Support Vector Machines

Machine Learning Course - CS-433
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Nicolas Flammarion

Vapnik's invention

A Training Algorithm for Optimal Margin Classifiers

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Support-Vector Networks

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

High generalization ability of support-vector networks uti
strated. We also compare the performance of the support-vec
that all took part in a benchmark study of Optical Character R

GVB+92, Vap82, BH89, TLS89, Mac92] link the
zation of a classifier to the error on the training
es and the complexity of the classifier. Meth-
h as structural risk minimization [Vap82] vary
plexity of the classification function in order to
e the generalization.

paper we describe a training algorithm that au-
ally tunes the capacity of the classification func-
maximizing the margin between training exam-

Том XXIV «АВТОМАТИКА И ТЕЛЕМЕХАНИКА» № 6

1963

УДК 519.95

УЗНАВАНИЕ ОБРАЗОВ ПРИ ПОМОЩИ ОБОБЩЕННЫХ ПОРТРЕТОВ

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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:

$S = \{x_n, y_n\}_{n=1}^{N}$ $\quad$ $\mathcal{A}$ $\quad$ $f_S = \mathcal{A}(S)$

$\Uparrow$

$\{-1,1\}$

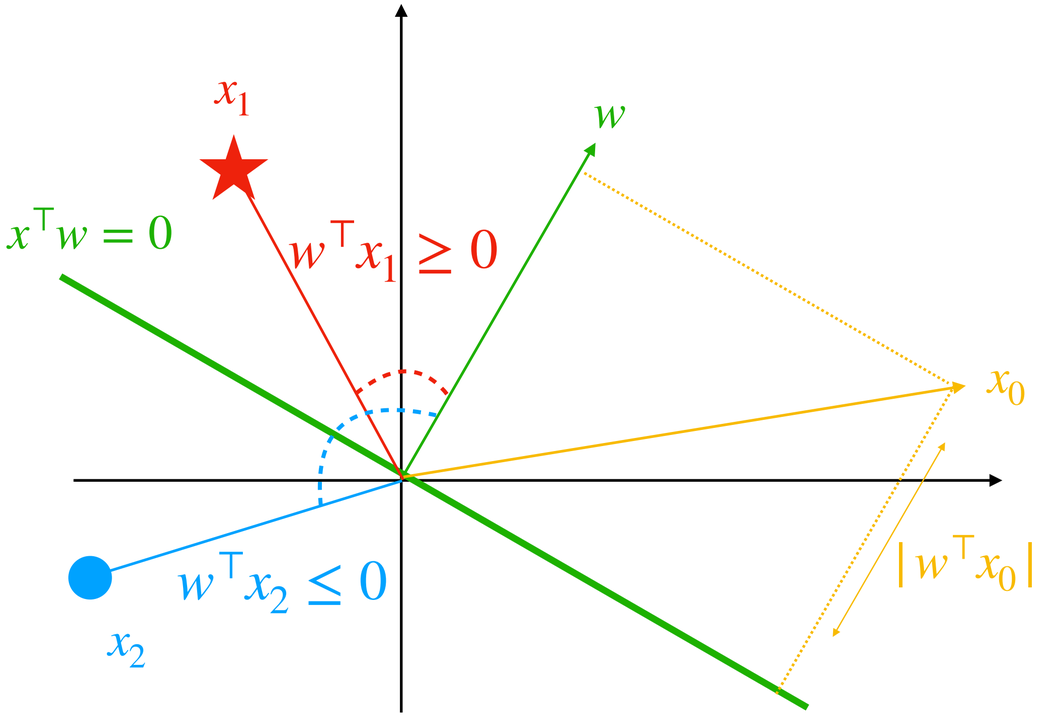
Linear Classifier

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

Prediction:

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

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

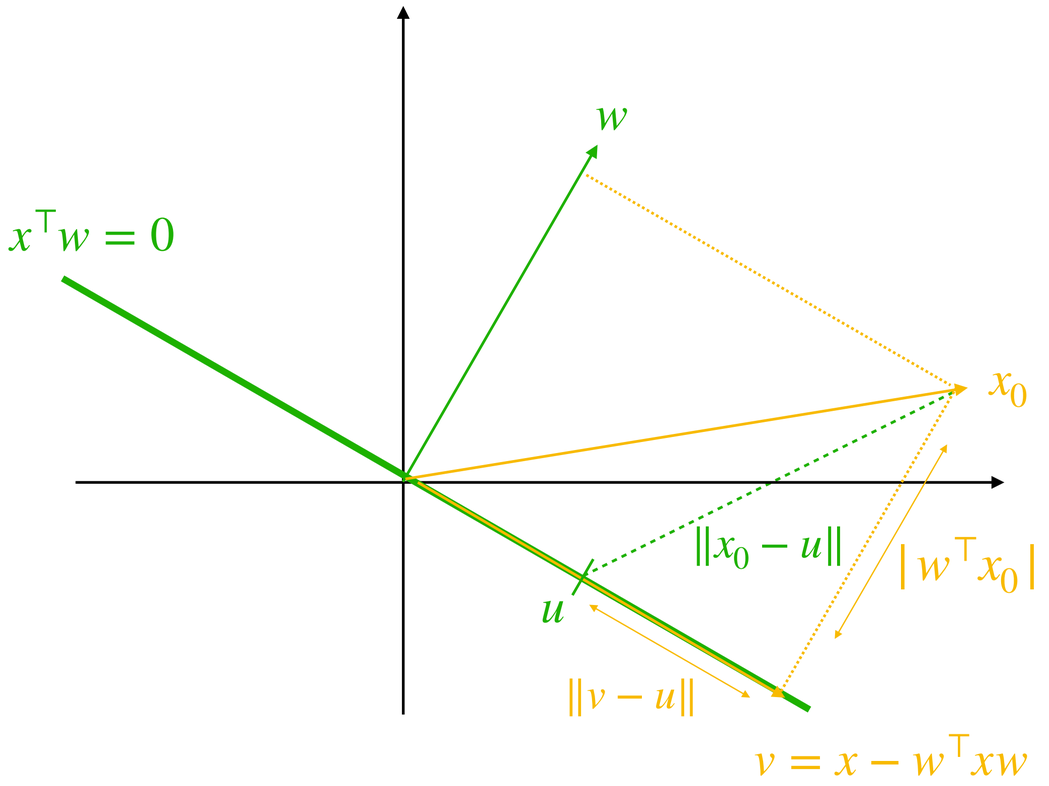


Linear Classifier

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

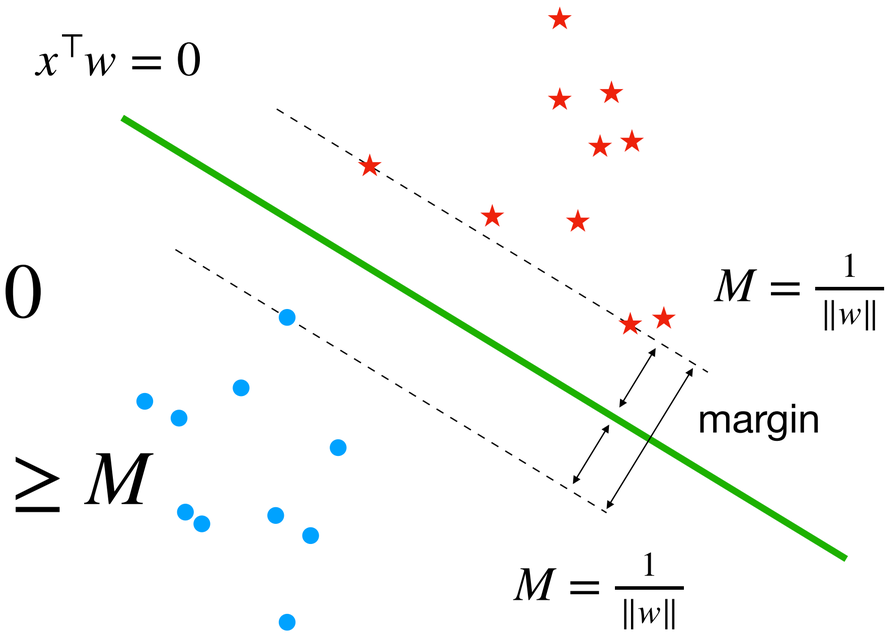
First assume the dataset $(x_n, y_n)_{n=1}^N$ is linearly separable

