Introductory Course: Machine Learning (WWI15B4)

Support Vector Machines

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DHBW Karlsruhe

Overview

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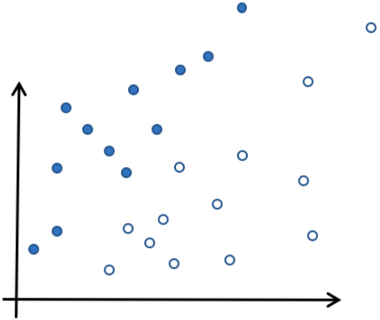
Recommended Literature

- V.N. Vapnik: "Statistical Learning Theory", Wiley, 1998
- B. Schoelkopf: "Support Vector Learning"
- Patrick Winston, MIT 6.034 Artificial Intelligence, Fall 2010, `https://www.youtube.com/watch?v=_PwhiWxHK8o`

Introduction

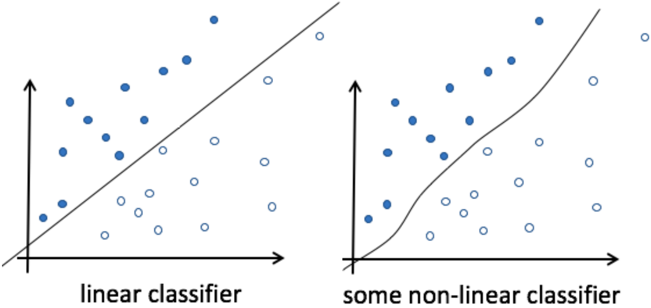
How to separate this space?



filled samples: positive, blank samples: negative

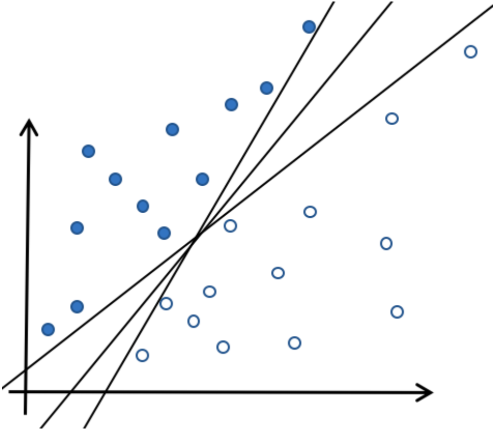
Introduction

Approaches we know so far would do something like this:

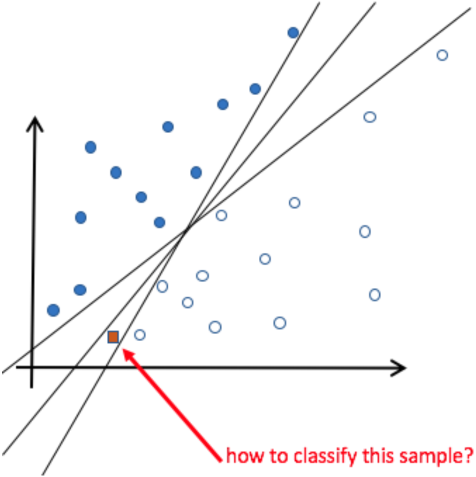


Introduction

There exist many hyperplanes that would correctly classify the data. Which one is the best?

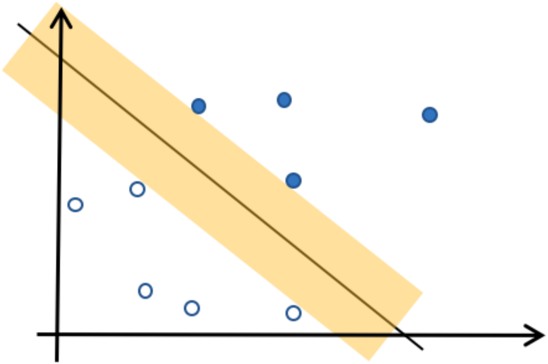


Introduction



Introduction

Let's choose a hyperplane so that it represents the largest separation (margin) between both classes.
This yields the task: maximize the distance from the *middle line* to the nearest data point on each side.



