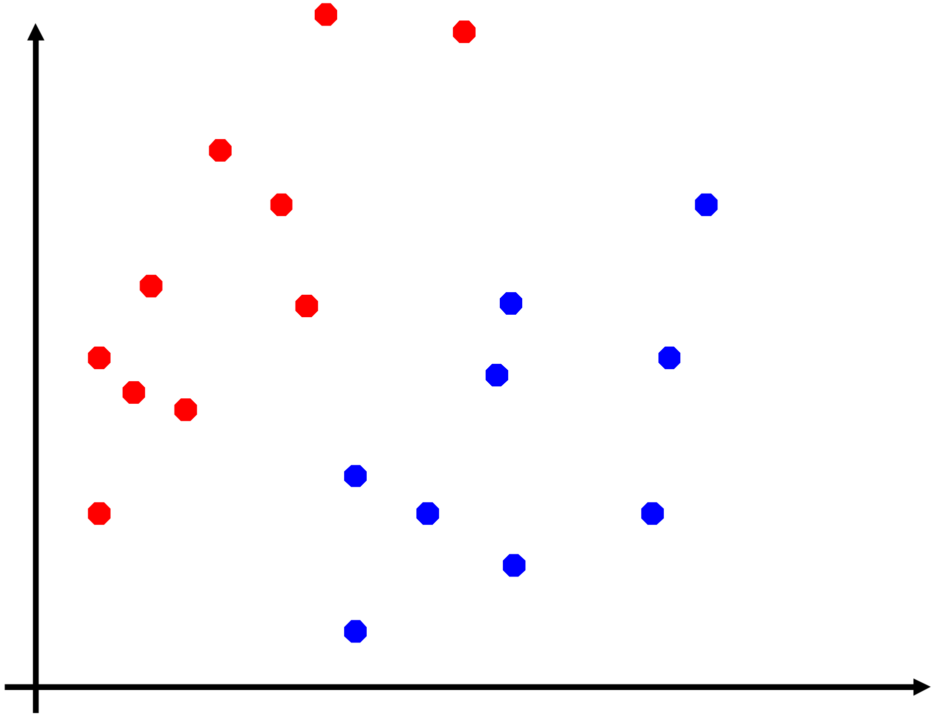
SVM - Support Vector Machines

- A new classification method for both linear and nonlinear data
- It uses a nonlinear mapping to transform the original training data into a higher dimension
- With the new dimension, it searches for the linear optimal separating hyperplane (i.e., “decision boundary”)
- With an appropriate nonlinear mapping to a sufficiently high dimension, data from two classes can always be separated by a hyperplane
- SVM finds this hyperplane using support vectors (“essential” training tuples) and margins (defined by the support vectors)

SVM - History and Applications

- Vapnik and colleagues (1992)—groundwork from Vapnik & Chervonenkis' statistical learning theory in 1960s
- Features: training can be slow but accuracy is high owing to their ability to model complex nonlinear decision boundaries (margin maximization)
- Used both for classification and prediction
- Applications:
  - handwritten digit recognition, object recognition, speaker identification, benchmarking time-series prediction tests

