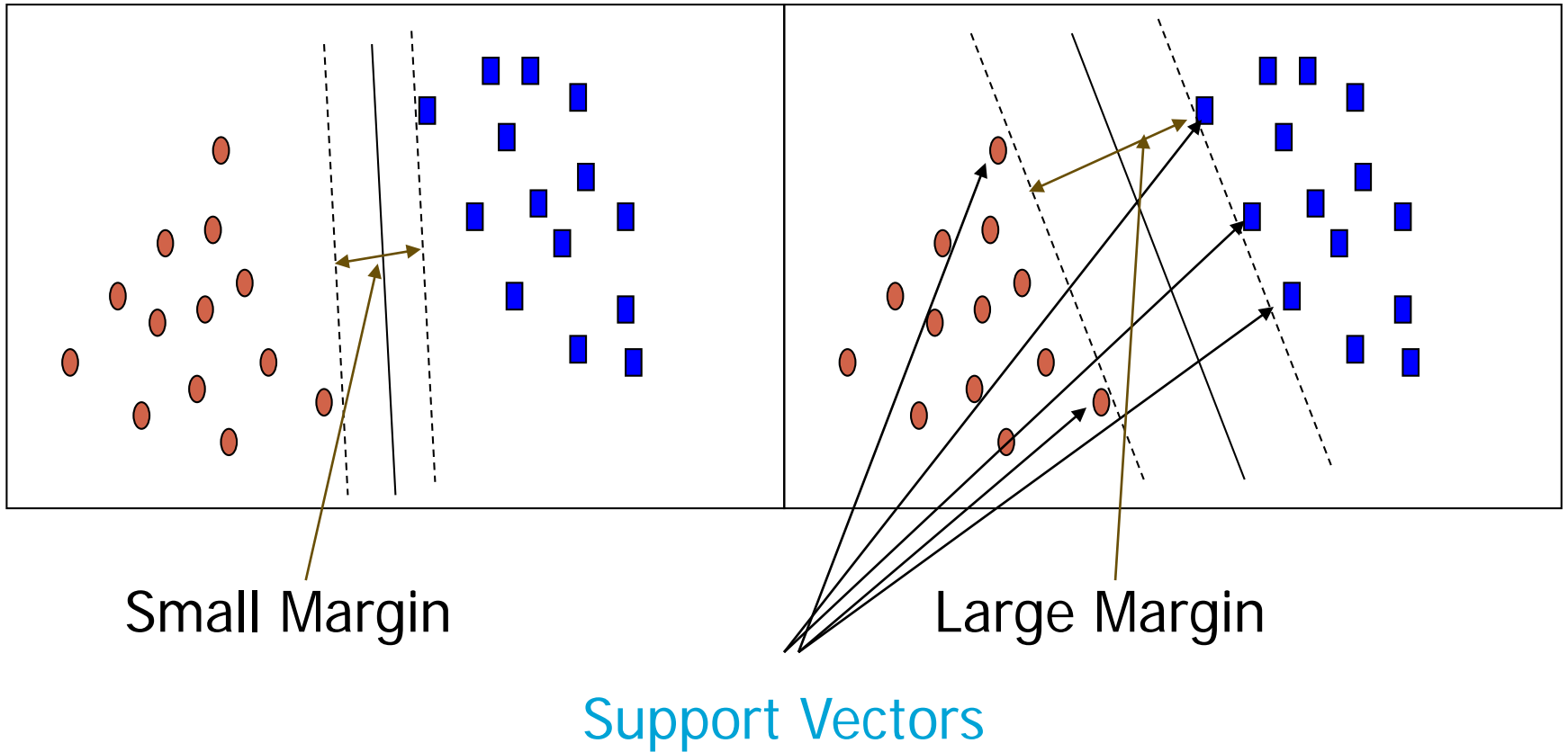
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Can we do better?

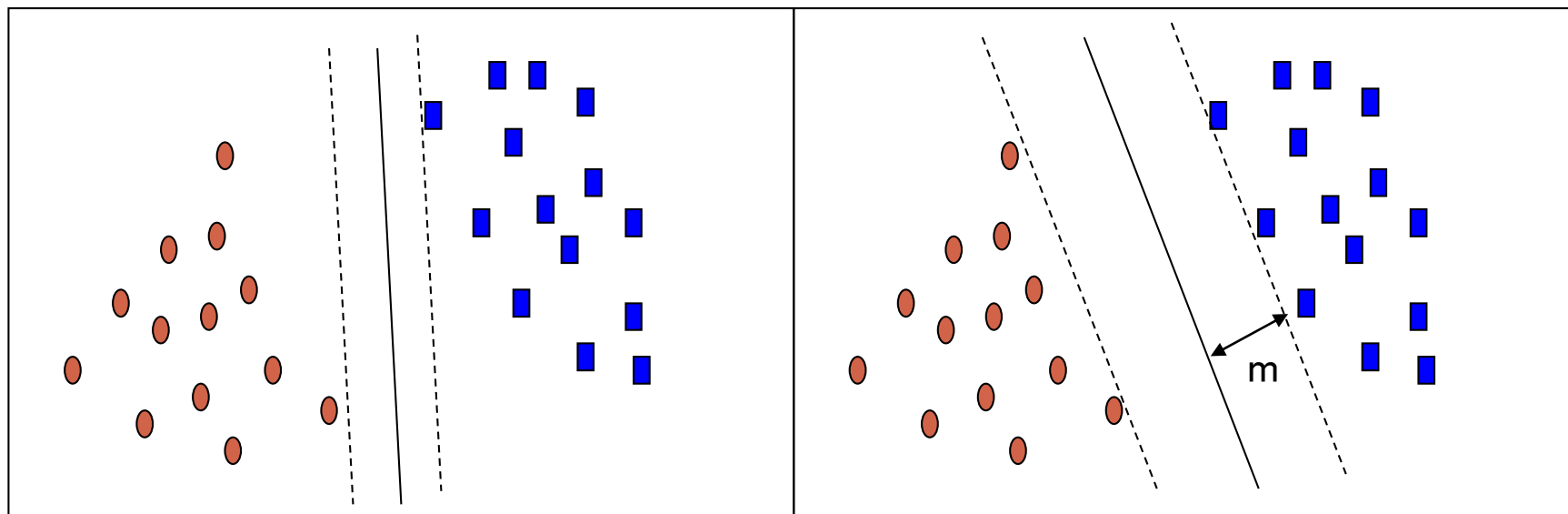
- Which hyperplane to choose?



