MADS-ML – Machine Learning

Support Vector Machines

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Moodle (WiSe 2024/25)

"The line must be drawn here!"

Motivation

- Find an actual model and learn its parameters (in contrast to kNN an decision trees)

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- important extensions: 1993 Soft Margin, 1995 Kernel Trick
- versatile, robust, effective in high-dimensional spaces

Outline

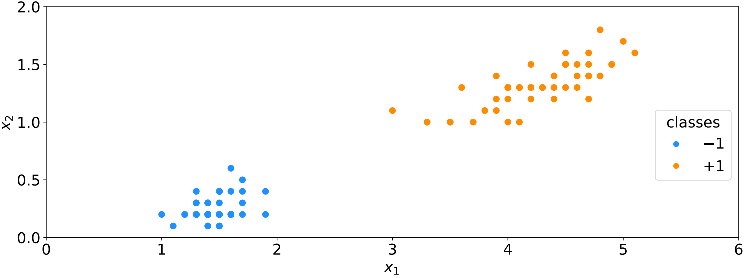
Basic Idea

Mathematical Description

Soft-Margin SVMs

Kernel Trick

Example Dataset 2D



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- two classes: $c_1 = -1$ und $c_2 = +1$ ➔ (binary classification)
- two features: x_1 and x_2
- data shows part of the Iris dataset

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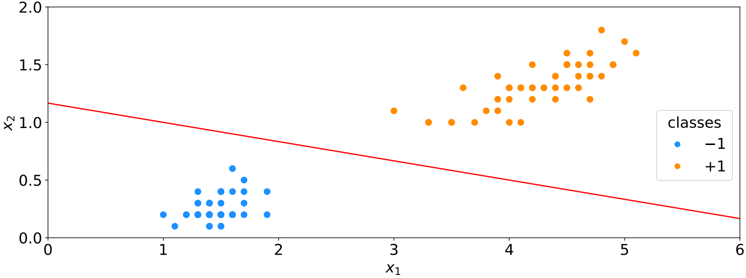

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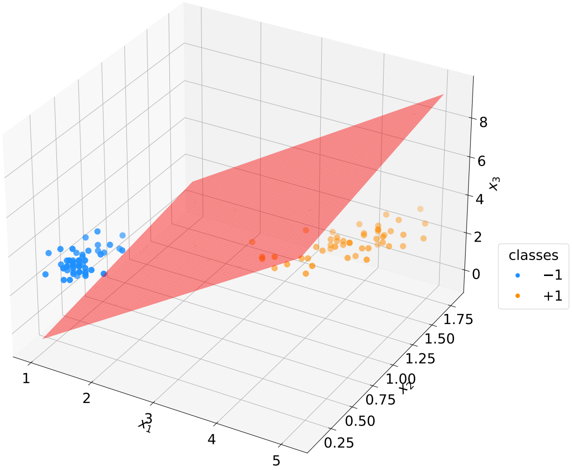

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- n=2 → line
- n=3 → (regular) plane

Hyperplane – Mathematical Representation

A hyperplane in $\mathbb{R}^n$ is described by a vector $\boldsymbol{w} \in \mathbb{R}^n$ of (**weights**), $\boldsymbol{w} \neq 0$, a scalar $b \in \mathbb{R}$ (**bias**) and the equation:

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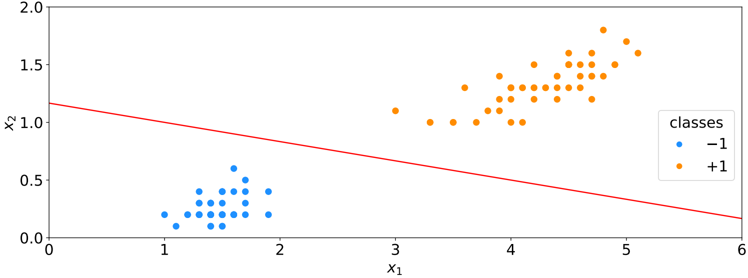
- denoted as $\mathcal{H}(\boldsymbol{w}, b)$
- $\langle \cdot, \cdot \rangle$ is the scalar product
- representation in coordinates::
  $w_1 x_1 + w_2 x_2 + \ldots + w_n x_n + b = 0$

Hyperplane – Mathematical Representation – Example



Description of the hyperplane $\mathcal{H}(\boldsymbol{w}, b)$:

- $\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b = 0$ with $\boldsymbol{w} = \begin{pmatrix} 1 \\ 6 \end{pmatrix}, b = -7$

Properties of a Hyperplane

Let $\mathcal{H}(\boldsymbol{w}, b)$ be the hyperplane $\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b = 0$ and define

$$f_{\boldsymbol{w},b} : \mathbb{R}^n \to \mathbb{R} : \boldsymbol{x} \mapsto \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b.$$

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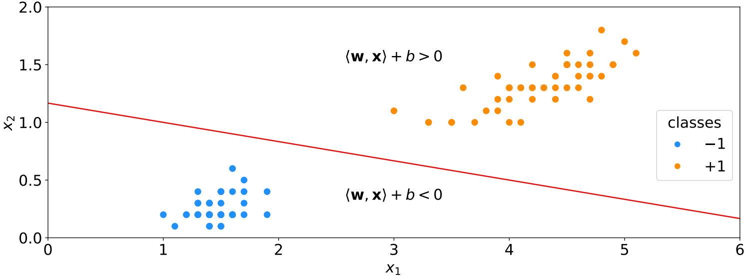
- $|f_{\boldsymbol{w},b}(\boldsymbol{x})|$ is called functional distance from $\boldsymbol{x}$ to $\mathcal{H}(\boldsymbol{w}, b)$.