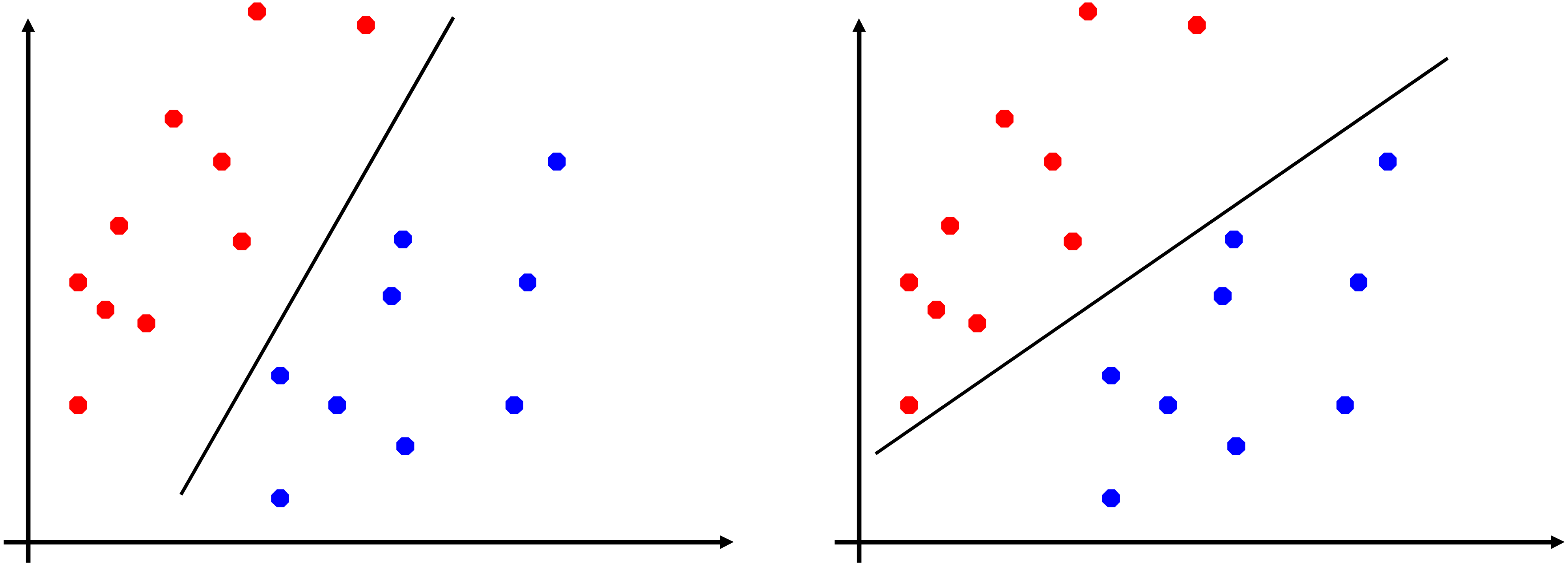
Linear Classifiers



Consider a two dimensional dataset with two classes

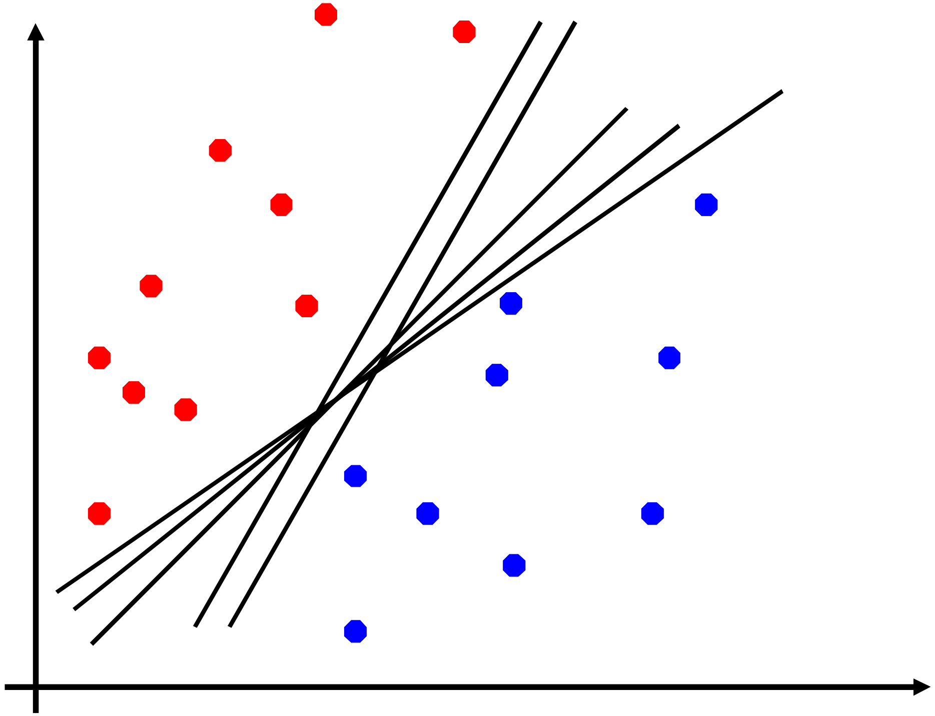
How would we classify this dataset?

Linear Classifiers



Both of the lines can be linear classifiers.

