Data Mining

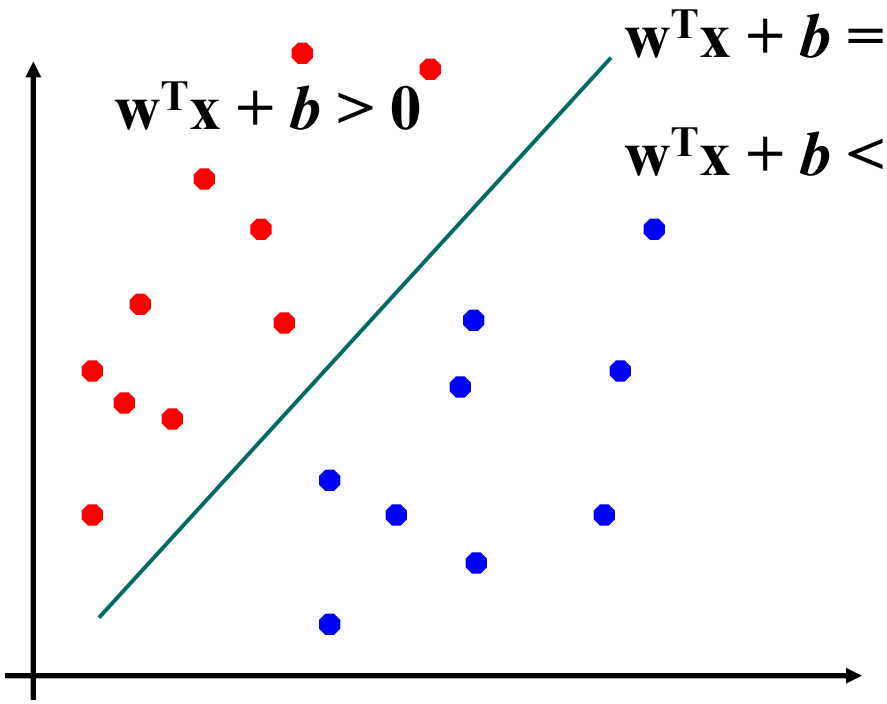
Support Vector Machines

Chris Ding

Most slides come from UT Austin, A. Moore (CMU) and book by Tan, Steinbach, Karpatne, Kumar

Perceptron Revisited: Linear Separators

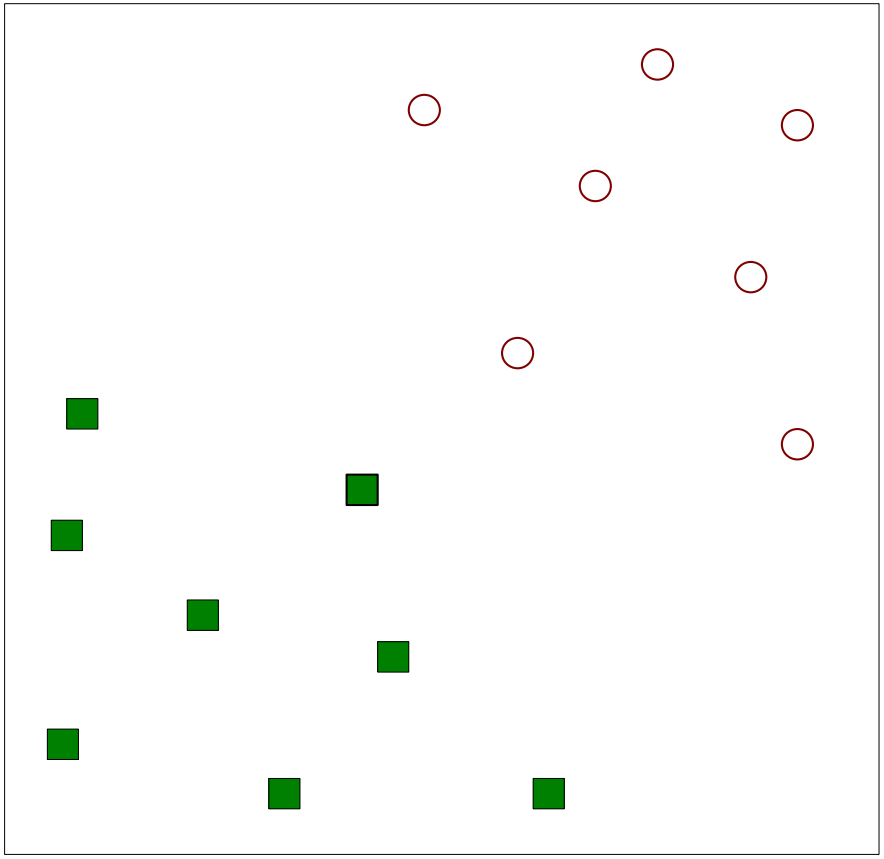
- Binary classification can be viewed as the task of separating classes in feature space:



$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

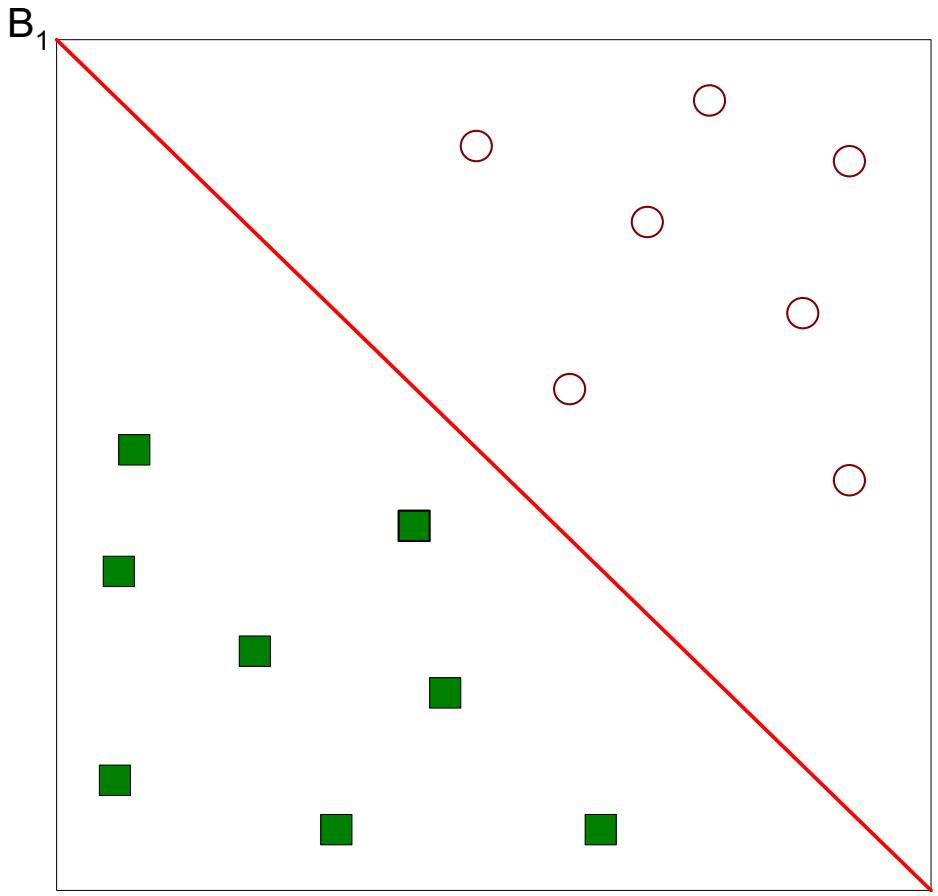
$$\mathbf{y}(\mathbf{x}) = sign(\mathbf{w}^T\mathbf{x} + b)$$