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

Max-margin separating hyperplane:

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

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



also equivalent to:

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

Proof of the equivalent formulations

Claim: The following optimization problems are equivalent

$$\max_{w,\|w\|=1} \min_{n\le N} |w^\top x_n| \quad \text{(I)}$$
$$\text{s.t. } \forall n,\ y_n x_n^\top w \ge 0$$

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

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

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

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

And the two problems are equivalent

Proof of the equivalent formulations

Claim: The following optimization problems are equivalent

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

$$\min_{w} \frac{1}{2}\|w\|^2 \quad \text{s.t. } \forall n, y_n x_n^\top w \geq 1 \qquad \text{(III)}$$

Proof: $\max_{M \in \mathbb{R}, w, \|w\|=1} M$ 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 $\xi_1, \cdots, \xi_N$ and replace the constraints with $y_n x_n^\top w \geq 1 - \xi_n$

Soft SVM:

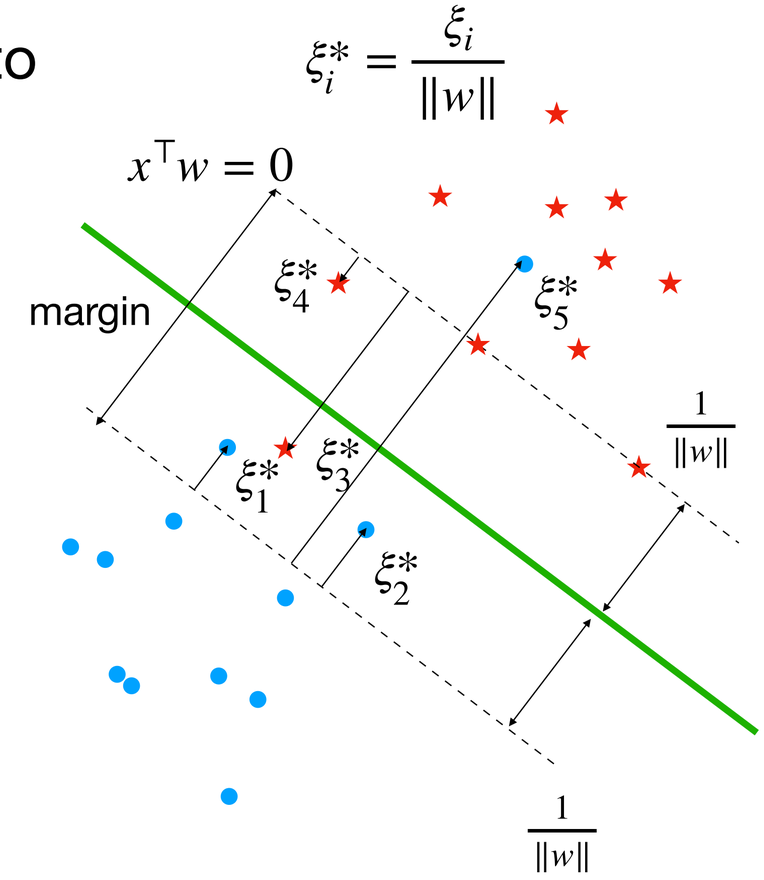
$$\min_{w,\xi} \frac{\lambda}{2}\|w\|^2 + \frac{1}{N}\sum_{n=1}^{N} \xi_n$$

$$\text{s.t. } \forall n, y_n x_n^\top w \geq 1 - \xi_n \quad \text{and} \quad \xi_n \geq 0$$

