Support Vector Machines Part 1

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Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Matt Gormley, Elad Hazan, Tom Dietterich, and Pedro Domingos.

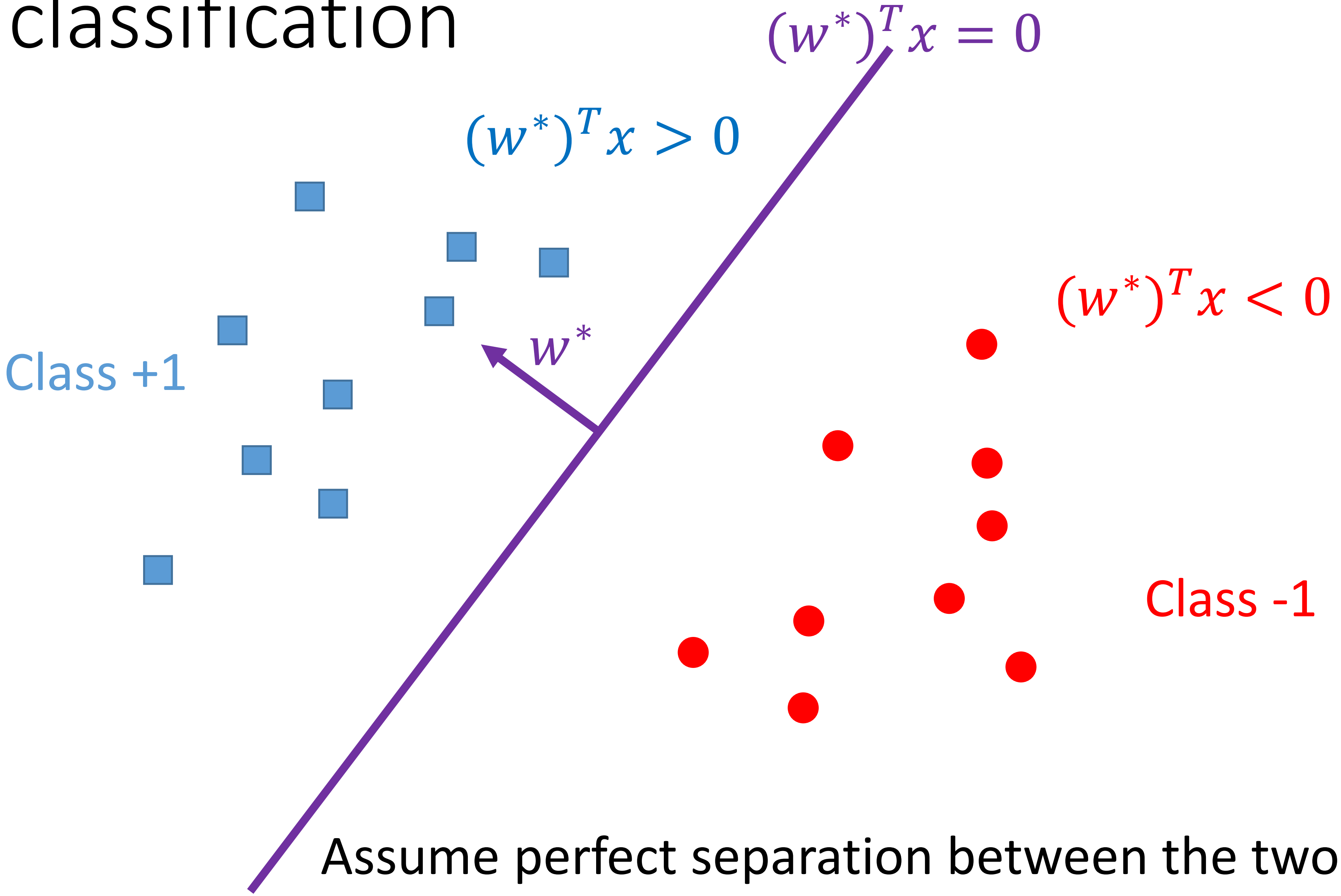
Goals for the lecture

you should understand the following concepts

- the margin
- the linear support vector machine
- the primal and dual formulations of SVM learning
- support vectors
- VC-dimension and maximizing the margin

