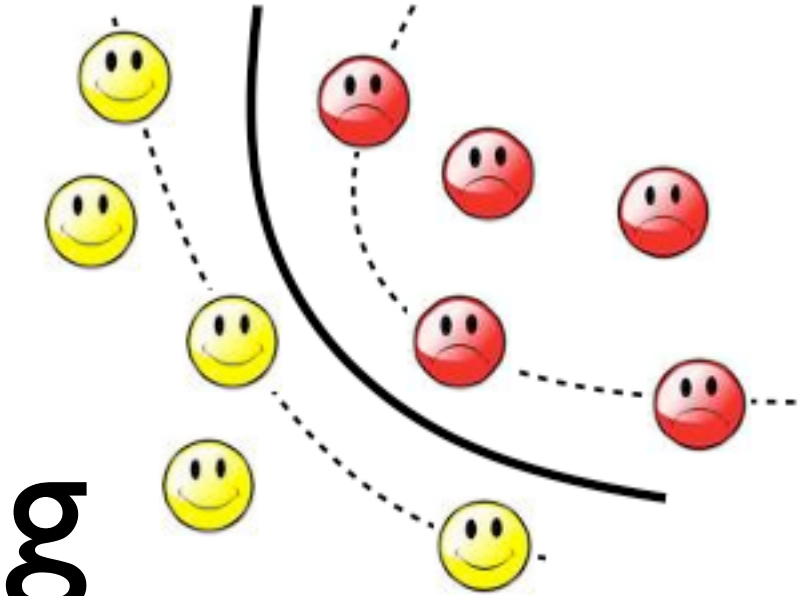

Machine Learning and Data Mining

(COMP 5318)

Support Vector Machines

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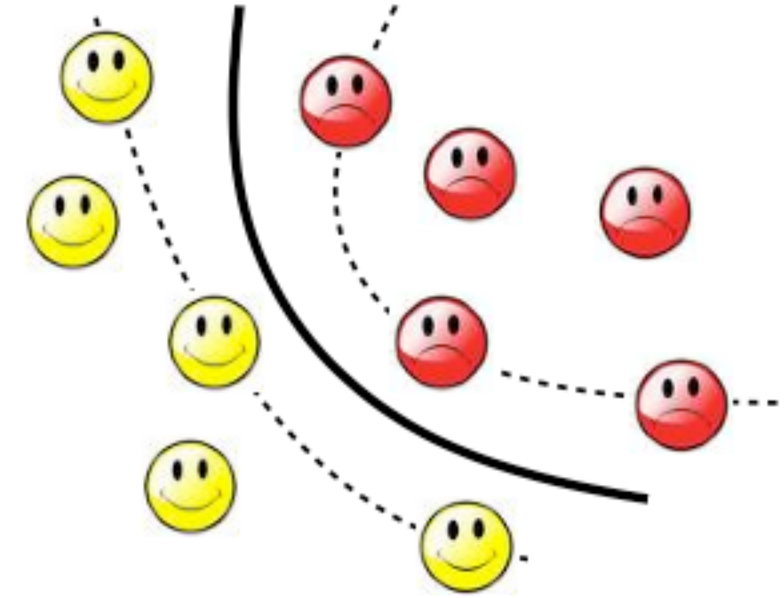
Announcements

- This lecture is based on:
  - Murphy's book: Chapters 8, 14
  - Ullman's book: Chapter 12