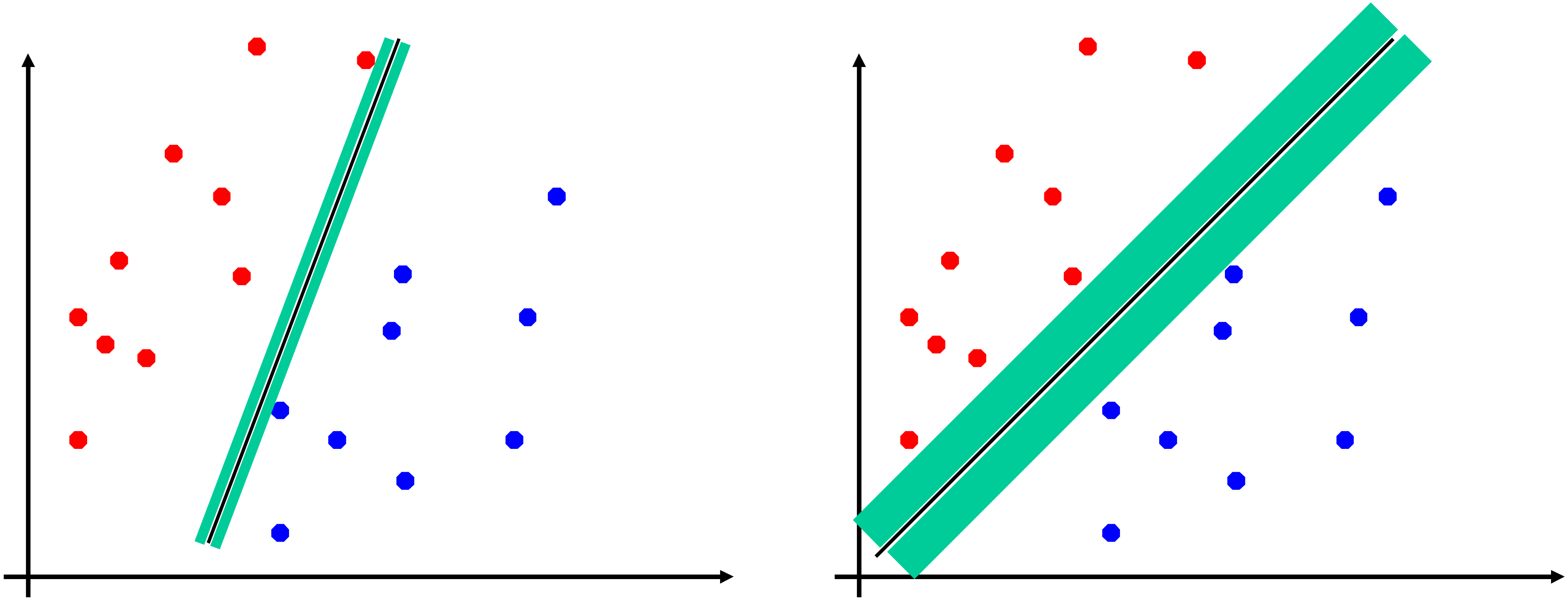
Linear Classifiers



There are many lines that can be linear classifiers.

Which one is the optimal classifier.

