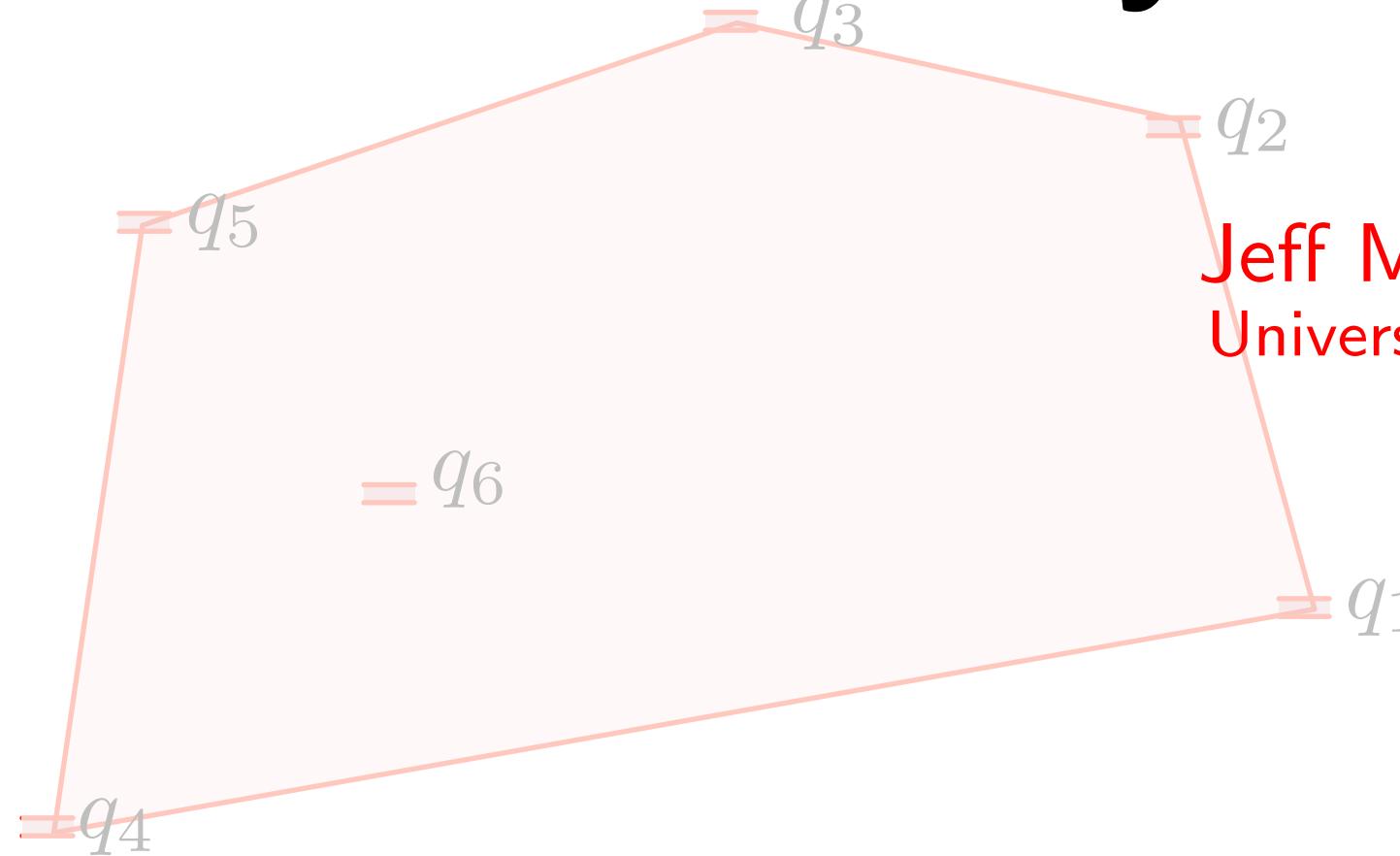


# A Primer on the Geometry in Machine Learning

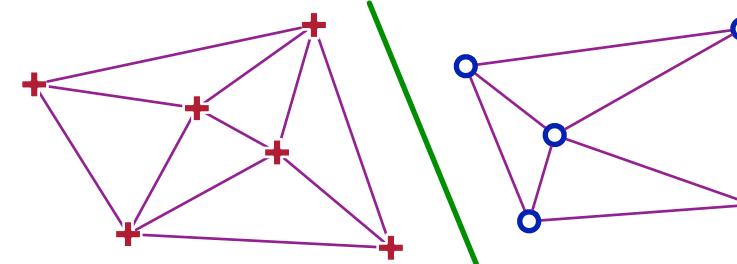
Jeff M. Phillips  
University of Utah



# What is Machine Learning?

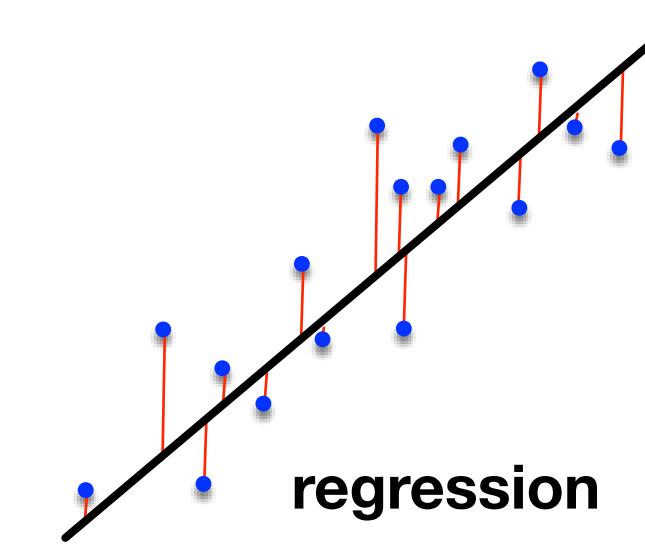
supervised (has labels)

class output

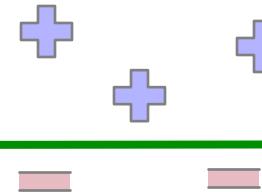


classification

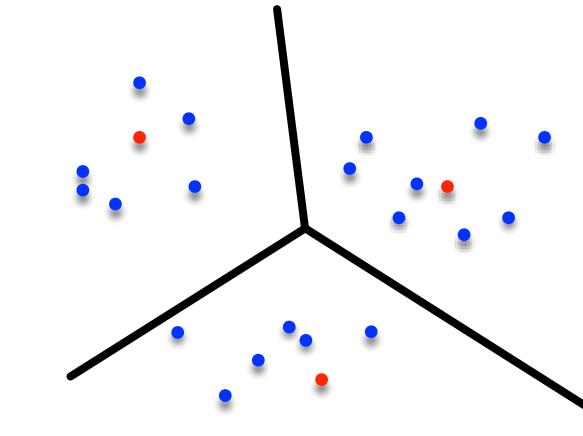
value output



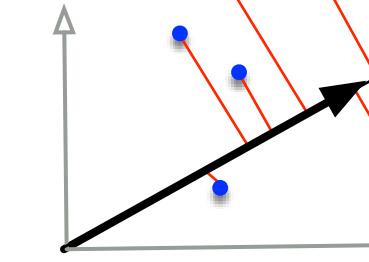
regression



unsupervised (no labels)



clustering

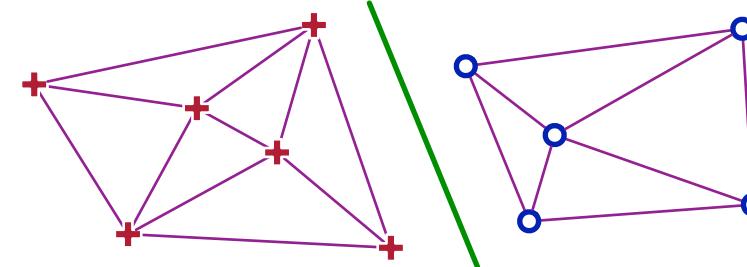


dimensionality reduction

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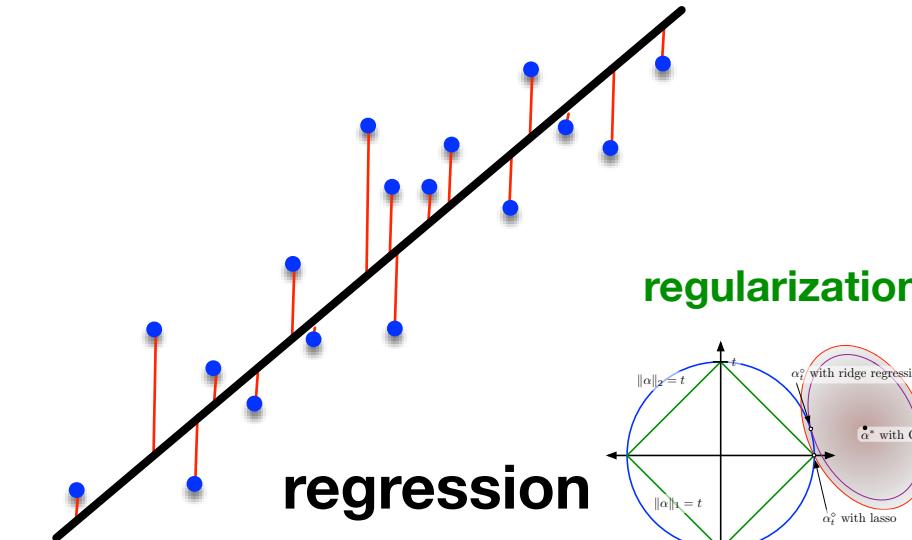
supervised (has labels)

class output

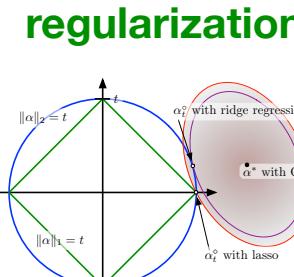


classification

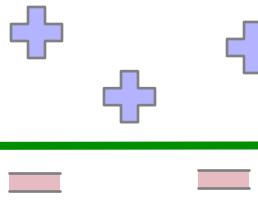
value output



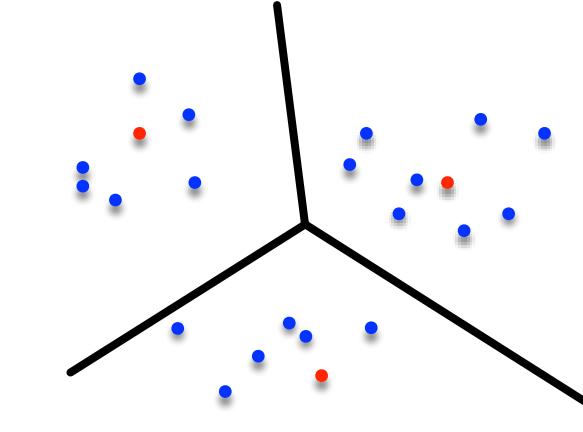
regression



regularization

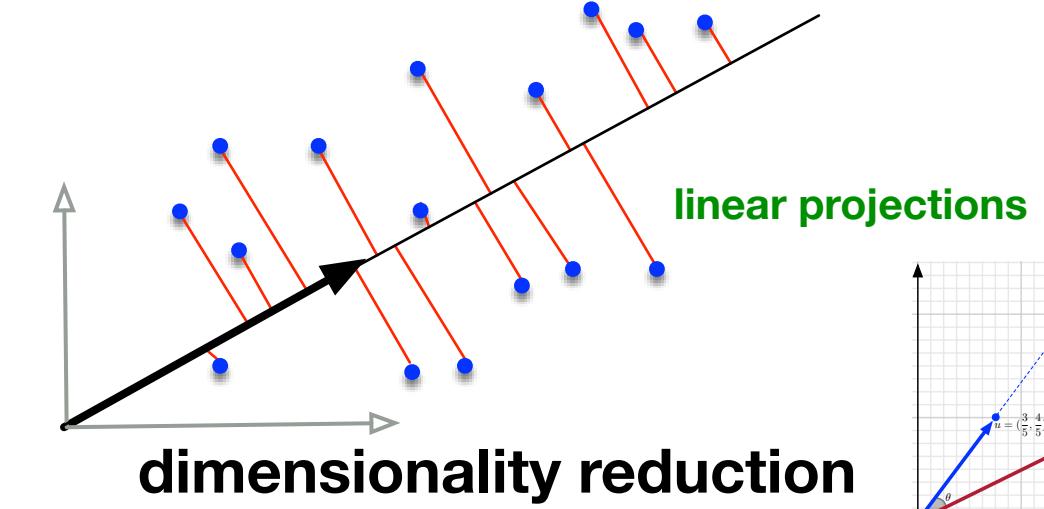
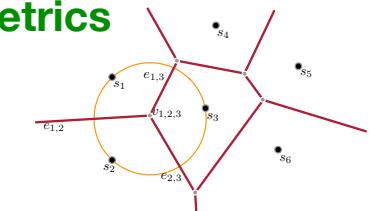


unsupervised (no labels)

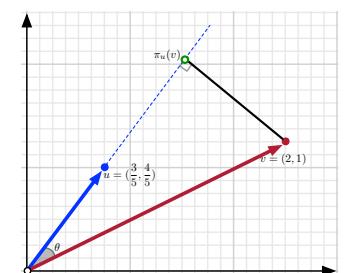


clustering

Voronoi  
metrics



dimensionality reduction



# MATHEMATICAL FOUNDATIONS FOR DATA ANALYSIS

## Implementation Hints:

To implement the Perceptron algorithm, inside the inner loop we need to find some misclassified point  $(x_i, y_i)$ , if one exists. This can require another implicit loop. A common approach would be to, for some ordering of points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  keep an iterator index  $i$  that is maintained outside the `repeat-until` loop. It is modularly incremented every step: it loops around to  $i = 1$  after  $i = n$ . That is, the algorithm keeps cycling through the data set, and updating  $w$  for each misclassified point it observes.

## Algorithm: Perceptron( $X, y$ )

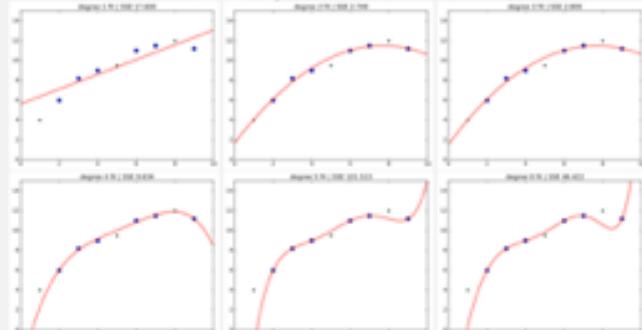
```
Initialize  $w = y_0 x_0$  for any  $(x_0, y_0) \in (X, y)$ ; Set  $i = 1; t = 0; \text{LAST-UPDATE} = 1$ 
repeat
    If  $y_i \langle x_i, w \rangle < 0$ 
         $w \leftarrow w + y_i x_i$ 
         $t = t + 1; \text{LAST-UPDATE} = i$ 
         $i = i + 1 \bmod n$ 
    until ( $t = T$  or  $\text{LAST-UPDATE} = i$ )
return  $w \leftarrow w/\|w\|$ 
```

## Example: Simple polynomial example with Cross Validation

Now split our data sets into a train set and a test set:

train:	$x$	2	3	4	6	7	8	test:	$x$	1	5	9
	$y$	6	8.2	9	11	11.5	12		$y$	4	9.5	11.2

With the following polynomial fits for  $p = \{1, 2, 3, 4, 5, 8\}$  generating model  $M_{\alpha_p}$  on the test data. We then calculate the  $\text{SSE}(x_{\text{test}}, M_{\alpha_p})$  score for each (as shown):



And the polynomial model with degree  $p = 2$  has the lowest SSE score of 2.749. It is also the simplest model that does a very good job by the "eye-ball" test. So we would choose this as our model.

# JEFF M. PHILLIPS

<http://www.cs.utah.edu/~jeffp/M4D/M4D.html>

In this illustration 6 elements with normalized weights  $w(\alpha_i)/\|w\|$  are depicted in a bar chart on the left. These bars are then stacked end-to-end in a unit interval on the right, the precisely stretch from 0.00 to 1.00. The  $t_i$  values mark the accumulation of probability that one of the first  $i$  values is chosen. Now when a random value  $u \sim \text{unif}[0, 1]$  is chosen at random, it maps into this "partition of unity" and selects an item. In this case it selects item  $\alpha_1$  since  $u = 0.68$  and  $t_1 = 0.58$  and  $t_2 = 0.74$  for  $t_1 < u \leq t_2$ .