Motivation

Linear classification



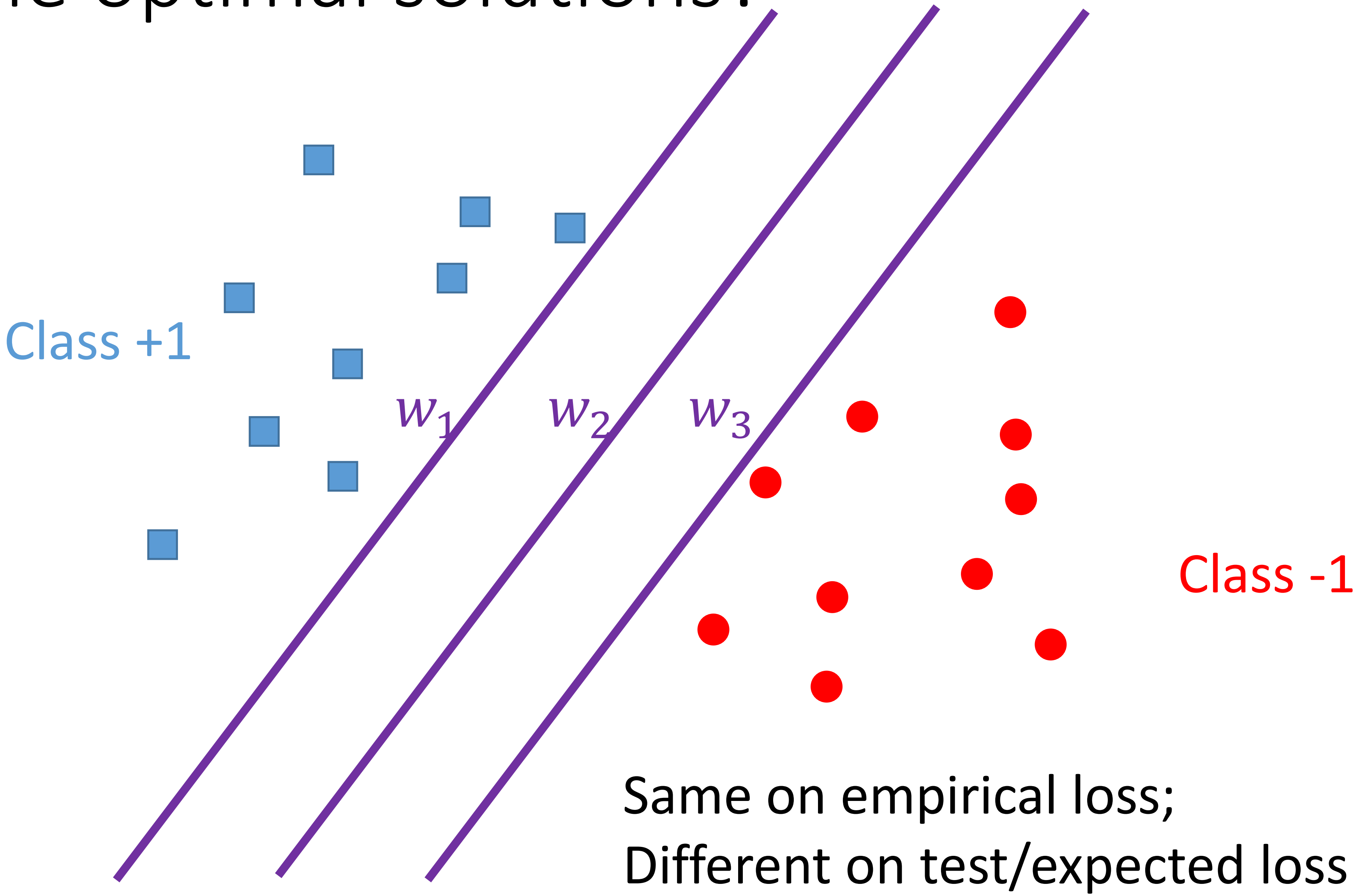
Assume perfect separation between the two classes

Attempt

- Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