Support Vector Machines



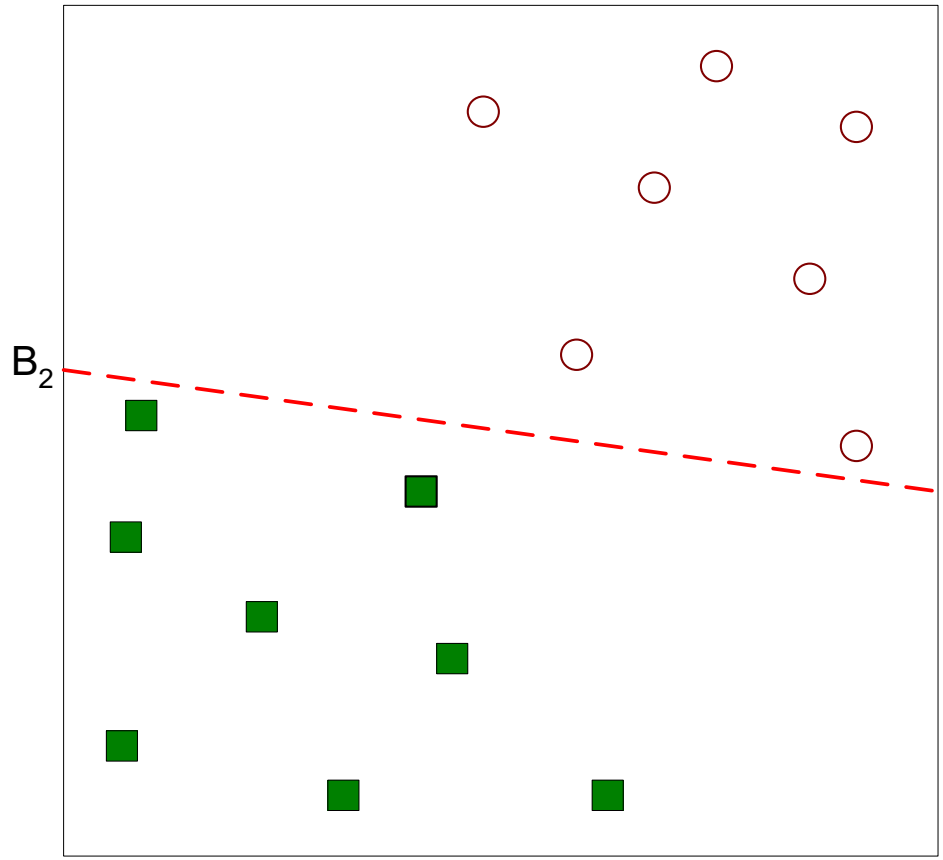
- Find a linear hyperplane (decision boundary) that will separate the data