Classifier Margin

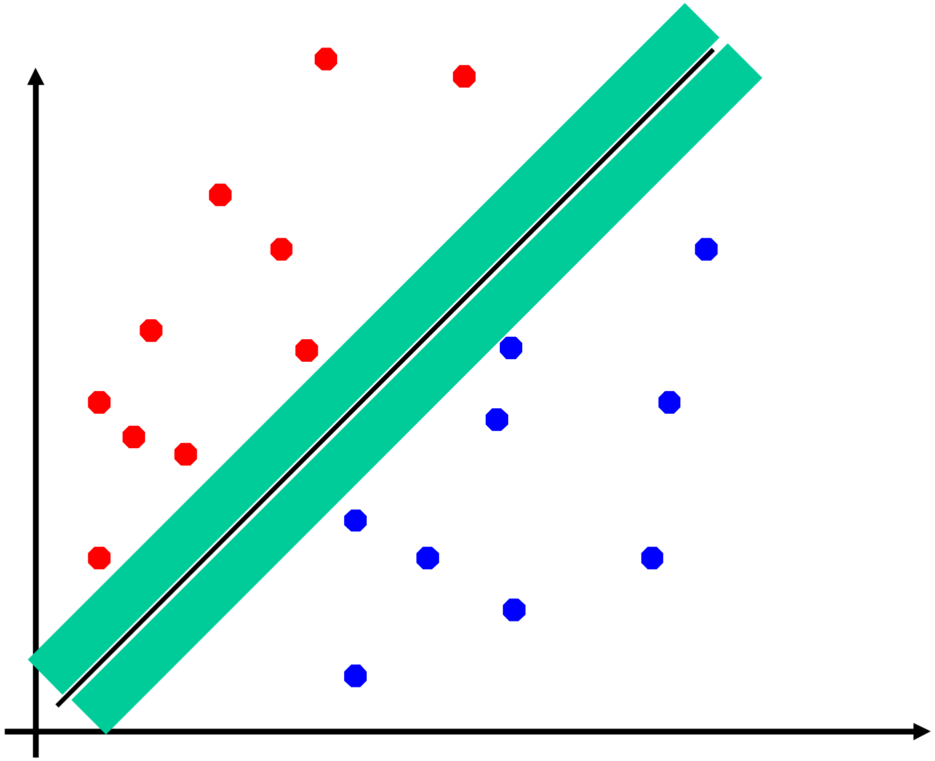


Define the **margin** of a linear classifier as the width that theboundary could be increased by before hitting a datapoint.

Maximum Margin

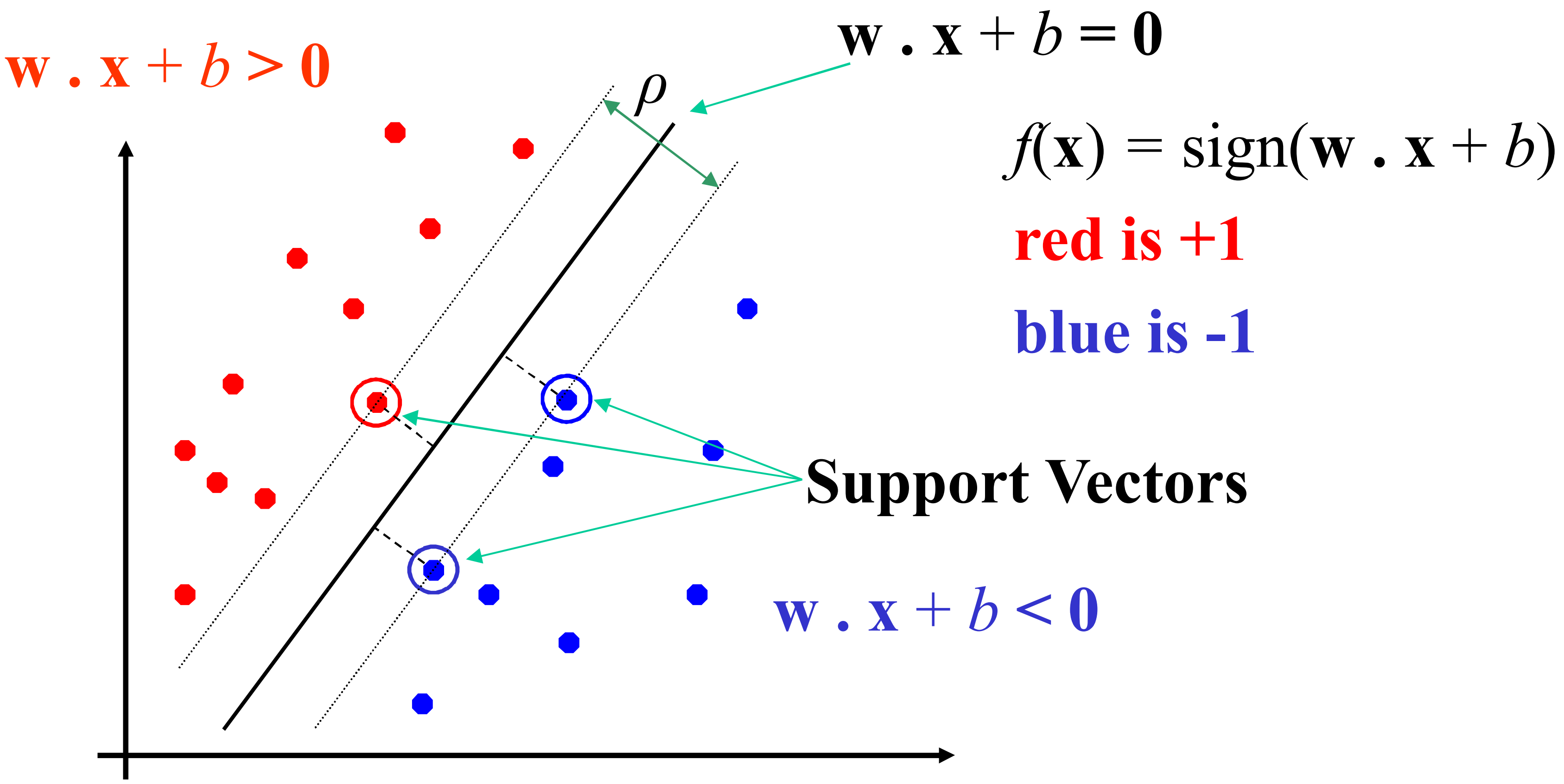
The **maximum margin linear classifier** is the linear classifier with the maximum margin.

