*** Applied Machine Learning Fundamentals ***
Support Vector Machines

M. Sc. Daniel Wehner

SAP SE

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Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	Classification I
Unit VII	Evaluation
Unit VIII	**Classification II**
Unit IX	Clustering
Unit X	Dimensionality Reduction

Agenda for this Unit

Section:

Linear SVMs

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What is a Support Vector Machine (SVM)?

- A support vector machine is a **binary classifier** [Vapnik and Chervonenkis]
  - The classes are denoted by $\{-1; +1\}$
  - Techniques for multi-class classification: One-vs-Rest and One-vs-One
- The algorithm was introduced in the 60s, extensions were made in the 90s
- An SVM finds the **best separating hyperplane**
- **Question:** *What is the best separating hyperplane?*
- Why is it called *'machine'*?
  - It's no physical machine, it's a mathematical construct
  - 'Machine' refers to 'Machine Learning'

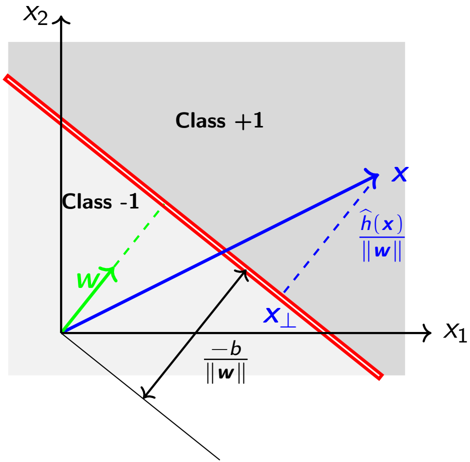
Discriminant Functions

- The simplest discriminant is a linear function of the form:

$$\widehat{h}(\boldsymbol{x}) = \boldsymbol{w}^\intercal \boldsymbol{x} + b = \sum_{j=1}^{m} w_j x_j + b = w_1 x_1 + w_2 x_2 + \cdots + w_m x_m + b \qquad (1)$$

- $\boldsymbol{\theta} = \{\boldsymbol{w}, b\}$: $\boldsymbol{w}$ is called the **weight vector** and b is the **bias**
- An input vector $\boldsymbol{x}$ is assigned class $\mathcal{C}_1$, if $\widehat{h}(\boldsymbol{x}) \geqslant 0$, class $\mathcal{C}_2$ otherwise
- The **decision boundary** is defined by the relation: $\widehat{h}(\boldsymbol{x}) = 0$
- The boundary is a $(D-1)$-dimensional hyperplane within the D-dimensional input space

Discriminant Functions (Ctd.)



Discriminant Functions (Ctd.)

- Consider two points, $\boldsymbol{x}_A$ and $\boldsymbol{x}_B$, which lie on the decision surface
- Since $\widehat{h}(\boldsymbol{x}_A) = \widehat{h}(\boldsymbol{x}_B) = 0$, we have $\boldsymbol{w}^\intercal(\boldsymbol{x}_A - \boldsymbol{x}_B) = 0$, hence $\boldsymbol{w}$ is **orthogonal** to every vector lying within the decision surface
- $\boldsymbol{w}$ determines the orientation of the decision surface
- Similarly, if $\boldsymbol{x}$ is a point on the decision surface, then $\widehat{h}(\boldsymbol{x}) = 0$ and the normal distance from the origin to the decision surface is given by:

$$\frac{\boldsymbol{w}^\intercal \boldsymbol{x} + b}{\|\boldsymbol{w}\|} = 0 \Leftrightarrow \frac{\boldsymbol{w}^\intercal \boldsymbol{x}}{\|\boldsymbol{w}\|} = -\frac{b}{\|\boldsymbol{w}\|} \tag{2}$$

- b controls the offset from the origin

Discriminant Functions (Ctd.)

- $\widehat{h}(\boldsymbol{x})$ gives a **signed measure** of the perp. distance of $\boldsymbol{x}$ to the boundary
- Consider an arbitrary point $\boldsymbol{x}$ and its orth. projection $\boldsymbol{x}_\perp$ onto the surface

$$\boldsymbol{x} = \boldsymbol{x}_\perp + r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|} \tag{3}$$

- Multiplying both sides by $\boldsymbol{w}^\intercal$ and adding b, and making use of:

$$\widehat{h}(\boldsymbol{x}) = \boldsymbol{w}^\intercal\boldsymbol{x} + b \qquad \text{and} \qquad \widehat{h}(\boldsymbol{x}_\perp) = \boldsymbol{w}^\intercal\boldsymbol{x}_\perp + b = 0$$

