Machine Learning

Lecture 7 – Support Vector Machine

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Today

- Linear Separable SVM
- Non-linear separable SVM

Linear Separable SVM

Linear Separable SVM

- Hard Margin Support Vector Machine
- Soft Margin Support Vector Machine

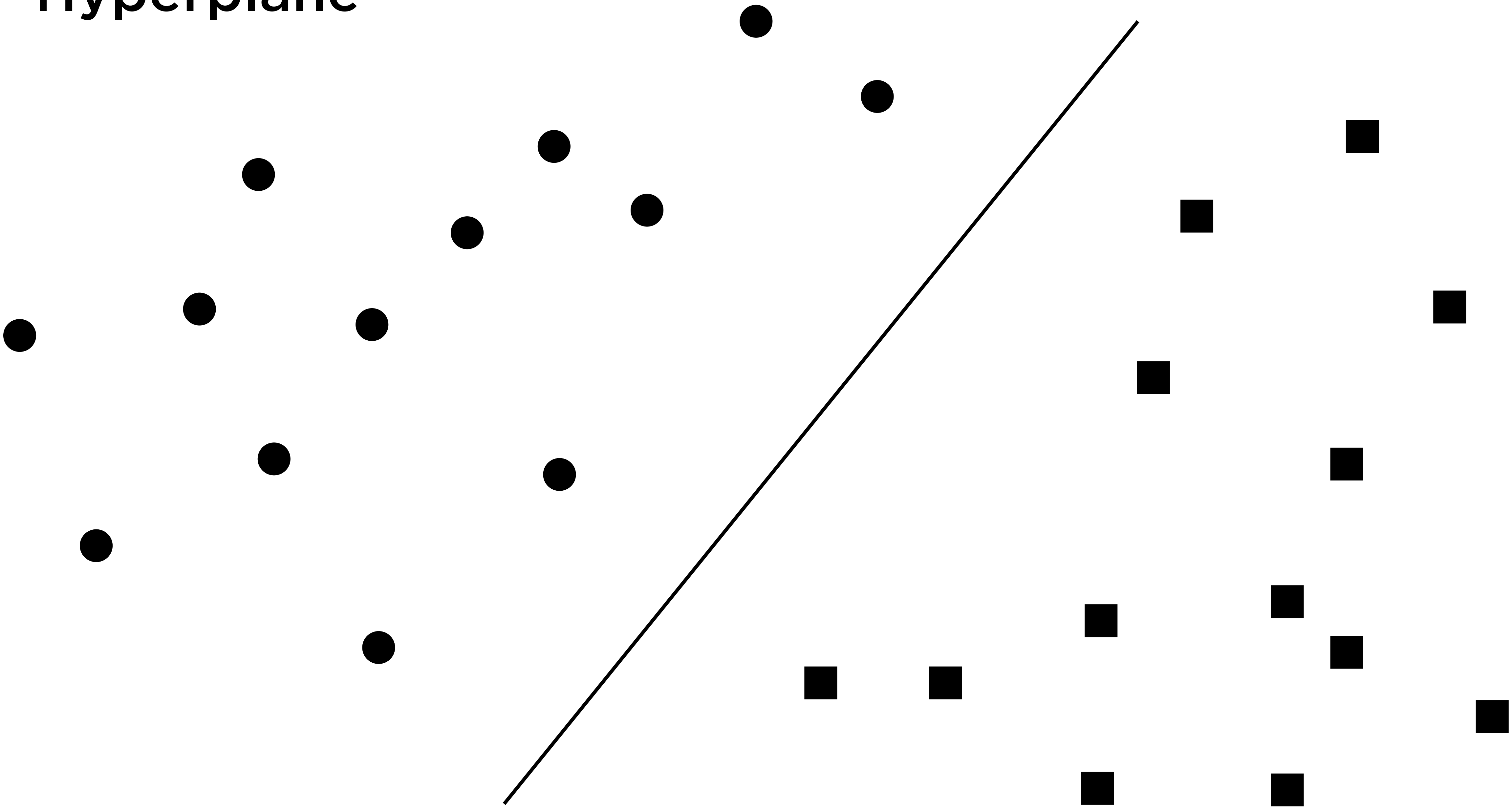
Hard Margin Support Vector Machine

Hyperplane

In geometry, a hyperplane is a subspace whose dimension is one less than its ambient space. For the context of this module, the ambient space is defined as the Hilbert space($\mathcal{H}$).

Hyperplane is a linear decision surface that can be used to separate and classify data points.

Hyperplane



Hard Margin Support Vector Machine

Intuition: an practical problem

Given training data (x_i, y_i) for $i = 1, \dots, N$ with $x_i \in \mathbb{R}^2$ and $y_i \in \{-1, +1\}$, learn a classifier $f(x)$ training such that:

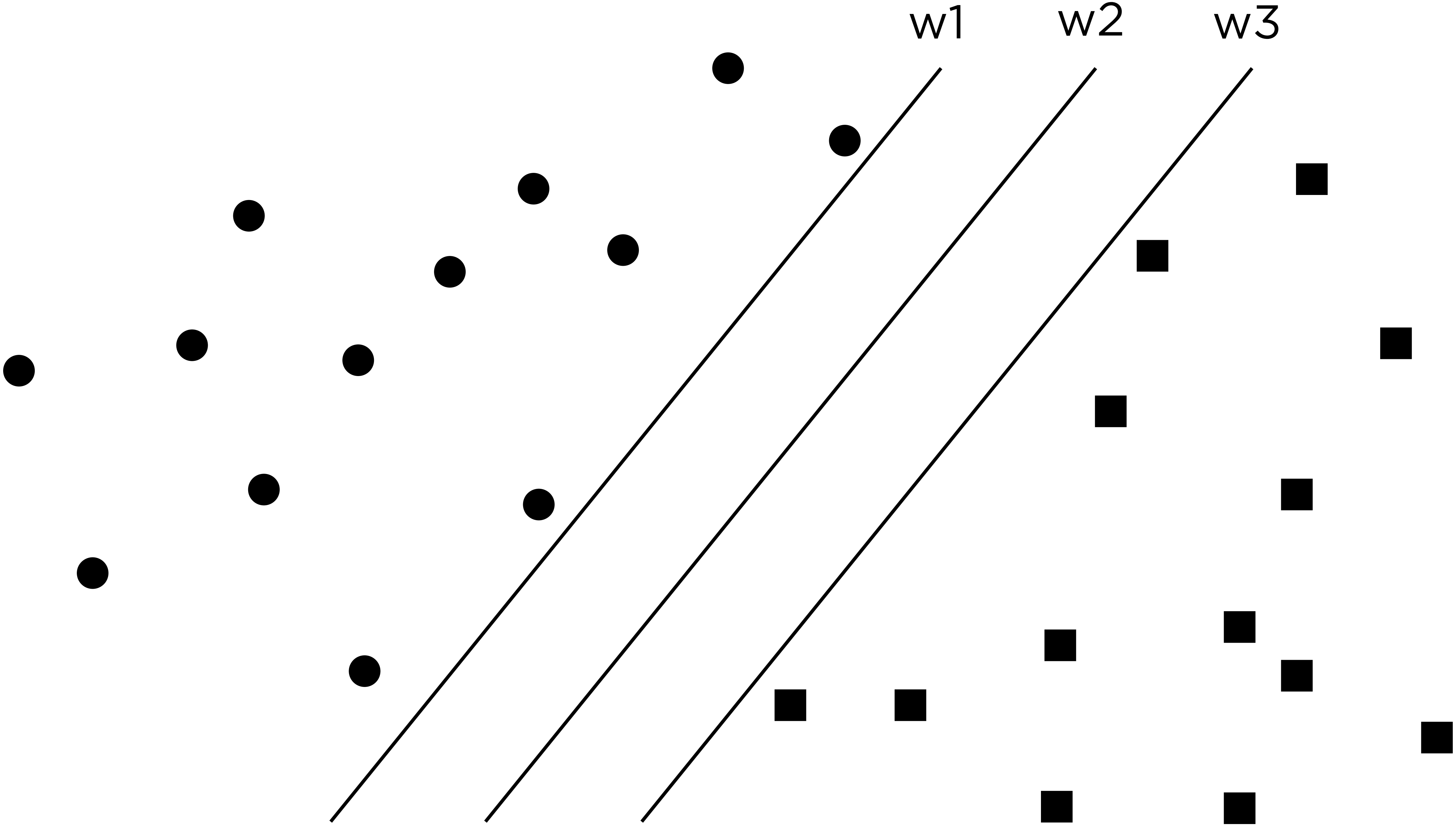
$$f(x_i) = \begin{cases} \geq 0, & y_i = +1 \\ < 0, & y_i = -1 \end{cases}$$

