NIO

Exercise 13: SVMs, Exam Hints

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Revision of Lecture

- What is the general idea of a Support Vector Machine?

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- What is the general idea of a Support Vector Machine?
  1) Find optimal hyperplane to linearly separate two classes
  2) Exactly the same as the perceptron
  3) Feature reduction
  4) Find optimal hyperplane for regression problems

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A: 1, 2, 3	B: all
C: 1	D: 1,4

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    (similar general idea as perceptron!)

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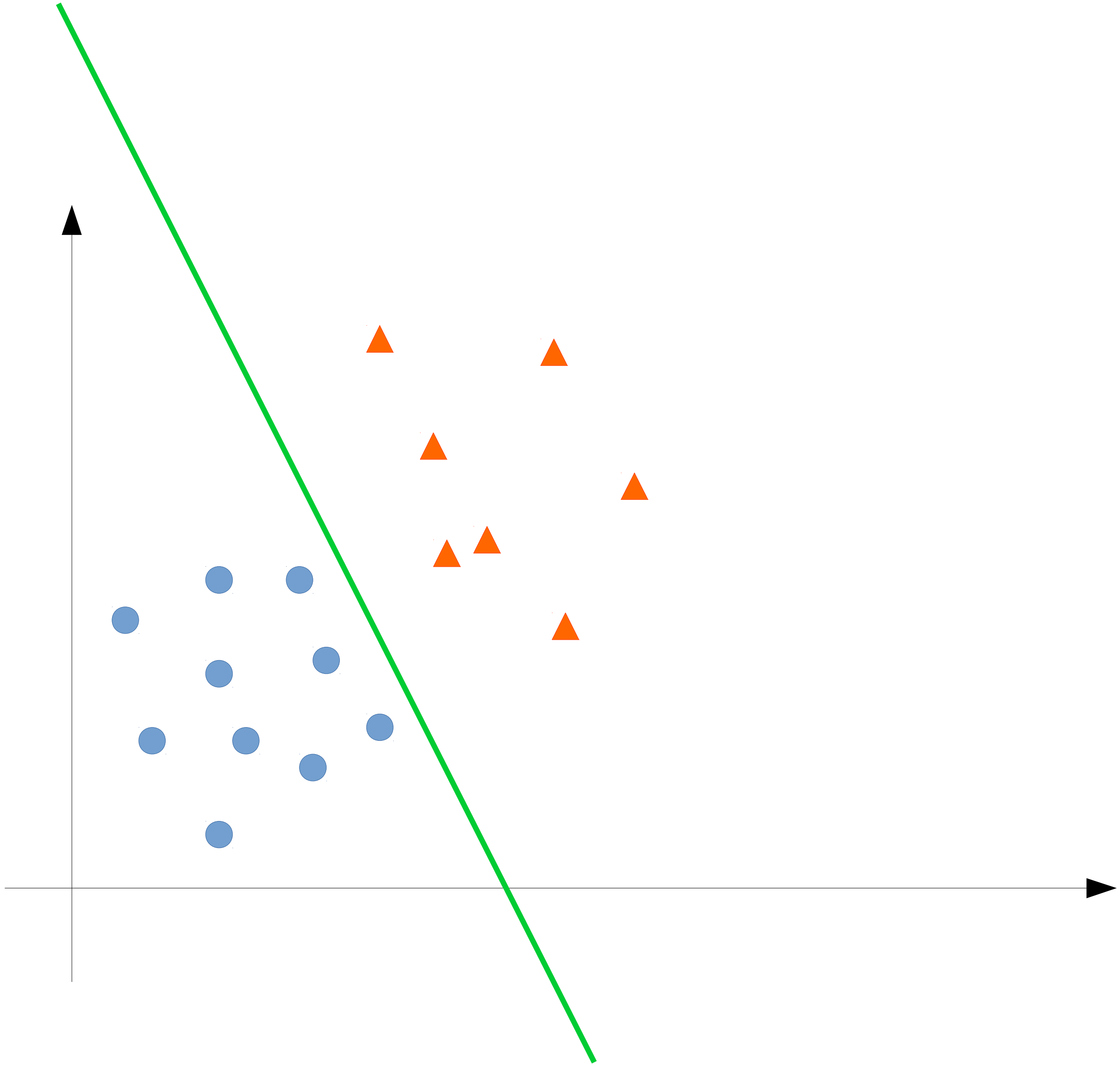
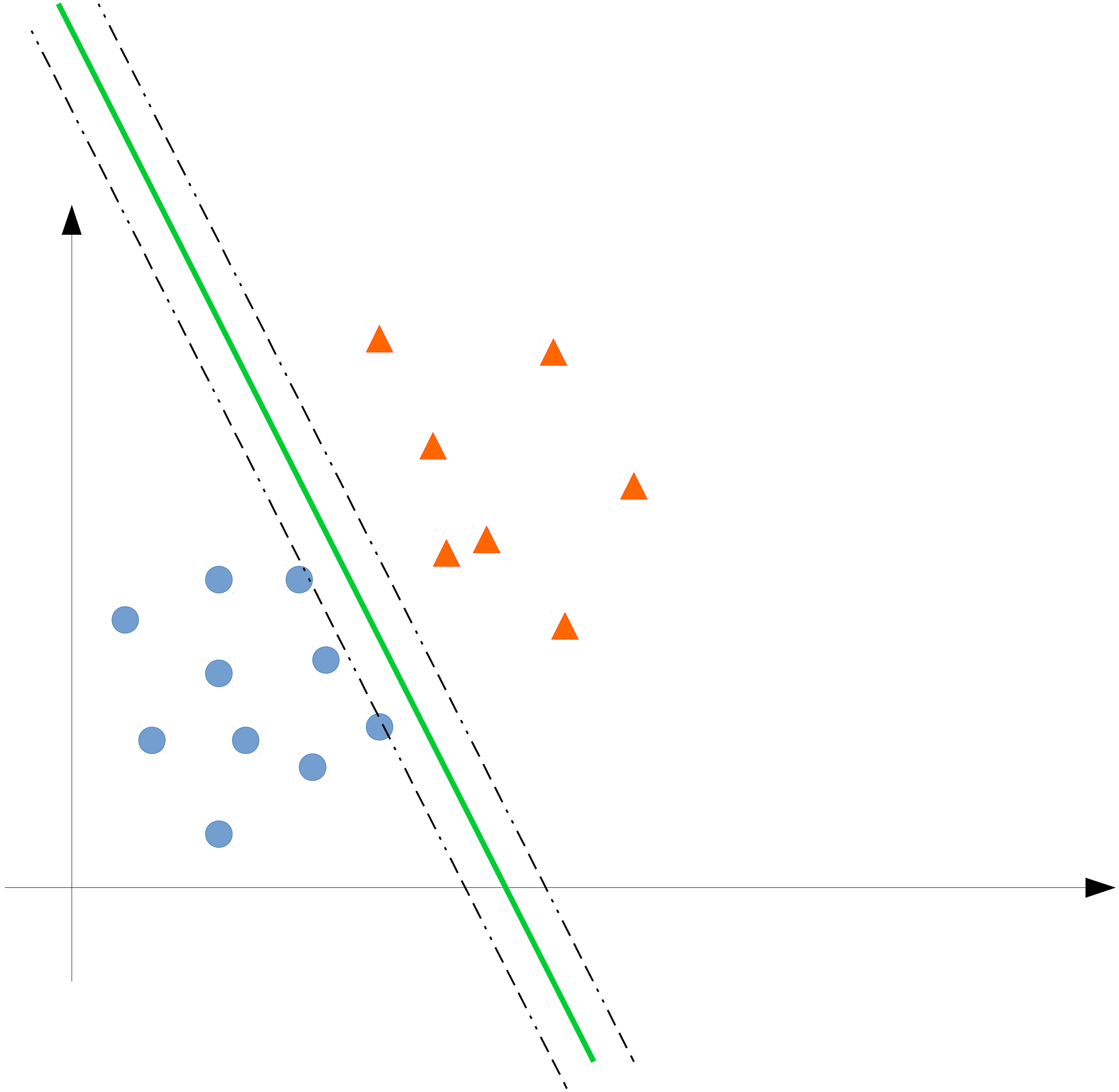
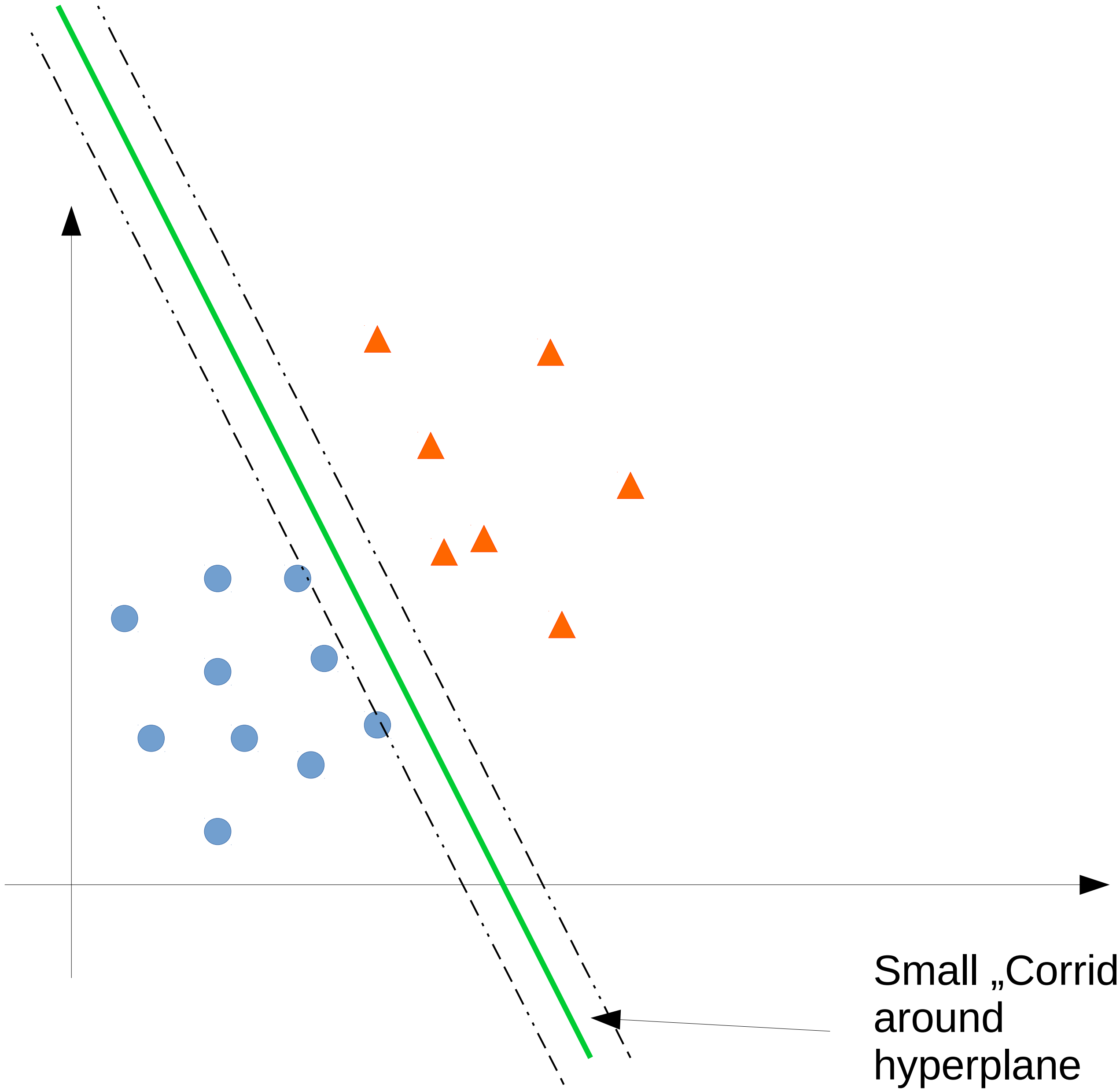
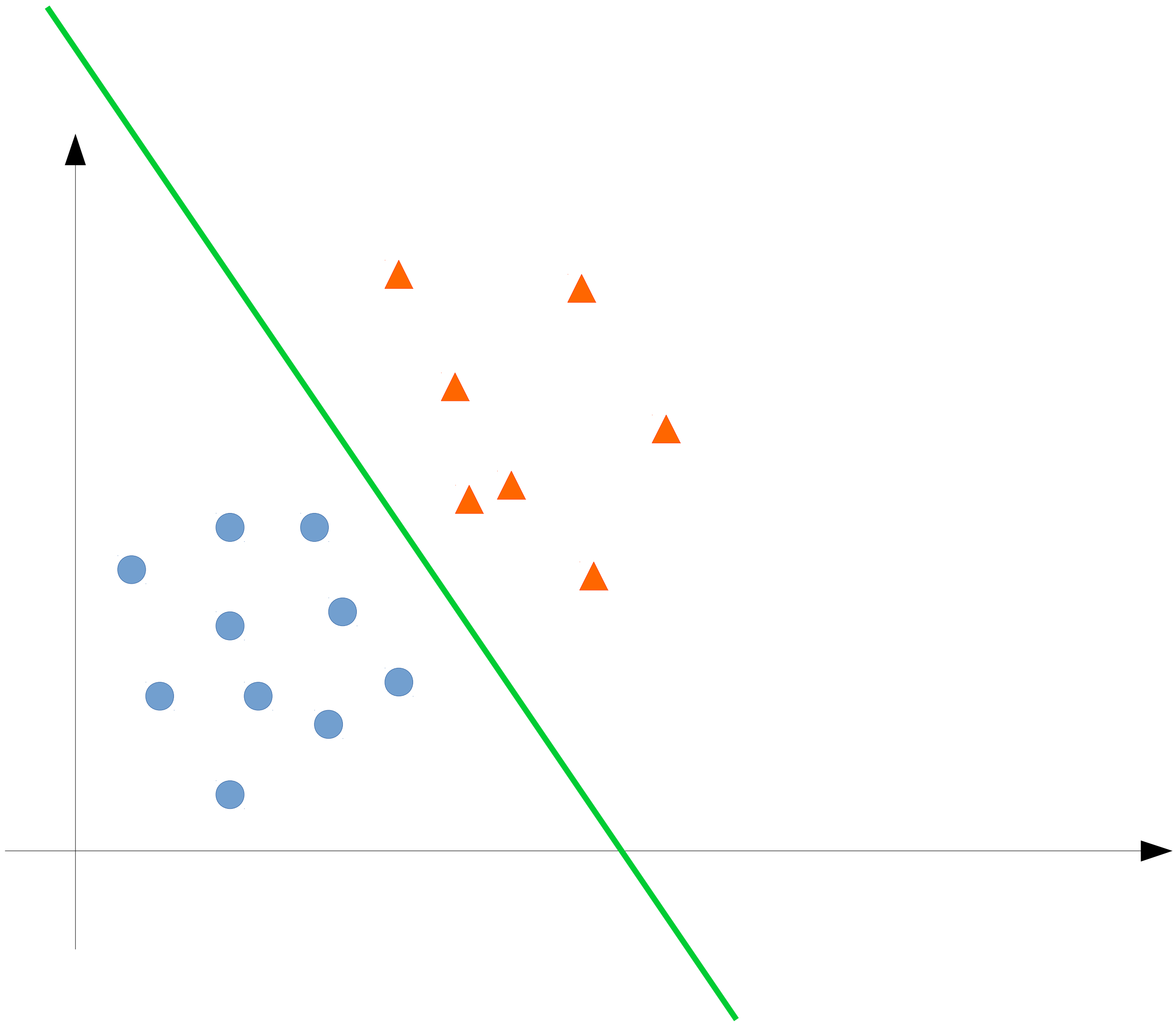
- What is the general idea of a Support Vector Machine?
  - Use „optimally“ positioned hyperplane to linearly separate two classes
    (similar general idea as perceptron!)
  - Maximize distance between hyperplane and both classes
    (maximize width of sample free „corridor“ [=functional margin] around hyperplane)