- We get:

$$r = \frac{\widehat{h}(\boldsymbol{x})}{\|\boldsymbol{w}\|} \tag{4}$$

Linear Separability

- We have n input vectors $\boldsymbol{X} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}\}$
- With corresponding target values $y^{(1)}, y^{(2)}, \dots, y^{(n)}$, where $y^{(i)} \in \{-1, +1\}$
- New data points are classified according to the sign of $\widehat{h}(\boldsymbol{x})$: $sign(\widehat{h}(\boldsymbol{x}))$

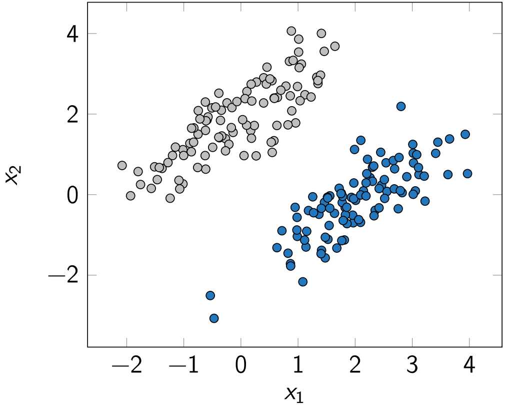
A data set is **linearly separable** in feature space, if $\exists(\boldsymbol{w}, b)$ such that

$$\widehat{h}(\boldsymbol{x}^{(i)}) = \boldsymbol{w}^\intercal \boldsymbol{x}^{(i)} + b > 0 \qquad \forall \boldsymbol{x}^{(i)} \text{ with } y^{(i)} = +1 \tag{5}$$

$$\widehat{h}(\boldsymbol{x}^{(i)}) = \boldsymbol{w}^\intercal \boldsymbol{x}^{(i)} + b < 0 \qquad \text{otherwise } (y^{(i)} = -1) \tag{6}$$

This can also be written as: $y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)}) > 0 \ \forall i$

Example Data Set (linearly separable)



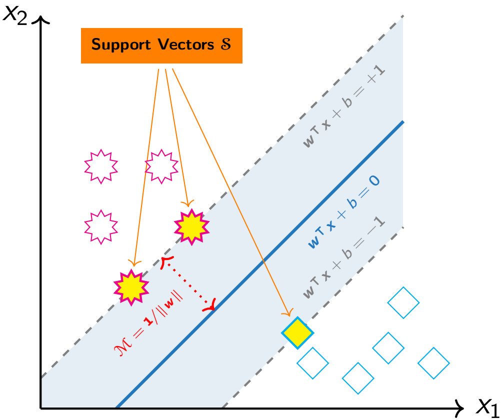
- This data set is **linearly separable** (you can find a straight line to separate the two classes)
- The possible number of hyperplanes is infinite...
- **Which hyperplane should be chosen?**

Maximum Margin Classifiers

- An SVM is a so-called **maximum margin classifier**
- It maximizes the margin $\mathcal{M}$

$$\max_{\boldsymbol{w},b} \mathcal{M}$$

- The larger $\mathcal{M}$ the less likely are false predictions
- Only the **support vectors** determine the hyperplane



Maximum Margin Classifiers (Ctd.)

- Recall the perpendicular distance of a point $\boldsymbol{x}$ to the hyperplane:

$$\frac{|\widehat{h}(\boldsymbol{x})|}{\|\boldsymbol{w}\|} \tag{7}$$

- Furthermore, we are only interested in solutions for which all data points are correctly classified, i. e. $y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)}) > 0 \ \forall i$, thus the distance is given by:

$$\frac{y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)})}{\|\boldsymbol{w}\|} = \frac{y^{(i)}(\boldsymbol{w}^\intercal\boldsymbol{x}^{(i)} + b)}{\|\boldsymbol{w}\|} \tag{8}$$

Maximum Margin Classifiers (Ctd.)

- The margin is given by the perp. distance to the closest data point $\boldsymbol{x}^{(i)}$
- We wish to optimize the parameters $\boldsymbol{w}$ and b to maximize this distance
- We have to solve:

$$\boldsymbol{w}^*, b^* = \arg\max_{\boldsymbol{w}, b} \overbrace{\left\{ \frac{1}{\|\boldsymbol{w}\|} \overbrace{\min_i \{ y^{(i)} (\boldsymbol{w}^\intercal \boldsymbol{x}^{(i)} + b) \}}^{\text{'closest data points'}} \right\}}^{\text{'maximize distance to closest data points'}} \tag{9}$$

- Note that $1/\|\boldsymbol{w}\|$ does not depend on i
- A direct solution of this optimization would be very complex $\Rightarrow$ rewrite!