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

raints to

d

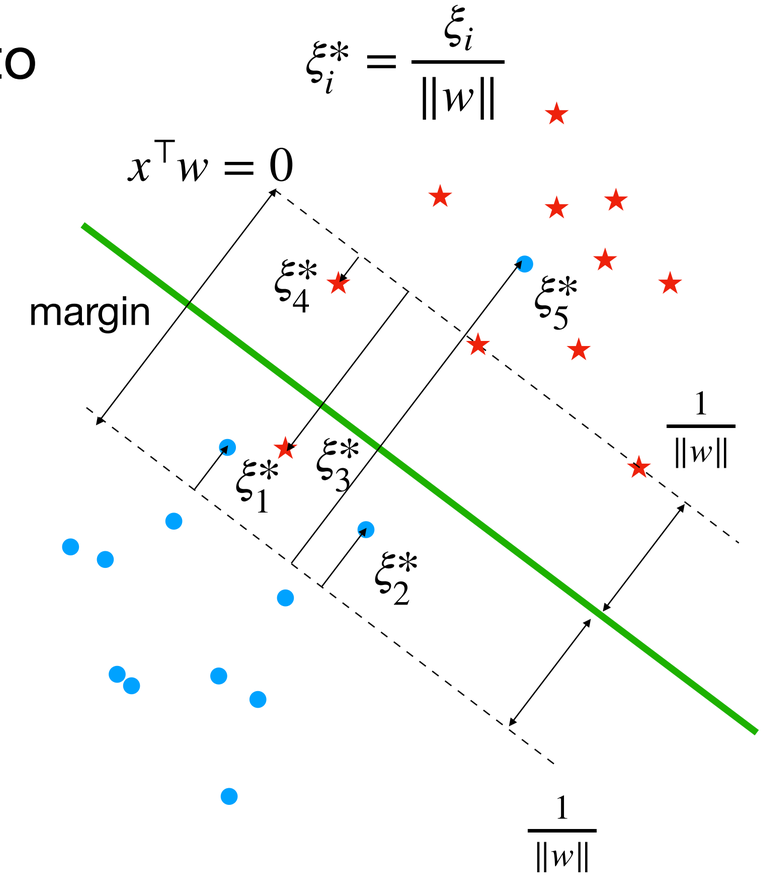
$$\min_{w,\xi} \frac{\lambda}{2}\|w\|^2 + \frac{1}{N}\sum_{n=1}^{N} \xi_n$$

$$\text{s.t. } \forall n, y_n x_n^\top w \geq 1 - \xi_n \quad \text{and} \quad \xi_n \geq 0$$

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 $f : \mathcal{X} \to \mathcal{Y}$ 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

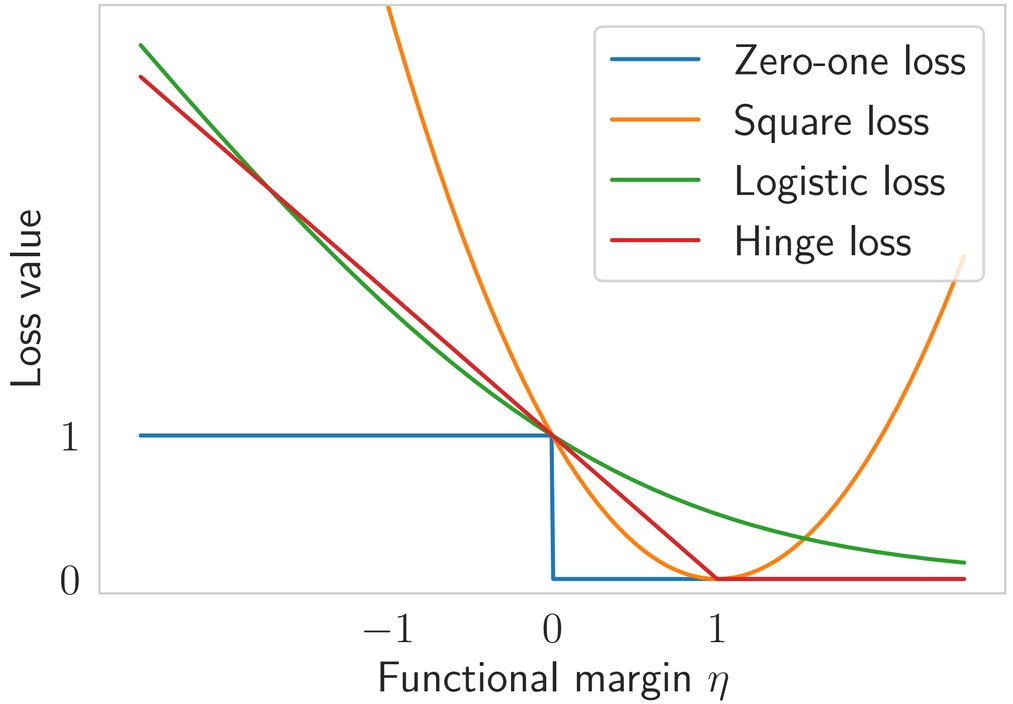
Examples of margin-based losses ($\eta = yx^\top w$):

