Support Vector Machines

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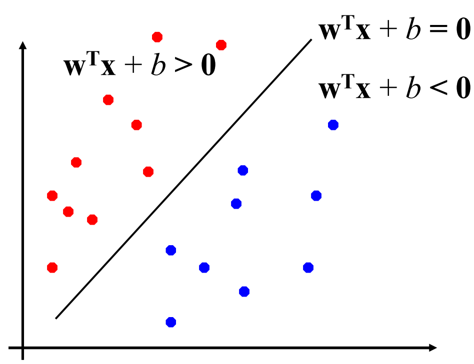
Perceptron Revisited: Linear Separators

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



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

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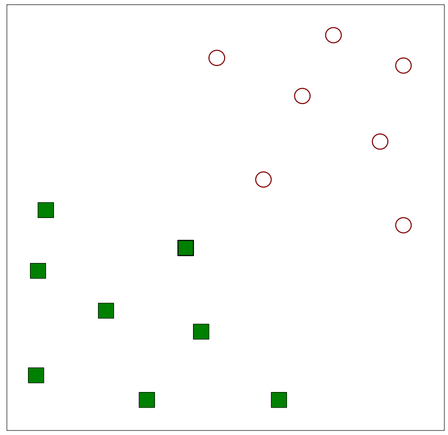
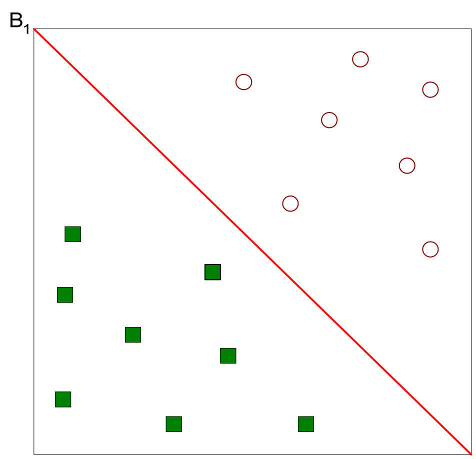


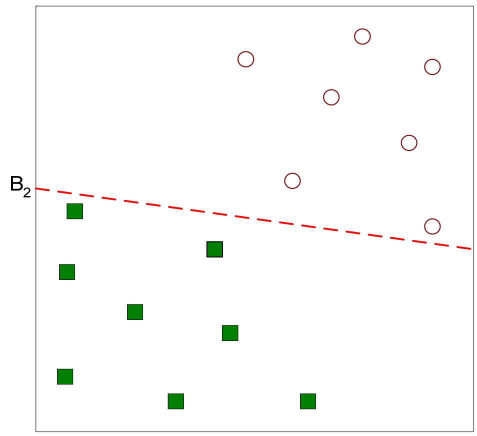
- Find a linear hyperplane (decision boundary) that will separate the data

Support Vector Machines



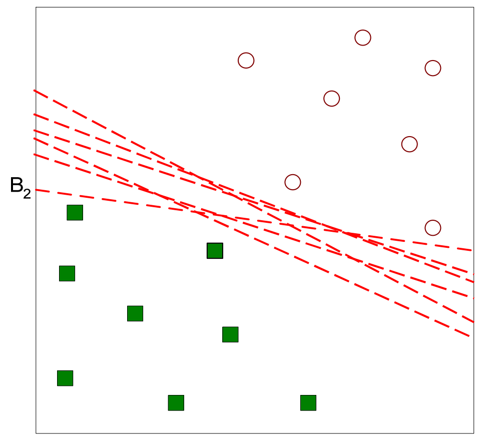
- One Possible Solution

Support Vector Machines



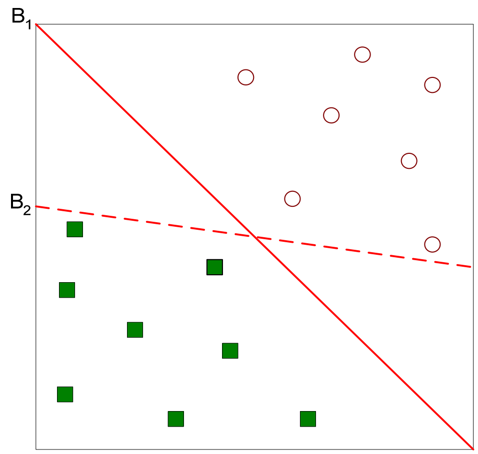
- Another possible solution

Support Vector Machines



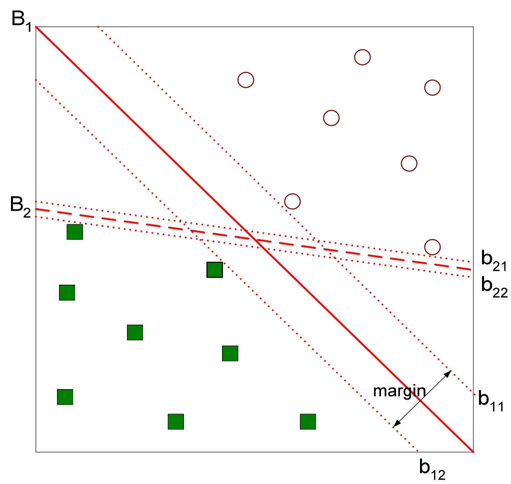
- Other possible solutions

Support Vector Machines



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

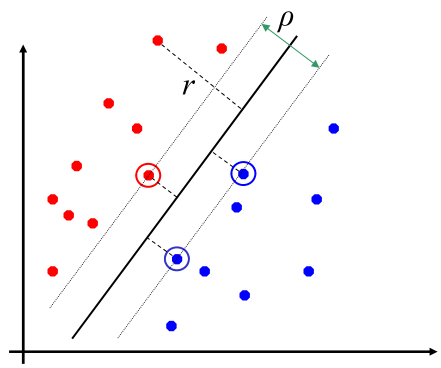
Support Vector Machines



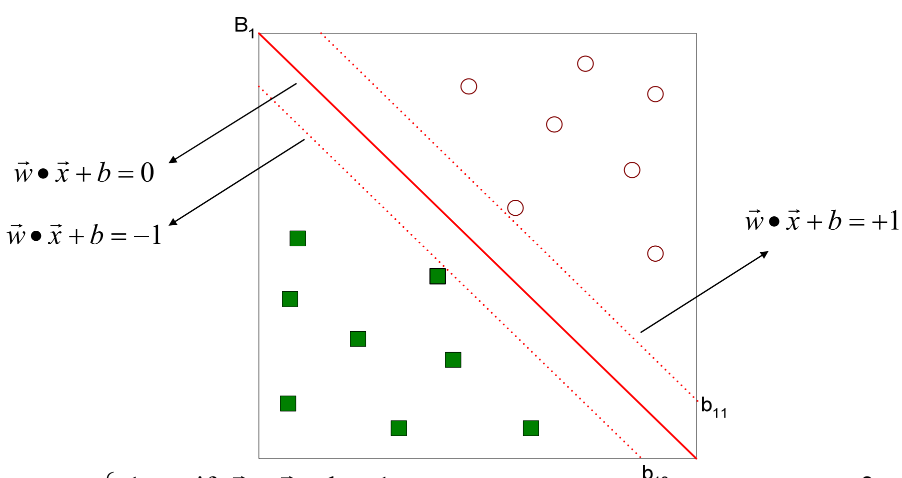
- Find hyperplane maximizes the margin => B1 is better than B2

Classification Margin

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



Support Vector Machines

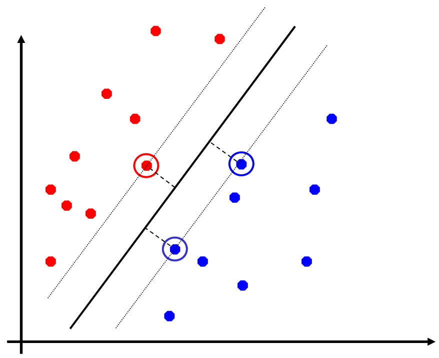


$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w}\bullet\vec{x}+b \ge 1 \\ -1 & \text{if } \vec{w}\bullet\vec{x}+b \le -1 \end{cases}$$

$$\text{Margin} = \frac{2}{\|\vec{w}\|}$$

Maximum Margin Classification

- Maximizing the margin is good according to intuition and PAC theory.
- Implies that only support vectors matter; other training examples are ignorable.



Support Vector Machines

- We want to maximize: $\text{Margin} = \dfrac{2}{\|\vec{w}\|}$
  - Which is equivalent to minimizing: $L(w) = \dfrac{\|\vec{w}\|^2}{2}$
  - But subjected to the following constraints:

$$f(\vec{x}_i) = \begin{cases} 1 & \text{if } \vec{\mathrm{w}} \bullet \vec{\mathrm{x}}_i + \mathrm{b} \geq 1 \\ -1 & \text{if } \vec{\mathrm{w}} \bullet \vec{\mathrm{x}}_i + \mathrm{b} \leq -1 \end{cases}$$

- This is a constrained optimization problem
  - Numerical approaches to solve it (e.g., quadratic programming)

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

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

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

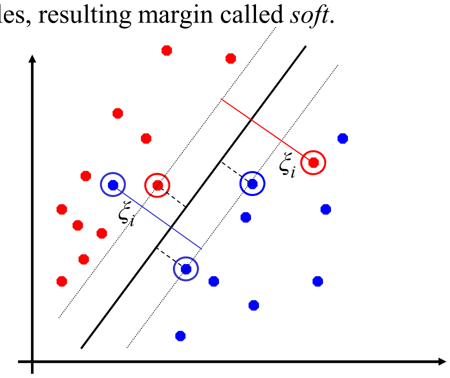
- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.
- Then the classifying function is (note that we don't need $\mathbf{w}$ explicitly):

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

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

- Modified formulation incorporates slack variables:

  Find **w** and b such that
  $\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w} + C\Sigma\xi_i$ 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):

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

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

Again, we don't need to compute $\mathbf{w}$ explicitly for classification:

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

Linear SVMs: Overview

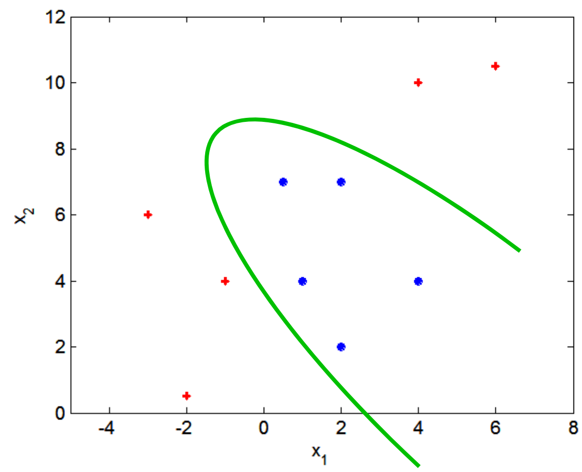
- The classifier is a *separating hyperplane.*
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation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

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

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

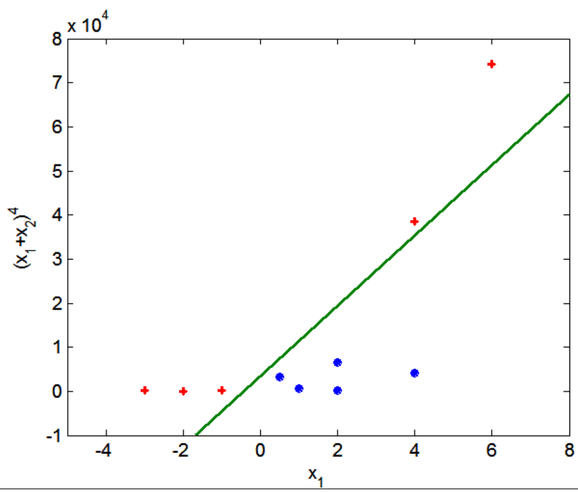
Nonlinear Support Vector Machines

- What if decision boundary is not linear?



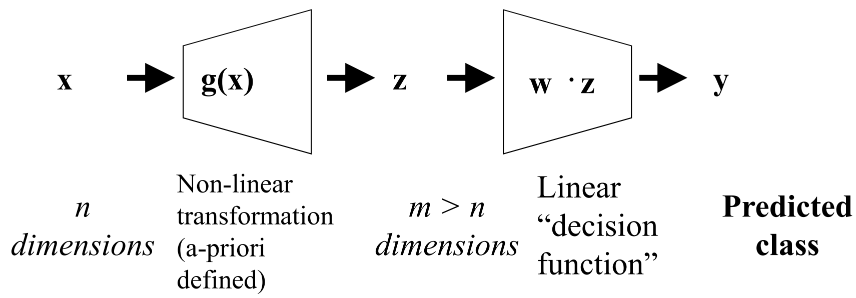
Nonlinear Support Vector Machines

- Transform data into higher dimensional space



What about the non-linear case?

- What if the classes are not linearly separable?
- Transform instances by introducing nonlinear combination "pseudo-attributes"



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: $\mathbf{x} \to \varphi(\mathbf{x})$, 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 eiquivalent to an inner product in some feature space.
- Example:

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

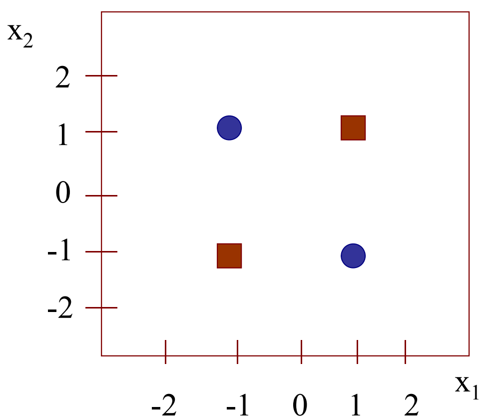
  Need to show that $K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$:

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

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

Exclusive-or problem

- A prototypical difficult case



Index i	x	y (class)
1	(1,1)	1
2	(1,-1)	-1
3	(-1,-1)	1
4	(-1,1)	-1

■ = class 1

● = class -1

Exclusive-or problem

- Not linearly separable in the input space
  - Needs a non-linear transformation
  - Recall decision tree for exclusive or
    - Maximal subtree repetition!
  - Overfitting a big danger
    - Handle each instance as a separate case
- Transform space by

$$H(x, x') = [(x \cdot x') + 1]^2$$

to get

$$[x_1^2 + x_2^2 + 1]^2$$

Solution

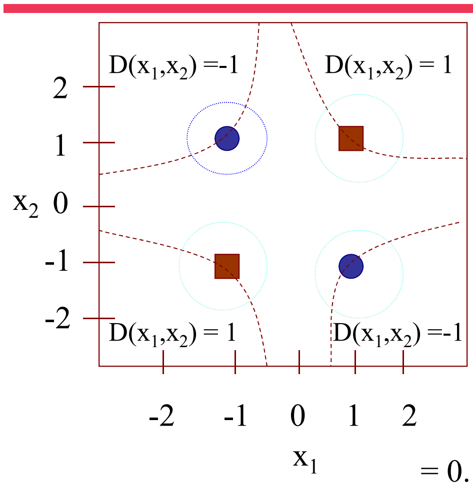
- The solution to the quadratic optimization problem is

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0.125$$

- All the points are support vectors
- The “decision function” is

$$D(\mathbf{x}) = (0.125)\, \Sigma_{i=1}^{4}\; y_i\, [\, (\mathbf{x_i} \cdot \mathbf{x}) + 1]^2$$

Solution



Decision on (1,1):

$$0.125(-1([-1\ 1]\begin{bmatrix}1\\1\end{bmatrix}+1)^2$$

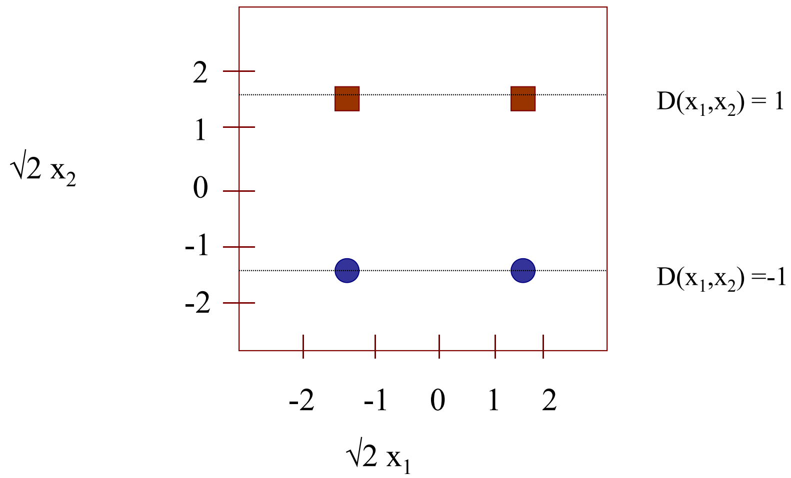
$$+1([1\ 1]\begin{bmatrix}1\\1\end{bmatrix}+1)^2$$

$$+(1([-1\ -1]\begin{bmatrix}1\\1\end{bmatrix}+1)^2\ \ )$$

$$+(-1([1\ -1]\begin{bmatrix}1\\1\end{bmatrix}+1)^2)))$$

$$= 0.125\,(-1 + 9 + 1 - 1) = 0.125(8) = 1$$

Transformed Space



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 $\alpha_1 \ldots \alpha_n$ 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!

Sparse data

- Sparse data has mostly 0 values
- SVM algorithms can be sped up dramatically on sparse data
  - Lots of dot products are 0
  - Iterate over the values that are not zero
- SVM algorithms can handle sparse datasets with tens of thousands of attributes

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.