Support Vector Machines



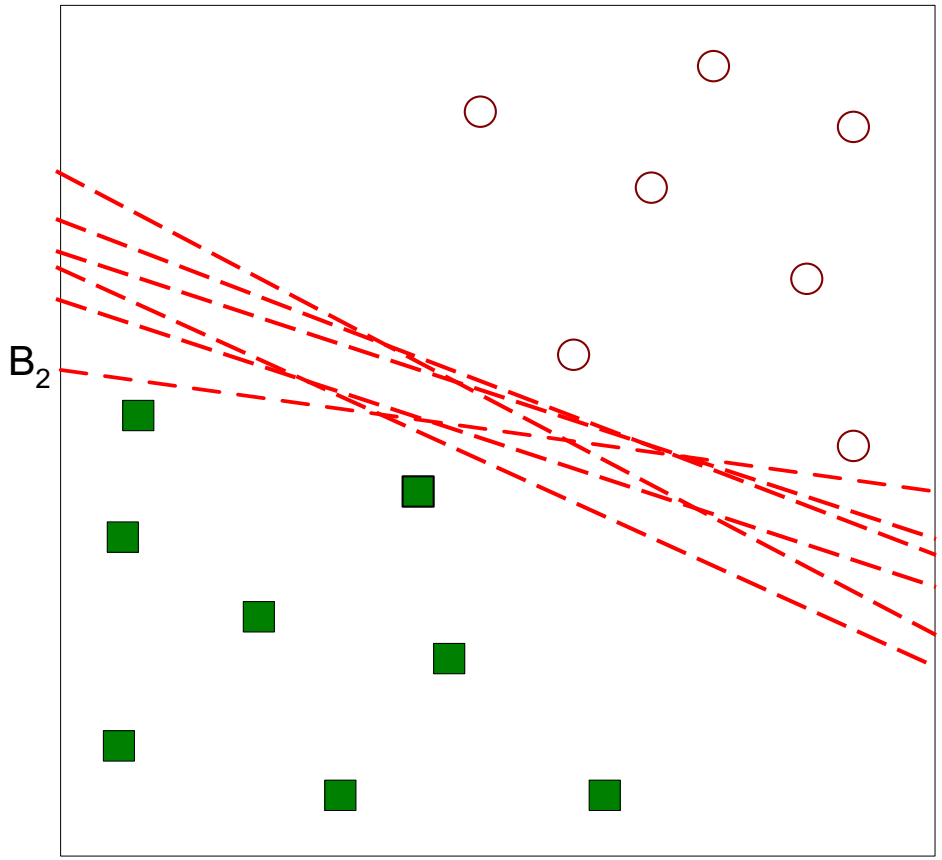
- One Possible Solution

Support Vector Machines



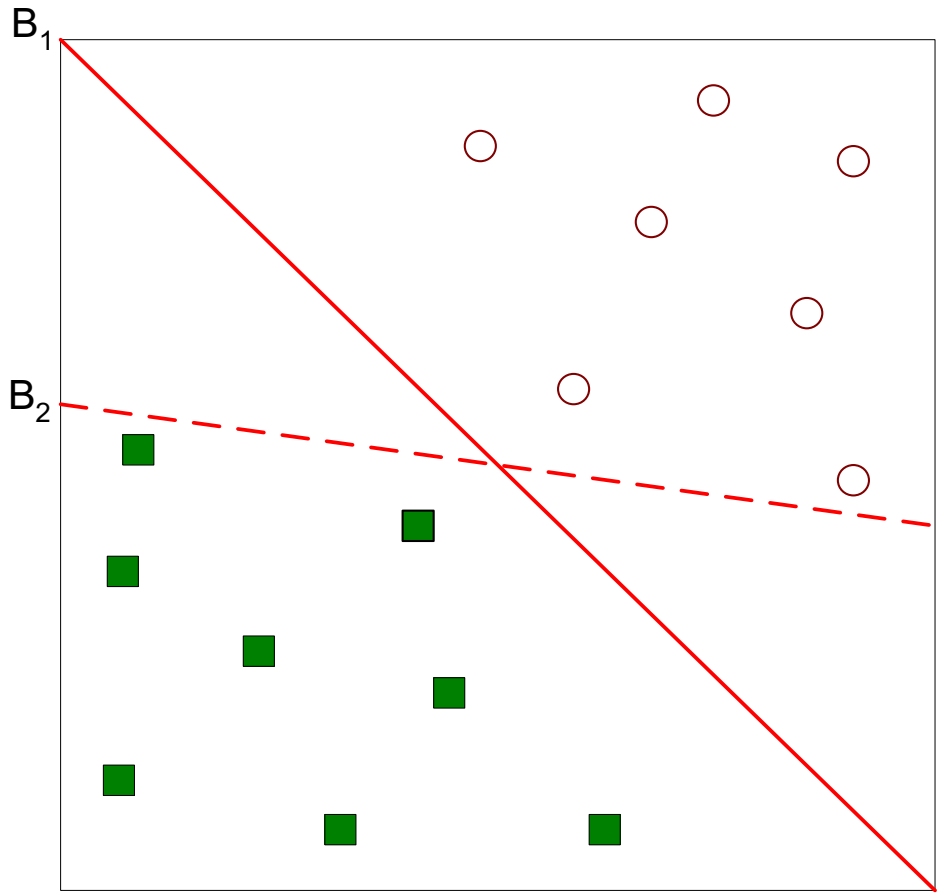
- Another possible solution

Support Vector Machines



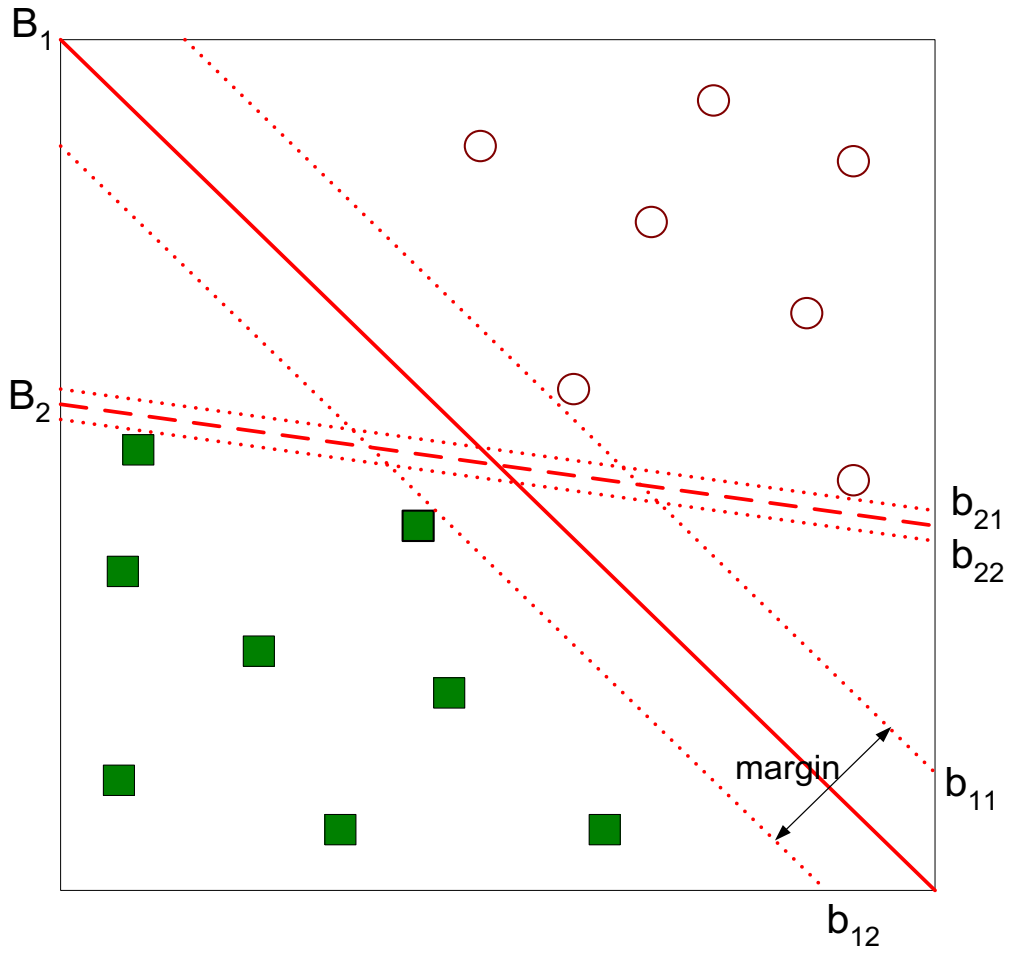
- Other possible solutions

Support Vector Machines



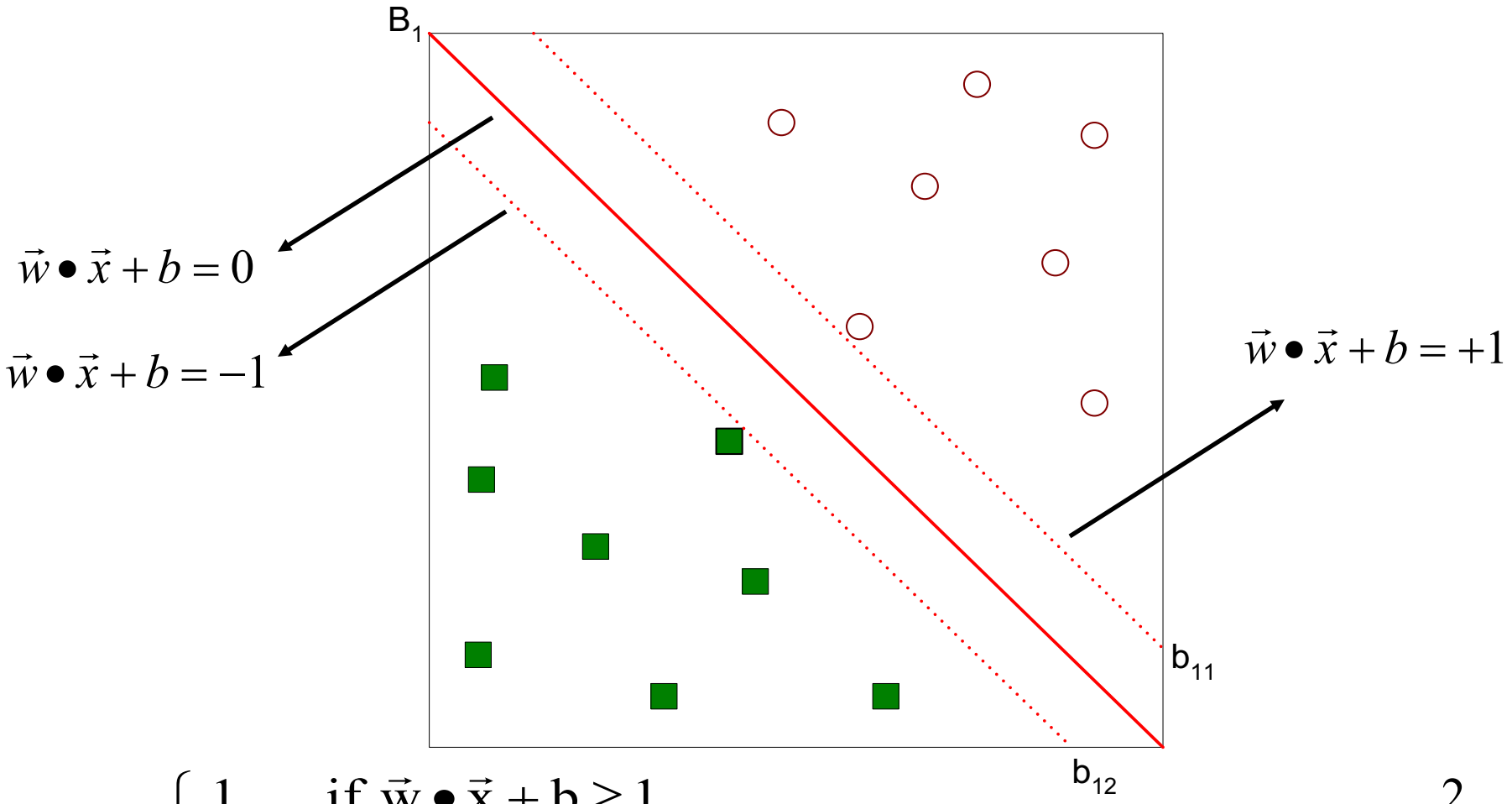
- Which one is better? B1 or B2?
- How do you define better?

Support Vector Machines