Maximum Margin Classifiers (Ctd.)

- We note that rescaling $\boldsymbol{w}$ and b by a factor ζ **does not change the distance** to the decision boundary
- Therefore, for the points that are closest to the surface, we can set:

$$y^{(i)}(\boldsymbol{w}^\intercal \boldsymbol{x}^{(i)} + b) = 1 \tag{10}$$

- In this case, all data points $\boldsymbol{x}^{(i)}$ satisfy the constraint:

$$y^{(i)}(\boldsymbol{w}^\intercal \boldsymbol{x}^{(i)} + b) \geqslant 1 \qquad i = 1, 2, \dots, n \tag{11}$$

- It is sufficient to solve: $\arg\min_{\boldsymbol{w},b} \frac{1}{2} \|\boldsymbol{w}\|^2$ ($1/2$ for mathematical convenience)

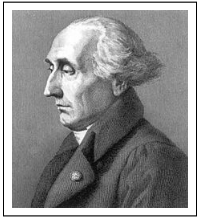
Maximum Margin Classifiers (Ctd.)

$$\boldsymbol{w}^*, b^* = \arg\min_{\boldsymbol{w}, b} \frac{1}{2} \|\boldsymbol{w}\|^2 \tag{12}$$

- This is a **quadratic optimization (QP)** problem
- A global optimum exists due to **convexity**
- How to solve such problems?

Lagrangian optimization

(named after Joseph-Louis Lagrange)



Lagrangian Optimization: A simple Example

- Lagrangian optimization is optimization **subject to constraints**
- **Example:**

$$\overbrace{f(x_1, x_2) = 1 - x_1^2 - x_2^2}^{\text{function to optimize } f(\boldsymbol{x})} \quad \text{s. t.} \quad \overbrace{g(x_1, x_2) = x_1 + x_2 - 1 = 0}^{\text{linear constraint } g(\boldsymbol{x}) = 0} \tag{13}$$

- To find a solution we have to formulate the Lagrangian equation:

General form: $\mathcal{L}(\boldsymbol{x}, \alpha) = f(\boldsymbol{x}) + \alpha g(\boldsymbol{x})$

$$\mathcal{L}(\boldsymbol{x}, \alpha) = 1 - x_1^2 - x_2^2 + \alpha(x_1 + x_2 - 1) \tag{14}$$

Lagrangian Optimization: A simple Example (Ctd.)

$$\mathcal{L}(\boldsymbol{x}, \alpha) = 1 - x_1^2 - x_2^2 + \alpha(x_1 + x_2 - 1)$$

We determine the partial derivatives w. r. t. x_1, x_2 and α and set them to zero:

$$\frac{\partial \mathcal{L}(\boldsymbol{x}, \alpha)}{\partial x_1} = -2x_1 + \alpha \overset{!}{=} 0 \tag{15}$$

$$\frac{\partial \mathcal{L}(\boldsymbol{x}, \alpha)}{\partial x_2} = -2x_2 + \alpha \overset{!}{=} 0 \tag{16}$$

$$\frac{\partial \mathcal{L}(\boldsymbol{x}, \alpha)}{\partial \alpha} = x_1 + x_2 - 1 \overset{!}{=} 0 \tag{17}$$

Lagrangian Optimization: A simple Example (Ctd.)

- Solving the first two equations for x_1 and x_2, respectively, we get:

$$x_1 = {}^1\!/\!{}_2\alpha \tag{18}$$
$$x_2 = {}^1\!/\!{}_2\alpha \tag{19}$$

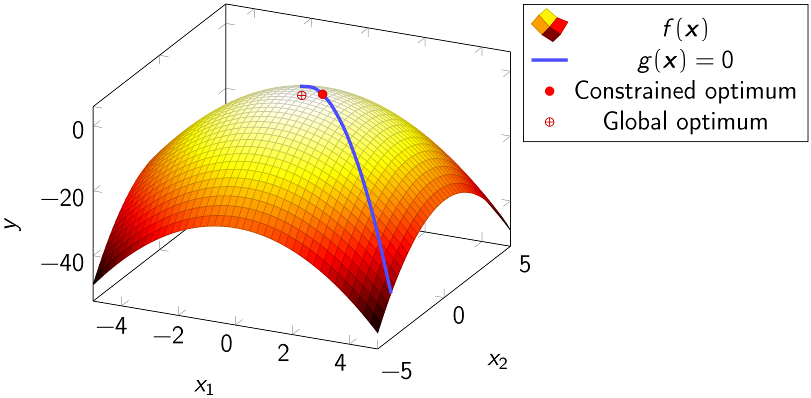
- Substitution into the third equation $x_1 + x_2 - 1 = 0$:

$$\widetilde{\mathcal{L}}(\alpha) = {}^1\!/\!{}_2\alpha + {}^1\!/\!{}_2\alpha - 1 = 0 \Leftrightarrow \alpha = 1 \tag{20}$$

- Finally, we get:

$$x_1 = {}^1\!/\!{}_2 \qquad x_2 = {}^1\!/\!{}_2$$

Lagrangian Optimization: A simple Example (Ctd.)



