INTRODUCTION TO MACHINE LEARNING

SUPPORT VECTOR MACHINE

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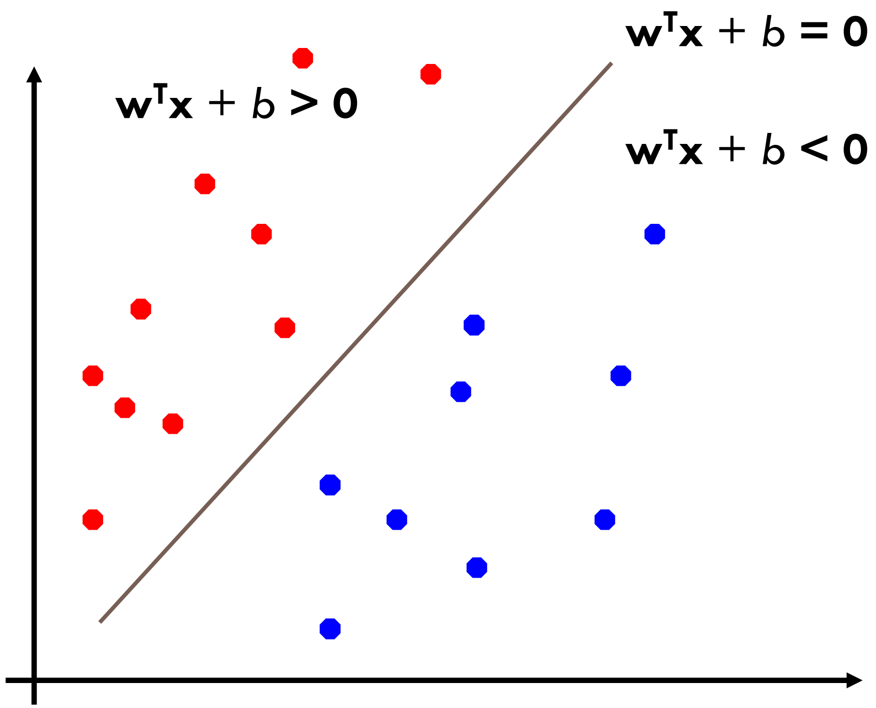
Linear Separators

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



Discriminant function:

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

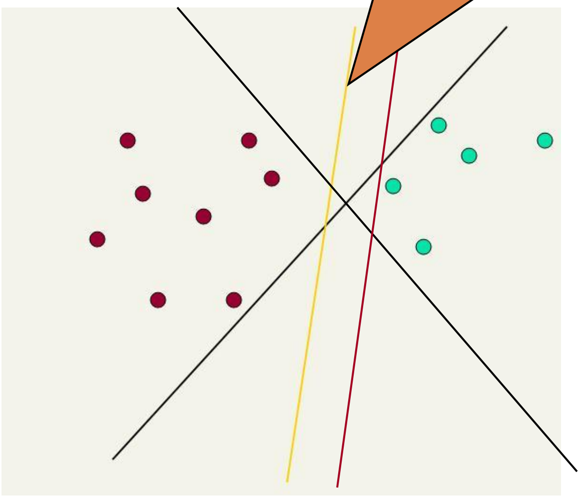
w: weight vector, normal to the line

b: bias

Linear classifiers: Which Hyperplane?

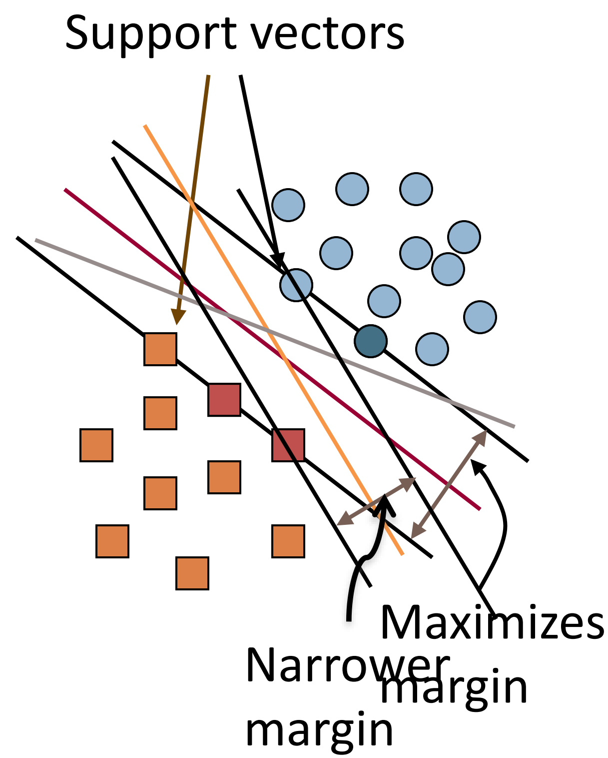
- Lots of possible choices for *a*, *b*, *c*.
- A Support Vector Machine (SVM) finds an optimal* solution.
  - Maximizes the distance between the hyperplane and the "difficult points" close to decision boundary
  - One intuition: if there are no points near the decision surface, then there are no very uncertain classification decisions