Separating Hyperplane



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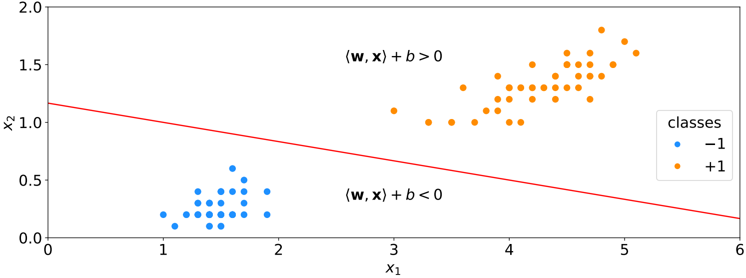

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$$\text{For } \boldsymbol{x} \in \mathbb{R}^n\text{:} \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b \begin{cases} = 0 \Rightarrow & \boldsymbol{x} \text{ in } \mathcal{H}(\boldsymbol{w}, b) \\ > 0 \Rightarrow & \boldsymbol{x} \text{ is in the positive half-space} \\ < 0 \Rightarrow & \boldsymbol{x} \text{ is in the negative half-space} \end{cases}$$

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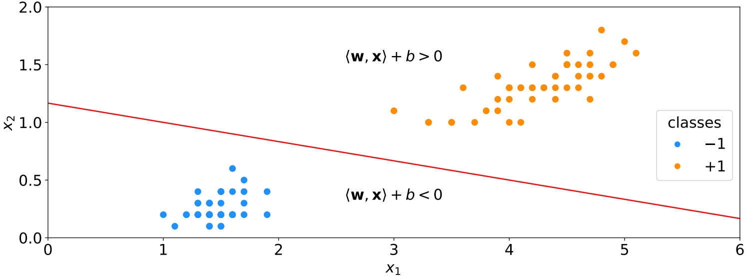
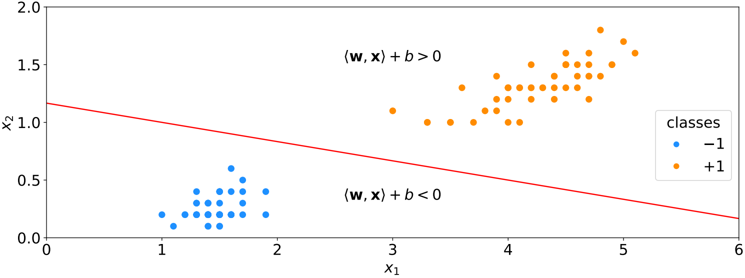


Definition 2 (Separating Hyperplane)

For a dataset D with two classes $(-1, +1)$, $\mathcal{H}(\boldsymbol{w}, b)$ is called a **separating hyperplane**, if for each instance $(\boldsymbol{x}, c) \in D$ holds

$$c = -1 \iff \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b < 0.$$

Binary Classification using a Hyperplane



Approach:

- learning phase: determine separating hyperplane $\mathcal{H}(\boldsymbol{w}, b)$
- classification: $\hat{c}(\boldsymbol{x}) := \begin{cases} +1 \text{ for } \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b \geq 0 \\ -1 \text{ for } \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b < 0 \end{cases}$

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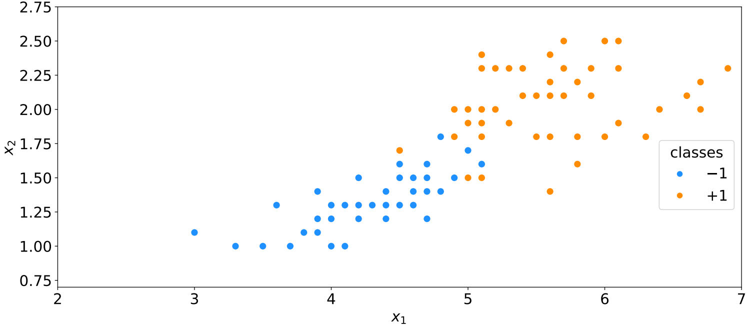
3. **Optimality:** Which is the best hyperplane?

Existence of a Separating Hyperplane



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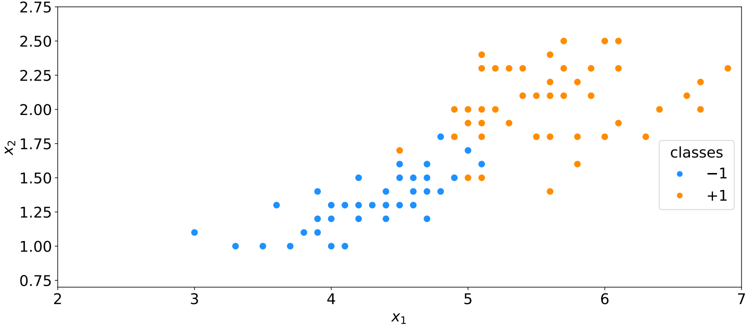

There are datasets for which no separating hyperplane exists.

