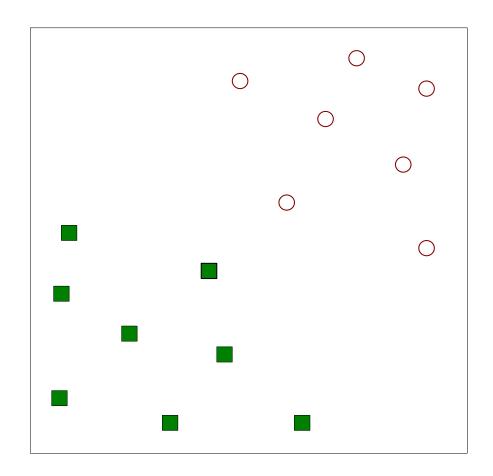
Data Mining

Support Vector Machines

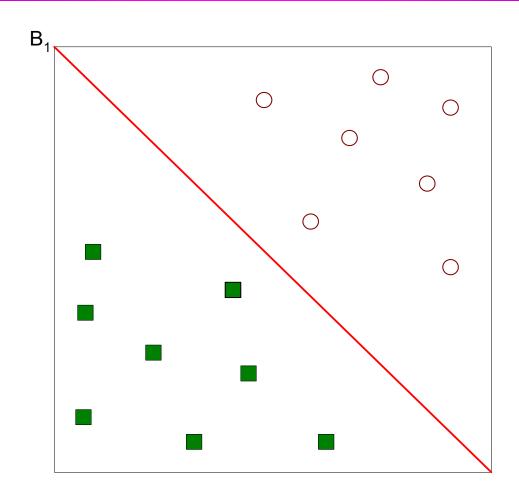
Introduction to Data Mining, 2nd Edition by

Tan, Steinbach, Karpatne, Kumar

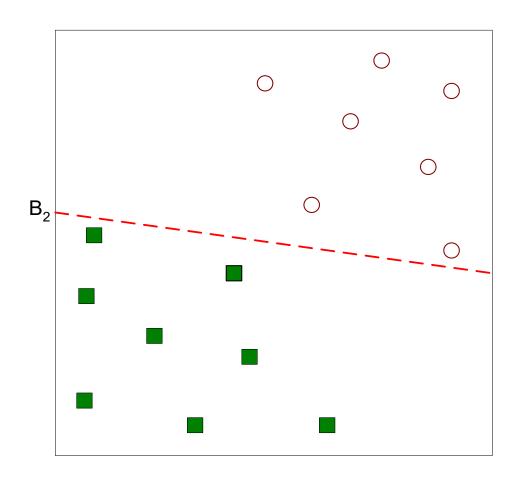


Find a linear hyperplane (decision boundary) that will separate the data

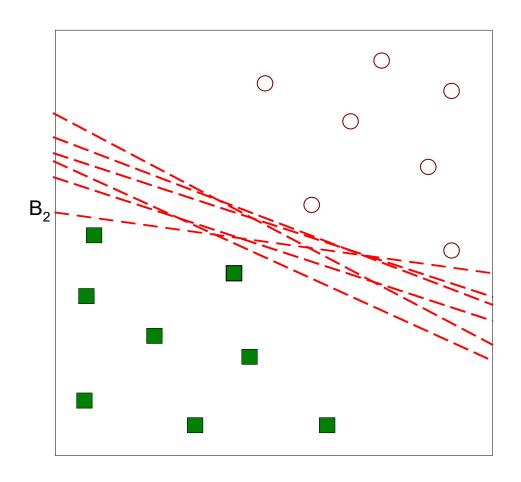
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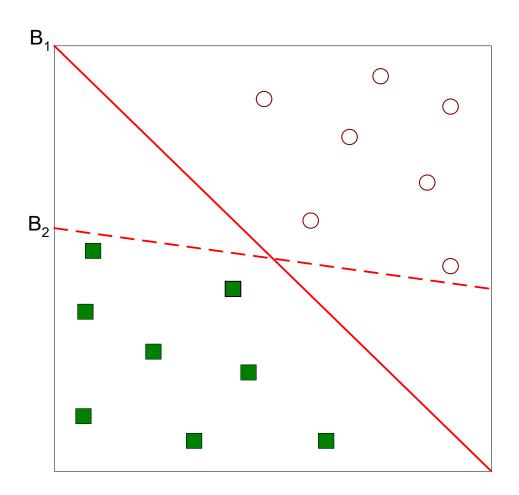
One Possible Solution