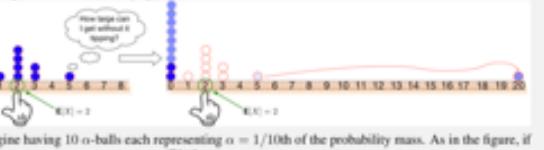


## Geometry of the Markov Inequality

Consider balancing the pdf of some random variable  $X$  on your finger at  $\mathbb{E}[X]$ , like a waitress balances a tray. If your finger is not under a value  $\mu$  so  $\mathbb{E}[X] = \mu$ , then the pdf (and the waitress's tray) will tip, and fall in the direction of  $\mu$  - the "center of mass". Now for some amount of probability  $\alpha$ , how large can we increase its location so we retain  $\mathbb{E}[X] = \mu$ . For each part of the pdf we increase, we must decrease some in proportion. However, by the assumption  $X \geq 0$ , the pdf must not be positive below 0. In the limit of this, we can set  $\Pr[X = 0] = 1 - \alpha$ , and then move the remaining  $\alpha$  probability as large as possible, to a location  $\delta$  so  $\mathbb{E}[X] = \mu$ . That is

$$\mathbb{E}[X] = 0 \cdot \Pr[X = 0] + \delta \cdot \Pr[X = \delta] = 0 \cdot (1 - \alpha) + \delta \cdot \alpha = \delta \cdot \alpha.$$

Solving for  $\delta$  we find  $\delta = \mathbb{E}[X]/\alpha$ .



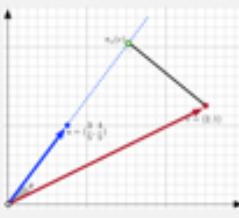
Imagine having 10  $\alpha$ -balls each representing  $\alpha = 1/10$ th of the probability mass. As in the figure, if these represent a distribution with  $\mathbb{E}[X] = 2$  and this must stay fixed, how far can one ball increase if all others balls must take a value at least 0? One ball can move to 20.

## Geometry of the Dot Product

A dot product is one of my favorite mathematical operations! It encodes a lot of geometry. Consider two vectors  $u = (\|u\|, \langle u, v \rangle)$  and  $v = (\|v\|, \langle u, v \rangle)$ , with an angle  $\theta$  between them. Then it holds

$$\langle u, v \rangle = \text{length}(u) \cdot \text{length}(v) \cdot \cos(\theta).$$

Here  $\text{length}(\cdot)$  measures the distance from the origin. We'll see how to measure length with a "norm"  $\|\cdot\|$  soon.



Moreover, since  $\|u\| = \text{length}(u) = 1$ , then we can also interpret  $\langle u, v \rangle$  as the length of  $v$  projected onto the line through  $u$ . That is, let  $v_\perp(v)$  be the closest point to  $v$  to the line through  $u$  (the line through  $u$  and the line segment from  $v$  to  $v_\perp(v)$  make a right angle). Then

$$\langle u, v \rangle = \text{length}(v_\perp(v)) = \|v_\perp(v)\|.$$

## Geometry of Why Perceptron Works

Here we will show that after at most  $T = (1/\gamma^*)^2$  steps (where  $\gamma^*$  is the margin of the maximum margin classifier), then there can be no more misclassified points.

To show this we will bound two terms as a function of  $t$ , the number of mistakes found. The term any  $\langle w, w^* \rangle$  and  $\|w\|^2 = \langle w, w \rangle$ ; this is before we ultimately normalize  $w$  in the return step.

First we can argue that  $\|w\|^2 \leq t$ , since each step increases  $\|w\|^2$  by at most 1:

$$\langle w + y_i x_i, w + y_i x_i \rangle = \langle w, w \rangle + \langle y_i \rangle^2 \langle x_i, x_i \rangle + 2y_i \langle w, x_i \rangle \leq \langle w, w \rangle + 1 + 0.$$

This is true since each  $\|x_i\| \leq 1$ , and if  $x_i$  is mis-classified, then  $y_i \langle w, x_i \rangle$  is negative.

Second, we can argue that  $\langle w, w^* \rangle \geq \gamma^*$  since each step increases it by at least  $\gamma^*$ . Recall that  $\|w^*\| = 1$

$$\langle w + y_i x_i, w^* \rangle = \langle w, w^* \rangle + \langle y_i \rangle \langle x_i, w^* \rangle \geq \langle w, w^* \rangle + \gamma^*.$$

The inequality follows from the margin of each point being at least  $\gamma^*$  with respect to the max-margin classifier  $w^*$ .

Combining these facts ( $\langle w, w^* \rangle \geq \gamma^*$  and  $\|w\|^2 \leq t$ ) together we obtain

$$\gamma^* \leq \langle w, w^* \rangle \leq \langle w, \frac{w}{\|w\|} \rangle = \|w\| \leq \sqrt{t}.$$

Solving for  $t$  yields  $t \leq (1/\gamma^*)^2$  as desired.

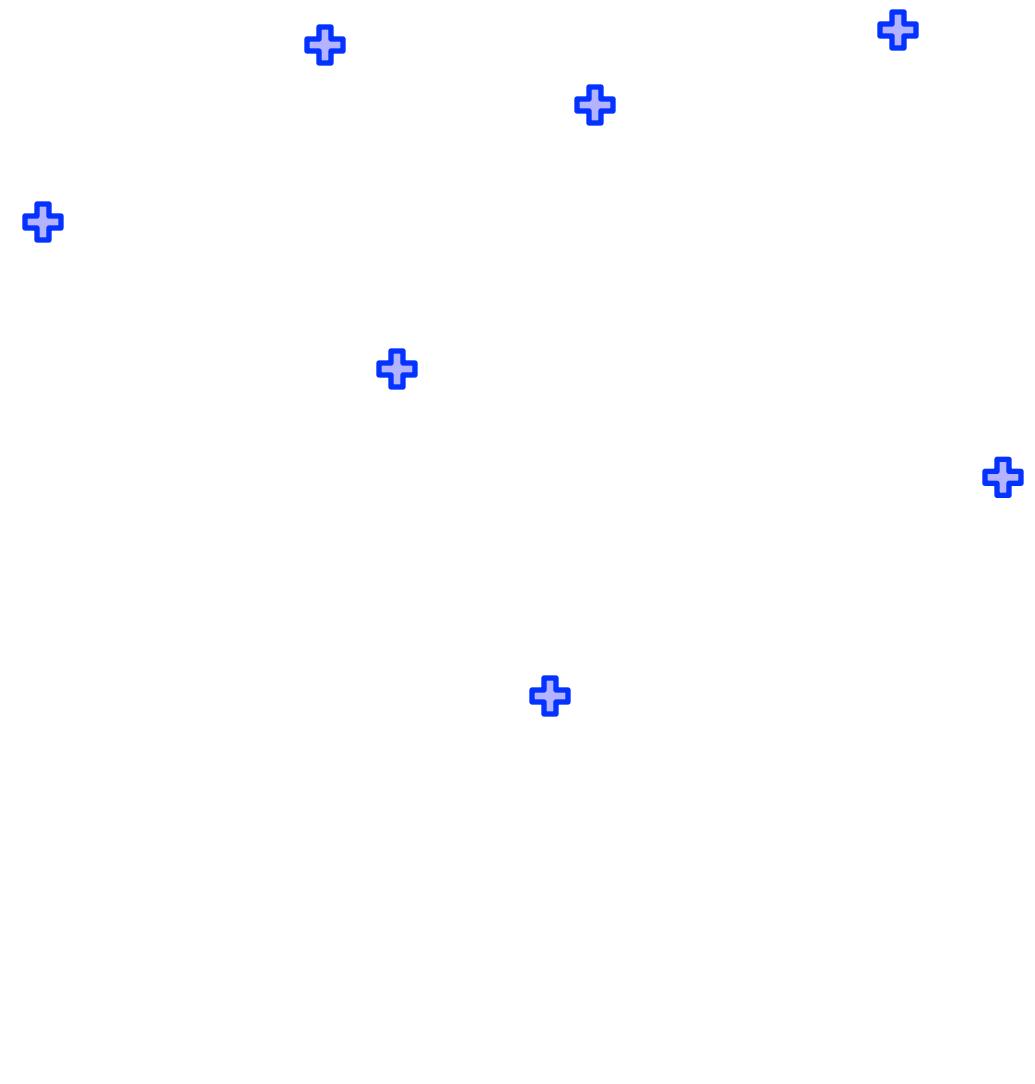
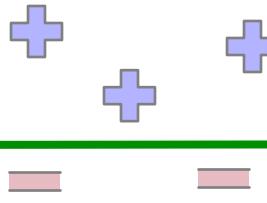


# What is Machine Learning?

Given  $X \in \mathbb{R}^d$  with sign  $\sigma : X \rightarrow \{-1, +1\}$ .

Find separating halfspace  $h \in \mathcal{H}$  so

$x \in h \Rightarrow \sigma(x) = +1$  and  $x \notin h \Rightarrow \sigma(x) = -1$ .

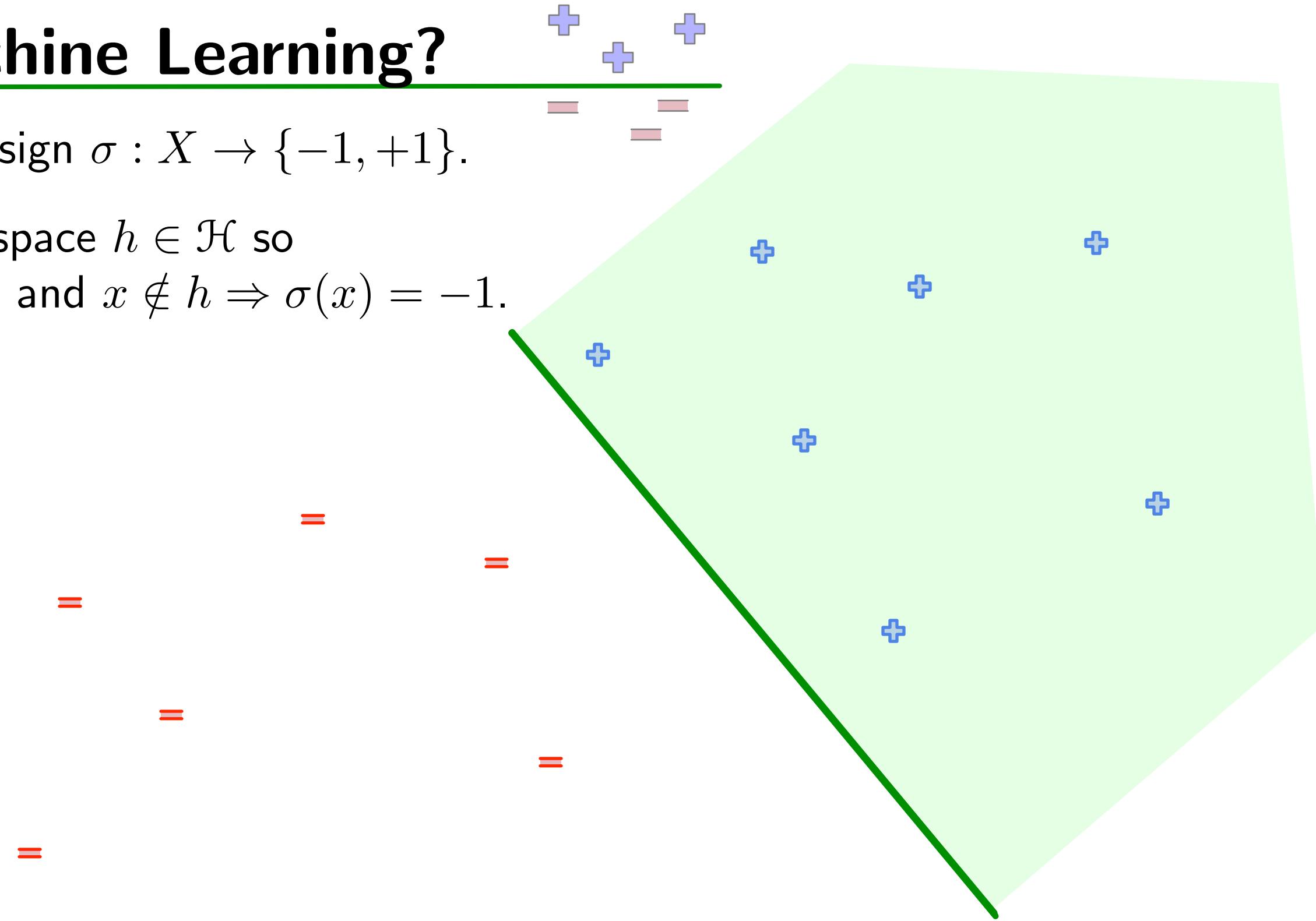


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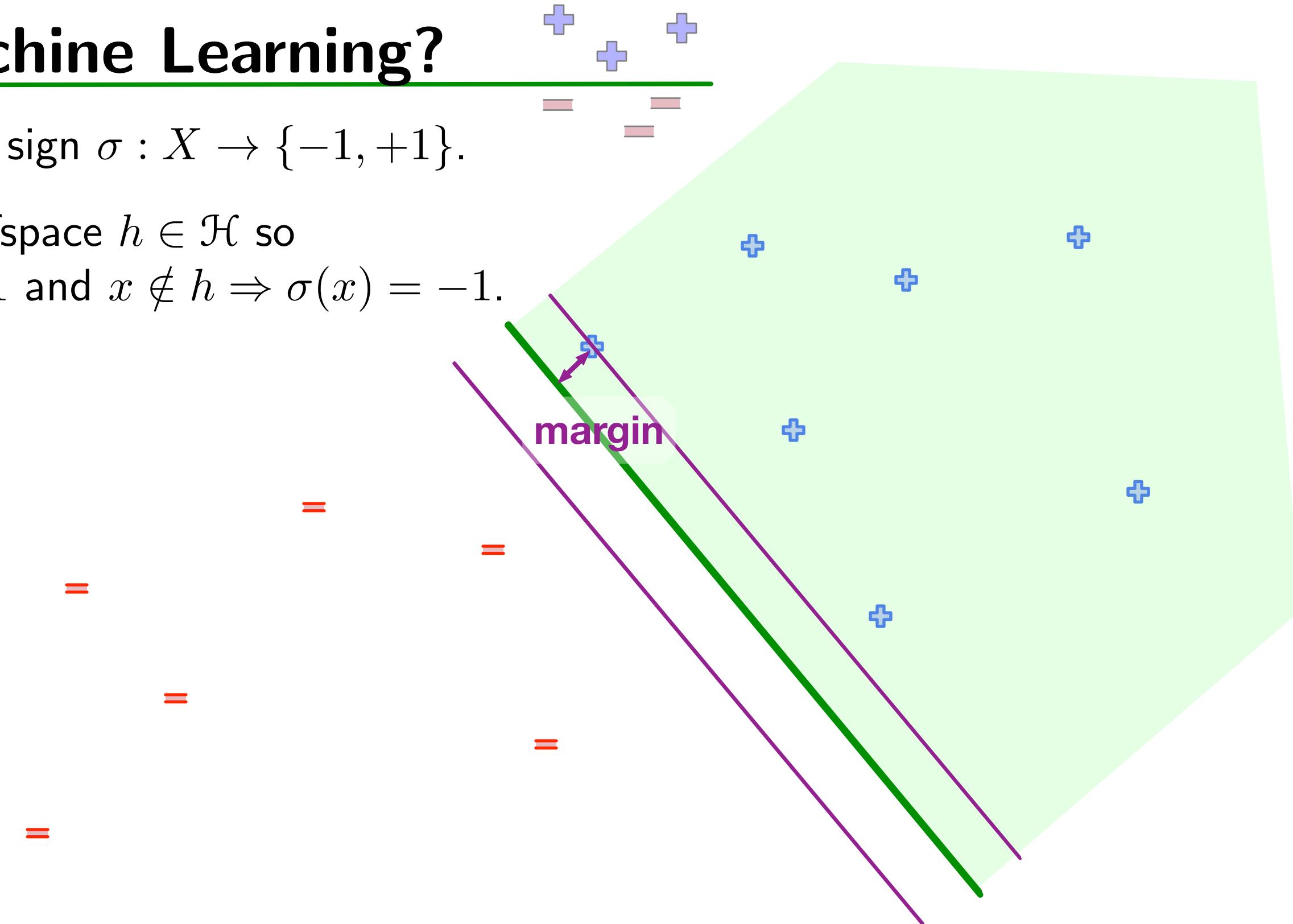