SVM Parameter Optimization

We have to solve the Lagrangian:

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \overbrace{1/2\|\boldsymbol{w}\|^2}^{f(\boldsymbol{x})} - \sum_{i=1}^{n} \alpha_i \overbrace{[y^{(i)} \cdot (\boldsymbol{w}^\intercal \boldsymbol{x}^{(i)} + b) - 1]}^{g(\boldsymbol{x})=0} \tag{21}$$

- $\boldsymbol{\alpha}$ is a vector of **Lagrangian multipliers**
- There is **one constraint per data point!**
- The Lagrangian multipliers will be non-zero for all support vectors

SVM Parameter Optimization (Ctd.)

We have to compute the partial derivatives w. r. t. $\boldsymbol{w}$ and b and set them to zero:

linear combination of input!

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i=1}^{n} \alpha_i y^{(i)} \boldsymbol{x}^{(i)} \stackrel{!}{=} 0 \Rightarrow \boxed{\boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y^{(i)} \boldsymbol{x}^{(i)}} \tag{22}$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^{n} \alpha_i y^{(i)} \stackrel{!}{=} 0 \quad \Rightarrow \boxed{\sum_{i=1}^{n} \alpha_i y^{(i)} = 0} \tag{23}$$

SVM Parameter Optimization (Ctd.)

As a next step the partial derivatives are substituted in into $\mathcal{L}$:

$$\widetilde{\mathcal{L}}(\boldsymbol{\alpha}) = \frac{1}{2}\left(\sum_{i=1}^{n} \alpha_i y^{(i)} \boldsymbol{x}^{(i)}\right)\left(\sum_{j=1}^{n} \alpha_j y^{(j)} \boldsymbol{x}^{(j)}\right) - \left(\sum_{i=1}^{n} \alpha_i y^{(i)} \boldsymbol{x}^{(i)}\right)\left(\sum_{j=1}^{n} \alpha_j y^{(j)} \boldsymbol{x}^{(j)}\right) - \sum_{i=1}^{n} \alpha_i y^{(i)} b + \sum_{i=1}^{n} \alpha_i \tag{24}$$

$$= \boxed{\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)} \rangle} \quad \text{s.t. } \alpha_i \geqslant 0 \ \forall i \text{ and } \sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \tag{25}$$

Wolfe dual

SVM Parameter Optimization (Ctd.)

- Once we know $\boldsymbol{\alpha}$, we can determine b by noting that any support vector satisfies $y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)}) = 1$: ($\mathcal{S} \equiv$ indices of support vectors)

$$y^{(i)}\left(\sum_{j\in\mathcal{S}} \alpha_j y^{(j)} \langle \boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)} \rangle + b\right) = 1 \tag{26}$$

- Average over all support vectors to compute b: ($n_{\mathcal{S}} \equiv$ number of support vectors)

$$b = \frac{1}{n_{\mathcal{S}}} \sum_{i\in\mathcal{S}} \left(y^{(i)} - \sum_{j\in\mathcal{S}} \alpha_j y^{(j)} \langle \boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)} \rangle \right) \tag{27}$$

Updated Decision Rule

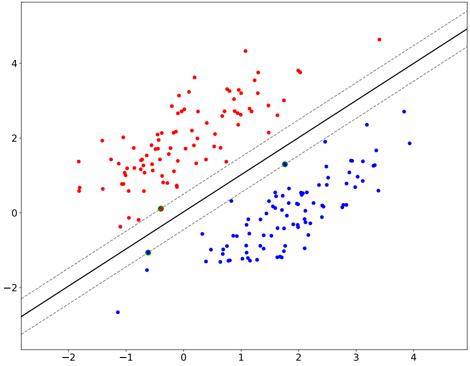
- Given our derivations, we can rewrite the SVM decision rule as follows:

$$h(\boldsymbol{x}) = sign\left(\sum_{i \in \mathcal{S}} \alpha_i y^{(i)} \langle \boldsymbol{x}^{(i)}, \boldsymbol{x} \rangle + b\right) \tag{28}$$