Linear Separable

Definition 3 (Linear Separable)

Two sets $A, B \subseteq \mathbb{R}^n$ are called **linear separable**, if there exist $\boldsymbol{w} \in \mathbb{R}^n$ and $b \in \mathbb{R}$, such that

- for all $\boldsymbol{x} \in A$ holds $\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b \geq 0$ and
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The requirement of linear separability is a strong restriction on the applicability of this approach.[1]

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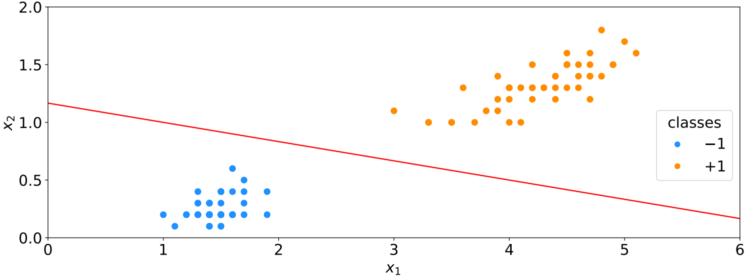
Uniqueness of a Separating Hyperplane



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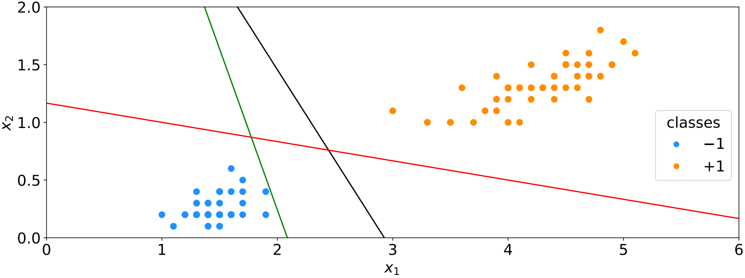

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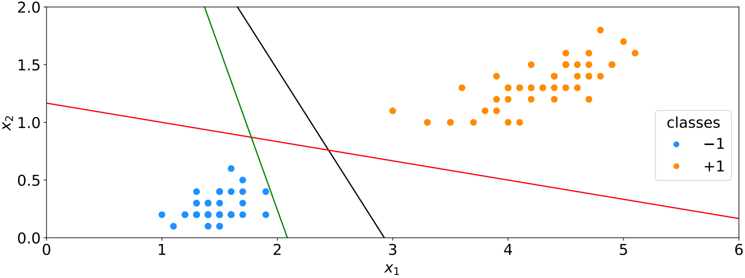

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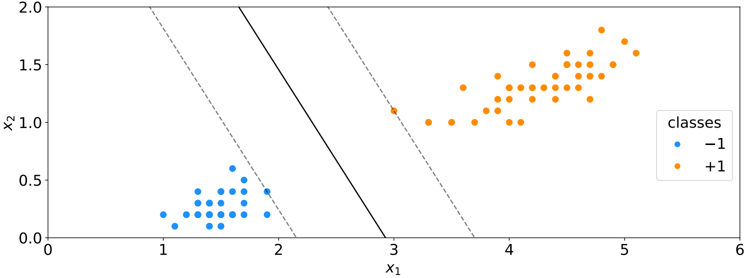
Which hyperplane is the best?

The Optimal Separating Hyperplane



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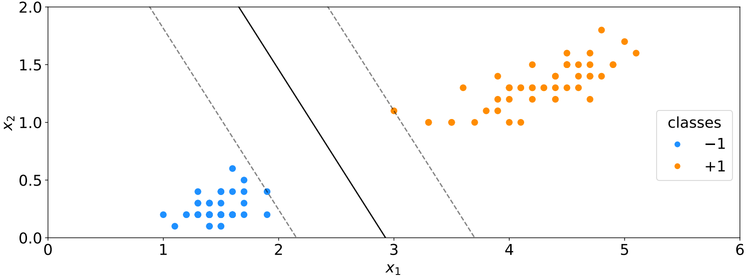

- **Generalization theory:** Estimate the risk of misclassification on unknown data

Risk of misclassification – Maximum Margin

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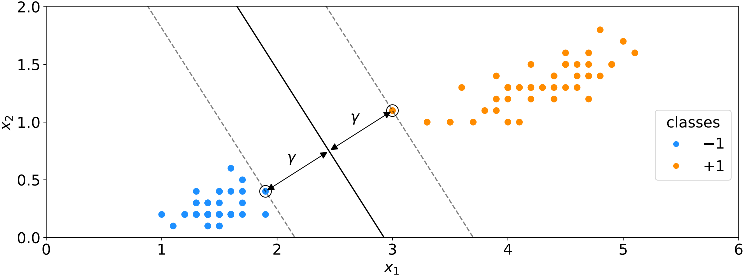
  - the probability of error δ (higher is better).
- **Result:** The higher the distance between hyperplane and data, the lower the risk.