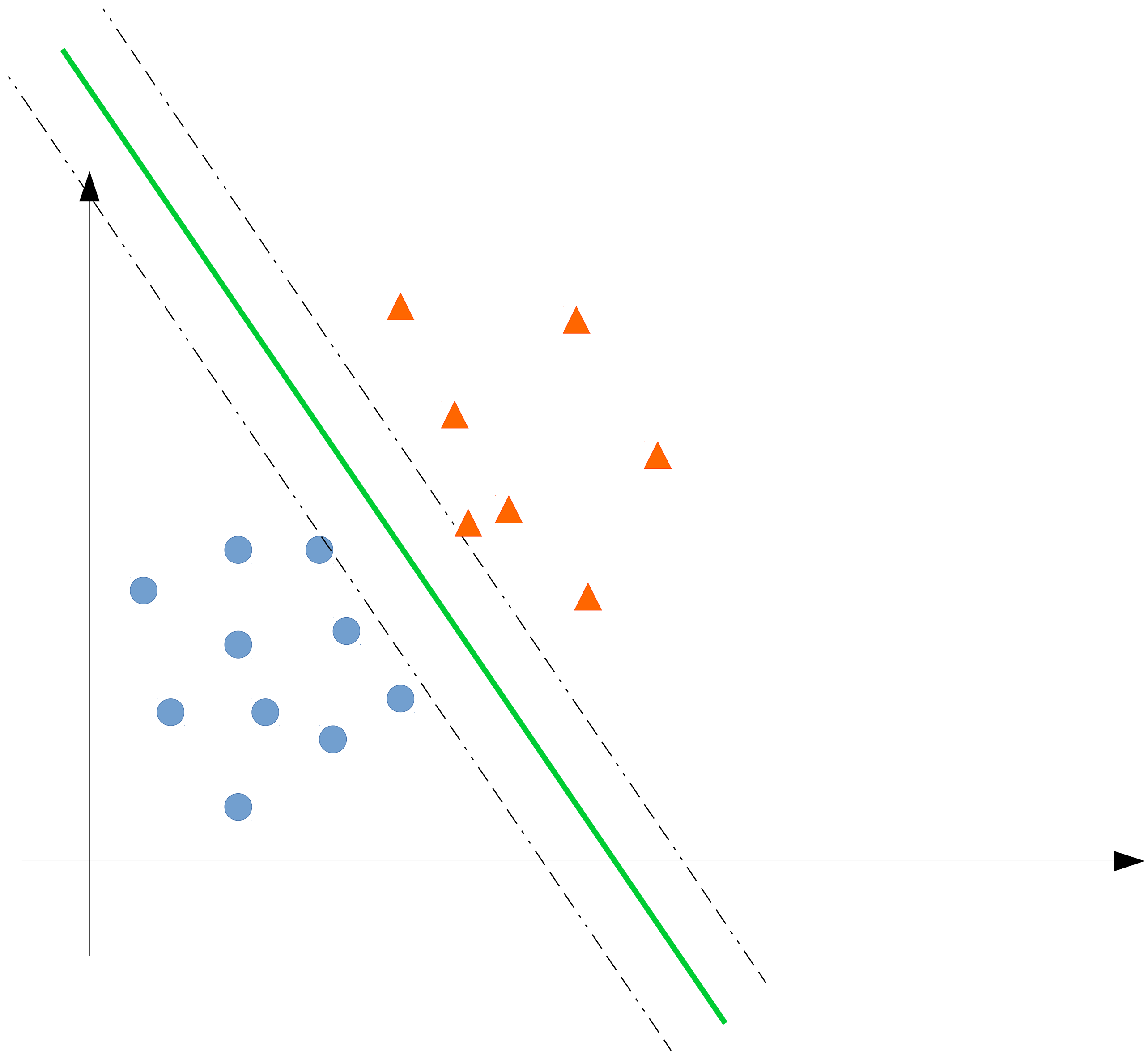


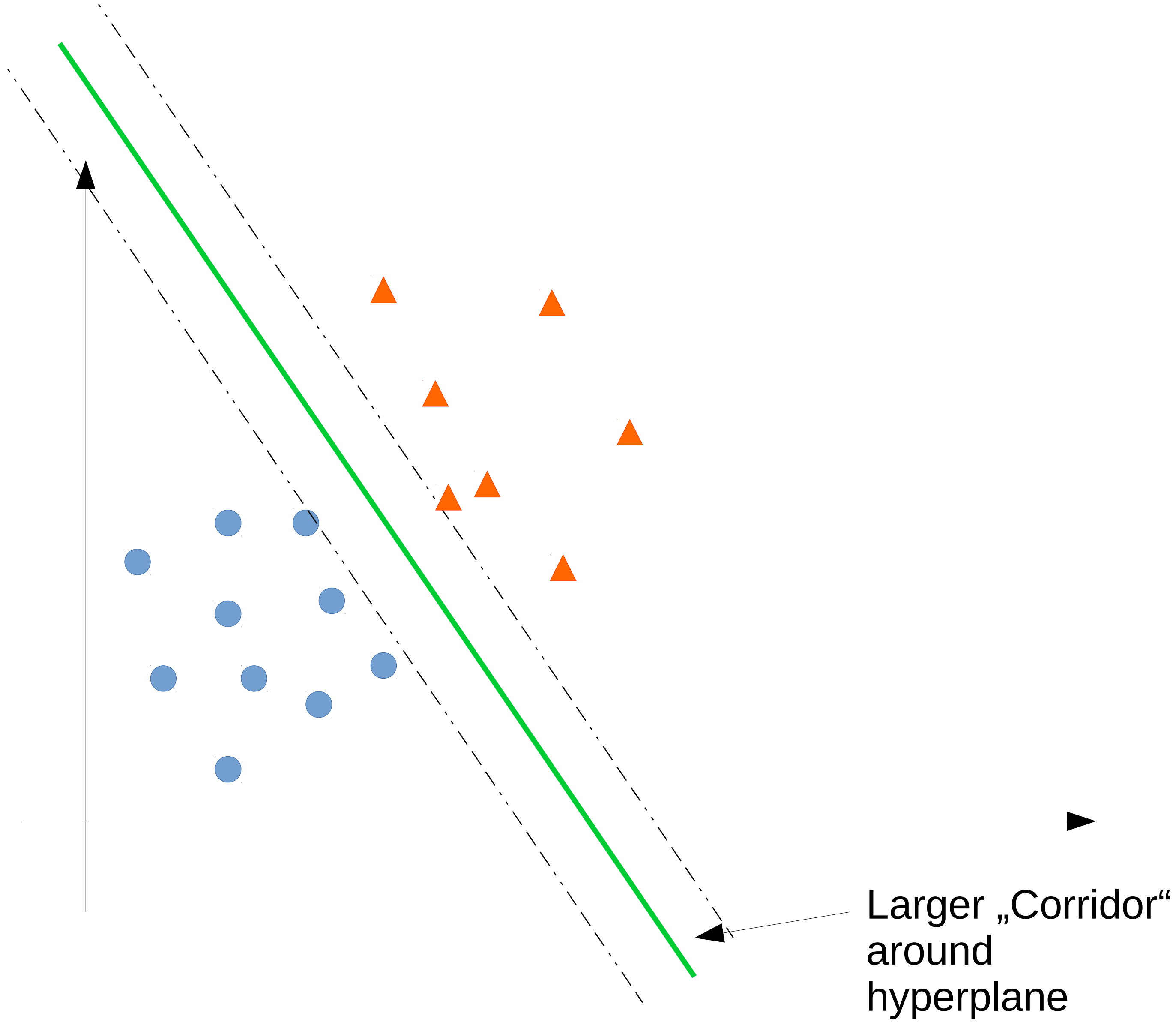




Small „Corridor“
around
hyperplane

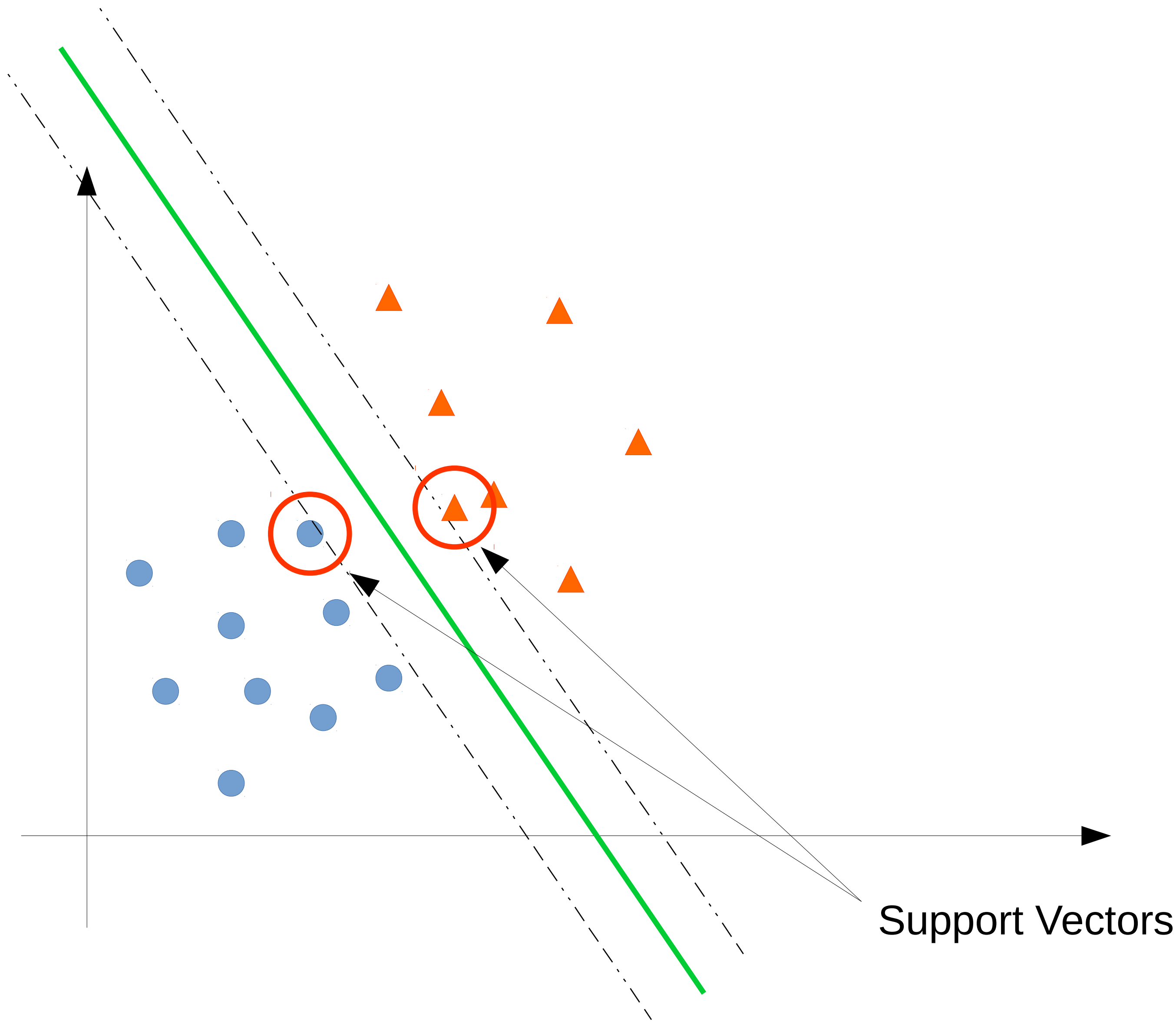


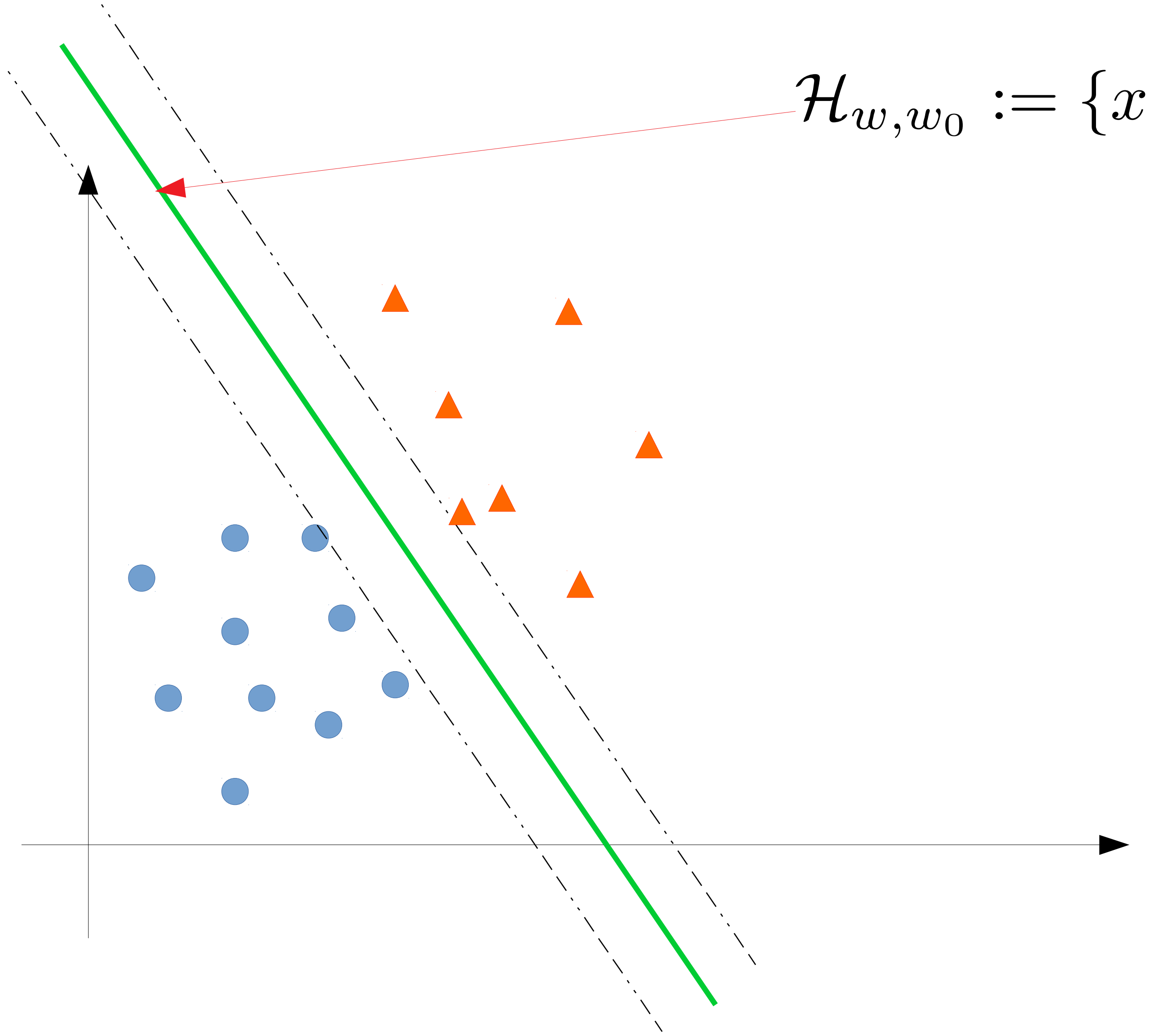



Larger „Corridor“
around
hyperplane

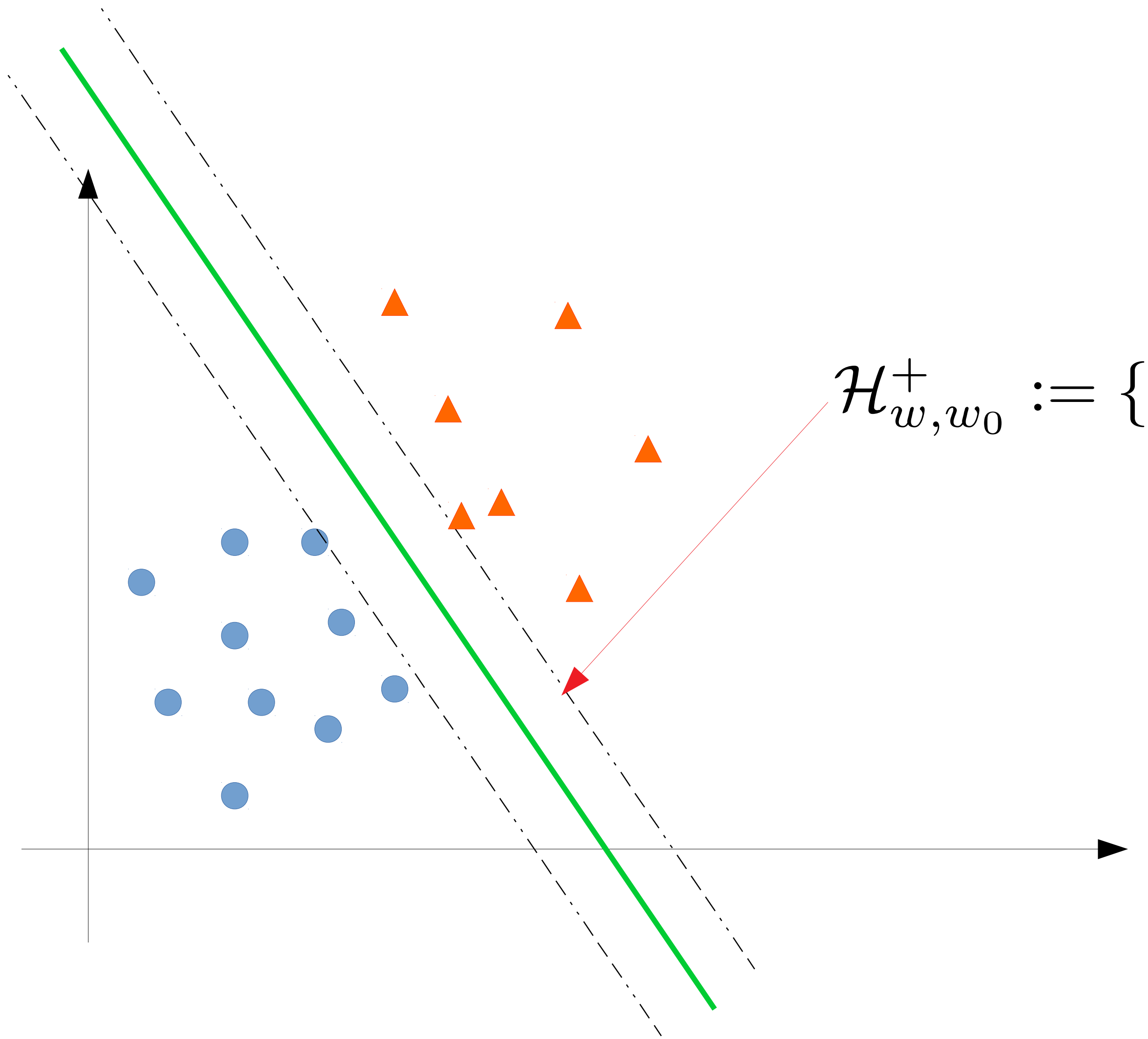
Revision of Lecture

- What are Support Vectors?
  - Support Vectors are the vectors that are on the margin of the corridor (functional margin)
  - They are the support/ the foundation of the margin hyperplanes
  - => functional margin width is restricted by Support Vectors