This is the simplest kind of SVM (Called Linear SVM)



Support Vectors

- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the distance between support vectors.



$\mathbf{w}\ .\ \mathbf{x} + b > 0$

ρ

$\mathbf{w}\ .\ \mathbf{x} + b = 0$

$f(\mathbf{x}) = \text{sign}(\mathbf{w}\ .\ \mathbf{x} + b)$

red is +1

blue is -1

Support Vectors

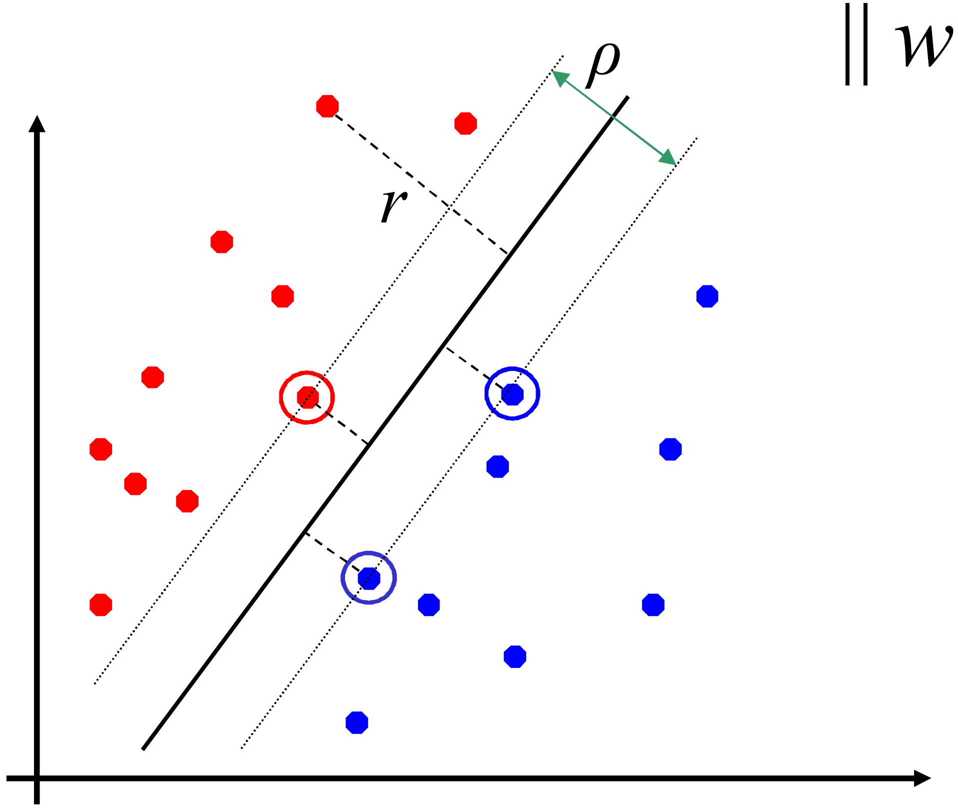
$\mathbf{w}\ .\ \mathbf{x} + b < 0$

Support Vectors

- Distance from example $\mathbf{x}_i$ to the separator is

$$r = \frac{\mathbf{w}.\mathbf{x}_i + b}{\|\mathbf{w}\|}$$

$$\| w \| \; is \; \sqrt{w_1^2 + \ldots + w_n^2}$$



SVM - Linearly Separable

- A separating hyperplane can be written as
  - $\mathbf{W} \bullet \mathbf{X} + b = 0$
  - where $\mathbf{W}=\{w_1, w_2, \ldots, w_n\}$ is a weight vector and b a scalar (bias)
- For 2-D it can be written as
  - $w_0 + w_1\, x_1 + w_2\, x_2 = 0$
- The hyperplane defining the sides of the margin:
  - H_1: $w_0 + w_1\, x_1 + w_2\, x_2 \geq 1$ for $y_i = +1$, and
  - H_2: $w_0 + w_1\, x_1 + w_2\, x_2 \leq -1$ 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**