SVM—Margins and Support Vectors



SVM—When Data Is Linearly Separable



Let data D be $(\mathbf{X}_1, y_1), \dots, (\mathbf{X}_{|D|}, y_{|D|})$, where \mathbf{X}_i is the set of training tuples associated with the class labels y_i

There are infinite lines (hyperplanes) separating the two classes but we want to find the best one (the one that minimizes classification error on unseen data)

*SVM searches for the hyperplane with the largest margin, i.e., **maximum marginal hyperplane** (MMH)*

SVM—Linearly Separable

- A separating hyperplane can be written as

$$\mathbf{W} \bullet \mathbf{X} + b = 0$$

- The hyperplane defining the sides of the margin, e.g.,:

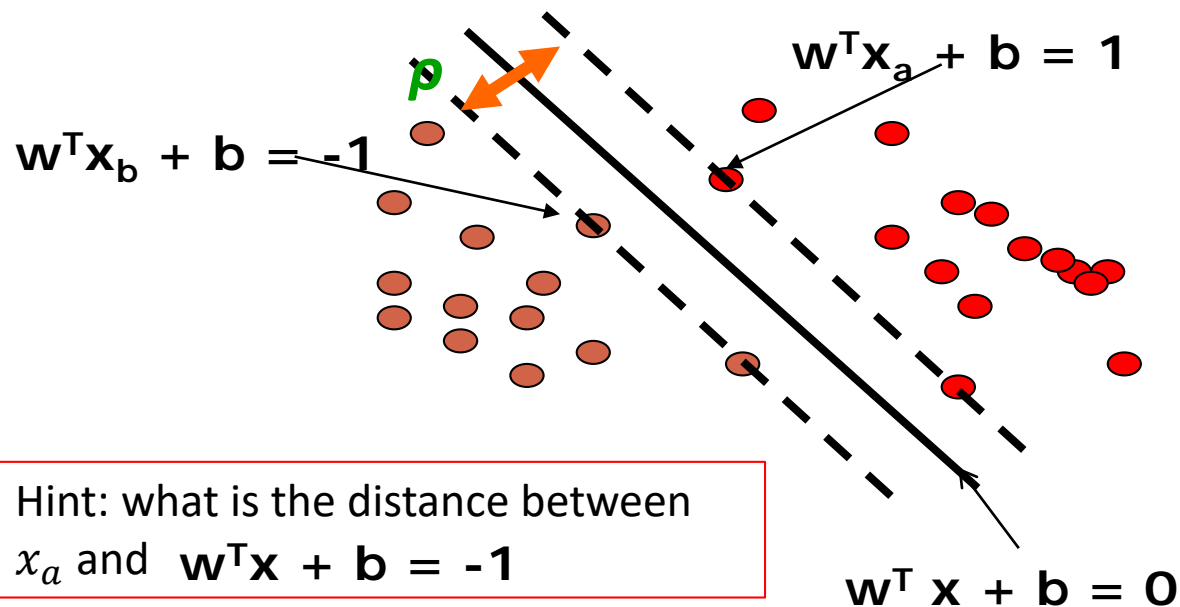
$$H_1: w_1 x_1 + w_2 x_2 + b \geq 1 \quad \text{for } y_i = +1, \text{ and}$$

$$H_2: w_1 x_1 + w_2 x_2 + b \leq -1 \quad \text{for } y_i = -1$$

- Any training tuples that fall on hyperplanes H_1 or H_2 (i.e., the sides defining the margin) are **support vectors**
- This becomes a **constrained (convex) quadratic optimization** problem: Quadratic objective function and linear constraints → *Quadratic Programming (QP)* → Lagrangian multipliers

Maximum Margin Calculation

- \mathbf{w} : decision hyperplane normal vector
- \mathbf{x}_i : data point i
- y_i : class of data point i (+1 or -1)



$$\text{margin: } \rho = \frac{2}{\|\mathbf{w}\|}$$

SVM as a Quadratic Programming

- QP

Objective: Find \mathbf{w} and b such that $\rho = \frac{2}{\|\mathbf{w}\|}$ is maximized;