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

Support Vector Machines



$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x} + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x} + b \leq -1 \end{cases}$$

$$\text{Margin} = \frac{2}{\| \vec{w} \|}$$

Linear SVM

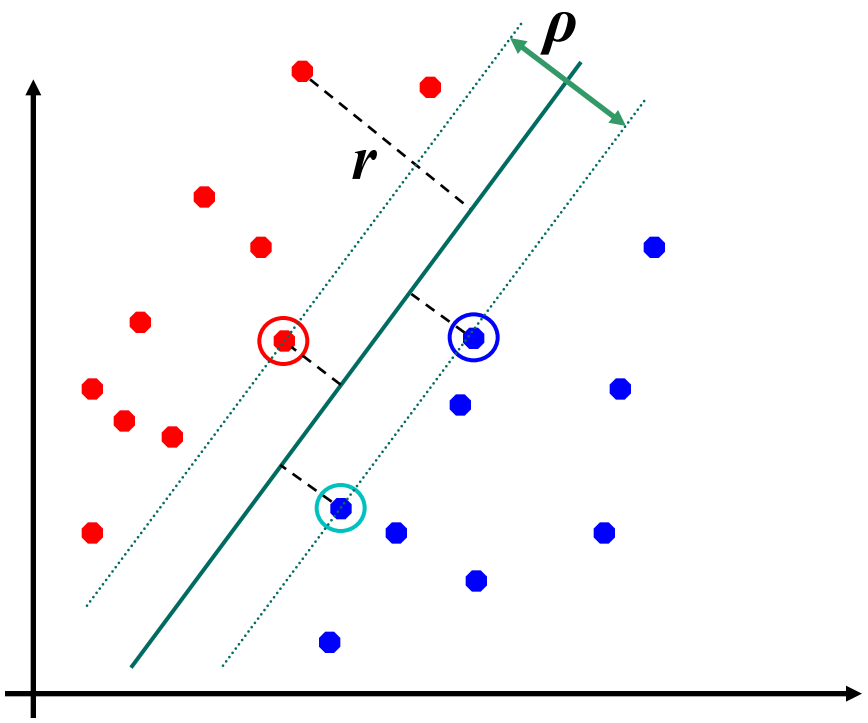
- Linear model:

$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x} + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x} + b \leq -1 \end{cases}$$

