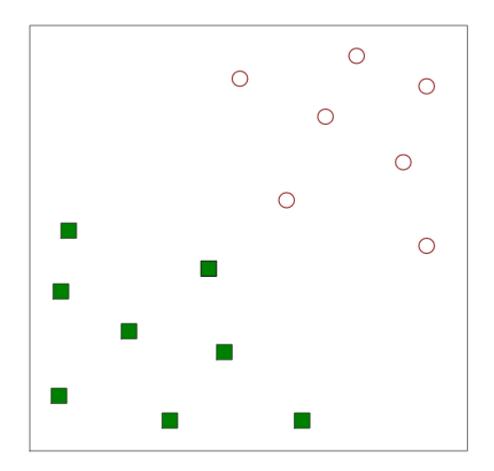
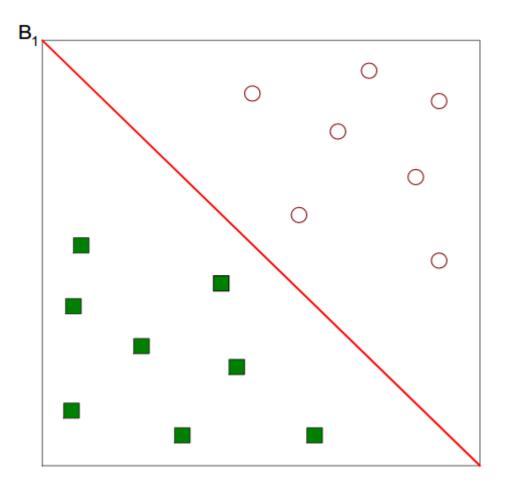
Introduction to Data Mining, 2nd Edition by Tan, Steinbach, Karpatne, Kumar



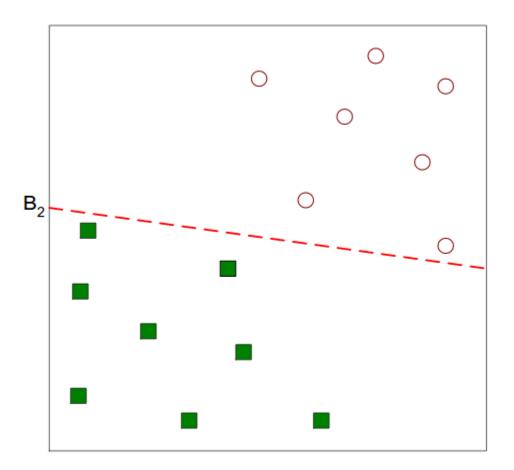
Find a linear hyperplane (decision boundary) that will separate the data

02/14/2018



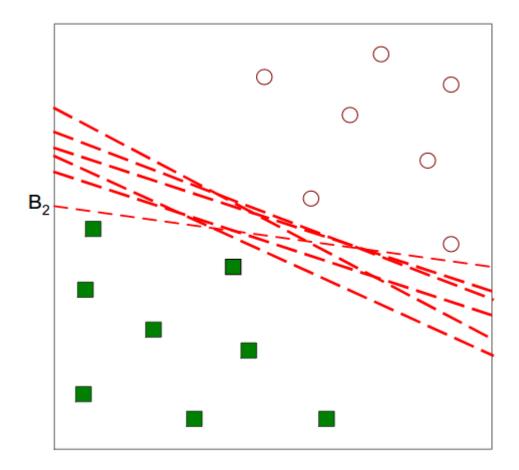
One Possible Solution

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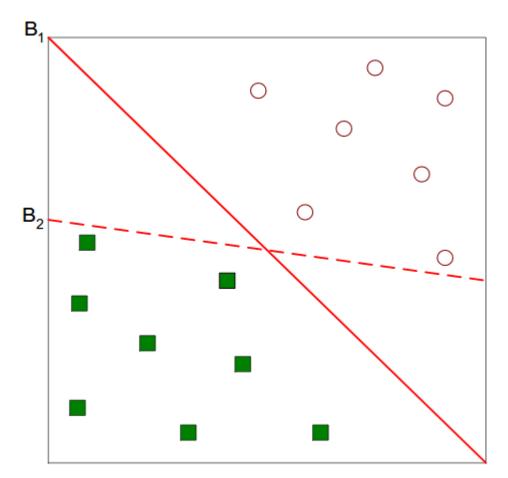
Another possible solution