Constraints: For all $\{(\mathbf{x}_i, y_i)\}$

$$\mathbf{w}^T \mathbf{x}_i + b \geq 1 \text{ if } y_i = 1;$$

$$\mathbf{w}^T \mathbf{x}_i + b \leq -1 \text{ if } y_i = -1$$

- A better form

Objective: Find \mathbf{w} and b such that $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w}$ is minimized;

Constraints: for all $\{(\mathbf{x}_i, y_i)\}$: $y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$

Solve QP

- This is now optimizing a *quadratic* function subject to *linear* constraints
- Quadratic optimization problems are a well-known class of mathematical programming problem, and many (intricate) algorithms exist for solving them (with many special ones built for SVMs)
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_j is associated with every constraint in the primary problem:

Lagrange Formulation

- Introducing Lagrange multipliers $\alpha_i \geq 0$ for each constraint

Minimize

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^N \alpha_i (y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1)$$

Take the partial derivatives w.r.t \mathbf{w}, b :

$$\nabla_{\mathbf{w}} L = \mathbf{w} - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i = 0 \implies \mathbf{w} = \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i$$

$$\frac{\partial L}{\partial b} = - \sum_{i=1}^N \alpha_i y_i = 0$$

Primal Form and Dual Form

Primal

Objective: Find \mathbf{w} and b such that $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w}$ is minimized;

Constraints: for all $\{(\mathbf{x}_i, y_i)\}$: $y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$

Equivalent under some conditions; also w, b, α satisfy KKT conditions

Dual

Objective: Find $\alpha_1 \dots \alpha_n$ such that $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

Constraints

(1) $\sum \alpha_i y_i = 0$

(2) $\alpha_i \geq 0$ for all α_i

- More derivations:

<http://cs229.stanford.edu/notes/cs229-notes3.pdf>

The Optimization Problem Solution

- The solution has the form:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i \quad b = y_k - \mathbf{w}^T \mathbf{x}_k \text{ for any } \mathbf{x}_k \text{ such that } \alpha_k \neq 0$$

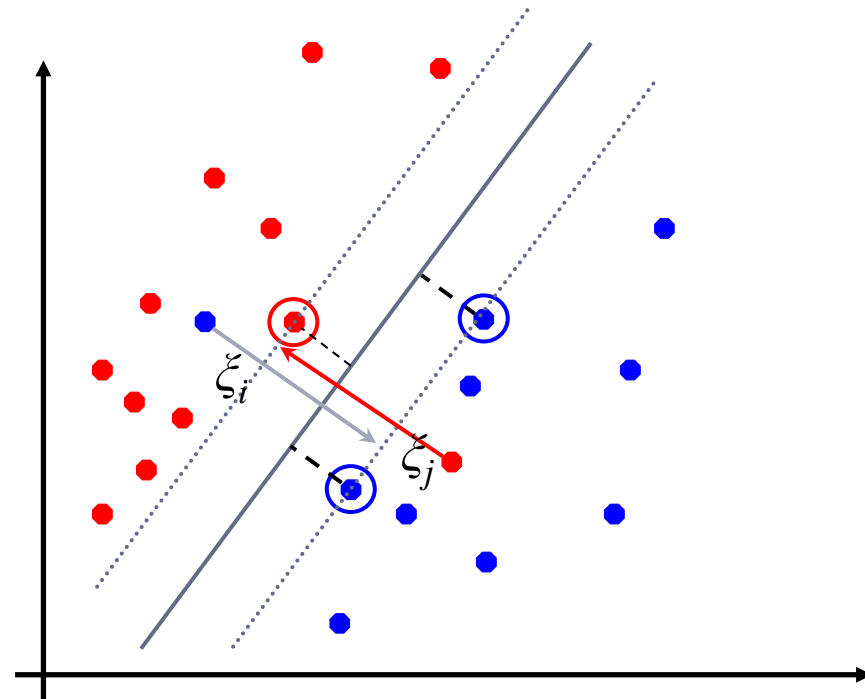
- Each non-zero α_i indicates that corresponding \mathbf{x}_i is a **support vector**.
- Then the classifying function will have the form:

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

- Notice that it relies on an *inner product* between the test point \mathbf{x} and the support vectors \mathbf{x}_i
 - We will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x}_i^T \mathbf{x}_j$ between all pairs of training points.

Soft Margin Classification

- If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.
- Allow some errors
 - Let some points be moved to where they belong, at a cost
- Still, try to minimize training set errors, and to place hyperplane “far” from each class (large margin)



Soft Margin Classification

Mathematically

- The old formulation:

Find \mathbf{w} and b such that

$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} \text{ is minimized and for all } \{(\mathbf{x}_i, y_i)\}$$
$$y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$$

- The new formulation incorporating slack variables:

Find \mathbf{w} and b such that

$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum \xi_i \text{ is minimized and for all } \{(\mathbf{x}_i, y_i)\}$$
$$y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i \quad \text{and} \quad \xi_i \geq 0 \text{ for all } i$$

- Parameter C can be viewed as a way to control overfitting
 - A regularization term (L1 regularization)

Soft Margin Classification – Solution

- The dual problem for soft margin classification:

Find $\alpha_1 \dots \alpha_N$ such that

$Q(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

(1) $\sum \alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ for all α_i

- Neither slack variables ξ_i nor their Lagrange multipliers appear in the dual problem!
- Again, \mathbf{x}_i with non-zero α_i will be **support vectors**.
 - If $0 < \alpha_i < C$, $\xi_i = 0$
 - If $\alpha_i = C$, $\xi_i > 0$
- Solution to the problem is:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i$$

$$b = y_k - \mathbf{w}^T \mathbf{x}_k \text{ for any } \mathbf{x}_k \text{ such that } 0 < \alpha_k < C$$

\mathbf{w} is not needed explicitly for classification!