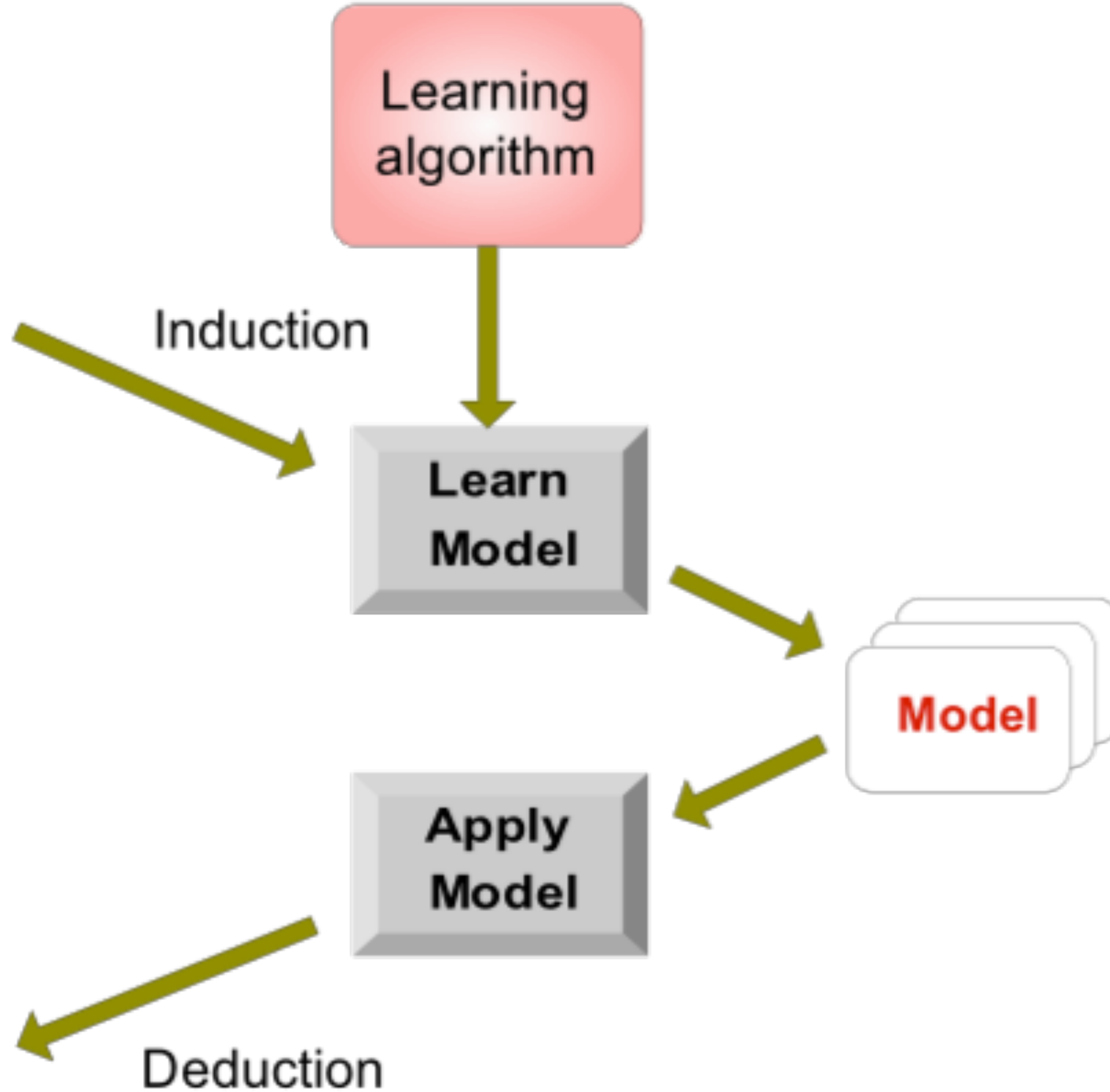


Quick Review

Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set



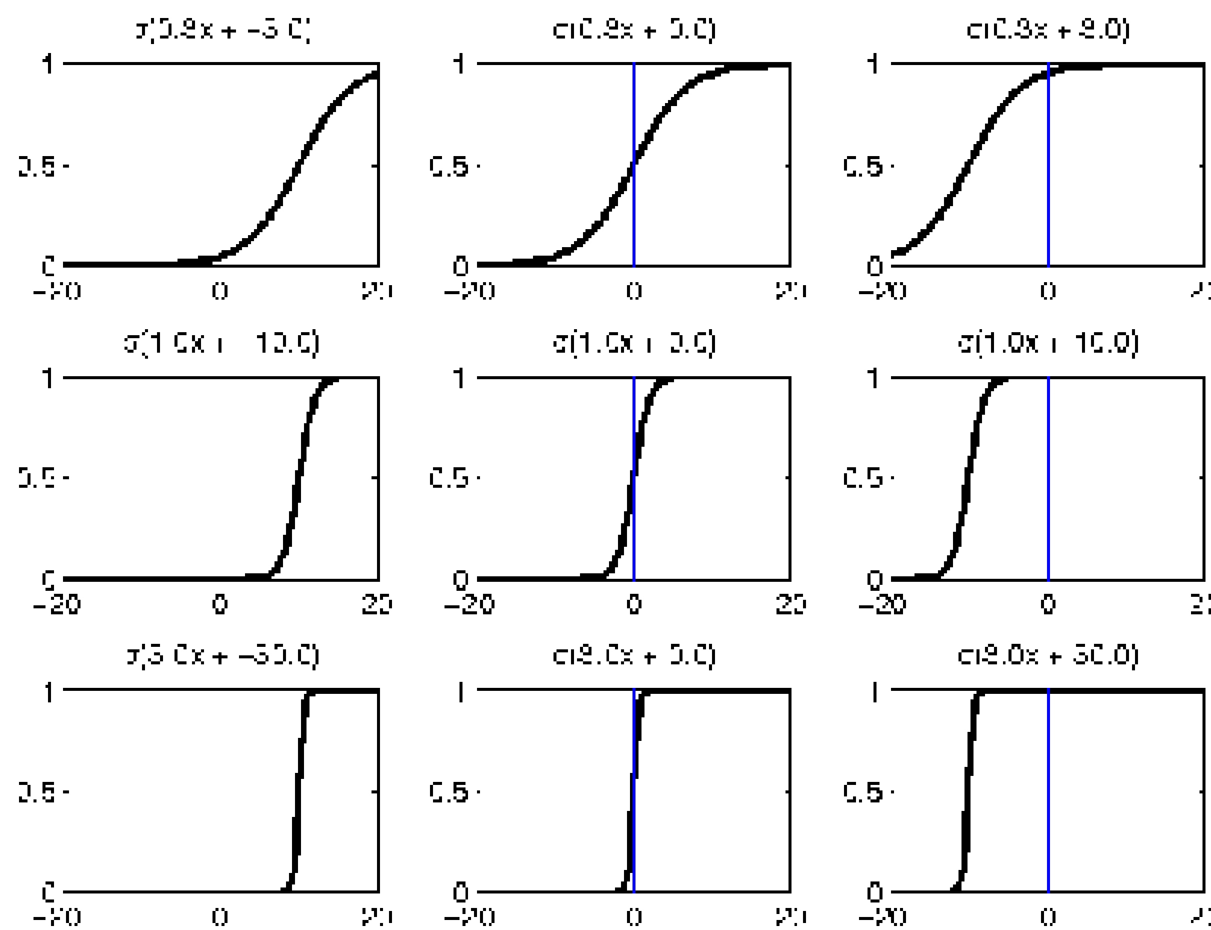
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Logistic Regression

- Discriminative model for binary classification

$$
\begin{aligned}
p(y|\mathbf{x}, \mathbf{w}) &= \mathrm{Ber}(y|\sigma(\eta)) = \sigma(\eta)^y(1-\sigma(\eta))^{1-y} \\
\eta &= \mathbf{w}^T\mathbf{x} \\
\sigma(\eta) &\stackrel{\text{def}}{=} \frac{1}{1+\exp(-\eta)} = \frac{e^\eta}{e^\eta + 1}
\end{aligned}
$$



Sigmoid or Logistic function

Logistic Regression

- Assumes a parametric form for directly estimating P(Y | X). For binary concepts, this is:

$$P(Y = 0|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

$$P(Y = 1|X) = 1 - P(Y = 0|X)$$

$$= \frac{\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}{1 + \exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

- Equivalent to a one-layer backpropagation neural net.
- Logistic regression is the source of the sigmoid function used in backpropagation.
- Objective function for training is somewhat different.