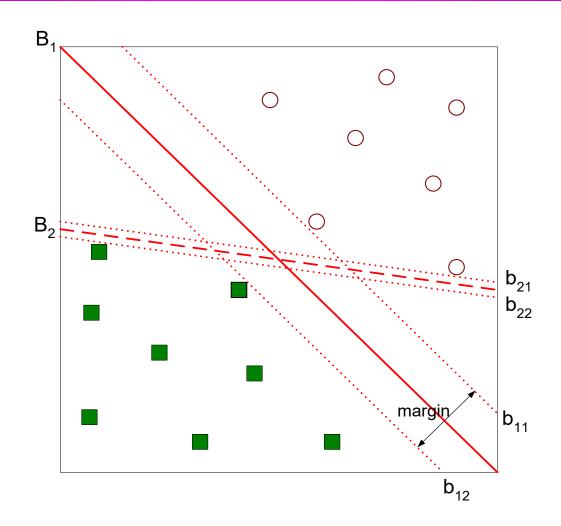
Another possible solution



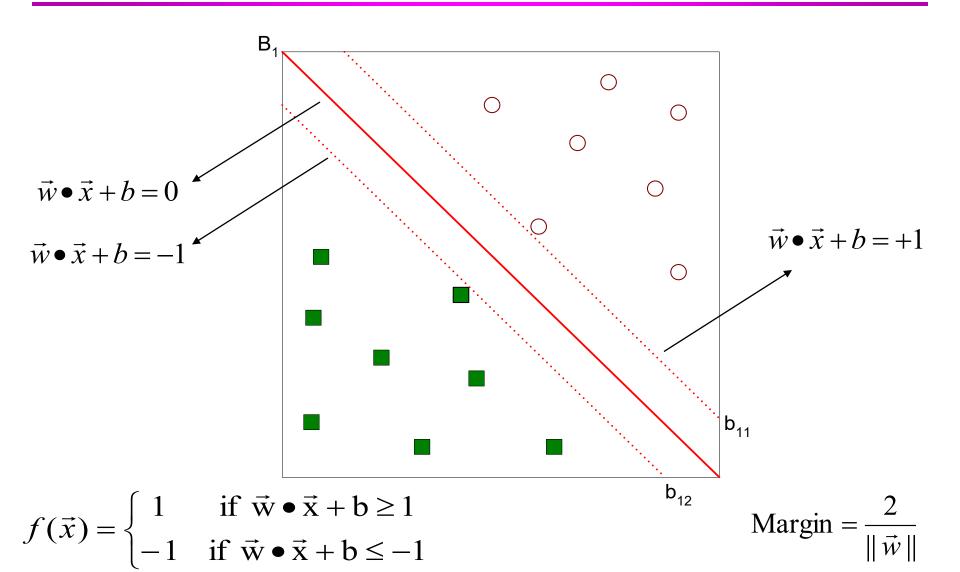
Other possible solutions



- Which one is better? B1 or B2?
- How do you define better?



Find hyperplane that maximizes the margin → B1 is better than B2



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Introduction to Data Mining, 2nd Edition

Linear SVM

Linear model:

$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x} + b \ge 1 \\ -1 & \text{if } \vec{w} \cdot \vec{x} + b \le -1 \end{cases}$$

- Learning the model is equivalent to determining the values of \vec{w} and b
 - How to find \vec{w} and \vec{b} from training data?

Learning Linear SVM

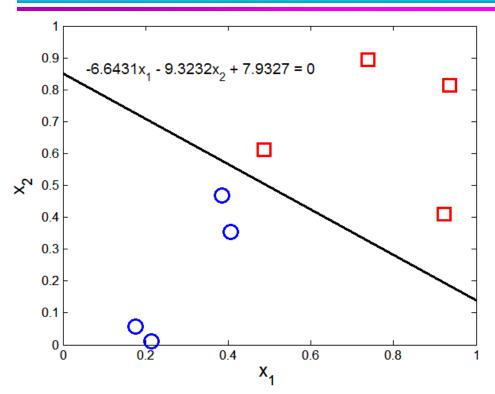
- Objective is to maximize: Margin = $\frac{2}{\|\vec{w}\|}$
 - Which is equivalent to minimizing: $L(\vec{w}) = \frac{\|\vec{w}\|^2}{2}$
 - Subject to the following constraints:

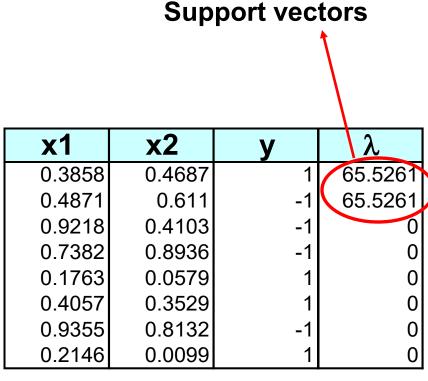
$$y_i = \begin{cases} 1 & \text{if } \vec{\mathbf{w}} \bullet \vec{\mathbf{x}}_i + b \ge 1 \\ -1 & \text{if } \vec{\mathbf{w}} \bullet \vec{\mathbf{x}}_i + b \le -1 \end{cases}$$