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

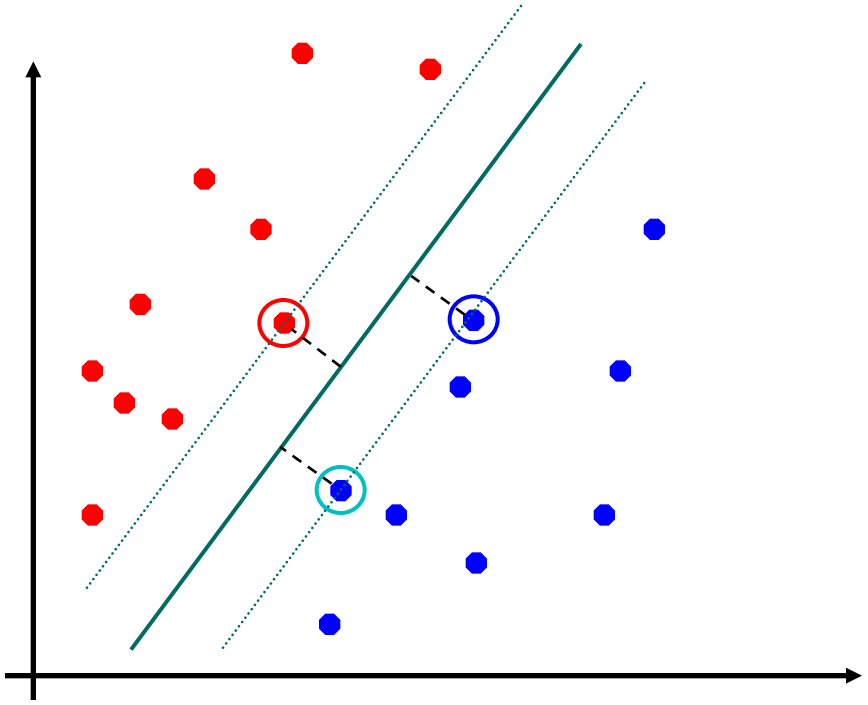
Classification Margin

- Distance from example $\mathbf{x}_i$ to the separator is $r = \dfrac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|}$
- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the distance between support vectors.



Maximum Margin Classification

- Maximizing the margin is good according to intuition and PAC theory.
- Implies that only support vectors matter; other training examples are ignorable.



Learning Linear SVM

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

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

or

$$y_i(\mathbf{w} \bullet \mathbf{x}_i + b) \geq 1, \quad i = 1,2,\ldots,N$$

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

Linear SVMs Mathematically (cont.)

- Then we can formulate the *quadratic optimization problem:*

Find w and *b* such that

$$\rho = \frac{2}{\|\mathbf{w}\|}$$ **is maximized**

and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

Which can be reformulated as:

Find w and *b* such that

$\Phi(\mathbf{w}) = \|\mathbf{w}\|^2 = \mathbf{w}^T\mathbf{w}$ **is minimized**

and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

Primal Problem

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

$$\text{subject to} \quad y_i(\mathbf{w}\cdot\mathbf{x_i}+b)\geq 1, \quad i=1,2,\ldots,N.$$

Lagrangian function

$$L_P = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N}\lambda_i\Big(y_i(\mathbf{w}\cdot\mathbf{x_i}+b)-1\Big)$$

Calculating derivatives

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \Longrightarrow \mathbf{w} = \sum_{i=1}^{N}\lambda_i y_i \mathbf{x}_i$$

$$\frac{\partial L_p}{\partial b} = 0 \Longrightarrow \sum_{i=1}^{N}\lambda_i y_i = 0.$$

Dual Problem

$$L_D = \sum_{i=1}^{N}\lambda_i - \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x_i}\cdot\mathbf{x_j}.$$

KKT condition

$$\lambda_i \geq 0,$$

$$\lambda_i\big[y_i(\mathbf{w}\cdot\mathbf{x}_i+b)-1\big]=0.$$

Solving the Optimization Problem

Find w and b such that
$\Phi(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ is minimized
and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems for which several (non-trivial) algorithms exist.
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every inequality constraint in the primal (original) problem:

Find $\alpha_1 \ldots \alpha_n$ such that
$Q(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- Given a solution $\alpha_1 \ldots \alpha_n$ to the dual problem, solution to the primal is:

$$\mathbf{w} = \Sigma \alpha_i y_i \mathbf{x}_i \qquad b = y_k - \Sigma \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_k \quad \text{for any } \alpha_k > 0$$

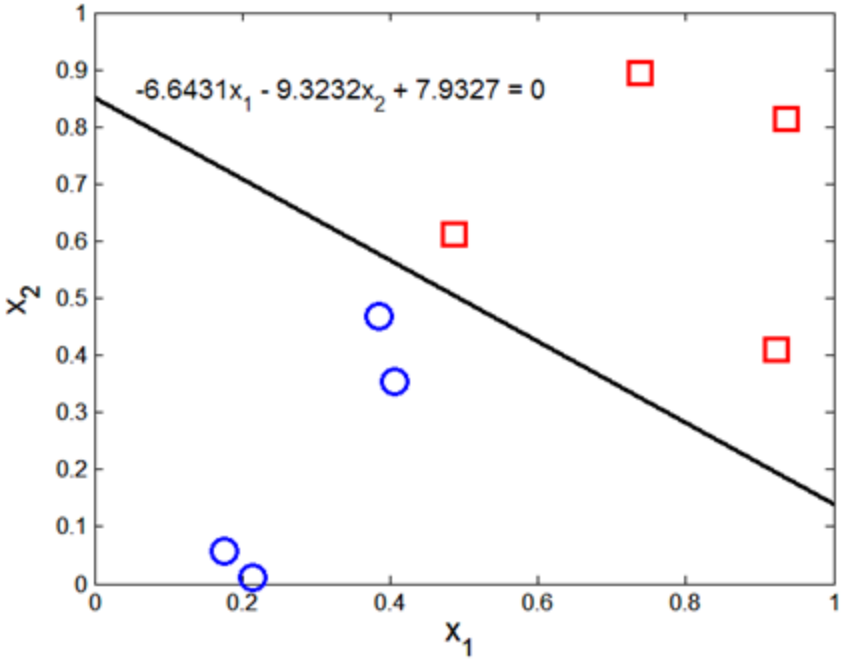
- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.

- Then the classifying function is (note that we don't need **w** explicitly):

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

- Notice that it relies on an *inner product* between the test point **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 $\mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j$ between all training points.