This line represents the decision boundary:
$ax + by - c = 0$



Support Vector Machine (SVM)

- SVMs maximize the *margin* around the separating hyperplane.
  - A.k.a. large margin classifiers
- The decision function is fully specified by a subset of training samples, *the support vectors.*
- Solving SVMs is a *quadratic programming* problem

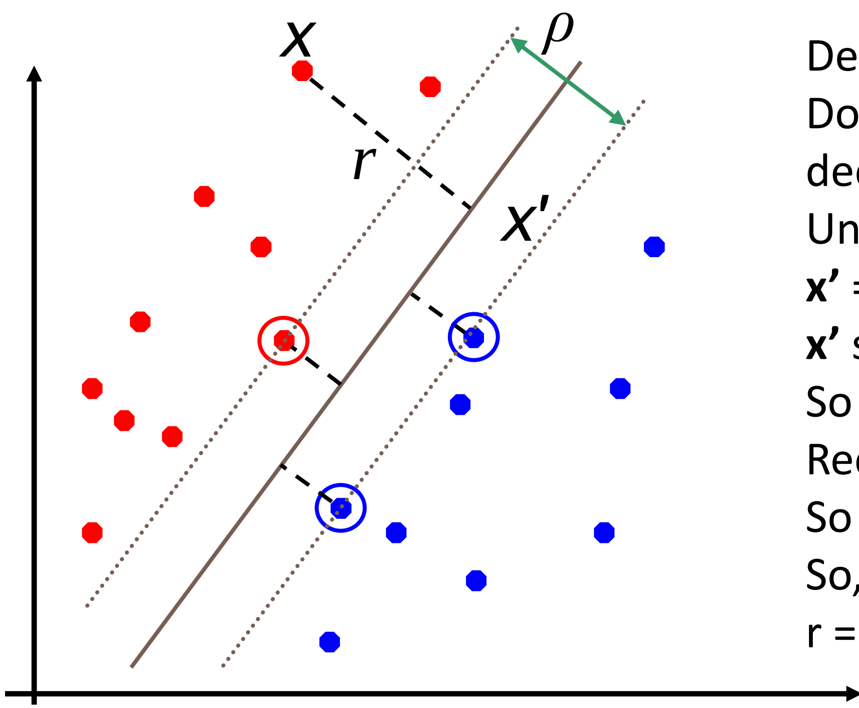


Maximum Margin: Formalization

- **w**: decision hyperplane normal vector
- $\mathbf{x}_i$: data point *i*
- y_i: class of data point *i* (+1 or -1)
- Classifier is: $f(\mathbf{x}_i) = \text{sign}(\mathbf{w}^T\mathbf{x}_i + b)$
- Functional margin of $\mathbf{x}_i$ is: $y_i\,(\mathbf{w}^T\mathbf{x}_i + b)$
- The functional margin of a dataset is twice the minimum functional margin for any point
  - The factor of 2 comes from measuring the whole width of the margin
- **Problem:** we can increase this margin simply by scaling **w**, **b**….

Geometric Margin

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



Derivation of finding *r:*
Dotted line **x’** − **x** is perpendicular to decision boundary so parallel to **w**.
Unit vector is **w**/|**w**|, so line is r**w**/|**w**|.
x’ = **x** – yr**w**/|**w**|.
x’ satisfies $\mathbf{w}^T\mathbf{x}'$ + b = 0.
So $\mathbf{w}^T(\mathbf{x} - yr\mathbf{w}/|\mathbf{w}|) + b = 0$
Recall that |**w**| = sqrt($\mathbf{w}^T\mathbf{w}$).
So $\mathbf{w}^T\mathbf{x} - yr|\mathbf{w}| + b = 0$
So, solving for r gives:
$r = y(\mathbf{w}^T\mathbf{x} + b)/|\mathbf{w}|$