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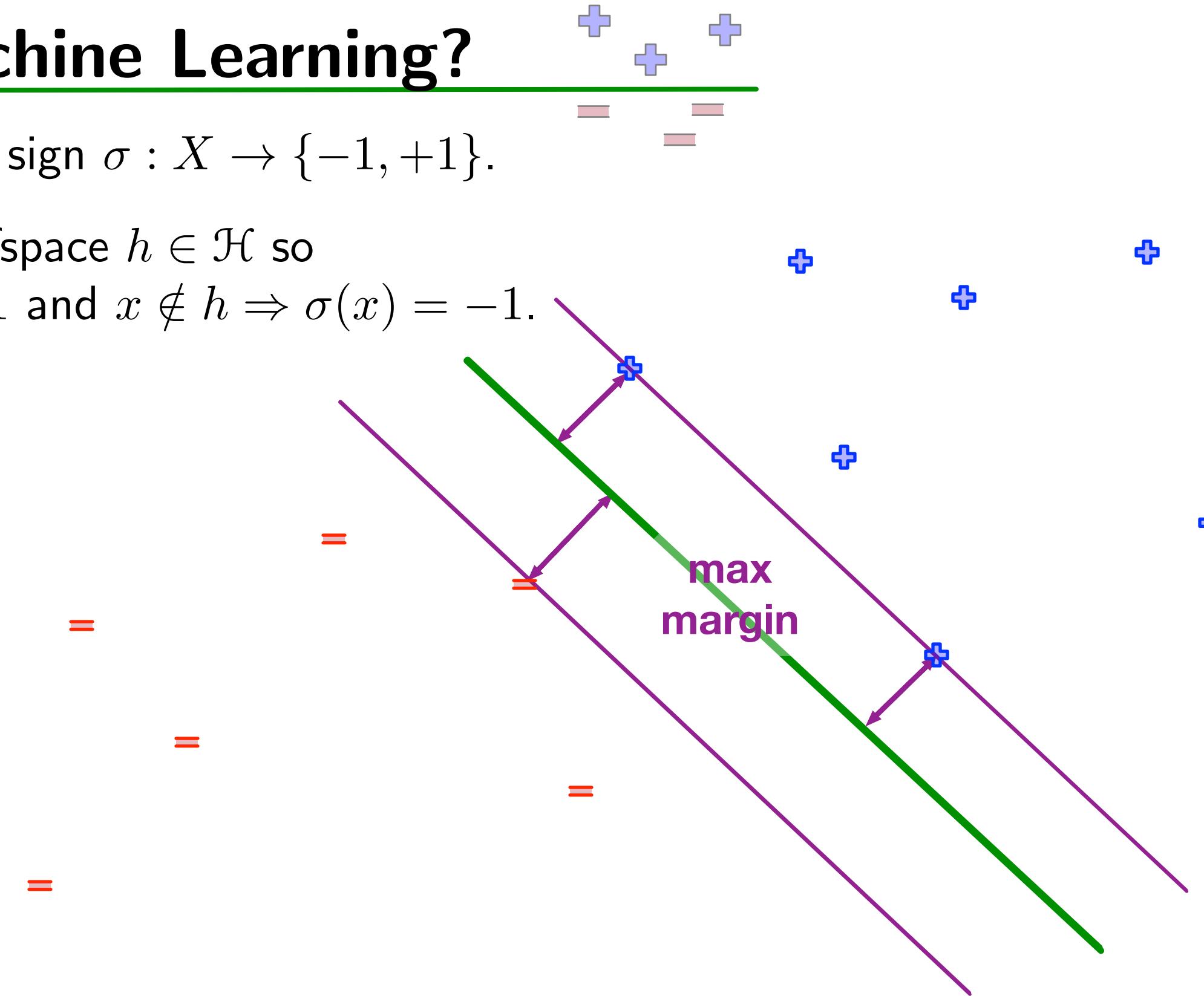


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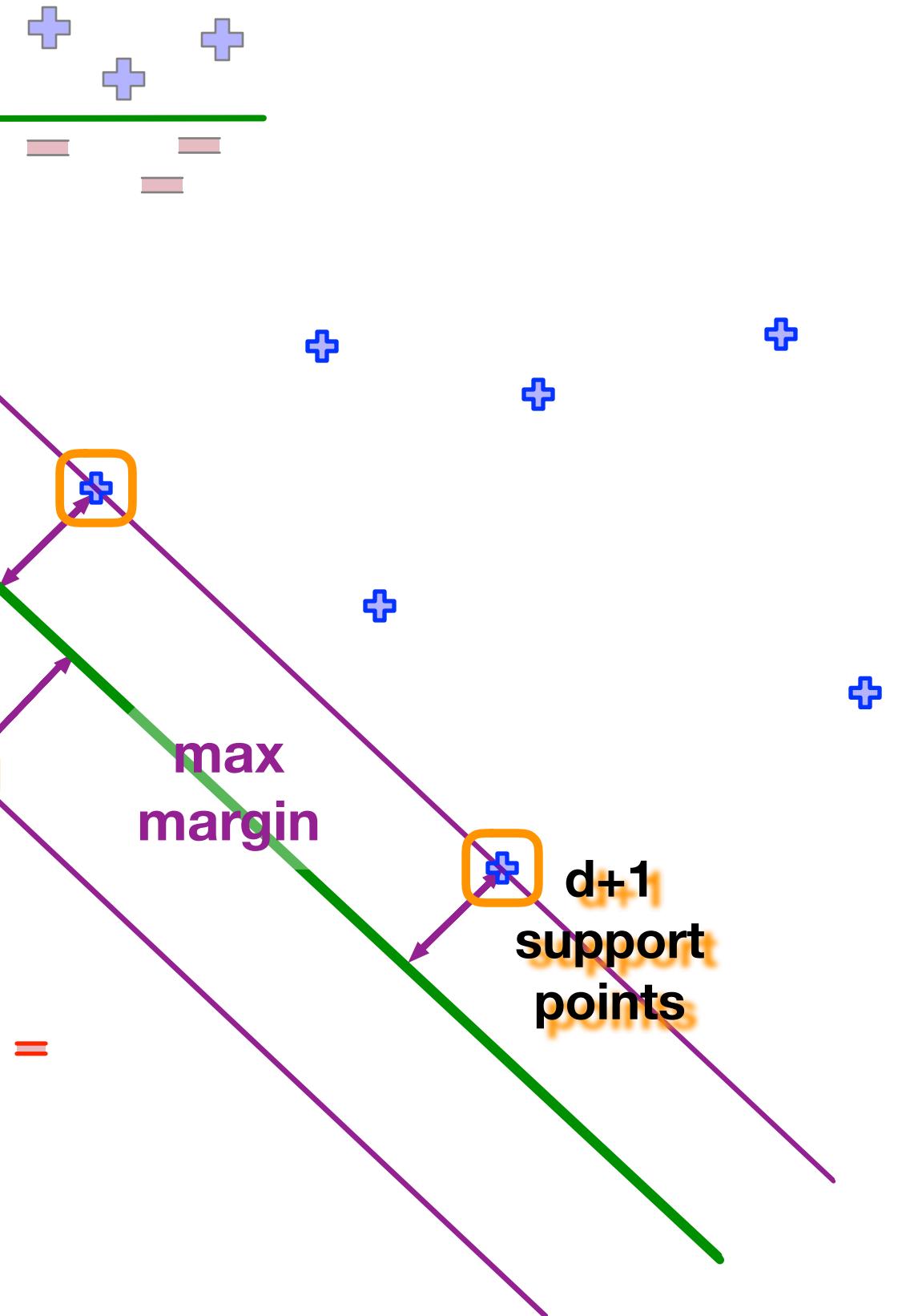


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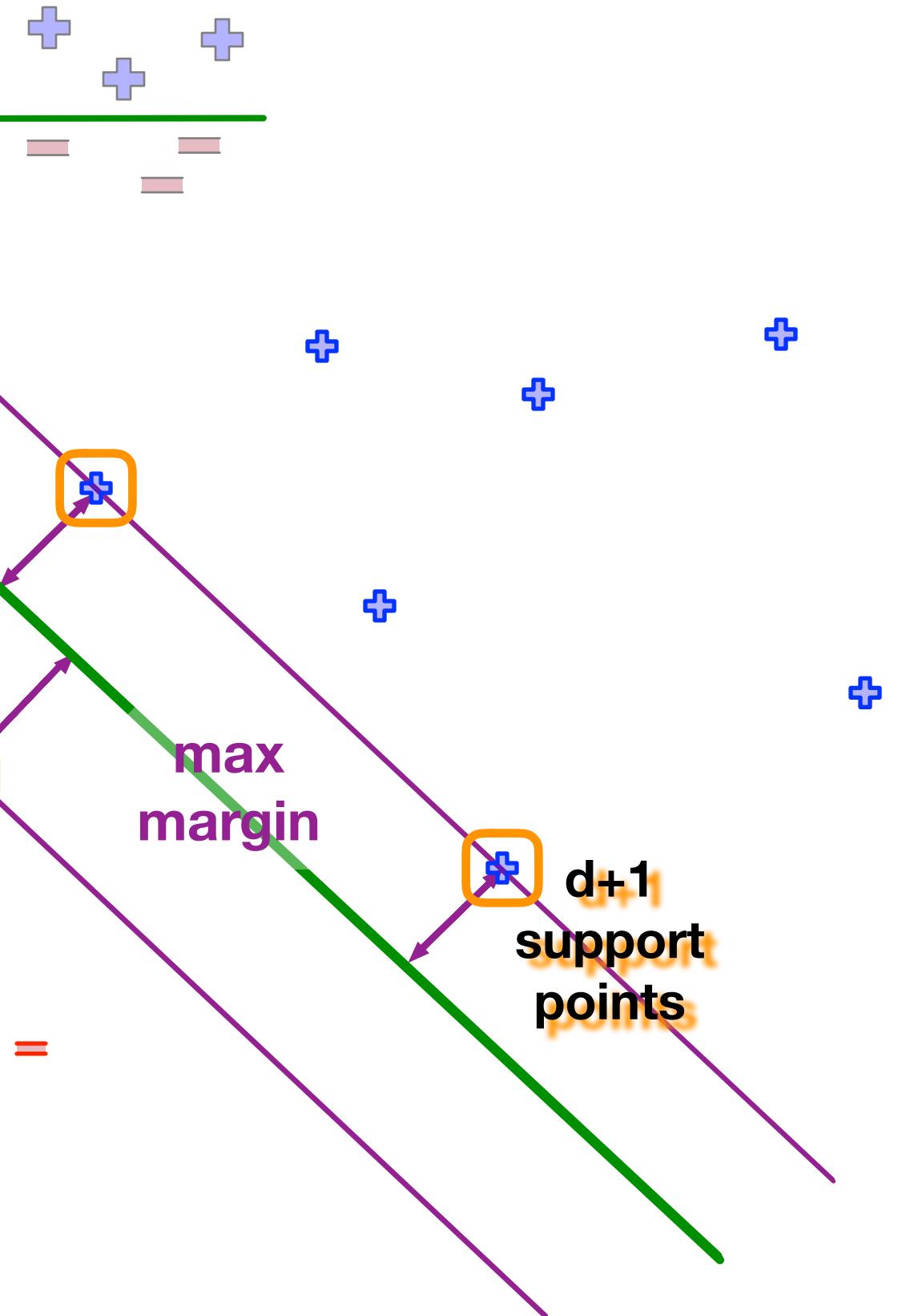
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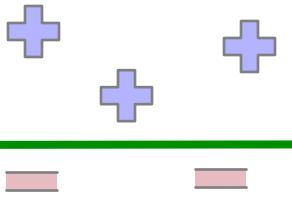
How do we solve this problem?



# Polytope Distance

Define polytopes  $P = \text{CH}(x \in X \mid \sigma(x) = +1)$

$Q = \text{CH}(x \in X \mid \sigma(x) = -1)$



$+ p_1$

$+ p_3$

$+ p_2$

$+ p_4$

$+ p_6$

$+ p_5$

$= q_3$

$= q_2$

$= q_5$

$= q_6$

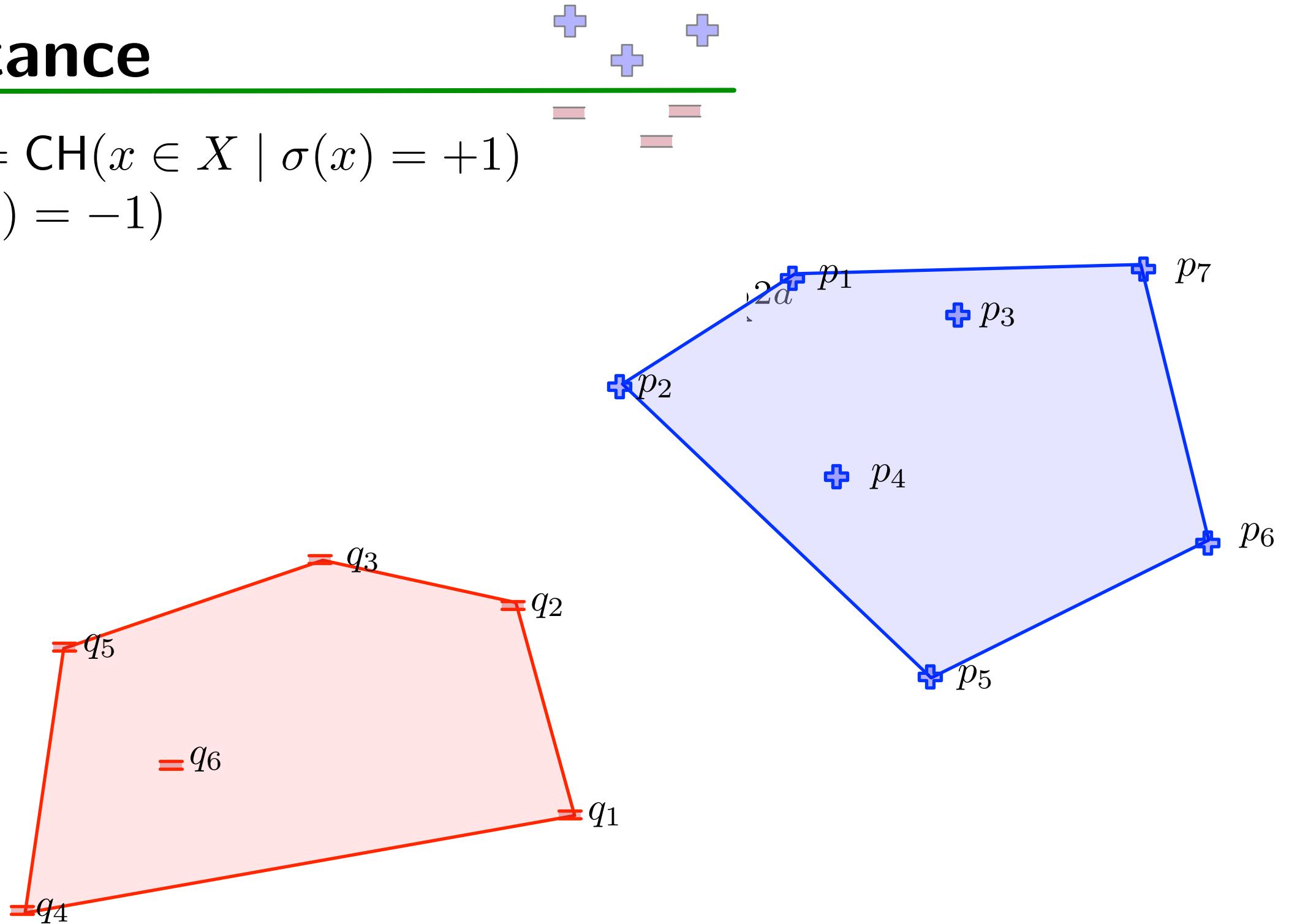
$= q_1$

$= q_4$

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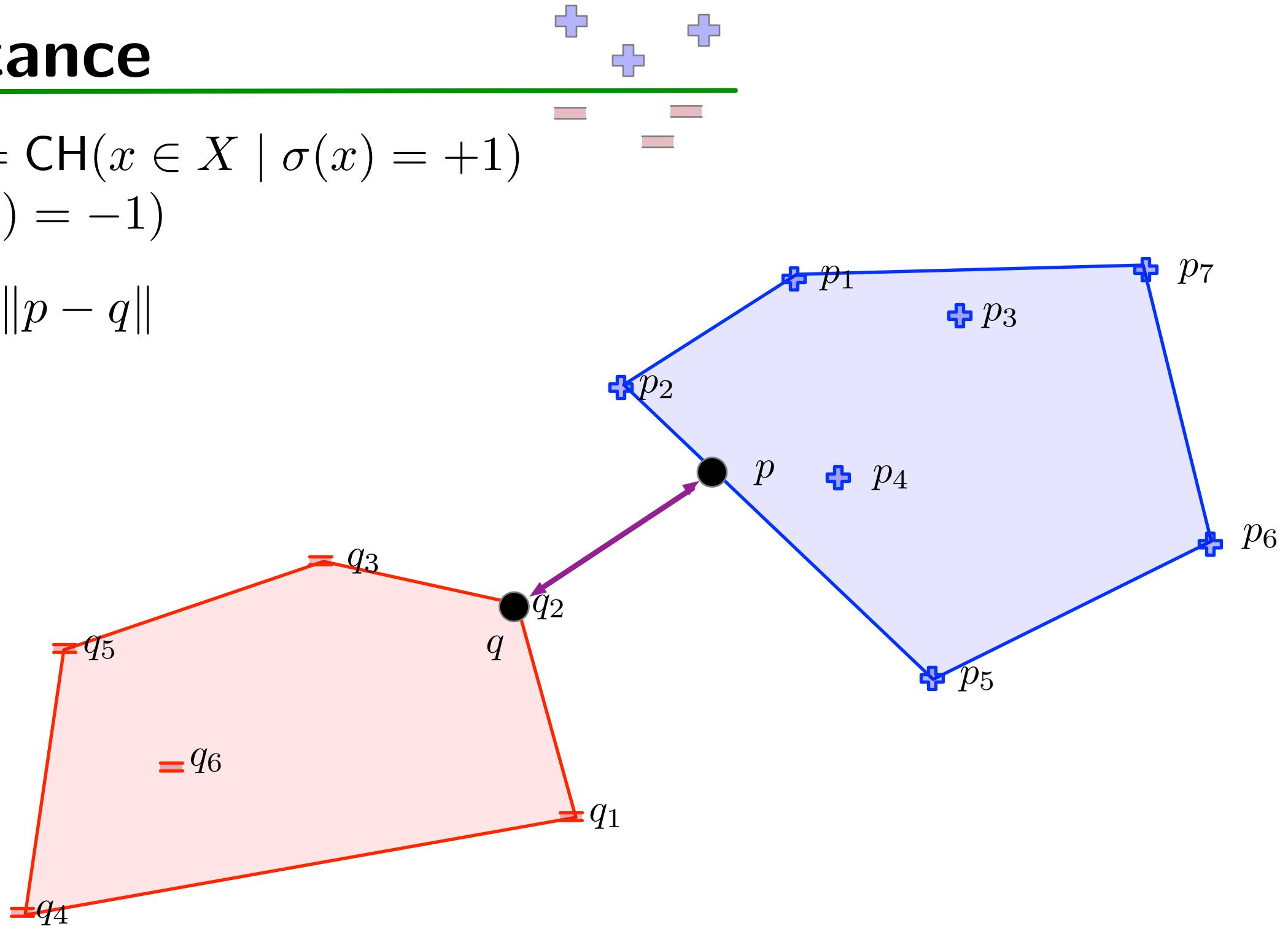