The Optimal Separating Hyperplane



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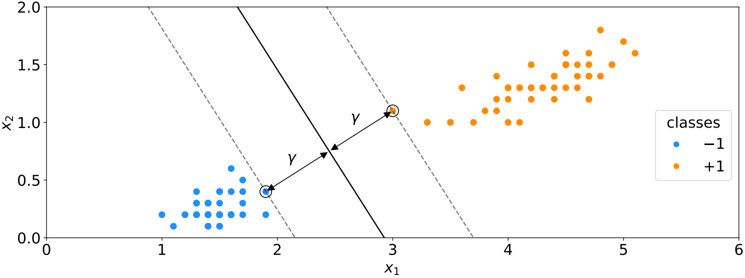

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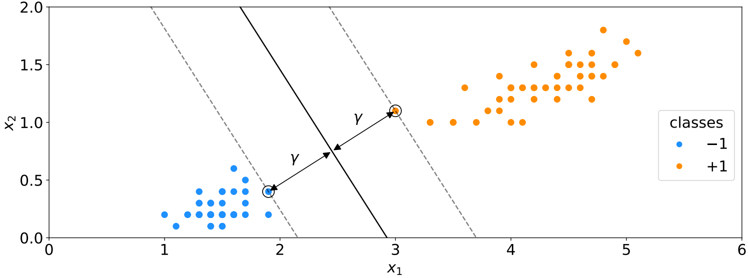

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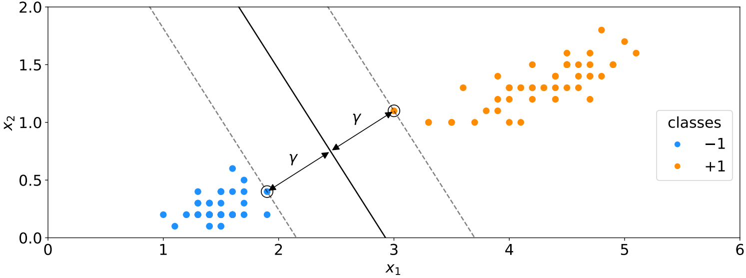
- Optimize $\gamma \to \max$

The distance γ



- $\lambda \in \mathbb{R}, \lambda > 0 : \mathcal{H}(\lambda \boldsymbol{w}, \lambda b) = \mathcal{H}(\boldsymbol{w}, b)$

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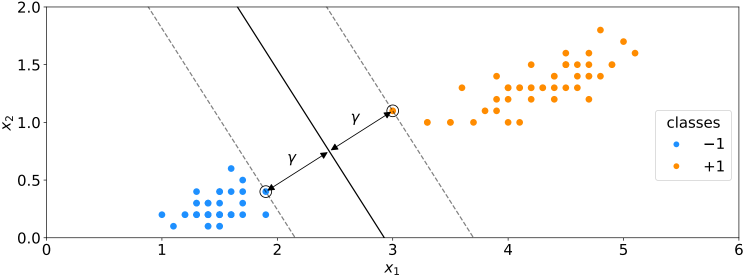

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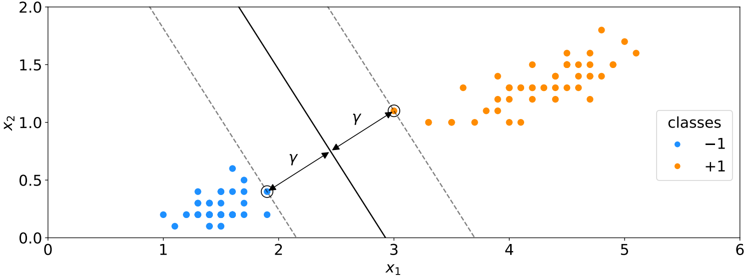

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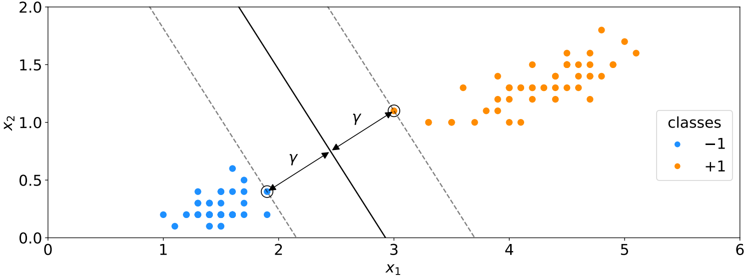

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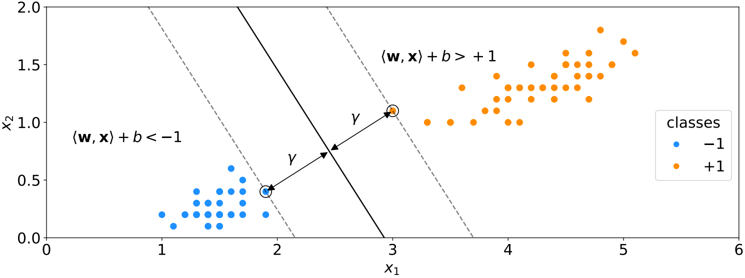
Optimization task for the Maximum Distance Classifier