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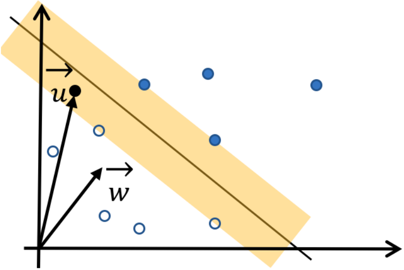
Linear Maximum Margin Classifier: Decision Rule

Considering a vector pointing to an unknown sample $\vec{u}$ and a vector $\vec{w}$ of arbitrary length constrained to be perpendicular to the middle line. **Task:** Determine if $\vec{u}$ is on the right or left side of the hyperplane



Idea: project $\vec{u}$ onto $\vec{w}$ with some constant $c \in \mathbb{R}$:

$$\vec{w} \cdot \vec{u} \geq c$$

or

$$\vec{w} \cdot \vec{u} + b \geq 0, c = -b$$

Decision rule: if this inequality holds then $\vec{u}$ is a positive sample

Linear Maximum Margin Classifier: Constraints

Remember the decision rule: $\vec{w} \cdot \vec{u} + b \geq 0 \Rightarrow$ positive sample
Idea: if some unknown sample is a positive sample, we insist the decision rule yields ≥ 1 (otherwise ≤ -1.)

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Mathematically:

- for positive samples: $\vec{w} \cdot \vec{x}_+ + b \geq 1$
- for negative samples: $\vec{w} \cdot \vec{x}_- + b \leq -1$

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For convenience we introduce a variable y_i s.t.:

- $y_i = 1$ for positive samples and $y_i = -1$ for negative samples

The comfort we gain: only one inequality that holds for x_i laying outside of the margin boundaries

$$\boxed{y_i(\vec{x}_i \cdot \vec{w} + b) \geq 1}$$

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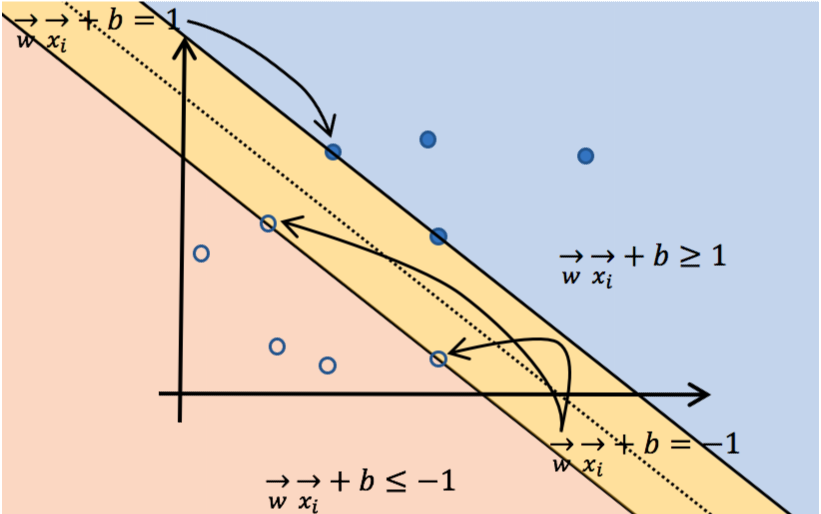
and we add one additional constraint for x_i placed on the margin boundaries:

$$\boxed{y_i(\vec{x}_i \cdot \vec{w} + b) - 1 = 0}$$

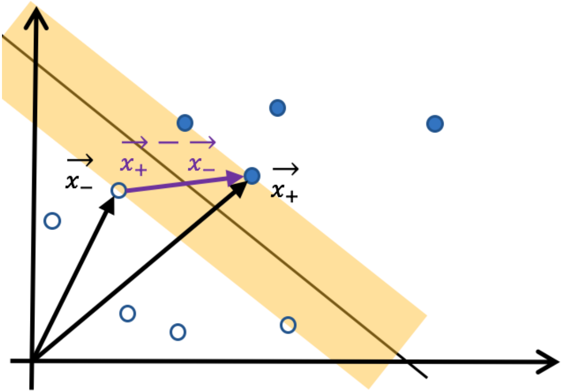
Linear Maximum Margin Classifier: Constraints