- 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:

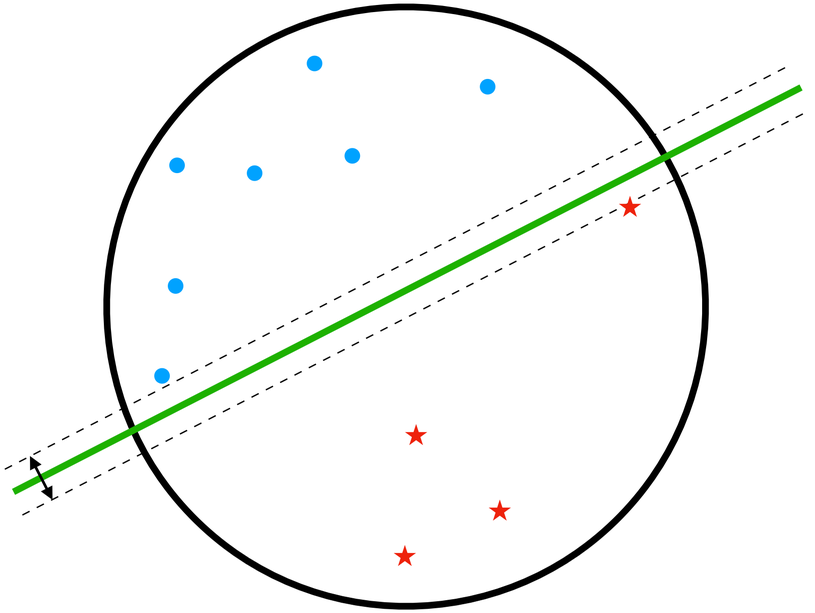
- **MSE:** Penalizes any deviation from 1
- **Logistic Loss:** Asymmetric cost – a penalty is always incurred.
- **Hinge Loss:** A penalty is applied if the prediction is incorrect or lacks confidence



Summary

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

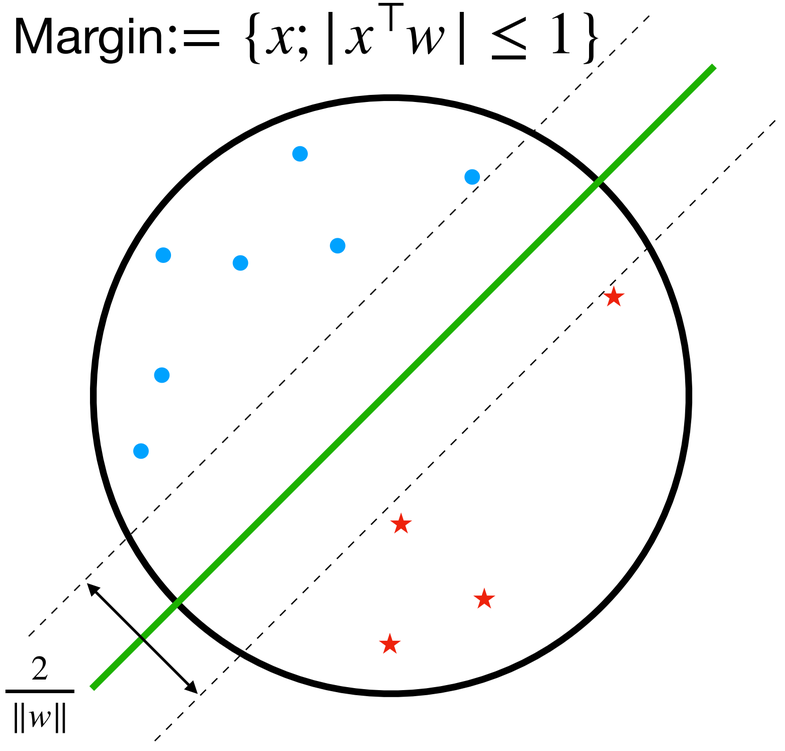
ERM for the hinge loss with ridge regularization



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

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



Optimization: How to get w?