- $\boldsymbol{x}$ is an unknown instance for which the class label is not known

Since all α_i will be zero for non-support vectors, the decision for a class depends on the support vectors only! This makes predictions fast, even for large data sets. **The number of support vectors can also be used as an evaluation criterion.**

Linear SVM: Example



Section:

Non-linear / Kernel SVMs

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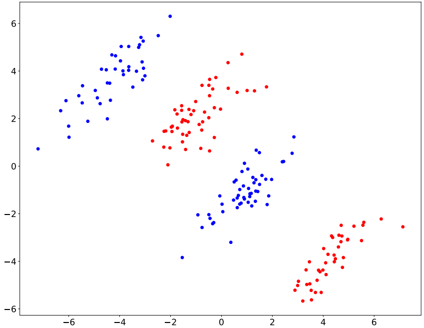
Non-Linear SVMs / Non-Linear Separability

- So far we have assumed **linear separability** of the data
- **What if the data is not linearly separable?**
  (which will be the case in practice...)
- We cannot find a straight line...
- $\overset{\textit{Remedy}}{\Longrightarrow}$ **Feature maps**, **Kernels**

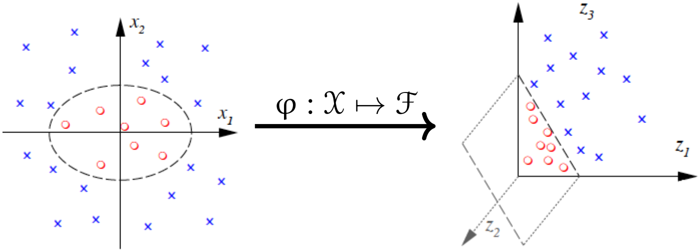


Feature Mapping

The mapping function φ maps from input space $\mathcal{X}$ to feature space $\mathcal{F}$:

$\mathcal{X}$

Input space



$\mathcal{F}$

Feature space

$$\varphi(x_1, x_2) \mapsto \left(x_1^2, \sqrt{2}x_1 x_2, x_2^2\right) = (z_1, z_2, z_3)$$

Feature Mapping (Ctd.)

- A **feature map** **explicitly** transforms the data to a higher dimension where classification becomes easier
- Computing the feature map can – from a computational point of view – become very expensive
- And how do you know how many dimensions to add? What transformations should be used?
- **A more tractable solution is required $\Rightarrow$ Kernels**

What is a Kernel?

- A kernel can be considered a **similarity function**
- Many algorithms have been *'kernelized'*, e. g. *Kernel PCA*, *Kernel SVM*
- Think of it as projecting the data in a higher dimensional space to make it linearly separable

A kernel allows the SVM to operate in a **high-dimensional, implicit feature space** without ever computing the coordinates of the data in that space, but rather by simply computing the **inner products** between the images of **all pairs of data** in the feature space. $\Rightarrow$ **Kernel trick** [Wikipedia]

What is a Kernel? (Ctd.)

- The explicit computation of a feature map $\varphi(\boldsymbol{x})$ is avoided...
- ...by replacing the dot product with the kernel $\mathcal{K}$:

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') \Leftrightarrow \varphi(\boldsymbol{x})^\intercal \varphi(\boldsymbol{x}') \tag{29}$$

- Instead of mapping features explicitly, we calculate the **Gram matrix** $\boldsymbol{K} \in \mathbb{R}^{n \times n}$, where:

$$K_{ij} = \mathcal{K}(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) \tag{30}$$

Important

Well-known Kernels

- **Linear kernel**

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^\intercal \boldsymbol{x}' \tag{31}$$

- **Polynomial kernel**

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^\intercal \boldsymbol{x}' + c)^p \tag{32}$$

- **Radial-Basis-Function (RBF) kernel**

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = \exp\left\{-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|^2}{2\sigma^2}\right\} = \exp\{-\gamma\|\boldsymbol{x} - \boldsymbol{x}'\|^2\} \tag{33}$$

Power of Kernels

- Suppose $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^m$ with $m = 2$
- Polynomial feature mapping ($c = 0$):

$$\varphi(\boldsymbol{x}) = [x_1 x_1, x_1 x_2, x_2 x_1, x_2 x_2]^\intercal \qquad \varphi(\boldsymbol{x}') = [x_1' x_1', x_1' x_2', x_2' x_1', x_2' x_2']^\intercal \tag{34}$$

- Using a polynomial kernel:

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^\intercal \boldsymbol{x}')^2 = \left(\sum_{i=1}^{m} x_i x_i'\right)\left(\sum_{j=1}^{m} x_j x_j'\right) = \sum_{i=1}^{m}\sum_{j=1}^{m}(x_i x_j)(x_i' x_j') = \varphi(\boldsymbol{x})^\intercal \varphi(\boldsymbol{x}') \tag{35}$$