Logistic Regression as a Log-Linear Model

- Logistic regression is basically a linear model, which is demonstrated by taking logs.

$$\text{Assign label } Y = 0 \text{ iff } 1 < \frac{P(Y=0 \mid X)}{P(Y=1 \mid X)}$$

$$1 > \exp(w_0 + \sum_{i=1}^{n} w_i X_i)$$

$$0 > w_0 + \sum_{i=1}^{n} w_i X_i$$

- Also called a **maximum entropy model** (**MaxEnt**) because it can be shown that standard training for logistic regression gives the distribution with maximum entropy that is consistent with the training data.

Loss for density estimation

- Suppose output is $\hat{p}(y|\mathbf{x})$, truth is $p(y|\mathbf{x})$
- Use KL (Kullback-Leibler) divergence

$$L(p(y|\mathbf{x}), \hat{p}(y|\mathbf{x})) = KL(p(y|\mathbf{x}), \hat{p}(y|\mathbf{x})) = \sum_y p(y|\mathbf{x}) \log \frac{p(y|\mathbf{x})}{\hat{p}(y|\mathbf{x})}$$

- Risk is expected negative log likelihood

$$R(\hat{p}) = -E_{\mathbf{x}} \sum_y p(y|\mathbf{x}) \log \hat{p}(y|\mathbf{x}) = -E_{\mathbf{x},y} \log \hat{p}(y|\mathbf{x})$$

Logistic Regression Training

- Weights are set during training to maximise the **conditional data likelihood** :

$$W \leftarrow \arg\max_W \prod_{d \in D} P(Y^d \mid X^d, W)$$

where D is the set of training examples and Y^d and X^d denote, respectively, the values of Y and X for example d.

- Equivalently viewed as maximising the **conditional log likelihood** (CLL)

$$W \leftarrow \arg\max_W \sum_{d \in D} \ln P(Y^d \mid X^d, W)$$

Preventing Overfitting in Logistic Regression

- To prevent overfitting, one can use **regularisation** (a.k.a. smoothing) by penalising large weights by changing the training objective:

$$W \leftarrow \underset{W}{\operatorname{argmax}} \sum_{d \in D} \ln P(Y^d \mid X^d, W) - \frac{\lambda}{2} \|W\|^2$$

Where λ is a constant that determines the amount of smoothing

- This can be shown to be equivalent to assuming a Gaussian prior for *W* with zero mean and a variance related to $1/\lambda$.

Relation Between NB and Logistic Regression

- Naïve Bayes with Gaussian distributions for features (GNB), can be shown to give the same functional form for the conditional distribution $P(Y \mid X)$.
  - But converse is not true, so Logistic Regression makes a weaker assumption.
- Logistic regression is a **discriminative** rather than generative model, since it models the conditional distribution $P(Y \mid X)$ and directly attempts to fit the training data for predicting Y from X. Does not specify a full joint distribution.

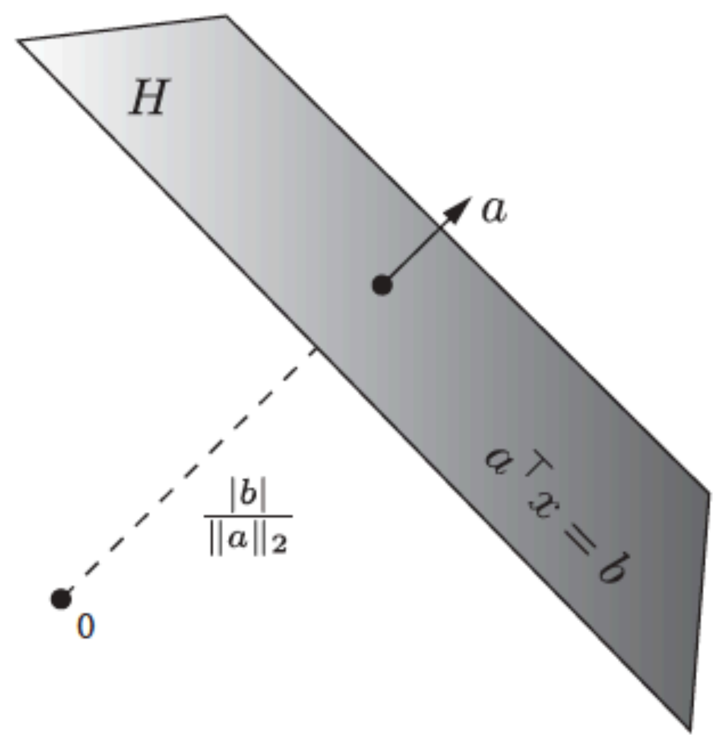
Support Vector Machines

Hyperplanes and Halfspaces

- A hyperplane in $\mathbb{R}^n$ is a set of the form

$$H = \left\{ x \in \mathbb{R}^n \, : \, a^\top x = b \right\},$$

where $a \in \mathbb{R}^n$, $a \neq 0$, and $b \in \mathbb{R}$ are given.

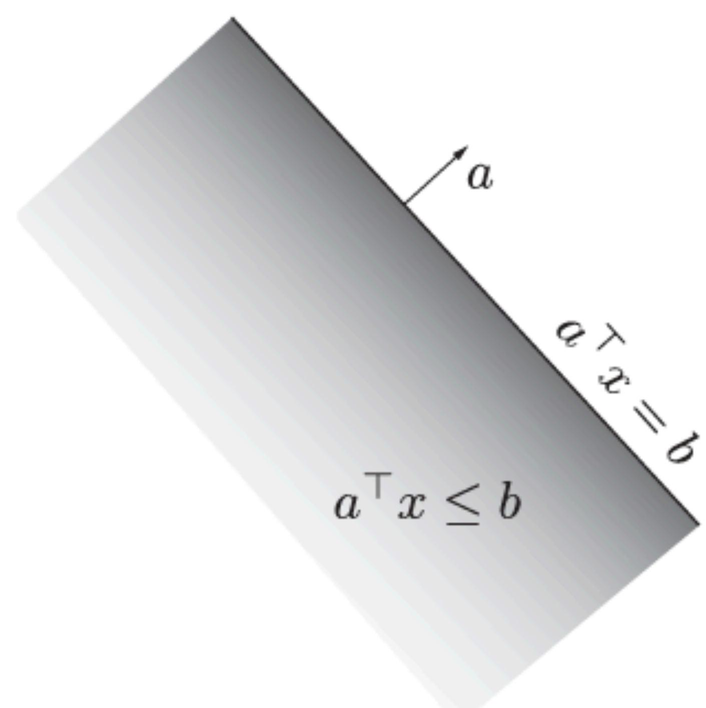


Hyperplanes and Halfspaces

- An hyperplane H separates the whole space in two regions:

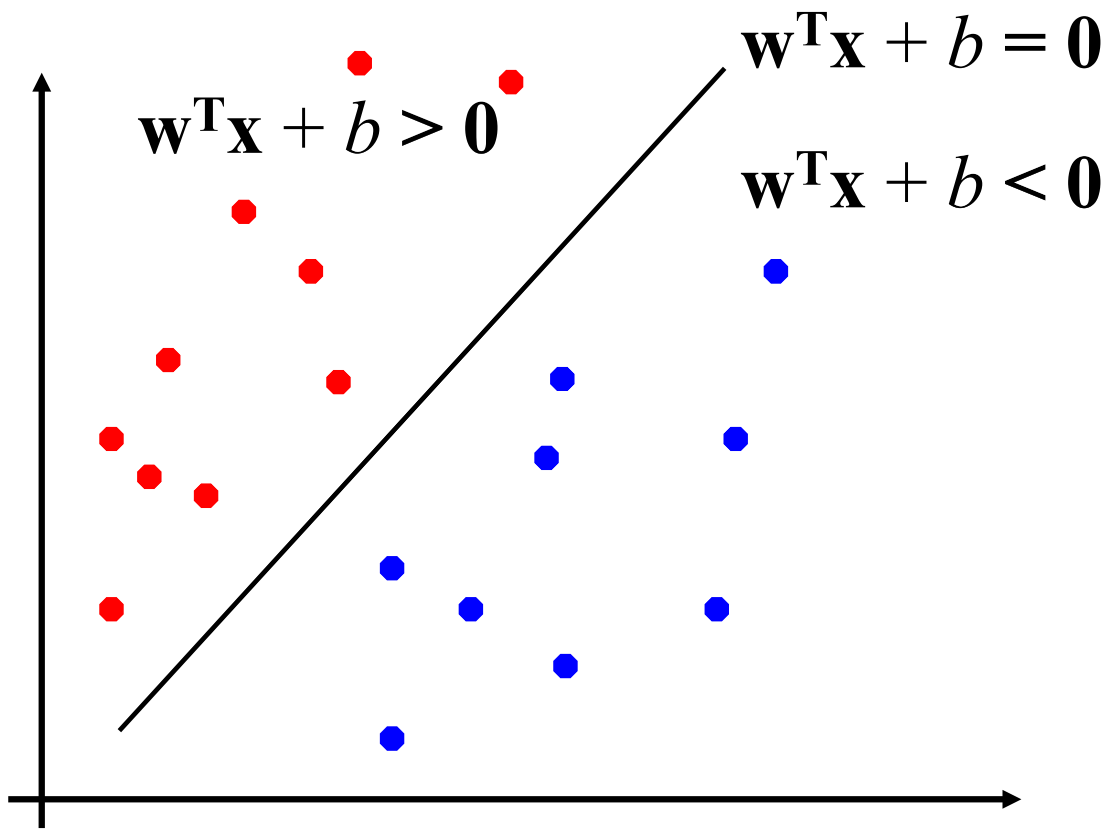
$$H_{-} = \left\{x \,:\, a^{\top}x \leq b\right\}, \quad H_{++} = \left\{x \,:\, a^{\top}x > b\right\}.$$

- These regions are called halfspaces (H_{-} is a closed halfspace, H_{++} is an open halfspace).
- the halfspace H_{-} is the region delimited by the hyperplane $H = \{a^{\top}x = b\}$ and lying in the direction opposite to vector a. Similarly, the halfspace H_{++} is the region lying above (i.e., in the direction of a) the hyperplane.