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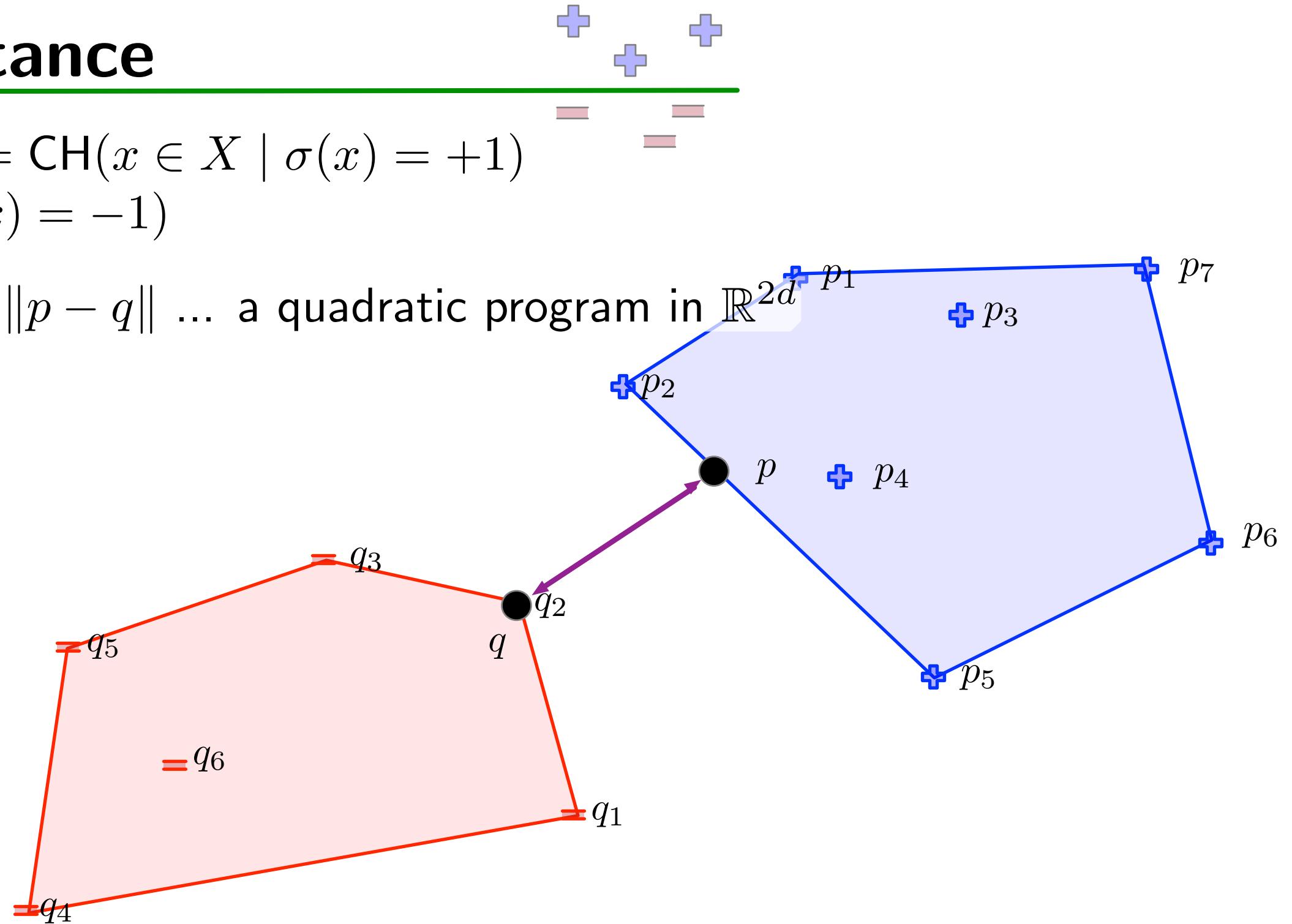


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Find  $\arg \min_{p \in P, q \in Q} \|p - q\|$  ... a quadratic program in  $\mathbb{R}^{2d}$



# Polytope Distance

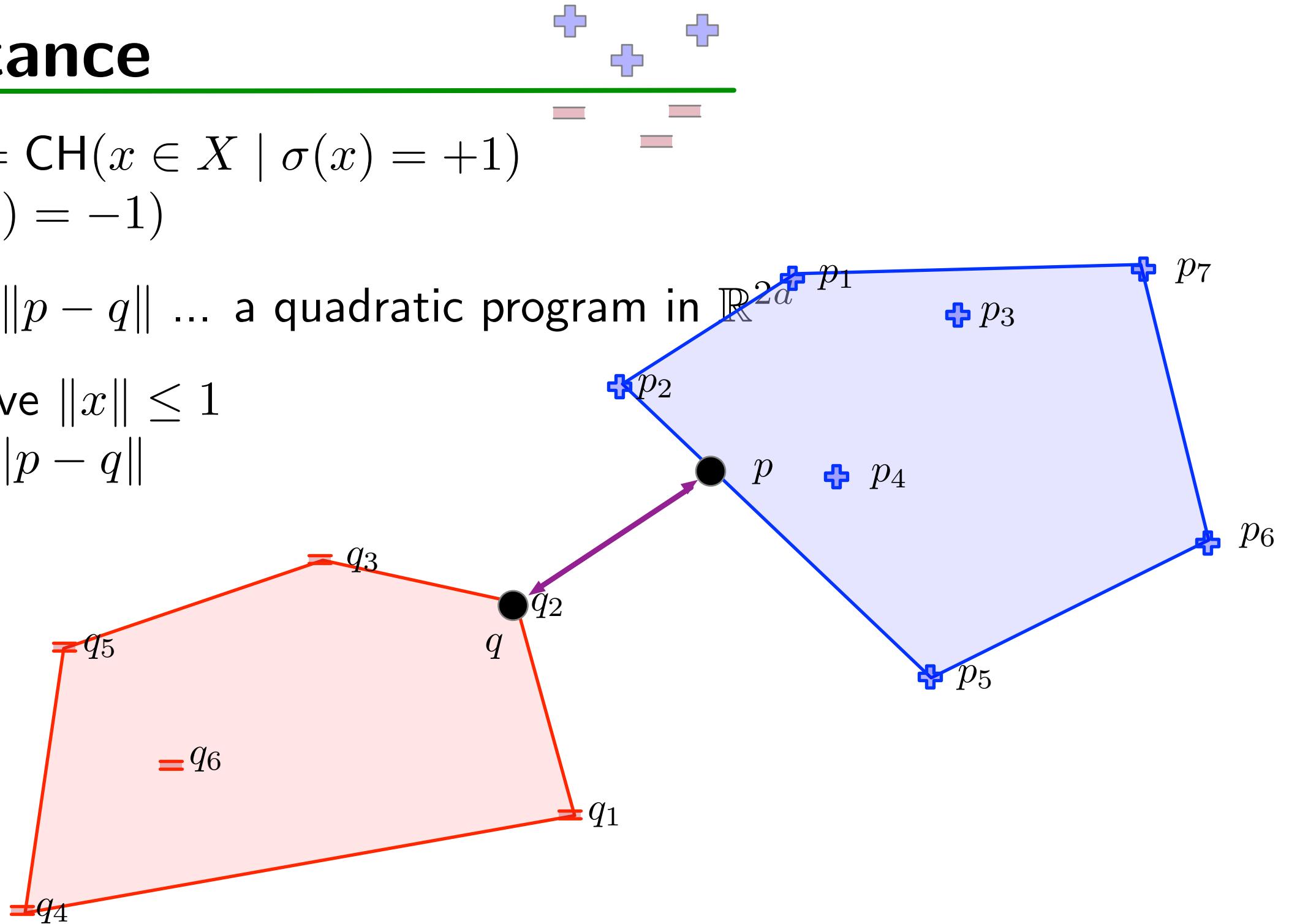
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Assume all  $x \in X$  have  $\|x\| \leq 1$

Let  $\gamma = \min_{p \in P, q \in Q} \|p - q\|$



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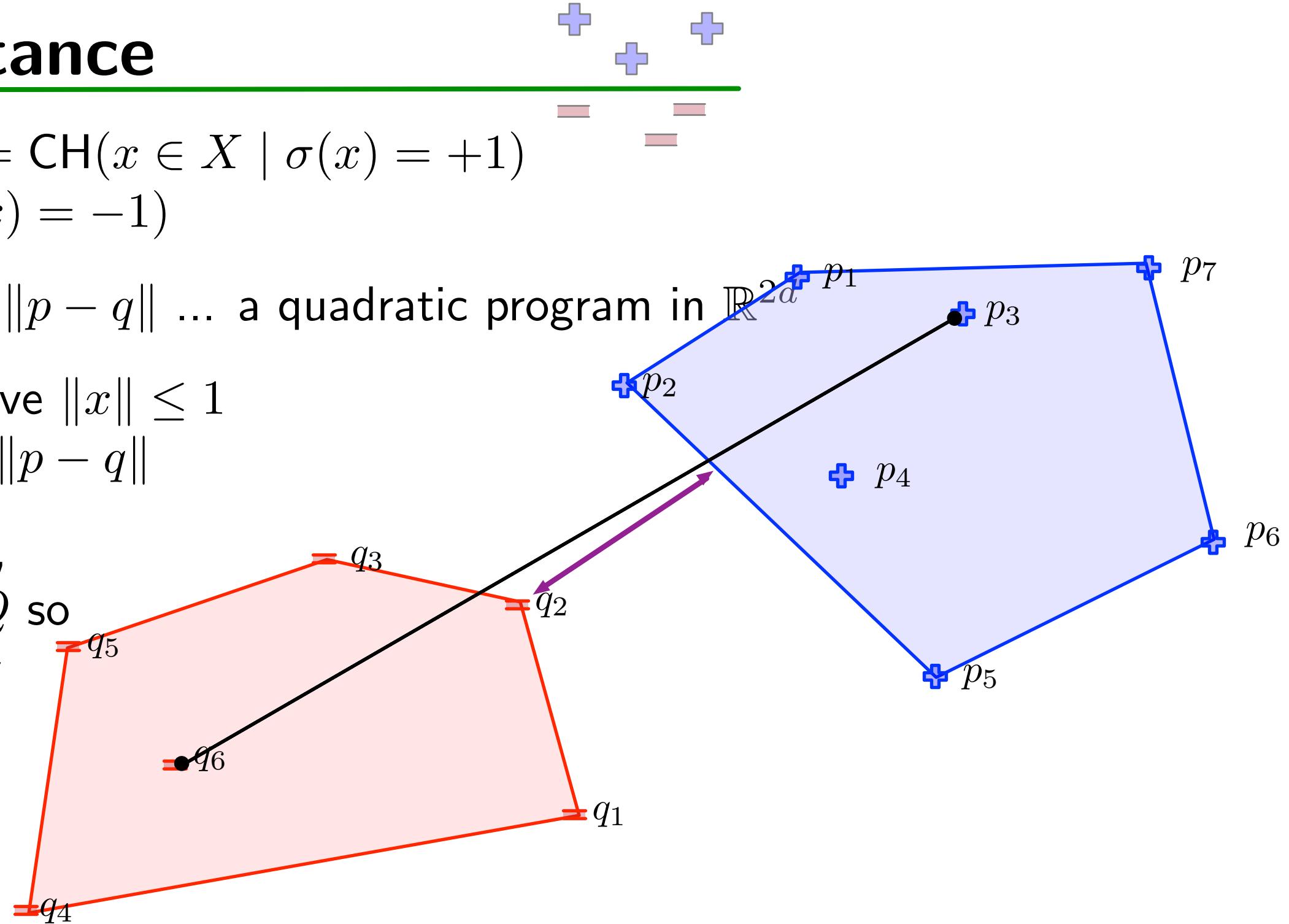
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Let  $\gamma = \min_{p \in P, q \in Q} \|p - q\|$

