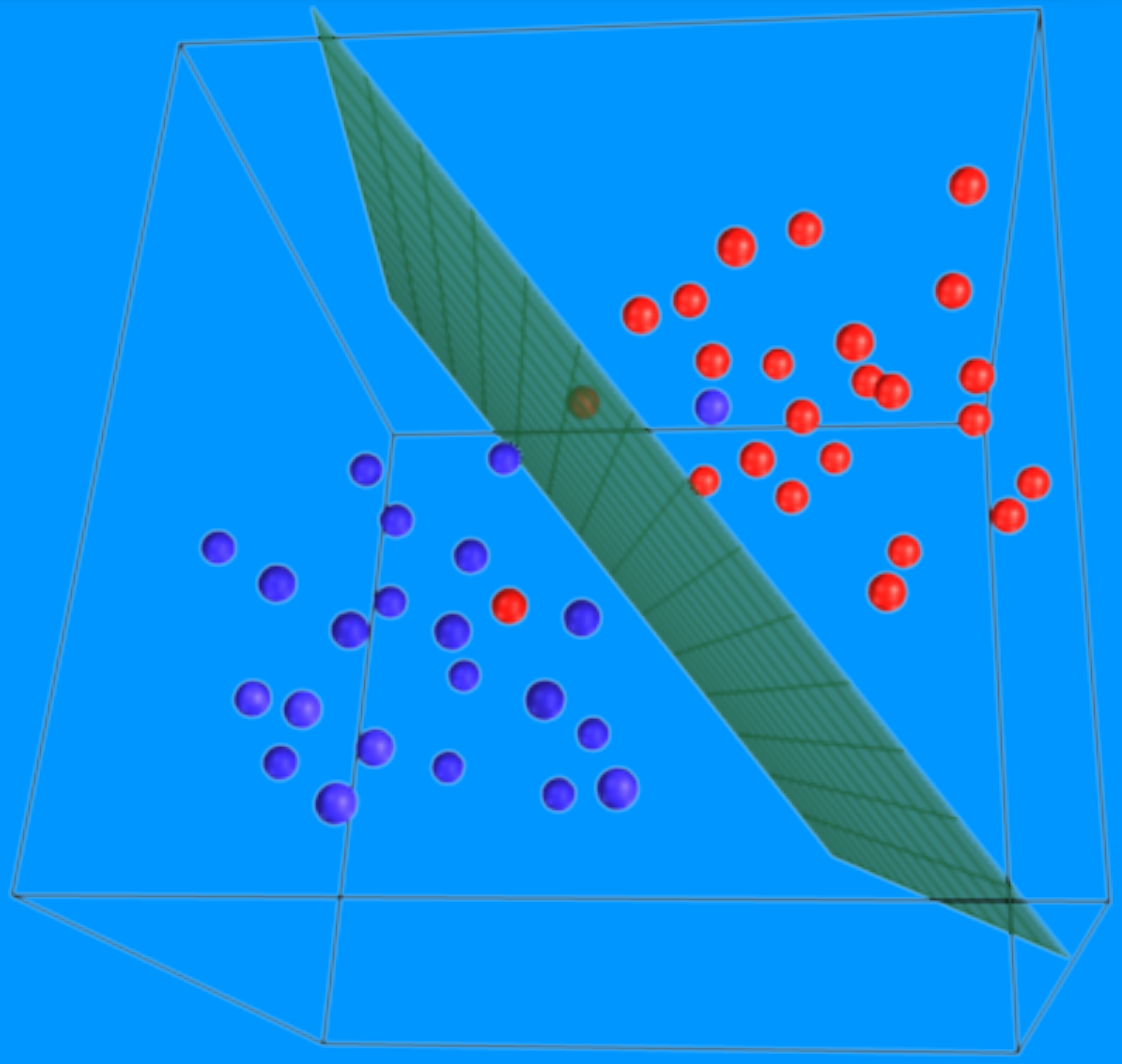
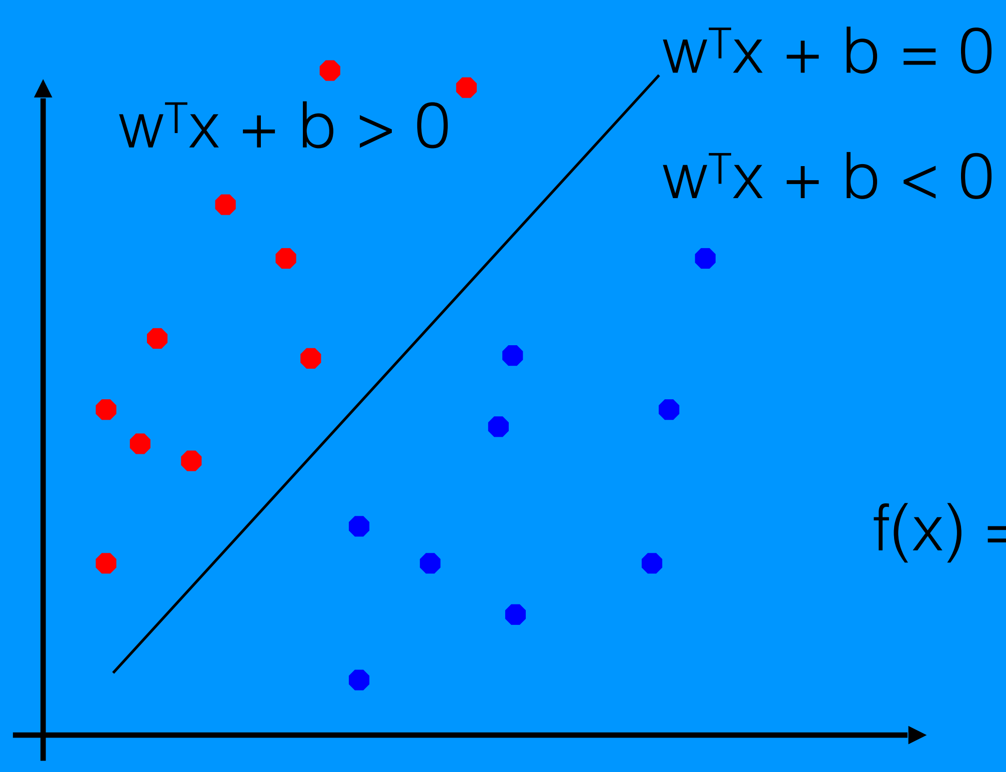
Support Vector Machines





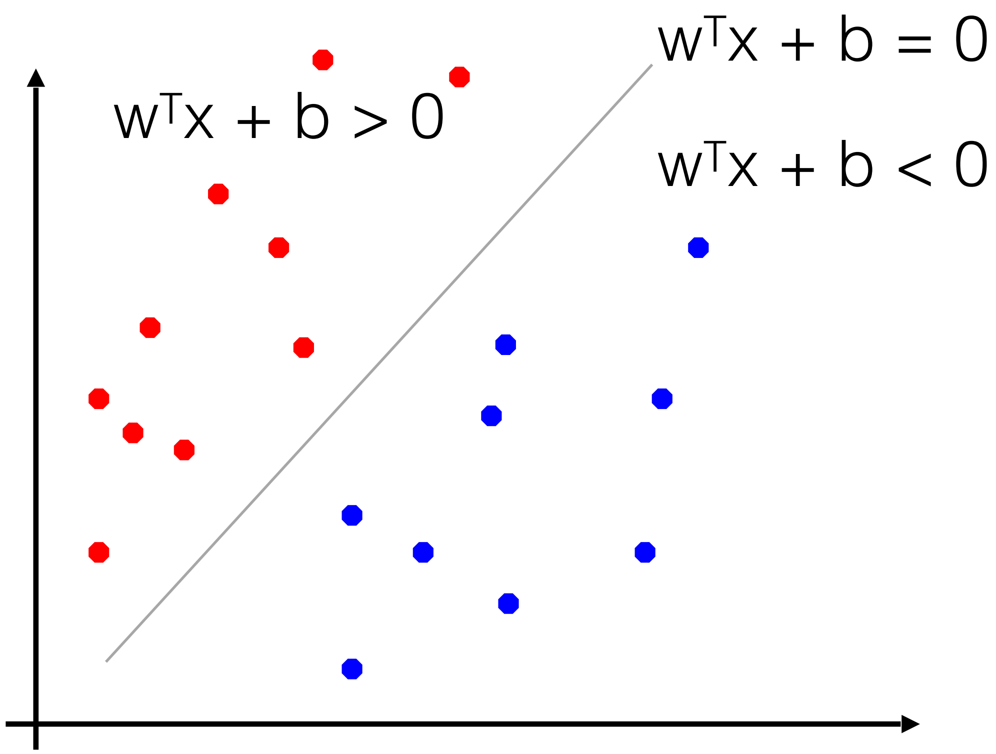
$f(x) = \text{sign}(w^Tx + b)$

Instructor

Mousum Dutta
Chief Data Scientist, Spotle.ai
Computer Science, IIT KGP

Perceptron Revisited: Linear Separators

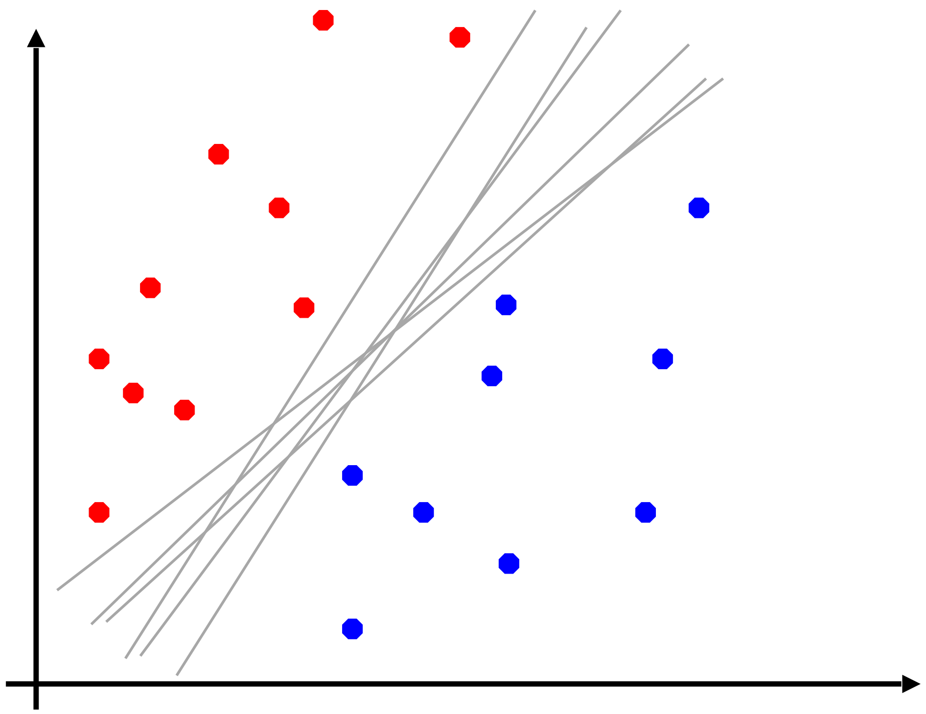
Binary classification can be viewed as the task of separating classes in feature space:



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

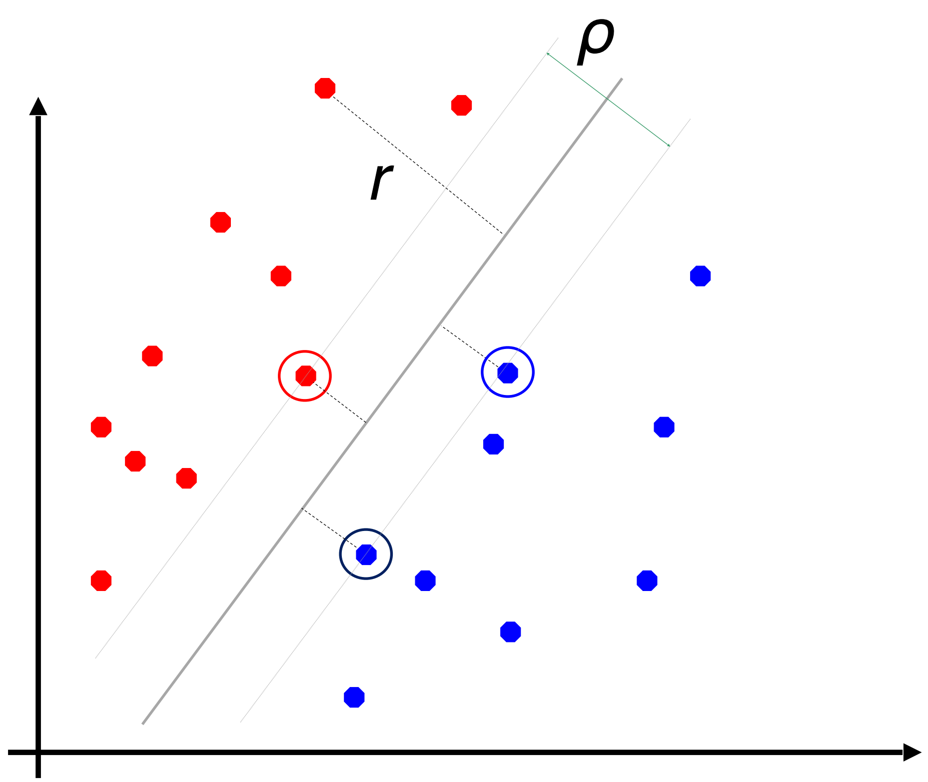
Linear Separators

Which of the linear separators is optimal?



Classification Margin

- Distance from example 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.



Linear SVM Mathematically

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

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

- For every support vector $\mathbf{x}_s$ the above inequality is an equality. After rescaling **w** and **b** by **ρ/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) **w** and **b** as:

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

Linear SVM Mathematically

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

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

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

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

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

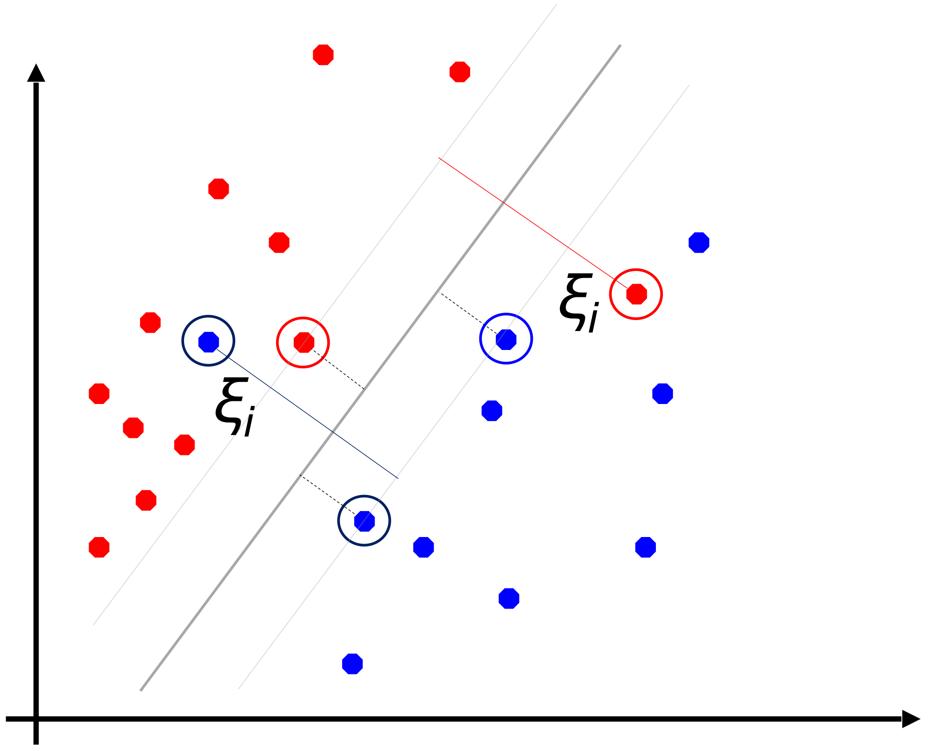
- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.
- Then the classifying function is (note that we don't need **w** explicitly):

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

- 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 $\mathbf{x}_i^{\mathsf{T}}\mathbf{x}_j$ 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
$\mathbf{\Phi(w)} = \mathbf{w}^T\mathbf{w}$ 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 $\mathbf{w}$ and b such that
$\mathbf{\Phi(w)} = \mathbf{w}^T\mathbf{w} + C\Sigma\xi_i$ 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.