- Hypothesis $y = \text{sign}(f_w(x)) = \text{sign}(w^T x)$
  - $y = +1$ if $w^T x > 0$
  - $y = -1$ if $w^T x < 0$

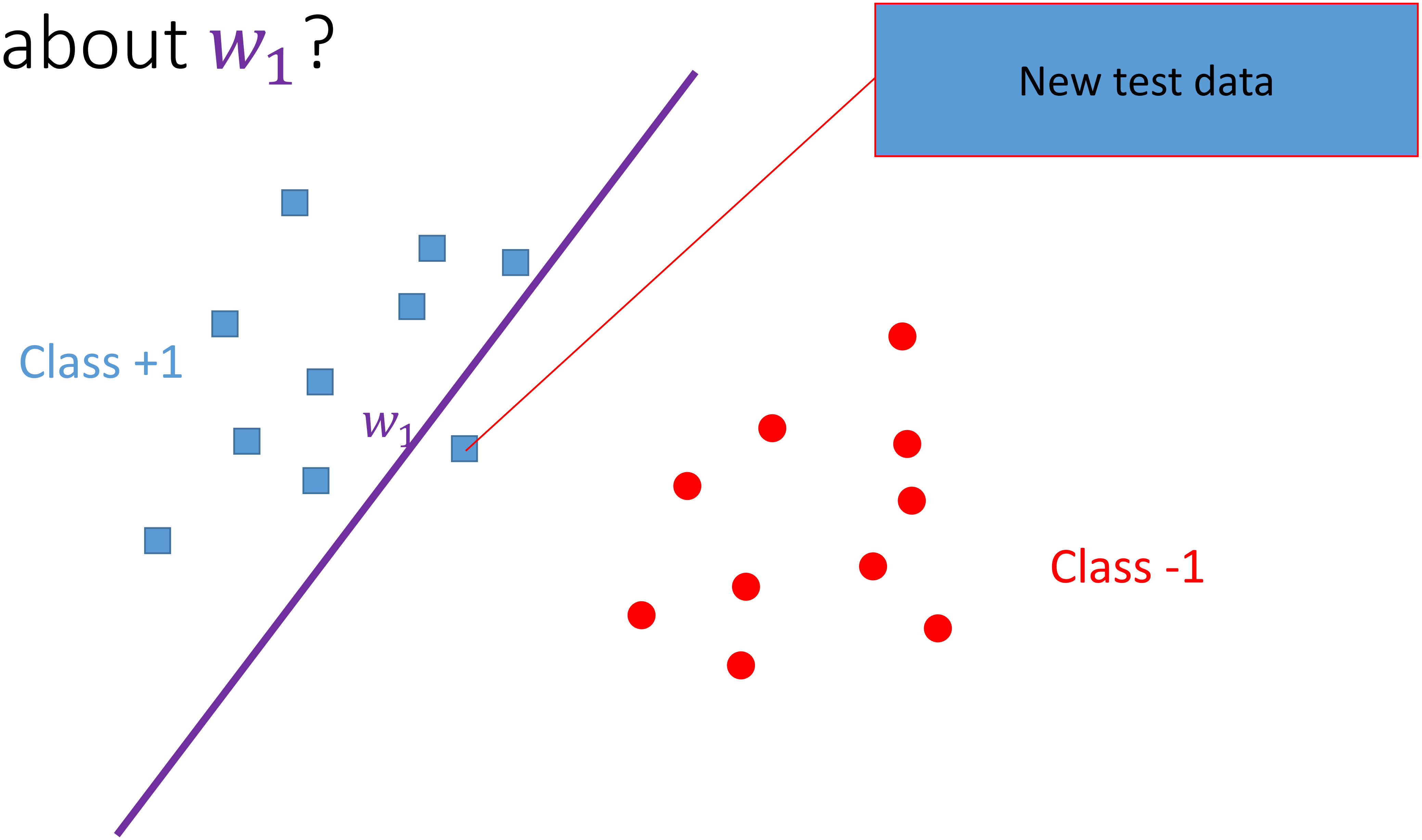
- Let's assume that we can optimize to find w