Linear SVM Mathematically

The linearly separable case

- Assume that the functional margin of each data item is at least 1, then the following two constraints follow for a training set $\{(\mathbf{x_i}, y_i)\}$

$$\mathbf{w^T x_i} + b \geq 1 \quad \text{if } y_i = 1$$

$$\mathbf{w^T x_i} + b \leq -1 \quad \text{if } y_i = -1$$

- For support vectors, the inequality becomes an equality
- Then, since each example's distance from the hyperplane is

$$r = y\frac{\mathbf{w}^T\mathbf{x} + b}{\|\mathbf{w}\|}$$

- The functional margin is:

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

Linear Support Vector Machine (SVM)

- **Hyperplane**

  $\mathbf{w}^T \mathbf{x} + b = 0$

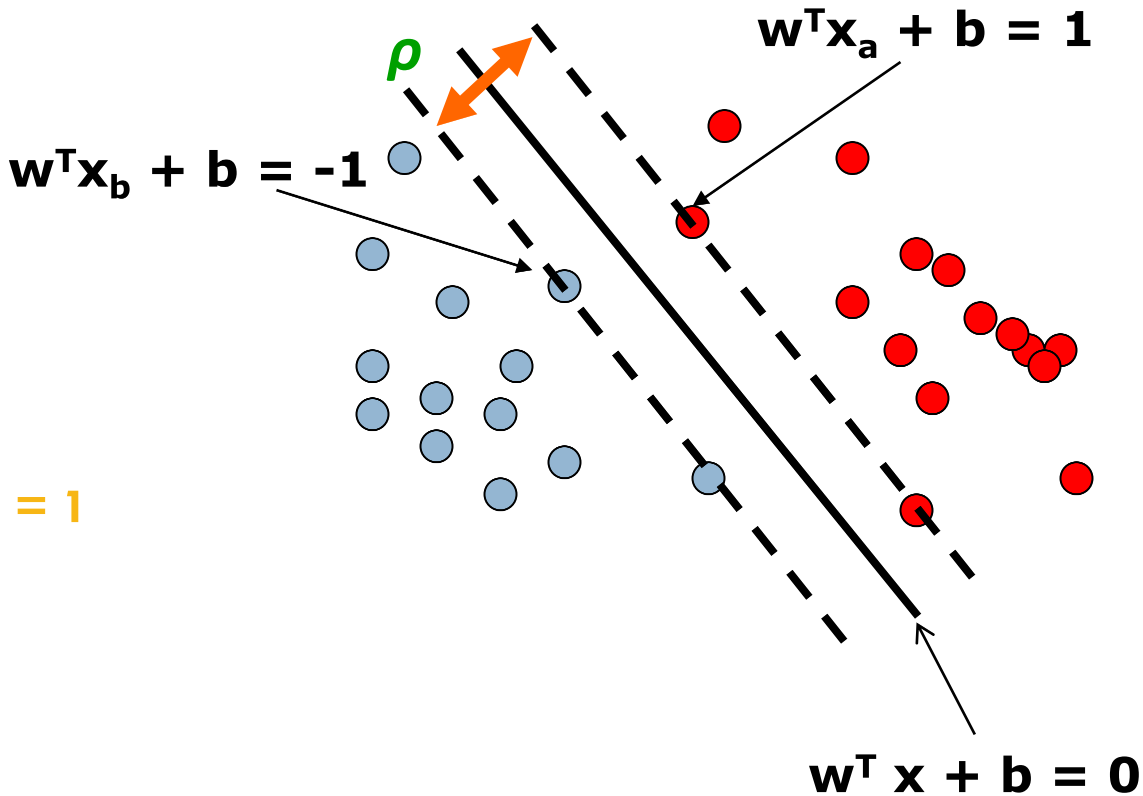
- **Extra scale constraint:**

  $\min_{i=1,\ldots,n} |\mathbf{w}^T\mathbf{x}_i + \mathbf{b}| = 1$

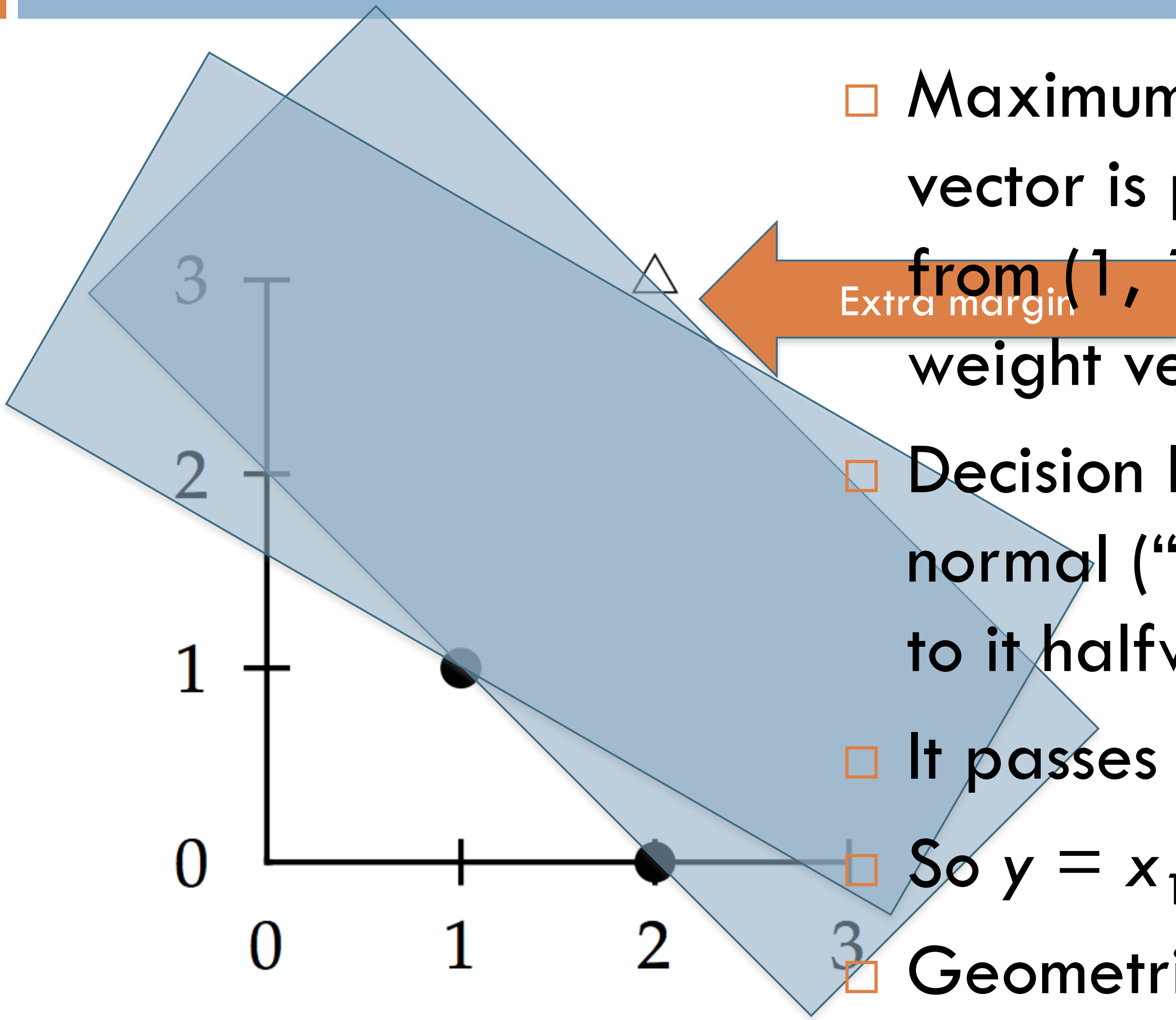
- This implies:

  $w^T(x_a - x_b) = 2$

  $\rho = \|x_a - x_b\|_2 = 2/\|\mathbf{w}\|_2$

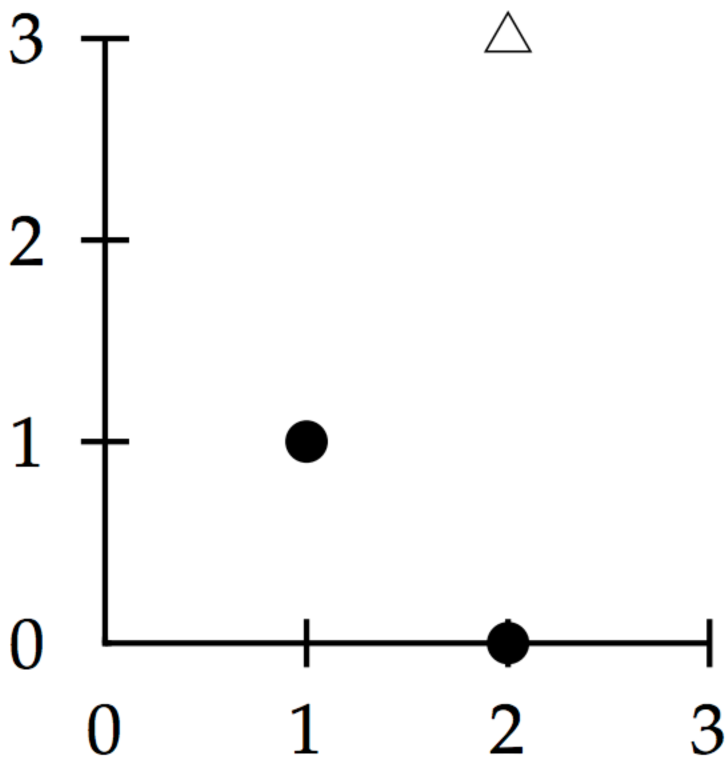


Worked example: Geometric margin



- Maximum margin weight vector is parallel to line from (1, 1) to (2, 3). So weight vector is (1, 2).
- Decision boundary is normal ("perpendicular") to it halfway between.
- It passes through (1.5, 2)
- So $y = x_1 + 2x_2 - 5.5$
- Geometric margin is $\sqrt{5}$

Worked example: Functional margin



- Let's minimize w given that $y_i(w^T x_i + b) \geq 1$
- Constraint has = at SVs; $w = (a, 2a)$ for some a
- $a+2a+b = -1$ $2a+6a+b = 1$
- So, $a = 2/5$ and $b = -11/5$
  Optimal hyperplane is: $w = (2/5, 4/5)$ and $b = -11/5$
- Margin ρ is $2/|w|$
  $= 2/\sqrt{(4/25+16/25)}$
  $= 2/(2\sqrt{5}/5) = \sqrt{5}$

Linear SVMs Mathematically (cont.)

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

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

$r = \dfrac{2}{\|\mathbf{w}\|}$ is maximized; and for all $\{(\mathbf{x_i}, y_i)\}$

$\mathbf{w}^T\mathbf{x_i} + b \geq 1$ if $y_i = 1$; $\mathbf{w}^T\mathbf{x_i} + b \leq -1$ if $y_i = -1$

- A better formulation (min $\|\mathbf{w}\|$ = max $1/\|\mathbf{w}\|$):

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

$\mathbf{\Phi}(\mathbf{w}) = \frac{1}{2}\,\mathbf{w}^T\mathbf{w}$ is minimized;

and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i\,(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

Solving the Optimization Problem

Find $\mathbf{w}$ and b such that
$\boldsymbol{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^T\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w^T x_i} + b) \geq 1$

- This is now optimizing a *quadratic* function subject to *linear* constraints
- Quadratic optimization problems are a well-known class of mathematical programming problem, and many (intricate) algorithms exist for solving them (with many special ones built for SVMs)
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every constraint in the primary problem:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- The solution has the form:

$$\mathbf{w} = \Sigma \alpha_i y_i \mathbf{x_i} \qquad b = y_k - \mathbf{w^T x_k} \text{ for any } \mathbf{x_k} \text{ such that } \alpha_k \neq 0$$