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

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:

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

The function G is convex in w and concave in α

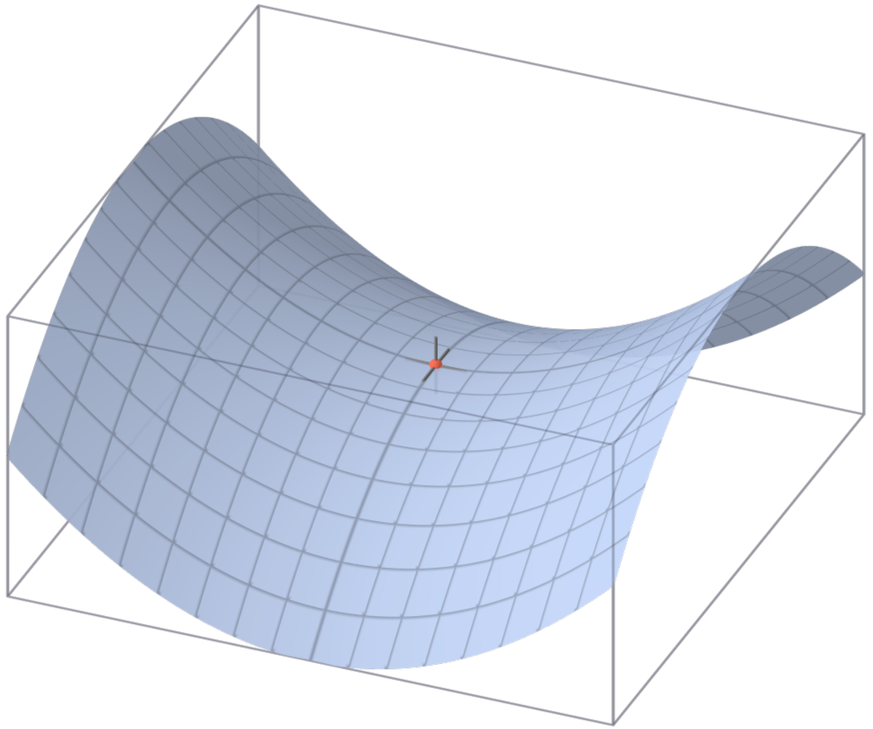
Q2: Can the min and max be interchanged?

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:

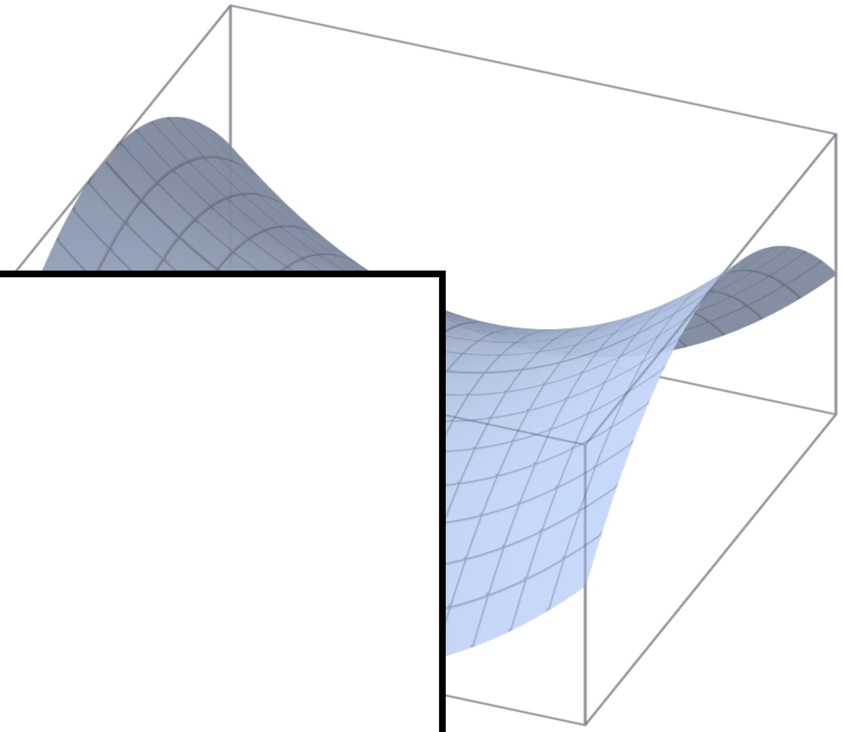
$$\max_{\alpha} \min_{w} G(w, \alpha) = \min_{w} \max_{\alpha} G(w, \alpha)$$



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:

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

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

Dual optimization problem:

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

Q3: Why?