We need $\mathcal{O}(n^2)$ to compute $\varphi(\boldsymbol{x})$ and $\varphi(\boldsymbol{x}')$, but $\mathcal{O}(n)$ to compute $\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}')$

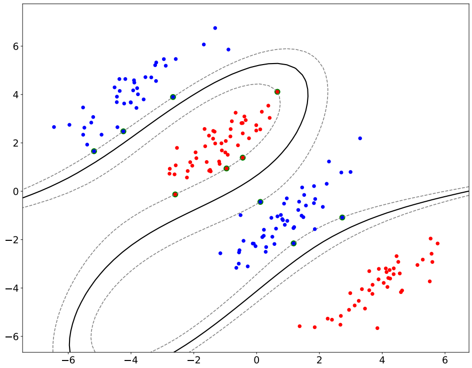
Incorporating the Kernel Function

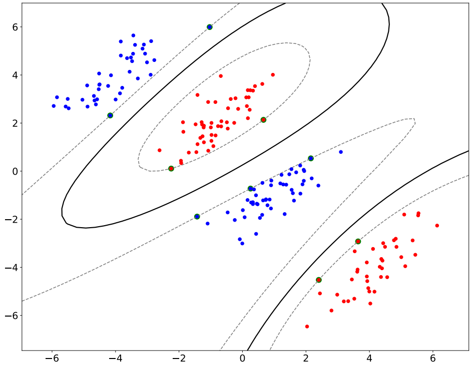
- The kernel function $\mathcal{K}$ replaces each occurrence of $\boldsymbol{x}^\intercal \boldsymbol{x}'$
- **Example:**

$$\widetilde{\mathcal{L}} = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} \mathcal{K}(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) \tag{36}$$

$$h(\boldsymbol{x}) = sign\left(\sum_{i \in \mathcal{S}} \alpha_i y^{(i)} \mathcal{K}(\boldsymbol{x}^{(i)}, \boldsymbol{x}) + b \right) \tag{37}$$

Polynomial Kernel vs. RBF Kernel





Mercer's Condition

- A kernel is valid, if it fulfills Mercer's condition
- This is the case, if for all **square-integrable functions** $g(\boldsymbol{x})$...

$$\int_{-\infty}^{\infty} |g(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} < \infty \tag{38}$$

- ...it holds:

$$\int\int g(\boldsymbol{x})\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}')g(\boldsymbol{x}') \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{x}' \geqslant 0 \tag{39}$$

Mercer's Condition (Ctd.)

- Suppose $\mathcal{K}$ is a valid kernel and let $\boldsymbol{X} = \{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)}\}$ be given
- For any vector $\boldsymbol{z} \in \mathbb{R}^n$:

$$\boldsymbol{z}^\intercal \boldsymbol{K}\boldsymbol{z} = \sum_i \sum_j z_i K_{ij} z_j = \sum_i \sum_j z_i \varphi(\boldsymbol{x}^{(i)})^\intercal \varphi(\boldsymbol{x}^{(j)}) z_j \tag{40}$$

$$= \sum_i \sum_j z_i \sum_k (\varphi(\boldsymbol{x}^{(i)}))_k (\varphi(\boldsymbol{x}^{(j)}))_k z_j = \sum_k \sum_i \sum_j z_i (\varphi(\boldsymbol{x}^{(i)}))_k (\varphi(\boldsymbol{x}^{(j)}))_k z_j \tag{41}$$

$$= \sum_k \left(\sum_i z_i \varphi(\boldsymbol{x}^{(i)})_k \right)^2 \geqslant 0 \Longrightarrow \boldsymbol{K} \geqslant 0 \tag{42}$$

- $\boldsymbol{K} \geqslant 0$ means that matrix $\boldsymbol{K}$ must be positive semi-definite (psd)

Mercer's Condition (Ctd.)

Mercer's Theorem:
$\mathcal{K}$ is a valid kernel, iff for any set of n training examples $\boldsymbol{X} = \{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}\}$ kernel matrix $\boldsymbol{K} \in \mathbb{R}^{n \times n}$ is **positive semi-definite**. The kernel is then called **Mercer kernel**.

