Support Vector Machine

Support Vector Machines

- Linear models can be used to implement nonlinear class boundaries using space transformations
  - The instance space is transformed into a new space using a nonlinear mapping
  - A straight line in the new space can represent a nonlinear decision boundary in the original space
- What kind of transformations?
  - Polynomials of sufficiently high degree can approximate arbitrary decision boundaries to any required accuracy

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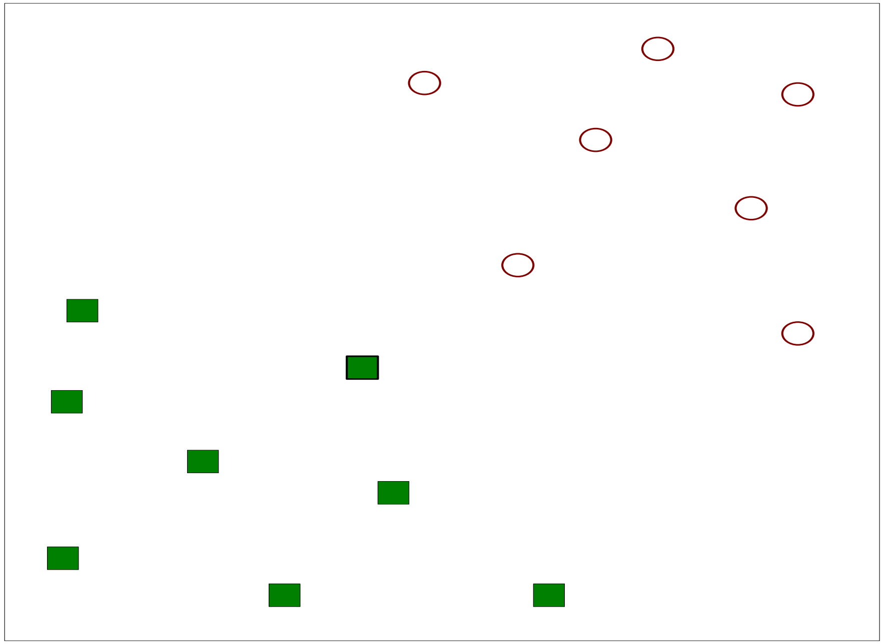

Find a linear hyperplane (decision boundary) that will separate the data

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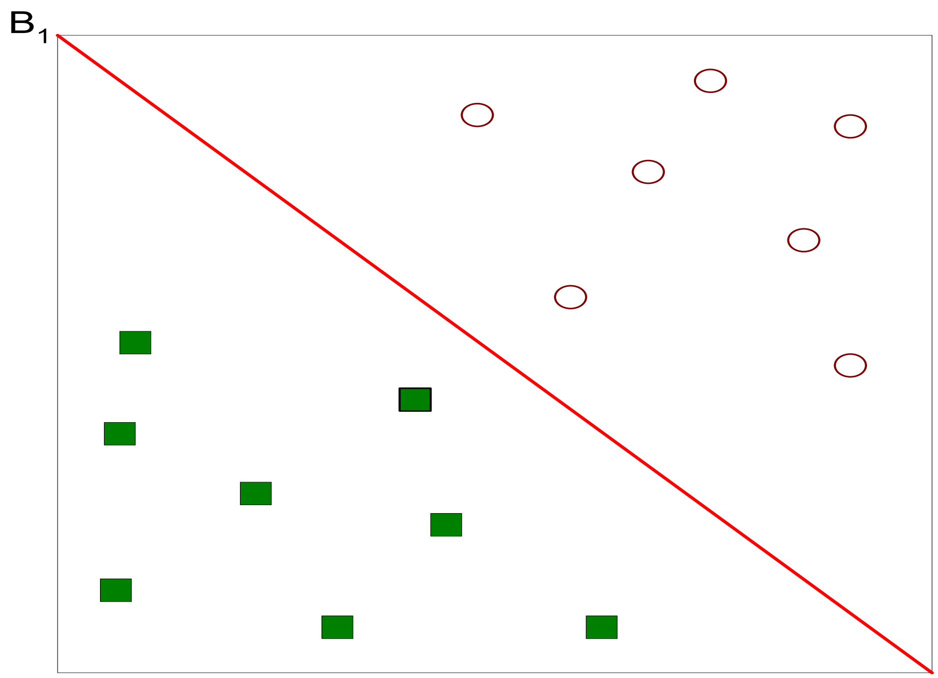