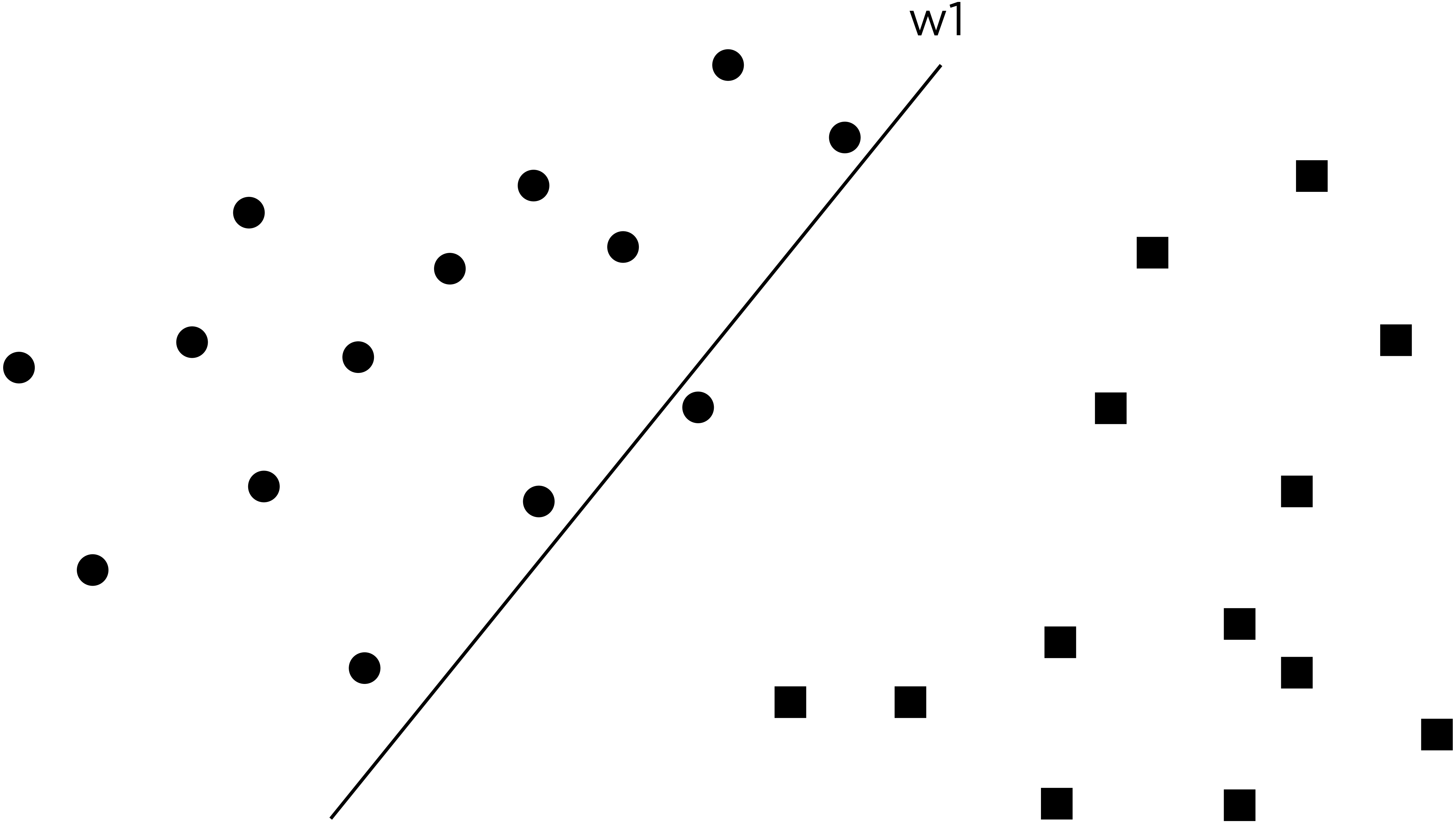
i.e. $y_i f(x_i) > 0$ for a correct classification.

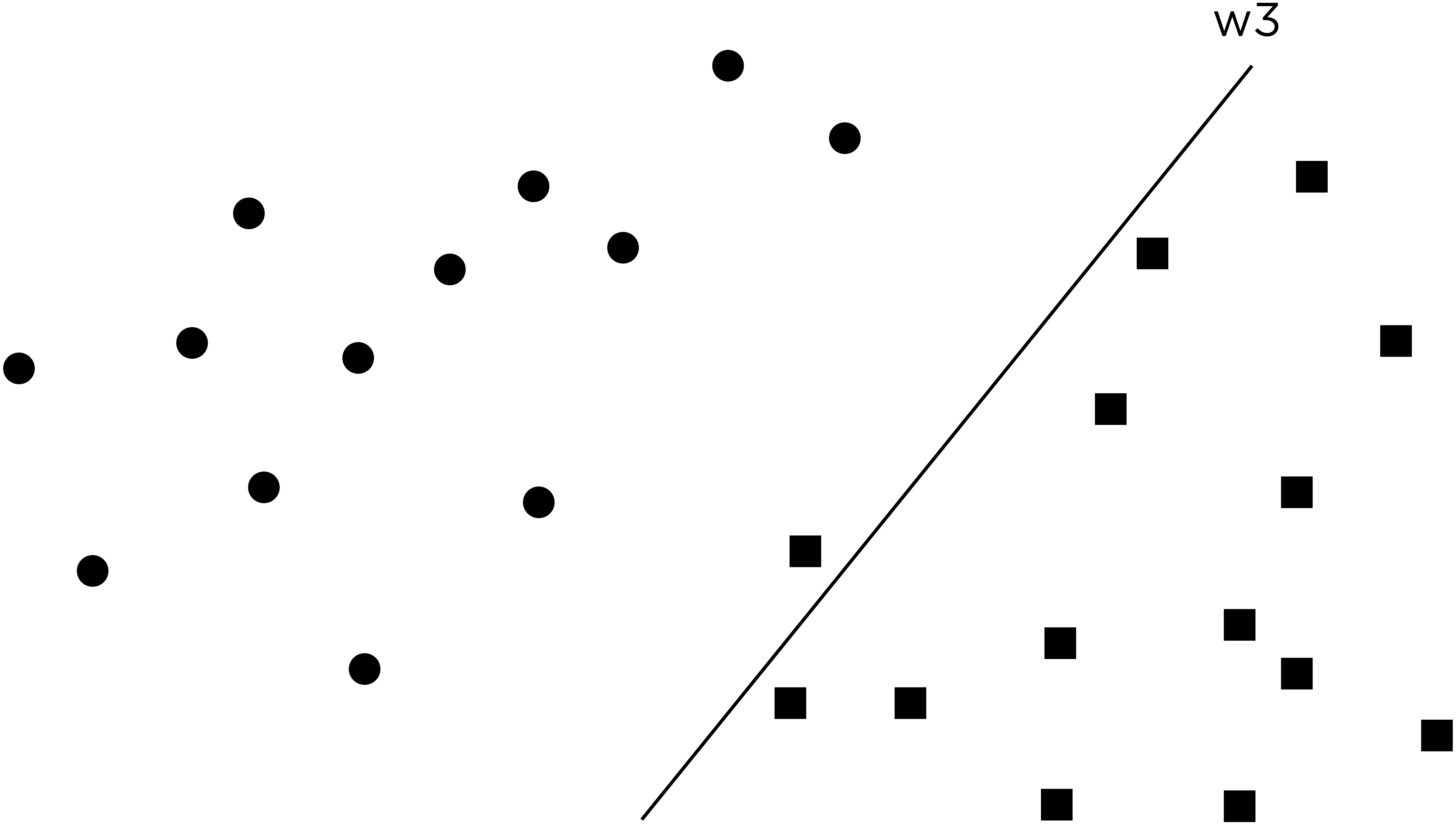
What is the problem with this solution?

Hard Margin Support Vector Machine

There is no optimal solution of Hyperplane given the training data points. Hyperplane here can alternatively be named **decision boundary**. An example solution could be either $w1$,$w2$, or $w3$.