Multiple optimal solutions?

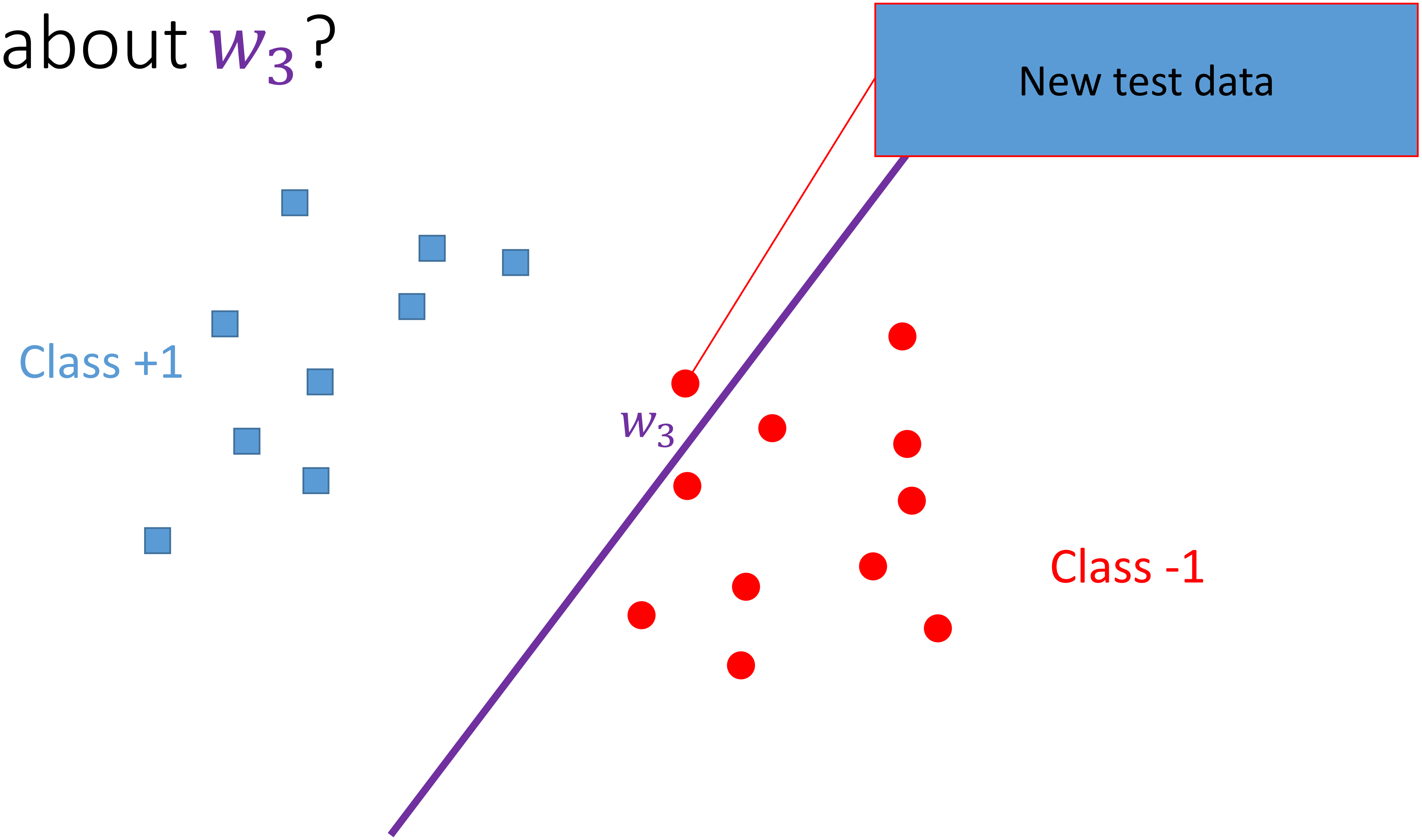


Same on empirical loss;
Different on test/expected loss

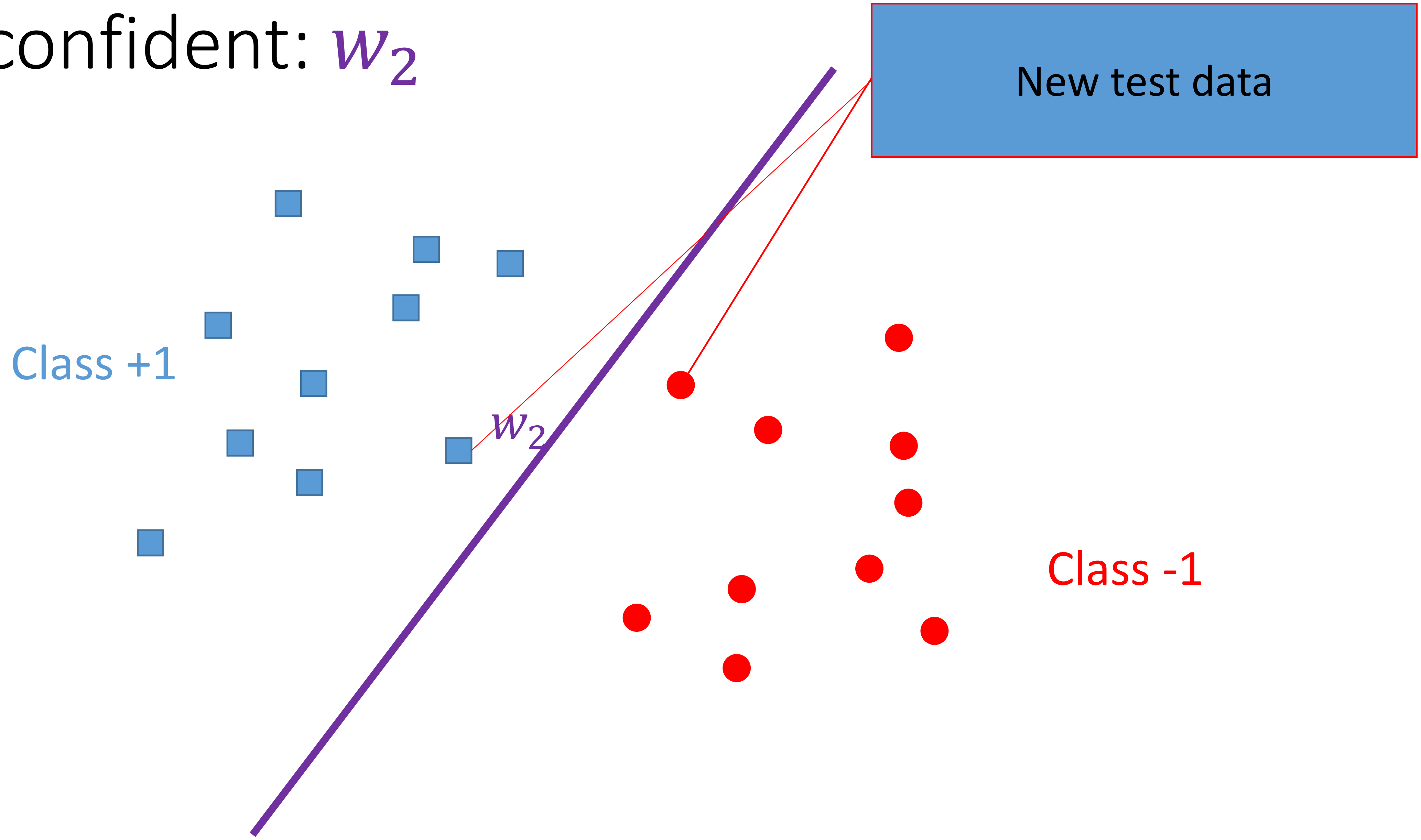
What about w_1?