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

A Different View of Soft Margin SVM

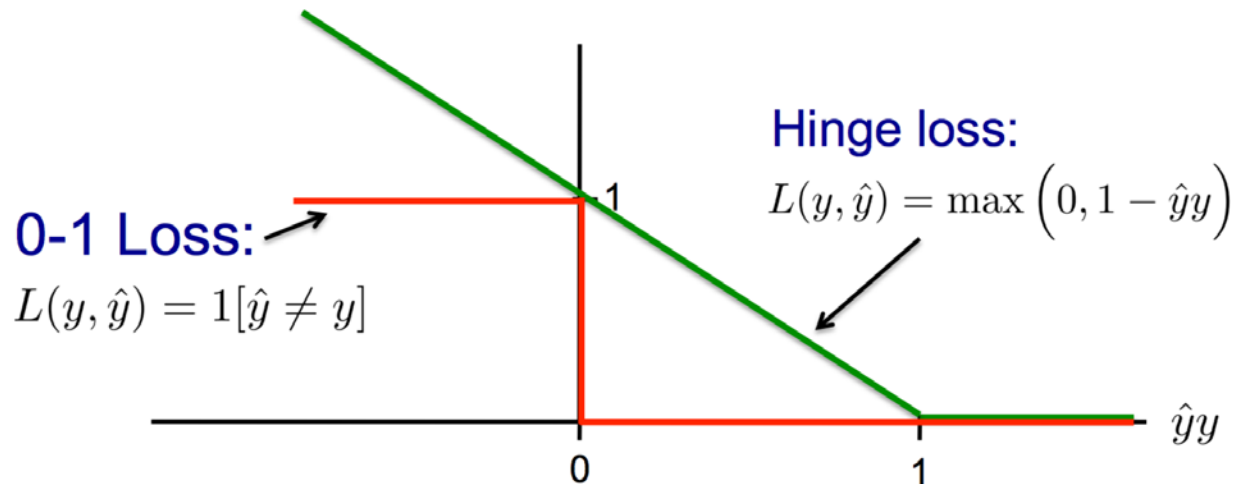
- Hinge loss with regularization terms

- $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum \xi_i$

$$= \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum \max(0, 1 - y_i (\mathbf{w}^T \mathbf{x}_i + b))$$

L2 regularization

Hinge loss



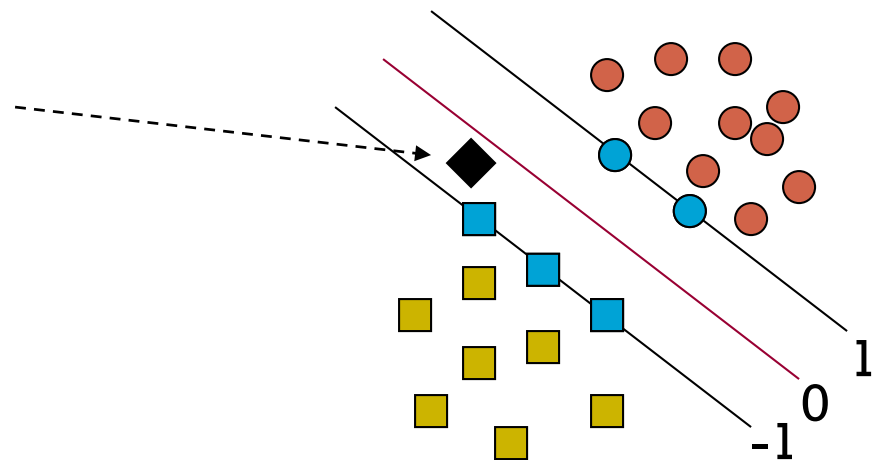
Classification with SVMs

- Given a new point \mathbf{x} , we can score its projection onto the hyperplane normal:
 - I.e., compute score: $\mathbf{w}^T \mathbf{x} + b = \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$
 - Decide class based on whether $<$ or $>$ 0
- Can set confidence threshold t .