Geometrically this gives us:



Linear Maximum Margin Classifier: Margin Width

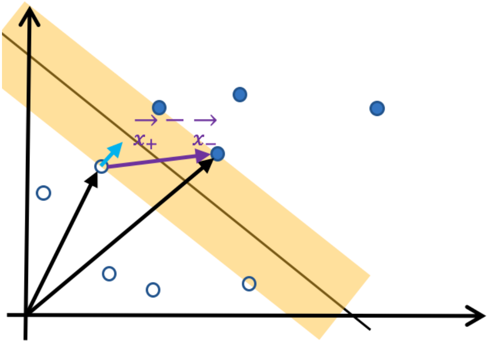
Recall: we want to maximize the distance between points of two different classes. This raises the question: how to express the distance between the two margin boundaries?



Linear Maximum Margin Classifier: Margin Width

How to express the distance between the two margin boundaries?

One solution: compute the width with a unit vector (light blue) and project the purple vector on that unit vector



$$width = (\vec{x}_+ - \vec{x}_-) \cdot \frac{\vec{w}}{||\vec{w}||}$$

Linear Maximum Margin Classifier: Margin Width

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now use $y_i(\vec{x}_i \cdot \vec{w} + b) - 1 = 0$ from before for to get:

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$$width = \frac{(1 - b + 1 + b)}{\|\vec{w}\|} = \frac{2}{\|\vec{w}\|}$$

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our goal now is:

$$\max \frac{2}{\|\vec{w}\|} = \max \frac{1}{\|\vec{w}\|} = \min \|\vec{w}\| \rightsquigarrow \min \frac{1}{2}\|\vec{w}\|^2$$

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find extremum of a function with constraints

$\rightarrow$ use Lagrangian optimization (method of Lagrange multipliers)

$\rightarrow$ yields a new (closed) expression with the constraints included

Linear Maximum Margin Classifier: Lagrangian Multipliers

Recall: we had defined a constraint for x_i placed directly on the margin boundaries: $y_i(\vec{x_i} \cdot \vec{w} + b) - 1 = 0 \rightarrow$ re-use it for the Lagrangian for m samples:

$$L(\vec{w}, \vec{\alpha}, b) = \frac{1}{2}\|\vec{w}\|^2 - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1] \qquad (1)$$

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compute the minimum/first partial derivatives of L w.r.t. $\vec{w}$ and b:

$$\frac{\partial L}{\partial \vec{w}} = \vec{w} - \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i = 0 \Rightarrow \boxed{\vec{w} = \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i} \tag{2}$$

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$$\frac{\partial L}{\partial \vec{b}} = -\sum_{i=1}^{m} \alpha_i y_i = 0 \Rightarrow \boxed{\sum_{i=1}^{m} \alpha_i y_i = 0} \tag{3}$$

Linear Maximum Margin Classifier: Lagrangian Multipliers

now we plug eq. 2 into eq. 1, simplify it and get:

$$W(\vec{\alpha}) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j \vec{x_i} \cdot \vec{x_j} \tag{4}$$

[1] note that W is a quadratic function $\Rightarrow$ convex problem

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- Those $\vec{x_i}$ with $\alpha_i > 0$ we call **support vectors** which all lie perpendicular to the margin line