Linear SVM Mathematically

- Let training set $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$, $\mathbf{x}_i \in \mathbf{R}^d$, $y_i \in \{-1, 1\}$ be separated by a hyperplane with margin ρ. Then for each training example $(\mathbf{x}_i, y_i)$:

$$\begin{array}{ll} \mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b \leq -\rho/2 & \text{if } y_i = -1 \\ \mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b \geq \rho/2 & \text{if } y_i = 1 \end{array} \quad \Leftrightarrow \quad y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b) \geq \rho/2$$

- For every support vector $\mathbf{x}_s$ the above inequality is an equality. After rescaling $\mathbf{w}$ and b by $\rho/2$ in the equality, we obtain that distance between each $\mathbf{x}_s$ and the hyperplane is $r = \dfrac{\mathrm{y}_s(\mathbf{w}^T\mathbf{x}_s + b)}{\|\mathbf{w}\|} = \dfrac{1}{\|\mathbf{w}\|}$

- Then the margin can be expressed through (rescaled) $\mathbf{w}$ and b as:

$$\rho = 2r = \frac{2}{\|\mathbf{w}\|}$$

Linear SVMs Mathematically (cont.)

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

Find $\mathbf{w}$ and b such that

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

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

Which can be reformulated as:

Find $\mathbf{w}$ and b such that

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

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

Solving the Optimization Problem

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

- 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
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$ 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 $\alpha_1 \dots \alpha_n$ to the dual problem, solution to the primal is:

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

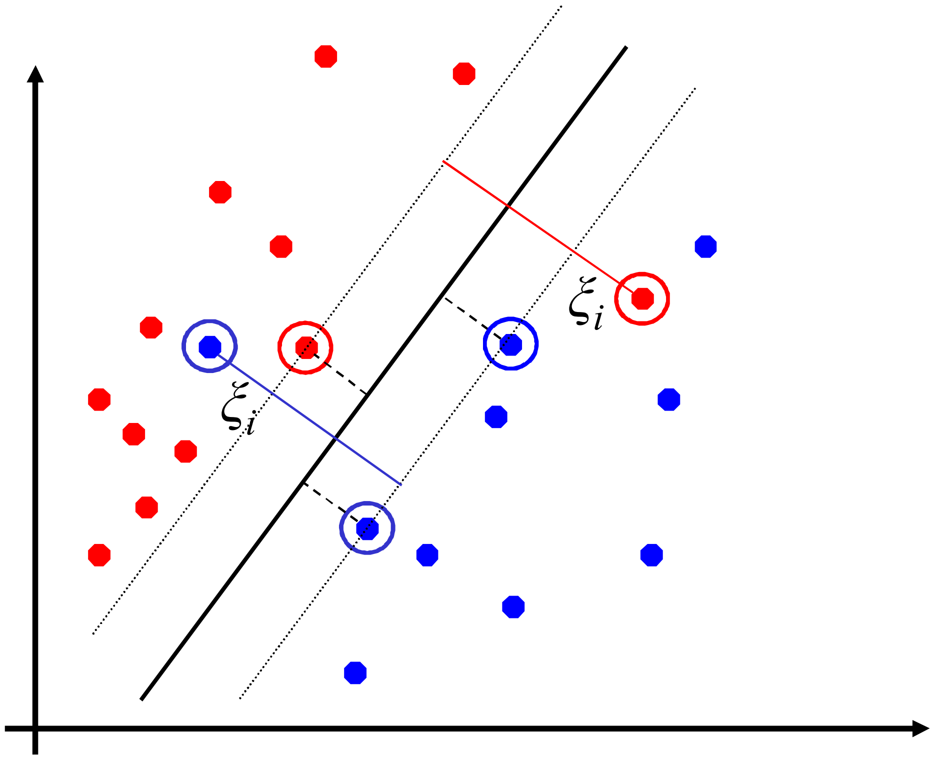
- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.
- Then the classifying function is (note that we don't need **w** explicitly):

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

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

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*.



Soft Margin Classification Mathematically

- The old formulation:

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

- Modified formulation incorporates slack variables:

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

- 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.

Soft Margin Classification – Solution

- 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
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

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

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

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

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

Theoretical Justification for Maximum Margins

- Vapnik has proved the following:

  The class of optimal linear separators has VC dimension h bounded from above as

  $$h \leq \min\left\{ \left\lceil \frac{D^2}{\rho^2} \right\rceil, m_0 \right\} + 1$$

  where ρ is the margin, D is the diameter of the smallest sphere that can enclose all of the training examples, and m_0 is the dimensionality.