- This entails: $K_{ij} \geqslant 0 \; \forall i, j$
- **Example**:
  - $\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}) = -1 \neq \varphi(\boldsymbol{x})^\intercal \varphi(\boldsymbol{x})$
  - $\mathcal{K}$ cannot be a valid kernel

Constructing new Kernels

- It is not always easy to check if Mercer's condition is satisfied, but it is possible to construct **new kernels out of known ones**
- If $\mathcal{K}_1(\boldsymbol{x}, \boldsymbol{x}')$ and $\mathcal{K}_2(\boldsymbol{x}, \boldsymbol{x}')$ are valid kernels, so are:

  - $c \cdot \mathcal{K}_1(\boldsymbol{x}, \boldsymbol{x}')$
  - $\mathcal{K}_1(\boldsymbol{x}, \boldsymbol{x}') + \mathcal{K}_2(\boldsymbol{x}, \boldsymbol{x}')$
  - $\mathcal{K}_1(\boldsymbol{x}, \boldsymbol{x}') \cdot \mathcal{K}_2(\boldsymbol{x}, \boldsymbol{x}')$
  - $f(\boldsymbol{x}) \cdot \mathcal{K}_1(\boldsymbol{x}, \boldsymbol{x}') \cdot f(\boldsymbol{x}')$
  - etc.

Section:

Soft-Margin SVMs

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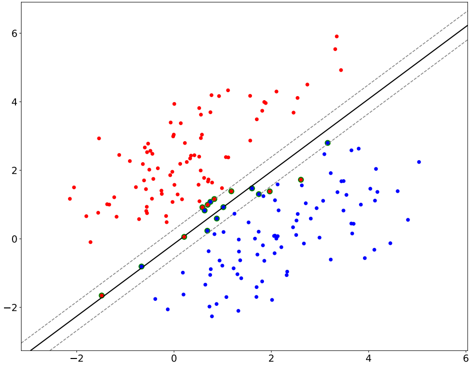
Overlapping Distributions

- We assumed linearly separable data
  $\Rightarrow$ **SVM gives exact solution**
- **But:** The classes may overlap
  $\Rightarrow$ **Exact separation leads to poor generalization**
- **Soft-margin SVM:** Allow some data points to be misclassified
- To this end, a penalty is introduced:
  - Misclassifications are penalized
  - This penalty increases linearly with the distance from the decision boundary
- This is done using **slack variables**

Overlapping Distributions: Example



Slack Variables

- The slack is denoted by ξ_i (where $\xi_i \geqslant 0; i = 1, \dots, n$), one per data point
- **Different cases**:

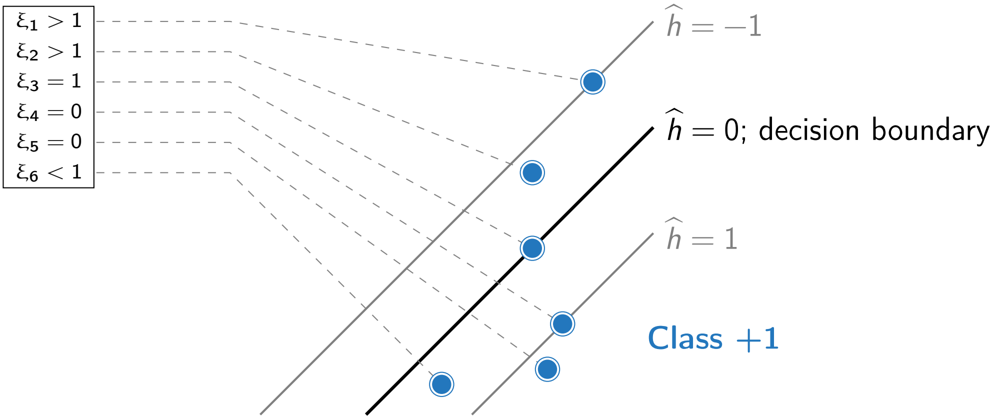
$\xi_i = 0$	if $\boldsymbol{x}^{(i)}$ is on or inside the correct margin boundary
$0 < \xi_i < 1$	if $\boldsymbol{x}^{(i)}$ lies inside the margin, but on the correct side
$\xi_i = 1$	if $\boldsymbol{x}^{(i)}$ is on the decision boundary
$\xi_i > 1$	if $\boldsymbol{x}^{(i)}$ lies on the wrong side of the decision boundary (misclassification)

- The classification constraints are replaced with:

$$y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)}) \geqslant 1 - \xi_i \qquad i = 1, \dots, n \tag{43}$$

- We get a soft-margin classifier

Slack Variables (Ctd.)



Soft SVM Parameter Optimization

- We want to maximize the margin, while softly **penalizing points which lie on the wrong side of the boundary**:

$$\frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{n}\xi_i \quad \text{s. t.} \quad y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)}) \geqslant 1 - \xi_i \text{ and } \xi_i \geqslant 0 \;\forall i \tag{44}$$

- $C > 0$ controls the *'degree of softness'*, the larger C the more we penalize
- The Lagrangian function:

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\{y^{(i)}\widehat{h}(\boldsymbol{x}^{(i)}) - 1 + \xi_i\} - \sum_{i=1}^{n}\mu_i\xi_i \tag{45}$$

Soft SVM Parameter Optimization (Ctd.)