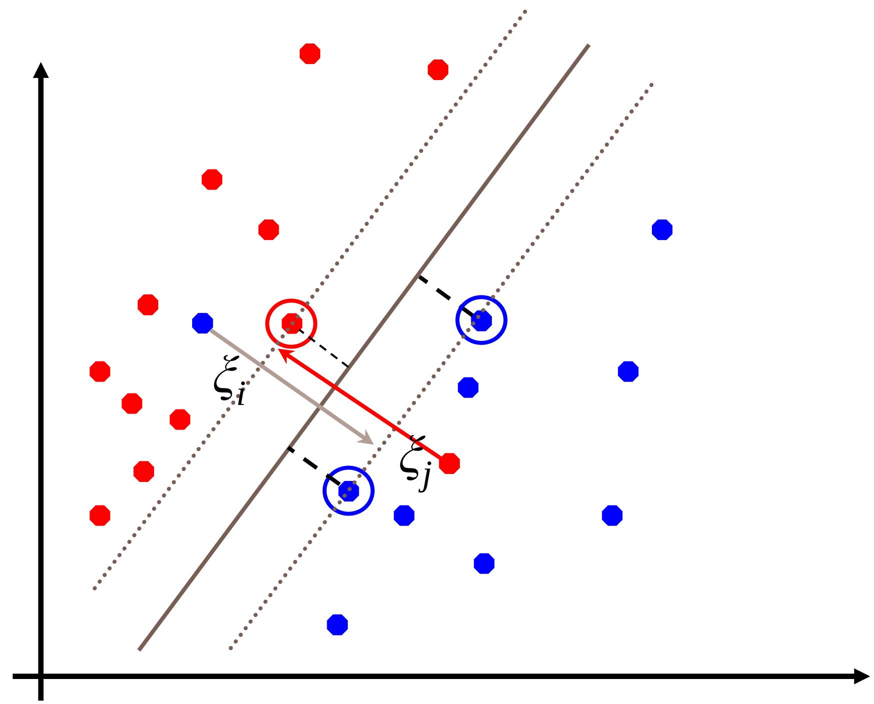
- Each non-zero α_i indicates that corresponding $\mathbf{x_i}$ is a support vector.
- Then the classifying function will have the form:

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

- Notice that it relies on an *inner product* between the test point $\mathbf{x}$ 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 pairs of training points.

Soft Margin Classification

- If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.
- Allow some errors
  - Let some points be moved to where they belong, at a cost
- Still, try to minimize training set errors, and to place hyperplane "far" from each class (large margin)



Soft Margin Classification Mathematically

- The old formulation:

> Find $\mathbf{w}$ and b such that
> $\boldsymbol{\Phi}(\mathbf{w}) = \frac{1}{2}\, \mathbf{w}^{T}\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
> $y_i\, (\mathbf{w^T x_i} + \mathrm{b}) \geq 1$

- The new formulation incorporating slack variables:

> Find $\mathbf{w}$ and b such that
> $\boldsymbol{\Phi}(\mathbf{w}) = \frac{1}{2}\, \mathbf{w}^{T}\mathbf{w} + C\Sigma\xi_i$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
> $y_i\, (\mathbf{w^T x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

- Parameter C can be viewed as a way to control overfitting
  - A regularization term

Soft Margin Classification – Solution

- The dual problem for soft margin classification:

$$
\begin{aligned}
&\text{Find } \alpha_1 \ldots \alpha_N \text{ such that} \\
&\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \tfrac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^{\mathbf{T}}\mathbf{x_j} \text{ is maximized and} \\
&(1)\ \ \Sigma\alpha_i y_i = 0 \\
&(2)\ \ 0 \leq \alpha_i \leq C \text{ for all } \alpha_i
\end{aligned}
$$

- Neither slack variables ξ_i nor their Lagrange multipliers appear in the dual problem!
- Again, $\mathbf{x_i}$ with non-zero α_i will be support vectors.
- Solution to the dual problem is:

$$
\begin{aligned}
&\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x_i} \\
&b = y_k(1-\xi_k) - \mathbf{w}^{\mathbf{T}}\mathbf{x}_k \text{ where } k = \underset{k'}{\operatorname{argmax}}\ \alpha_{k'}
\end{aligned}
$$

w is not needed explicitly for classification!

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

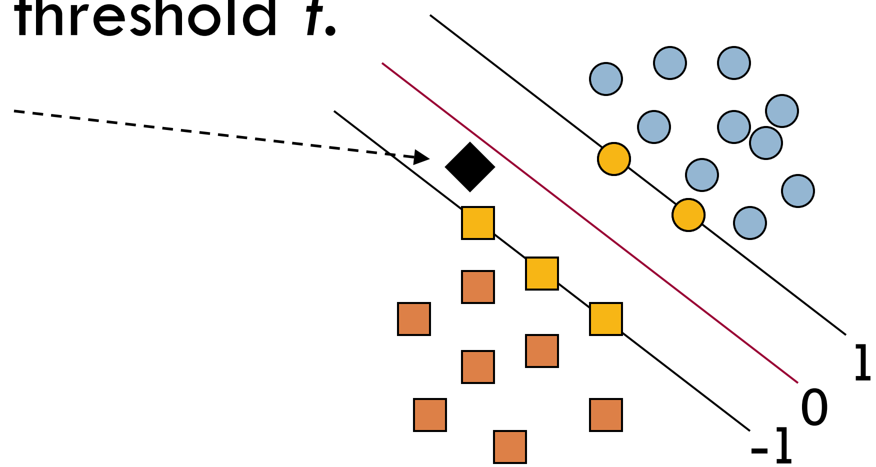
Classification with SVMs

- Given a new point **x**, we can score its projection onto the hyperplane normal:
  - I.e., compute score: $\mathbf{w}^T\mathbf{x} + b = \Sigma\alpha_i y_i \mathbf{x_i}^T\mathbf{x} + b$
    - Decide class based on whether < or > 0
  - Can set confidence threshold *t*.