Given: linear separable dataset $\{(\boldsymbol{x}_1, c_1), (\boldsymbol{x}_2, c_2), \ldots, (\boldsymbol{x}_\ell, c_\ell)\}$

Target: Minimize $\langle \boldsymbol{w}, \boldsymbol{w} \rangle$

- for $c_i = +1 : \langle \boldsymbol{w}, \boldsymbol{x_i} \rangle + b \geq +1$
- for $c_i = -1 : \langle \boldsymbol{w}, \boldsymbol{x_i} \rangle + b \leq -1$

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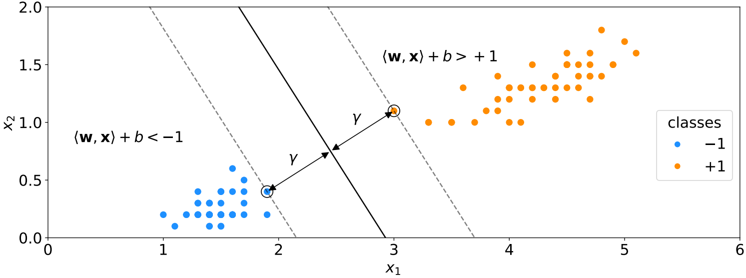

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Conditions: $c_i(\langle \boldsymbol{w}, \boldsymbol{x_i} \rangle + b) - 1 \geq 0$ for $i = 1, ..., \ell$

Solution of the Optimization Task

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- problem is convex → globally optimal solution

Solution of the Optimization Task

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- mathematical background: Lagrange-Theory, Karush-Kuhn-Tucker-Conditions
- problem is convex ➔ globally optimal solution
- Lagrange function:

$$L(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\langle \boldsymbol{w}, \boldsymbol{w} \rangle - \sum_{i=1}^{\ell} \alpha_i \left[c_i(\langle \boldsymbol{w}, \boldsymbol{x_i} \rangle + b) - 1 \right] \rightarrow \min$$

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- Result: $\boldsymbol{w}^*, b^*, \boldsymbol{\alpha}^*$

Observations 1/2

- b can be computed as

$$b^* := -\frac{\max_{c_i=-1}(\langle \boldsymbol{w}^*, \boldsymbol{x_i} \rangle) + \min_{c_i=1}(\langle \boldsymbol{w}^*, \boldsymbol{x_i} \rangle)}{2}$$

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- the distance γ between hyperplane and data is

$$\gamma = \left(\sum_{i:\alpha_i \neq 0} \alpha_i^* \right)^{-\frac{1}{2}} .$$

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- In the solution, we yield

$$\alpha_i^*(c_i(\langle \boldsymbol{w^*}, \boldsymbol{x_i} \rangle + b^*) - 1) = 0 \text{ for } 1 \leq i \leq \ell,$$

and thus $\alpha_i^* \neq 0 \implies \langle \boldsymbol{w^*}, \boldsymbol{x_i} \rangle + b^* = \pm 1$ ($\boldsymbol{x_i}$ has minimum distance γ).

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- usually, the number of support vectors is way smaller than the number of training instances ℓ

Classification

To classify an instance $\boldsymbol{x}$, we compute

$$\hat{c}(\boldsymbol{x}) := \begin{cases} +1 \text{ for } \langle \boldsymbol{w^*}, \boldsymbol{x} \rangle + b^* \geq 0 \\ -1 \text{ for } \langle \boldsymbol{w^*}, \boldsymbol{x} \rangle + b^* < 0 \end{cases}$$

$$\langle \boldsymbol{w^*}, \boldsymbol{x} \rangle = \langle \sum_{i:\alpha_i^* \neq 0} c_i \alpha_i^* \boldsymbol{x_i}, \boldsymbol{x} \rangle = \sum_{i:\alpha_i^* \neq 0} c_i \alpha_i^* \langle \boldsymbol{x_i}, \boldsymbol{x} \rangle$$

Thus, classification is computed directly by computing a couple of scalar products between the instance to classify and only those instances of the training data that are support vectors.

Achievements (so far)

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SVMs learn parameters for a linear function

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Stability:
Solution depends only on the support vectors ➔ very stable against perturbation of the training set

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Notebook 05_1_Iris_23, Cells 1–12

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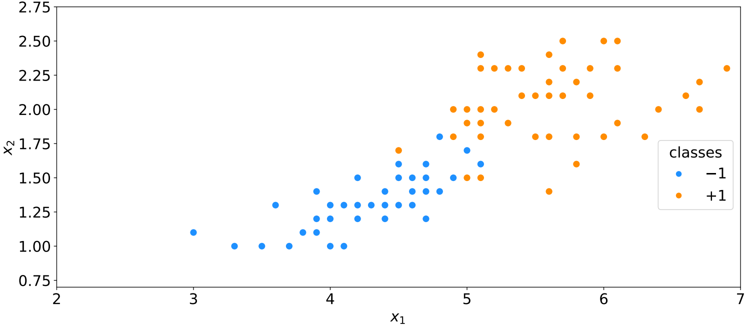
Notebook 05_1_Iris_23, Cells 1–12