w1
w2
w3


w1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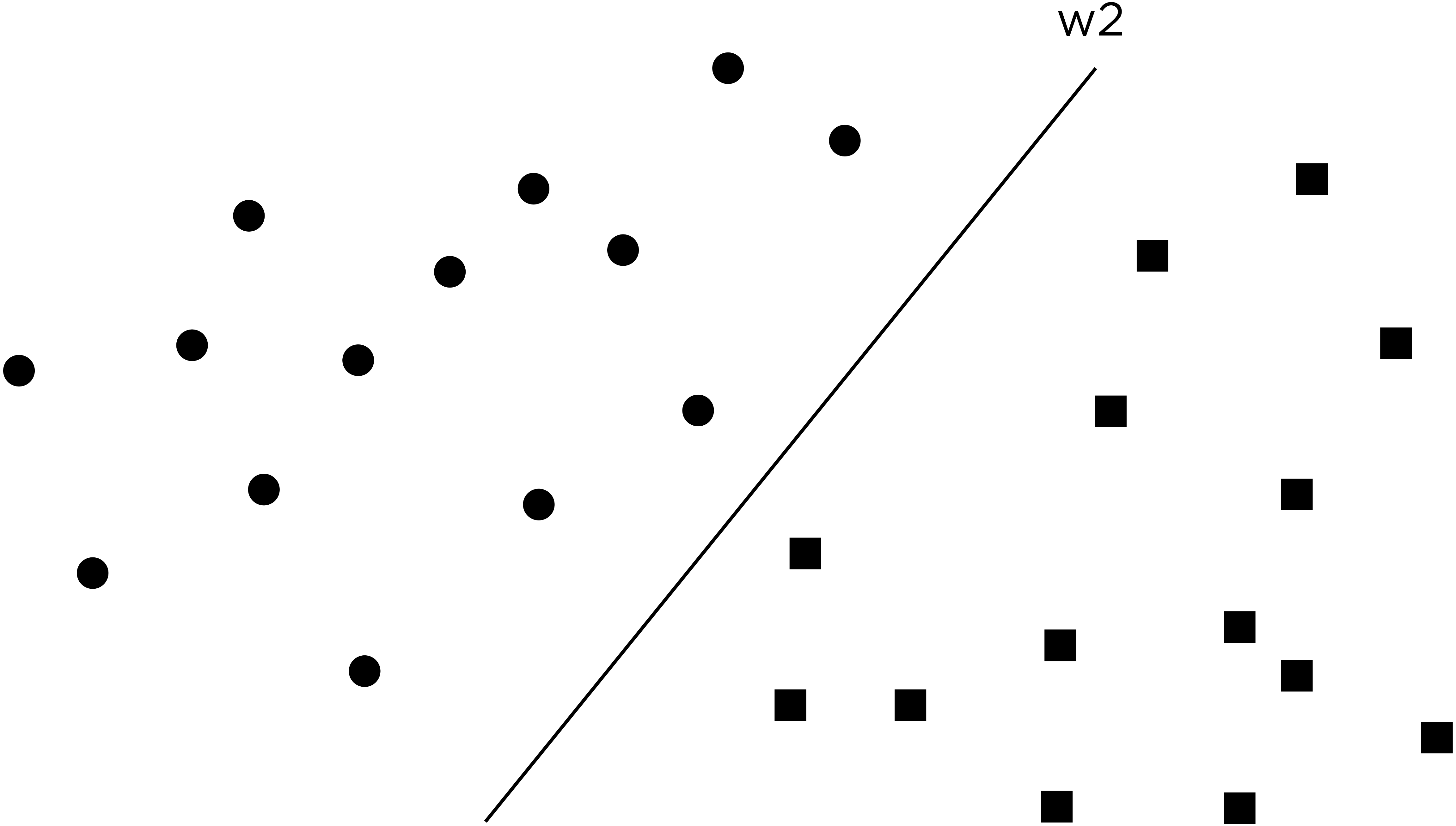
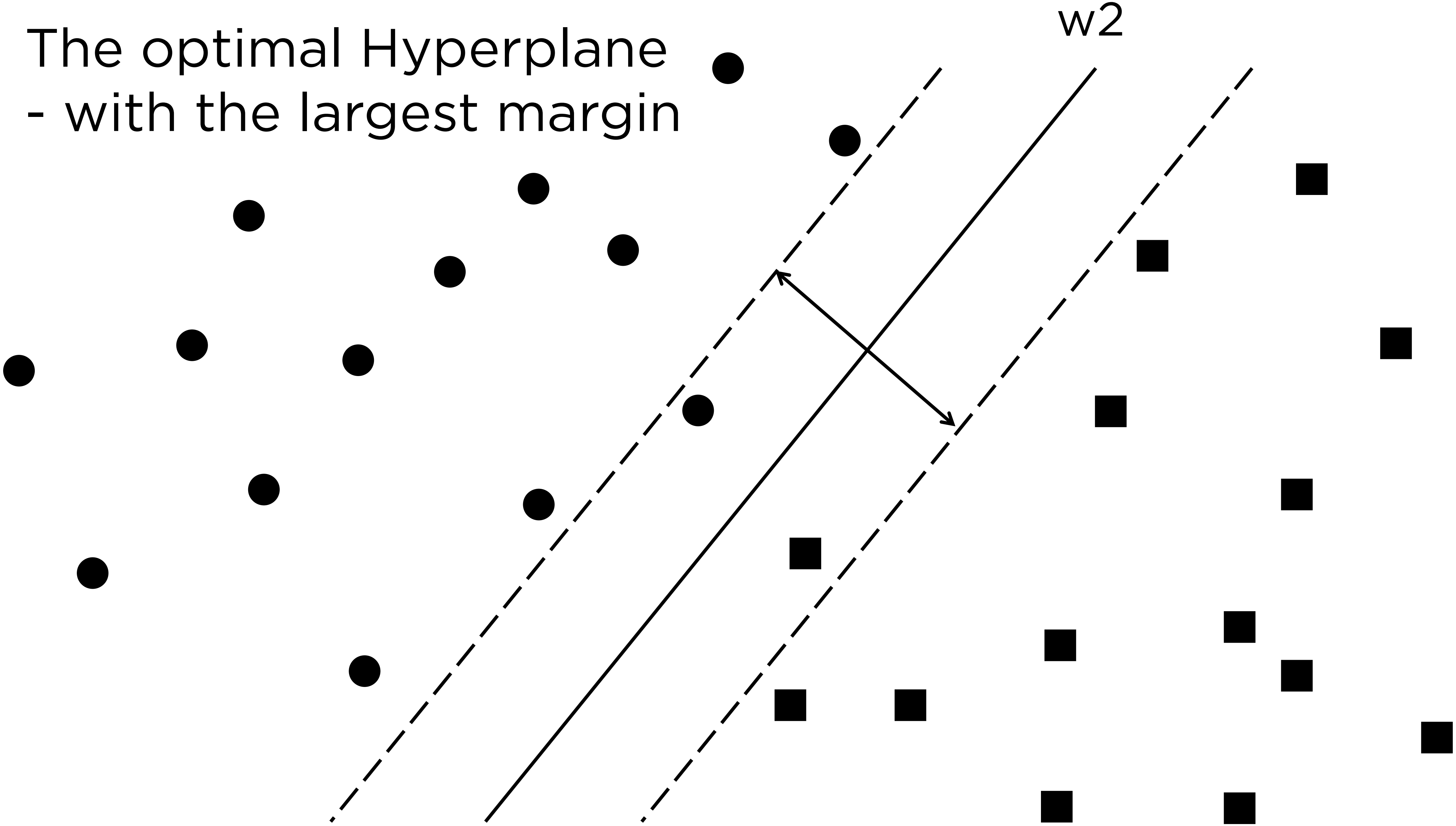

w2

The optimal Hyperplane
- with the largest margin



Hard Margin Support Vector Machine

Definition: Separating Hyperplane

Let $S = \{(x_i, y_i)\}_{i=1}^{m} \in \mathbb{R}^d \times \{-1, +1\}$ be a training set.

By a hyperplane we mean a set of Hilbert space $\mathcal{H}_{w,b} = \{x \in \mathbb{R}^d : w^T x + b = 0\}$ parameterized by $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$

We assume that the data are linearly separable, that is, there exist $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that $y_i(w^T x_i + b) > 0,\ i = 1, \dots, m$

In which case we call $\mathcal{H}_{w,b}$ a **separating hyperplane**

Note that we require the inequality to be strict (we do not admit that the data lie on a hyperplane).

Hard Margin Support Vector Machine

Definition: Distance & Margin

The **distance** $\rho_x(w, b)$ of a point x from a hyperplane $\mathcal{H}_{w,b}$ is:

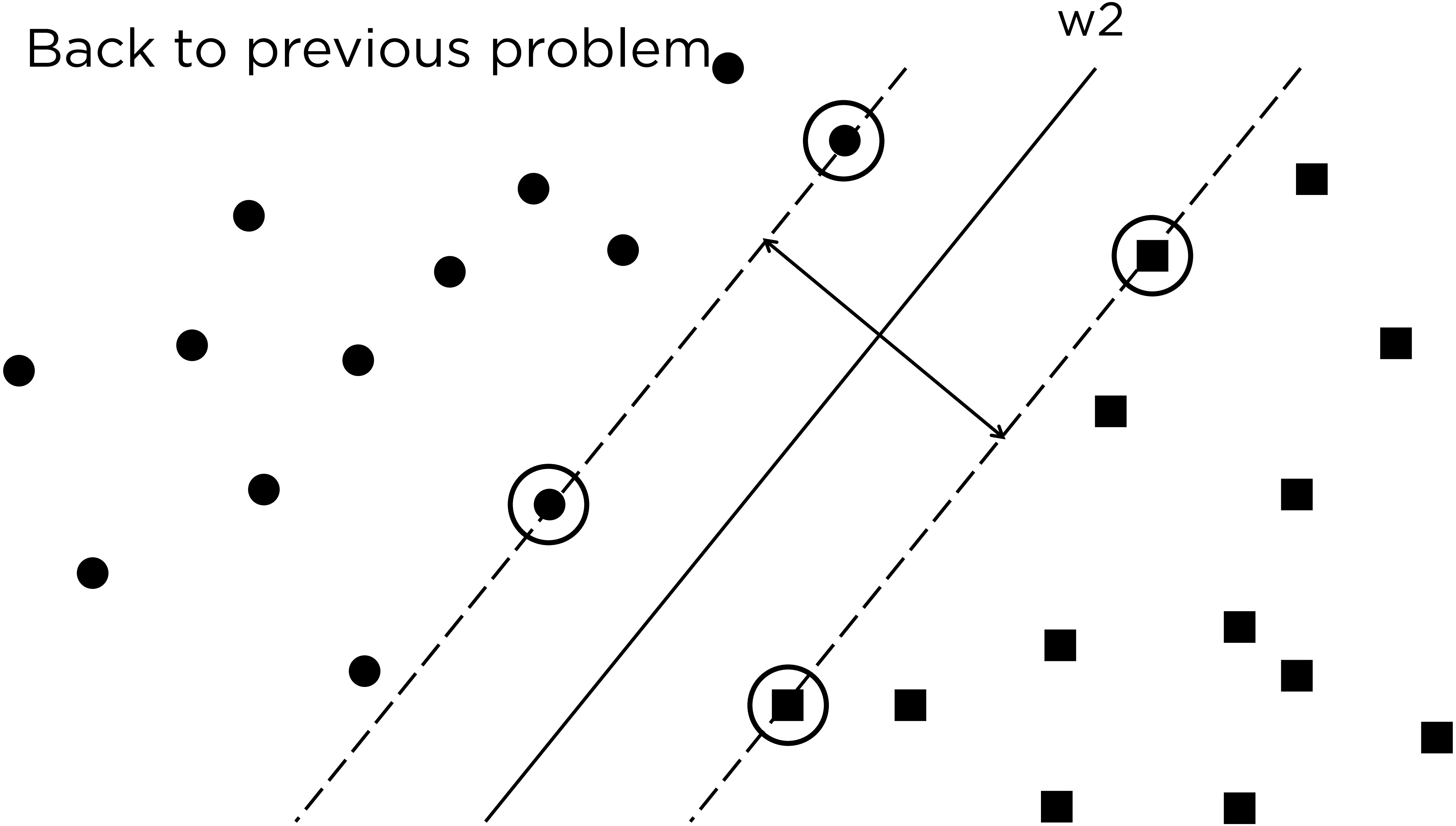
$$\rho_x(w, b) = \frac{|w^T x + b|}{||w||}$$

If $\mathcal{H}_{w,b}$ separates the training set S we define its **margin** as:

$$\rho_x(w, b) = \min_{i=1:m} \rho_{x_i}(w, b)$$

If $\mathcal{H}_{w,b}$ is a hyperplane (separating or not) we also define the margin of a point x as $w^T x + b$ (note that this can be positive)

Back to previous problem



Hard Margin Support Vector Machine

Optimal separating hyperplane (OSH)

The separating hyperplane with maximum margin can be solved with the following optimization problem

$$\rho(S) = \max_{w,b} \min_{i} \{ \frac{y_i(w^T x_i + b)}{\|w\|} : \ y_i(w^T x_i + b) \geq 0, \qquad i = 1, \dots, m\} > 0$$

A separating hyperplane is parameterised by (w, b), but this choice is not unique (rescaling with a positive constant gives the same separating hyperplane).

Hard Margin Support Vector Machine

Optimal separating hyperplane (OSH)

Two possible ways to fix the parameterisation:

- **Normalised hyperplane**: set $\|w\| = 1$, in which case $\rho_x(w, b) = |w^T x + b|$ and $\rho_S(w, b) = \min_{i=1:m} y_i(w^T x_i + b)$
- **Canonical hyperplane**: choose $\|w\|$ such that $\rho_S(w, b) = \frac{1}{\|w\|}$, i.e. we require that $\min_{i=1:m} y_i(w^T x_i + b) = 1$ (a data –dependent parameterization)

We will mainly work with the second parameterisation and it is also the most common version of SVM mentioned in the literature.

Hard Margin Support Vector Machine

Optimal separating hyperplane (OSH)

Given the canonical hyperplane, we have

$$\rho(S) = \max_{w,b}\left\{\frac{1}{\|w\|} : \min_i\{y_i(w^T x_i + b)\} = 1, \qquad y_i(w^T x_i + b) \geq 0\right\} > 0$$

$$= \max_{w,b}\left\{\frac{1}{\|w\|} :\ y_i(w^T x_i + b) \geq 1\right\}$$

$$= \frac{1}{\min_{w,b}\{\|w\| : y_i(w^T x_i + b) \geq 1\}}$$

Hard Margin Support Vector Machine

Optimisation problem (primal form)

The problem thus can be defined as

Minimise $\frac{1}{2}w^T w$

Subject to $y_i(w^T x_i + b) \geq 1,\ i = 1, \ldots, m$

Hard Margin Support Vector Machine

Saddle point

To determine the saddle point of the Lagrangian function

$$L(w, b; \alpha) = \frac{1}{2}w^T w - \sum_{i=1}^{m} \alpha_i \{y_i(w^T x_i + b) - 1\}$$

where $\alpha_i \geq 0$ are the Lagrange multipliers

We minimise L over (w, b) and maximize over α. Differentiating w.r.t w and b we obtain:

$$\frac{\partial L}{\partial b} = -\sum_{i=1}^{m} y_i \alpha_i = 0$$

$$\frac{\partial L}{\partial w} = w - \sum_{i=1}^{m} \alpha_i y_i x_i = 0 \;\Rightarrow w = \sum_{i=1}^{m} \alpha_i y_i x_i$$

Hard Margin Support Vector Machine

Optimization problem (dual form)

Substituting the solution of $w = \sum_{i=1}^{m} \alpha_i y_i x_i$ leads to the dual problem

Maximise $\quad \mathrm{Q}(\alpha) = -\frac{1}{2}\alpha^T A\alpha + \sum_{i=1}^{m} \alpha_i$

Subject to $\quad \sum_{i=1}^{m} y_i \alpha_i = 0$

$\quad \alpha_i \geq 0,\ i = 1, \dots, m$

where A is an $m{\times}m$ matrix $A = (y_i y_i x_i^T x_j \colon i, j = 1, \dots, m)$

Note the complexity of this problem depends on $\boldsymbol{m}$, not on the number of data point dimension $\mathbb{R}^{\boldsymbol{d}}$.

Hard Margin Support Vector Machine

Karush-Kuhn-Tucker conditions and support vectors

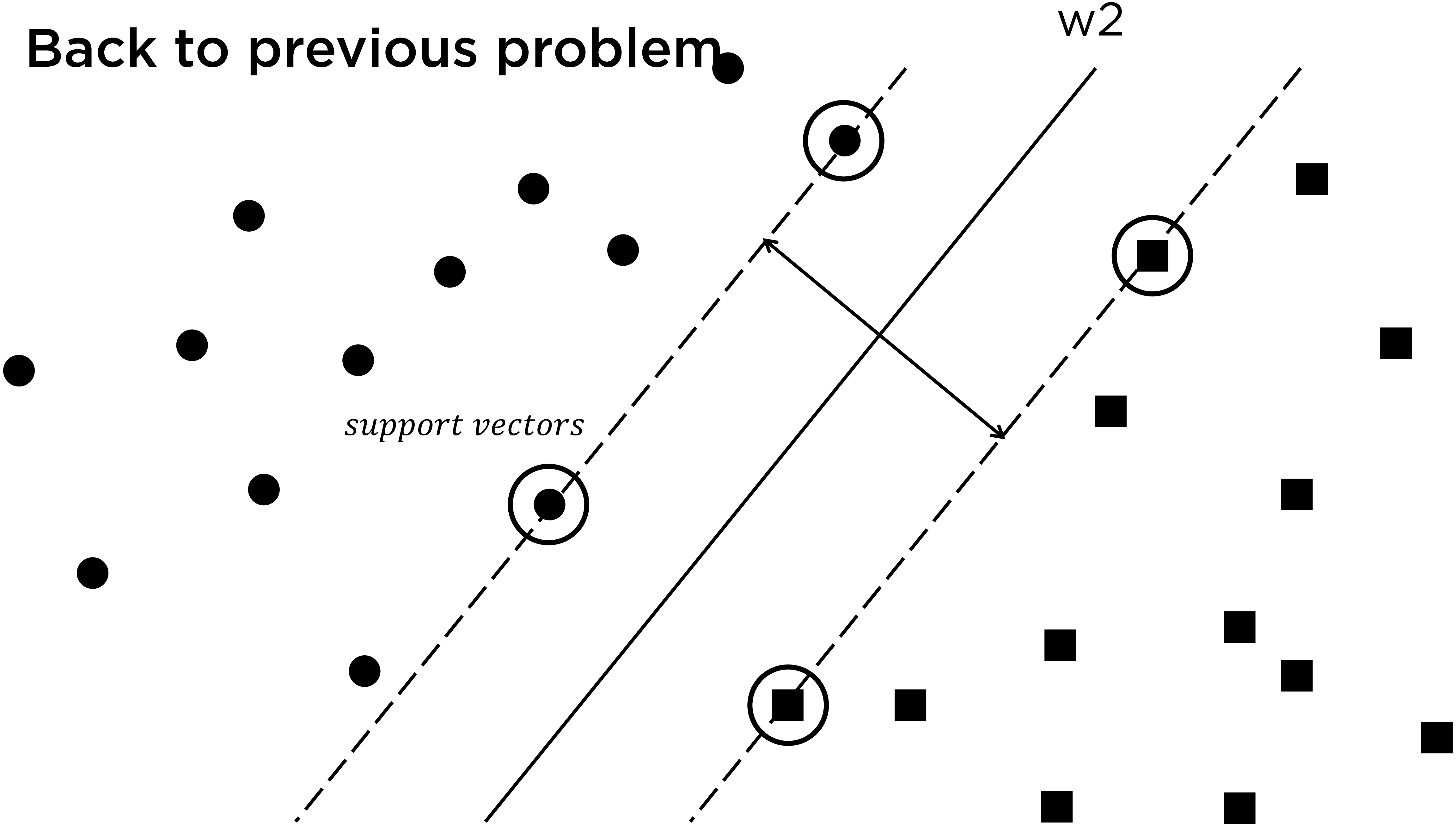
In optimisation theory, the dual form solution (d^*) serves as the lower bound of the primal solution (p^*). i.e. $d^* \leq p^*$

When $d^* = p^*$, the solution satisfy Karush-Kuhn-Tucker (KKT) condition and we have the maximum margin for SVM constructed by **support vectors.** The optimal solution is given by

$$\bar{w} = \sum_{i=1}^{m} \bar{\alpha}_i y_i x_i$$

This $\bar{w}$ is a linear combination of only the x_i for which $\bar{\alpha}_i > 0$. These x_i are termed **support vectors.**

Back to previous problem



Hard Margin Support Vector Machine

Some conclusions

- The most remarkable fact about OSH is that it is determined only by support vectors, which is usually a subset of the training data
- All the information contained in the data points is summarized by the support vectors: The whole data set could be replaced by only these points and the same hyperplane would be found
- A new point x is classified as $sgn(\sum_{i=1}^{m} y_i \bar{\alpha}_i {x_i}^T x + \bar{b})$

Linear Separable SVM

- Hard Margin Support Vector Machine
- Soft Margin Support Vector Machine

Soft Margin Support Vector Machine

Motivation

- In ideal cases, we show that if data is completely linearly separable without any errors (noise or outliers). Support Vector Machine is an efficient algorithm for these data points.
- However, what if the data is not strictly linearly separable?

Soft Margin Support Vector Machine

If the data is not linearly separable, the previous analysis can be generalized as the following problem:

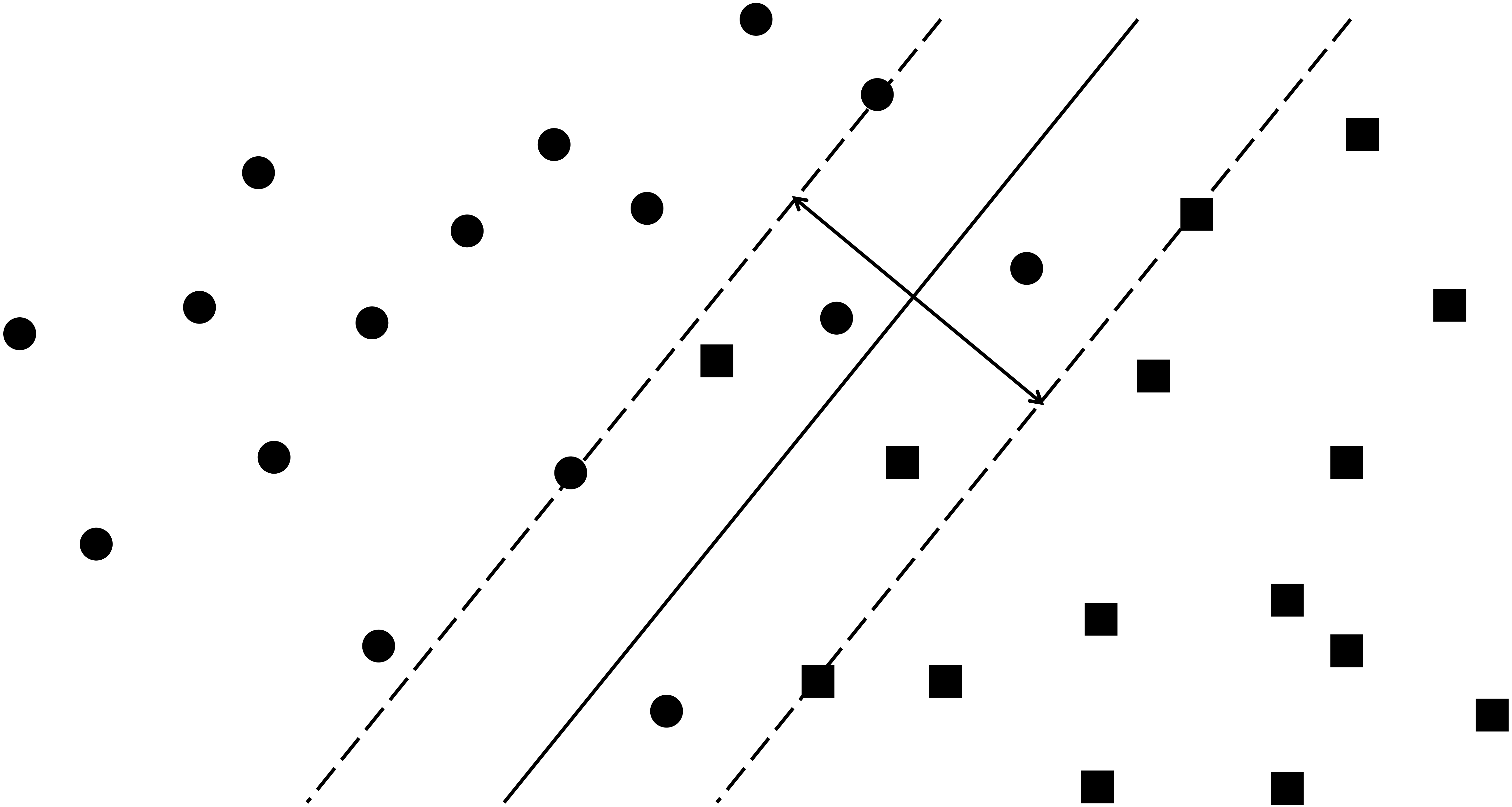
Minimise $\frac{1}{2}w^T w + C\sum_{i=1}^{m}\xi_i$

Subject to $y_i(w^T x_i + b) \geq 1 - \xi_i,$

$$\xi_i \geq 0, \qquad i = 1, \ldots, m$$

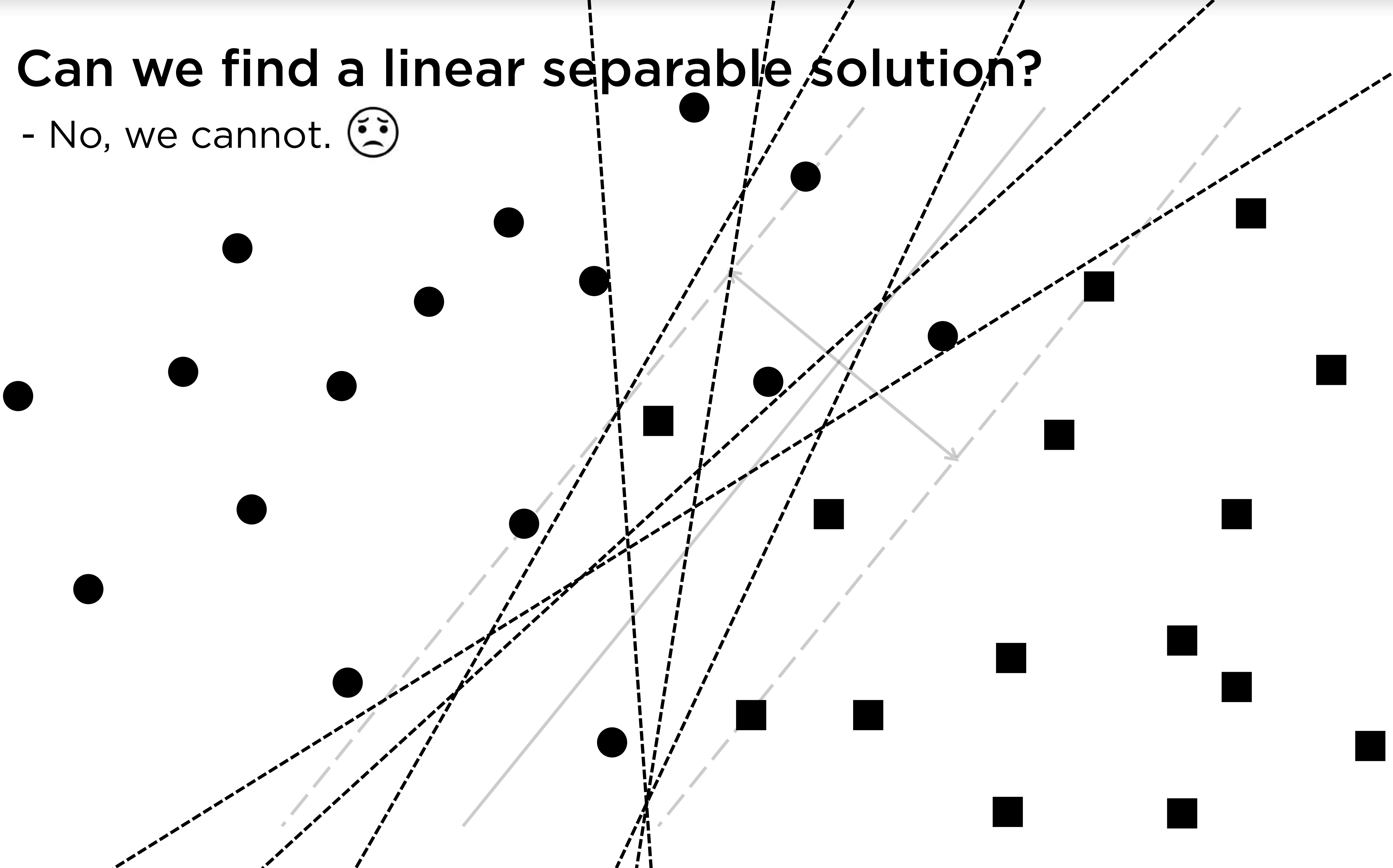
The idea is to introduce the **slack variable** ξ_i to relax the separation constraints ($\xi_i > 0$)

How do we relax the constrains?

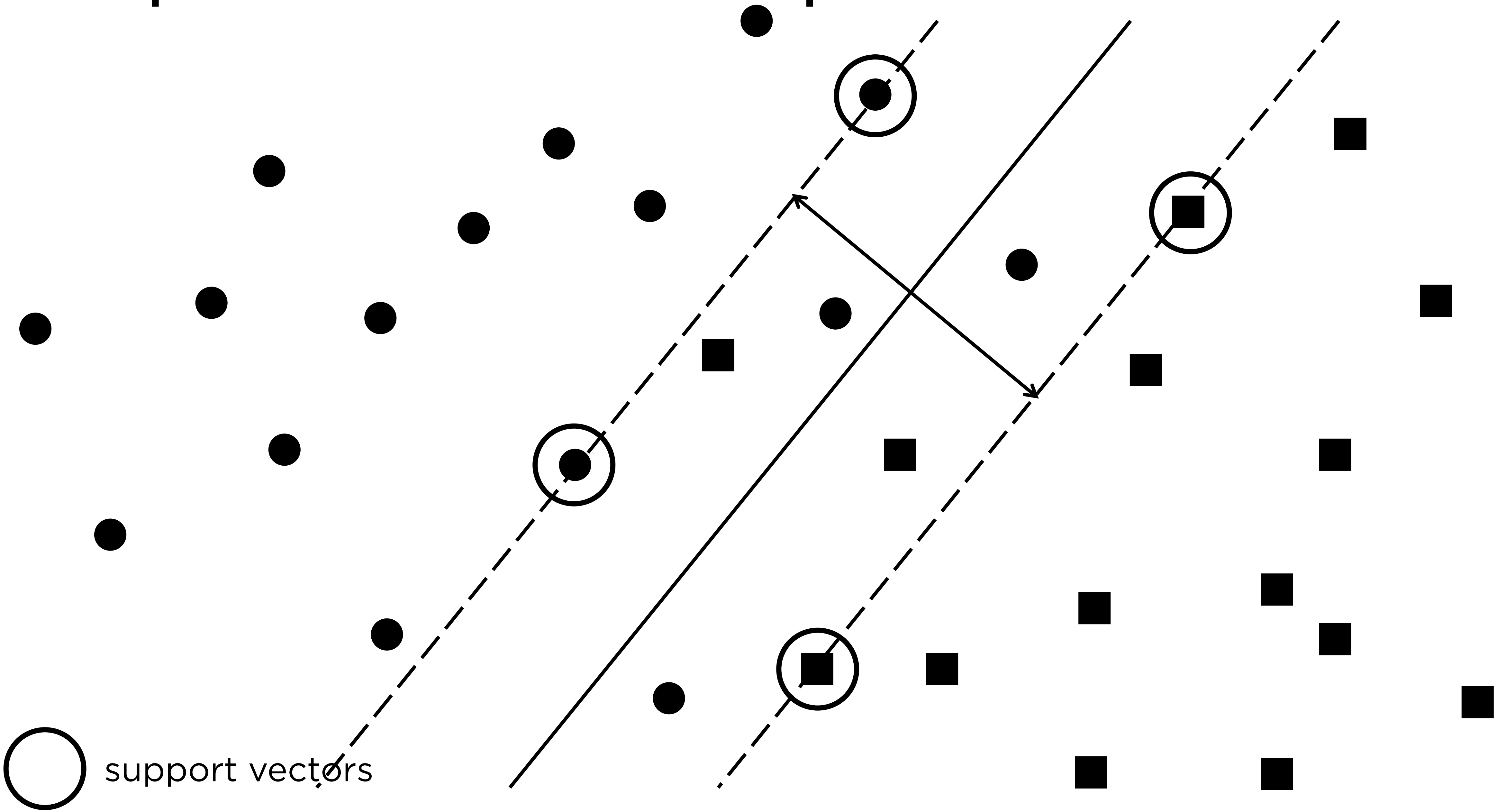


Can we find a linear separable solution?

- No, we cannot. 😟



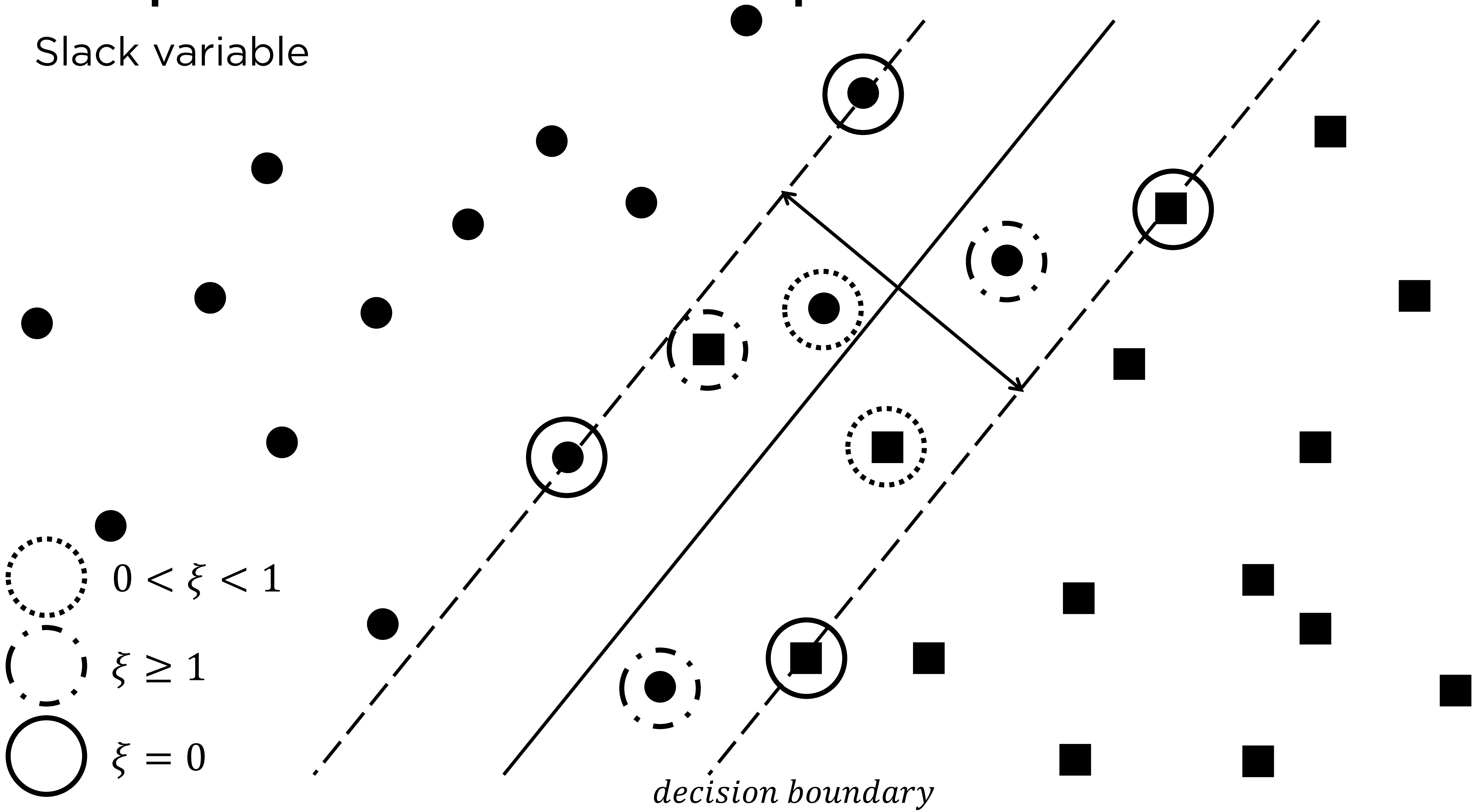
Old problem with new data points



○ support vectors

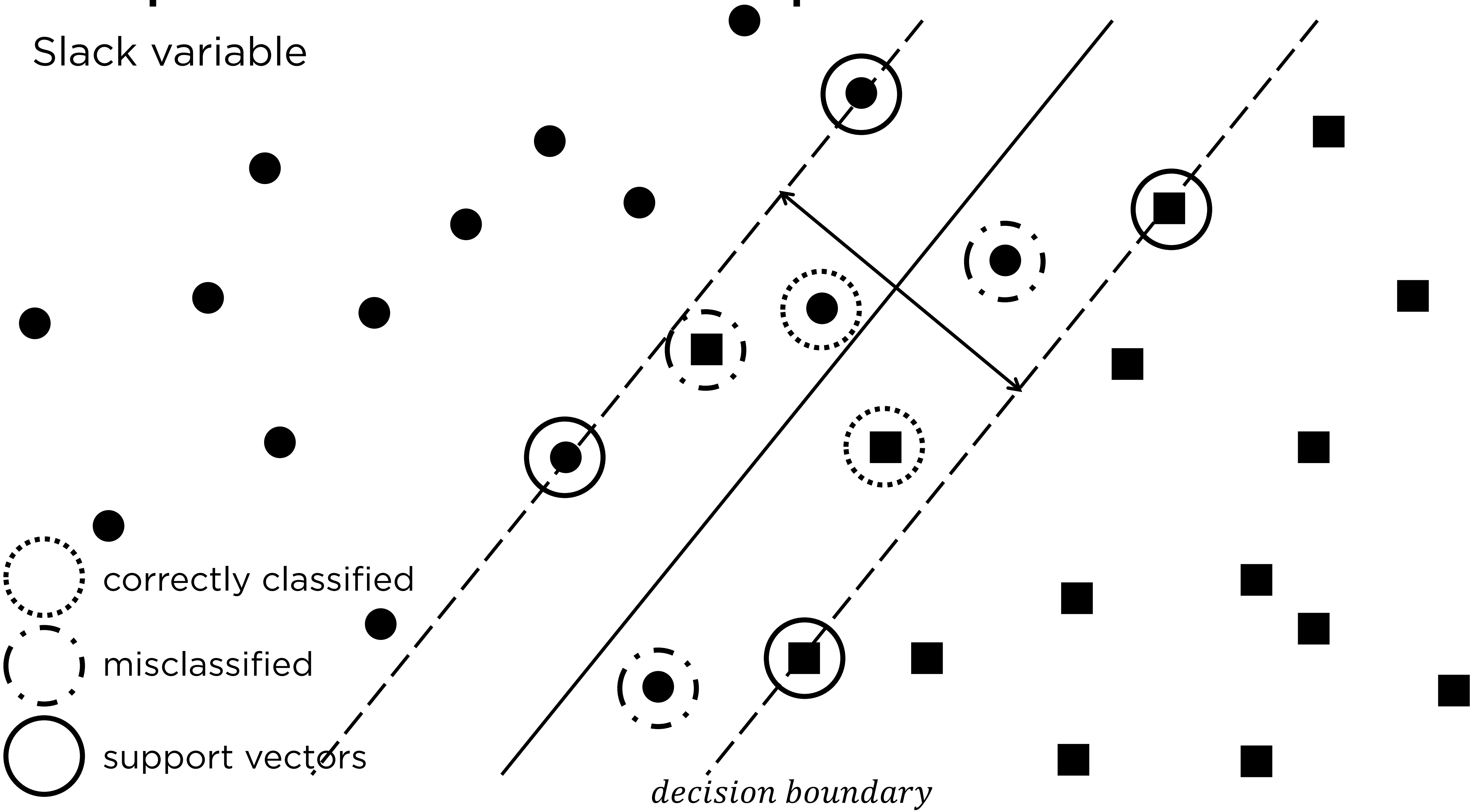
Old problem with new data points

Slack variable



Old problem with new data points

Slack variable



Soft Margin Support Vector Machine

The role of the parameter C

C is a regularization parameter:

- Small C allows constraints to be easily ignored, hence results in large margin.
- Large C makes constraints hard to ignore, hence results in narrow margin.
- When $C = \infty$, it enforces all constraints to become hard margin problem.

Today

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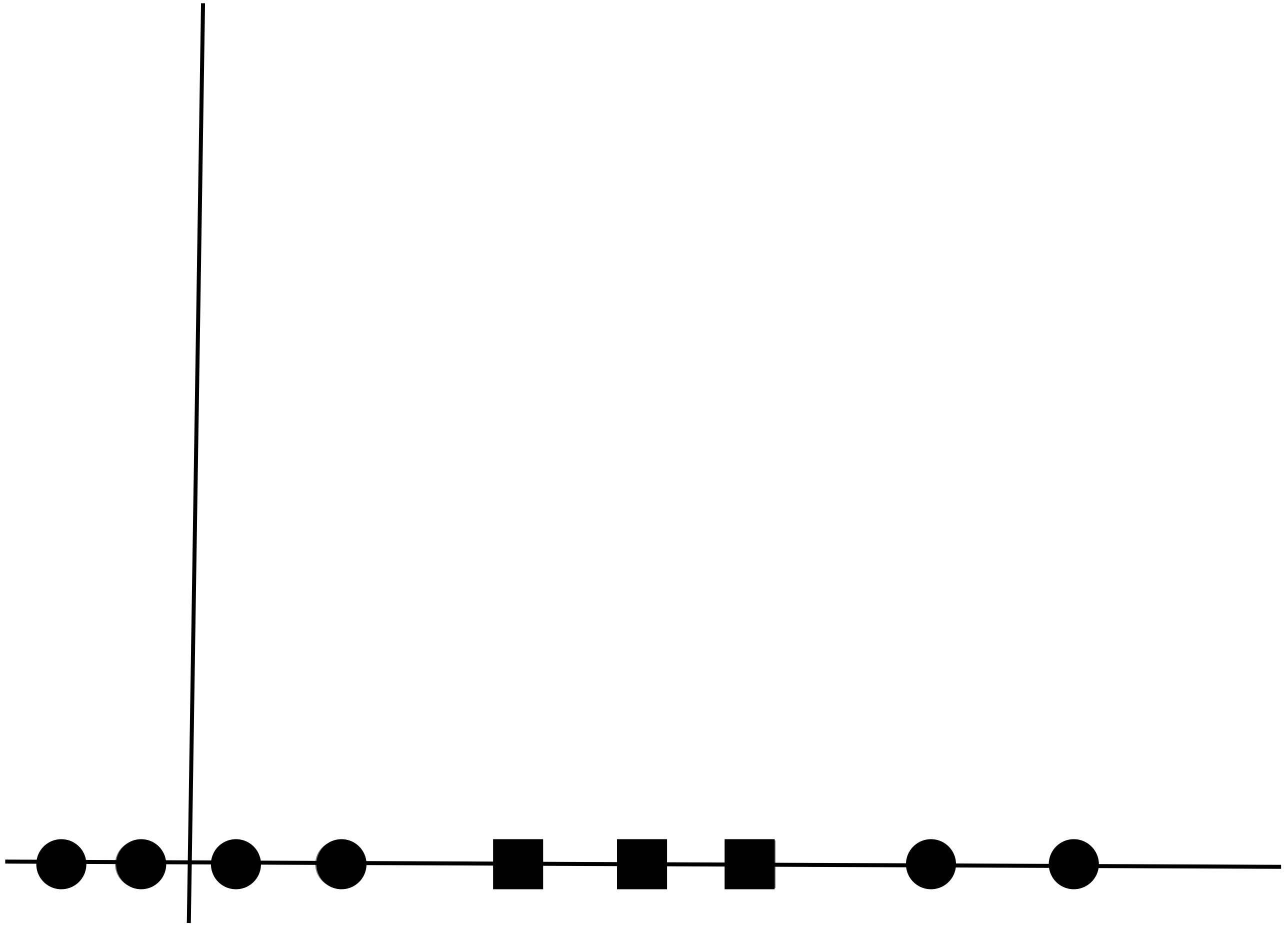
- Non-Linear Separable SVM

Non-Linear Separable SVM

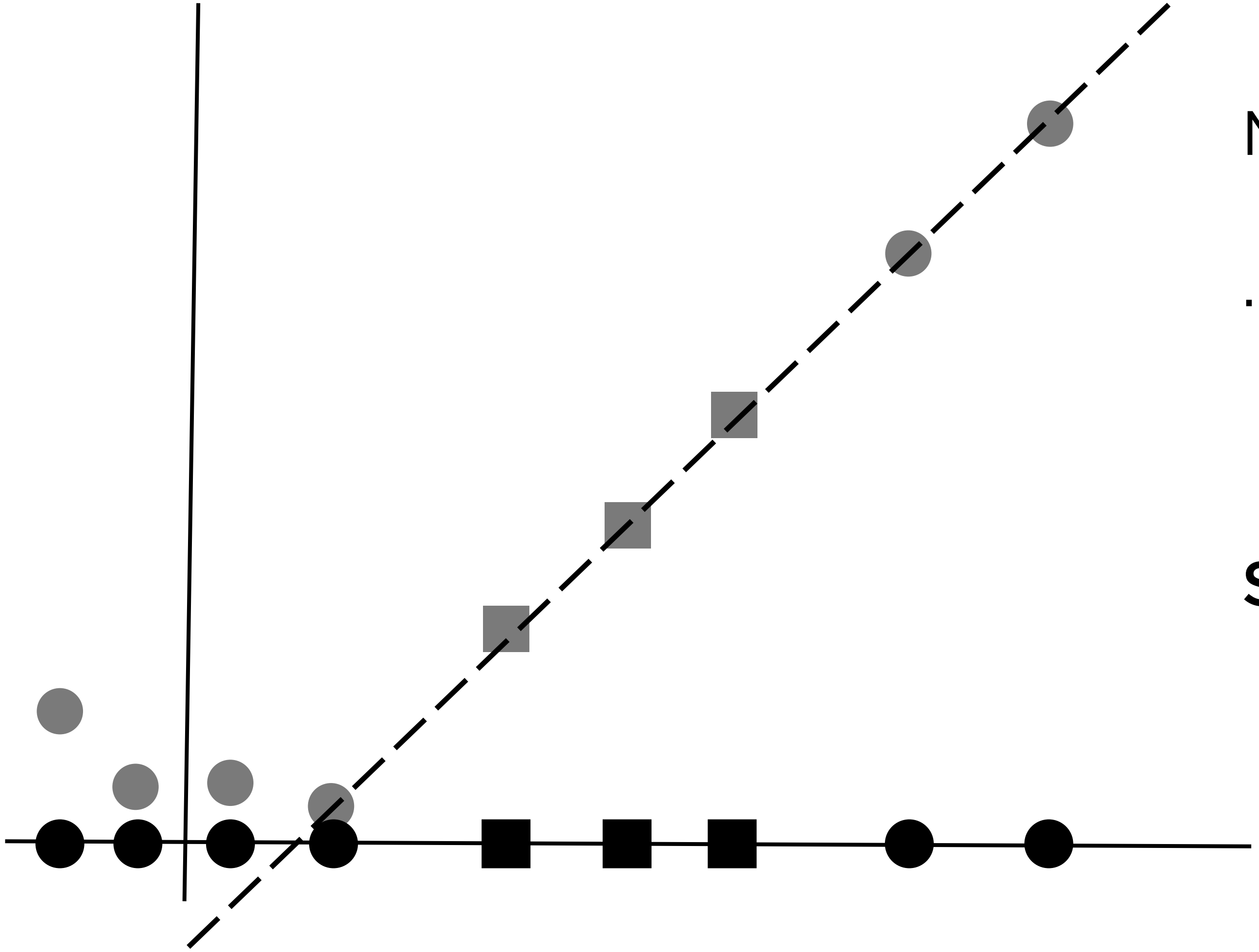
Non-Linear Separable SVM

Hard 1-dimensional Dataset Solution



Non-Linear Separable SVM

Hard 1-dimensional Dataset Solution



Make up a new feature!

…Computed from original feature(s)

$$y_k = (x_k, {x_k}^2)$$

Separable. 😉

Non-Linear Separable SVM

Feature Vector and Feature Space

Let $\vec{x} = [\overrightarrow{x_1}] \in \mathbb{R}$ be a vector representation of object $x \in X$

Let $\Phi: X \longrightarrow K \in \mathbb{R}^2$ feature map given by

$$\Phi(\vec{x}) = [\overrightarrow{x_1}, \overrightarrow{x_1}^2] \in \mathbb{R}^2$$

K is refers to as **feature space** and $\Phi(\vec{x}) = [\Phi_1(\vec{x}), \Phi_2(\vec{x})]$, vector

$\Phi(\vec{x})$ is called the **feature vector.**

Non-Linear Separable SVM

Feature Map and Kernel Function

A **feature map** refers to a function $\Phi\colon \mathbb{R}^n \longrightarrow \mathbb{R}^N$

$$\Phi(\vec{x}) = \left(\Phi_1(\vec{x}), \dots, \Phi_N(\vec{x})\right)^T, \vec{x} \in \mathbb{R}^n$$

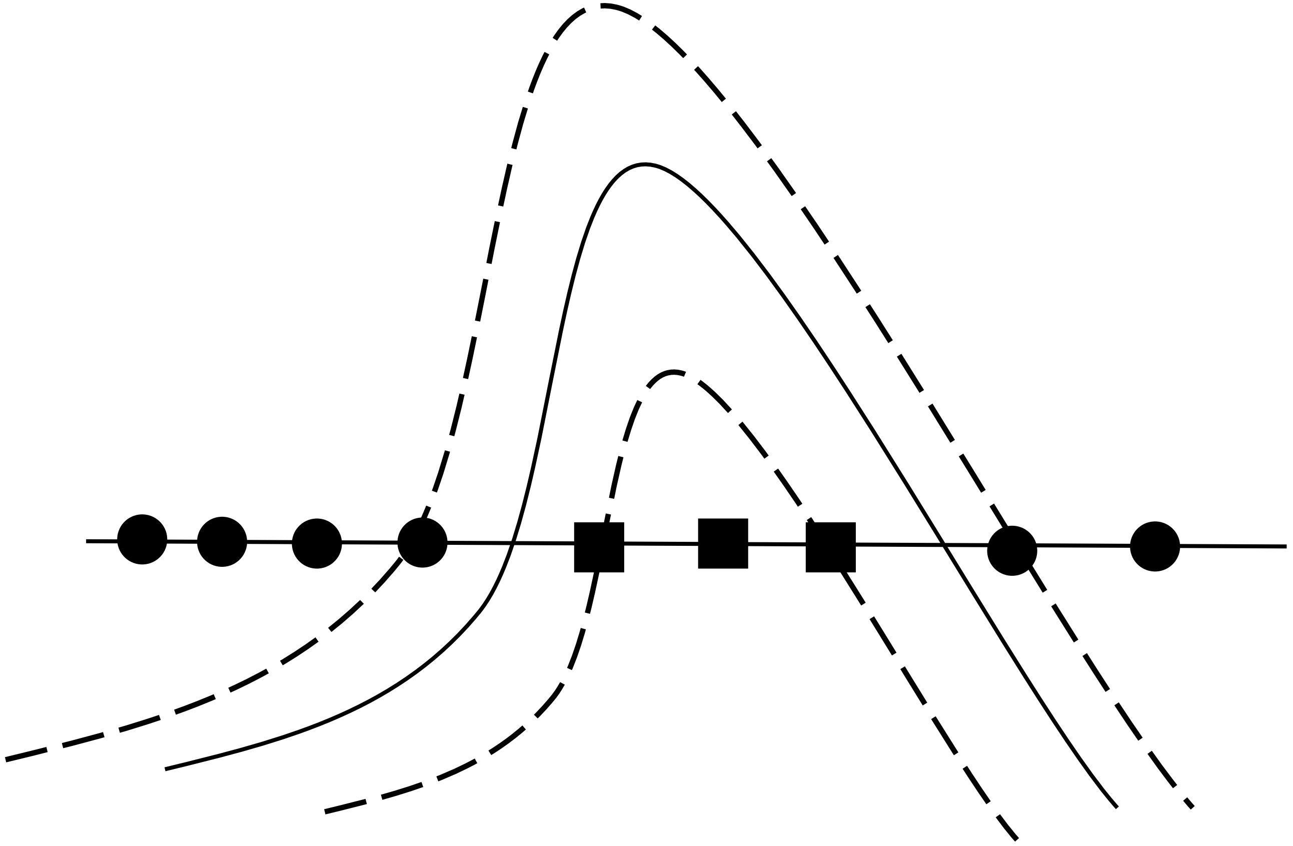
The $\Phi_1, .., \Phi_N$ are called **basis functions**, given a feature map Φ

we define its associated kernel function $\mathrm{K}\colon \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}$ as

$$\boldsymbol{K}(\boldsymbol{x}, \boldsymbol{t}) =< \Phi(\boldsymbol{x}), \Phi(\boldsymbol{t}) >, \qquad \boldsymbol{x}, \boldsymbol{t} \in \mathbb{R}^n$$

Non-Linear Separable SVM

What is the decision boundary for this data?



The least polynomial degree equal to 2 for this example since that is the highest polynomial degree in our basis functions, we can also called it quadratic kernels

Today

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- Non-Linear Separable SVM

Questions?

Further Reading

The Elements of Statistical Learning Chapter 6 and Chapter 12

https://web.stanford.edu/~hastie/Papers/ESLII.pdf