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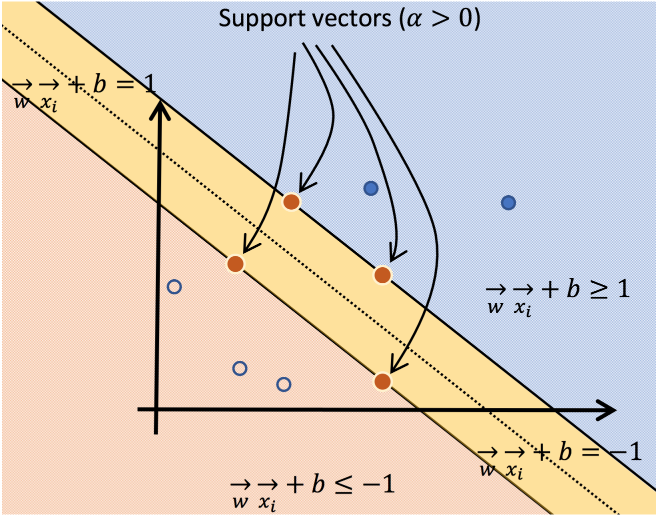
Linear Maximum Margin Classifier: Support Vectors



Linear Maximum Margin Classifier: Lagrangian Multipliers

Recall the the **decision rule** $\vec{w} \cdot \vec{u} + b \geq 0$ for positive samples, insert $\vec{w} = \sum_{i=1}^{m} \alpha_i y_i \vec{x_i}$ (eq. 2) and we get:

$$\sum_{i=1}^{m} \alpha_i y_i \vec{x_i} \cdot \vec{u} + b \geq 0$$

for a positive (unknown) sample $\vec{u}$. The decision rule now also **only depends on α_i and on the the dot product between $\vec{x_i}$ and $\vec{u}$**

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for a positive (unknown) sample $\vec{u}$. The decision rule now also **only depends on α_i and on the the dot product between $\vec{x_i}$ and $\vec{u}$**
This lets us specify a classification rule:

$$f(\vec{u}) = sgn(\vec{w} \cdot \vec{u} + b) = \boxed{sgn\left(\sum_{i=1}^{m} \alpha_i y_i \vec{x_i} \cdot \vec{u} + b\right)}$$

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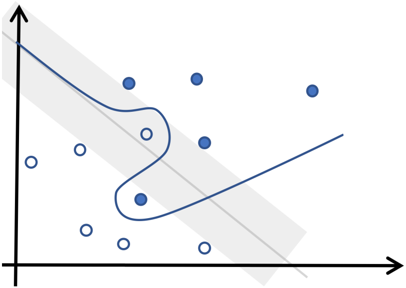
Non-linear separable data

What if the data is not linearly separable (as in most practical cases)?



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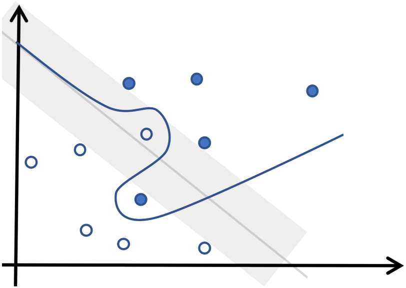

⇒ linear SVM won't converge. Two common solutions:

- adjust SVM specification to use a soft margin
- apply kernel methods
- (or both)

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Soft Margin

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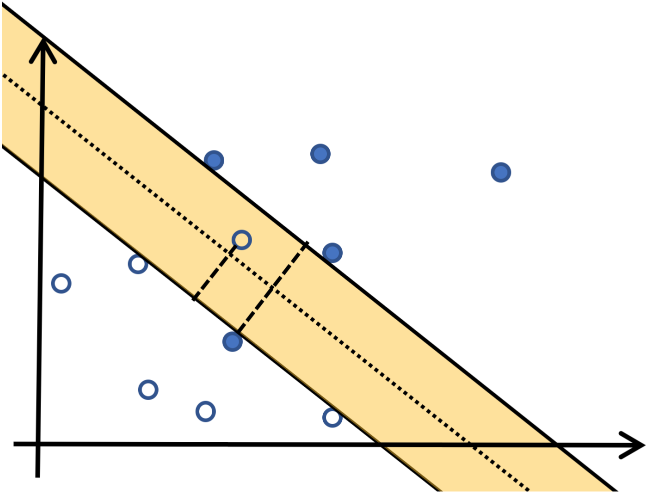
- if C small $\Rightarrow$ more misclassified samples allowed