Exercises 1–3

Outline

The Maximum Distance Classifier



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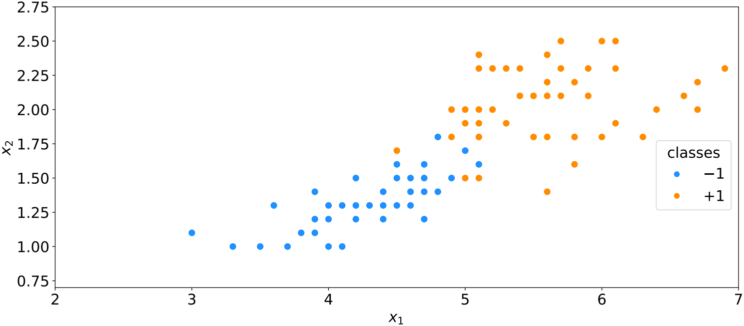

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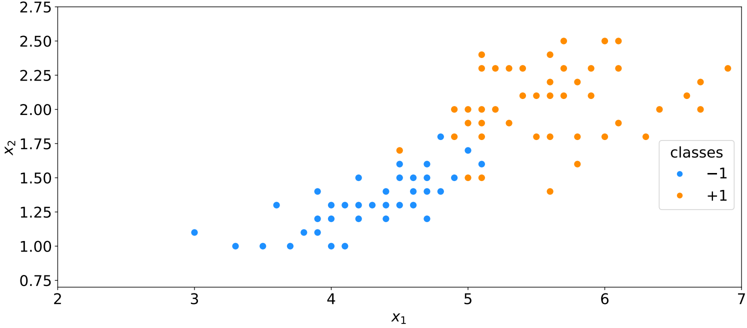

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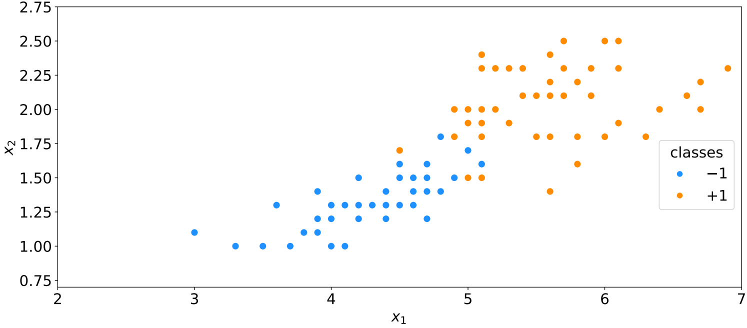

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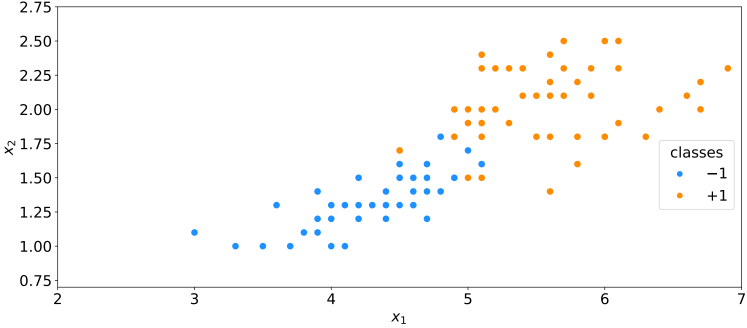

Given: dataset, not linear separable

Idea: modify the optimization problem

- to allow some digressions
- optimize a trade-off between digression and margin

Soft-Margin Optimization

$$\frac{1}{2}\langle \boldsymbol{w}, \boldsymbol{w} \rangle + C \sum_{i=1}^{\ell} \xi_i \to \min$$

with

$$c_i(\langle \boldsymbol{w}, \boldsymbol{x_i} \rangle + b) \geq 1 - \xi_i \text{ und } \xi_i \geq 0 \text{ for } i = 1, \ldots, \ell.$$

- the ξ_i are called **slack variables**.
- C is a hyperparameter, controlling the trade-off between margin and slack – between generalization and bias
  - higher C punishes digression harder (thus lower misclassification probability)

Soft-Margin – Lagrange Approach

Lagrange-Approach:

$$L(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{r}) = \frac{1}{2}\langle \boldsymbol{w}, \boldsymbol{w}\rangle + C\sum_{i=1}^{\ell}\xi_i$$
$$-\sum_{i=1}^{\ell}\alpha_i\left[c_i(\langle \boldsymbol{w}, \boldsymbol{x_i}\rangle + b) - 1 + \xi_i\right]$$
$$-\sum_{i=1}^{\ell} r_i\xi_i$$
$$\rightarrow \min$$

with $\alpha_i \geq 0$ and $r_i \geq 0$ for $1 \leq i \leq \ell$.