Example of Linear SVM



Support vectors

x1	x2	y	λ
0.3858	0.4687	1	65.5261
0.4871	0.611	-1	65.5261
0.9218	0.4103	-1	0
0.7382	0.8936	-1	0
0.1763	0.0579	1	0
0.4057	0.3529	1	0
0.9355	0.8132	-1	0
0.2146	0.0099	1	0

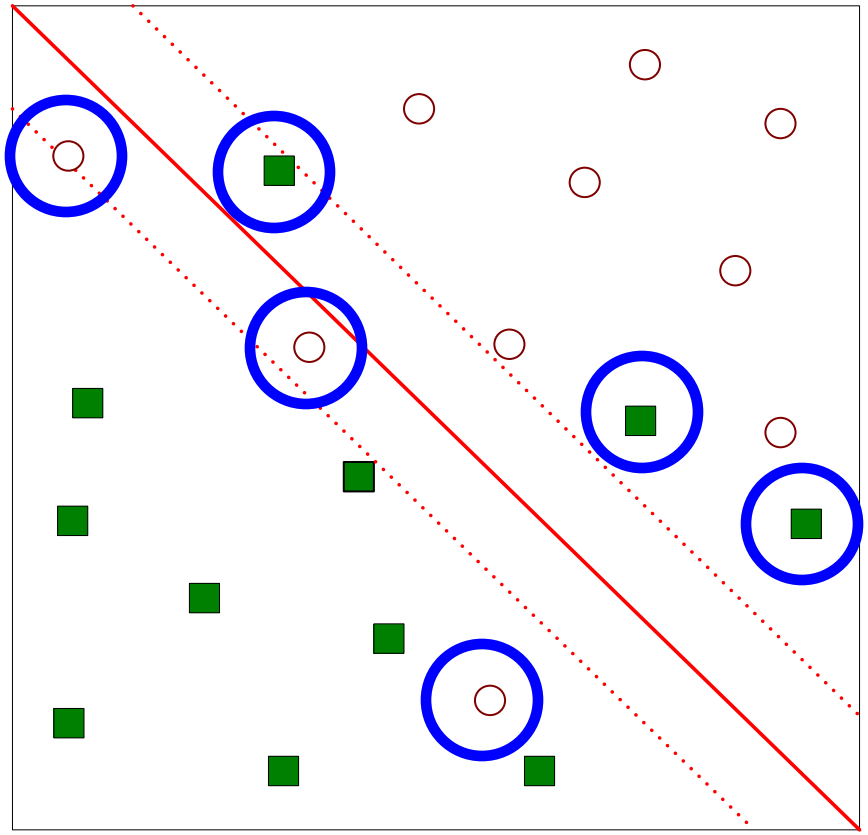
Learning Linear SVM

- 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

$$f(\vec{x}_i) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x}_i + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x}_i + b \leq -1 \end{cases}$$

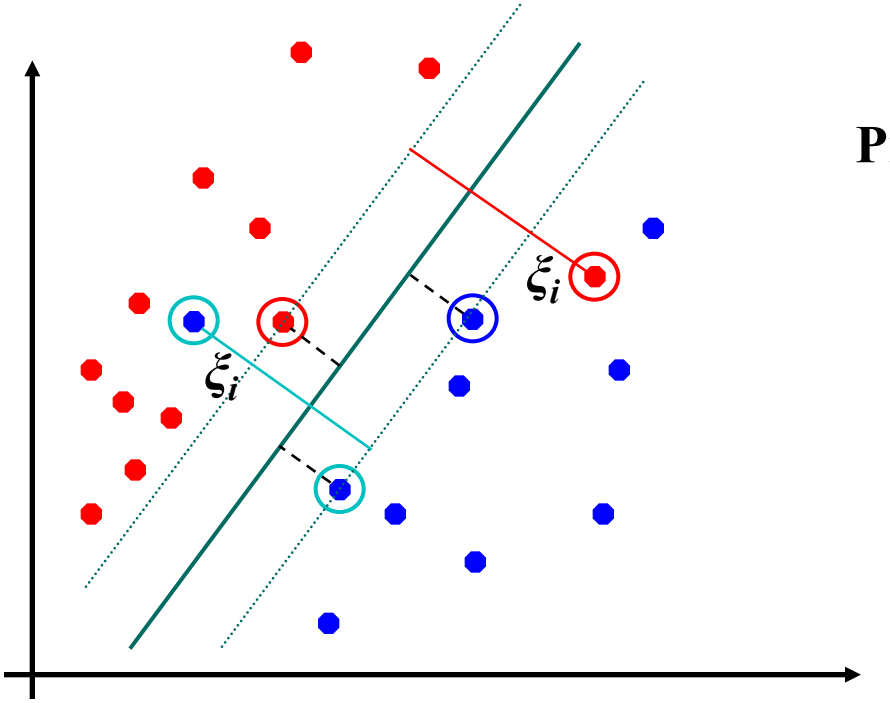
Support Vector Machines

- What if the problem is not linearly separable?



Soft Margin Classification

- What if the training set is not linearly separable?
- *Slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples, resulting margin called *soft*.



Proposed in 1970s

Support Vector Machines

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

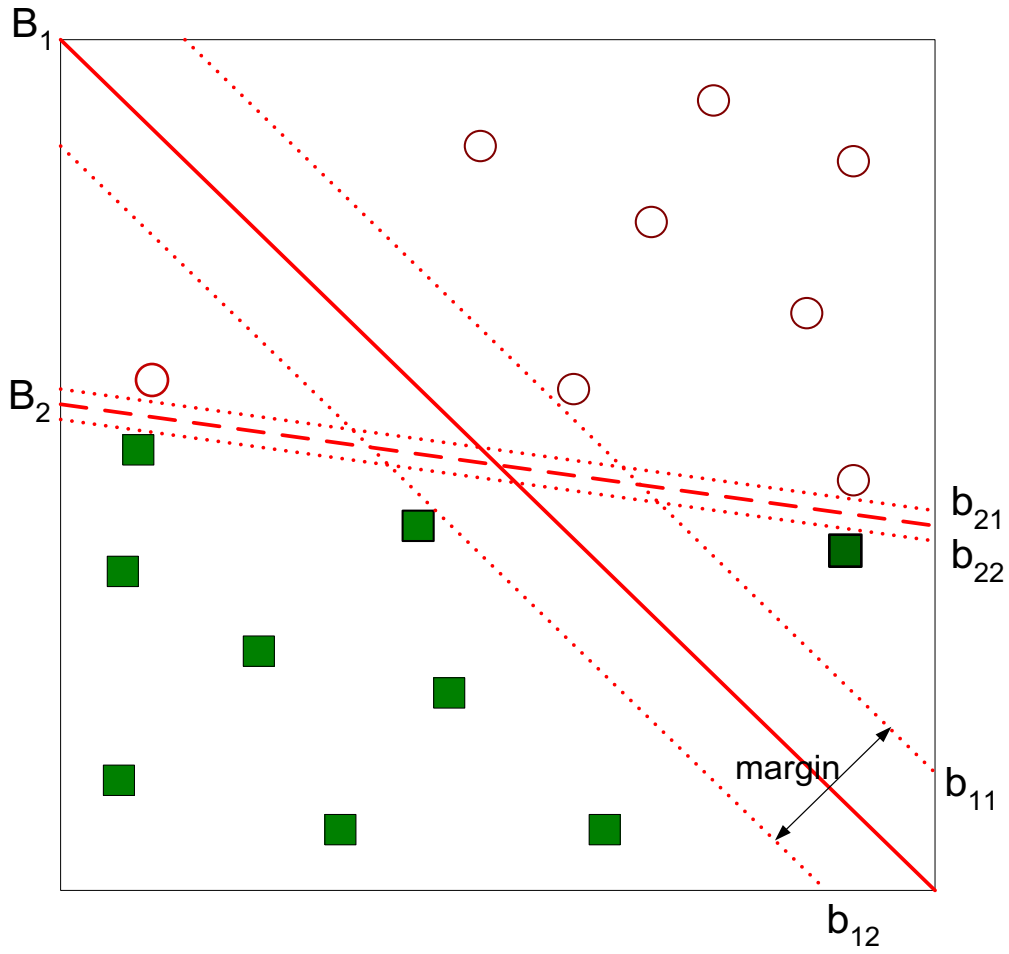
$$L(w) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k \right)$$