Score $> t$: yes

Score $< -t$: no

Else: don't know



Linear SVMs: Summary

- The classifier is a *separating hyperplane*.
- The most “important” training points are the support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points \mathbf{x}_i are support vectors with non-zero Lagrangian multipliers α_i .
- Both in the dual formulation of the problem and in the solution, training points appear only inside inner products:

Find $\alpha_1 \dots \alpha_N$ such that


$\mathbf{Q}(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

(1) $\sum \alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ for all α_i

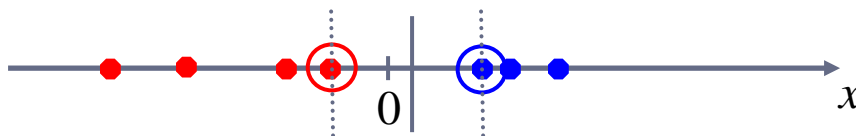
$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

Support Vector Machine

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Non-linear SVMs

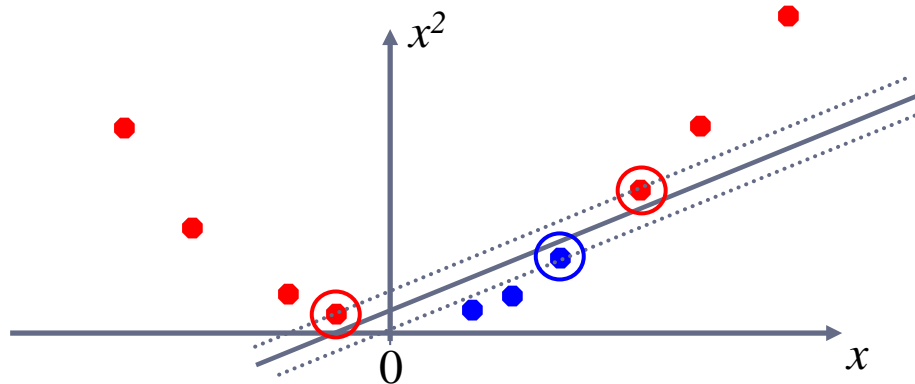
- Datasets that are linearly separable (with some noise) work out great:



- But what are we going to do if the dataset is just too hard?

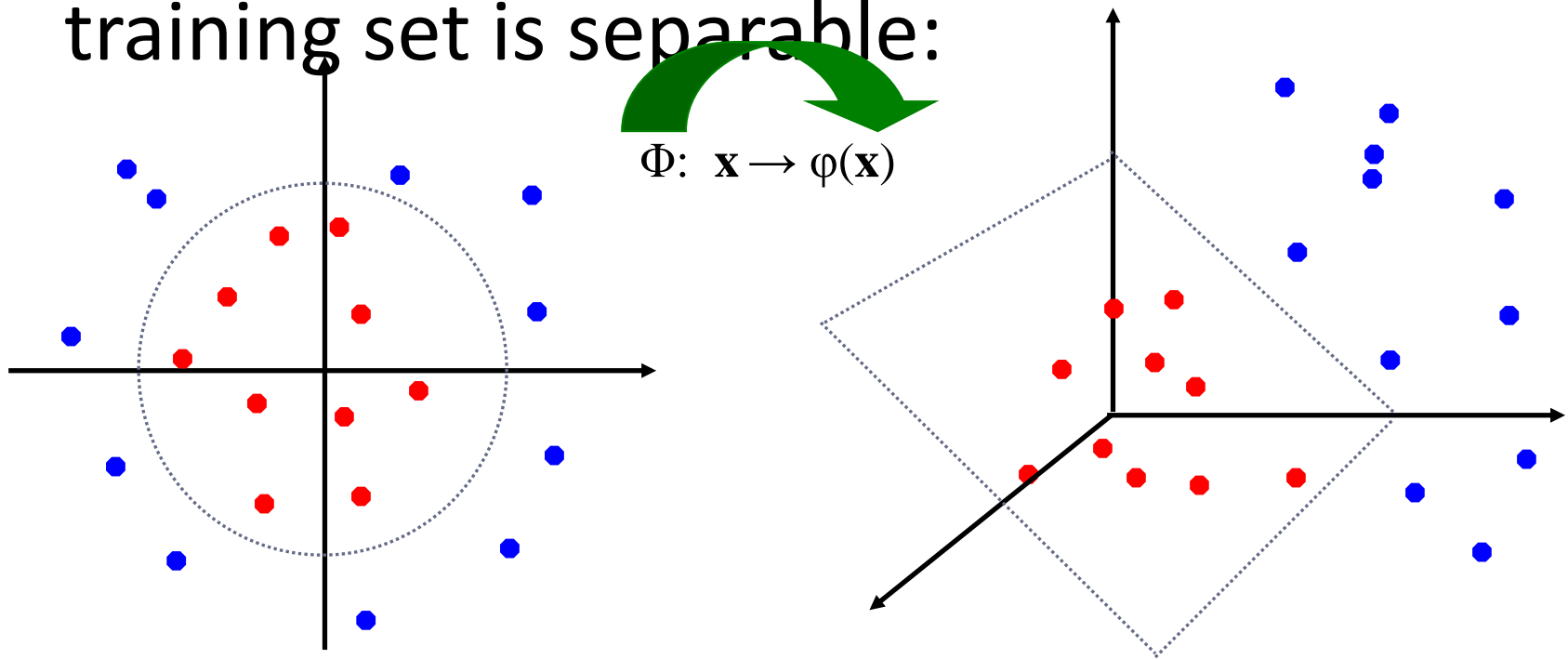


- How about ... mapping data to a higher-dimensional space:



Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



The “Kernel Trick”

- The linear classifier relies on an inner product between vectors $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
- If every data point is mapped into high-dimensional space via some transformation $\Phi: \mathbf{x} \rightarrow \phi(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

- A *kernel function* is some function that corresponds to an inner product in some expanded feature space.