Soft-Margin Dual

In the solution of the optimization task, we yield $\boldsymbol{w}^* := \sum_{i=1}^{\ell} c_i \alpha_i^* \boldsymbol{x_i}$ and the margin

$$\gamma = \left(\sum_{i,j \in sv} c_i c_j \alpha_i^* \alpha_j^* \langle \boldsymbol{x_i}, \boldsymbol{x_j} \rangle \right)^{-\frac{1}{2}}$$

with the Box Constraint: $0 \leq \boldsymbol{\alpha} \leq \boldsymbol{C}$

Soft-Margin KKT Conditions

$$\alpha_i \left[c_i(\langle \boldsymbol{w}, \boldsymbol{x_i} \rangle) - 1 + \xi_i\right] = 0, \quad i = 1, \ldots, \ell,$$
$$\xi_i(\alpha_i - C) = 0, \quad i = 1, \ldots, \ell,$$

Thus follows:

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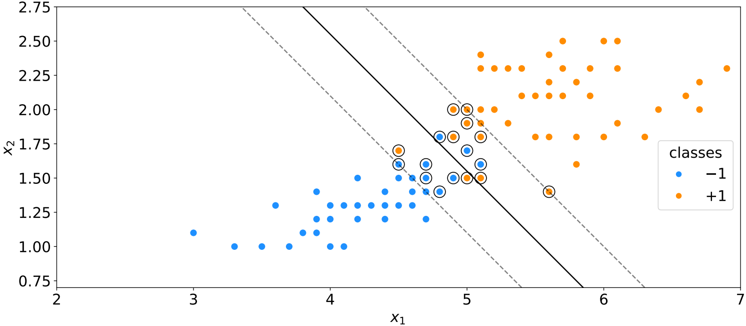
  - $0 < \alpha_i < C \Rightarrow \boldsymbol{x_i}$ is on the border of the margin
  - $\alpha_i = C \Rightarrow \boldsymbol{x_i}$ is either correctly classified but within the margin ($\xi_i < 1$), on the hyperplane ($\xi_i = 1$), or misclassified ($\xi_i > 1$)

The Maximum Distance Classifier



In this example, we yield 17 support vectors, most of them within the margin.

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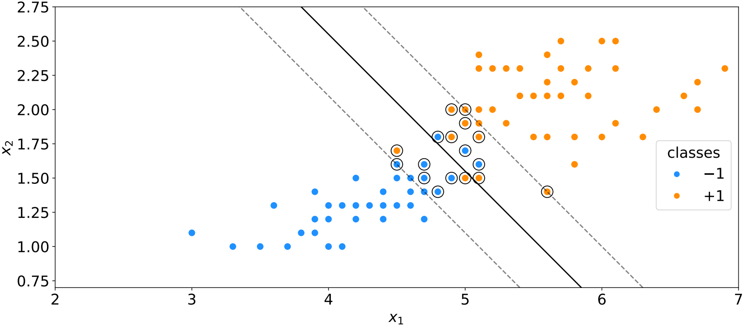

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Notebook 05_1_Iris_23, Cells 13–31

Outline

Basic Idea

Mathematical Description

Soft-Margin SVMs

Kernel Trick

Embedding into higher-dimensional spaces

Problem: Datasets are rarely linear separable

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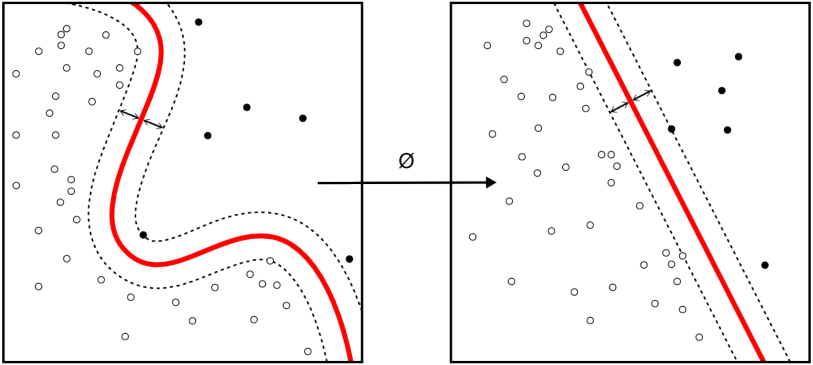

Embedding: Example

Given a non-separable dataset in $\mathbb{R}^3$.
1.) Choose embedding $\phi : \mathbb{R}^3 \to \mathbb{R}^6$:

$$\begin{aligned} \phi_1(\boldsymbol{x}) &= x_1 & \phi_2(\boldsymbol{x}) &= x_2 & \phi_3(\boldsymbol{x}) &= x_3 \\ \phi_4(\boldsymbol{x}) &= x_1^2 & \phi_5(\boldsymbol{x}) &= x_1 x_2 & \phi_6(\boldsymbol{x}) &= x_1 x_3 \end{aligned}$$

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Note, that the classification function allows us to consider features combined, e.g. $x_1 x_2$.

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Observation:
in the classifier and in the actual optimization, the training data occur only in scalar products, e.g.

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- optimization and classification work with all kinds of scalar products

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SVMs:

The full construction of the SVM classifier works, if regular scalar product is replaced by some kernel function.