One possible solution

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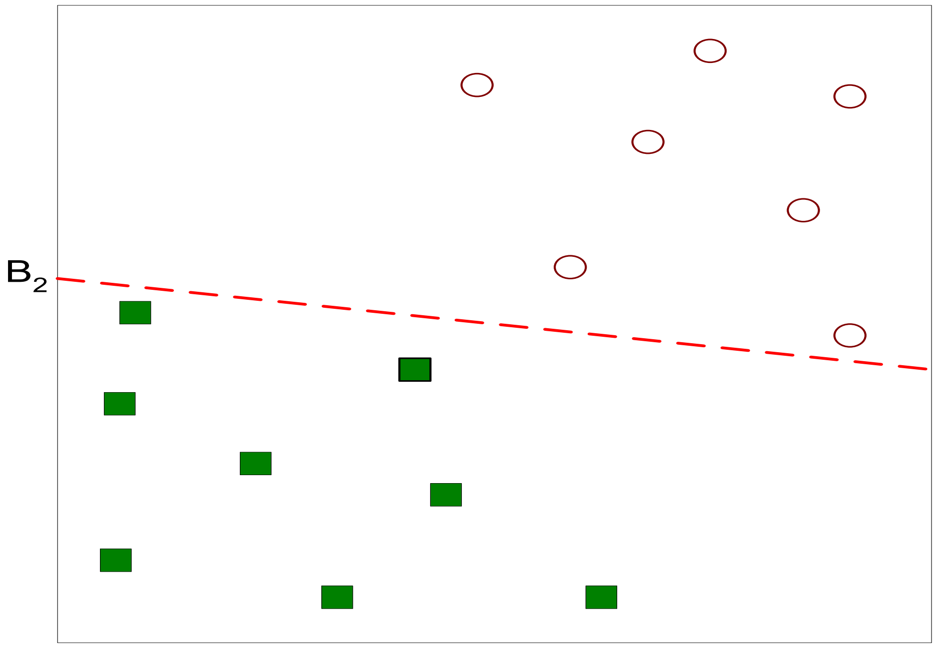

Another solution

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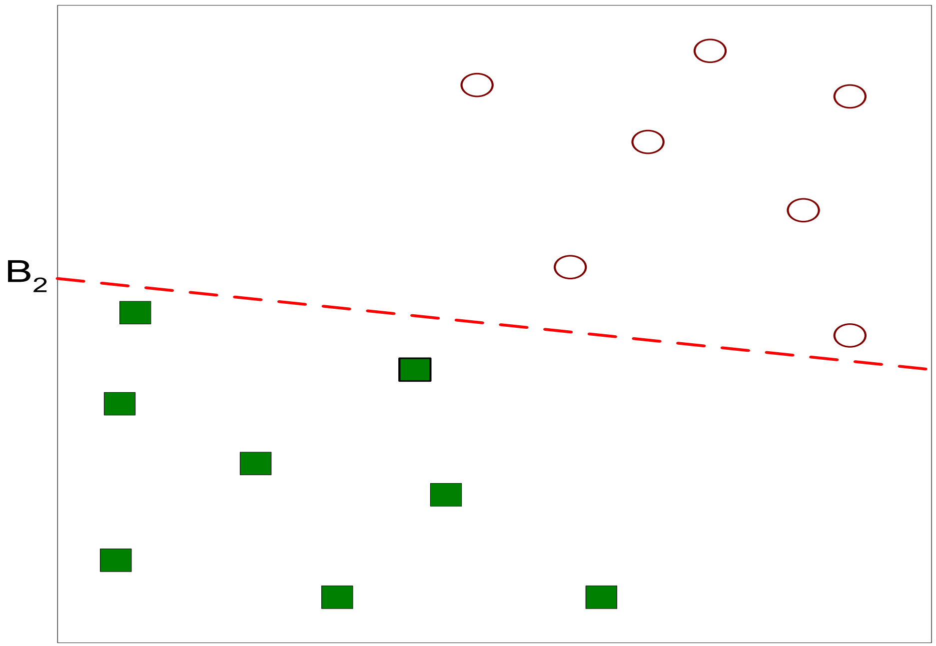