Support Vectors

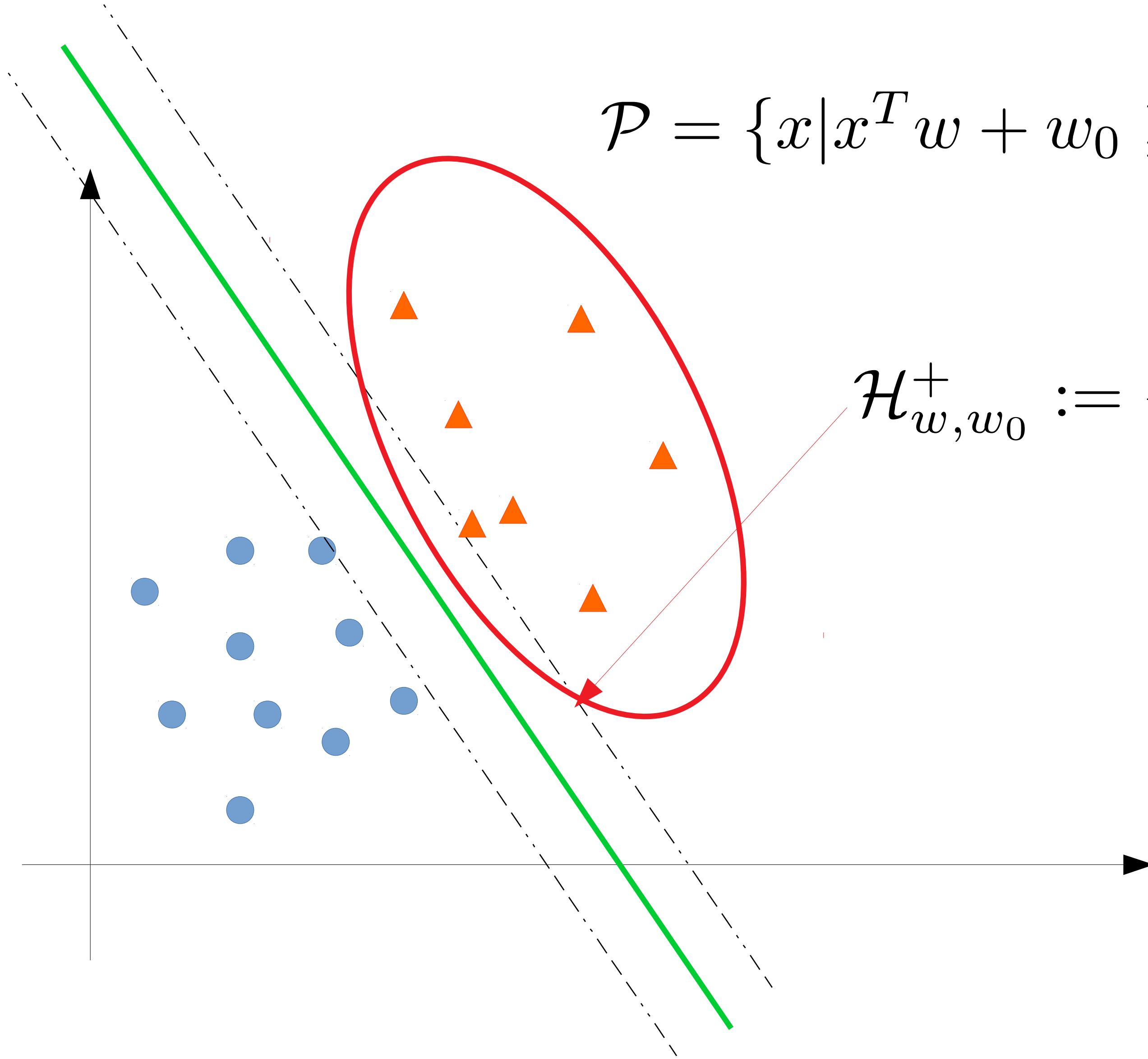


$$\mathcal{H}_{w,w_0} := \{x | x^T w + w_0 = 0\}$$

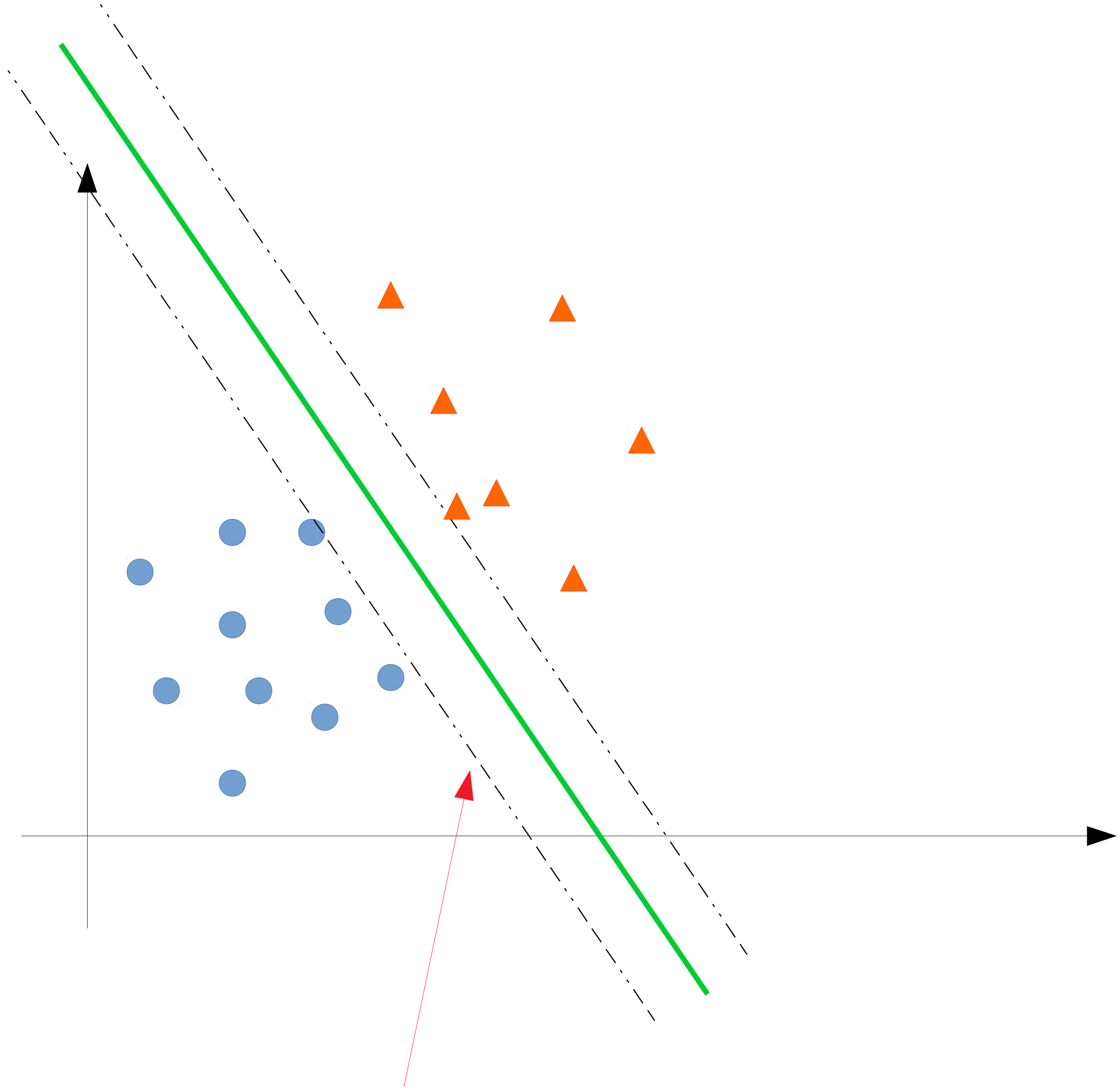


$$\mathcal{H}^{+}_{w,w_0} := \{x | x^T w + w_0 = 1\}$$

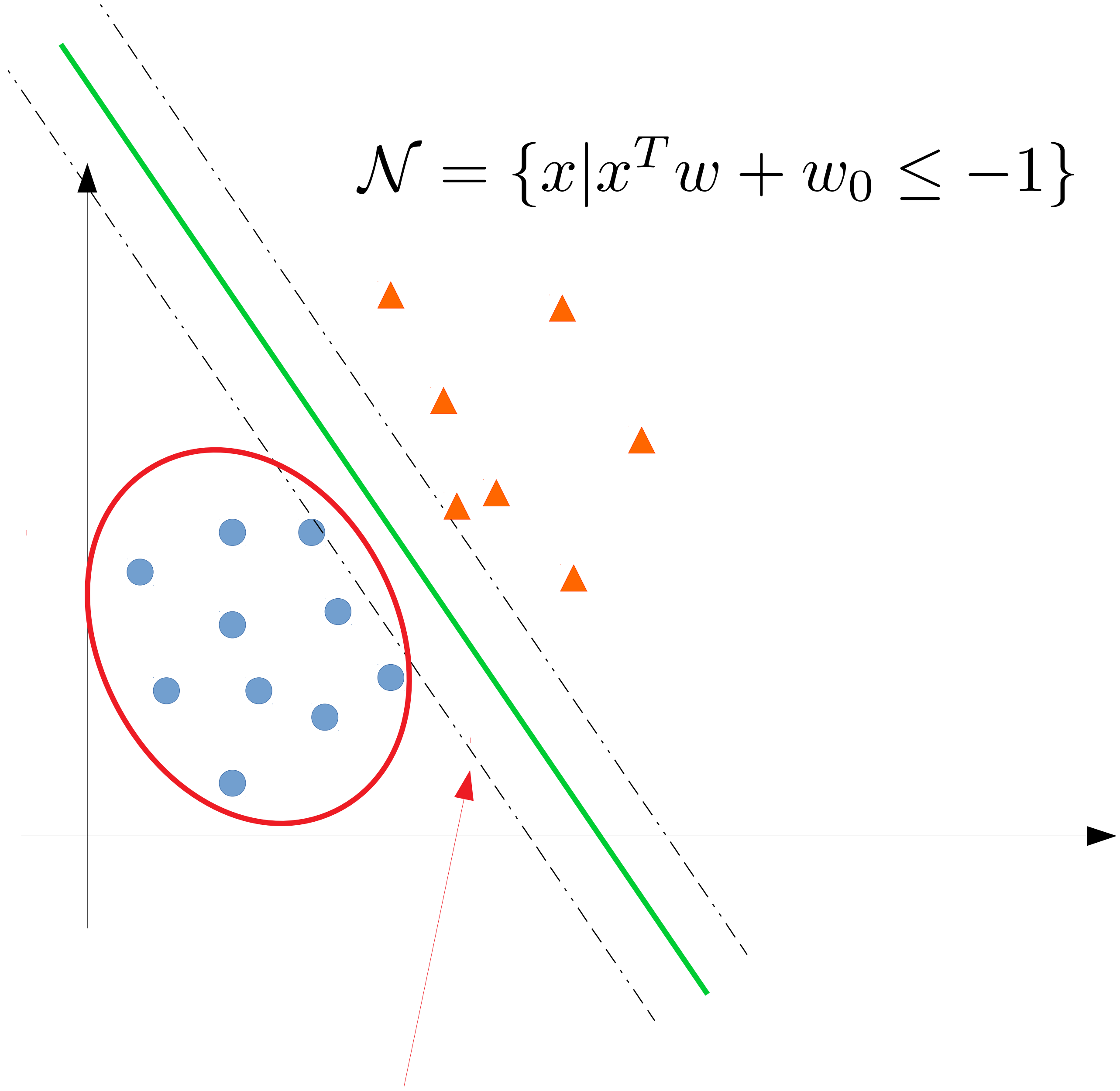
$$\mathcal{P} = \{x | x^T w + w_0 \geq 1\}$$



$$\mathcal{H}^{+}_{w,w_0} := \{x | x^T w + w_0 = 1\}$$



$$\mathcal{H}^{-}_{w,w_0} := \{x | x^T w + w_0 = -1\}$$



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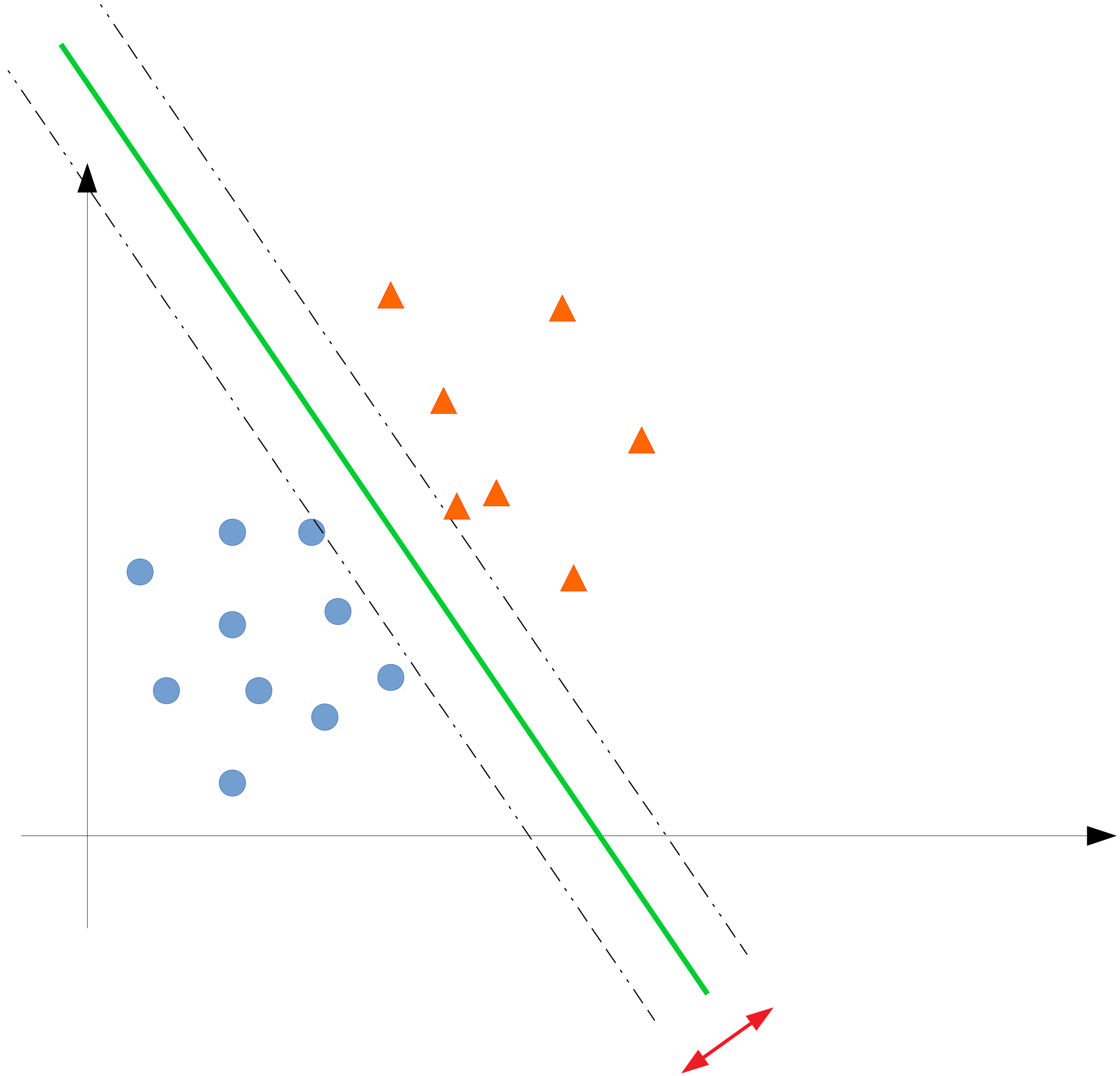

$$d_{w,w_0} = \left| \frac{1-w_0}{||w||} - \frac{-1-w_0}{||w||} \right| = \frac{2}{||w||}$$

Formalization of SVM goal

- Maximize $d_{w,w_0} = \left| \frac{1-w_0}{||w||} - \frac{-1-w_0}{||w||} \right| = \frac{2}{||w||}$
- Subject to:
  - $x^T w + w_0 \geq 1 \qquad \forall x \in \mathcal{P}$
  - $x^T w + w_0 \leq -1 \quad \forall x \in \mathcal{N}$

Formalization of SVM goal

- Minimize $\frac{1}{d_{w,w_0}} = \frac{||w||}{2} = \frac{1}{2} w^T w$
- Subject to:
  - $x^T w + w_0 \geq 1 \qquad \forall x \in \mathcal{P}$
  - $x^T w + w_0 \leq -1 \quad \forall x \in \mathcal{N}$

Formalization of SVM goal

- Minimize $\frac{1}{d_{w,w_0}} = \frac{||w||}{2} = \frac{1}{2} w^T w$
- Subject to:
  - $r_x \cdot (x^T w + w_0) \geq 1 \quad \forall x \in \mathcal{P} \cup \mathcal{N}$

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Formalization of SVM goal

- Minimize $$\frac{1}{d_{w,w_0}} = \frac{||w||}{2} = \frac{1}{2}w^T w$$
- Subject to:
  - $$r_x \cdot (x^T w + w_0) \geq 1 \quad \forall x \in \mathcal{P} \cup \mathcal{N}$$

$$(r_x = 1 \text{ if } x \in \mathcal{P})$$

$$(r_x = -1 \text{ if } x \in \mathcal{N})$$

Now use Lagrange Multipliers!