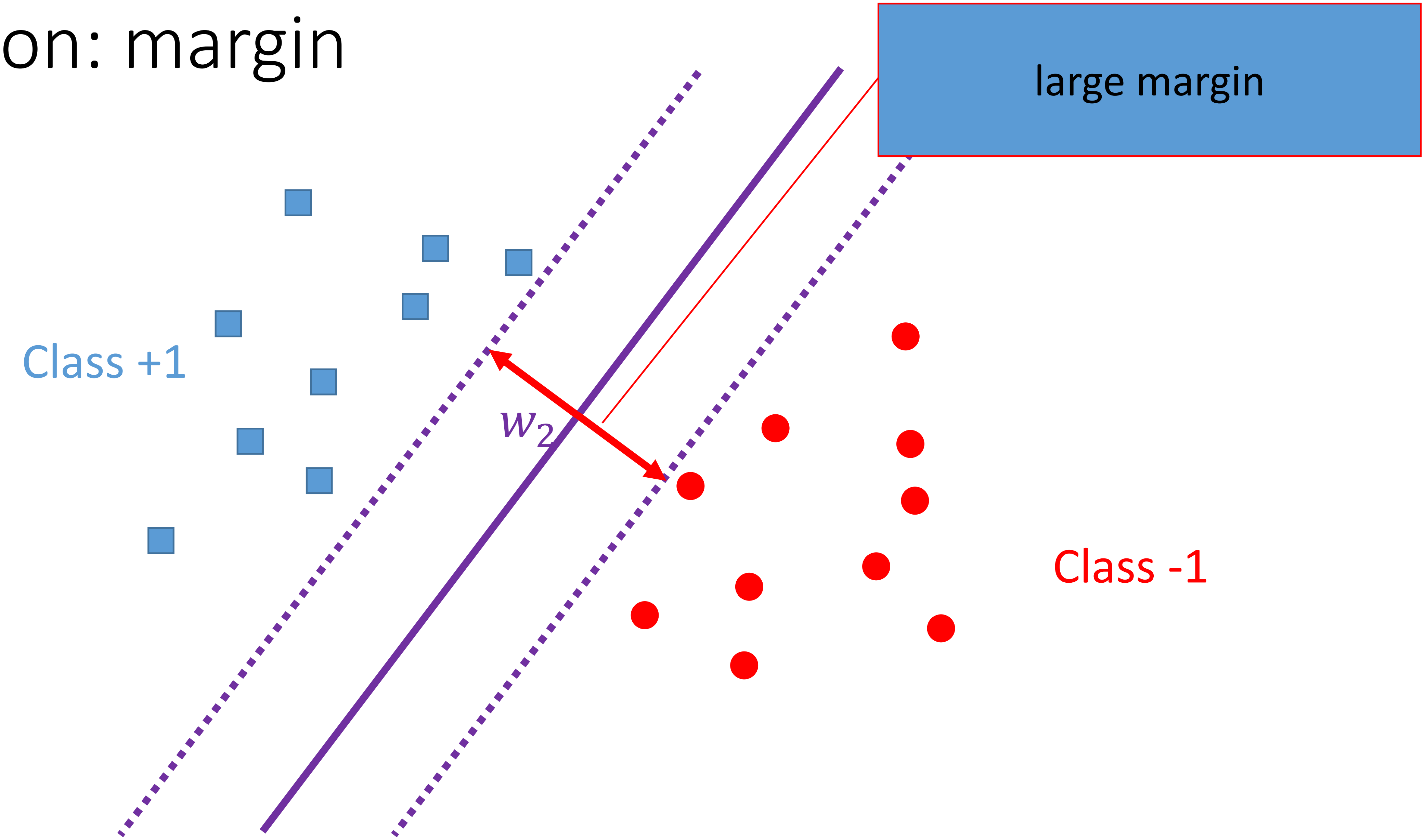
What about w_3?



Most confident: w_2



Intuition: margin



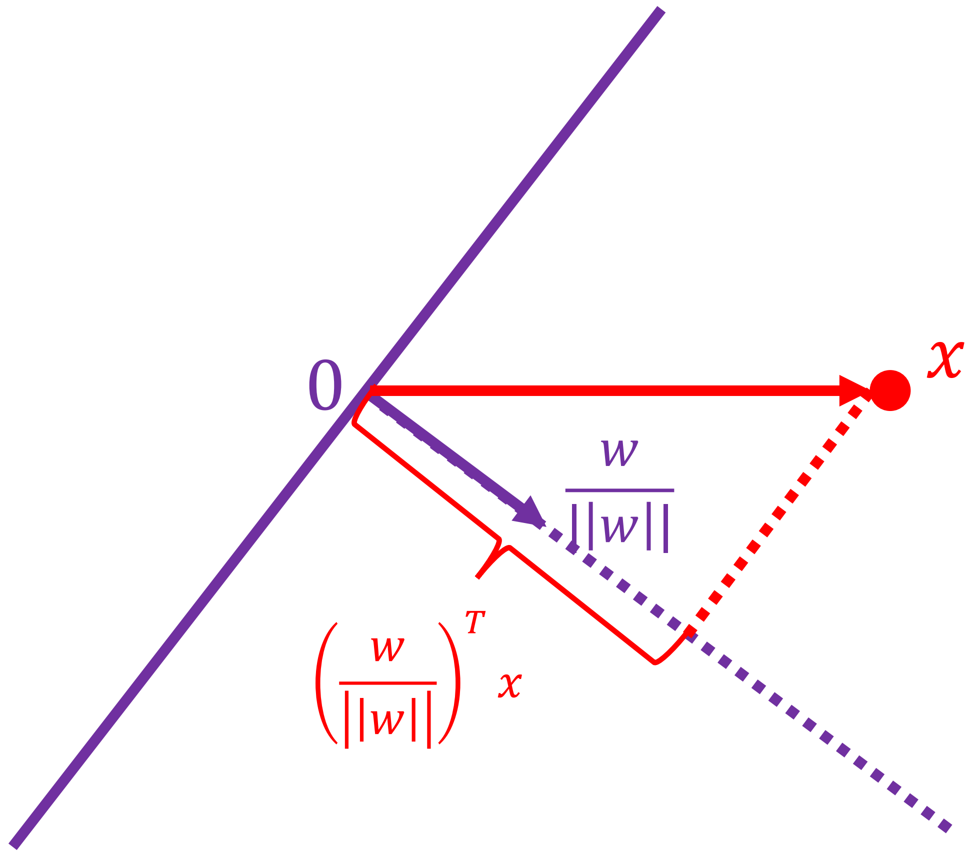
Margin

Margin

- Lemma 1: x has distance $\frac{|f_w(x)|}{||w||}$ to the hyperplane $f_w(x) = w^T x = 0$

Proof:

- w is orthogonal to the hyperplane
- The unit direction is $\frac{w}{||w||}$
- The projection of x is $\left(\frac{w}{||w||}\right)^T x = \frac{f_w(x)}{||w||}$