Soft Margin Example



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Example

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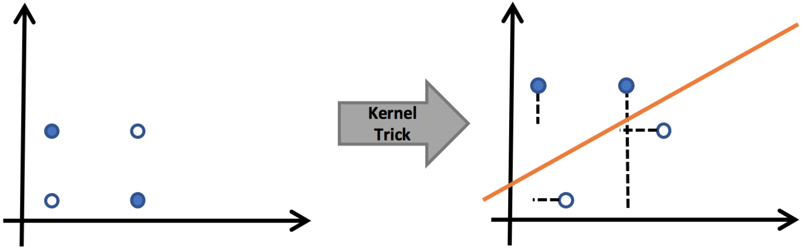
use the *kernel trick* for projecting into such higher-dimensional space, for example:



Kernel Trick

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The approach of transforming data into an **implicitly** higher-dimensional space without computing coordinates of the data in that space, but rather by computing pairwise inner products of the samples. Typically $K(\vec{x}_i, \vec{x}_j) = \phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$ [Wikipedia]

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Some clarification:

- the kernel trick **does not** produce a **mapping** from low to high-dimensional space
- it does provide a solution to compute inner products of samples in high-dim. space **without knowing the mapping**

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Some clarification:

- the kernel trick **does not** produce a **mapping** from low to high-dimensional space
- it does provide a solution to compute inner products of samples in high-dim. space **without knowing the mapping**
- Advantages: low-cost computation, operating in infinite spaces (e.g. Gaussian kernel) possible

Kernel Trick Example

Example for $K(\vec{x}, \vec{z}) = (\vec{x} \cdot \vec{z})^2$
without using the kernel trick (explicit mapping):

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_{\mathbb{R}^3} \qquad \phi(x) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_1 x_3 \\ \vdots \\ x_3 x_3 \end{bmatrix}_{\mathbb{R}^9}$$

$\Rightarrow$ 18 multiplications (project x and $z : \mathbb{R}^3 \rightarrow \mathbb{R}^9$) + 9 multiplications + 8 additions (inner product) = 35 operations

Kernel Trick Example

Example for $K(\vec{x}, \vec{z}) = (\vec{x} \cdot \vec{z})^2$
using the kernel trick:

$$\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_1 \\ z_1 \end{bmatrix} \right)^2 = (x_1 z_1 + x_2 z_2 + x_3 z_3)^2$$

$\Rightarrow$ 3 multiplications + 2 additions + 1 multiplication $((\cdot)^2)$
$=$ 6 operations

Kernel Trick in the SVM

Where the kernel trick is used in the SVM:

$$W(\vec{\alpha}) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j \boxed{\vec{x_i} \cdot \vec{x_j}}$$

[2] must fulfill the Mercer theorem

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Note: not all functions $\phi : \mathrm{I\!R}^{\mathrm{n}} \rightarrow \mathrm{I\!R}^{\mathrm{m}}, (n, m) \in \mathrm{I\!R}$ are valid kernel functions[2].

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Popular kernel functions are:

- inner product: $K(\vec{x}, \vec{z}) = \vec{x} \cdot \vec{z}$
- degree-d polynomial: $K(\vec{x}, \vec{z}) = (\vec{x} \cdot \vec{z} + c)^d, c \geq 0$

---

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Kernel Trick in the SVM

Where the kernel trick is used in the SVM:

$$W(\vec{\alpha}) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j \boxed{\vec{x_i} \cdot \vec{x_j}}$$

Note: not all functions $\phi : \mathbb{R}^n \to \mathbb{R}^m, (n, m) \in \mathbb{R}$ are valid kernel functions[2].