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

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

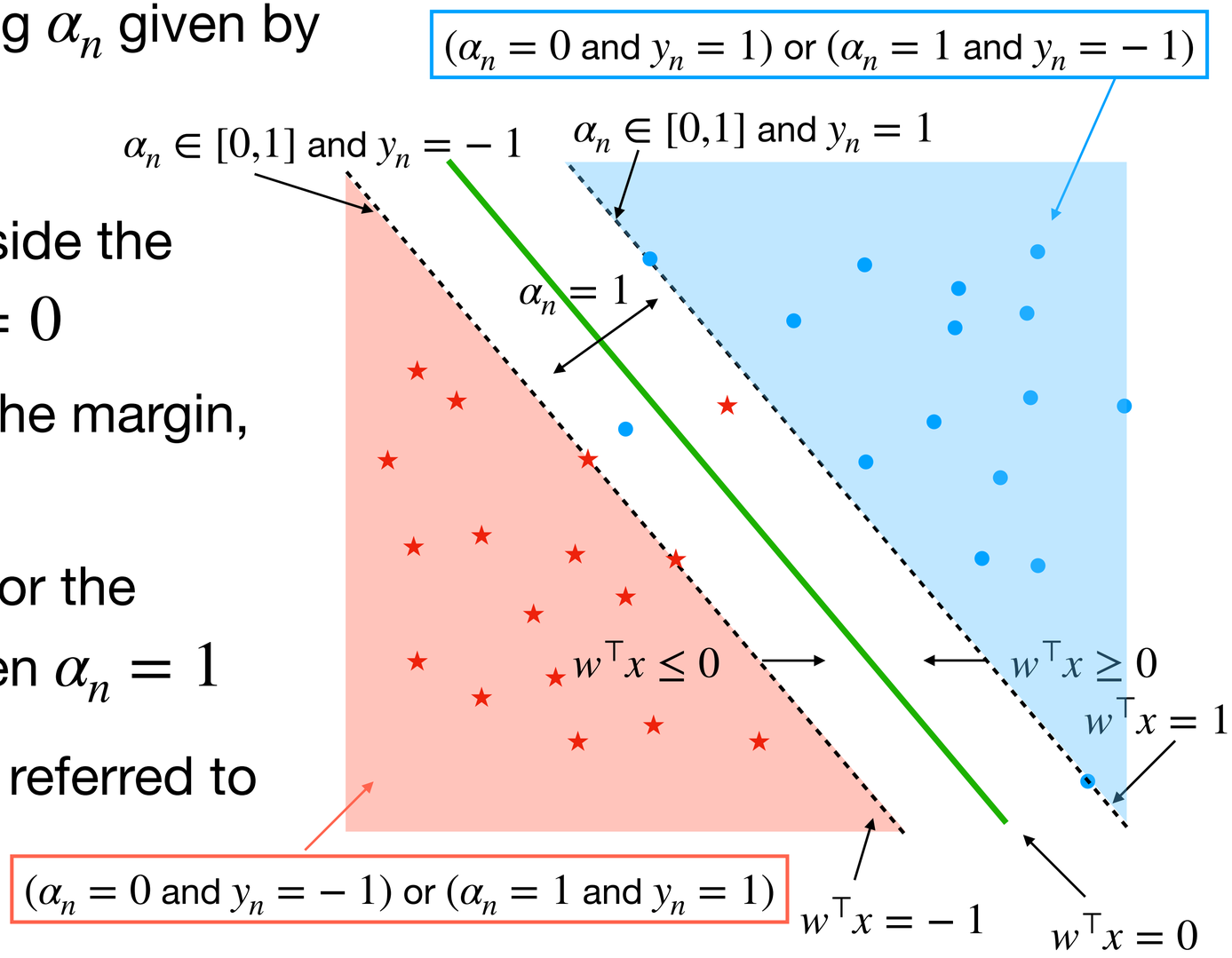
Interpretation of the dual formulation

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 or the incorrect side, $1 - y_n x_n^\top w > 0$, then $\alpha_n = 1$

