

Support Vector Machines

Machine Learning Course - CS-433

Oct 15, 2024

Nicolas Flammarion

EPFL

Vapnik's invention

A Training Algorithm for Optimal Margin Classifiers

Bernhard E. Boser*
EECS Department
University of California
Berkeley, CA 94720
boser@eecs.berkeley.edu

Isabelle M. Guyon
AT&T Bell Laboratories
50 Fremont Street, 6th Floor
San Francisco, CA 94105
isabelle@neural.att.com

Vladimir N. Vapnik
AT&T Bell Laboratories
Crawford Corner Road
Holmdel, NJ 07733
vlad@neural.att.com

Support-Vector Networks

CORINNA CORTES
VLADIMIR VAPNIK
AT&T Bell Labs., Holmdel, NJ 07733, USA

Editor: Lorenza Saitta

Abstract. The *support-vector network* is a new learning machine conceptually implements the following idea: input dimension feature space. In this feature space a linear decision surface ensures high generalization ability of the learning network was previously implemented for the restricted case of linearly separable data. We here extend this result to non-separable training data.

High generalization ability of support-vector networks utilized. We also compare the performance of the support-vector network that all took part in a benchmark study of Optical Character Recognition.

Machine Learning, 20, 273–297 (1995)

© 1995 Kluwer Academic Publishers, Boston. Manufactured in The Netherlands.

GVB⁺92, Vap82, BH89, TLS89, Mac92] link the generalization of a classifier to the error on the training set and the complexity of the classifier. Methods such as structural risk minimization [Vap82] vary the complexity of the classification function in order to improve the generalization.

In this paper we describe a training algorithm that automatically tunes the capacity of the classification function maximizing the margin between training examples.

corinna@neural.att.com

Том XXIV «АВТОМАТИКА И ТЕЛЕМЕХАНИКА» № 6
1963

УДК 519.95

УЗНАВАНИЕ ОБРАЗОВ ПРИ ПОМОЩИ ОБОБЩЕННЫХ ПОРТРЕТОВ

В. Н. ВАПНИК, А. Я. ЛЕРНЕР
(Москва)

Дается аксиоматическое определение образа. Вводятся понятия «обобщенный портрет», «различение» и «узнавание». Предлагаются алгоритмы обучения узнаванию и различению, основанные на нахождении обобщенных портретов образов.

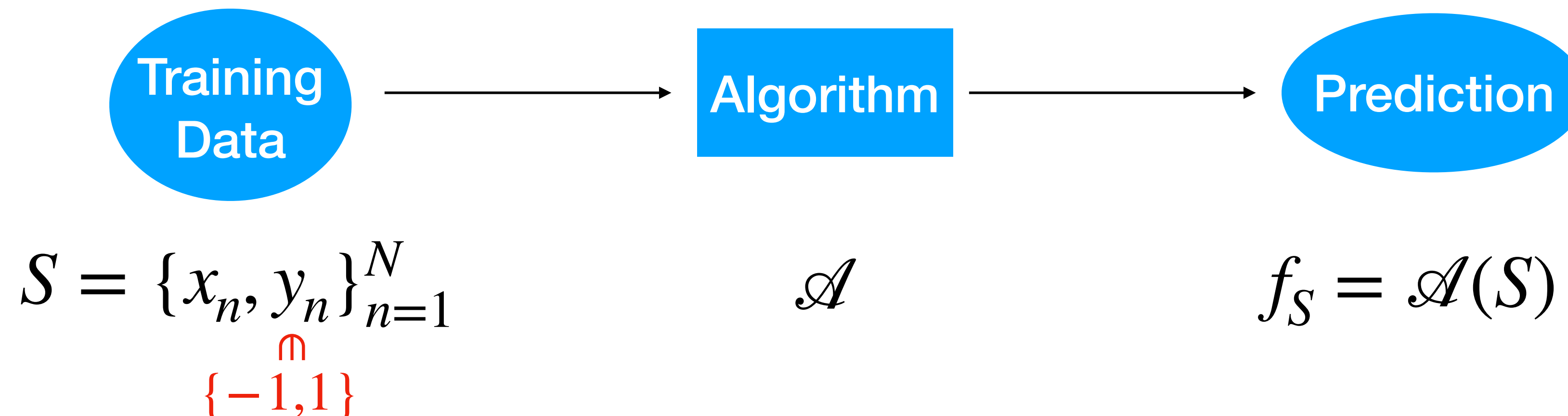


Binary classification

We observe some data $S = \{x_n, y_n\}_{n=1}^N \in \mathcal{X} \times \{-1, 1\}$

Goal: given a new observation x , we want to predict its label y

How:



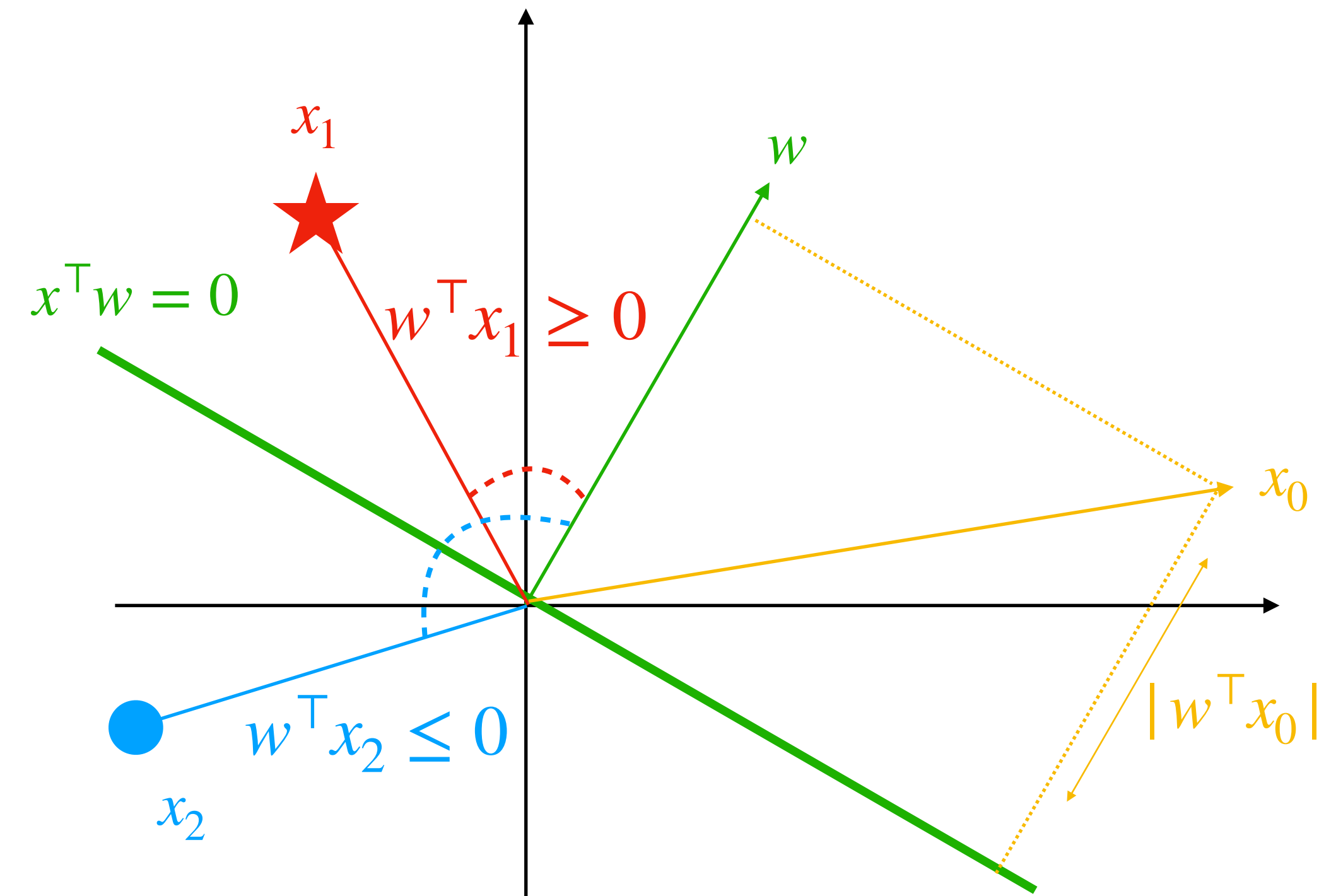
Linear Classifier

Define a hyperplane as $\{x : w^\top x = 0\}$
where $\|w\| = 1$

Prediction:

$$f(x) = \text{sign}(x^\top w)$$

Claim: The distance between a point x_0 and the hyperplane defined by w is $|w^\top x_0|$



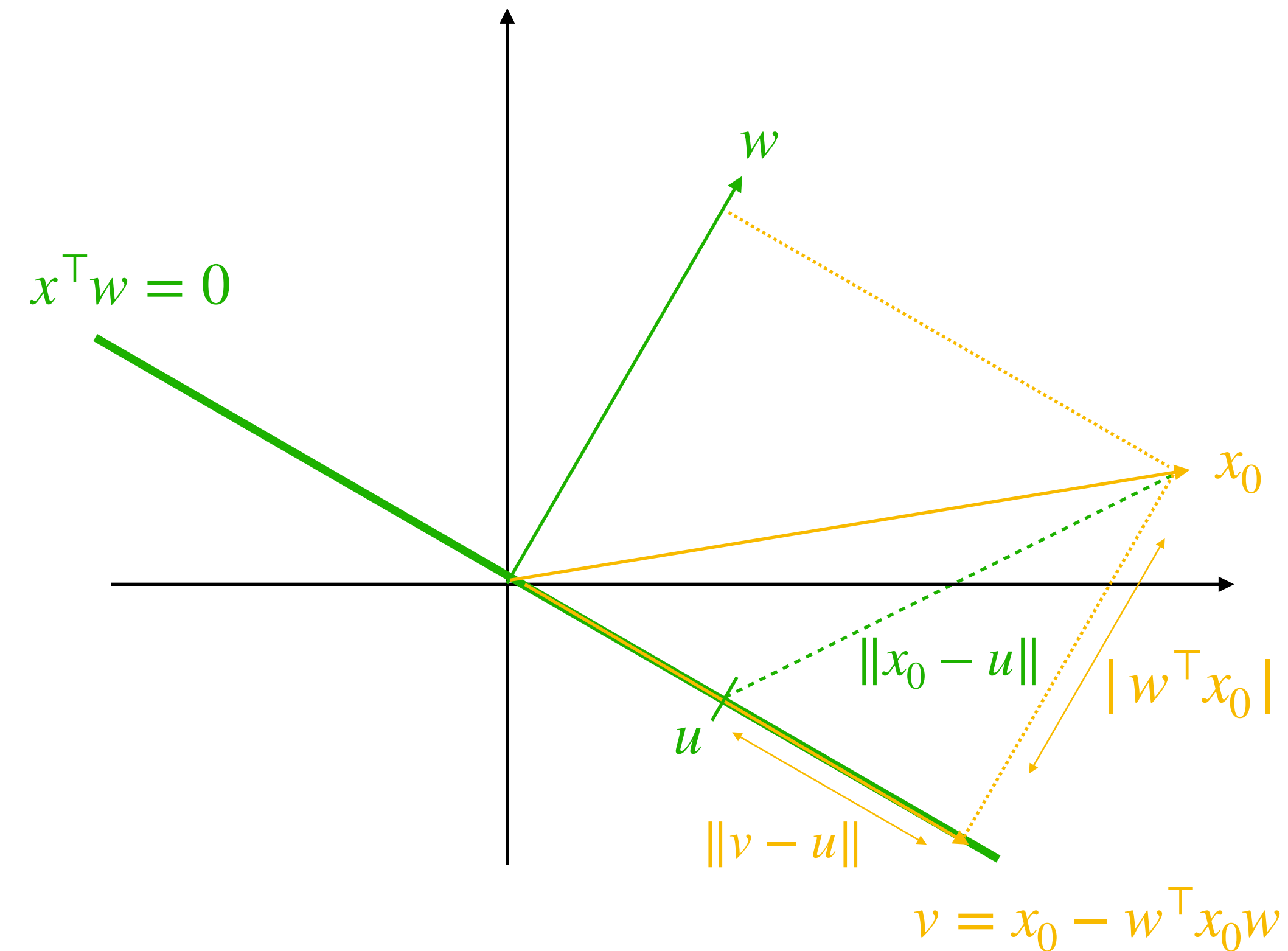
Linear Classifier

Proof: The distance between x_0 and the hyperplane is given by $\min_{u:w^\top u=0} \|x_0 - u\|$

Let $v = x_0 - w^\top x_0 w$ then by the Pythagorean theorem for any u s.t. $w^\top u = 0$

$$\|x_0 - u\|^2 = (w^\top x_0)^2 + \|v - u\|^2 \geq (w^\top x_0)^2$$

Claim: The distance between a point x_0 and the hyperplane defined by w is $|w^\top x_0|$



Hard-SVM rule: max-margin separating hyperplane

First assume the dataset $(x_n, y_n)_{n=1}^N$ is linearly separable

Margin of a hyperplane: $\min_{n \leq N} |w^\top x_n|$

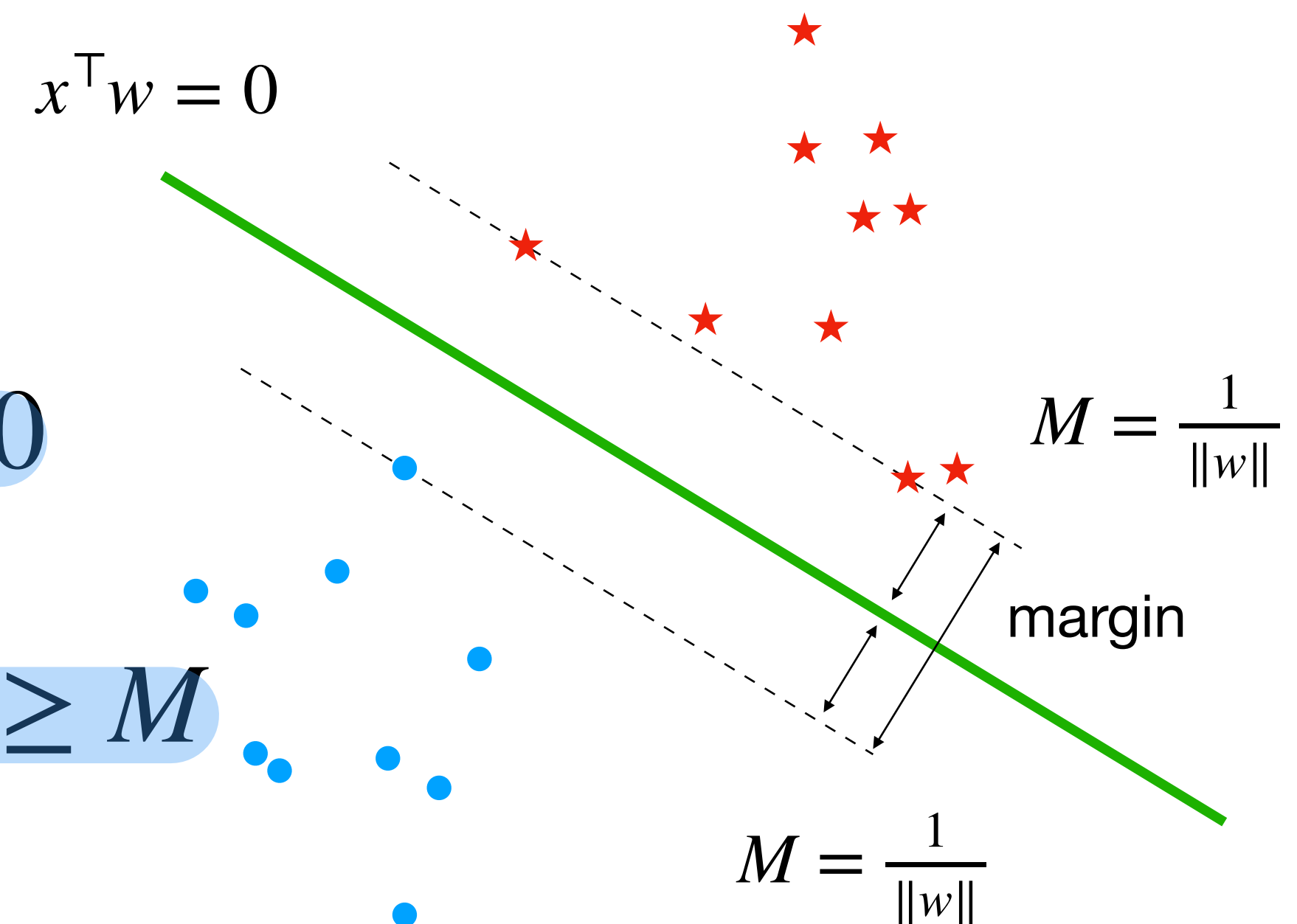
Max-margin separating hyperplane:

$$\max_{w, \|w\|=1} \min_{n \leq N} |w^\top x_n| \text{ such that } \forall n, y_n x_n^\top w \geq 0$$

Equivalent to $\max_{M \in \mathbb{R}, w, \|w\|=1} M$ such that $\forall n, y_n x_n^\top w \geq M$

also equivalent to:

$$\min_w \frac{1}{2} \|w\|^2 \text{ such that } \forall n, y_n x_n^\top w \geq 1$$



Proof of the equivalent formulations

Claim: The following optimization problems are equivalent

$$\begin{aligned} & \max_{w, \|w\|=1} \min_{n \leq N} |w^\top x_n| \\ & \text{s.t. } \forall n, y_n x_n^\top w \geq 0 \end{aligned} \quad (\text{I})$$

$$\begin{aligned} & \max_{M \in \mathbb{R}, w, \|w\|=1} M \\ & \text{s.t. } \forall n, y_n x_n^\top w \geq M \end{aligned} \quad (\text{II})$$

Proof: Let w_1 be a solution of (I) and $M_1 = \min_{n \leq N} |w_1^\top x_n|$ and let w_2 and M_2 be solutions of (II)

- (w_1, M_1) is admissible for (II) so $M_1 \leq M_2$
- w_2 is admissible for (I) so $\min_{n \leq N} |w_2^\top x_n| \leq \min_{n \leq N} |w_1^\top x_n|$
- $\forall n, y_n x_n^\top w_2 \geq M_2$ implies that $\forall n, |x_n^\top w_2| \geq M_2$ and $\min_{n \leq N} |x_n^\top w_2| \geq M_2$

Therefore $M_1 = \min_{n \leq N} |w_1^\top x_n| \geq \min_{n \leq N} |w_2^\top x_n| \geq M_2 \geq M_1$

And the two problems are equivalent

Proof of the equivalent formulations

Claim: The following optimization problems are equivalent

$$\begin{aligned} \max_{M \in \mathbb{R}, w, \|w\|=1} \quad & M \\ \text{s.t.} \quad & \forall n, y_n x_n^\top w \geq M \end{aligned} \quad (\text{II})$$

$$\begin{aligned} \min_w \quad & \frac{1}{2} \|w\|^2 \\ \text{s.t.} \quad & \forall n, y_n x_n^\top w \geq 1 \end{aligned} \quad (\text{III})$$

Proof:

$$\max_{M \in \mathbb{R}, w, \|w\|=1} M \text{ such that } \forall n, y_n x_n^\top w \geq M$$

$$\iff \max_{M \in \mathbb{R}, w} M \text{ such that } \forall n, y_n x_n^\top \frac{w}{\|w\|} \geq M$$

The constraints are independent of the scale of w . Set $\|w\| = 1/M$:

$$\iff \max_w 1/\|w\| \text{ such that } \forall n, y_n x_n^\top w \geq 1$$

$$\iff \min_w \frac{1}{2} \|w\|^2 \text{ such that } \forall n, y_n x_n^\top w \geq 1$$

Soft SVM: a relaxation of the Hard-SVM rule that can be applied even if the training set is not linearly separable

Idea: Maximize the margin while allowing some constraints to be violated

How: Introduce positive slack variables ξ_1, \dots, ξ_N and replace the constraints with $y_n x_n^\top w \geq 1 - \xi_n$

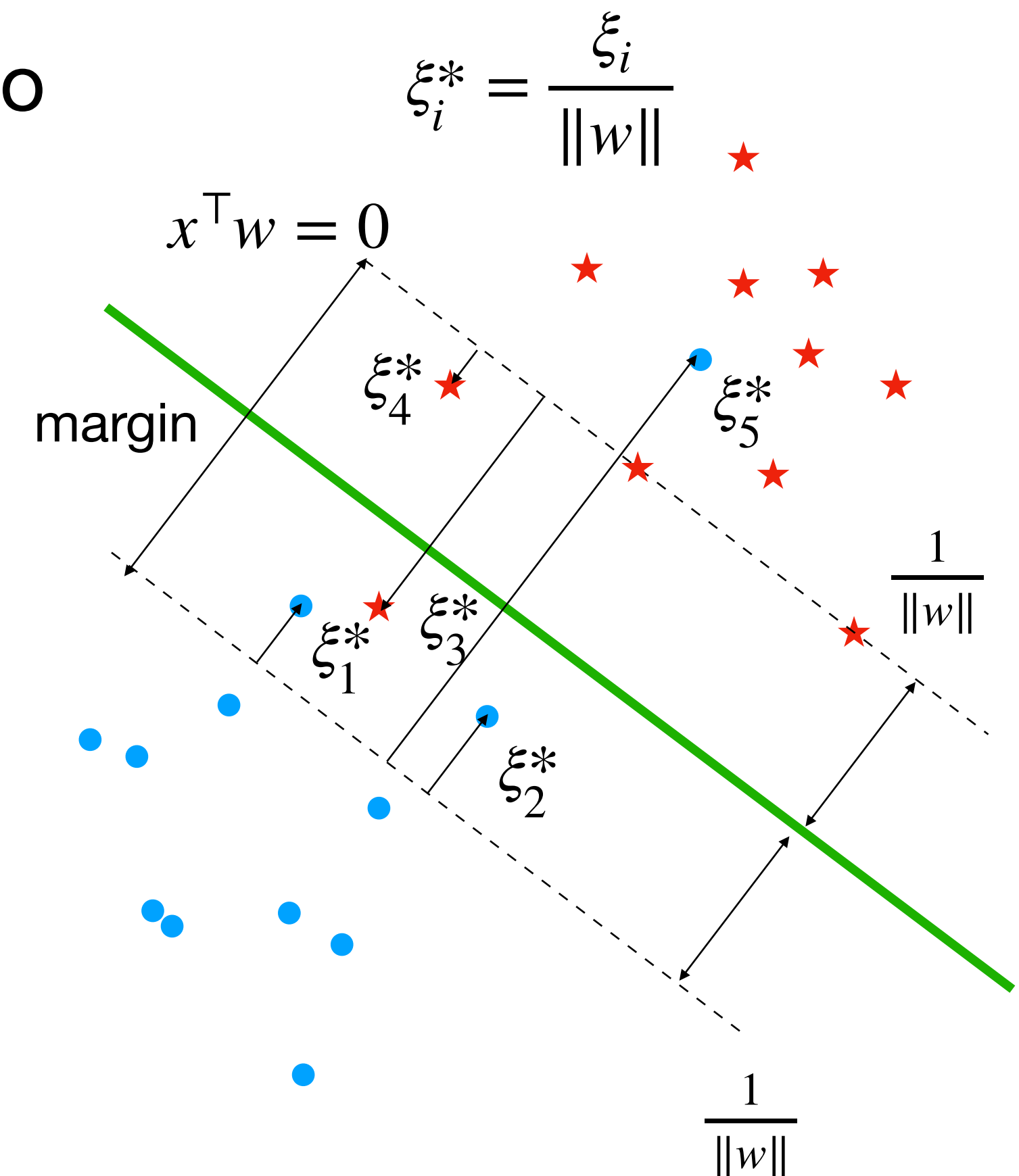
Soft SVM:

$$\begin{aligned} \min_{w, \xi} \quad & \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N \xi_n \\ \text{s.t.} \quad & \forall n, y_n x_n^\top w \geq 1 - \xi_n \text{ and } \xi_n \geq 0 \end{aligned}$$

which is equivalent to

$$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N [1 - y_n x_n^\top w]_+$$

$[\alpha]_+ = \max\{0, \alpha\}$



Soft SVM: a relaxation of the Hard-SVM rule that can be applied even if the training set is not linearly separable

Proof: Fix w and consider the minimization over ξ :

- If $y_n x_n^\top w \geq 1$, then $\xi_n = 0$
- If $y_n x_n^\top w < 1$, $\xi_n = 1 - y_n x_n^\top w$

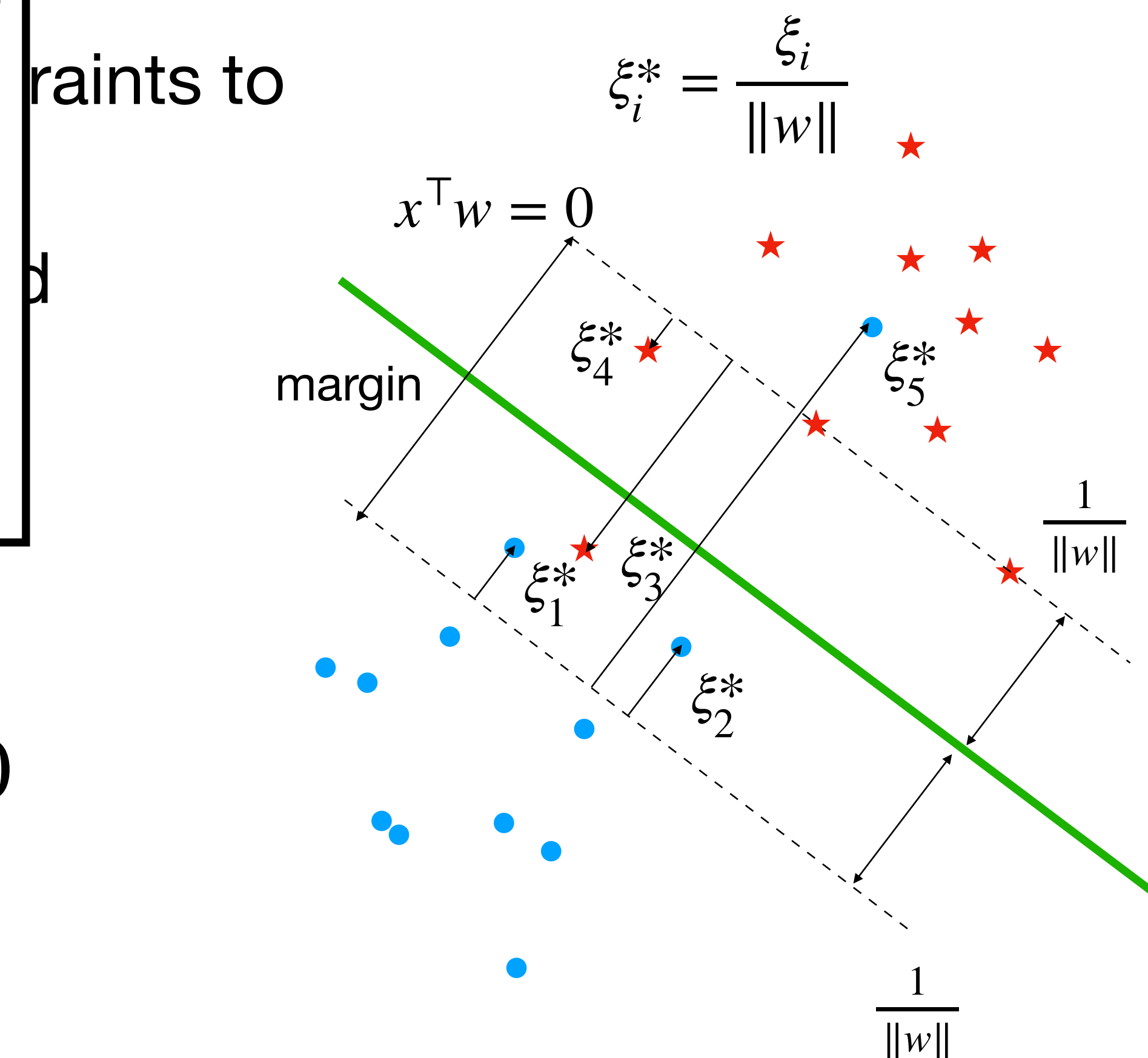
Therefore $\xi_n = [1 - y_n x_n^\top w]_+$

$$\begin{aligned} \min_{w, \xi} \quad & \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N \xi_n \\ \text{s.t.} \quad & \forall n, y_n x_n^\top w \geq 1 - \xi_n \quad \text{and} \quad \xi_n \geq 0 \end{aligned}$$

which is equivalent to

$$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N [1 - y_n x_n^\top w]_+$$

$$[\alpha]_+ = \max\{0, \alpha\}$$



Classification by risk minimization

Setting: $(X, Y) \sim \mathcal{D}$ with ranges \mathcal{X} and $\mathcal{Y} = \{-1, 1\}$

Goal: Find a classifier $f: \mathcal{X} \rightarrow \mathcal{Y}$ that minimizes the true risk

$$L(f) = \mathbb{E}_{\mathcal{D}}(1_{Y \neq f(X)})$$

How: Through Empirical Risk Minimization (ERM):

$$\min_w L_{\text{train}}(w) = \frac{1}{N} \sum_{n=1}^N \phi(y_n w^\top x_n)$$

ϕ represents the loss function of the functional margin $y_n x_n^\top w$

ϕ also serves as a convex surrogate for the 0-1 loss

Losses for Classification

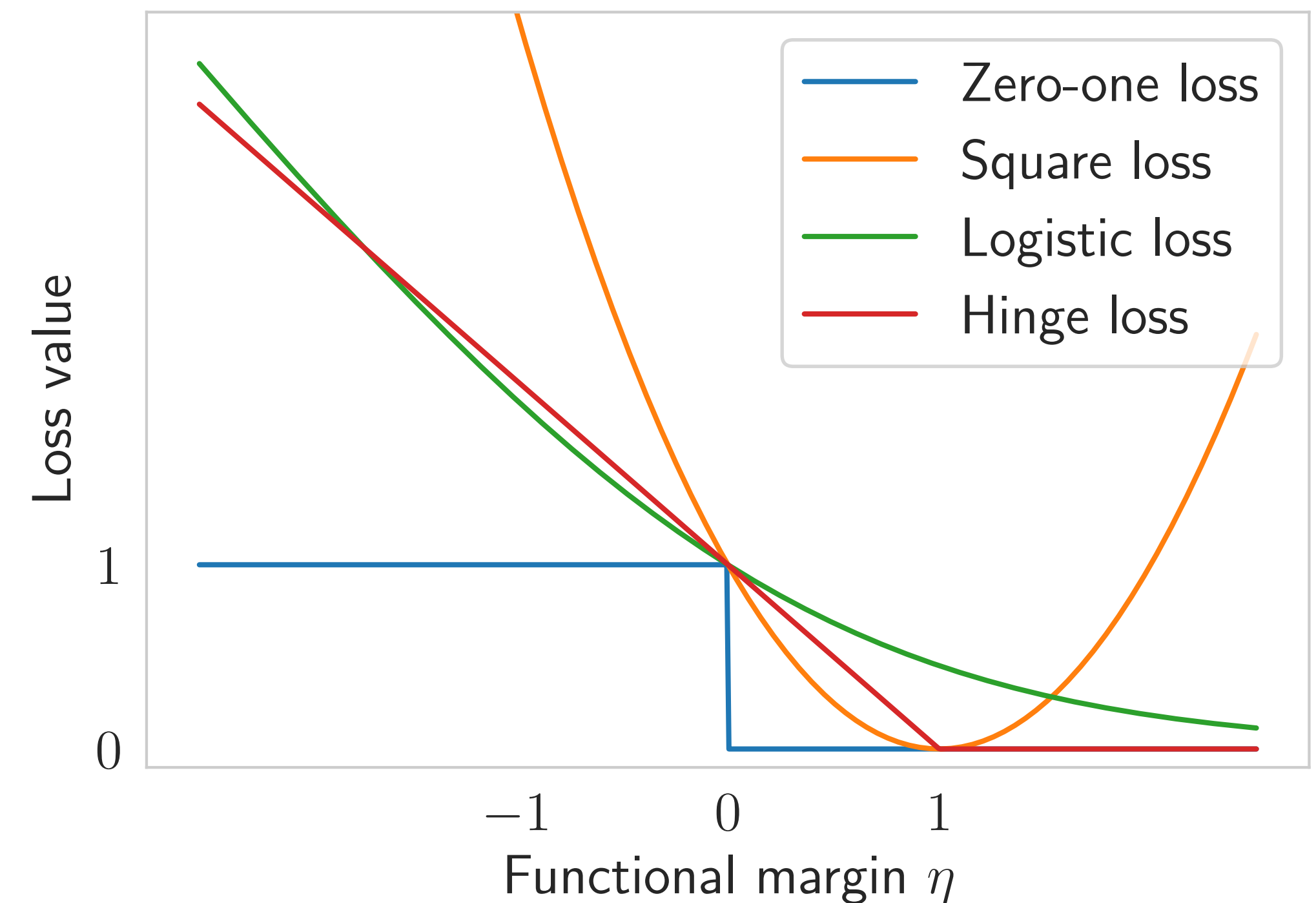
Examples of margin-based losses ($\eta = yx^T w$):

- Quadratic loss: $\text{MSE}(\eta) = (1 - \eta)^2$
- Logistic loss: $\text{Logistic}(\eta) = \frac{\log(1 + \exp(-\eta))}{\log(2)}$
- Hinge loss: $\text{Hinge}(\eta) = [1 - \eta]_+$

Common features: these losses are convex and provide an upper bound for the zero-one loss

Behavioral differences:

- **MSE:** Penalizes any deviation from 1
- **Logistic Loss:** Asymmetric cost – a penalty is always incurred.
- **Hinge Loss:** A penalty is applied if the prediction is incorrect or lacks confidence



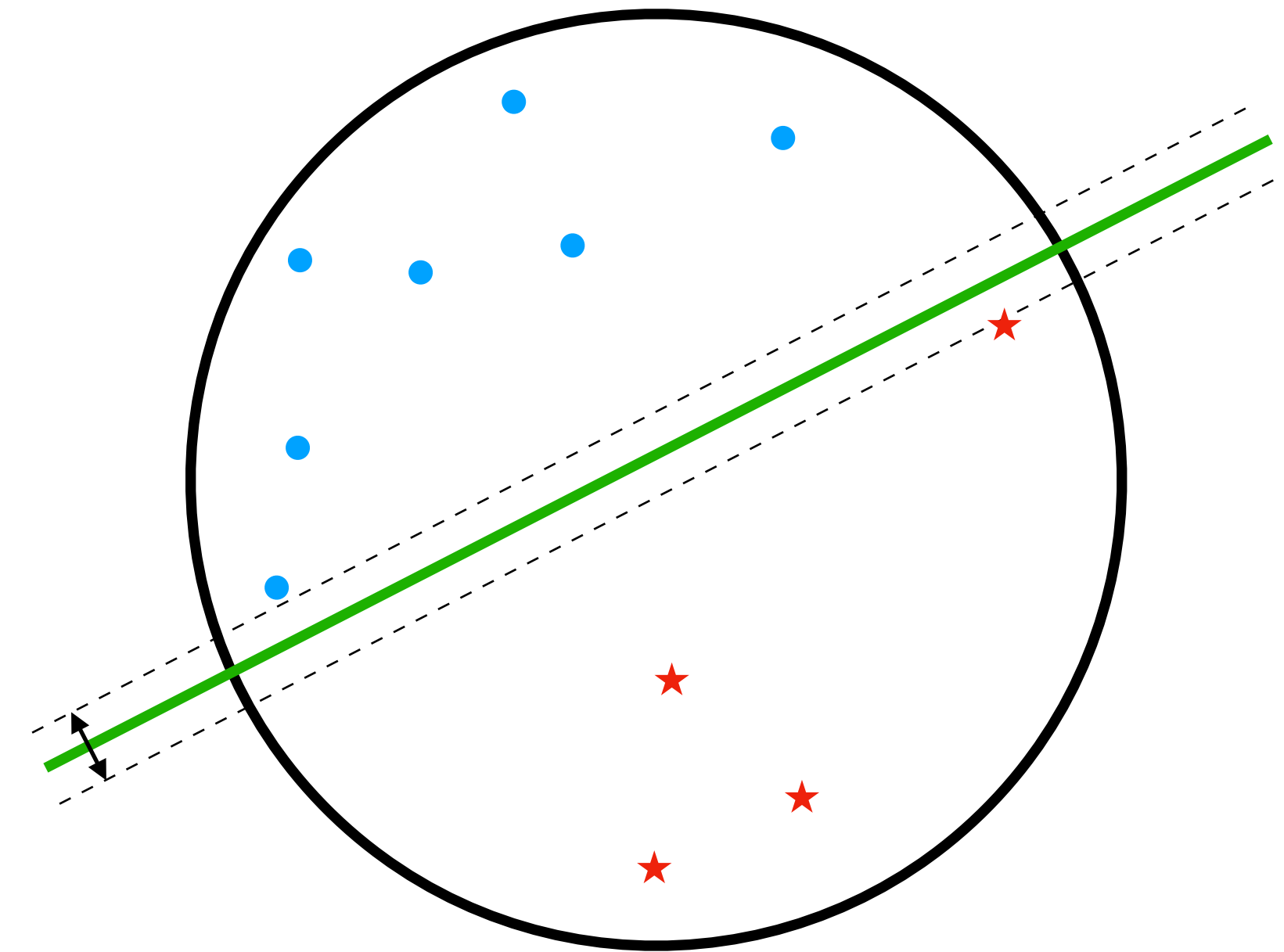
Summary

$$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N [1 - y_n x_n^\top w]_+$$

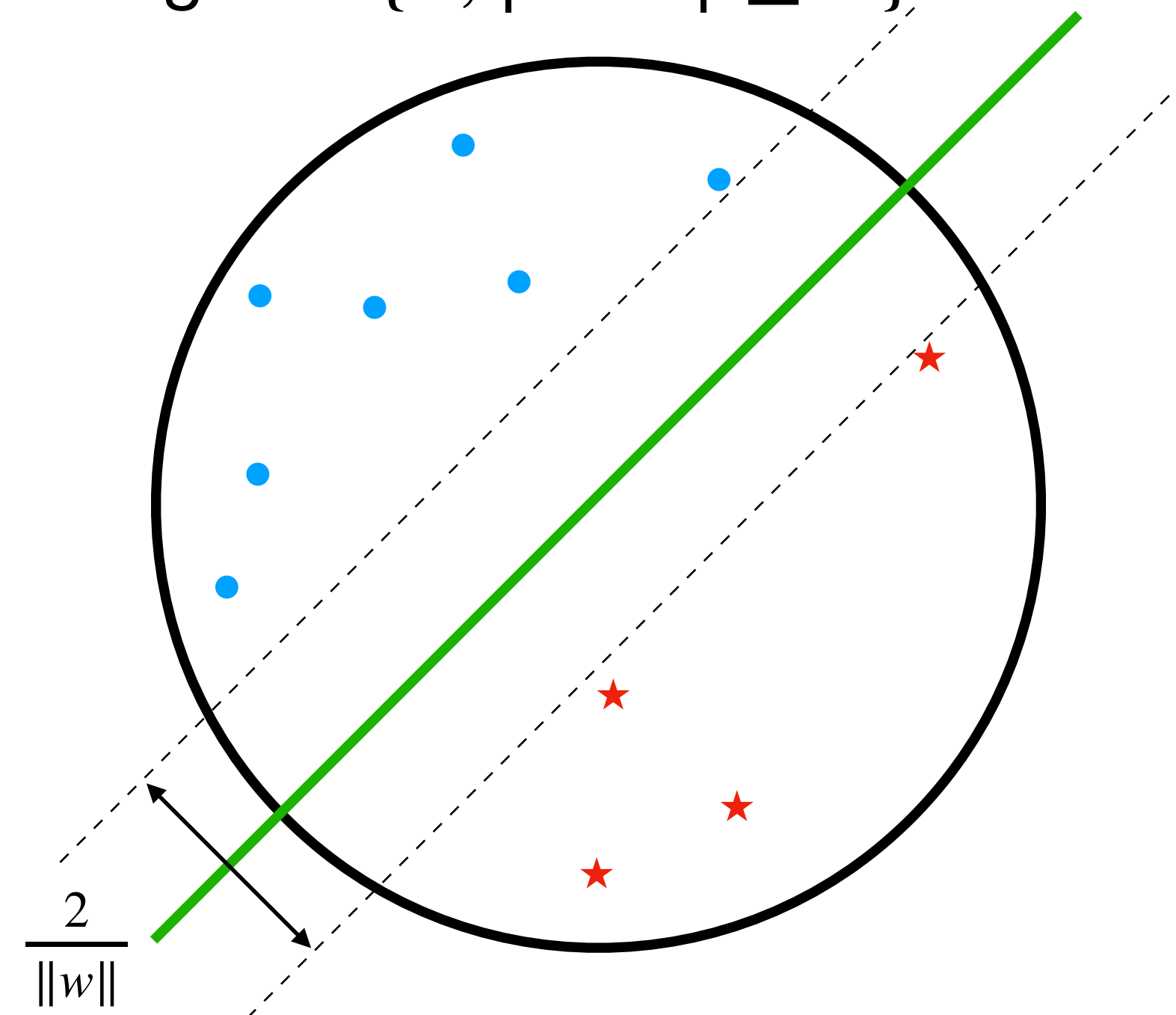
ERM for the hinge loss with ridge regularization

Interpretation for separable data with small λ :

1. Choose the direction of w such that w^\perp acts as a separating hyperplane
2. Adjust the scale of w to ensure that no point lies with the margin
3. Select the hyperplane with the largest margin



Margin: $= \{x; |x^\top w| \leq 1\}$



Optimization: How to get w ?

$$\min_w \frac{1}{N} \sum_{n=1}^N [1 - y_n x_n^\top w]_+ + \frac{\lambda}{2} \|w\|^2$$

Convex (but non-smooth) objective which can be minimized with:

- Subgradient method
- Stochastic Subgradient method

Convex duality

Assume you can define an auxiliary function $G(w, \alpha)$ such that

$$\min_w L(w) = \min_w \max_{\alpha} G(w, \alpha)$$

Primal problem: $\min_w \max_{\alpha} G(w, \alpha)$

Dual problem: $\max_{\alpha} \min_w G(w, \alpha)$

➡ Sometimes, the dual problem is easier to solve than the primal problem.

Questions:

1. How do we identify a suitable $G(w, \alpha)$?
2. Under what conditions can the min and max be interchanged?
3. When is the dual problem more tractable than the primal problem?

Q1: How do we find a suitable $G(w, \alpha)$?

$$[z]_+ = \max(0, z) = \max_{\alpha \in [0, 1]} \alpha z$$

Therefore $[1 - y_n x_n^\top w]_+ = \max_{\alpha_n \in [0, 1]} \alpha_n (1 - y_n x_n^\top w)$

The SVM problem is equivalent to:

$$\min_w L(w) = \min_w \max_{\alpha \in [0, 1]^n} \underbrace{\frac{1}{N} \sum_{n=1}^N \alpha_n (1 - y_n x_n^\top w)}_{G(w, \alpha)} + \frac{\lambda}{2} \|w\|_2^2$$

The function G is convex in w and concave in α

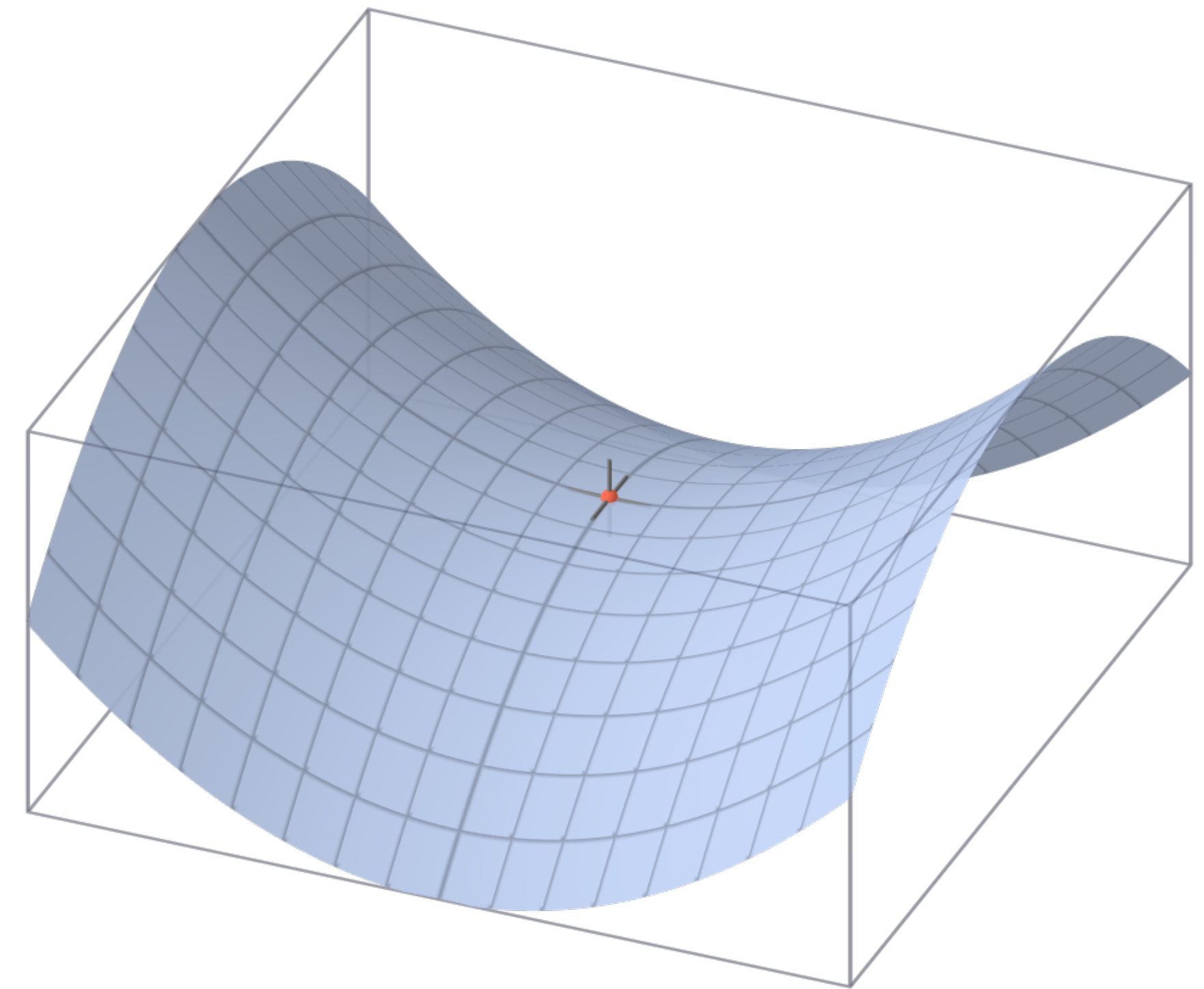
Q2: Can the min and max be interchanged?

Always true:

$$\max_{\alpha} \min_w G(w, \alpha) \leq \min_w \max_{\alpha} G(w, \alpha)$$

Equality if G is convex in w , concave in α and the domains of w and α are convex and compact:

$$\max_{\alpha} \min_w G(w, \alpha) = \min_w \max_{\alpha} G(w, \alpha)$$



Q2: Can the min and max be interchanged?

Always true:

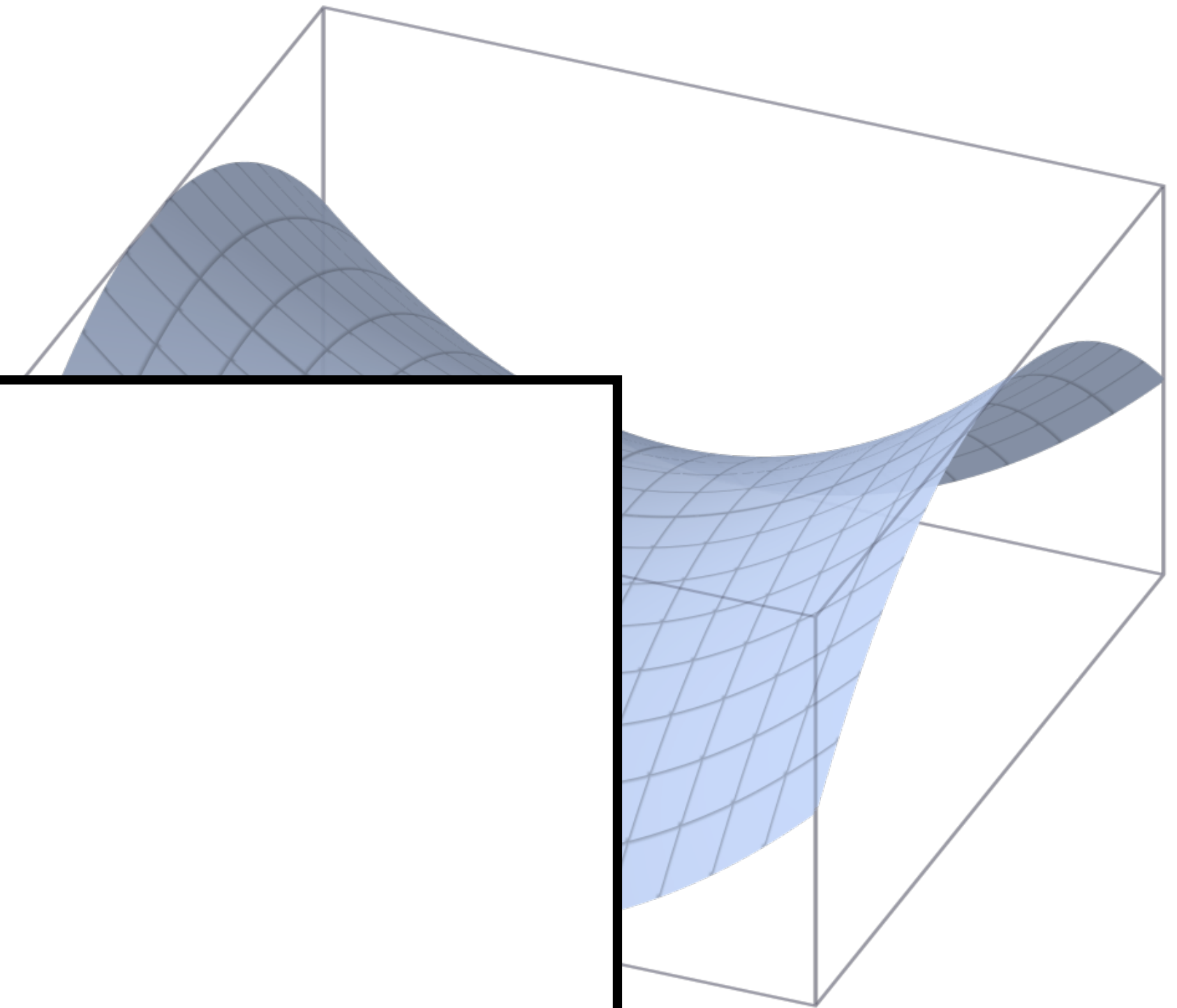
$$\max_{\alpha} \min_w G(w, \alpha) \leq \min_w \max_{\alpha} G(w, \alpha)$$

Proof:

$$\min_w G(\alpha, w) \leq G(\alpha, w') \text{ for any } w'$$

$$\max_{\alpha} \min_w G(\alpha, w) \leq \max_{\alpha} G(\alpha, w') \text{ for any } w'$$

$$\max_{\alpha} \min_w G(\alpha, w) \leq \min_{w'} \max_{\alpha} G(\alpha, w')$$



Application to SVM

For SVM, the condition is met, allowing us to interchange min and max:

$$\min_w L(w) = \max_{\alpha \in [0,1]^n} \min_w \frac{1}{N} \sum_{n=1}^N \alpha_n (1 - y_n x_n^\top w) + \frac{\lambda}{2} \|w\|_2^2$$

Minimizer computation:

$$\nabla_w G(w, \alpha) = -\frac{1}{N} \sum_{n=1}^N \alpha_n y_n x_n + \lambda w = 0 \implies w(\alpha) = \frac{1}{\lambda N} \sum_{n=1}^N \alpha_n y_n x_n = \frac{1}{\lambda N} \mathbf{X}^\top \mathbf{Y} \alpha$$

$\mathbf{Y} = \text{diag}(\mathbf{y})$
↓

Dual optimization problem:

$$\begin{aligned} \min_w L(w) &= \max_{\alpha \in [0,1]^n} \frac{1}{N} \sum_{n=1}^N \alpha_n \left(1 - \frac{1}{\lambda N} y_n x_n^\top \mathbf{X}^\top \mathbf{Y} \alpha\right) + \frac{1}{2\lambda N^2} \|\mathbf{X}^\top \mathbf{Y} \alpha\|_2^2 \\ &= \max_{\alpha \in [0,1]^n} \frac{1^\top \alpha}{N} - \frac{1}{\lambda N^2} \alpha^\top \mathbf{Y} \mathbf{X} \mathbf{X}^\top \mathbf{Y} \alpha + \frac{1}{2\lambda N^2} \|\mathbf{X}^\top \mathbf{Y} \alpha\|_2^2 \\ &= \max_{\alpha \in [0,1]^n} \frac{1^\top \alpha}{N} - \frac{1}{2\lambda N^2} \alpha^\top \underbrace{\mathbf{Y} \mathbf{X} \mathbf{X}^\top \mathbf{Y}}_{\text{PSD matrix}} \alpha \end{aligned}$$

PSD matrix

Q3: Why?

$$\max_{\alpha \in [0,1]^n} \alpha^\top \mathbf{1} - \frac{1}{2\lambda N} \alpha^\top \underbrace{\mathbf{Y} \mathbf{X} \mathbf{X}^\top \mathbf{Y}}_{\text{PSD matrix}} \alpha$$

1. **Differentiable Concave Problem:** Efficient solutions can be achieved using
 - Quadratic programming solvers
 - Coordinate ascent
2. **Kernel Matrix Dependency:** The cost function only depends on the data via the *kernel matrix* $K = \mathbf{X} \mathbf{X}^\top \in \mathbb{R}^{N \times N}$ - no dependency on d
3. **Dual Formulation Insight:** α is typically sparse and non-zero exclusively for the training examples that are crucial in determining the decision boundary

Interpretation of the dual formulation

For any (x_n, y_n) , there is a corresponding α_n given by

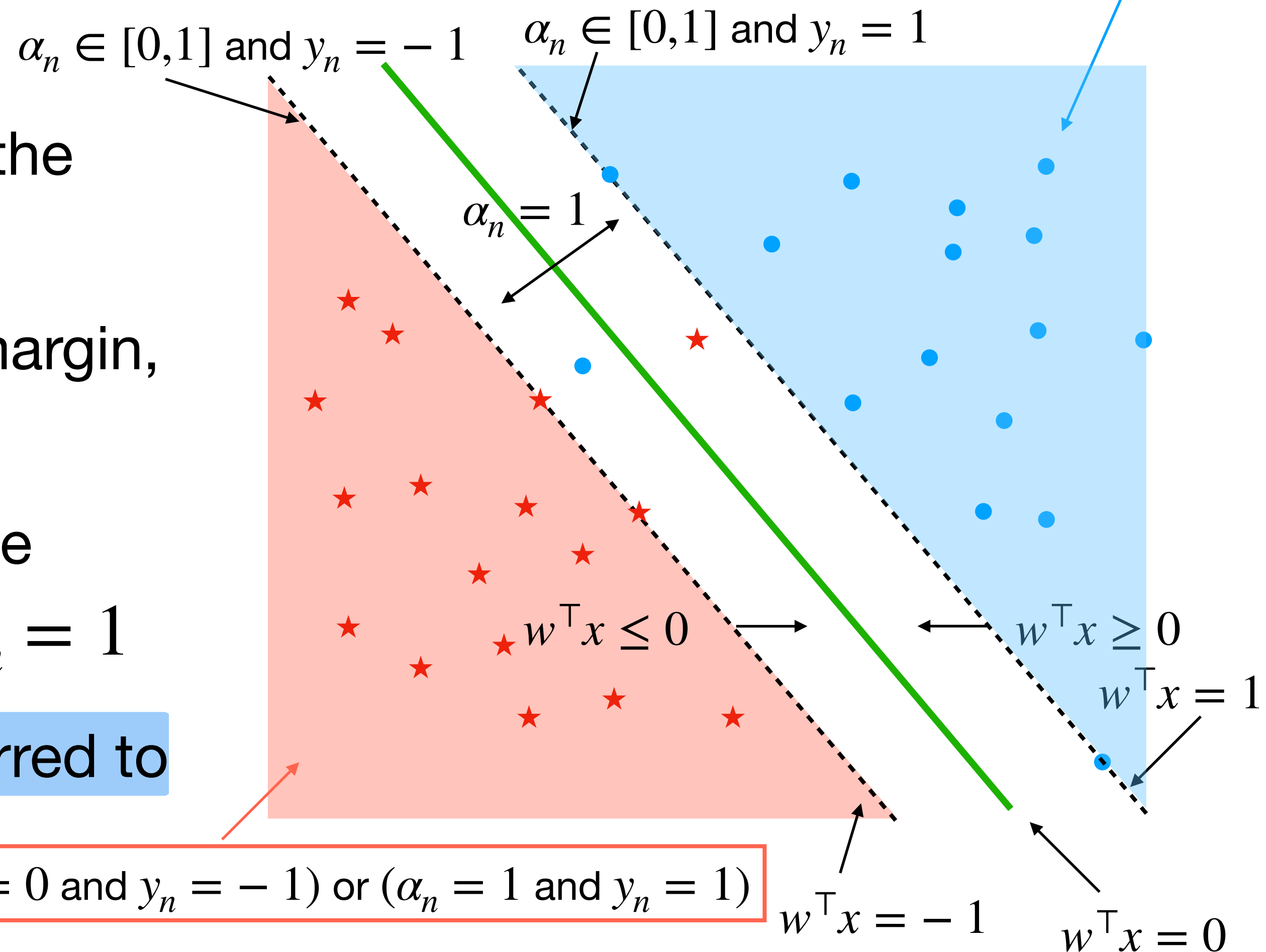
$$\max_{\alpha_n \in [0,1]} \alpha_n (1 - y_n x_n^\top w)$$

- If x_n is on the correct side and outside the margin, $1 - y_n x_n^\top w < 0$, then $\alpha_n = 0$
- If x_n is on the correct side and on the margin, $1 - y_n x_n^\top w = 0$, then $\alpha_n \in [0,1]$
- If x_n is strictly inside the margin or on the incorrect side, $1 - y_n x_n^\top w > 0$, then $\alpha_n = 1$

➡ The points for which $\alpha_n > 0$ are referred to as support vectors

$$(\alpha_n = 0 \text{ and } y_n = -1) \text{ or } (\alpha_n = 1 \text{ and } y_n = 1)$$

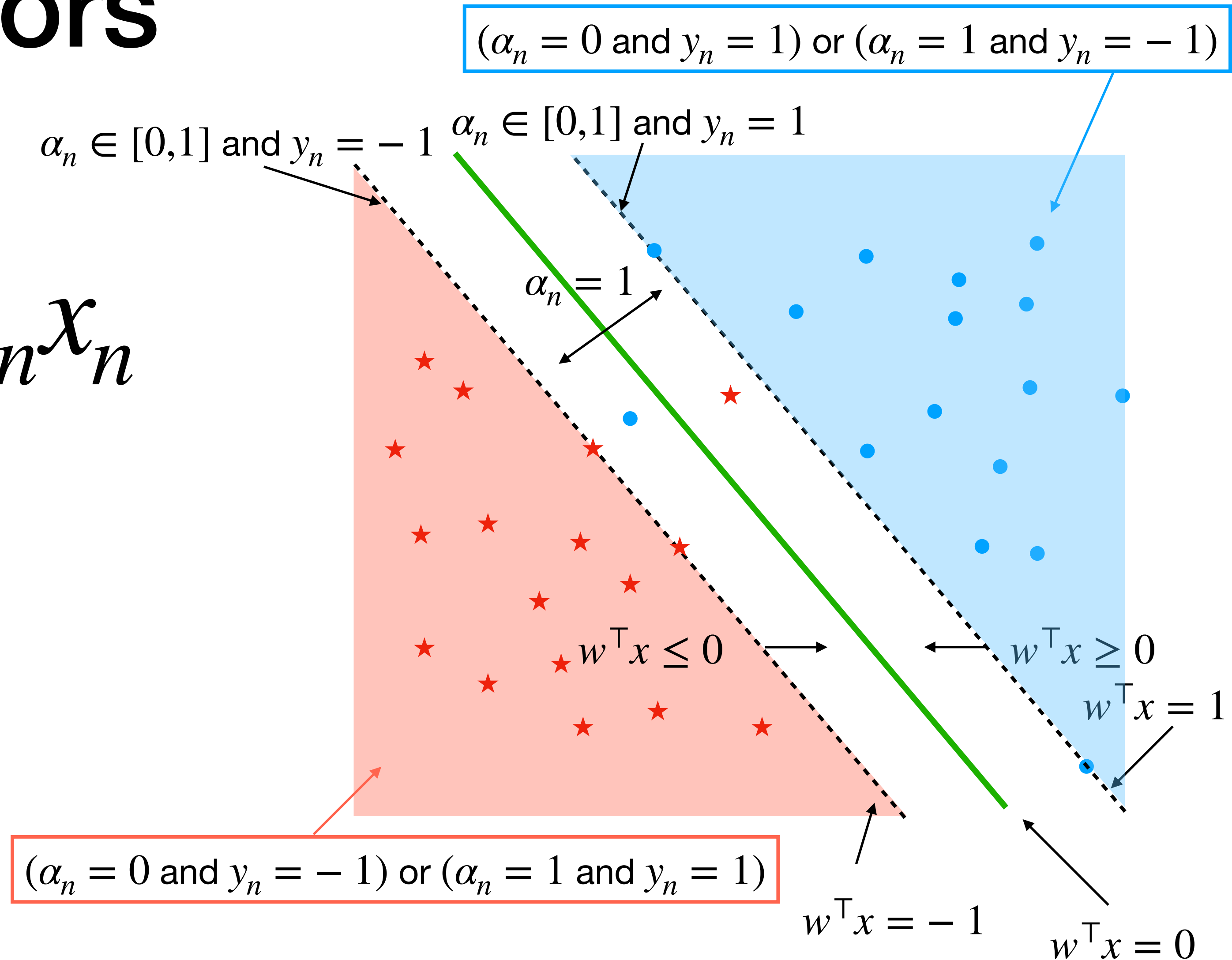
$$(\alpha_n = 0 \text{ and } y_n = 1) \text{ or } (\alpha_n = 1 \text{ and } y_n = -1)$$



The SVM hyperplane is supported by the support vectors

$$w = \frac{1}{\lambda N} \sum_{n=1}^N \alpha_n y_n x_n$$

➔ w does not depend on the observation (x_n, y_n) if $\alpha_n = 0$



Recap

- Hard SVM - finds max-margin separating hyperplane

$$\min_w \frac{1}{2} \|w\|^2 \text{ such that } \forall n, y_n x_n^\top w \geq 1$$

- Soft SVM - relax the constraint for non-separable data

$$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N [1 - y_n x_n^\top w]_+$$

- Hinge loss can be optimized with (stochastic) sub-gradient method
- Duality: min max problem is equivalent to max min (convex-concave objective)
 - Efficient solutions with quadratic programming and coordinate ascent
 - The cost depends on the data via the *kernel matrix* (no dependency on d)