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1, \qquad i = 1, 2, \dots, N$$

- This is a constrained optimization problem
 - Solve it using Lagrange multiplier method

Example of Linear SVM



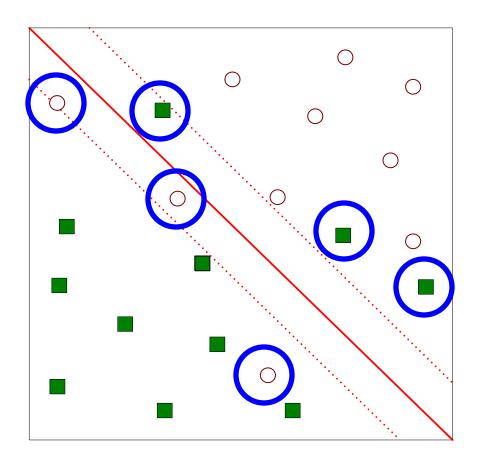


Learning Linear SVM

- Decision boundary depends only on support vectors
 - If you have data set with same support vectors, decision boundary will not change
 - How to classify using SVM once w and b are found? Given a test record, x_i

$$f(\vec{x}_i) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x}_i + b \ge 1 \\ -1 & \text{if } \vec{w} \cdot \vec{x}_i + b \le -1 \end{cases}$$

What if the problem is not linearly separable?



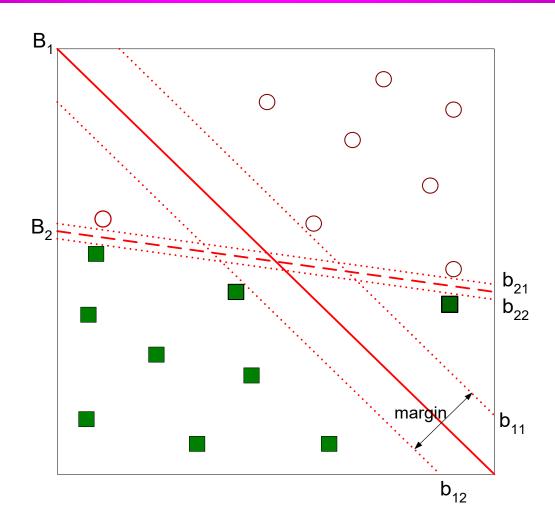
- What if the problem is not linearly separable?
 - Introduce slack variables
 - Need to minimize:

$$L(w) = \frac{\|\vec{w}\|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k\right)$$

Subject to:

$$y_i = \begin{cases} 1 & \text{if } \vec{\mathbf{w}} \bullet \vec{\mathbf{x}}_i + \mathbf{b} \ge 1 - \xi_i \\ -1 & \text{if } \vec{\mathbf{w}} \bullet \vec{\mathbf{x}}_i + \mathbf{b} \le -1 + \xi_i \end{cases}$$

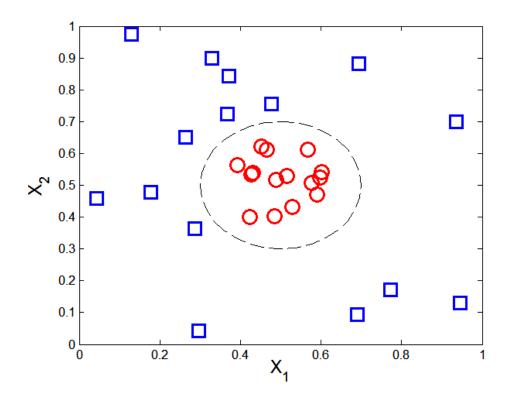
◆ If k is 1 or 2, this leads to similar objective function as linear SVM but with different constraints (see textbook)



Find the hyperplane that optimizes both factors

Nonlinear Support Vector Machines

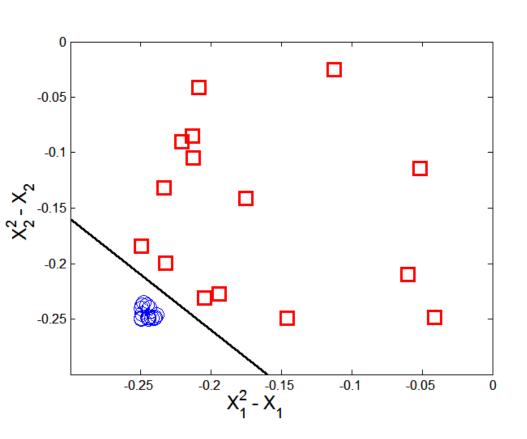
What if decision boundary is not linear?