- Intuitively, this implies that regardless of dimensionality m_0 we can minimize the VC dimension by maximizing the margin *ρ*.

- Thus, complexity of the classifier is kept small regardless of dimensionality.

Linear SVMs: Overview

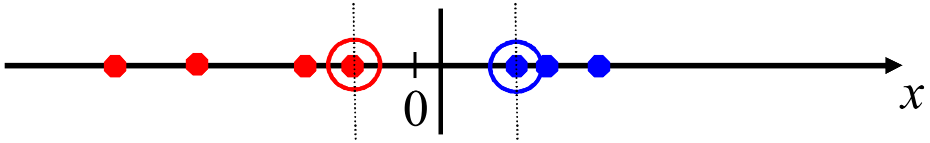
- The classifier is a *separating hyperplane.*
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation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

Find $\alpha_1 \dots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$ is maximized
and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

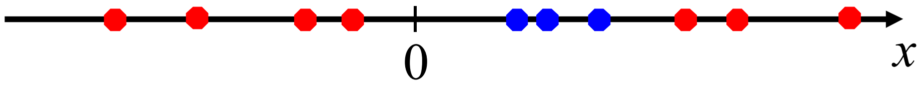
$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x}_i^{\mathbf{T}}\mathbf{x} + b$

Non-linear SVMs

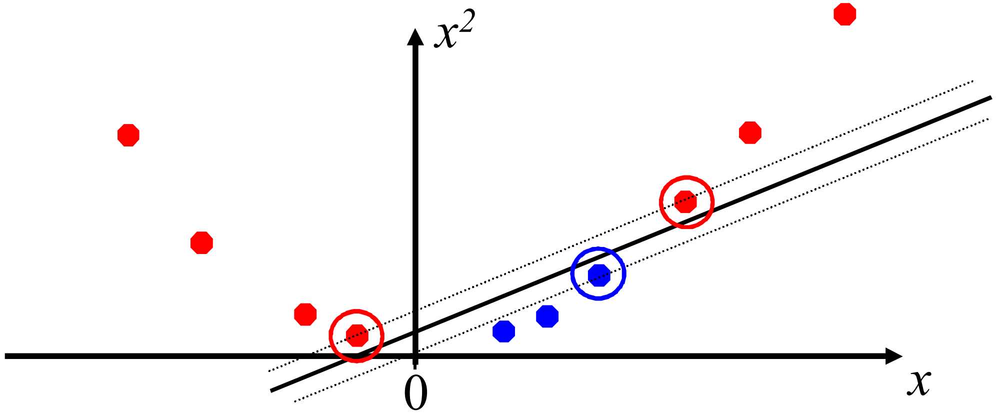
- Datasets that are linearly separable with some noise work out great:



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

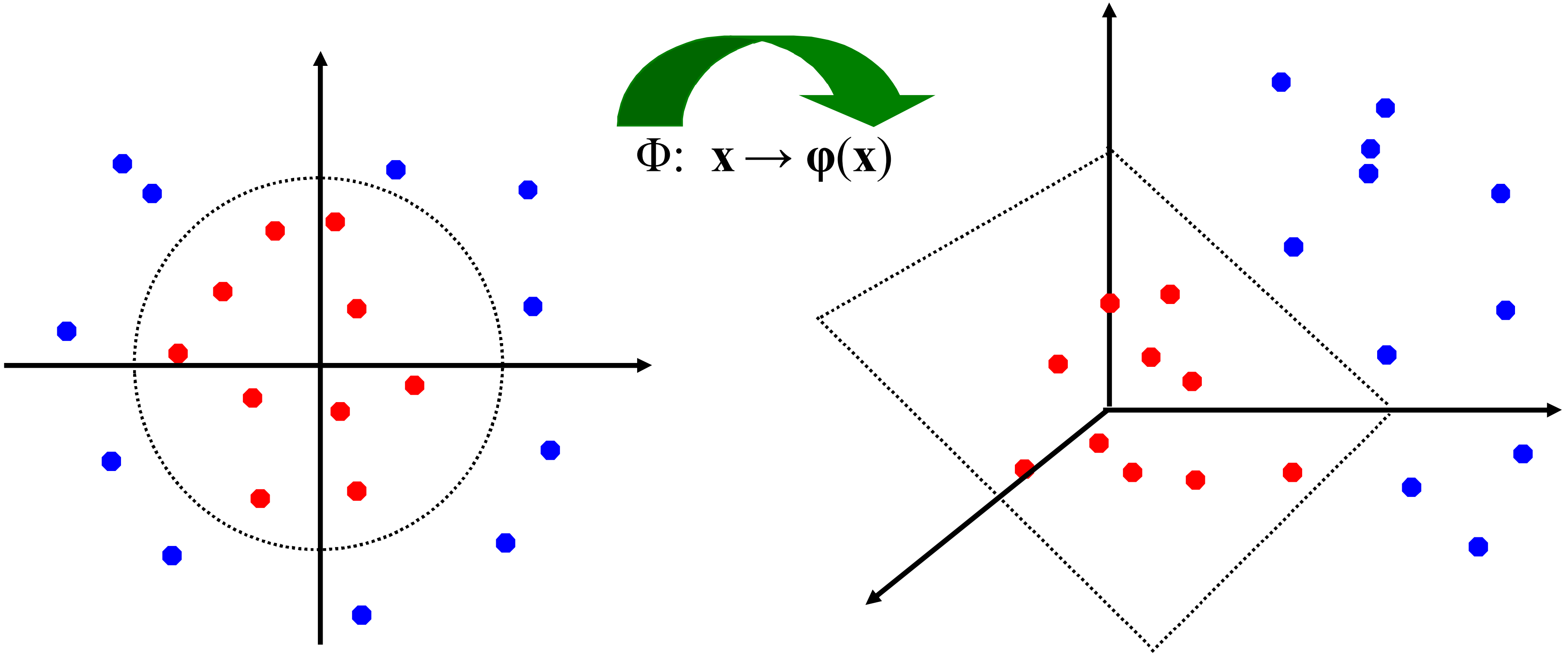


- How about… mapping data to a higher-dimensional space



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 inner product between vectors $K(\mathbf{x}_i,\mathbf{x}_j)=\mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
- If every datapoint is mapped into high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$, the inner product becomes:

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

- A *kernel function* is a function that is eqiuvalent to an inner product in some feature space.
- Example:

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

  Need to show that $K(\mathbf{x}_i,\mathbf{x}_\mathbf{j})= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$:

$$K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^2{}_,= 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}=$$

$$= [1\ \ x_{i1}^2\ \sqrt{2}\, x_{i1}x_{i2}\ \ x_{i2}^2\ \sqrt{2}x_{i1}\ \sqrt{2}x_{i2}]^{\mathbf{T}}\, [1\ \ x_{j1}^2\ \sqrt{2}\, x_{j1}x_{j2}\ \ x_{j2}^2\ \sqrt{2}x_{j1}\ \sqrt{2}x_{j2}] =$$

$$= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j), \quad \text{where } \boldsymbol{\varphi}(\mathbf{x}) = [1\ \ x_1^2\ \sqrt{2}\, x_1x_2\ \ x_2^2\ \ \sqrt{2}x_1\ \sqrt{2}x_2]$$

- Thus, a kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\boldsymbol{\varphi}(\mathbf{x})$ explicitly).

Examples of Kernel Functions

- Linear: $K(\mathbf{x}_i,\mathbf{x}_j)= \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is $\mathbf{x}$ itself

- Polynomial of power p: $K(\mathbf{x}_i,\mathbf{x}_j)= (1+ \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^p$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ has $\binom{d+p}{p}$ dimensions

- Gaussian (radial-basis function): $K(\mathbf{x}_i,\mathbf{x}_j) = e^{-\frac{\left\|\mathbf{x}_i-\mathbf{x}_j\right\|^2}{2\sigma^2}}$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is *infinite-dimensional*: every point is mapped to *a function* (a Gaussian); combination of functions for support vectors is the separator.

- Higher-dimensional space still has *intrinsic* dimensionality d (the mapping is not *onto*), but linear separators in it correspond to *non-linear* separators in original space.

Non-linear SVMs Mathematically

- Dual problem formulation:

Find $\alpha_1 \ldots \alpha_n$ such that

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

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

(2) $\alpha_i \geq 0$ for all α_i

- The solution is:

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

- Optimization techniques for finding α_i's remain the same!

SVM applications

- SVMs were originally proposed by Boser, Guyon and Vapnik in 1992 and gained increasing popularity in late 1990s.
- SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
- SVM techniques have been extended to a number of tasks such as regression [Vapnik *et al.* '97], principal component analysis [Schölkopf *et al.* '99], etc.
- Most popular optimization algorithms for SVMs use *decomposition* to hill-climb over a subset of α_i's at a time, e.g. SMO [Platt '99] and [Joachims '99]
- Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner.