SUPPORT VECTOR MACHINES

Concha Bielza, Pedro Larrañaga

Computational Intelligence Group
Departmento de Inteligencia Artificial
Universidad Politécnica de Madrid

Machine Learning

Outline

Outline

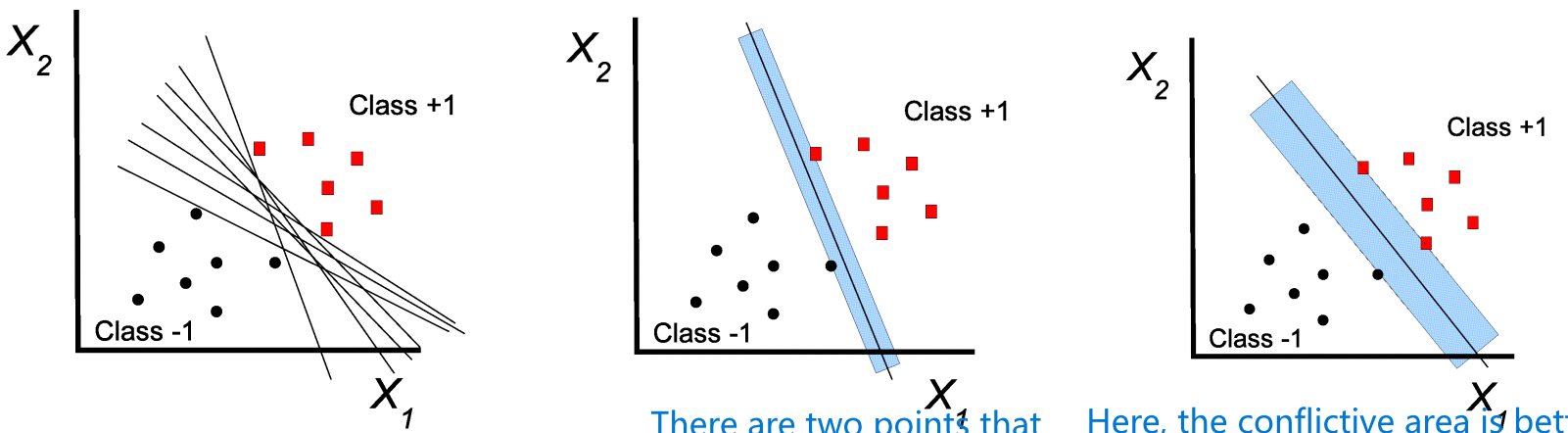
Motivation: linear SVM

- Data set $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$
- Assume $c^i \in \Omega_C = \{-1, 1\}$ and data is linearly separable:

We are looking for a hyperplane that separates the two classes

We work in a vectorial space

(a) (b) (c)



There are two points that are very close to the line

Here, the conflictive area is better
conflictive -> this separation is better -
we take the one with the bigger margi
The margin is the space between the line and the closest point

(a) Infinite possible separating lines

(b) Margin $\rightarrow$ width that the line can be increased before hitting a data point

(c) Simplest (linear) SVM $\rightarrow$ the linear classifier with the maximum margin

Choose the line as far as possible from the closest points –called **support vectors**– of both classes

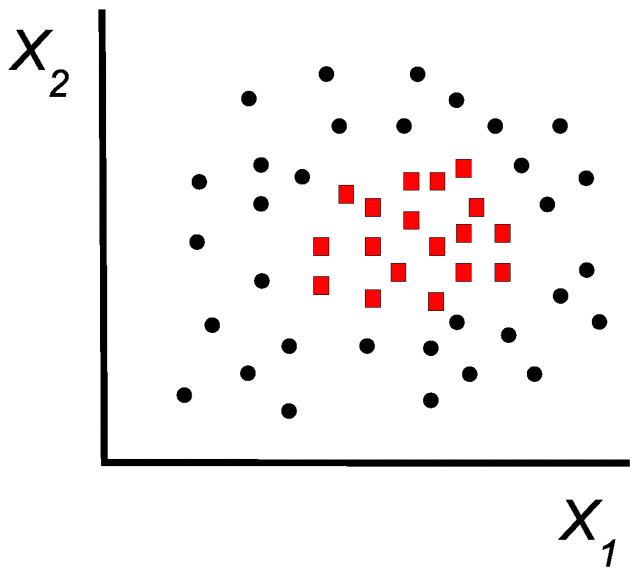
Motivation: nonlinear SVM

(a) If such linear decision boundary does not exist...??

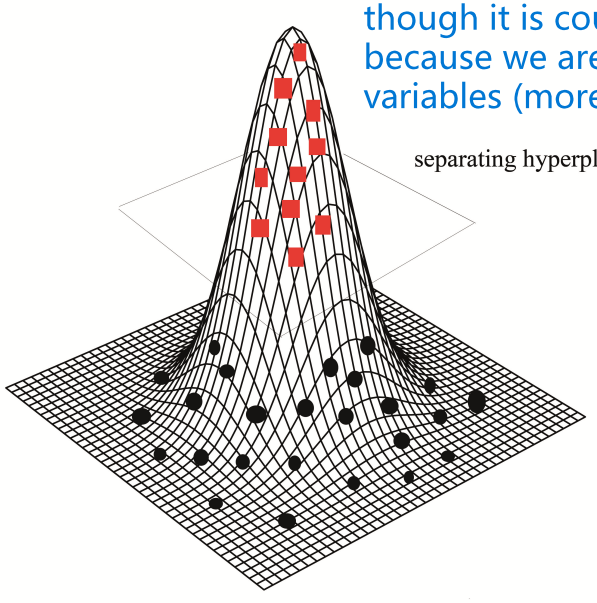
$\Rightarrow$ Solution 1) Allow a few points to be on the wrong side (by using **slack variables**)

$\Rightarrow$ Solution 2) Map the data to a much higher dimensional space where a linear decision rule is found, *see (b)*
Construct the new space via clever mathematical projection known as "kernel trick"

(a)



(b)



Solution 2 is the most general even though it is counter intuitive because we are using more variables (more dimensions)

Outline

Linearly separable data: "Hard-margin" linear SVM

- Assume linear SVM trained on linearly separable data, i.e.,
  - There exists a hyperplane $\mathcal{H}$: $\mathbf{w}^T\mathbf{x} + b = 0$ which separates positive from negative instances
- The distance d between two parallel hyperplanes, $\mathbf{w}^T\mathbf{x} + b_1 = 0$ and $\mathbf{w}^T\mathbf{x} + b_2 = 0$, is $d = |b_1 - b_2|/||\mathbf{w}||$: *see figure*

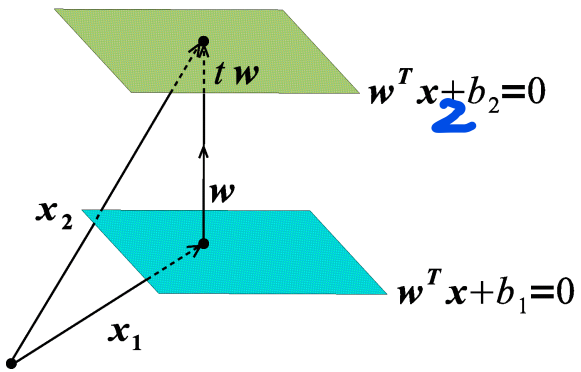
w = the normal vect

x \in R^n; b \in R

$d = |t| \cdot ||\mathbf{w}||$,
take $\mathbf{x}_1$ and $\mathbf{x}_2$, a point on each hyperplane, $\mathbf{x}_2 = \mathbf{x}_1 + t\mathbf{w} \Rightarrow$

$$0 = \mathbf{w}^T\mathbf{x}_2 + b_2 = \mathbf{w}^T(\mathbf{x}_1 + t\mathbf{w}) + b_2 = \mathbf{w}^T\mathbf{x}_1 + t||\mathbf{w}||^2 + b_2 = -b_1 + t||\mathbf{w}||^2 + b_2$$

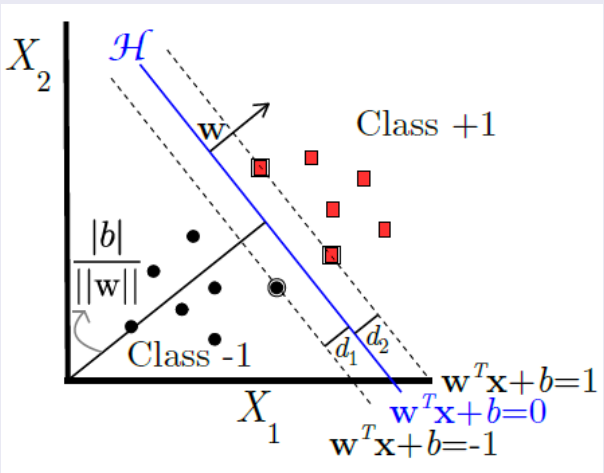
Se despeja t y se sustituye en



Linearly separable data: "Hard-margin" linear SVM

- Let d_2 (d_1) be the distance from $\mathcal{H}$ to the closest positive (negative) instance
- **Margin** of $\mathcal{H}$ is defined as $d_1 + d_2$
- Linear SVM looks for $\mathcal{H}$ with **largest margin** $\Rightarrow$ how to find it?

- Points above (below) $\mathcal{H}$ should have label 1 (-1);
  decision rule is: $\phi(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$ Over the line, when we evaluate on the hyperplane we get 0. Above >0 and below <0
- Assume $\mathbf{w}^T\mathbf{x}^i + b \geq 1$ for $c^i = +1$ and $\mathbf{w}^T\mathbf{x}^i + b \leq -1$ for $c^i = -1$
  $\Leftrightarrow c^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1, \quad i = 1, ..., N$ As many constraints as points
- For the support vectors the equality holds
- Dist. from support hyperplanes to $\mathcal{H}$ is $d_1 = d_2 = 1/||\mathbf{w}||$ $\Rightarrow$ Margin is $2/||\mathbf{w}||$



- No training points fall between the three hyperplanes
- $\mathcal{H}$ must be as far from the support vectors (+ difficult points to classify) as possible
- Support vectors: influence on the optimum location of the decision boundary; if removed, the solution changes

Primal and dual forms

- Max $\frac{2}{||\mathbf{w}||} \Leftrightarrow$ Min $\frac{1}{2}||\mathbf{w}||^2$ (allows quadratic programming optimization)

$$\text{Primal: } \min_{\mathbf{w},b} \frac{1}{2}||\mathbf{w}||^2 \quad \text{subject to} \quad 1 - c^i(\mathbf{w}^T\mathbf{x}^i + b) \leq 0, \quad \forall i = 1, ..., N \tag{1}$$

$\Rightarrow$ Solved by allocating each constraint a Lagrange multiplier or dual variable $\lambda_i \geq 0$ and then obtaining the dual form (with N variables rather than n)

$$\text{Dual: } \max_{\boldsymbol{\lambda}} L_D(\boldsymbol{\lambda}) = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j c^i c^j (\mathbf{x}^i)^T\mathbf{x}^j + \sum_{i=1}^{N}\lambda_i$$

subject to

$$\lambda_i \geq 0, \quad \forall i = 1, ..., N$$

$$\sum_{i=1}^{N}\lambda_i c^i = 0 \tag{2}$$

Solving the dual is the same as solving the primal, but this is one is easier

- Solving dual $\Leftrightarrow$ Solving primal
- Problem (2) is a convex quadratic optimization problem: A global maximum can always be found (many methods available, like Seq. Min. Optimization (SMO))

Procedure

- Points $\mathbf{x}^i$ for which $\lambda_i > 0$ are called support vectors
- All other points have $\lambda_i = 0$

Algorithm 1: Classification with hard margin linear SVM: Linearly sep. data

Input : A data set $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$ with $c^i \in \{-1, +1\}$
Output: Classification c^* of each new observation $\mathbf{x}$

1. Solve problem (1) by solving problem (2) and obtain $\lambda_i, i = 1, ..., N$
2. Find set S, the indices i of support vectors such that $\lambda_i > 0$
3. Calculate $\mathbf{w} = \sum_{i \in S} \lambda_i c^i \mathbf{x}^i$
4. Calculate $b = \frac{1}{|S|} \sum_{s \in S} (c^s - \sum_{i \in S} \lambda_i c^i (\mathbf{x}^i)^T \mathbf{x}^s)$
5. Classify each new point $\mathbf{x}$ as $c^* = \phi(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$

Outline

Non-linearly sep. data: "Soft-margin" linear SVM

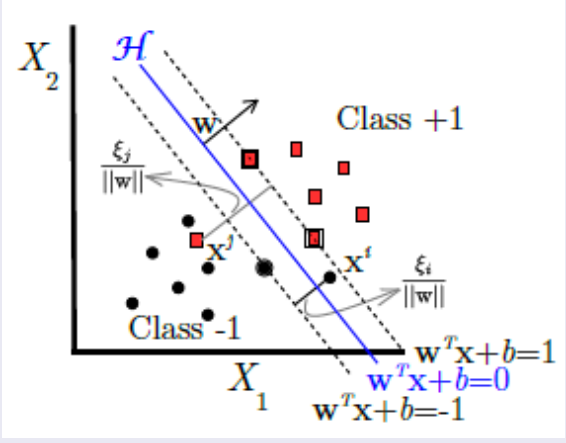
- Assume non-linearly separable data, e.g., there are outliers, noise or slightly non-linear data
- Aim: handle this case without changing the family of decision functions

⇒ Relax the constraints slightly to allow for misclassifications, although with a cost

⇒ Can be done by introducing slack variables $\xi_i \geq 0, i = 1, ..., N$ in the constraints

$$c^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1 - \xi_i$$ Relax the inequation

Chi_i is some kind of measurement of the error



- Points on the wrong side of $\mathcal{H}$ will have a penalty that increases with the distance from it
- ξ_i can be thought of as the distance from the support hyperplane for misclassified instances and 0 for correct classifications
- ξ_i thereby measures the degree of misclassification of $\mathbf{x}^i$

Primal and dual

$$\text{Primal: } \min_{\mathbf{w},b,\boldsymbol{\xi}} \frac{1}{2}||\mathbf{w}||^2 + M\sum_{i=1}^{N}\xi_i \quad \text{(Sum of the errors)}$$

$$\text{subject to} \qquad 1 - c^i(\mathbf{w}^T\mathbf{x}^i + b) - \xi_i \leq 0 \qquad (3)$$

$$-\xi_i \leq 0, \quad \forall i = 1, ..., N$$

- $M > 0$: fixed by the user. A larger M assigns a higher penalty to errors. M controls the trade-off between the slack variable penalty or errors and the size of the margin

$$\text{Dual: } \max_{\boldsymbol{\lambda}} L_D(\boldsymbol{\lambda}) = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j c^i c^j (\mathbf{x}^i)^T\mathbf{x}^j + \sum_{i=1}^{N}\lambda_i \quad \text{(Same equation as in the hard SVM)}$$

$$\text{subject to} \qquad 0 \leq \lambda_i \leq M, \quad \forall i = 1, ..., N \qquad (4)$$

$$\sum_{i=1}^{N}\lambda_i c^i = 0$$

Procedure

Algorithm 2: Classification with soft margin linear SVM: Non-linearly sep. data

Input : A data set $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$ with $c^i \in \{-1, +1\}$, a constant $M > 0$

Output: Classification c^* of each new observation $\mathbf{x}$

1 Solve problem (3) by solving problem (4) and obtain $\lambda_i, i = 1, ..., N$

2 Find set S, the indices i of support vectors such that $0 < \lambda_i < M$

3 Calculate $\mathbf{w} = \sum_{i \in S} \lambda_i c^i \mathbf{x}^i$

4 Calculate $b = \frac{1}{|S|} \sum_{s \in S} (c^s - \sum_{i \in S} \lambda_i c^i (\mathbf{x}^i)^T \mathbf{x}^s)$

5 Classify each new point $\mathbf{x}$ as $c^* = \phi(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$

Outline

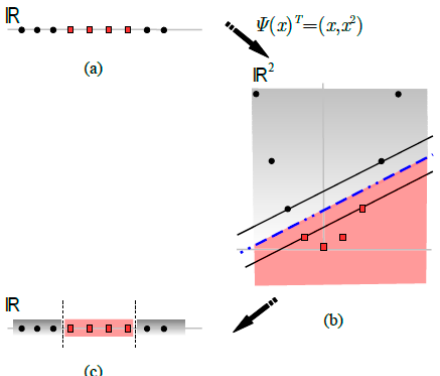
Non linearly separable data: nonlinear SVM

- Idea from **Cover's theorem**: given a set of training data that is non-linearly separable, it can be transformed with high probability into linearly separable by projecting it into a higher-dimensional space via some non-linear transformation
- Assume we map the data to some other (possibly infinite dimensional) feature space $\mathcal{F}$ via a non-linear mapping

$$\begin{aligned} \psi : \mathbb{R}^n &\mapsto \mathcal{F} \\ \mathbf{x} &\mapsto \psi(\mathbf{x}) \end{aligned}$$

- Data can be linearly separable in the new feature space. When the classifier is seen from the original input space it is non-linear

Example: map data x from $\mathbb{R}$ to $\mathbb{R}^2$ by using $\psi(x) = (x, x^2)^T$



- We obtain the points in (b)
- (bottom): Original space with the classification and the associated nonlinear boundaries

Primal and dual forms

- Replace $\mathbf{x}$ everywhere by their mapped versions $\psi(\mathbf{x})$
- A new instance is assigned the label $c^* = \phi(\mathbf{x}) = \text{sign}(\mathbf{w}^T \psi(\mathbf{x}) + b)$, with

We even substitute x hei

The expression of w is not needed

$$\mathbf{w} = \sum_{i \in S} \lambda_i c^i \psi(\mathbf{x}^i)$$

Al sustituir esto en la expresión del signo, también aparece un producto escalar entre chi(x_i) y chi(x_s)

$$b = \frac{1}{|S|} \sum_{s \in S} (c^s - \sum_{i \in S} \lambda_i c^i \psi(\mathbf{x}^i)^T \psi(\mathbf{x}^s))$$

where S contains the indices i such that $0 < \lambda_i < M$

- Dual problem only requires the inner products $\psi(\mathbf{x}^i)^T \psi(\mathbf{x}^j)$ of mapped points
- A smart way to compute such inner product is known as **kernel**
  $\Rightarrow$ kernel trick enters into play, allowing to recast the problem efficiently without using $\mathbf{w}$ or even $\psi(\mathbf{x})$ alone

The kernel mapping

- A **kernel function** or simply a **kernel** K is a symmetric function of two arguments that returns in $\mathbb{R}$ the value of the inner product of the mapped two arguments
$$K(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x})^T \psi(\mathbf{x}')$$
- Computing $K(\mathbf{x}^i, \mathbf{x}^j)$ directly can be less costly than $\psi(\mathbf{x}^i)^T \psi(\mathbf{x}^j)$ and avoids computing ψ explicitly

Example

- $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$
- $\psi(\mathbf{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2, x_1^2, x_2^2)^T \in \mathbb{R}^6$
- $\Rightarrow \psi(\mathbf{x})^T \psi(\mathbf{x}') = 1 + 2x_1 x_1' + 2x_2 x_2' + 2x_1 x_1' x_2 x_2' + x_1^2 x'^2_1 + x_2^2 x'^2_2$
- If we define $K(\mathbf{x}, \mathbf{x}') = (1 + x_1 x_1' + x_2 x_2')^2 = (1 + \mathbf{x}^T \mathbf{x}')^2 \ldots = \psi(\mathbf{x})^T \psi(\mathbf{x}')$
- ...it operates on the lower dimension vectors $\mathbf{x}$ and $\mathbf{x}'$ to produce a value equivalent to the inner product of the higher-dimensional vectors
- Neither the mapping ψ nor the space $\mathcal{F}$ are unique for a given kernel:

$\Rightarrow$ Example: $\psi_2(\mathbf{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1 x_2, x_1 x_2, x_1^2, x_2^2)^T \in \mathbb{R}^7$ is such that $\psi_2(\mathbf{x})^T \psi_2(\mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^2$ too

The kernel mapping

- A **kernel function** or simply a **kernel** K is a symmetric function of two arguments that returns in $\mathbb{R}$ the value of the inner product of the mapped two arguments
$$K(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x})^T \psi(\mathbf{x}') \quad \text{It is a number}$$
- Computing $K(\mathbf{x}^i, \mathbf{x}^j)$ directly can be less costly than $\psi(\mathbf{x}^i)^T \psi(\mathbf{x}^j)$ and avoids computing ψ explicitly

Example

- $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$
- $\psi(\mathbf{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2, x_1^2, x_2^2)^T \in \mathbb{R}^6$
- $\Rightarrow \psi(\mathbf{x})^T \psi(\mathbf{x}') = 1 + 2x_1 x_1' + 2x_2 x_2' + 2x_1 x_1' x_2 x_2' + x_1^2 x'^2_1 + x_2^2 x'^2_2$
- If we define $K(\mathbf{x}, \mathbf{x}') = (1 + x_1 x_1' + x_2 x_2')^2 = (1 + \mathbf{x}^T \mathbf{x}')^2 \ldots = \psi(\mathbf{x})^T \psi(\mathbf{x}')$
- ...it operates on the lower dimension vectors $\mathbf{x}$ and $\mathbf{x}'$ to produce a value equivalent to the inner product of the higher-dimensional vectors
- Neither the mapping ψ nor the space $\mathcal{F}$ are unique for a given kernel:

$\Rightarrow$ Example: $\psi_2(\mathbf{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1 x_2, x_1 x_2, x_1^2, x_2^2)^T \in \mathbb{R}^7$ is such that $\psi_2(\mathbf{x})^T \psi_2(\mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^2$ too

Procedure

Algorithm 3: Classification with nonlinear SVM

Input : A data set $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$ with $c^i \in \{-1, +1\}$, a constant $M > 0$

Output: Classification c^* of each new observation $\mathbf{x}$

1. Solve problem (4) with $K(\mathbf{x}^i, \mathbf{x}^j)$ instead of $(\mathbf{x}^i)^T\mathbf{x}^j$ in the objective function, and obtain $\lambda_i, i = 1, ..., N$
2. Find set S, the indices i of support vectors such that $0 < \lambda_i < M$
3. Calculate $b = \frac{1}{|S|} \sum_{s \in S}(c^s - \sum_{i \in S} \lambda_i c^i K(\mathbf{x}^i, \mathbf{x}^s))$
4. Classify each new point $\mathbf{x}$ as $c^* = \phi(\mathbf{x}) = \text{sign}(\sum_{i \in S} \lambda_i c^i K(\mathbf{x}^i, \mathbf{x}) + b)$

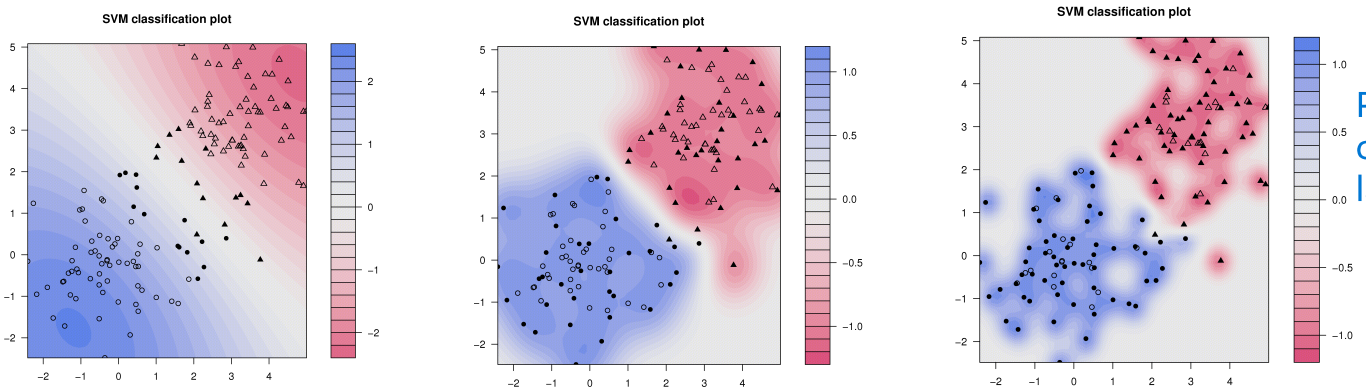
Which is a valid kernel?

- It needs to satisfy the **Mercer's condition**: the $N \times N$ kernel matrix (also called the Gram matrix) $\mathbf{K}$ in which the (i, j) entry is $K(\mathbf{x}^i, \mathbf{x}^j)$ is always positive-semidefinite, i.e., $\mathbf{x}^T\mathbf{K}\mathbf{x} \geq 0, \forall \mathbf{x} \neq 0$ in the training set
- Popular kernels:

Once you decide the kernel, optimize the parameter

Name	$K(\mathbf{x}, \mathbf{x}')$	Parameters
Polynomial	$(\mathbf{x}^T\mathbf{x}')^p$	degree $p \in \mathbb{N}$
Inhomogeneous polynomial	$(1 + \mathbf{x}^T\mathbf{x}')^p$	degree $p \in \mathbb{N}$
Gaussian RBF (radial basis function)	$e^{-\frac{1}{2\sigma^2}\|\|\mathbf{x}-\mathbf{x}'\|\|^2}$	width $\sigma > 0$
Sigmoidal	$\tanh(\kappa\mathbf{x}^T\mathbf{x}' - \theta)$	κ, θ

Gaussian RBF: As σ decreases (center and right) the flexibility of the decision boundary increases and can lead to overfitting (color gradient is the decision value)



Perhaps we are overfitting on the last one

Points in solid black are the support vectors. Note that a smaller σ demands more support vectors

Outline

Conclusions

Summary

- Linear (hard and soft) SVM
- Kernel trick for the nonlinear SVM
- Multi-class SVM: $\Omega_C = \{1, ..., R\}$: build many binary SVMs and then combine them

In Weka

SMO within *Functions*

Bibliography

Texts

- Bielza, C., Larrañaga, P. (2021) *Data-Driven Computational Neuroscience. Machine Learning and Statistical Models*, Cambridge University Press [Chap. 7]
- Burges, C.J.C. (1998) A tutorial on support vector machines for pattern recognition, *Data Mining and Knowledge Discovery*, 2, 2, 121-167
- Cristianini, N., Shawe-Taylor, J. (2000) *An Introduction to Support Vector Machines and Other Kernel-Based Learning Methods*, Cambridge University Press
- Platt, J.C. (1999) Fast training of support vector machines using sequential minimal optimization, In *Advances in Kernel Methods - Support Vector Learning*, pp. 185-208, The MIT Press
- Vapnik, V.N. (1998) *Statistical Learning Theory*, Wiley