    - Subject to:

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

    - If k =1 , this leads to same objective function as linear SVM but with different constraints (see textbook)

Support Vector Machines



- Find the hyperplane that optimizes both factors

Soft Margin Classification Mathematically

- The old formulation:

Find w and b such that
$\Phi(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ **is minimized**
and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

- Modified formulation incorporates slack variables:

Find w and b such that
$\Phi(\mathbf{w}) = \mathbf{w}^T\mathbf{w} + C\Sigma\xi_i$ **is minimized**
and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i$, $\xi_i \geq 0$

- Parameter *C* can be viewed as a way to control overfitting: it "trades off" the relative importance of maximizing the margin and fitting the training data.

Primal Problem

$$\min_{\mathbf{w}} \quad \frac{\|\mathbf{w}\|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i\right)$$

$$\text{subject to} \qquad y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1 - \xi_i \qquad \xi_i > 0$$

Lagrangian function

$$L_P = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \lambda_i\{y_i(\mathbf{w} \cdot \mathbf{x_i} + b) - 1 + \xi_i\} - \sum_{i=1}^{N} \mu_i \xi_i$$

Calculating derivatives

$$\frac{\partial L}{\partial w_j} = w_j - \sum_{i=1}^{N} \lambda_i y_i x_{ij} = 0 \implies w_j = \sum_{i=1}^{N} \lambda_i y_i x_{ij}.$$

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

$$\frac{\partial L}{\partial \xi_i} = C - \lambda_i - \mu_i = 0 \implies \lambda_i + \mu_i = C.$$

Dual Problem

$$
\begin{aligned}
L_D &= \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x}_i\cdot\mathbf{x}_j + C\sum_i \xi_i \\
&\quad -\sum_i \lambda_i\{y_i(\sum_j \lambda_j y_j \mathbf{x}_i\cdot\mathbf{x}_j + b) - 1 + \xi_i\} \\
&\quad -\sum_i (C-\lambda_i)\xi_i \\
&= \sum_{i=1}^{N}\lambda_i - \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x_i}\cdot\mathbf{x_j},
\end{aligned}
$$

KKT condition

$$
\begin{aligned}
&\xi_i \geq 0, \quad \lambda_i \geq 0, \quad \mu_i \geq 0, \\
&\lambda_i\{y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \xi_i\} = 0, \\
&\mu_i\xi_i = 0.
\end{aligned}
$$

Soft Margin Classification – Solution

Invented 1992

- Dual problem is identical to separable case (would *not* be identical if the 2-norm penalty for slack variables $C\Sigma\xi_i^2$ was used in primal objective, we would need additional Lagrange multipliers for slack variables):

Find $\alpha_1 \ldots \alpha_N$ such that
$Q(\alpha) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \le \alpha_i \le C$ for all α_i

- Again, $\mathbf{x}_i$ with non-zero α_i will be support vectors.
- Solution to the dual problem is:

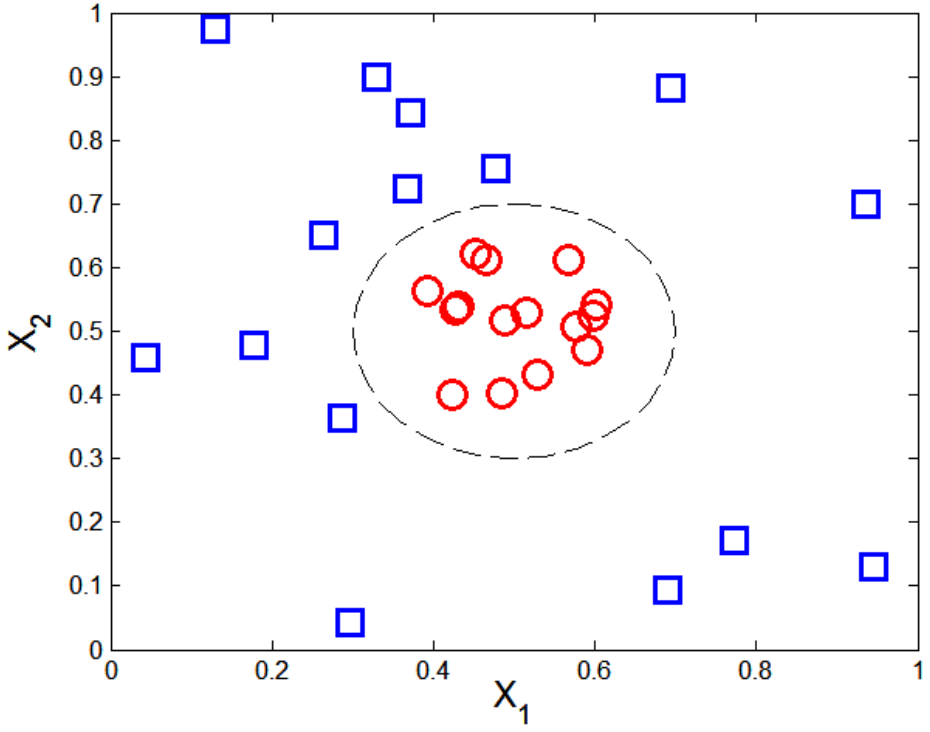
$$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x}_i$$
$$b = y_k(1 - \xi_k) - \Sigma\alpha_i y_i \mathbf{x}_i^T \mathbf{x}_k \quad \text{for any } k \text{ s.t. } \alpha_k > 0$$

Again, we don't need to compute w explicitly for classification:

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

Nonlinear Support Vector Machines

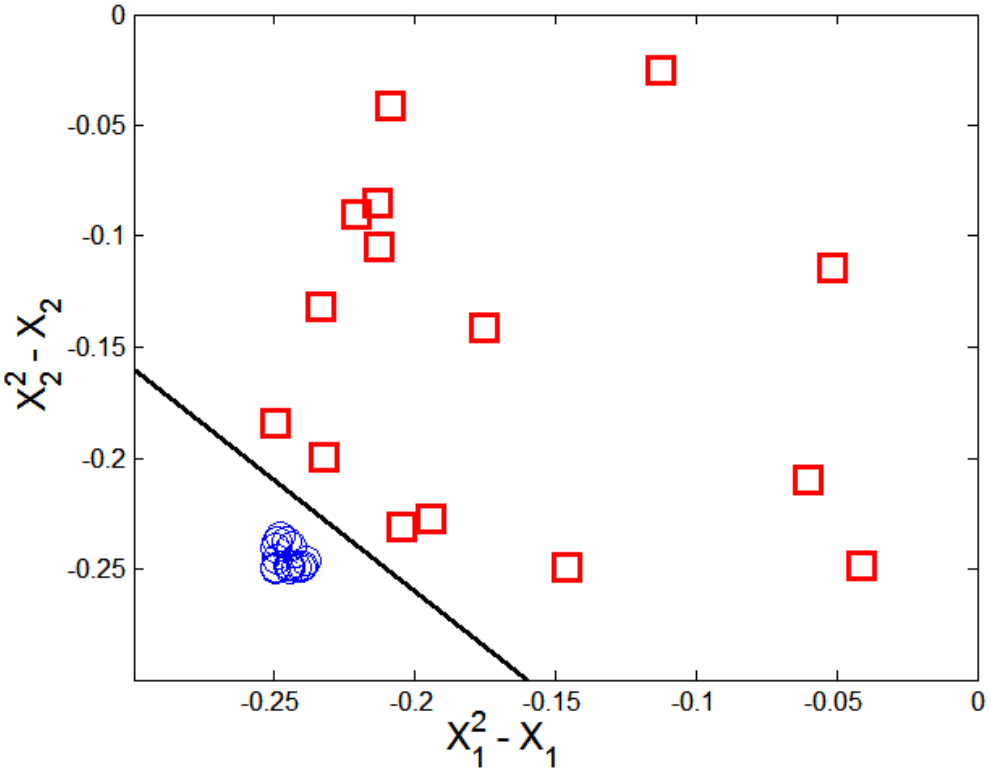
- What if decision boundary is not linear?



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

Nonlinear Support Vector Machines

- 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:

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

Learning Nonlinear SVM

- Optimization problem:

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

- Which leads to the same set of equations (but involve $\Phi(x)$ instead of x)

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

$$\lambda_i \{ y_i (\sum_j \lambda_j y_j \Phi(\mathbf{x}_j) \cdot \Phi(\mathbf{x}_i) + b) - 1 \} = 0,$$

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

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 $\Phi(x_i) \bullet \Phi(x_j)$
    - Curse of dimensionality?

Learning Nonlinear SVM

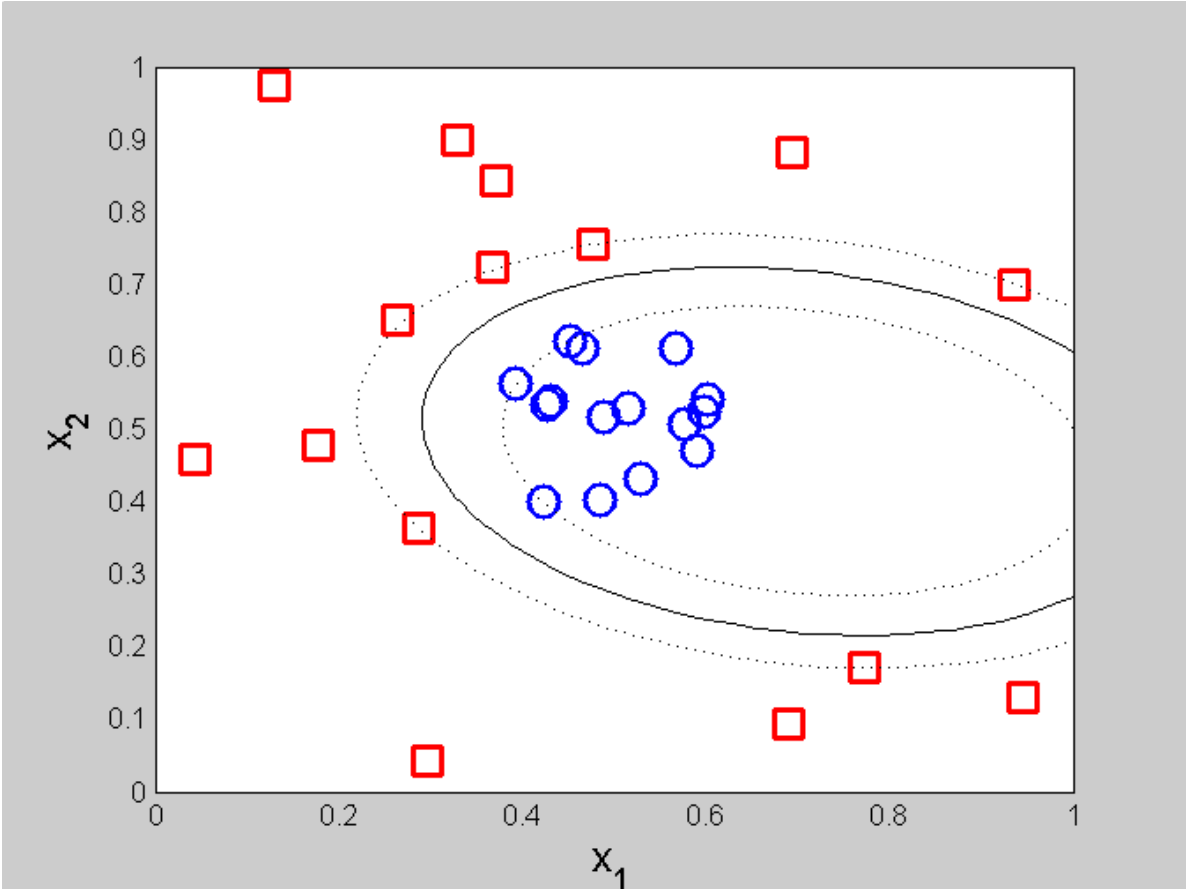
- Kernel Trick:
  - $\Phi(x_i) \bullet \Phi(x_j) = K(x_i, x_j)$
  - $K(x_i, x_j)$ is a kernel function (expressed in terms of the coordinates in the original space)
    - Examples:

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

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

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

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

- 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