Score > *t*: yes

Score < -*t*: no

Else: don't know



Linear SVMs: Summary

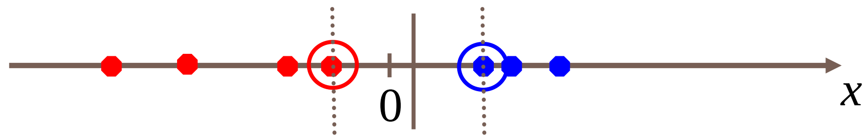
- The classifier is a *separating hyperplane.*
- The most "important" training points are the support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the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

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

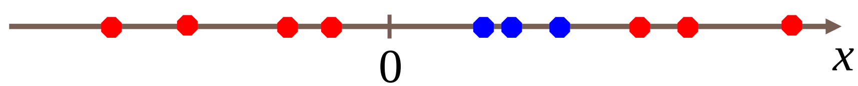
$$f(\mathbf{x}) = \Sigma\alpha_i y_i \boxed{\mathbf{x_i}^{\mathbf{T}}\mathbf{x}} + b$$

Non-linear SVMs

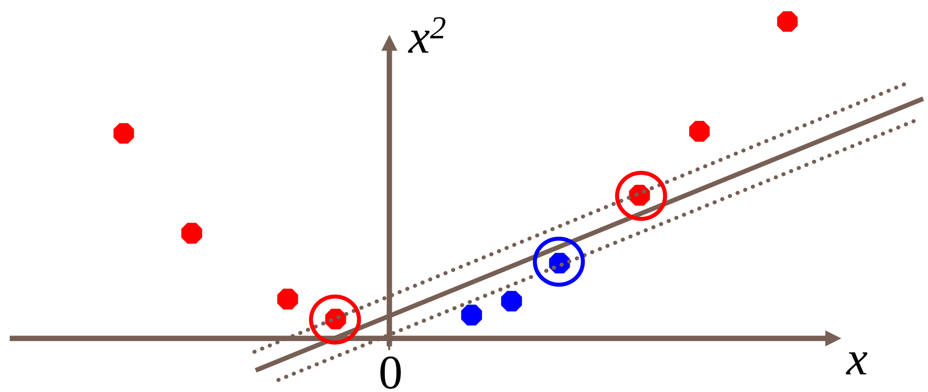
- Datasets that are linearly separable (with some noise) work out great:



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

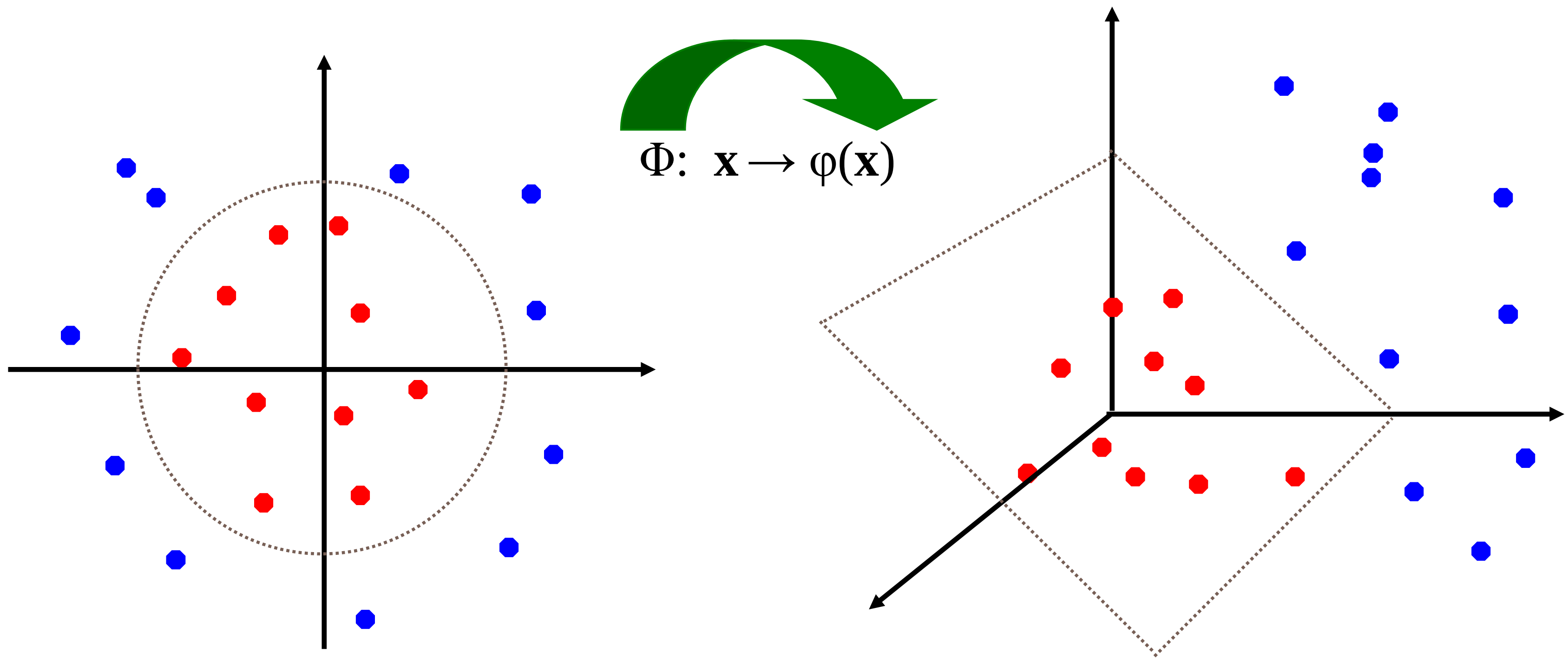


- How about … mapping data to a higher-dimensional space:



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:



Non-linear SVMs: Feature spaces

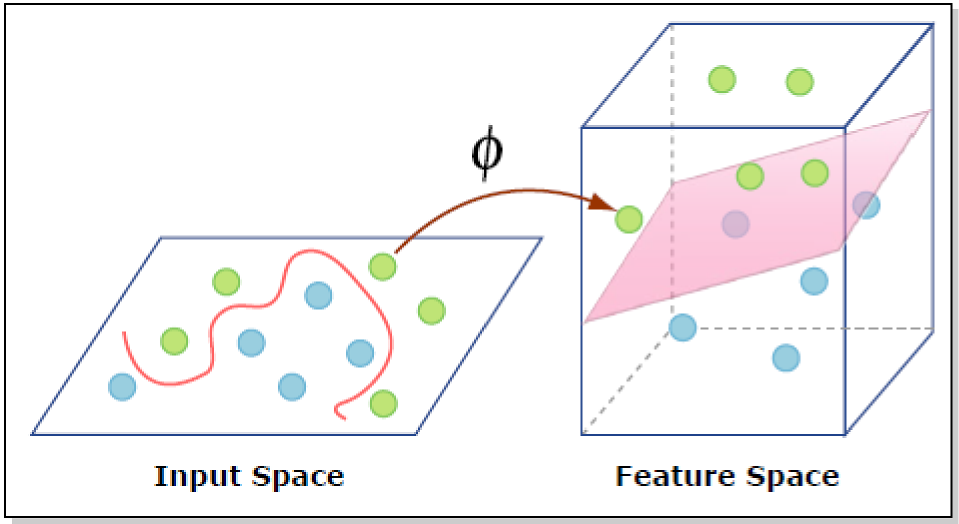


Image by MIT OpenCourseWare.

The “Kernel Trick”

- The linear classifier relies on an 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: $\mathbf{x} \rightarrow \phi(\mathbf{x})$, the inner product becomes:

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

- A *kernel function* is some function that corresponds to an inner product in some expanded 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 $K(\mathbf{x}_i,\mathbf{x}_j)= \phi(\mathbf{x}_i)^{\mathbf{T}}\phi(\mathbf{x}_j)$:

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

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

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

Kernels

- Why use kernels?
  - Make non-separable problem separable.
  - Map data into better representational space
- Common kernels
  - Linear
  - Polynomial **$K(x,z) = (1+x^T z)^d$**
    - Gives feature conjunctions
  - Radial basis function (infinite dimensional space)

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