Popular kernel functions are:

- inner product: $K(\vec{x}, \vec{z}) = \vec{x} \cdot \vec{z}$
- degree-d polynomial: $K(\vec{x}, \vec{z}) = (\vec{x} \cdot \vec{z} + c)^d, c \geq 0$
- Gaussian radial basis function[3]: $K(\vec{x}, \vec{z}) = \exp(-\frac{\|\vec{x}-\vec{z}\|^2}{2\sigma^2})$

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[2] must fulfill the Mercer theorem

[3] also called Gaussian kernel

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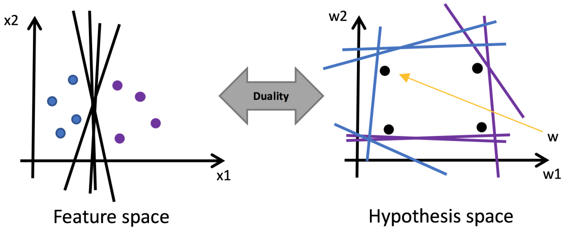
Duality of feature and hypothesis space

Points in the feature space correspond to hyperplanes in the hypothesis space and vice versa ("Statistical Learning Theory", Vapnik, 1998).



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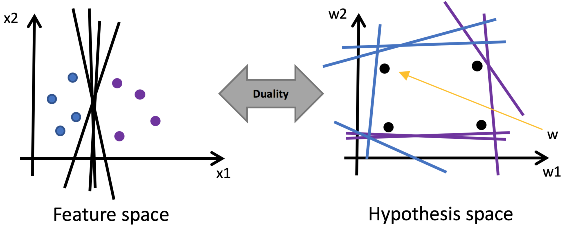
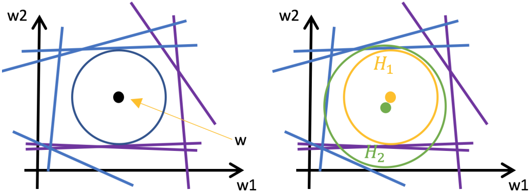


Implications:

- the more data points, the more the hypothesis space will be constrained
- maximum margin search means searching for hyper planes with largest distance to data points $\Rightarrow$ center point of hyper sphere

Structural Risk Minimization



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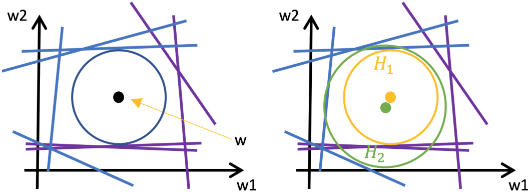
Structural Risk Minimization



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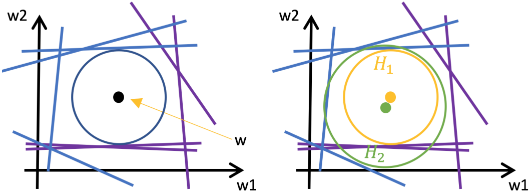

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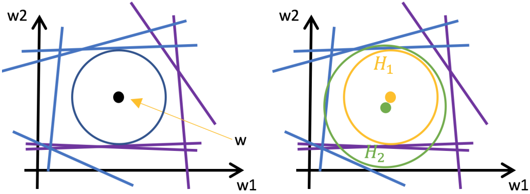

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- then, the best hyper plane with the smallest empirical error is chosen (center point of hyper sphere)
- recall from concept learning lecture: this is **Structural Risk Minimization** e.g. $\ldots H_3 \subset H_2 \subset H_1$

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Advantages

- SVM optimization problem is convex (no local minima)
- can handle high-dimensional data well
- fast test time execution (usually few $\alpha_i > 0 \Rightarrow$ few inner products, if linear SVM: $\vec{w}$ can always be pre-computed [use eq. 2], if non-linear SVM: no pre-computation of $\vec{w}$ guaranteed [e.g. Gaussian kernel] but computing inner products between support vector train samples and a new sample is still relatively cheap)

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Disadvantages

- data samples have to be stored (space complexity not negligible, however, SVM is still not a lazy-learner since it learns a decision boundary $\Rightarrow$ eager-learner)
- number of support vectors depend on problem
- no pre-processing of the data in the SVM approach included
- finding optimal kernel can be tedious

Reading Assignment

Use the Internet to gain knowledge about the following topics:

- multi-class SVM (one-vs-all and one-vs-one)
- where the kernel trick is further applied (in addition to the SVM)