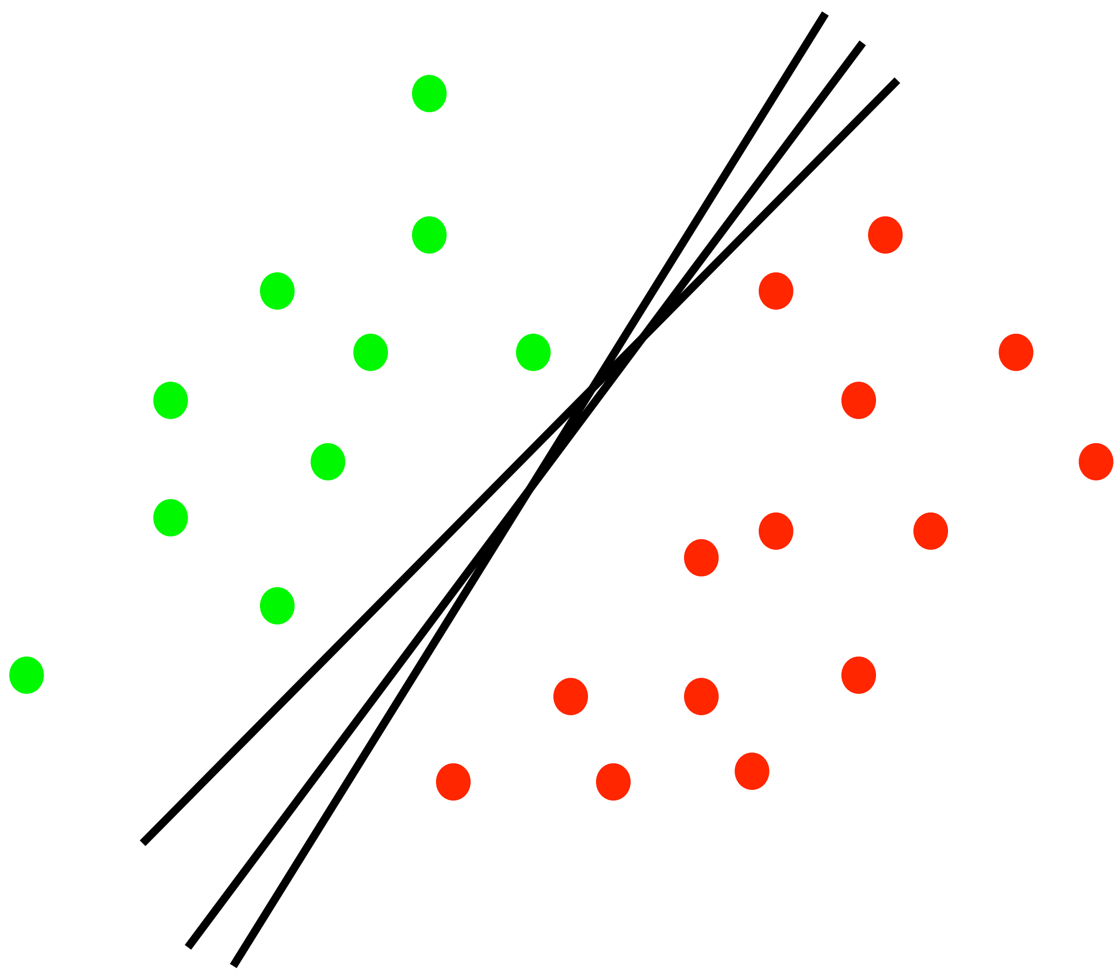
Linear Classifiers

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



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

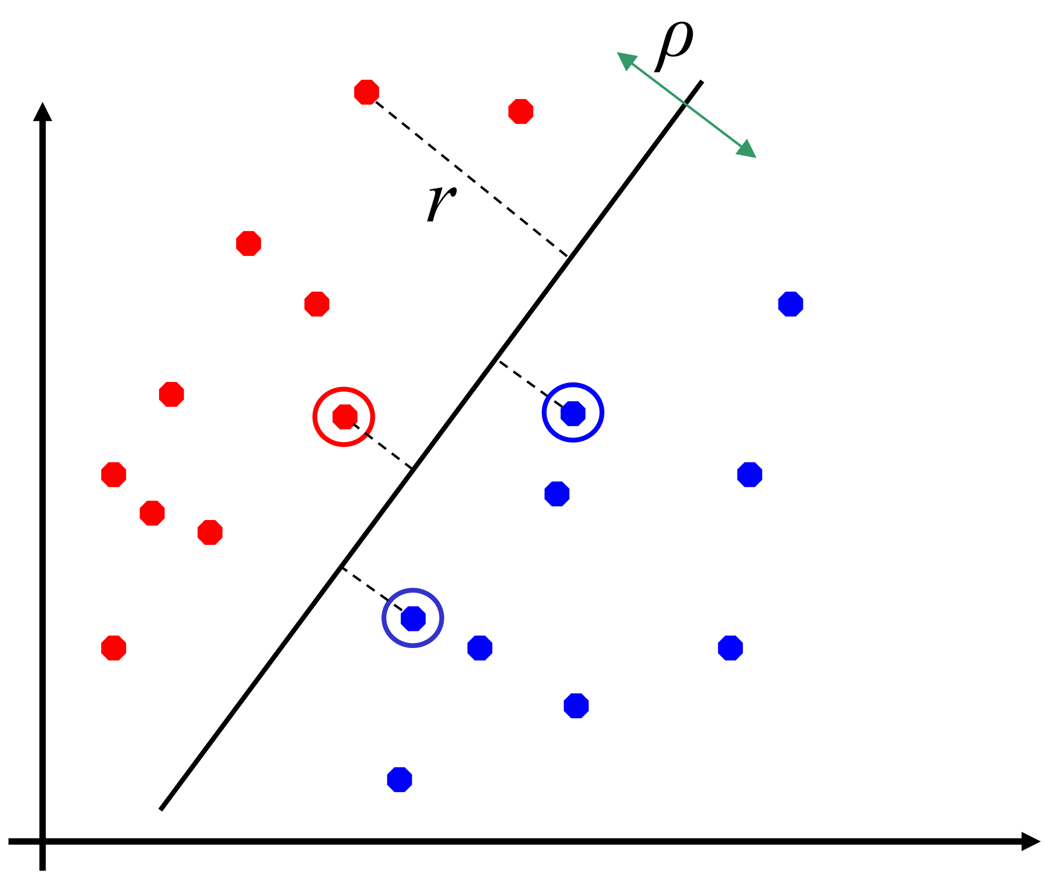
Linear classifiers



Which line is better?