Classification Model

Regular classification function in input space $\mathcal{I}$

$$f_{\boldsymbol{w},b}(\boldsymbol{x}) = \sum_{i:\alpha_i^{\mathcal{I}*} \neq 0} c_i \alpha_i^{\mathcal{I}*} \langle \boldsymbol{x_i}, \boldsymbol{x} \rangle_{\mathcal{I}} + \boldsymbol{b}^{\mathcal{I}}$$

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Transformation into the feature space $\mathcal{F}$

$$f_{\boldsymbol{w},b} \circ \phi(\boldsymbol{x}) = \sum_{i:\alpha_i^{\mathcal{F}*} \neq 0} c_i \alpha_i^{\mathcal{F}*} \langle \phi(\boldsymbol{x_i}), \phi(\boldsymbol{x}) \rangle_{\mathcal{F}} + \boldsymbol{b}^{\mathcal{F}}$$

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Transformation into the feature space $\mathcal{F}$

$$f_{\boldsymbol{w},b} \circ \phi(\boldsymbol{x}) = \sum_{i:\alpha_i^{\mathcal{F}*} \neq 0} c_i \alpha_i^{\mathcal{F}*} \langle \phi(\boldsymbol{x_i}), \phi(\boldsymbol{x}) \rangle_{\mathcal{F}} + \boldsymbol{b}^{\mathcal{F}}$$

Using a kernel function $K(x, y) \coloneqq \langle \phi(\boldsymbol{x_i}), \phi(\boldsymbol{x}) \rangle_{\mathcal{F}}$

$$f_{\boldsymbol{w},b} \circ \phi(\boldsymbol{x}) = \sum_{i:\alpha_i^{\mathcal{F}*} \neq 0} c_i \alpha_i^{\mathcal{F}*} K(\boldsymbol{x_i}, \boldsymbol{x}) + \boldsymbol{b}^{\mathcal{F}}$$

Kernel Functions – Example

Kernel function $K : \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R} : (\boldsymbol{x}, \boldsymbol{y}) \mapsto (\langle \boldsymbol{x}, \boldsymbol{y} \rangle_2 + 1)^2$

$$\begin{aligned} K(\boldsymbol{x}, \boldsymbol{y}) &= (\langle \boldsymbol{x}, \boldsymbol{y} \rangle_2 + 1)^2 \\ &= (x_1 y_1 + x_2 y_2 + 1)^2 \end{aligned}$$

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&= \langle (x_1^2,\, x_2^2,\, 1,\, \sqrt{2} x_1 x_2,\, \sqrt{2} x_1,\, \sqrt{2} x_2)^T, \\
&\qquad\quad (y_1^2,\, y_2^2,\, 1,\, \sqrt{2} y_1 y_2,\, \sqrt{2} y_1,\, \sqrt{2} y_2)^T \rangle_6
\end{aligned}$$

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With $\phi : \mathbb{R}^2 \to \mathbb{R}^6 : x \mapsto (x_1^2,\, x_2^2,\, 1,\, \sqrt{2}x_1 x_2,\, \sqrt{2}x_1,\, \sqrt{2}x_2)^T$:

$$K(\boldsymbol{x}, \boldsymbol{y}) = \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{y}) \rangle_6$$

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$$K(\boldsymbol{x}, \boldsymbol{y}) = \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{y}) \rangle_6$$

Computation: scalar product in $\mathbb{R}^2$, sum, multiplication
Result: polynomial embedding, scalar product in $\mathbb{R}^6$

Kernel Trick: discussion

Achievement:

Kernels make SVMs powerful and efficient

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Kernels have their own parameters (see below) which become hyperparameters of the algorithm

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- Select a function K that is known to be a kernel function.
  - neither ϕ nor the feature space are considered explicitly
  - kernel property is verified mathematically (Mercer Theorem)
  - kernel functions can be found by combining known kernel functions

Mercer Theorem – finite

Theorem 4

Let X be a finite subset of $\mathbb{R}^n$ and K a symmetrical function on X. Then, K is a kernel function if and only if matrix

$$\left(K(\boldsymbol{x_i} \boldsymbol{x_j})\right)_{i,j}^{n}$$

is positive semidefinite (no negative eigenvalues).

Popular Kernels – The Polynomial Kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = (\gamma\langle \boldsymbol{x}, \boldsymbol{y}\rangle + r)^d$$

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$n_\mathcal{O}$	d	$n_\mathcal{F}$
2	2	6
2	3	10
10	2	66
1,000	2	501,501

Popular Kernels – The Radial-Basis-Function Kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{y}\|^2)$$

- a.k.a. Gaussian Kernel (for $\gamma = \frac{1}{2\sigma^2}$)

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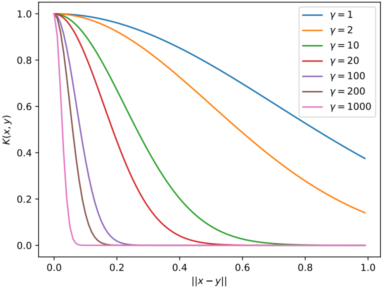

Notebook 05_1_Iris_23, Cells 24–26

Exercises 4