Margin: with bias

- Claim 1: w is orthogonal to the hyperplane $f_{w,b}(x) = w^T x + b = 0$

Proof:

- pick any x_1 and x_2 on the hyperplane
- $w^T x_1 + b = 0$
- $w^T x_2 + b = 0$

- So $w^T (x_1 - x_2) = 0$

Margin: with bias

- Claim 2: 0 has distance $\frac{-b}{||w||}$ to the hyperplane $w^T x + b = 0$

Proof:

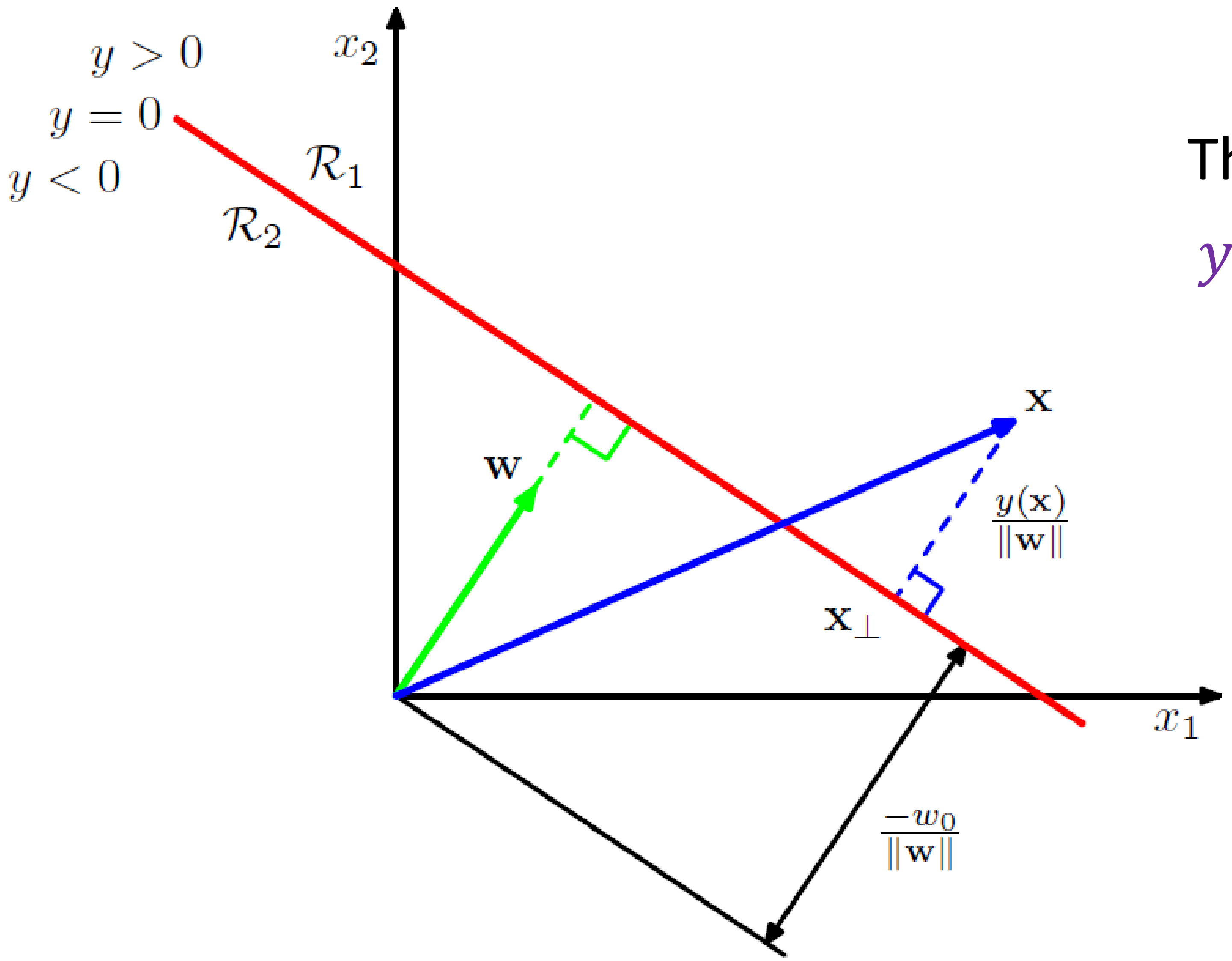
- pick any x_1 the hyperplane
- Project x_1 to the unit direction $\frac{w}{||w||}$ to get the distance
- $\left(\frac{w}{||w||}\right)^T x_1 = \frac{-b}{||w||}$ since $w^T x_1 + b = 0$

Margin: with bias

- Lemma 2: x has distance $\frac{|f_{w,b}(x)|}{||w||}$ to the hyperplane $f_{w,b}(x) = w^T x + b = 0$

Proof:

- Let $x = x_{\perp} + r\frac{w}{||w||}$, then $|r|$ is the distance
- Multiply both sides by w^T and add b
- Left hand side: $w^T x + b = \ f_{w,b}(x)$
- Right hand side: $w^T x_{\perp} + r\frac{w^T w}{||w||} + b = 0 + r||w||$



The notation here is:

$$y(x) = w^T x + w_0$$

Figure from *Pattern Recognition and Machine Learning*, Bishop

Support Vector Machine (SVM)