$$y(x_1, x_2) = \begin{cases} 1 & \text{if } \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} > 0.2 \\ -1 & \text{otherwise} \end{cases}$$

Nonlinear Support Vector Machines

Transform data into higher dimensional space



$$x_1^2 - x_1 + x_2^2 - x_2 = -0.46.$$

$$\Phi:(x_1,x_2) \longrightarrow (x_1^2,x_2^2,\sqrt{2}x_1,\sqrt{2}x_2,1).$$

$$w_4x_1^2 + w_3x_2^2 + w_2\sqrt{2}x_1 + w_1\sqrt{2}x_2 + w_0 = 0.$$

Decision boundary:

$$\vec{w} \bullet \Phi(\vec{x}) + b = 0$$

Learning Nonlinear SVM

Optimization problem:

$$\min_{\mathbf{w}} \frac{\|\mathbf{w}\|^2}{2}$$
subject to $y_i(\mathbf{w} \cdot \Phi(\mathbf{x}_i) + b) \ge 1, \ \forall \{(\mathbf{x}_i, y_i)\}$

 Which leads to the same set of equations (but involve Φ(x) instead of x)

$$\begin{split} L_D &= \sum_{i=1}^n \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j) \qquad \mathbf{w} = \sum_i \lambda_i y_i \Phi(\mathbf{x}_i) \\ & \lambda_i \{ y_i (\sum_j \lambda_j y_j \Phi(\mathbf{x}_j) \cdot \Phi(\mathbf{x}_i) + b) - 1 \} = 0, \end{split}$$

$$f(\mathbf{z}) = sign(\mathbf{w} \cdot \Phi(\mathbf{z}) + b) = sign(\sum_{i=1}^{n} \lambda_i y_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{z}) + b).$$

Learning NonLinear SVM

Issues:

- What type of mapping function ⊕ should be used?
- How to do the computation in high dimensional space?
 - Most computations involve dot product Φ(x_i)• Φ(x_j)
 - Curse of dimensionality?

Learning Nonlinear SVM

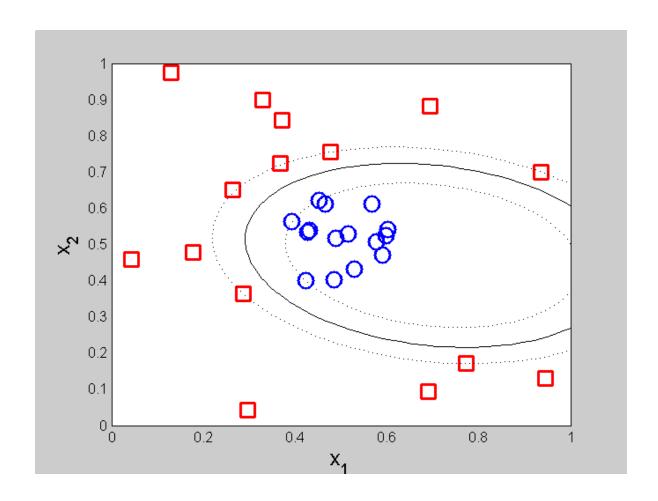
- Kernel Trick:
 - $\Phi(x_i) \bullet \Phi(x_i) = K(x_i, x_i)$
 - K(x_i, x_j) is a kernel function (expressed in terms of the coordinates in the original space)
 - Examples:

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y} + 1)^{p}$$

$$K(\mathbf{x}, \mathbf{y}) = e^{-\|\mathbf{x} - \mathbf{y}\|^{2}/(2\sigma^{2})}$$

$$K(\mathbf{x}, \mathbf{y}) = \tanh(k\mathbf{x} \cdot \mathbf{y} - \delta)$$

Example of Nonlinear SVM



SVM with polynomial degree 2 kernel

Learning Nonlinear SVM

- Advantages of using kernel:
 - Don't have to know the mapping function Φ
 - Computing dot product $\Phi(x_i) \bullet \Phi(x_j)$ in the original space avoids curse of dimensionality
- Not all functions can be kernels
 - Must make sure there is a corresponding Φ in some high-dimensional space
 - Mercer's theorem (see textbook)

Characteristics of SVM

- The learning problem is formulated as a convex optimization problem
 - Efficient algorithms are available to find the global minima
 - Many of the other methods use greedy approaches and find locally optimal solutions
 - High computational complexity for building the model
- Robust to noise
- Overfitting is handled by maximizing the margin of the decision boundary,
- SVM can handle irrelevant and redundant attributes better than many other techniques
- The user needs to provide the type of kernel function and cost function
- Difficult to handle missing values
- What about categorical variables?