Example

- 2-dimensional vectors $\mathbf{x}=[x_1 \ x_2]$, let $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$
- show that $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$:

$$\begin{aligned} K(\mathbf{x}_i, \mathbf{x}_j) &= (1 + \mathbf{x}_i^T \mathbf{x}_j)^2 = 1 + x_{i1}^2 x_{j1}^2 + 2 x_{i1} x_{j1} x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2 x_{i1} x_{j1} + 2 x_{i2} x_{j2} = \\ &= [1 \ x_{i1}^2 \ \sqrt{2} x_{i1} x_{i2} \ x_{i2}^2 \ \sqrt{2} x_{i1} \ \sqrt{2} x_{i2}]^T [1 \ x_{j1}^2 \ \sqrt{2} x_{j1} x_{j2} \ x_{j2}^2 \ \sqrt{2} x_{j1} \ \sqrt{2} x_{j2}] \\ &= \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) \end{aligned}$$

$$\text{where } \phi(\mathbf{x}) = [1 \ x_1^2 \ \sqrt{2} x_1 x_2 \ x_2^2 \ \sqrt{2} x_1 \ \sqrt{2} x_2]$$

SVM: Different Kernel functions

- Instead of computing the dot product on the transformed data, it is math. equivalent to applying a kernel function $K(\mathbf{X}_i, \mathbf{X}_j)$ to the original data, i.e., $K(\mathbf{X}_i, \mathbf{X}_j) = \Phi(\mathbf{X}_i)^\top \Phi(\mathbf{X}_j)$
- Typical Kernel Functions

Polynomial kernel of degree h : $K(\mathbf{X}_i, \mathbf{X}_j) = (\mathbf{X}_i \cdot \mathbf{X}_j + 1)^h$

Gaussian radial basis function kernel : $K(\mathbf{X}_i, \mathbf{X}_j) = e^{-\|\mathbf{X}_i - \mathbf{X}_j\|^2 / 2\sigma^2}$

Sigmoid kernel : $K(\mathbf{X}_i, \mathbf{X}_j) = \tanh(\kappa \mathbf{X}_i \cdot \mathbf{X}_j - \delta)$

- *SVM can also be used for classifying multiple (> 2) classes and for regression analysis (with additional parameters)

Non-linear SVM

- Replace inner-product with kernel functions
 - Optimization problem

Find $\alpha_1 \dots \alpha_N$ such that

$Q(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{K}(\mathbf{x}_i, \mathbf{x}_j)$ is maximized and


(1) $\sum \alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ for all α_i

- Decision boundary

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{K}(\mathbf{x}_i, \mathbf{x}) + b$$

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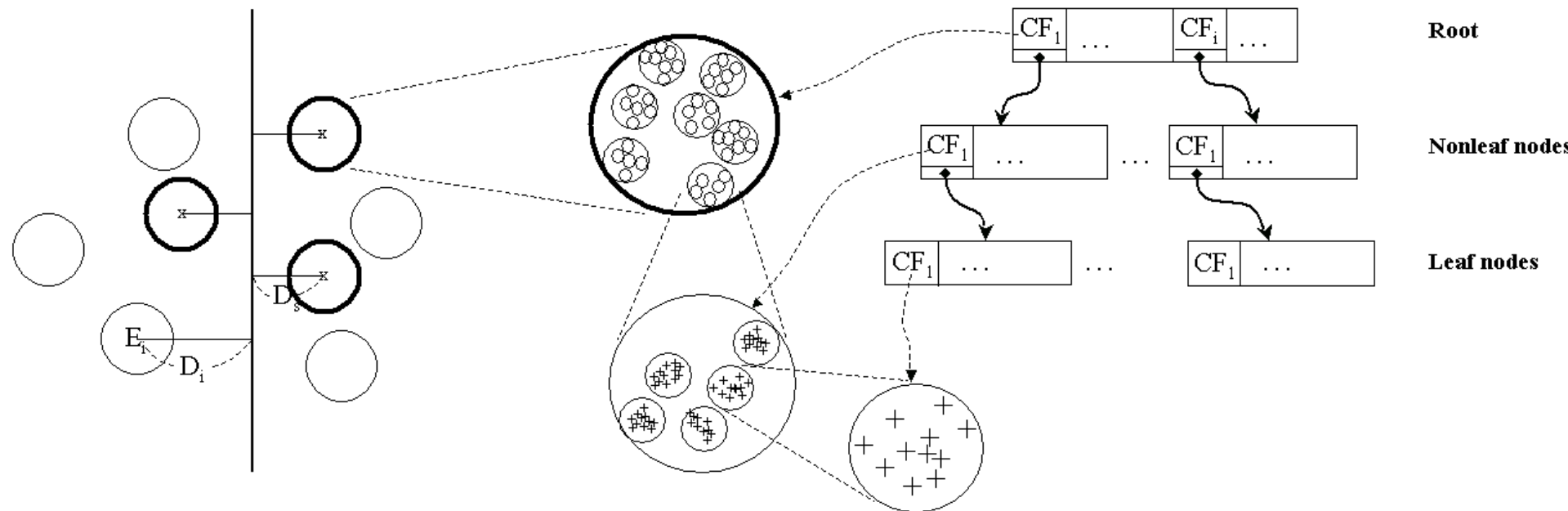
*Scaling SVM by Hierarchical Micro-Clustering