SVM: objective

- Margin over all training data points:

$$\gamma = \min_i \frac{|f_{w,b}(x_i)|}{||w||}$$

- Since only want correct $f_{w,b}$, and recall $y_i \in \{+1, -1\}$, we have

$$\gamma = \min_i \frac{y_i f_{w,b}(x_i)}{||w||}$$

- If $f_{w,b}$ incorrect on some x_i, the margin is negative

SVM: objective

- Maximize margin over all training data points:

$$\max_{w,b} \gamma = \max_{w,b} \min_{i} \frac{y_i f_{w,b}(x_i)}{||w||} = \max_{w,b} \min_{i} \frac{y_i(w^T x_i + b)}{||w||}$$

- A bit complicated …

SVM: simplified objective

- Observation: when (w, b) scaled by a factor c, the margin unchanged

$$\frac{y_i(cw^T x_i + cb)}{||cw||} = \frac{y_i(w^T x_i + b)}{||w||}$$

- Let's consider a fixed scale such that

$$y_{i^*}(w^T x_{i^*} + b) = 1$$

where x_{i^*} is the point closest to the hyperplane

SVM: simplified objective

- Let's consider a fixed scale such that

$$y_{i^*}(w^T x_{i^*} + b) = 1$$

  where x_{i^*} is the point closet to the hyperplane
- Now we have for all data

$$y_i(w^T x_i + b) \geq 1$$

  and at least for one i the equality holds
- Then the margin is $\frac{1}{||w||}$

SVM: simplified objective

- Optimization simplified to

$$\min_{w,b} \frac{1}{2}||w||^2$$

$$y_i(w^T x_i + b) \geq 1, \forall i$$

- How to find the optimum $\hat{w}^*$?
- Solved by Lagrange multiplier method

Lagrange multiplier

Lagrangian

- Consider optimization problem:

$$\min_{w} \; f(w)$$

$$h_i(w) = 0, \forall 1 \leq i \leq l$$

- Lagrangian:

$$\mathcal{L}(w, \boldsymbol{\beta}) = f(w) + \sum_{i} \beta_i h_i(w)$$

where β_i's are called Lagrange multipliers

Lagrangian

- Consider optimization problem:

$$\min_{w} \; f(w)$$

$$h_i(w) = 0, \forall 1 \leq i \leq l$$

- Solved by setting derivatives of Lagrangian to 0

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0; \quad \frac{\partial \mathcal{L}}{\partial \beta_i} = 0$$

Generalized Lagrangian

- Consider optimization problem:

$$\min_w f(w)$$

$$g_i(w) \leq 0, \forall 1 \leq i \leq k$$

$$h_j(w) = 0, \forall 1 \leq j \leq l$$

- Generalized Lagrangian:

$$\mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(w) + \sum_i \alpha_i g_i(w) + \sum_j \beta_j h_j(w)$$

where α_i, β_j's are called Lagrange multipliers

Generalized Lagrangian

- Consider the quantity:

$$\theta_P(w) := \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} \mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- Why?

$$\theta_P(w) = \begin{cases} f(w), & \text{if } w \text{ satisfies all the constraints} \\ +\infty, & \text{if } w \text{ does not satisfy the constraints} \end{cases}$$

- So minimizing $f(w)$ is the same as minimizing $\theta_P(w)$

$$\min_w f(w) = \min_w \theta_P(w) = \min_w \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} \mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

Lagrange duality

- The primal problem

$$p^* := \min_w f(w) = \min_w \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} \mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- The dual problem

$$d^* := \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} \min_w \mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- Always true:

$$d^* \leq p^*$$

Lagrange duality

- The primal problem

$$p^* := \min_w f(w) = \min_w \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} \mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- The dual problem

$$d^* := \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} \min_w \mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- Interesting case: when do we have

$$d^* = p^*?$$

Lagrange duality

- Theorem: under proper conditions, there exists $(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ such that

$$d^* = \mathcal{L}(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*) = p^*$$

  Moreover, $(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ satisfy Karush-Kuhn-Tucker (KKT) conditions:

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0, \qquad \alpha_i g_i(w) = 0$$

$$g_i(w) \leq 0, \; h_j(w) = 0, \qquad \alpha_i \geq 0$$

Lagrange duality

dual complementarity

- Theorem: under proper conditions, there exists $(w$

$$d^* = \mathcal{L}(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*) = p^*$$

Moreover, $(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ satisfy Karush-Kuhn-Tucker (KKT) conditions:

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0, \qquad \alpha_i g_i(w) = 0$$

$$g_i(w) \le 0, \;\; h_j(w) = 0, \qquad \alpha_i \ge 0$$

Lagrange duality

primal constraints

… conditions, there exists $(w$ …

dual constraints

$$\ldots = \mathcal{L}(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*) = p^*$$

- Moreover, $(w^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ satisfy Karush-Kuhn-Tucker (KKT) conditions:

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0, \qquad \alpha_i g_i(w) = 0$$

$$g_i(w) \leq 0, \;\; h_j(w) = 0, \qquad \alpha_i \geq 0$$

Lagrange duality

- What are the proper conditions?
- A set of conditions (Slater conditions):
  - f, g_i convex, h_j affine, and exists w satisfying all $g_i(w) < 0$

- There exist other sets of conditions
  - Check textbooks, e.g., Convex Optimization by Boyd and Vandenberghe