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):

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

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

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

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

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

Justification for Maximum Margins

- Vapnik has proved the following:

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

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

  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

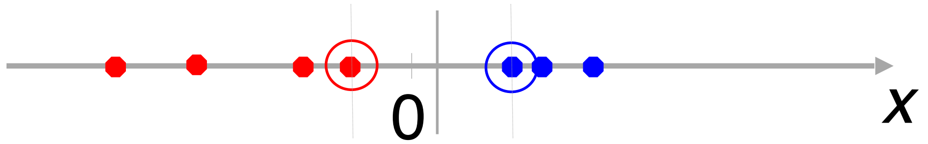
- The classifier is a separating hyperplane.
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation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

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

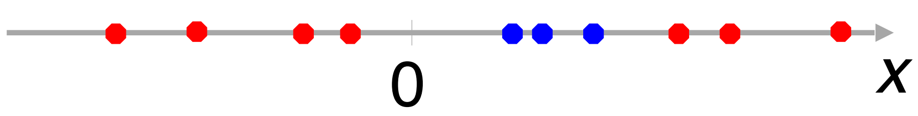
$f(\mathbf{x}) = \Sigma\alpha_i y_i \boxed{\mathbf{x}_i^T\mathbf{x}} + b$

Non-linear SVMs

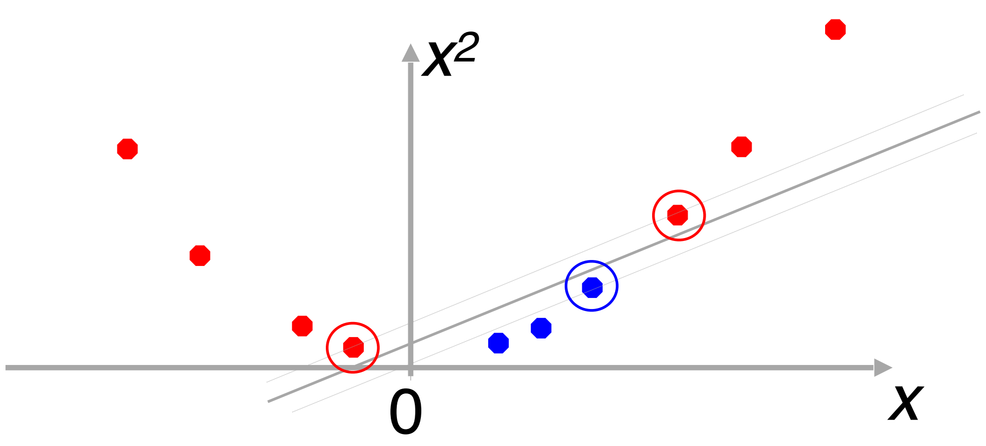
- Datasets that are linearly separable with some noise work out great:



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

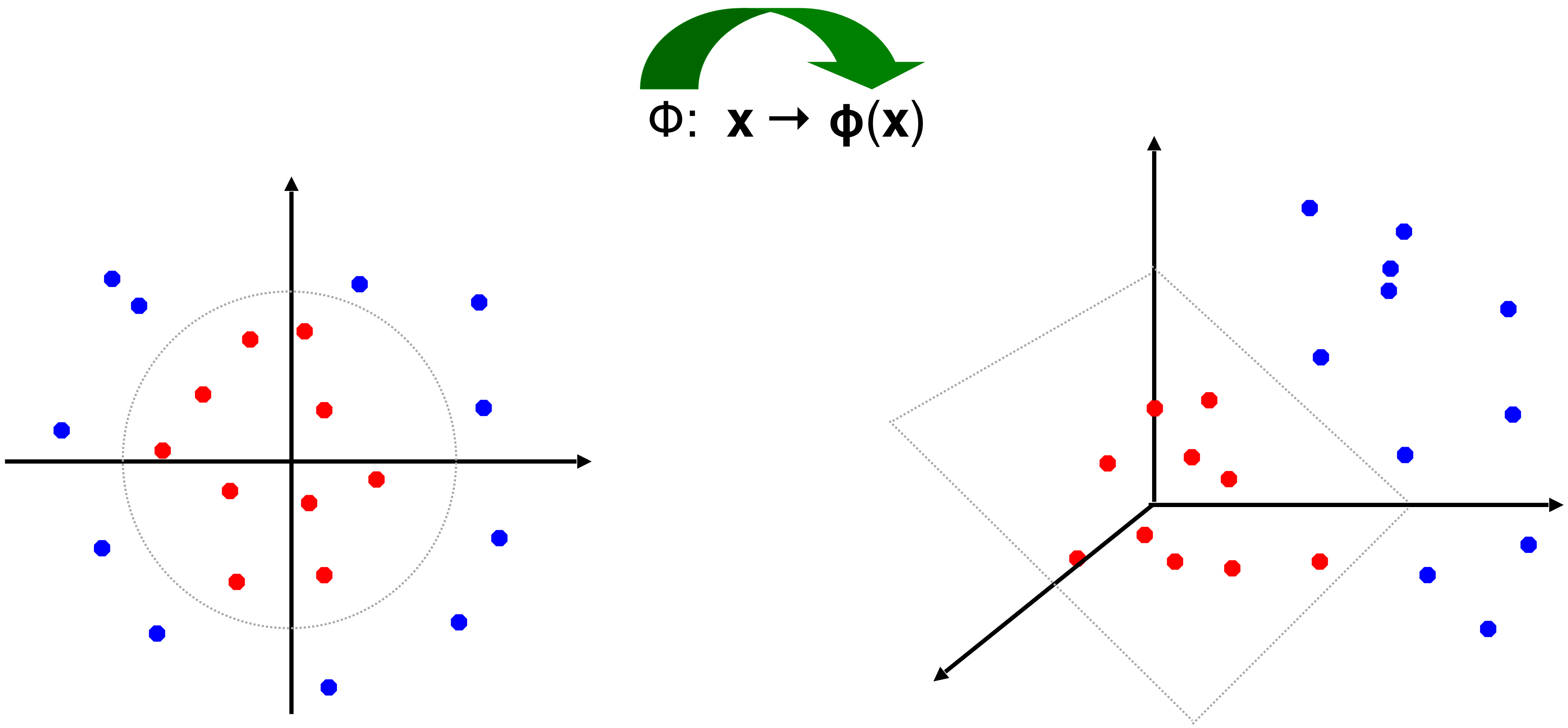


- How about… mapping data to a higher-dimensional space:



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 $K(x_i,x_j) = x_i^T x_j$
- If every data point is mapped into high-dimensional space via some transformation Φ: $x \rightarrow \phi(x)$, the inner product becomes:

$$K(x_i,x_j) = \phi(x_i)^T \phi(x_j)$$

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

The "Kernel Trick"

- Example:

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

We need to show that $K(\mathbf{x}_i,\mathbf{x}_j) = \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$

$$
\begin{aligned}
K(\mathbf{x}_i,\mathbf{x}_j) &= (1 + \mathbf{x}_i^T\mathbf{x}_j)^2 \\
&= 1 + x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2} + x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} \\
&= [1 \;\; x_{i1}^2 \;\; \sqrt{2}\, x_{i1}x_{i2} \;\; x_{i2}^2 \;\; \sqrt{2}x_{i1} \;\; \sqrt{2}x_{i2}]^T [1 \;\; x_{j1}^2 \;\; \sqrt{2}\, x_{j1}x_{j2} \;\; x_{j2}^2 \;\; \sqrt{2}x_{j1} \;\; \sqrt{2}x_{j2}] \\
&= \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j), \quad \text{where } \phi(\mathbf{x}) = [1 \;\; x_1^2 \;\; \sqrt{2}\, x_1x_2 \;\; x_2^2 \;\; \sqrt{2}x_1 \;\; \sqrt{2}x_2]
\end{aligned}
$$

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

What Functions are Kernels?

- It may be cumbersome to check that $K(x_i,x_j)= \phi(x_i)^T\phi(x_j)$ for some functions $K(x_i,x_j)$.
- **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: $K(x_i,x_j)= x_i^T x_j$
  - Mapping Φ: $x \rightarrow \phi(x)$, where $\phi(x)$ is x itself
- Polynomial of power p: $K(x_i,x_j)= (1+ x_i^T x_j)^p$
  - Mapping Φ: $x \rightarrow \phi(x)$, where $\phi(x)$ has $\binom{d+p}{p}$ dimensions
- Gaussian (radial-basis function): $K(x_i,x_j) = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}}$
  - Mapping Φ: $x \rightarrow \phi(x)$, where $\phi(x)$ 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
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$ 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 History

- 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.
- 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.