- It turns out that the dual objective function looks exactly the same:

$$\widetilde{\mathcal{L}}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)} \rangle \tag{46}$$

- But the constraints differ slightly:

$$1) \quad \sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \tag{47}$$

$$2) \quad \boxed{0 \leqslant \alpha_i \leqslant C \qquad i = 1, \dots, n} \tag{48}$$

- Constraint 2) is called **boxed constraint**

Section:

Multi-Class Classification

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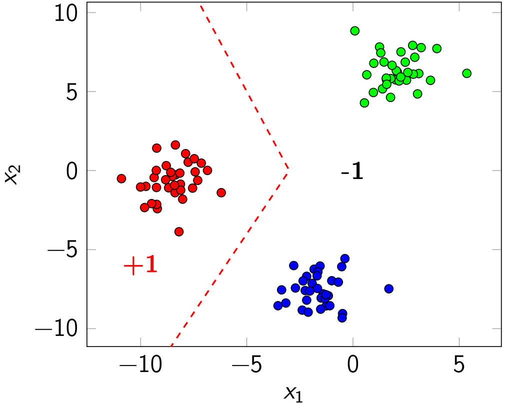
Multi-Class Classification

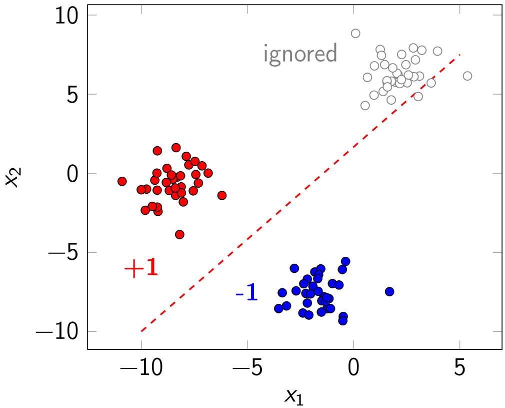
- An SVM can handle two classes only, namely **-1** and **+1**
- **What if there are more than two classes?**
- Two common techniques:
  - **One-vs-Rest (OVR)** ⇒ One-against-All
  - **One-vs-One (OVO)** ⇒ Pairwise classification
- Several classifiers are trained
- During prediction the classifiers **vote for the correct class**
- Such techniques can be used for all binary classifiers (e. g. logistic regression)

Multi-Class Classification: One-vs-Rest (OVR)

- **Train one classifier per class** (expert for that class)
- We get $|\mathcal{C}|$ classifiers
- The k-th classifier learns to distinguish the k-th class from all the others
- Set the labels of examples from class k to $+1$, all the others to -1



Multi-Class Classification: One-vs-One (OVO)



- **Train one classifier for each pair of classes**
- We get $\binom{|\mathcal{C}|}{2}$ classifiers
- Ignore all other examples that do not belong to either of the two classes
- **Voting**: Count how often each class wins; the class with the highest score is predicted

Section:

Wrap-Up

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Summary

- SVMs assume the data to be **linearly separable**
- **Generalization guarantee:** SVMs are **maximum margin** classifiers
- The set of **support vectors** defines the decision boundary
- We have to solve a quadratic optimization problem to obtain the support vectors which are needed for prediction
- **Important concept:** Kernels (cf. Mercer's condition)
- Slack variables allow for **soft-margin classification**
- Apply multi-class classification techniques like OVR / OVO if you have more than two classes

Important

Self-Test Questions

1. What is a maximum-margin classifier?
2. Which data points are needed for prediction? How do we get them?
3. What is a kernel? Can every function serve as a kernel?
4. What prerequisite allows for the usage of kernels?
5. Name famous kernels and write down the equation to compute them!
6. What is slack? What can we do with it?

What's next...?

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	Classification I
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	**Clustering**
Unit X	Dimensionality Reduction

Recommended Literature and further Reading I

[1] Pattern Recognition and Machine Learning
Christopher Bishop. Springer. 2006.
→ Link, cf. chapter 7

[2] Machine Learning: A Probabilistic Perspective
Kevin Murphy. MIT Press. 2012.
→ Link, cf. chapter 14.5

Meme of the Day

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Support Vector Machines
Term: Winter term 2019/2020

Contact:
M. Sc. Daniel Wehner
SAP SE
daniel.wehner@sap.com

Do you have any questions?