SVM: optimization

SVM: optimization

- Optimization (Quadratic Programming):

$$\min_{w,b} \frac{1}{2} ||w||^2$$

$$y_i(w^T x_i + b) \geq 1, \forall i$$

- Generalized Lagrangian:

$$\mathcal{L}(w, b, \boldsymbol{\alpha}) = \frac{1}{2} ||w||^2 - \sum_i \alpha_i [y_i(w^T x_i + b) - 1]$$

where $\boldsymbol{\alpha}$ is the Lagrange multiplier

SVM: optimization

- KKT conditions:

$$\frac{\partial \mathcal{L}}{\partial w} = 0, \rightarrow w = \sum_i \alpha_i y_i x_i \quad (1)$$

$$\frac{\partial \mathcal{L}}{\partial b} = 0, \rightarrow 0 = \sum_i \alpha_i y_i \quad (2)$$

- Plug into $\mathcal{L}$:

$$\mathcal{L}(w, b, \boldsymbol{\alpha}) = \sum_i \alpha_i - \frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j \quad (3)$$

combined with $0 = \sum_i \alpha_i y_i \,, \alpha_i \geq 0$

SVM: optimization

Only depend on inner products

- Reduces to dual problem:

$$\mathcal{L}(w, b, \boldsymbol{\alpha}) = \sum_i \alpha_i - \frac{1}{2}\sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

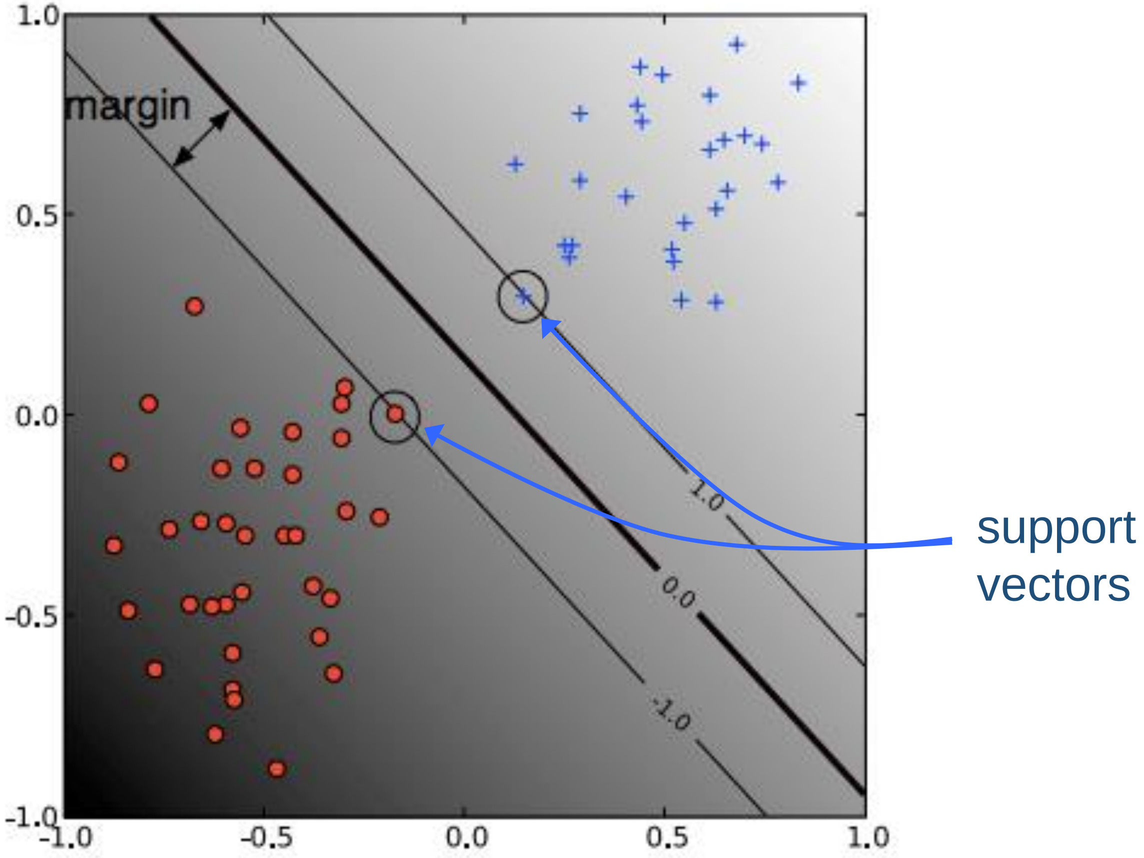
$$\sum_i \alpha_i y_i = 0, \alpha_i \geq 0$$

- Since $w = \sum_i \alpha_i y_i x_i$, we have $w^T x + b = \sum_i \alpha_i y_i x_i^T x + b$

Support Vectors

- final solution is a sparse linear combination of the training instances

- those instances with $\alpha_i > 0$ are called *support vectors*
  - they lie on the margin boundary
- solution NOT changed if delete the instances with $\alpha_i = 0$



Learning theory justification

$$error(h) \leq error_D(h) + \sqrt{\frac{VC\left(\log\frac{2m}{VC}+1\right)+\log\frac{4}{\delta}}{m}}$$

error on true distribution

training set error

VC: VC-dimension of hypothesis class

- Vapnik showed a connection between the margin and VC dimension

$$VC \leq \frac{4R^2}{margin_D(h)}$$

constant dependent on training data (i.e. $4R^2$)

- thus to minimize the VC dimension (and to improve the error bound) ➔ maximize the margin