- Objective Function: $\frac{1}{2}w^T w$
- Conditions:

$$r_x \cdot (x^T w + w_0) - 1 \geq 0 \qquad \forall x \in \mathcal{P} \cup \mathcal{N}$$

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$$f_{Lagr}(w, w_0, B) :=$$

$$\frac{1}{2}w^T w - \sum_{m=1}^{M} \beta^m (r^m (w^T x^m + w_0) - 1)$$

$$f_{Lagr}(w, w_0, B) :=$$

$$\frac{1}{2} w^T w - \sum_{m=1}^{M} \beta^m (r^m (w^T x^m + w_0) - 1)$$

Mimimize wrt w and w_0

Maximize wrt beta

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \;:=\; & \frac{1}{2} w^T w + \sum_{m=1}^{M} \beta^m - \\
& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
& \sum_{m=1}^{M} \beta^m r^m w^T x^m
\end{aligned}
$$

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\end{aligned}
$$

$$
\nabla_w f_{Lagr}(w, w_0, B) = w - \sum_{m=1}^{M} \beta^m r^m x^m \overset{!}{=} \vec{0}
$$

$$
\begin{aligned}
\boldsymbol{f}_{Lagr}(\boldsymbol{w}, \boldsymbol{w}_0, \boldsymbol{B}) \ := \ & \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \sum_{m=1}^{M} \boldsymbol{\beta}^m - \\
& \sum_{m=1}^{M} \boldsymbol{\beta}^m \boldsymbol{r}^m \boldsymbol{w}_0 - \\
& \sum_{m=1}^{M} \boldsymbol{\beta}^m \boldsymbol{r}^m \boldsymbol{w}^T \boldsymbol{x}^m
\end{aligned}
$$

$$
\nabla_{\boldsymbol{w}} \boldsymbol{f}_{Lagr}(\boldsymbol{w}, \boldsymbol{w}_0, \boldsymbol{B}) = \boldsymbol{w} - \sum_{m=1}^{M} \boldsymbol{\beta}^m \boldsymbol{r}^m \boldsymbol{x}^m \stackrel{!}{=} \vec{\mathbf{0}}
$$

$$
\Rightarrow \qquad \boldsymbol{w} := \sum_{m=1}^{M} \boldsymbol{\beta}^m \boldsymbol{r}^m \boldsymbol{x}^m
$$

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \;:=\; & \frac{1}{2} w^T w + \sum_{m=1}^{M} \beta^m - \\
& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
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\end{aligned}
$$

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\nabla_w f_{Lagr}(w, w_0, B) = w - \sum_{m=1}^{M} \beta^m r^m x^m \stackrel{!}{=} \vec{0}
$$

$$
\Rightarrow \quad \boxed{w := \sum_{m=1}^{M} \beta^m r^m x^m}
$$

Need Lagrange
Multipliers to get w!

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \; := \; & \frac{1}{2} w^T w + \sum_{m=1}^{M} \beta^m - \\
& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
& \sum_{m=1}^{M} \beta^m r^m w^T x^m
\end{aligned}
$$

$$
\nabla_w f_{Lagr}(w, w_0, B) = w - \sum_{m=1}^{M} \beta^m r^m x^m \stackrel{!}{=} \vec{0}
$$

$$
\Rightarrow \qquad w := \sum_{m=1}^{M} \beta^m r^m x^m
$$

$$
\frac{\partial f_{Lagr}(w, w_0, B)}{\partial w_0} = \sum_{m=1}^{M} \beta^m r^m \stackrel{!}{=} 0
$$

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \;:=\; & \frac{1}{2} w^T w + \sum_{m=1}^{M} \beta^m - \\
& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
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& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
& \sum_{m=1}^{M} \beta^m r^m w^T x^m
\end{aligned}
$$

$\boxed{w^T w}$

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \;:=\; & \frac{1}{2} w^T w + \sum_{m=1}^{M} \beta^m - \\
& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
& \sum_{m=1}^{M} \beta^m r^m w^T x^m
\end{aligned}
$$

$$
\begin{aligned}
= \; & \sum_{m=1}^{M} \beta^m - \\
& \frac{1}{2} \underbrace{(\sum_{m=1}^{M} \beta^m r^m x^m)}_{w}{}^T \underbrace{(\sum_{l=1}^{M} \beta^l r^l x^l)}_{w}
\end{aligned}
$$

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \;:=\; & \frac{1}{2}w^T w + \sum_{m=1}^{M} \beta^m - \\
& \sum_{m=1}^{M} \beta^m r^m w_0 - \\
& \sum_{m=1}^{M} \beta^m r^m w^T x^m
\end{aligned}
$$

$$
\begin{aligned}
= \; & \sum_{m=1}^{M} \beta^m - \\
& \frac{1}{2}(\underbrace{\sum_{m=1}^{M} \beta^m r^m x^m}_{w})^T(\underbrace{\sum_{l=1}^{M} \beta^l r^l x^l}_{w})
\end{aligned}
$$

Maximize this **Dual form** to get Lagrange Multipliers!
(Condition: Betas >= 0)

$$
\begin{aligned}
f_{Lagr}(w, w_0, B) \; &:= \; \frac{1}{2} w^T w + \sum_{m=1}^{M} \beta^m - \\
&\sum_{m=1}^{M} \beta^m r^m w_0 - \\
&\sum_{m=1}^{M} \beta^m r^m w^T x^m
\end{aligned}
$$

$$
= \sum_{m=1}^{M} \beta^m - \frac{1}{2} \underbrace{\left(\sum_{m=1}^{M} \beta^m r^m x^m \right)^T}_{w} \underbrace{\left(\sum_{l=1}^{M} \beta^l r^l x^l \right)}_{w}
$$

Maximize this **Dual form** to get Lagrange Multipliers!
(Condition: Betas >= 0)

From lecture:
x^m is support vector iff beta^m > 0!!!

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Berechnung von $\boldsymbol{w}_0^*$:

Sei $\boldsymbol{x}^m$ ein Support-Vektor, z.B. derjenigen Klasse mit $\boldsymbol{r}^m = \mathbf{1}$.

Dann gilt $\quad \boldsymbol{w}^{*,T}\boldsymbol{x}^m + \boldsymbol{w}_0 = \mathbf{1} \Rightarrow \boldsymbol{w}_0^* := \mathbf{1} - \boldsymbol{w}^{*,T}\boldsymbol{x}^m$

Summary

- How to get optimal weight vector?
  - Formulate Lagrange Approach
  - Calculate partial derivatives of Lagrange function wrt to weights
  - Optimal weight vector is dependant on Lagrange multipliers
  - Insert finding into formular to get Dual Form
  - (dual form is independent of weight vector)
  - Max Dual Form to get Lagrange Multipliers!
  - (Lagrange Multipliers determine optimal weight vector)
  - Positive Lagrange Multipliers indicate support vector
  - Use support vector to calculate offset w_0

Revision of Lecture

- What to do if classes are not linearly separable?

Revision of Lecture

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  - Apply Transformation (embedding function) f_{Tran} on input space to establish linear separability

Revision of Lecture

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  - Apply Transformation (embedding function) f_{Tran} on input space to establish linear separability
  - The discriminant function would then change to:

$$f_{Disk}(x) := \text{sign}(w^{*,T} f_{Tran}(x) + w_0^*)$$

$$w^* := \sum_{m=1}^{M} \beta^{*,m} r^m f_{Tran}(x^m)$$
$$\beta^{*,m} \neq 0$$

Revision of Lecture

- What to do if classes are not linearly separable?
  - Apply Transformation (embedding function) f_{Tran} on input space to establish linear separability
  - The discriminant function would then change to:

$$f_{Disk}(x) := \text{sign}(w^{*,T} f_{Tran}(x) + w_0^*)$$

Transformed input

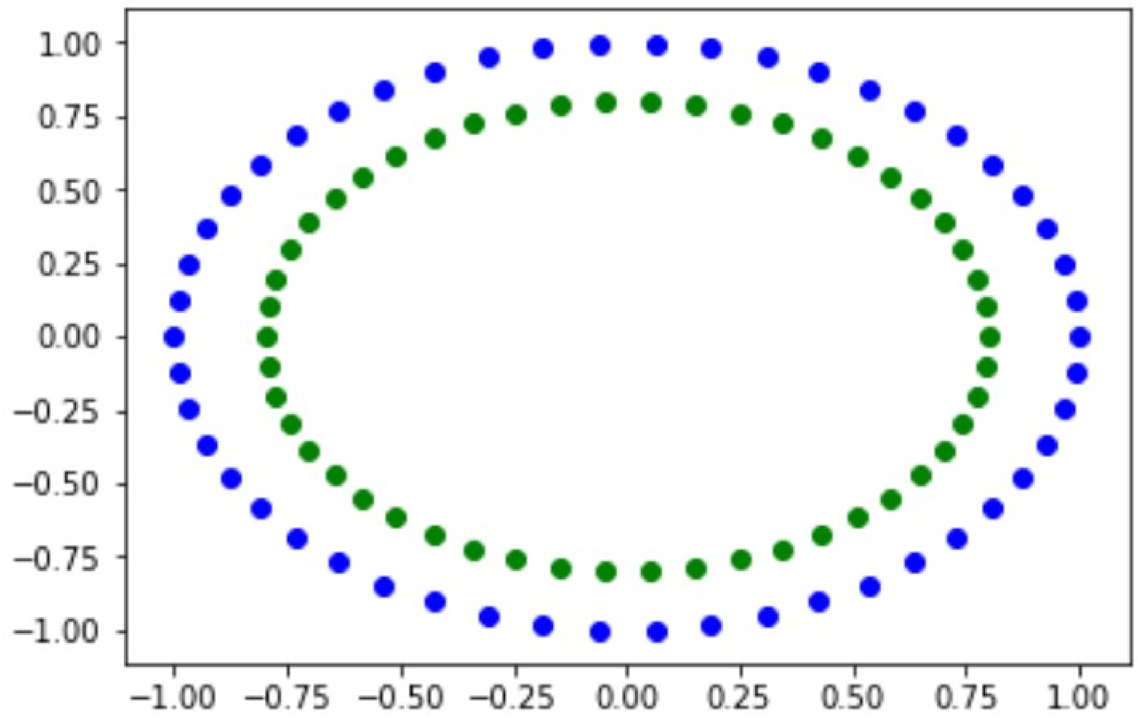
$$w^* := \sum_{m=1}^{M} \beta^{*,m} r^m f_{Tran}(x^m)$$

$$\beta^{*,m} \neq 0$$

Optimal weight vector for hyperplane
in transformed input space

(Lagrange coefficient)