02/14/2018



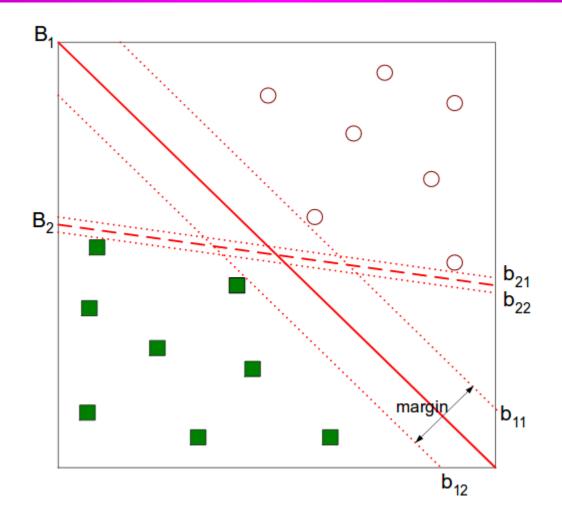
Other possible solutions

02/14/2018



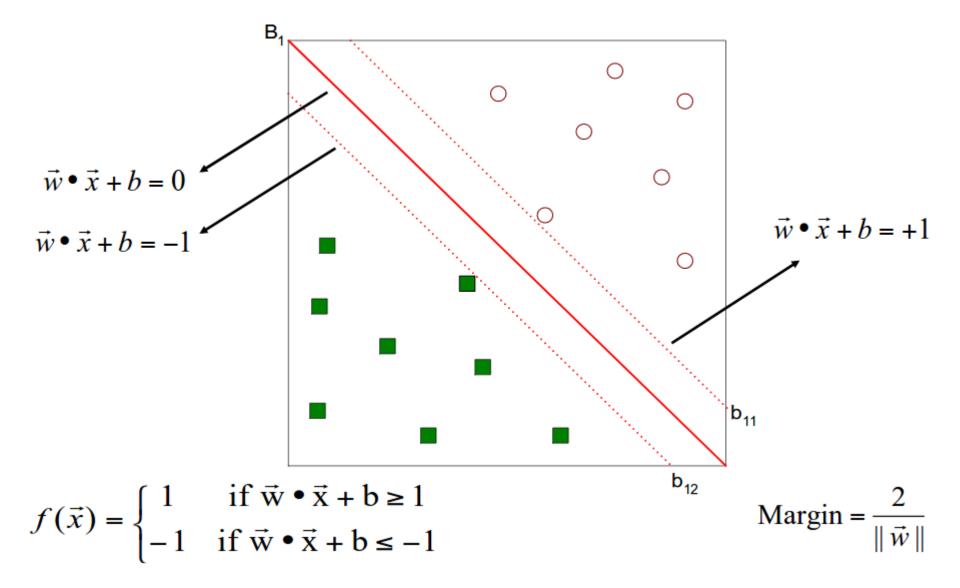
- Which one is better? B1 or B2?
- How do you define better?

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Find hyperplane maximizes the margin => B1 is better than B2

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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 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:

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

or $y_i(w \cdot x_i + b) \ge 1, \quad i = 1, 2, ..., N$

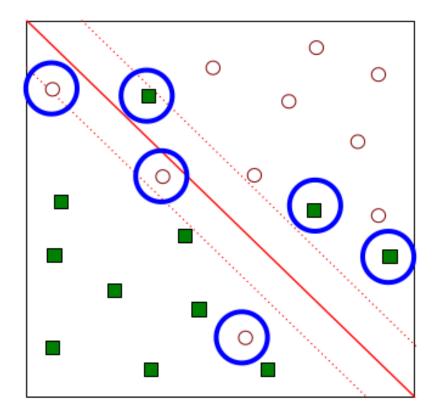
This is a constrained optimization problem – Solve it using Lagrange multiplier method

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

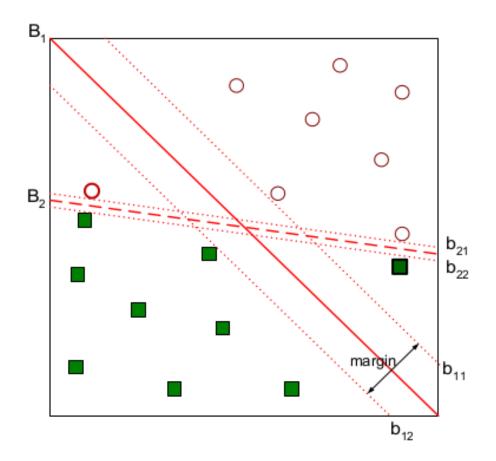
Need to minimize:

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

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 same objective function as linear SVM but with different constraints (see textbook)

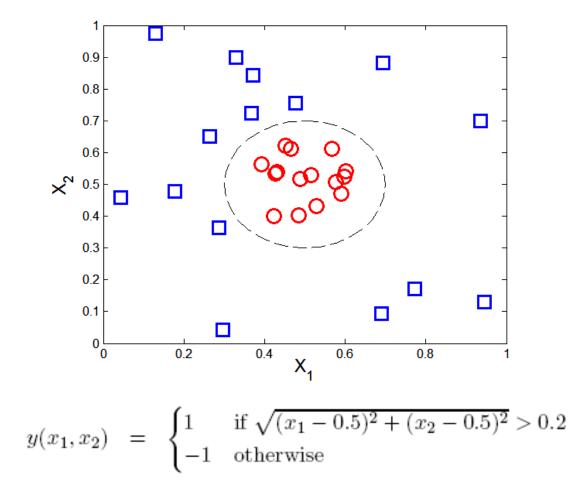


Find the hyperplane that optimizes both factors

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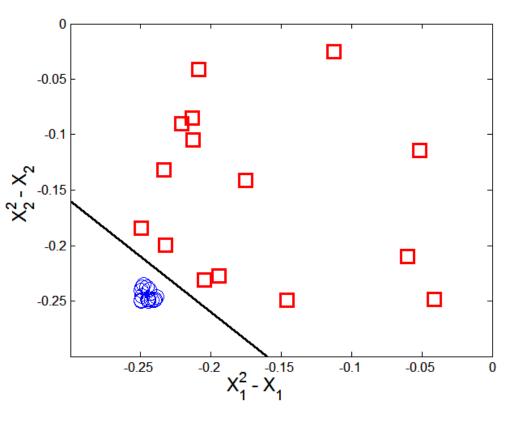
Nonlinear Support Vector Machines

• What if decision boundary is not linear?



Machines

Trick: Transform data into higher dimensional space



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

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

$$w_4 x_1^2 + w_3 x_2^2 + w_2 \sqrt{2}x_1 + w_1 \sqrt{2}x_2 + w_0 = 0.$$

Decision boundary:

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

Learning Nonlinear SVM

Optimization problem:

$$\min_{w} \frac{\|\mathbf{w}\|^2}{2}$$

subject to $y_i(w \cdot \Phi(x_i) + b) \ge 1, \ \forall \{(x_i, y_i)\}$

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

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

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

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Learning NonLinear SVM

Issues:

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

Learning Nonlinear SVM

Kernel Trick:

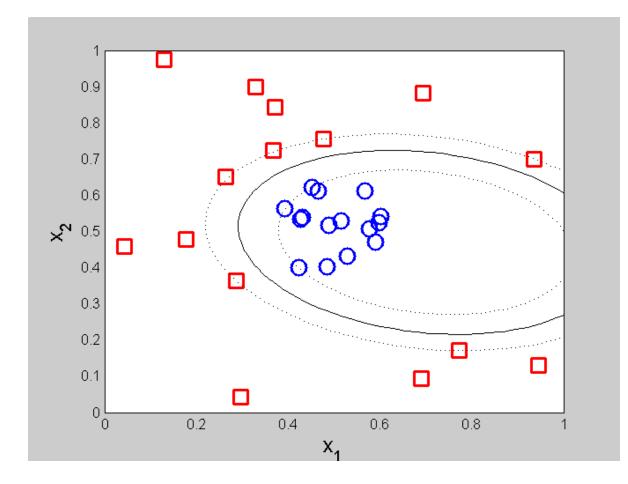
$$-\Phi(\mathbf{x}_i) \bullet \Phi(\mathbf{x}_j) = \mathsf{K}(\mathbf{x}_i, \mathbf{x}_j)$$

K(x_i, x_j) is a kernel function (expressed in terms of the coordinates in the original space)

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

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

Example of Nonlinear SVM



SVM with polynomial degree 2 kernel

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Learning Nonlinear SVM

- Advantages of using kernel:
 - Don't have to know the mapping function Φ
 - Computing dot product Φ(x_i)• Φ(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)

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Characteristics of SVM

- Since the learning problem is formulated as a convex optimization problem, efficient algorithms are available to find the global minima of the objective function (many of the other methods use greedy approaches and find locally optimal solutions)
- Overfitting is addressed by maximizing the margin of the decision boundary, but the user still needs to provide the type of kernel function and cost function
- Difficult to handle missing values
- Robust to noise
- High computational complexity for building the model