Iterate  $1/(\varepsilon\gamma^2)$  steps,

find  $\hat{p} \in P$  and  $\hat{q} \in Q$  so

$$(1 - \varepsilon)\|\hat{p} - \hat{q}\| \leq \gamma$$



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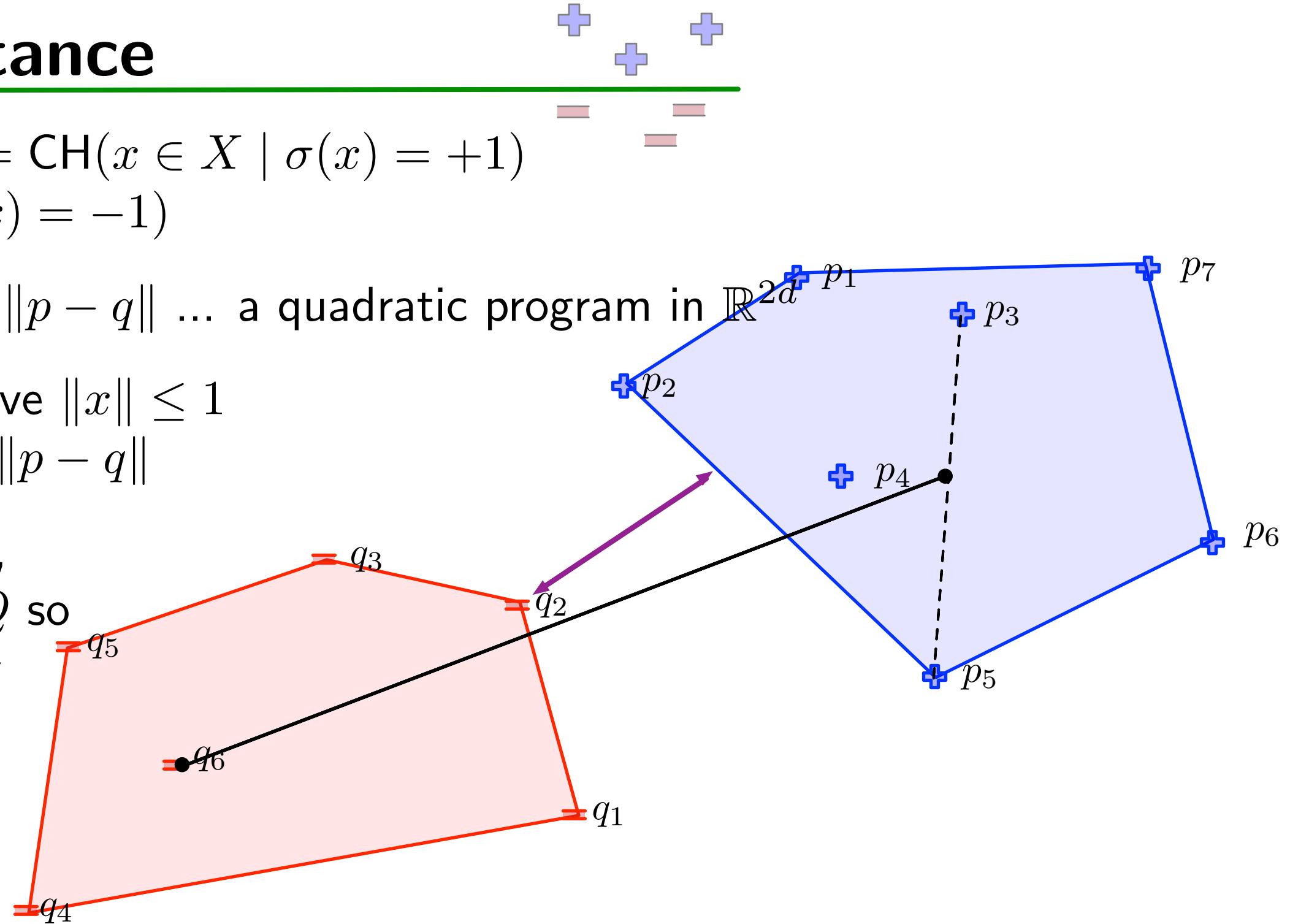
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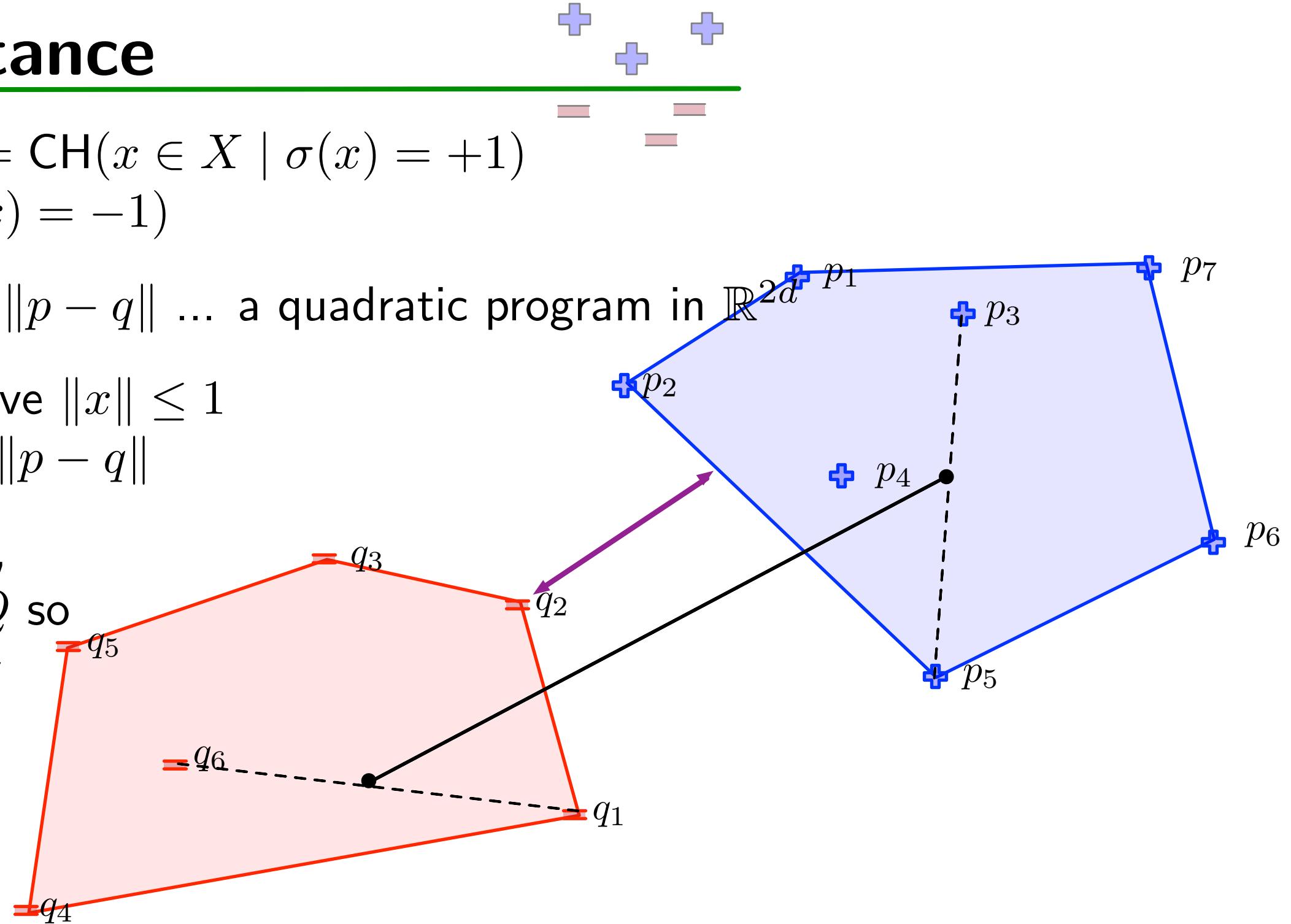
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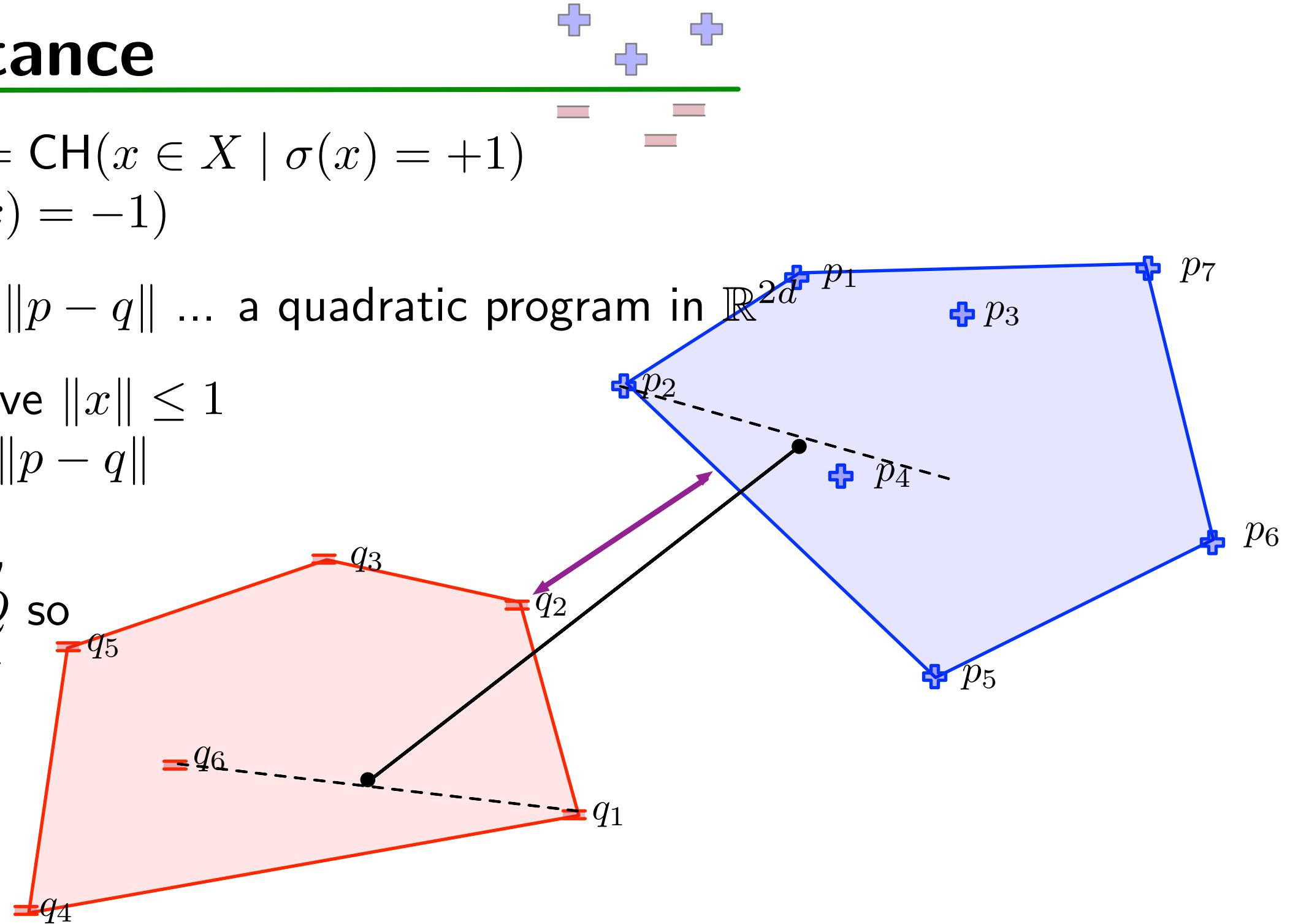
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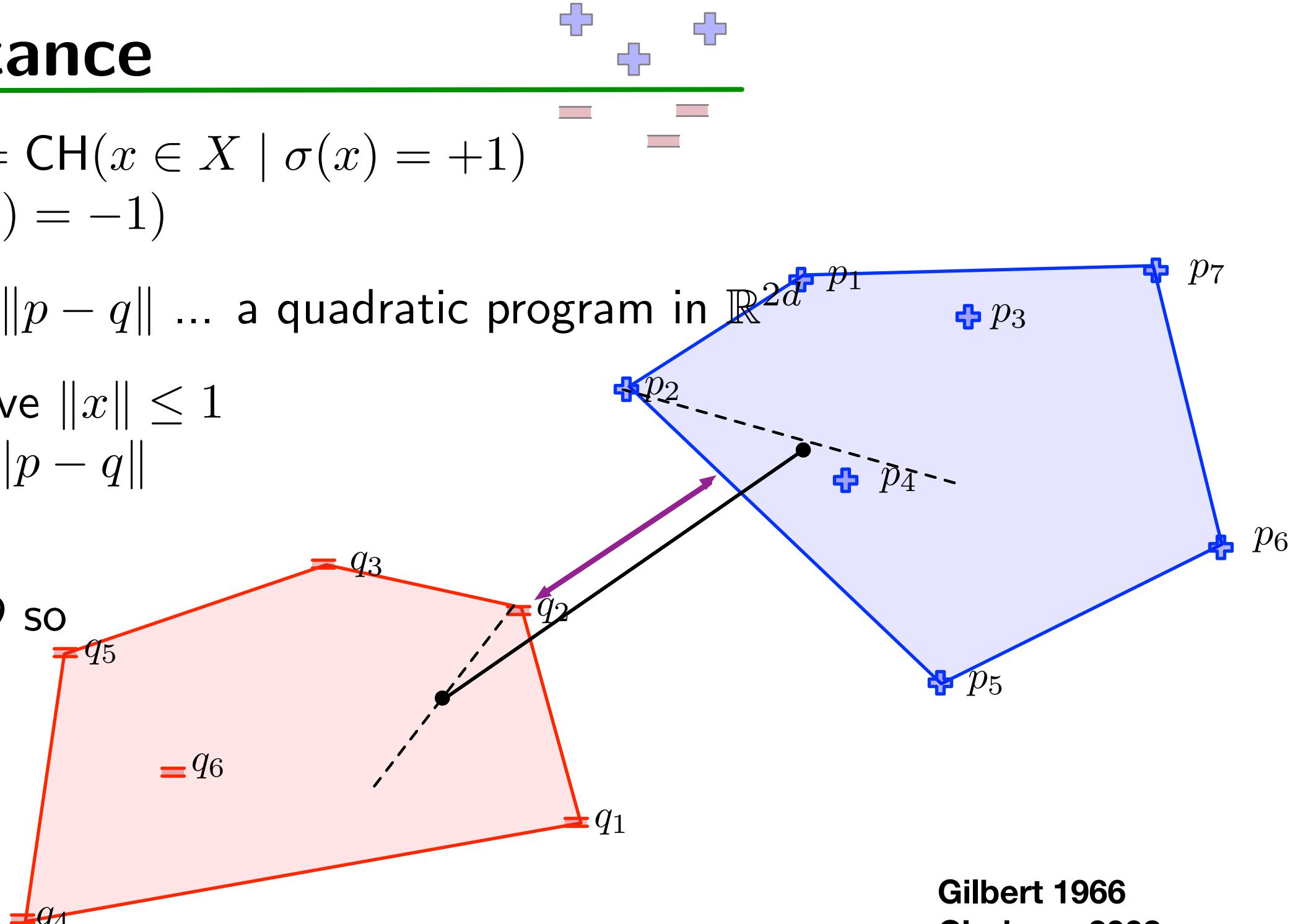
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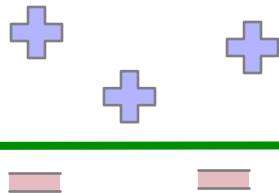
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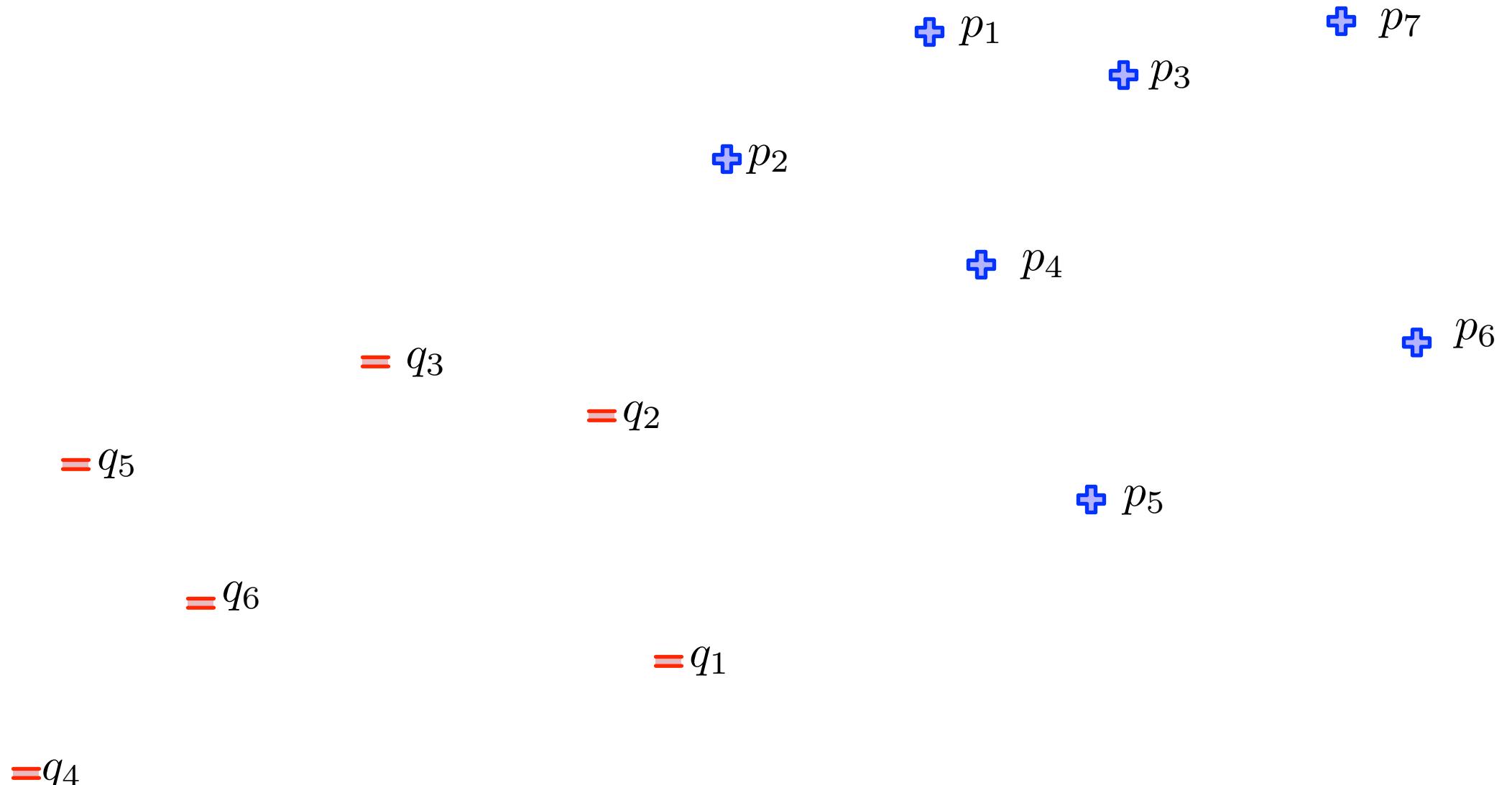


Gilbert 1966  
Clarkson 2008  
Gartner+Jaggi 2009

# Force $h$ through Origin

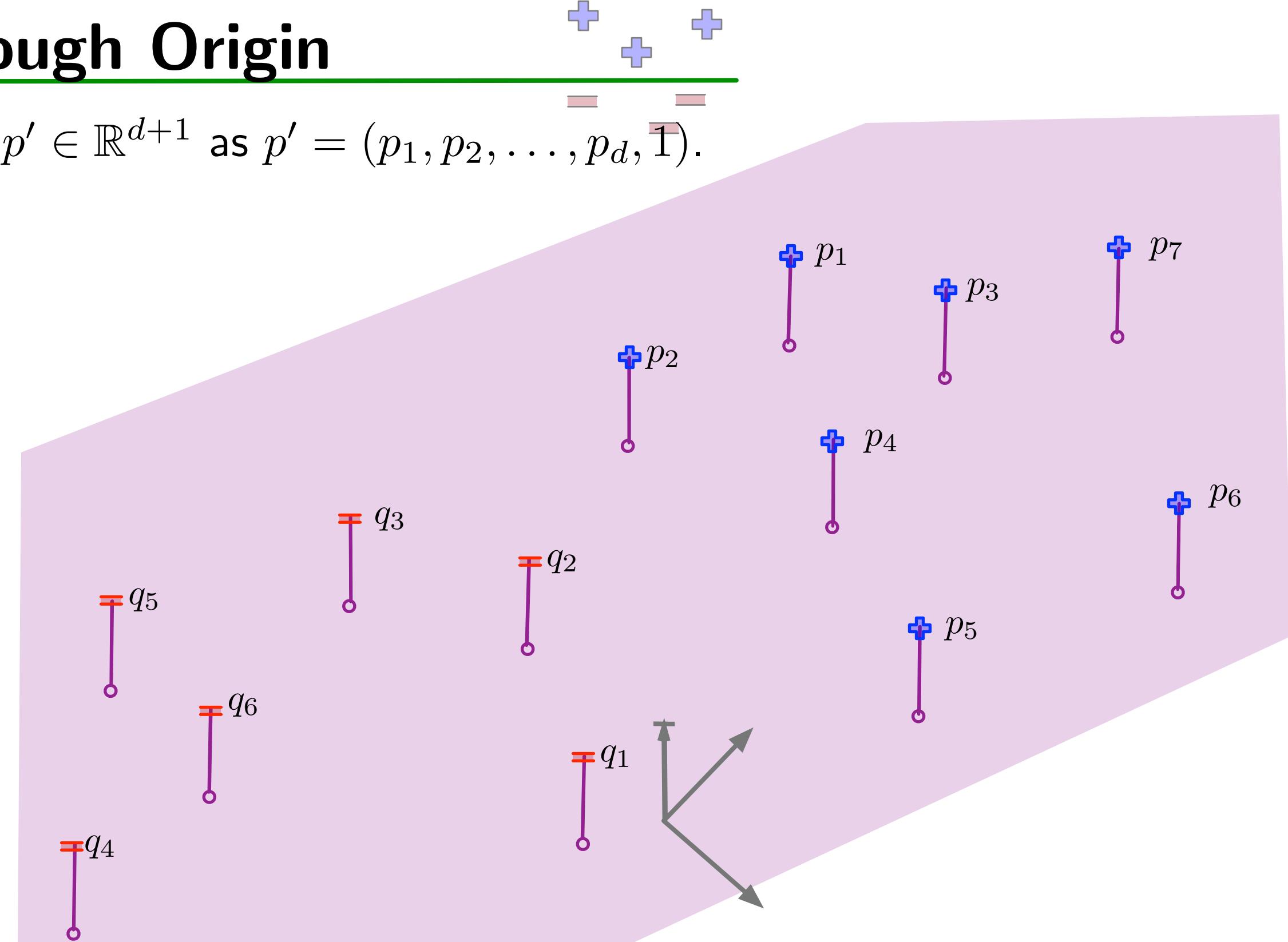


1: Map  $p \in \mathbb{R}^d$  to  $p' \in \mathbb{R}^{d+1}$  as  $p' = (p_1, p_2, \dots, p_d, 1)$ .



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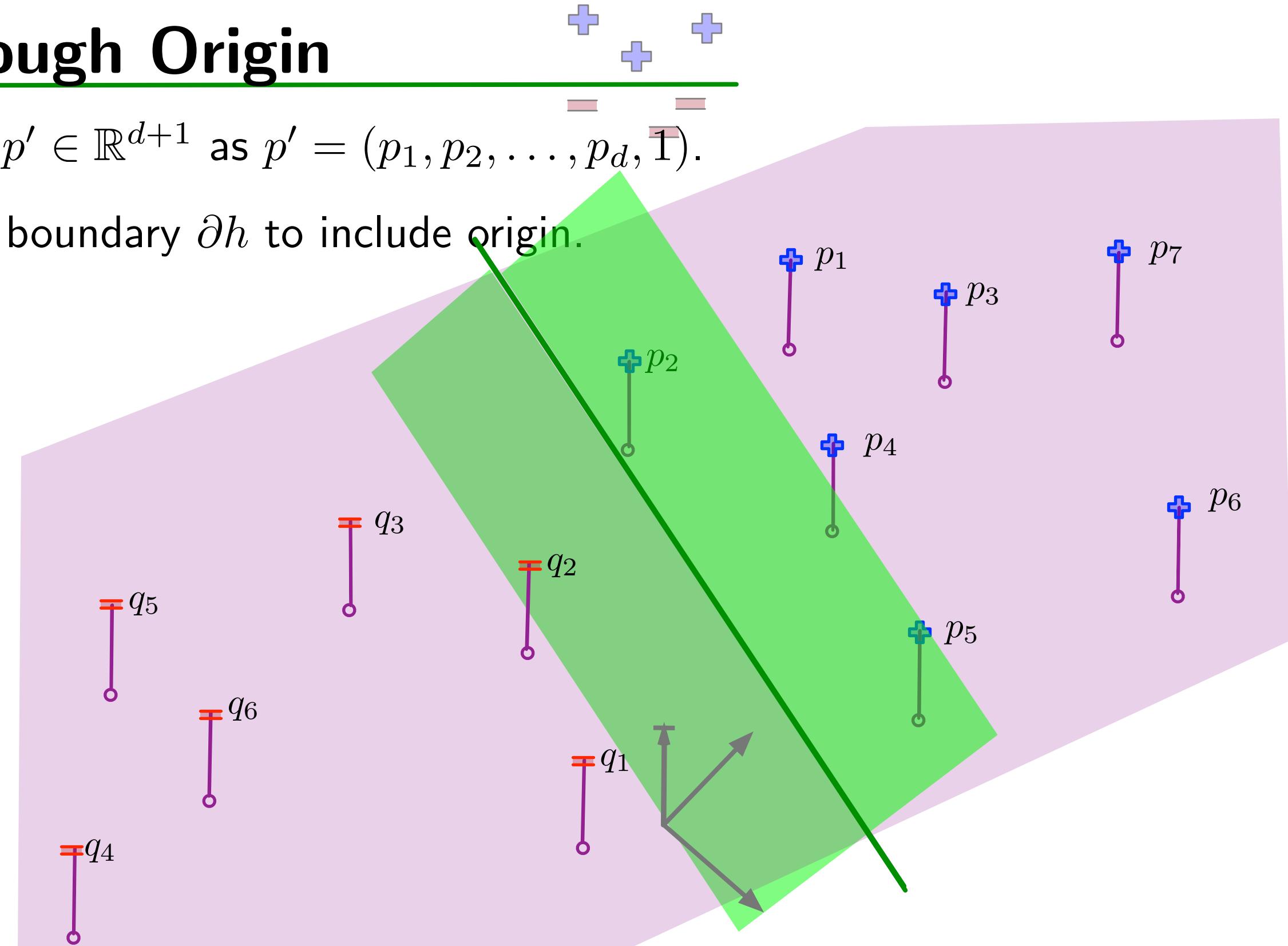
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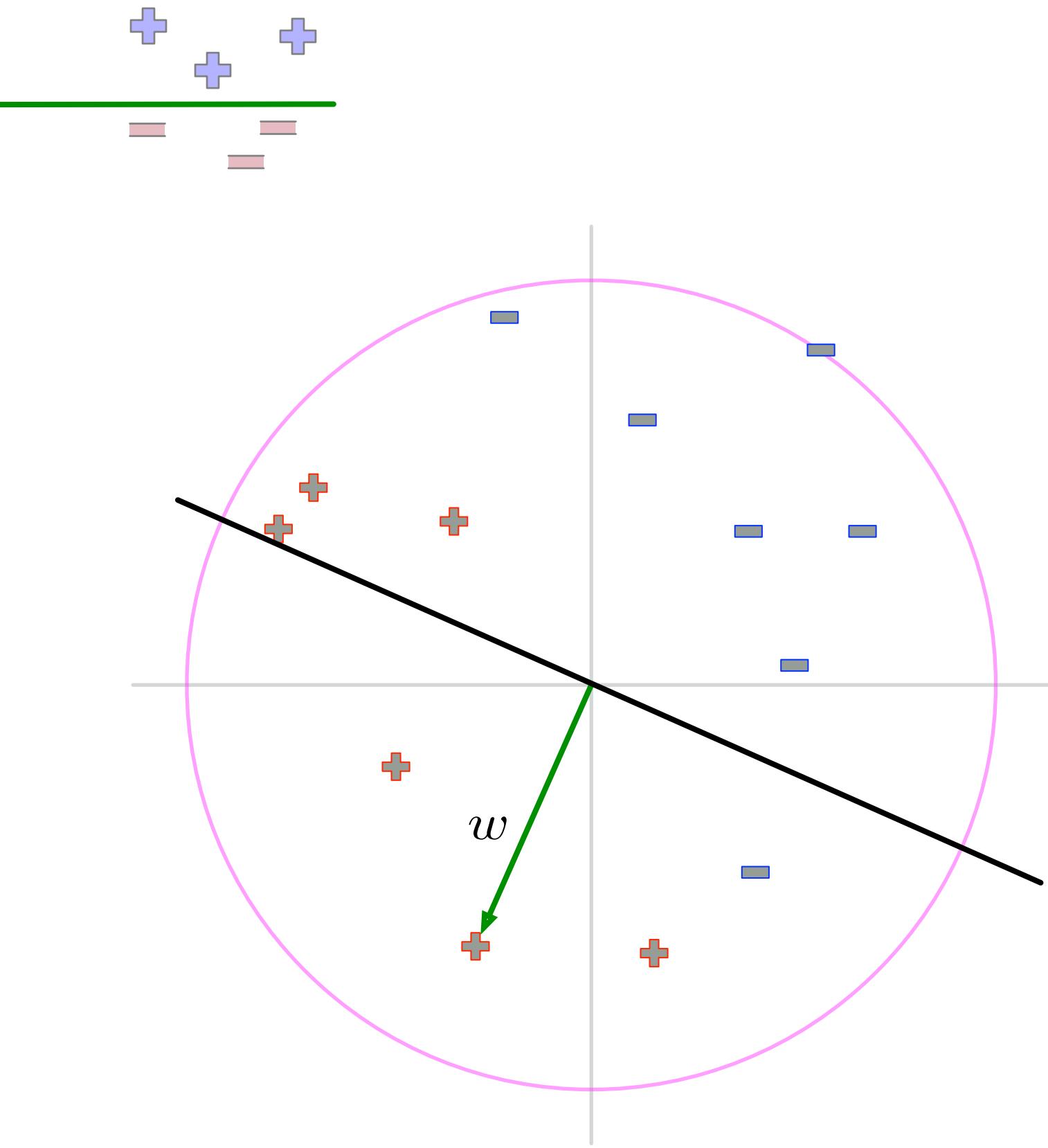
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2: Force halfspace boundary  $\partial h$  to include origin.



# Perceptron Algorithm

- Assume (1)  $x \in X \subset \mathbb{R}^d$  has  $\|x\| \leq 1$   
(2) halfspace  $h \in \mathcal{H}_0$  goes through origin



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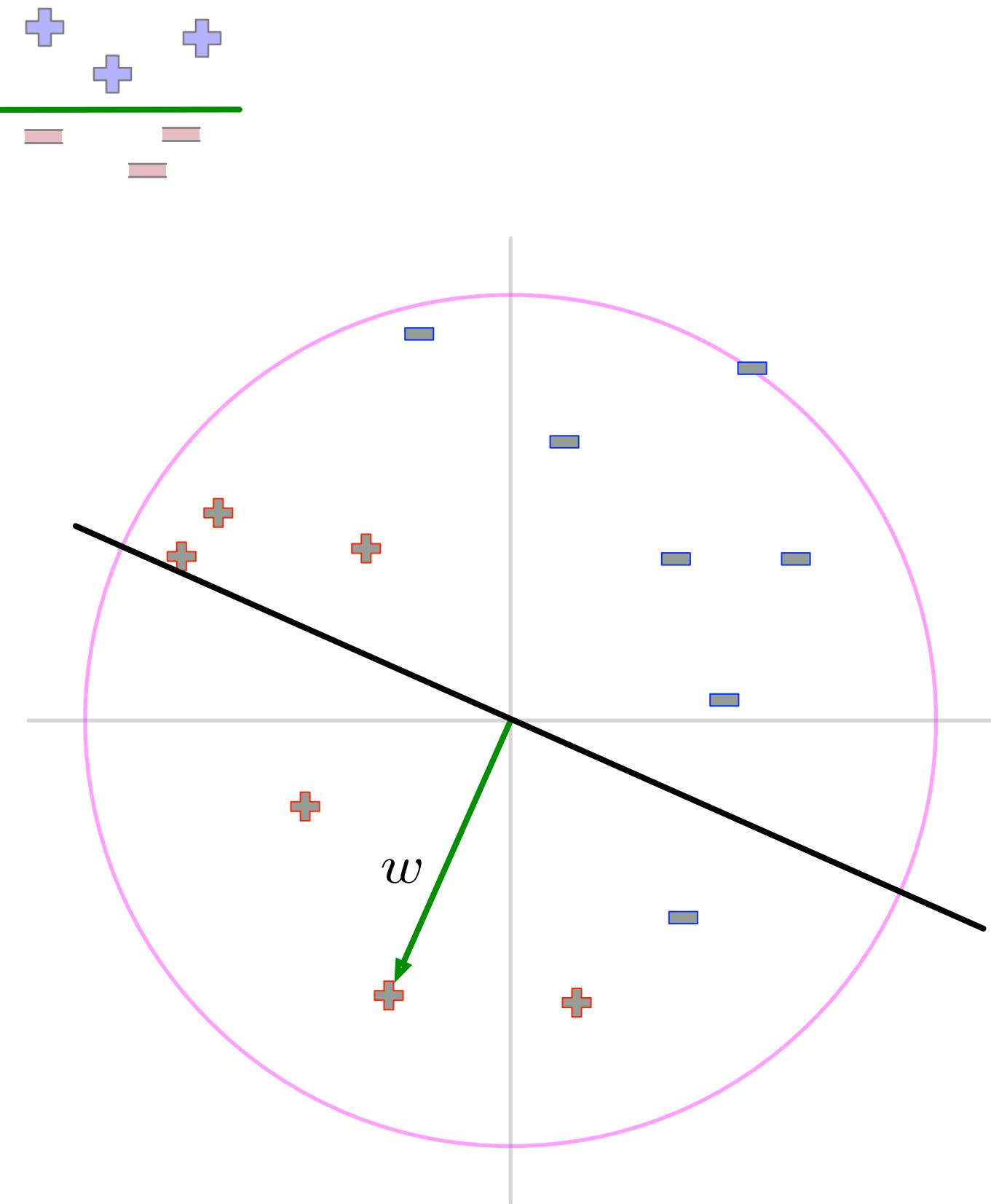
Algorithm: **(Rosenblatt 1958)**