(Desired ouput)


1.00
0.75
0.50
0.25
0.00
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−0.50
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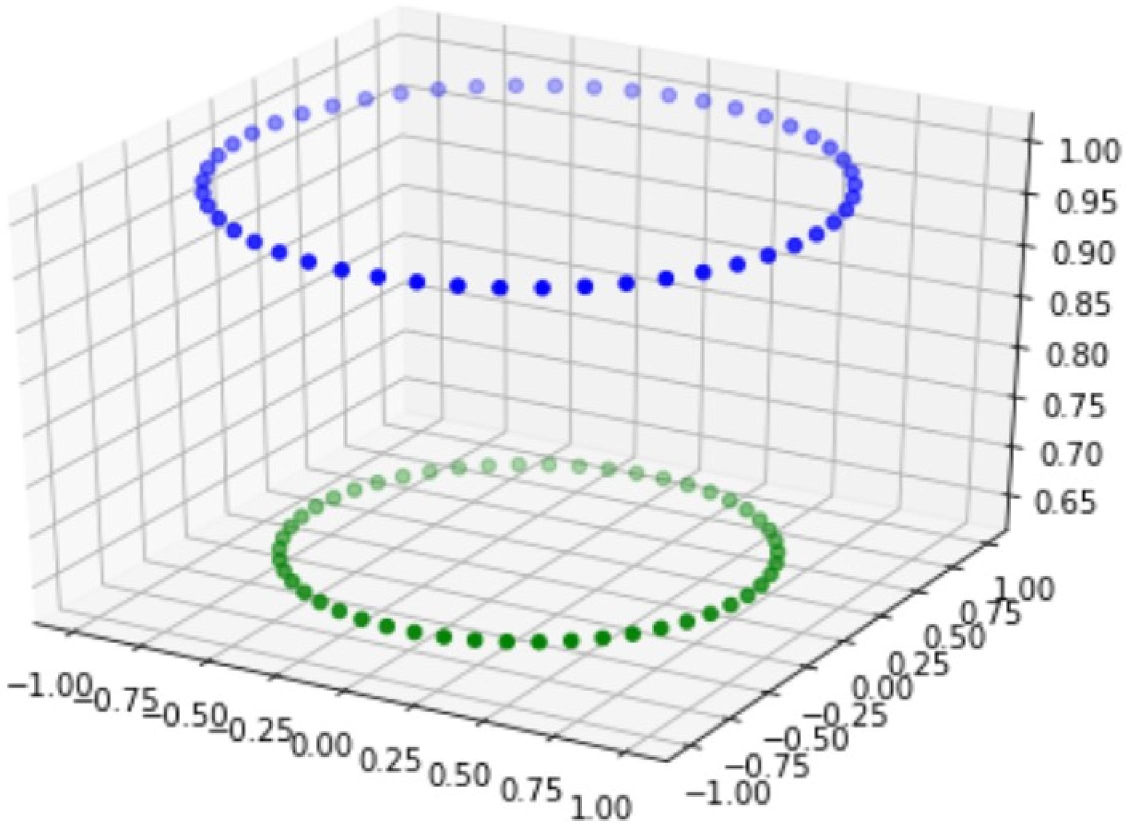
−1.00
−1.00 −0.75 −0.50 −0.25 0.00 0.25 0.50 0.75 1.00



$$f_{Tran}(x_1, x_2) := \begin{pmatrix} x_1 \\ x_2 \\ x_1^2 + x_2^2 \end{pmatrix}$$

Revision of Lecture

- What is the Kernel Trick?

Revision of Lecture

- What is the Kernel Trick?
  - Embeddings into very high dimensions demand more computational power and capacity for calculation of scalar product

$$\boldsymbol{w}^{*,T}\boldsymbol{f}_{Tran}(\boldsymbol{x}) = \sum \beta^{*,m} r^{m} \boldsymbol{f}_{Tran}(\boldsymbol{x}^{m})^{T} \boldsymbol{f}_{Tran}(\boldsymbol{x})$$

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Revision of Lecture

- What is the Kernel Trick?
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$$w^{*,T} f_{Tran}(x) = \sum \beta^{*,m} r^m \boxed{f_{Tran}(x^m)^T f_{Tran}(x)}$$

Revision of Lecture

- What is the Kernel Trick?
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$$\boldsymbol{w}^{*,T}\boldsymbol{f}_{Tran}(\boldsymbol{x}) = \sum \beta^{*,m} r^m \boxed{\boldsymbol{f}_{Tran}(\boldsymbol{x}^m)^T \boldsymbol{f}_{Tran}(\boldsymbol{x})}$$

  - There exist combination of embedding function f_{Tran} and kernel function f_{Kern} , such that Mercer condition holds:

$$\boldsymbol{f}_{Tran}(\boldsymbol{x}^m)^T \cdot \boldsymbol{f}_{Tran}(\boldsymbol{x}^\ell) = \boldsymbol{f}_{Kern}(\boldsymbol{x}^m, \boldsymbol{x}^\ell) \quad \forall \boldsymbol{x}^m, \boldsymbol{x}^\ell$$

Revision of Lecture

- What is the Kernel Trick?
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  - This way, we do not even need to compute the transformation! Only the <u>result</u> of the scalar product!

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Revision of Lecture

- Some Kernel functions:

$$f_{Kern}(x^m, x^\ell) := (x^{m,T} \cdot x^\ell)^2$$

$$f_{Kern}(x^m, x^\ell) := e^{-\frac{\|x^m - x^\ell\|^2}{2\sigma^2}}$$

$$f_{Kern}(x^m, x^\ell) := \tanh(x^{m,T} \cdot x^\ell)$$

$$f_{Kern}(x^m, x^\ell) := (x^{m,T} \cdot x^\ell + 1)^d$$

Topics covered in this course

- Neuroinformatics & Machine Learning Basics
- Statistical Decision Theory
  & Statistical Classifiers
- McCulloch Pitts Cell & Perceptron
  & Learning Algorithms
- Adaline
- Multi Layer Perceptron
- Convolutional Neural Networks
- Bias-Variance-Dilemma
  & Statistical Analyses (e.g. Precision/Recall)
- RBF- Nets
- SVMs

Exam hints

- No proofs!
- No programming tasks!
- Content from the tutorials is expected to be known (except for proofs and programming assignments!)
- It is more important to be able to accurately explain concepts and relationships than to learn complicated mathematical deriviations by heart.
- You should understand the derivations, though!
- Simple (usually short) formulas, introduced in the lecture, are expected to be known (e.g. Bayes etc...)

Exam hints

- These lecture topics are definitely not going to be in the exam:
  - Chapter 1 : slides 3-4
  - Chapter 3: slides 42-47
  - Chapter 5: slides 19-24, slides 29-32, slide 38
  - Chapter 6: slides 3-4, slide 10, slides 62-64
  - Chapter 7: slides 4-9
  - Chapter 8:
    - Do not learn formulas by heart, but rather understand them and know the meaning of the used symbols!

Types of Questions

- Definitions:
  - E.g.: When are two sets of classes said to be linearly separable?
  - Assume two sets: $\mathbf{P},\mathbf{N} \subset \mathbb{R}^N$
  - P, N linearly separable if there exists a weight vector $w \in \mathbb{R}^N$ and a threshold $\Theta \in \mathbb{R}$ such that

$$w^T x \geq \Theta \quad \forall x \in P$$

$$w^T x < \Theta \quad \forall x \in N$$

Types of Questions

- Calculations (only minor part of exam):
  - Some easy calculations
  - No calculator required
  - e.g. covariance matrix, bayes, conditional probabilities or something similarly easy
  - No calculations of inverse matrix expected

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Types of Questions

- Algorithms:
  - Description of algorithm
    - How does it work?
    - Do not leave out important aspects!
    - Make sure the corrector sees, that you know what you are talking about
    - (Do not just write down some formulas without any explanation!)
    - E.g. Perceptron learning algorithm

Types of Questions

- Algorithms:
  - Idea of algorithm
    - What is the general idea of this algorithm?
    - Explain it in an understandable fashion
      (like you would explain it to a collegue)
    - Draw sketches to illustrate your explanations
    -

Types of Questions

- Derivations:
  - Do not learn derivations/proofs by heart!
  - Make sure you understand WHY we had to make these derivations!
  - To which conclusions did these poofs/derivations lead us?

Types of Questions

- Formulas:
  - Do not learn very complex formulas by heart!
    (see list in previous slide)
  - Make sure you understand which components these formulas consist of!
  - Easier formulas are expected to be known!
  - (E.g. Bias, Variance, Definition of a hyperplane, linear associator, bayes, etc...)

Types of Questions

- Transfer of knowledge:
  - Get an overall understanding of which topics this course covers
  - What are the differences?
  - What are common properties?
  - Is there any relation between chapter X and Y?

Good luck in your exam!