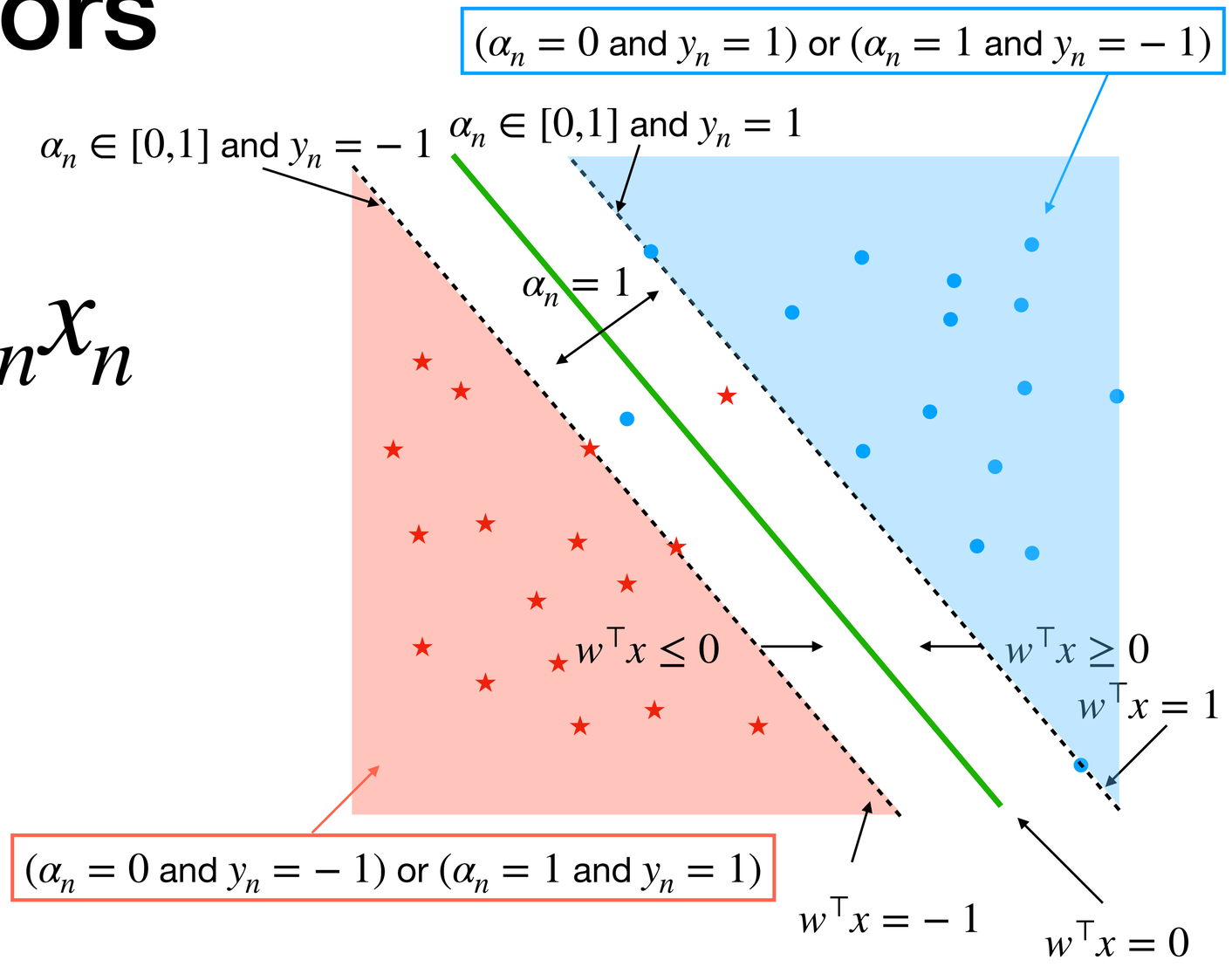
➡The points for which $\alpha_n > 0$ are referred to as support vectors



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

  $\min_w \frac{1}{2}\|w\|^2$ 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)