Classification Margin

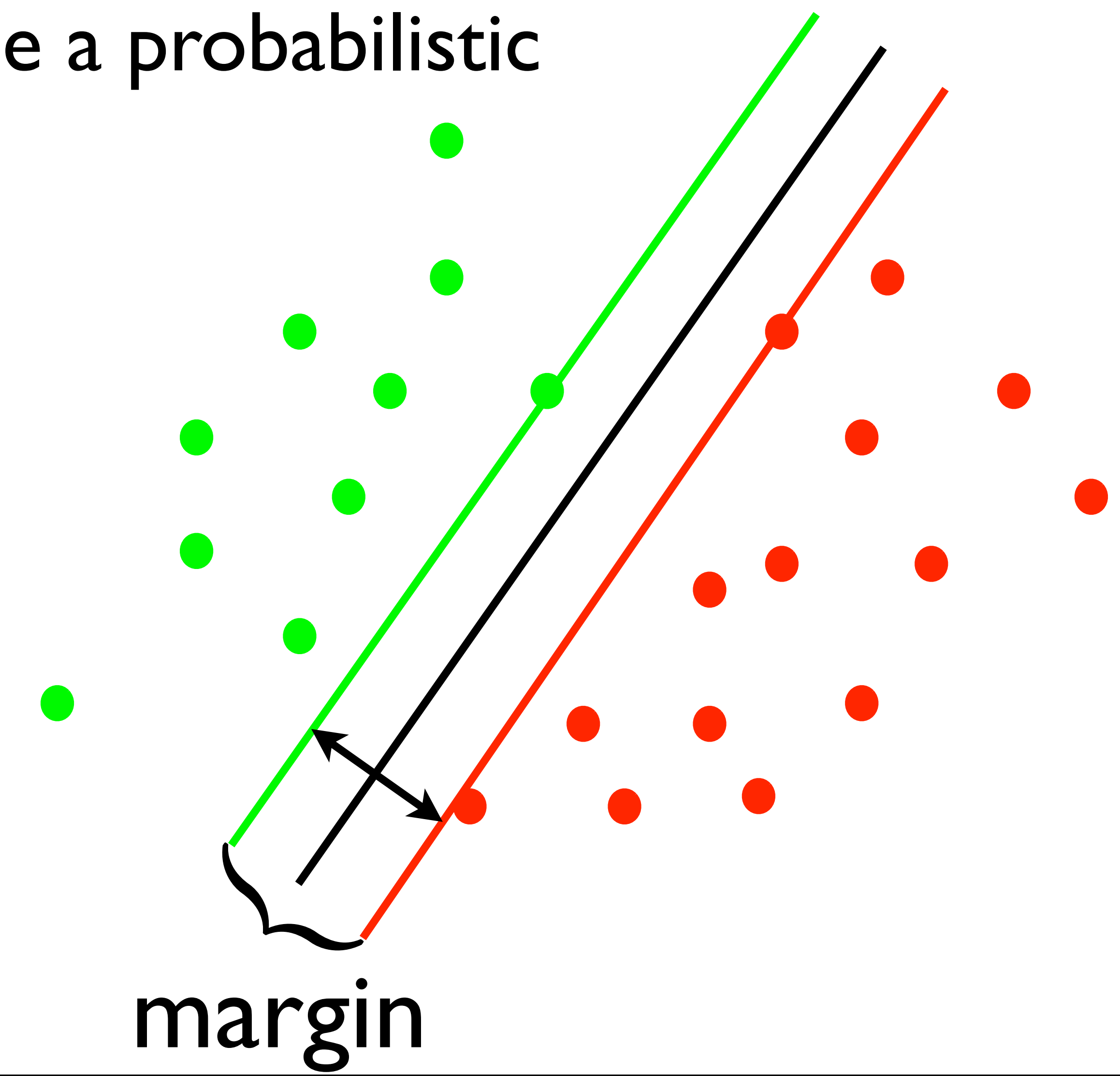
- Distance from example $\mathbf{x}_i$ to the separator is $r = \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|}$
- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the distance between support vectors.



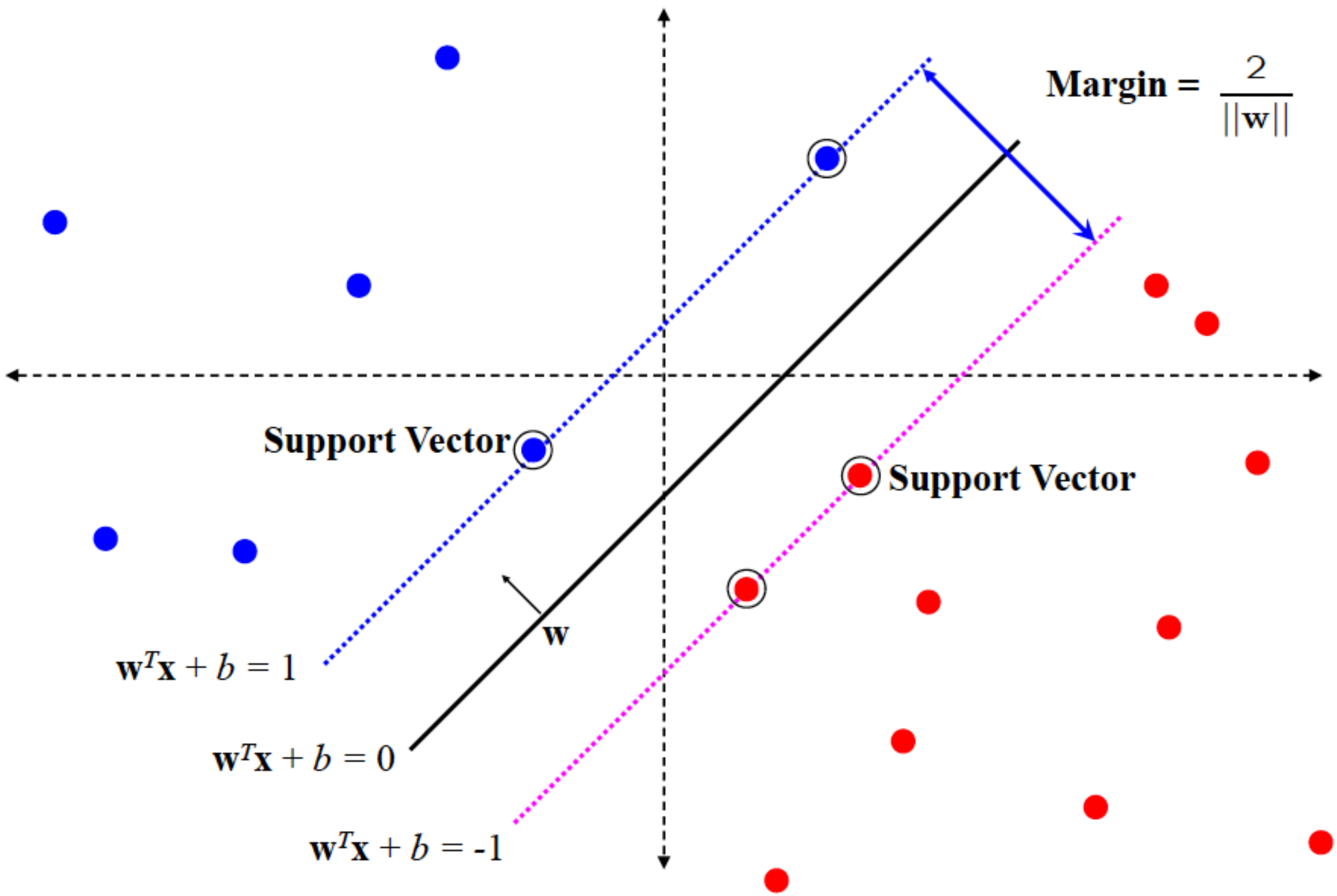
Maximum margin

Things to note

- The boundary is defined by only a few points (support vectors)
- Difficult to define a probabilistic explanation