Other possible solutions

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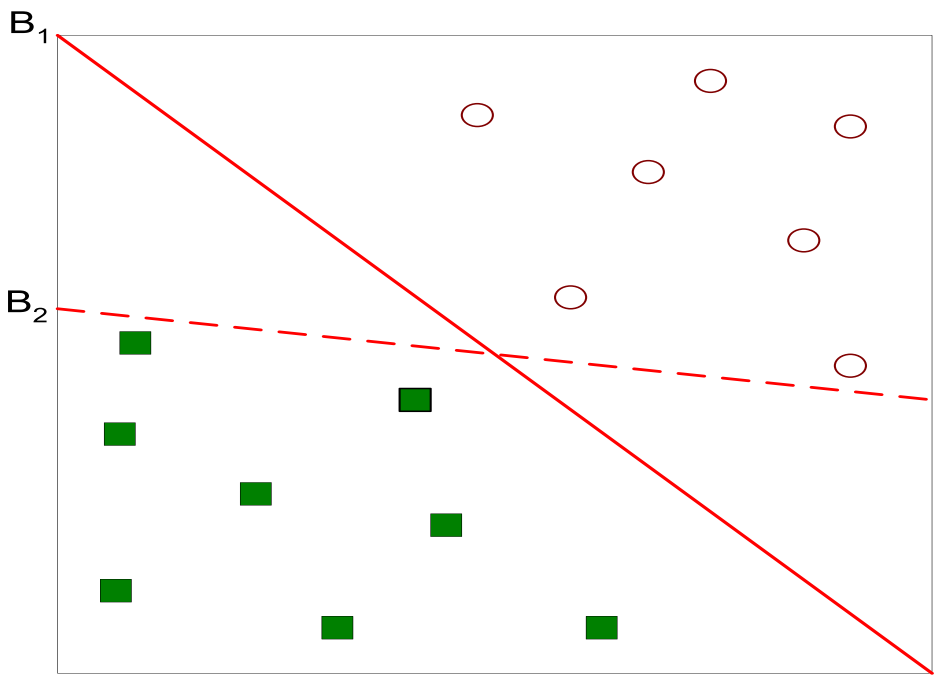

Which one is better? B1 or B2?
How do you define better?

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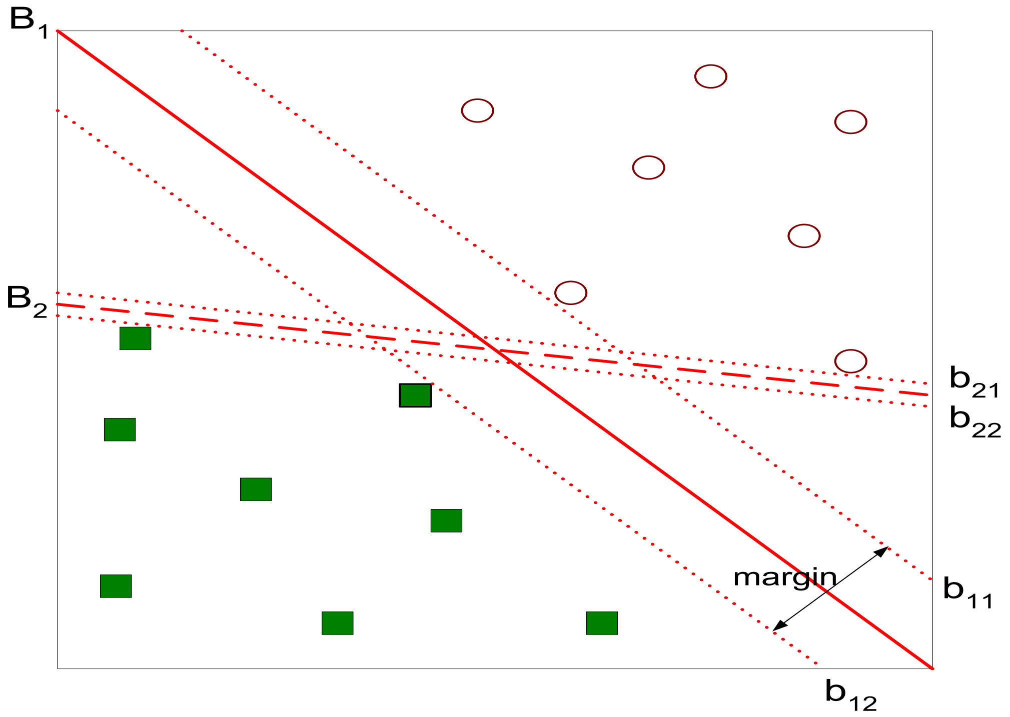
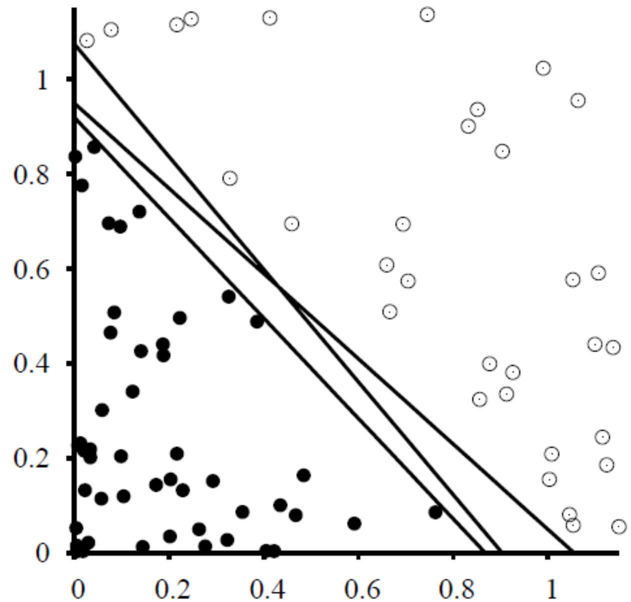


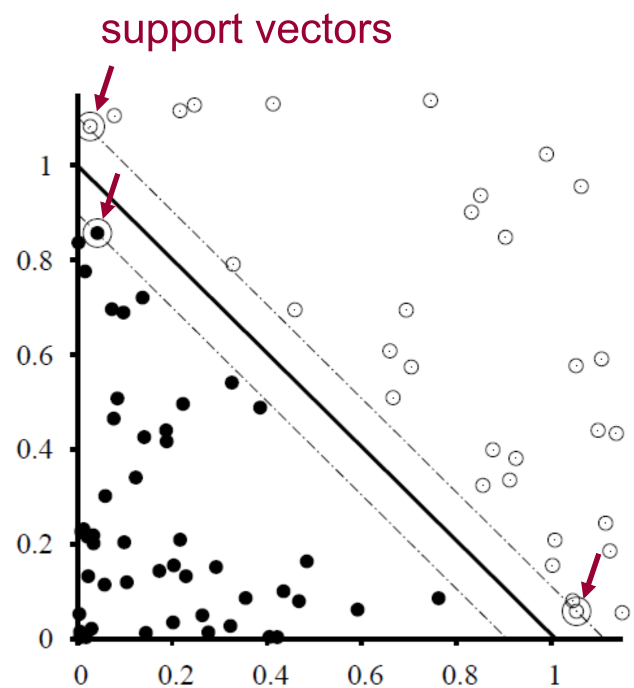
Find hyperplane maximizes the margin => B1 is better than B2

Support Vector Machines

- Attractive properties:
  - SVMs construct maximum margin separator
    - Minimize expected generalization loss rather than empirical loss



(a) candidate linear separators



(b) maximum margin separator

Support Vector Machines

- Attractive properties:
  - SVMs construct maximum margin separator ☞
    - Minimize expected generalization loss rather than empirical loss
  - SVMs map the data into a higher-dimensional space in which the data become linearly separable
  - SVMs are a nonparametric method retaining only a small fraction of training examples
    - Can represent complex functions but resistant to overfitting
- Key insight: maximum margin separator
  - Some examples are more important than the others
  - Only support vectors matter → better generalization

Support Vector Machines

- In the two-attribute case, a hyperplane separating the two classes (1 or –1) might be written as

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

  where x_1 and x_2 are the attribute values, and there are three weights w_i to be learned

- In general, for a training set $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$, we want to find $\mathbf{w}$ and w_0 such that

$$\mathbf{w}^T\mathbf{x}_i + w_0 \geq m \quad \text{if } y_i = 1$$

$$\mathbf{w}^T\mathbf{x}_i + w_0 \leq -m \quad \text{if } y_i = -1$$

  where m is the smallest margin of any positive or negative example

- The above can be rewritten as the following constraint

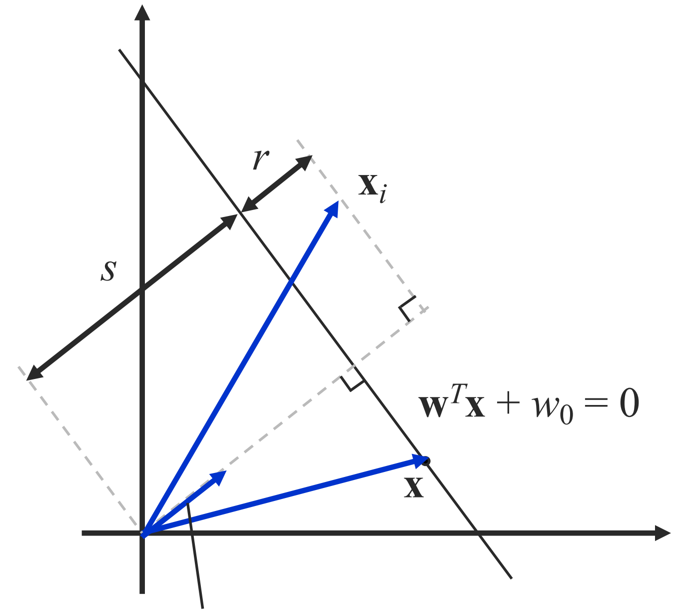
$$y_i\,(\mathbf{w}^T\mathbf{x}_i + w_0) \geq m$$

Support Vector Machines

- To calculate the distance from an example to the hyperplane, we need to know the distance from the origin to the hyperplane
- The distance s from the origin to the hyperplane can be obtained by the inner product of a point $\mathbf{x}$ on the hyperplane and the unit normal vector

$$s = \frac{\mathbf{w}^T}{\|\mathbf{w}\|} \cdot \mathbf{x} = \frac{\mathbf{w}^T \mathbf{x}}{\|\mathbf{w}\|} = \frac{-w_0}{\|\mathbf{w}\|}$$

because $\mathbf{x}$ satisfies $\mathbf{w}^T\mathbf{x} + w_0 = 0$, i.e., $\mathbf{w}^T\mathbf{x} = -w_0$



$\frac{\mathbf{w}^T}{\|\mathbf{w}\|}$: unit normal vector

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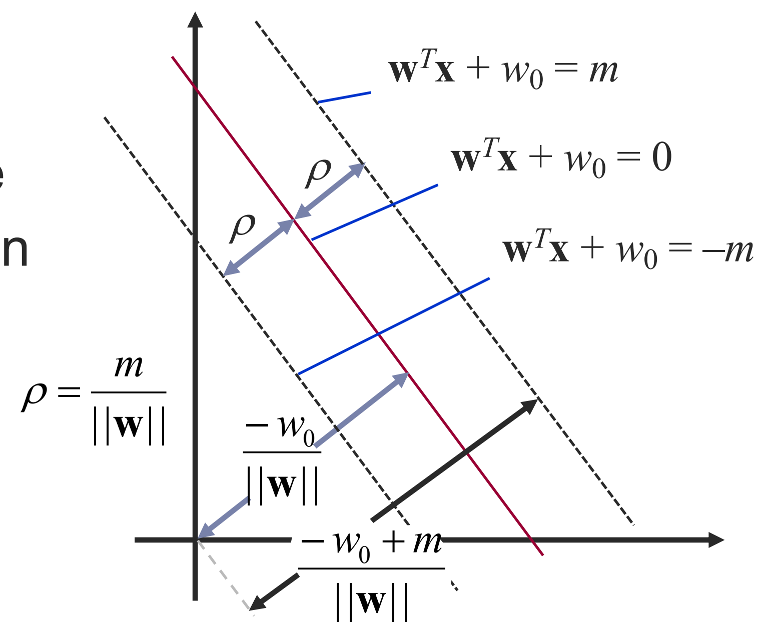
- Thus, the distance r from an example $\mathbf{x}_i$ to the hyperplane is

$$r = \left| \frac{\mathbf{w}^T \mathbf{x}_i}{\|\mathbf{w}\|} - s \right| = \left| \frac{\mathbf{w}^T \mathbf{x}_i}{\|\mathbf{w}\|} - \frac{-w_0}{\|\mathbf{w}\|} \right| = \frac{\left| \mathbf{w}^T \mathbf{x}_i + w_0 \right|}{\|\mathbf{w}\|} = \frac{y_i(\mathbf{w}^T \mathbf{x}_i + w_0)}{\|\mathbf{w}\|}$$

- We want this distance to be at least some value ρ for all i:

$$\frac{y_i(\mathbf{w}^T \mathbf{x}_i + w_0)}{\|\mathbf{w}\|} \geq \rho, \quad \forall i$$

- We want to maximize ρ but there are an infinite number of solutions we can get by scaling $\mathbf{w}$



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- For a unique solution, we fix $\rho\,||\mathbf{w}|| = 1$ (i.e., $m = 1$) and thus, to maximize ρ, we minimize $||\mathbf{w}||$, or more conveniently:

$$\min \frac{1}{2}||\mathbf{w}||^2 \text{ subject to } y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1,\ \forall i$$

  - This is a standard quadratic optimization problem and can be solved directly to find $\mathbf{w}$ and w_0 (numerical approaches can solve it)
  - The complexity depends on the input dimensionality d which can be quite large especially in the transformed space
  - Note that the instances are at least $\rho = 1/||\mathbf{w}||$ away from the hyperplane and the total margin becomes $2/||\mathbf{w}||$

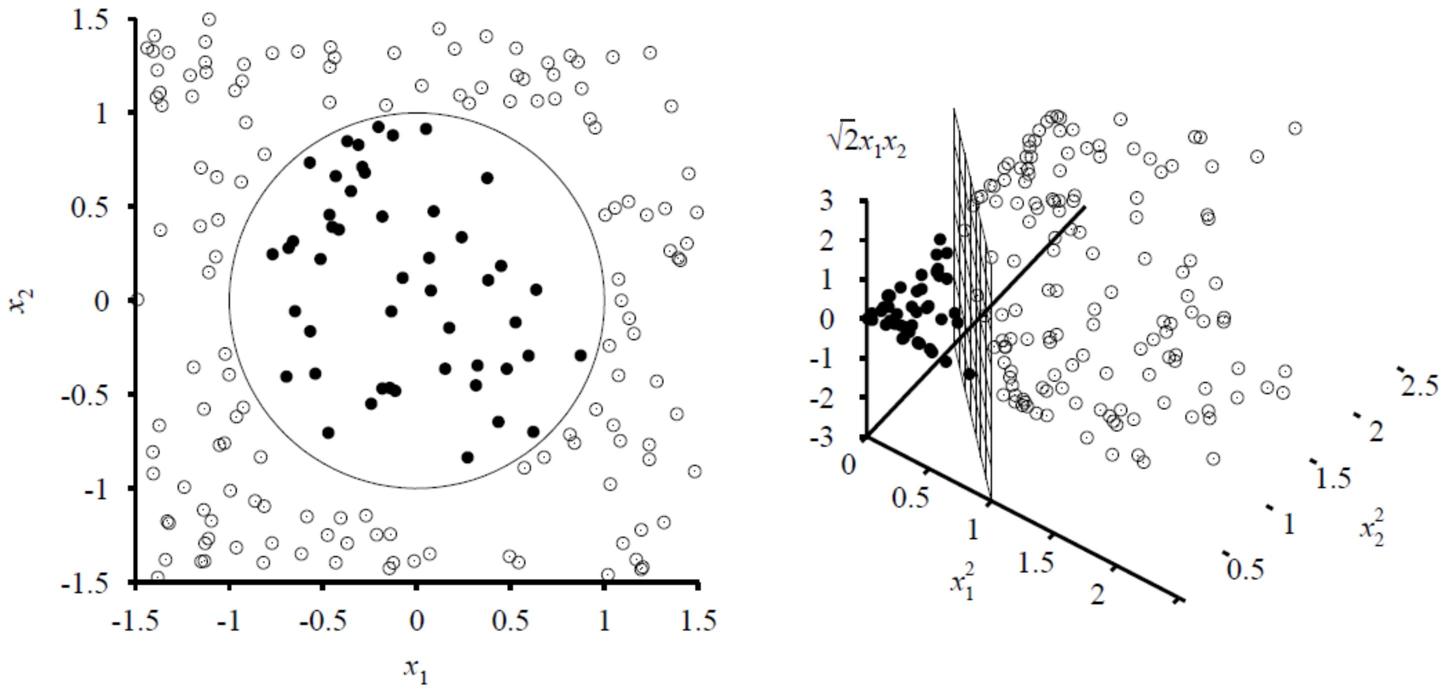
Support Vector Machines

- Now the classifying function becomes

$$g(\mathbf{x}) = \operatorname{sign}\left(\sum_j \alpha_j y_j (\mathbf{x} \cdot \mathbf{x}_j) + b \right)$$

- Properties:
  - The data enter the expression only in the form of dot products of pairs of points
  - $\alpha_j = 0$ except for the support vectors
    $\rightarrow$ SVMs gain some advantages of parametric models
- Nonlinear decision boundaries:
  - $\mathbf{x}_j \cdot \mathbf{x}_k$ can be replaced by a kernel function $K(\mathbf{x}_j \cdot \mathbf{x}_k)$ that is equivalent to $F(\mathbf{x}_j) \cdot F(\mathbf{x}_k)$
  - To find a linear separator not in the input space $\mathbf{x}$ but in the high-dimensional feature space $F(\mathbf{x})$

Support Vector Machines



(a) true decision boundary:

$$x_1^2 + x_2^2 \le 1$$

(b) after mapping to the space

$$(x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

$$F(\mathbf{x}_j) \cdot F(\mathbf{x}_k) = (\mathbf{x}_j \cdot \mathbf{x}_k)^2 = K(\mathbf{x}_j \cdot \mathbf{x}_k)$$

$$(a^2, b^2, \sqrt{2}ab) \cdot (c^2, d^2, \sqrt{2}cd) = a^2c^2 + b^2d^2 + 2acbd = (ac + bd)^2 = ((a, b) \cdot (c, d))^2$$

Support Vector Machines

- Kernel trick:
  - Polynomial kernel, $K(\mathbf{x}_j \cdot \mathbf{x}_k) = (1 + \mathbf{x}_j \cdot \mathbf{x}_k)^d$, corresponds to a feature space whose dimension increases fast with d
  - The dot product can be calculated before the nonlinear mapping is performed in the original feature space
    $\longrightarrow$ efficient computation

- Any algorithms for learning linear models can be upgraded by applying the kernel trick:
  - Reformulate to work only with dot products of pairs of data points
  - Replace the dot product by a kernel function

Support Vector Machines

- Soft margin classifier:
  - For noisy data, we want to find a decision surface in a lower-dimensional space that do not cleanly separate the classes
  - Examples on the wrong side are penalized