- SVM is not scalable to the number of data objects in terms of training time and memory usage
- H. Yu, J. Yang, and J. Han, “[Classifying Large Data Sets Using SVM with Hierarchical Clusters](#)”, KDD'03)
- CB-SVM (Clustering-Based SVM)
 - Given limited amount of system resources (e.g., memory), maximize the SVM performance in terms of accuracy and the training speed
 - Use micro-clustering to effectively reduce the number of points to be considered
 - At deriving support vectors, de-cluster micro-clusters near “candidate vector” to ensure high classification accuracy

*CF-Tree: Hierarchical Micro-cluster

Negative clusters

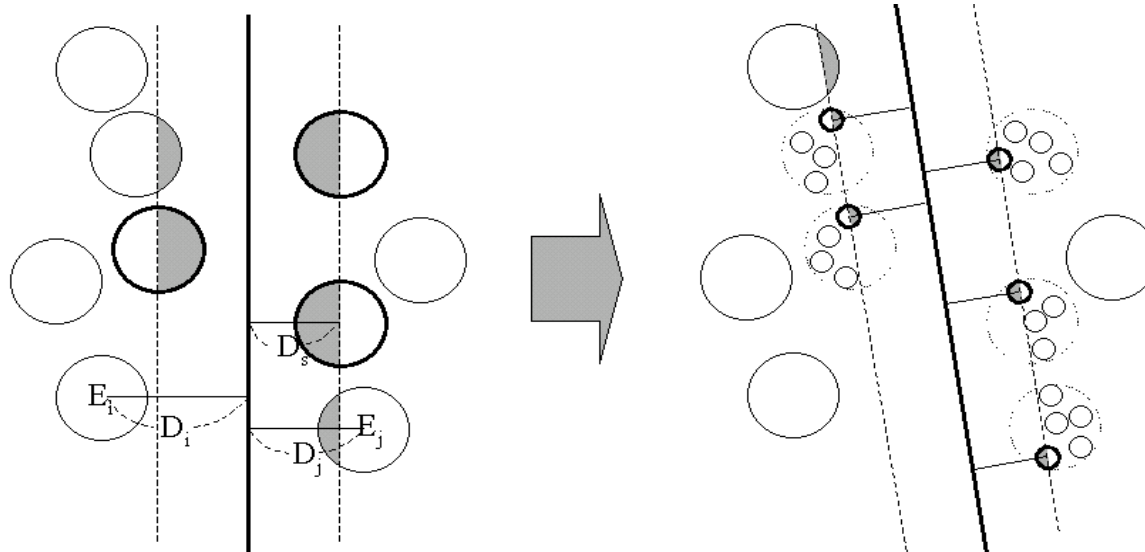
Positive clusters



- Read the data set once, construct a statistical summary of the data (i.e., hierarchical clusters) given a limited amount of memory
- Micro-clustering: Hierarchical indexing structure
 - provide finer samples closer to the boundary and coarser samples farther from the boundary

*Selective Declustering: Ensure High Accuracy

- CF tree is a suitable base structure for selective declustering
- De-cluster only the cluster E_i such that
 - $D_i - R_i < D_s$, where D_i is the distance from the boundary to the center point of E_i and R_i is the radius of E_i
 - Decluster only the cluster whose subclusters have possibilities to be the support cluster of the boundary
 - “Support cluster”: The cluster whose centroid is a support vector



*CB-SVM Algorithm: Outline

- Construct two CF-trees from positive and negative data sets independently
 - Need one scan of the data set
- Train an SVM from the centroids of the root entries
- De-cluster the entries near the boundary into the next level
 - The children entries de-clustered from the parent entries are accumulated into the training set with the non-declustered parent entries
- Train an SVM again from the centroids of the entries in the training set
- Repeat until nothing is accumulated

*Accuracy and Scalability on Synthetic Dataset

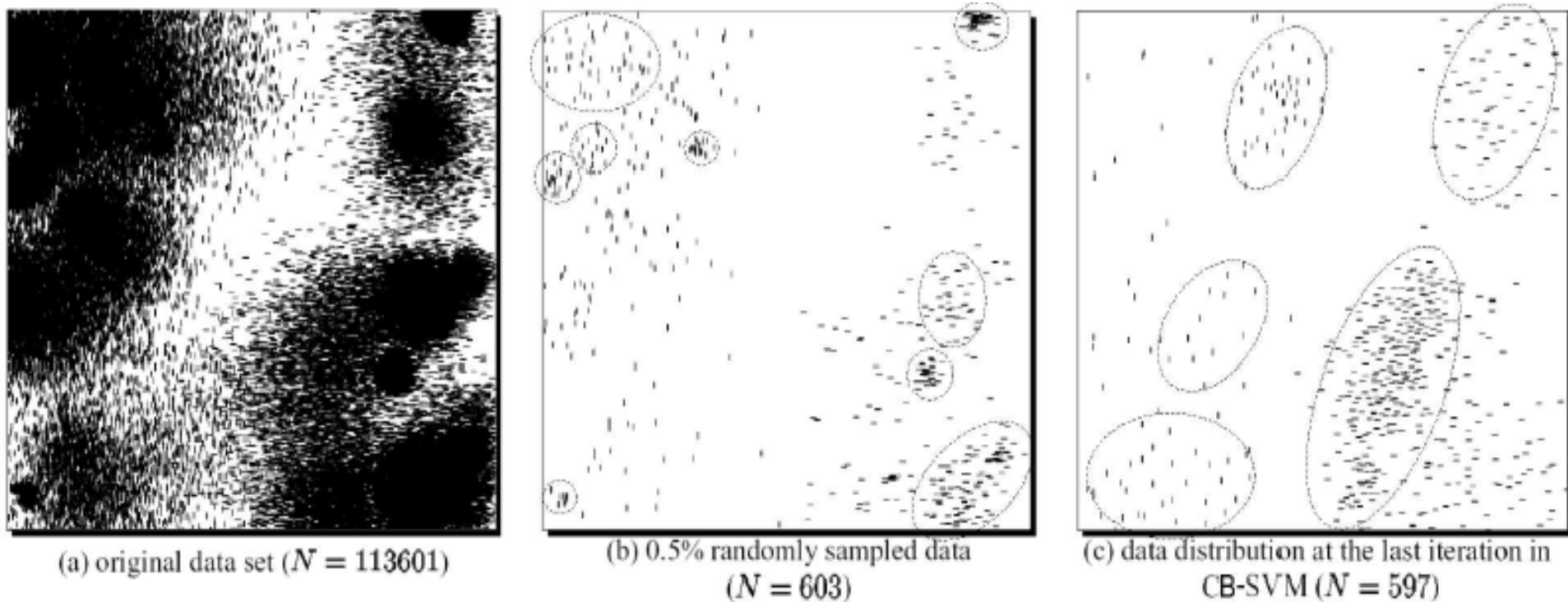



Figure 6: Synthetic data set in a two-dimensional space. ‘|’: positive data; ‘-’: negative data

- Experiments on large synthetic data sets shows better accuracy than random sampling approaches and far more scalable than the original SVM algorithm

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Summary

- Support Vector Machine
 - Linear classifier; support vectors; kernel SVM

SVM Related Links

- SVM Website: <http://www.kernel-machines.org/>
- Representative implementations
 - **LIBSVM**: an efficient implementation of SVM, multi-class classifications, nu-SVM, one-class SVM, including also various interfaces with java, python, etc.
 - **SVM-light**: simpler but performance is not better than LIBSVM, support only binary classification and only in C
 - **SVM-torch**: another recent implementation also written in C
- From classification to regression and ranking:
 - <http://www.dainf.ct.utfpr.edu.br/~kaestner/Mineracao/hwanjoyu-svmtutorial.pdf>

More about Lagrangian

- Objective with equality constraints

$$\min_w f(w)$$

s. t.

$$h_i(w) = 0, \text{ for } i = 1, 2, \dots, l$$

- Lagrangian:

- $L(w, \alpha) = f(w) + \sum_i \alpha_i h_i(w)$

- α_i : Lagrangian multipliers

- Solution: setting the derivatives of Lagrangian to be 0

- $\frac{\partial L}{\partial w} = 0$ and $\frac{\partial L}{\partial \alpha_i} = 0$ for every i

Generalized Lagrangian

- Objective with both equality and inequality constraints

$$\min_w f(w)$$

s. t.

$$h_i(w) = 0, \text{ for } i = 1, 2, \dots, l$$

$$g_j(w) \leq 0, \text{ for } j = 1, 2, \dots, k$$

- Lagrangian

- $L(w, \alpha, \beta) = f(w) + \sum_i \alpha_i h_i(w) + \sum_j \beta_j g_j(w)$

- α_i : Lagrangian multipliers

- $\beta_j \geq 0$: Lagrangian multipliers

Why It Works

- Consider function

$$\theta_p(w) = \max_{\alpha, \beta: \beta_j \geq 0} L(w, \alpha, \beta)$$

- $\theta_p(w) = \begin{cases} f(w), & \text{if } w \text{ satisfies all constraints} \\ \infty, & \text{if } w \text{ doesn't satisfy constraints} \end{cases}$

- Therefore, minimize $f(w)$ with constraints is equivalent to minimize $\theta_p(w)$

Lagrange Duality

- The primal problem

$$p^* = \min_w \max_{\alpha, \beta: \beta_j \geq 0} L(w, \alpha, \beta)$$

- The dual problem

$$d^* = \max_{\alpha, \beta: \beta_j \geq 0} \min_w L(w, \alpha, \beta)$$

- According to max-min inequality

$$p^* \leq d^*$$

- When does equation hold?

Primal = Dual

- $p^* = d^*$, under some proper condition (Slater conditions)
 - f, g_j convex, h_i affine
 - Exists w , such that all $g_j(w) < 0$
- (w^*, α^*, β^*) need to satisfy KKT conditions
 - $\frac{\partial L}{\partial w} = 0$
 - $\beta_j g_j(w) = 0$
 - $h_i(w) = 0, g_j(w) \leq 0, \beta_j \geq 0$