SVM



Margin = $\frac{2}{||\mathbf{w}||}$
Support Vector
Support Vector
$\mathbf{w}$
$\mathbf{w}^T\mathbf{x} + b = 1$
$\mathbf{w}^T\mathbf{x} + b = 0$
$\mathbf{w}^T\mathbf{x} + b = -1$

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 $r = \frac{y_s(\mathbf{w}^T\mathbf{x}_s + b)}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$

- 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
$\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ 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 $\alpha_1 \dots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ 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:

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

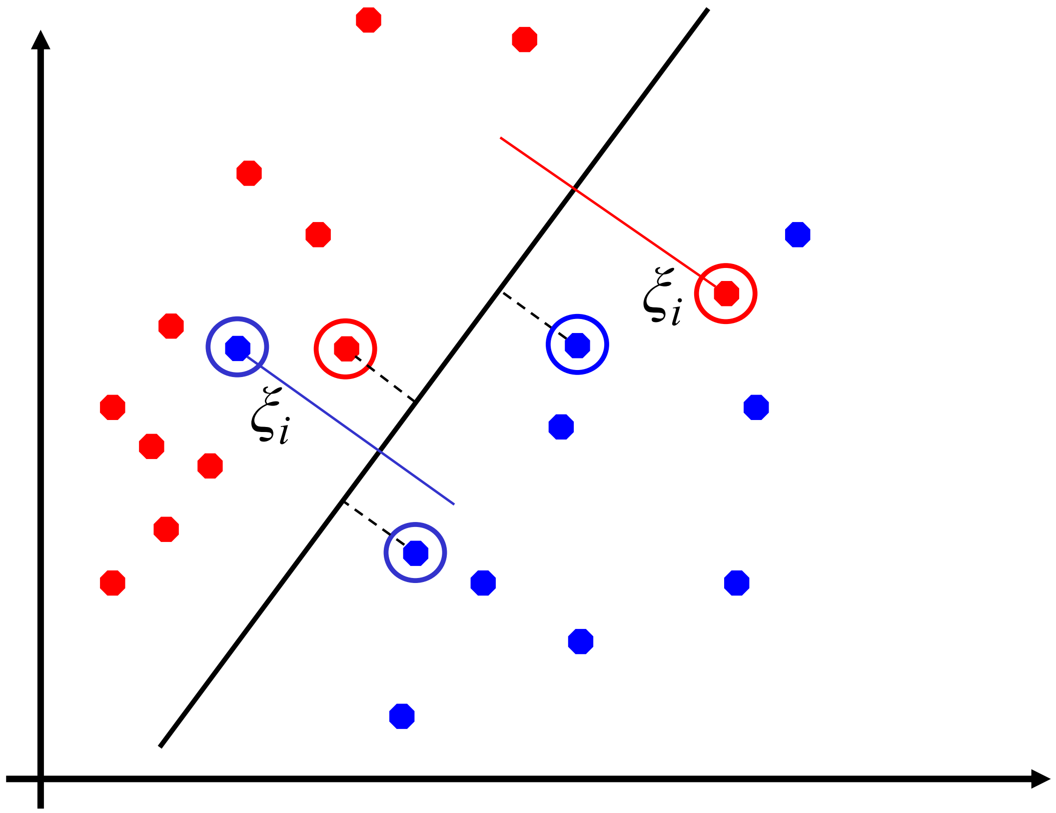
- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.
- Then the classifying function is (note that we don't need **w** explicitly):

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

- Notice that it relies on an *inner product* between the test point **x** and the support vectors $\mathbf{x}_i$ – we will return to this later.
- 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 $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b) \geq 1$

- 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 $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b) \geq 1 - \xi_i$, $\xi_i \geq 0$

- 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.

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 $\mathbf{w}$ explicitly for classification:

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

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.

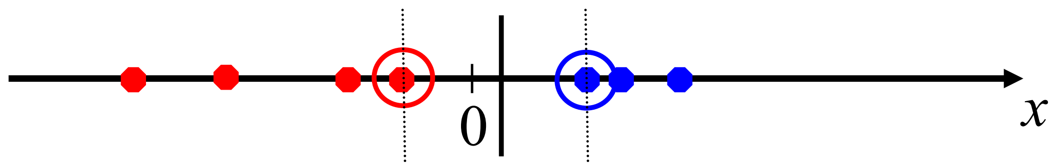
- Both in the dual formulation of the problem and in the solution training points appear only inside inner products:

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

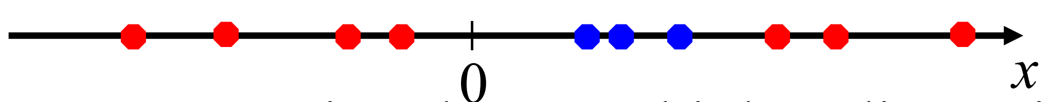
$$f(\mathbf{x}) = \Sigma\alpha_i y_i \boxed{\mathbf{x}_i^{\mathrm{T}}\mathbf{x}} + b$$

Non-linear SVMs

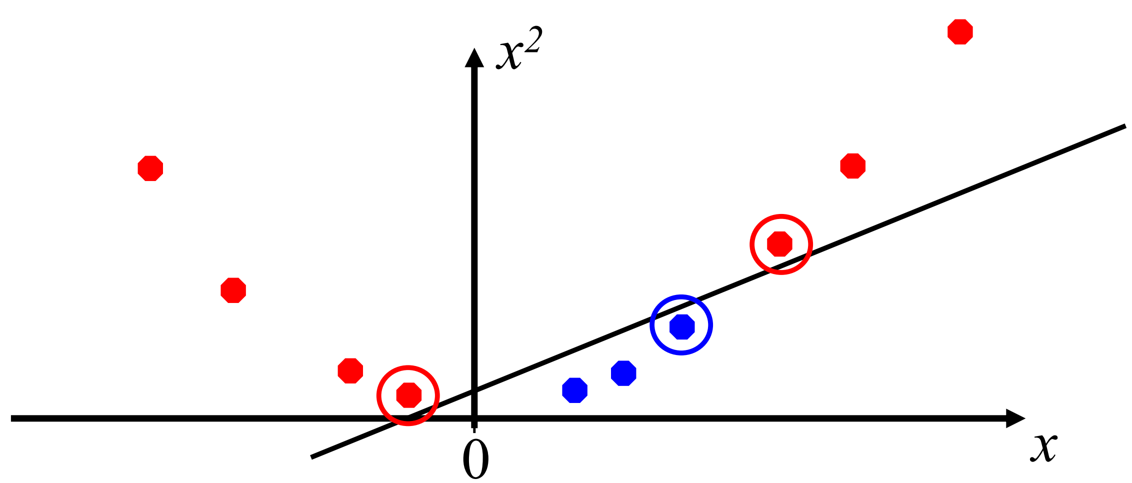
- Datasets that are linearly separable with some noise work out great:



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

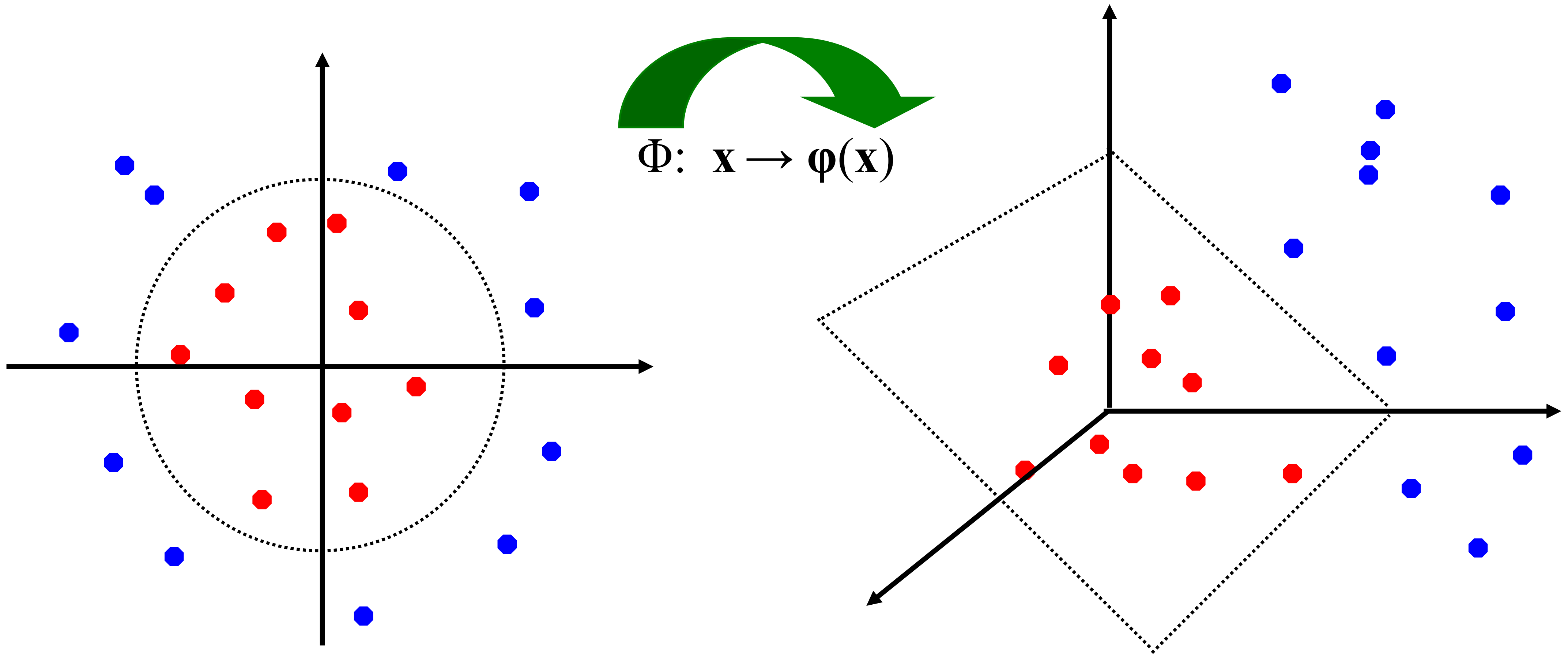


- How about… mapping data to a higher-dimensional space:



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 equivalent 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).

What Functions are Kernels?

- For some functions $K(\mathbf{x}_i,\mathbf{x}_j)$ checking that $K(\mathbf{x}_i,\mathbf{x}_j)= \varphi(\mathbf{x}_i)^{\mathbf{T}}\varphi(\mathbf{x}_j)$ can be cumbersome.
- Mercer's theorem:

  Every semi-positive definite symmetric function is a kernel

- Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

K=

$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x}_1,\mathbf{x}_2)$	$K(\mathbf{x}_1,\mathbf{x}_3)$	…	$K(\mathbf{x}_1,\mathbf{x}_n)$
$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_n)$
…	…	…	…	…
$K(\mathbf{x}_n,\mathbf{x}_1)$	$K(\mathbf{x}_n,\mathbf{x}_2)$	$K(\mathbf{x}_n,\mathbf{x}_3)$	…	$K(\mathbf{x}_n,\mathbf{x}_n)$

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): $K(\mathbf{x}_i,\mathbf{x}_j) = e^{-\frac{\|\mathbf{x}_i-\mathbf{x}_j\|^2}{2\sigma^2}}$
  - 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 $\alpha_1 \dots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$ 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

Overfitting

- Huge feature space with kernels, what about overfitting???
  - Maximising margin leads to sparse set of support vectors
  - Some interesting theory says that SVMs search for simple hypothesis with large margin
  - Often robust to overfitting

Summary

- SVM advantages
  - Efficient QP learning
  - Sparse
- SVM disadvantages
  - Not probabilistic
  - Do not directly handle multi-class problems
  - QP might struggle in very large datasets