choose  $w = \sigma(x)x$

**for**  $i = 1$  **to**  $1/\gamma^2$  steps

$x' = \text{any } x \in X \text{ s.t. } \langle \sigma(x)x, w \rangle < 0$

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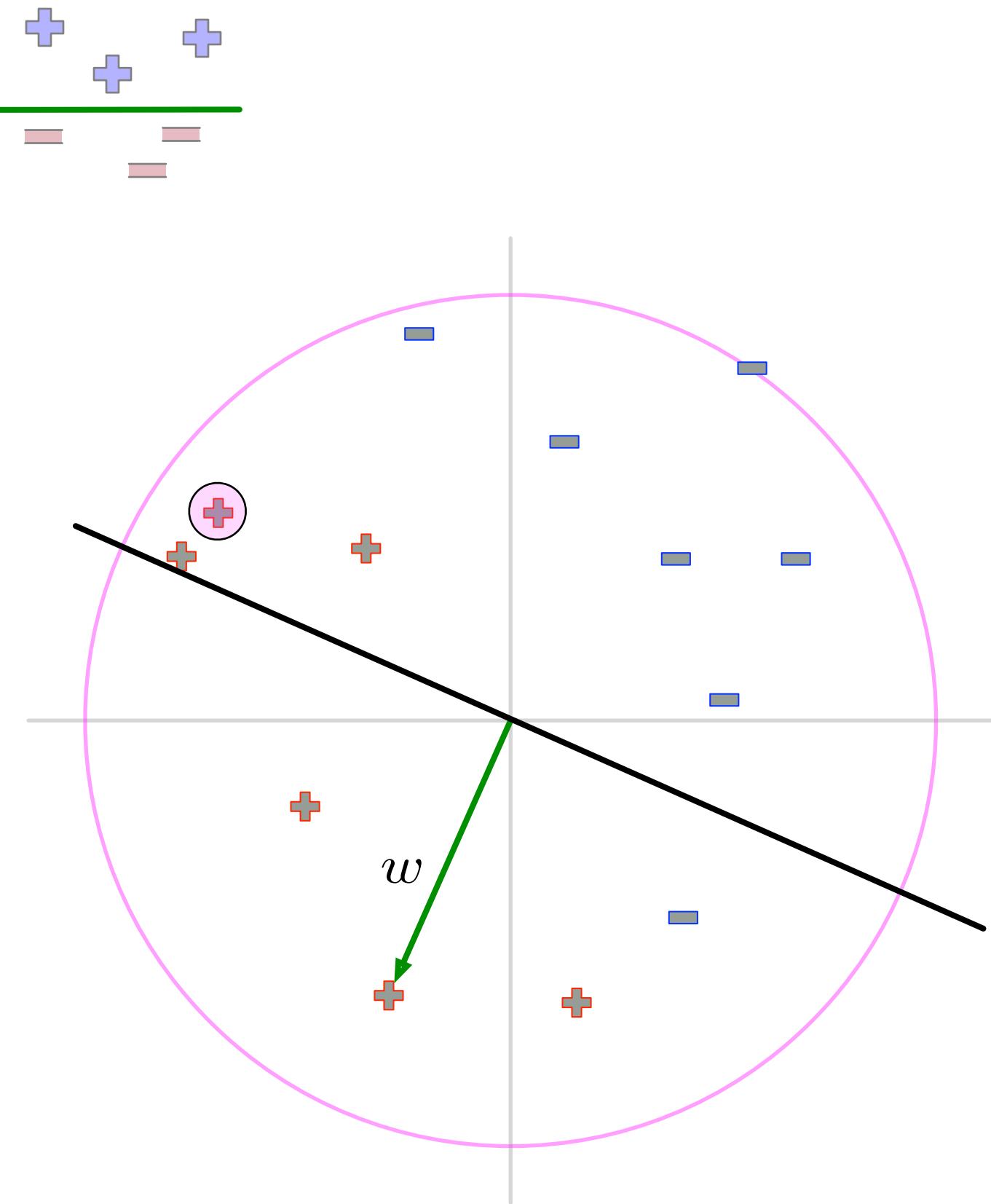
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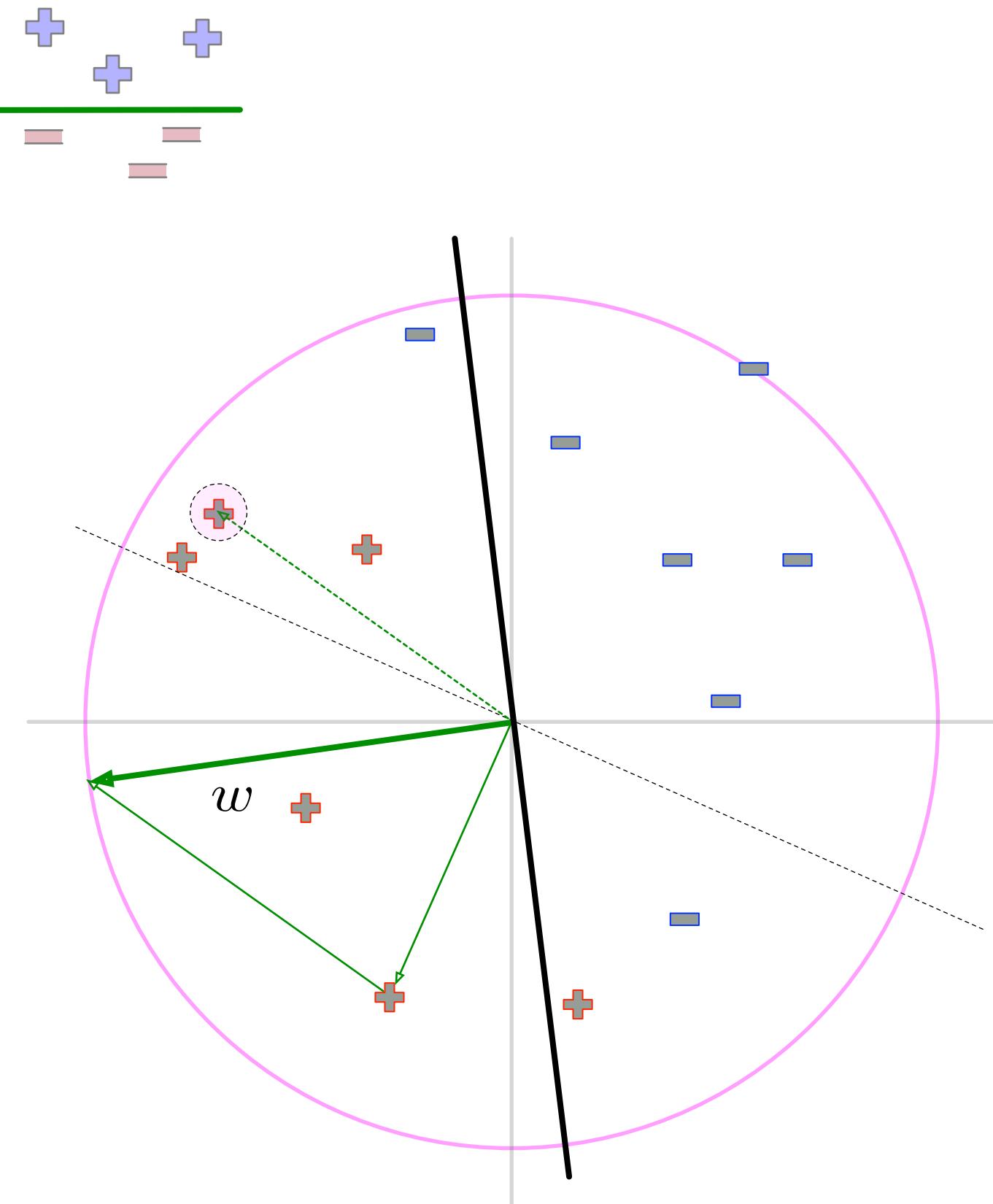
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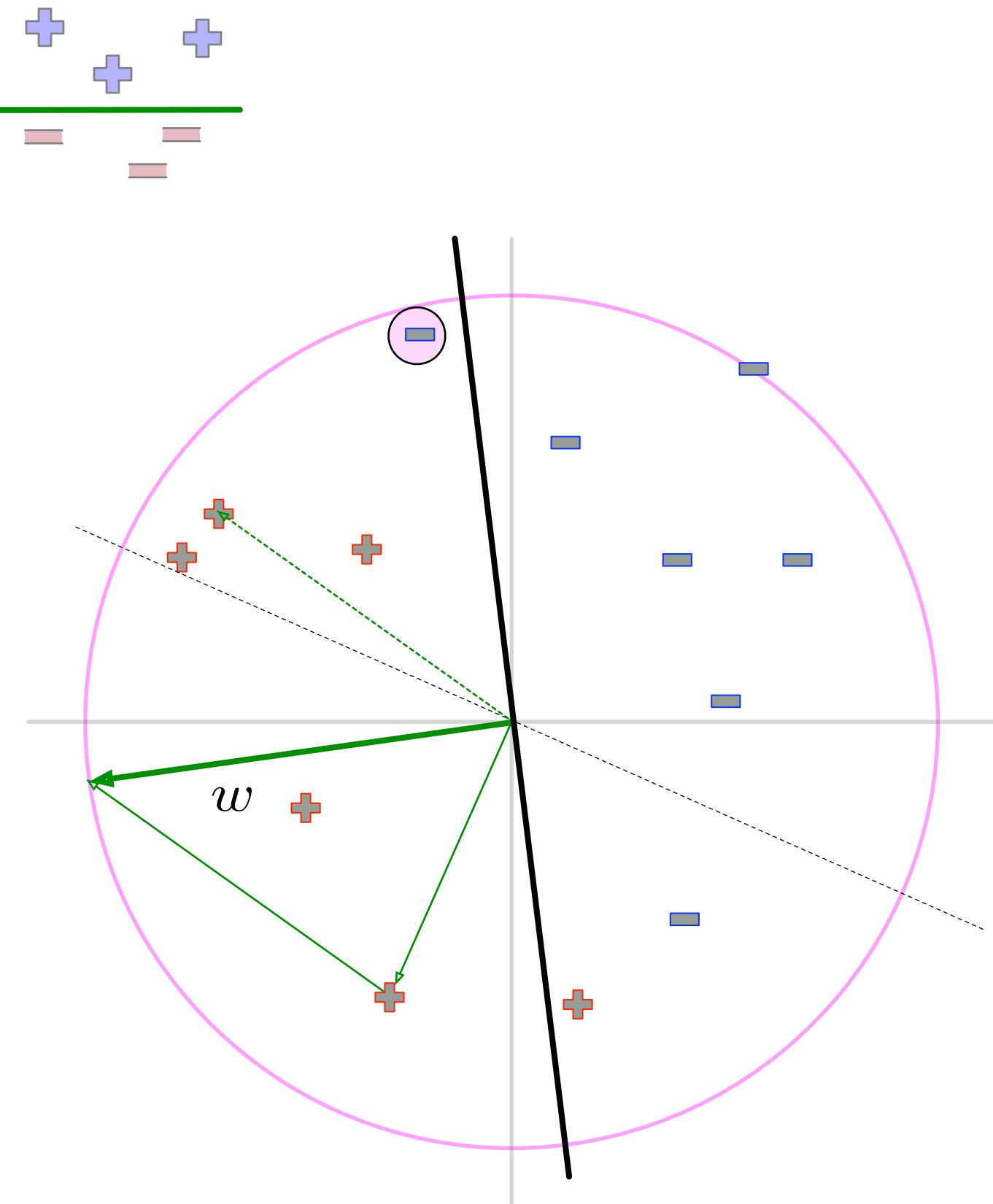
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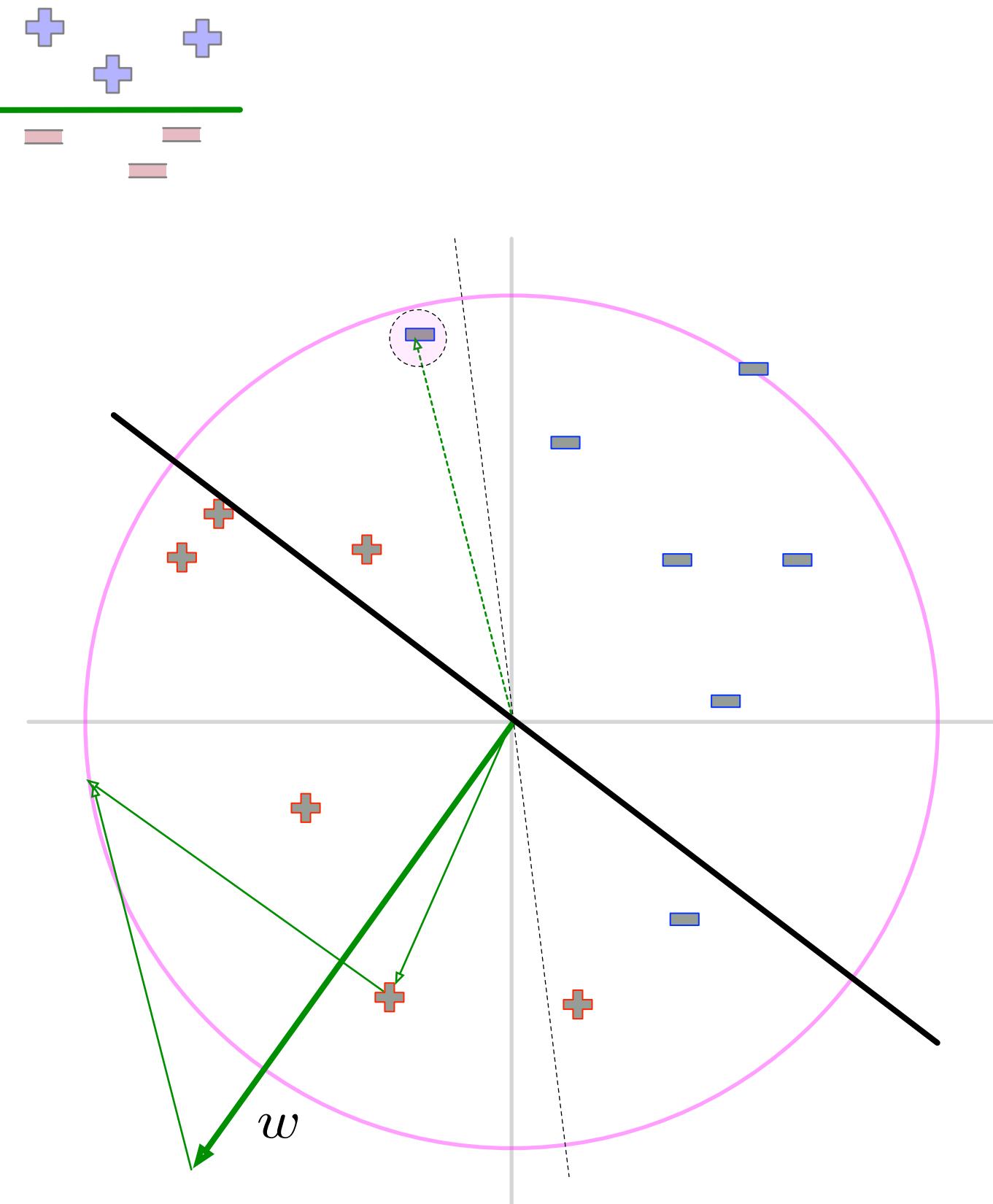
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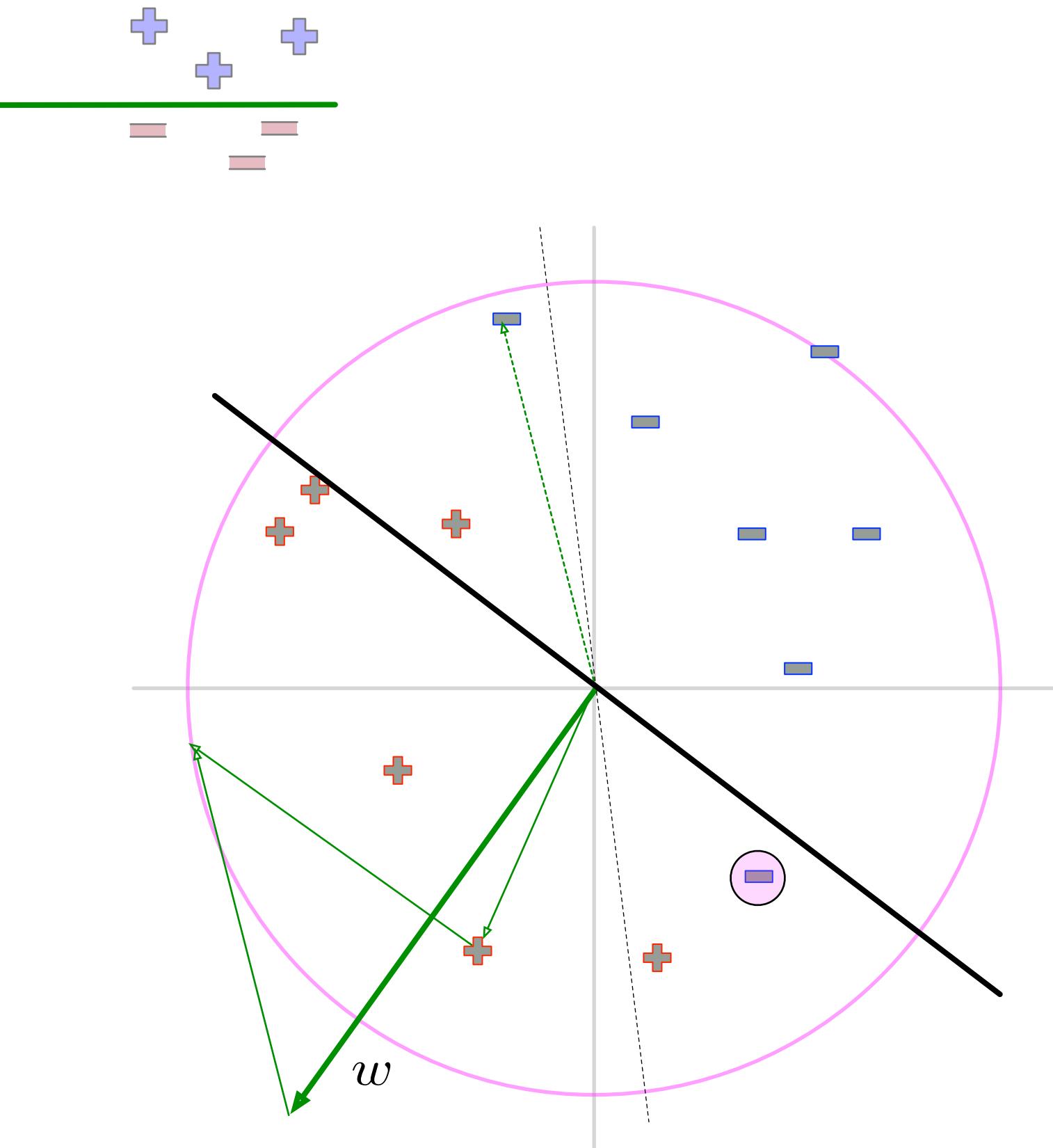
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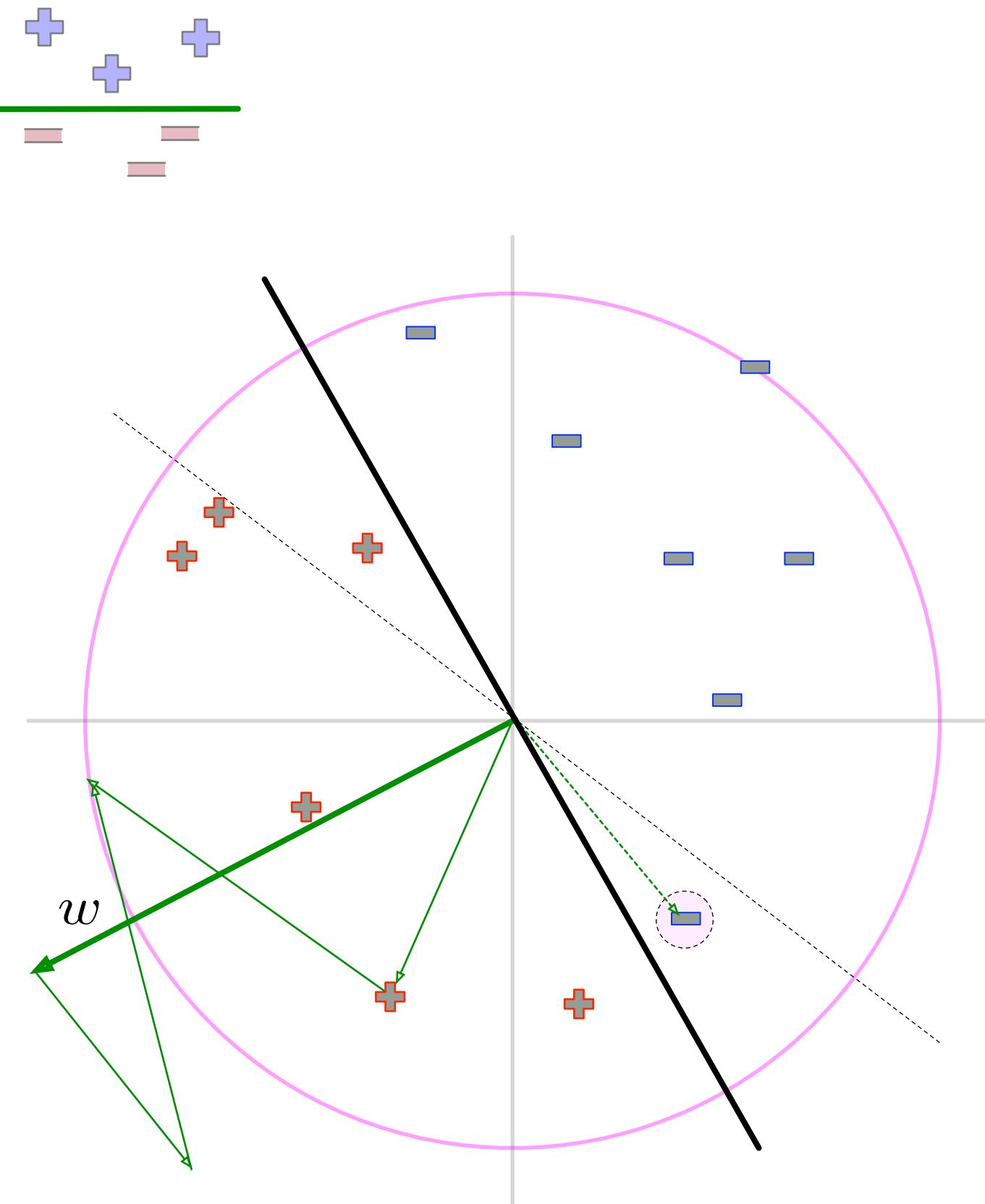
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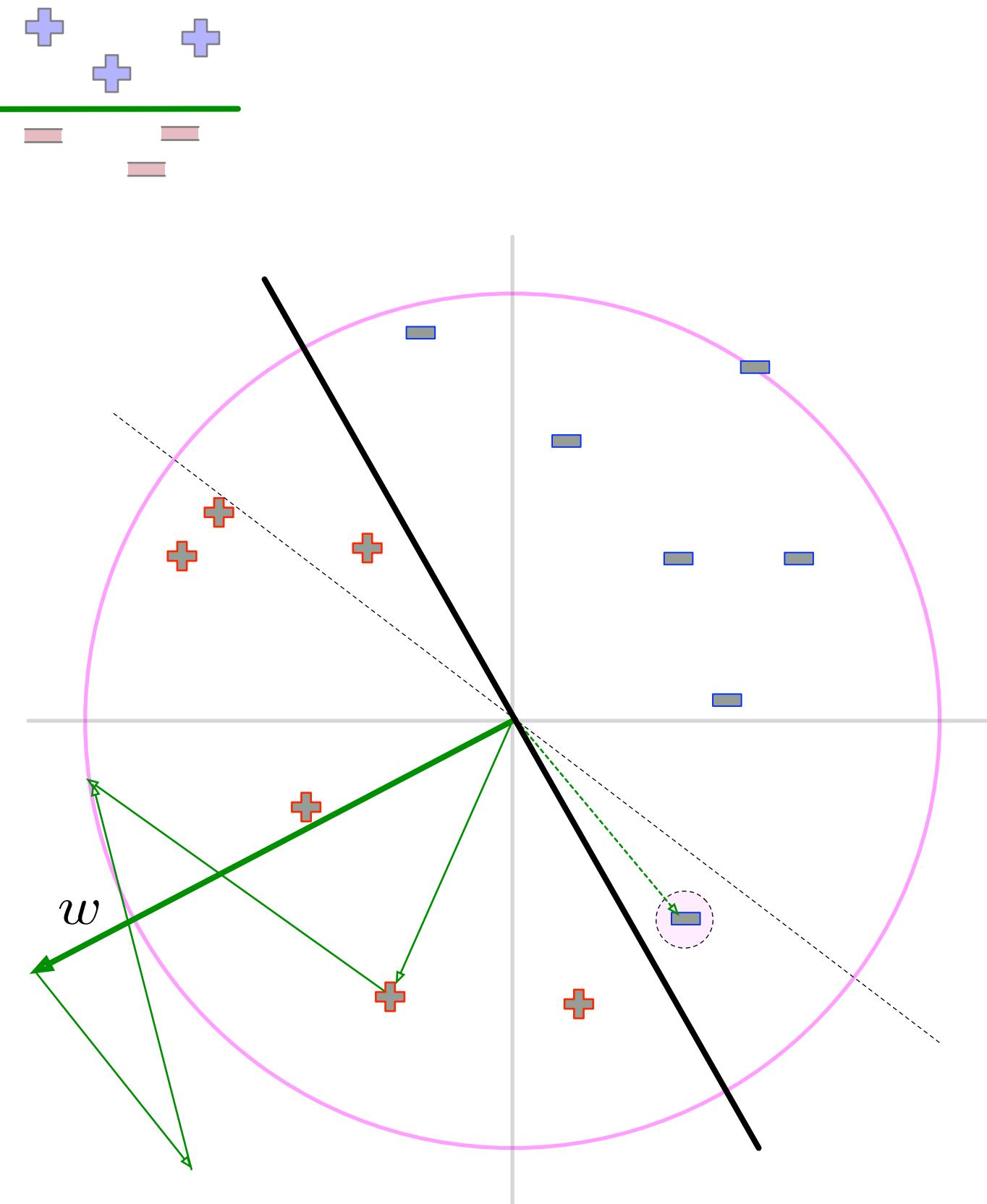
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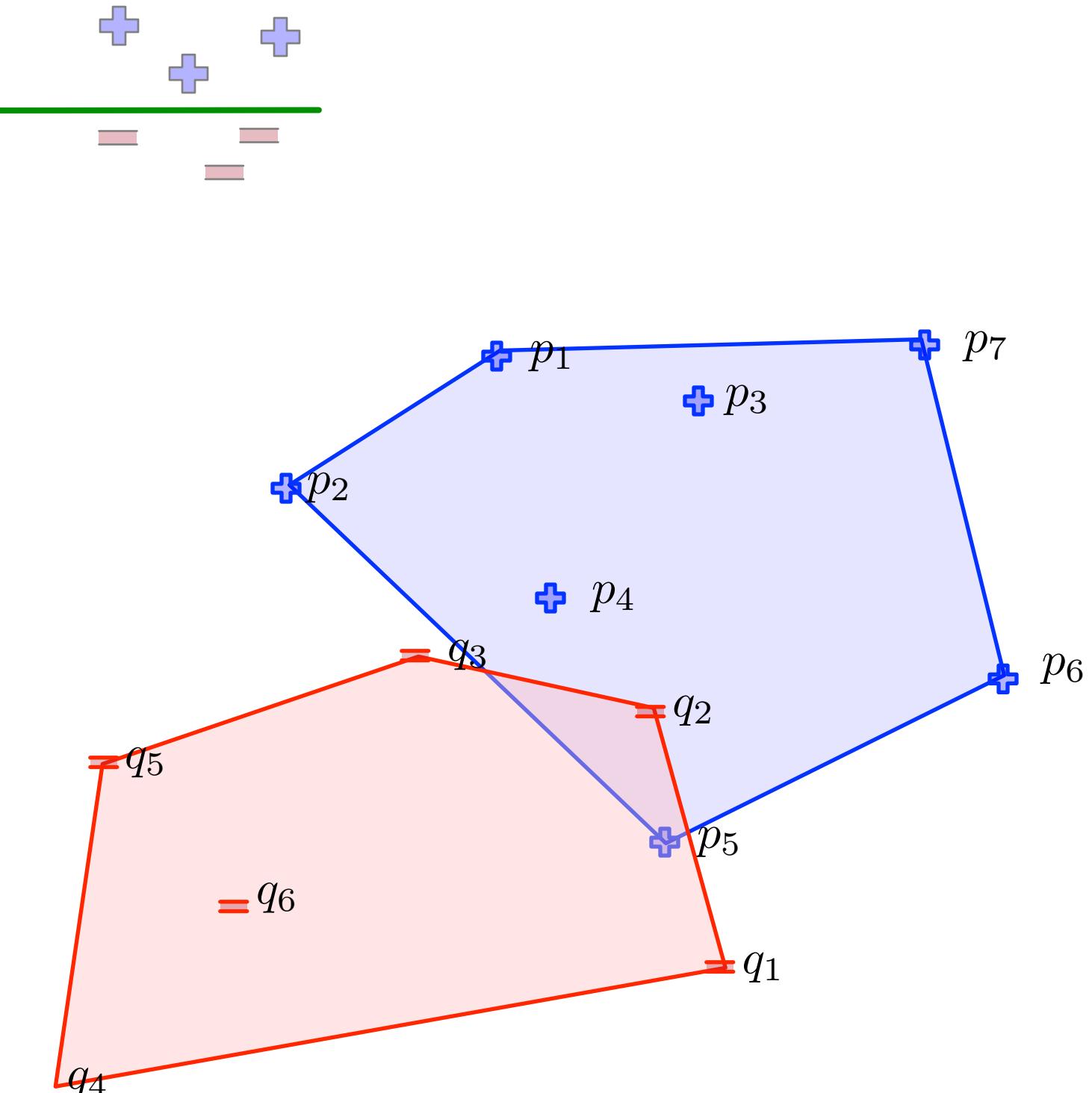
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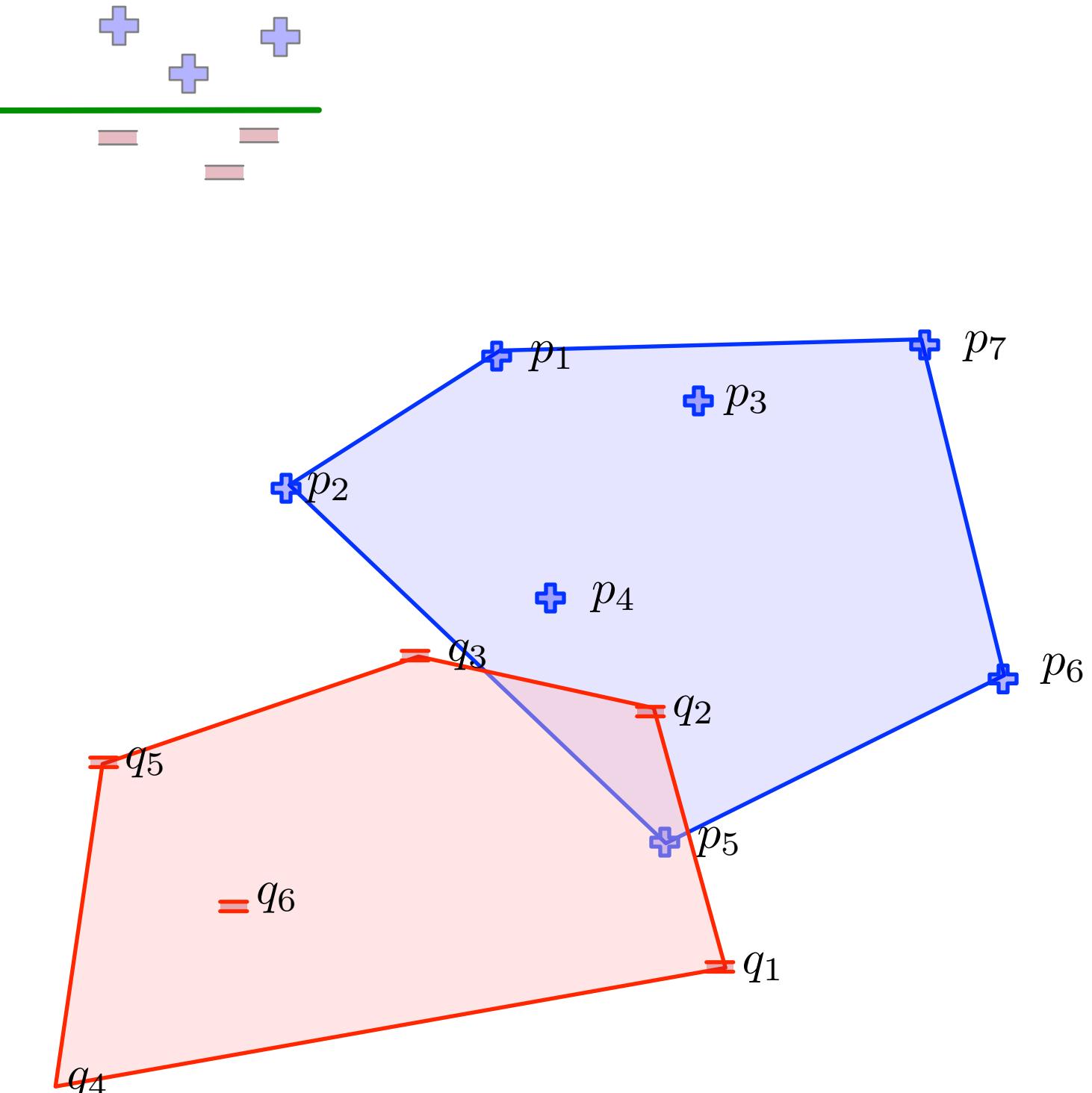
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**(1) kernels**

**(2) penalize it**



# Kernel Perceptron Algorithm

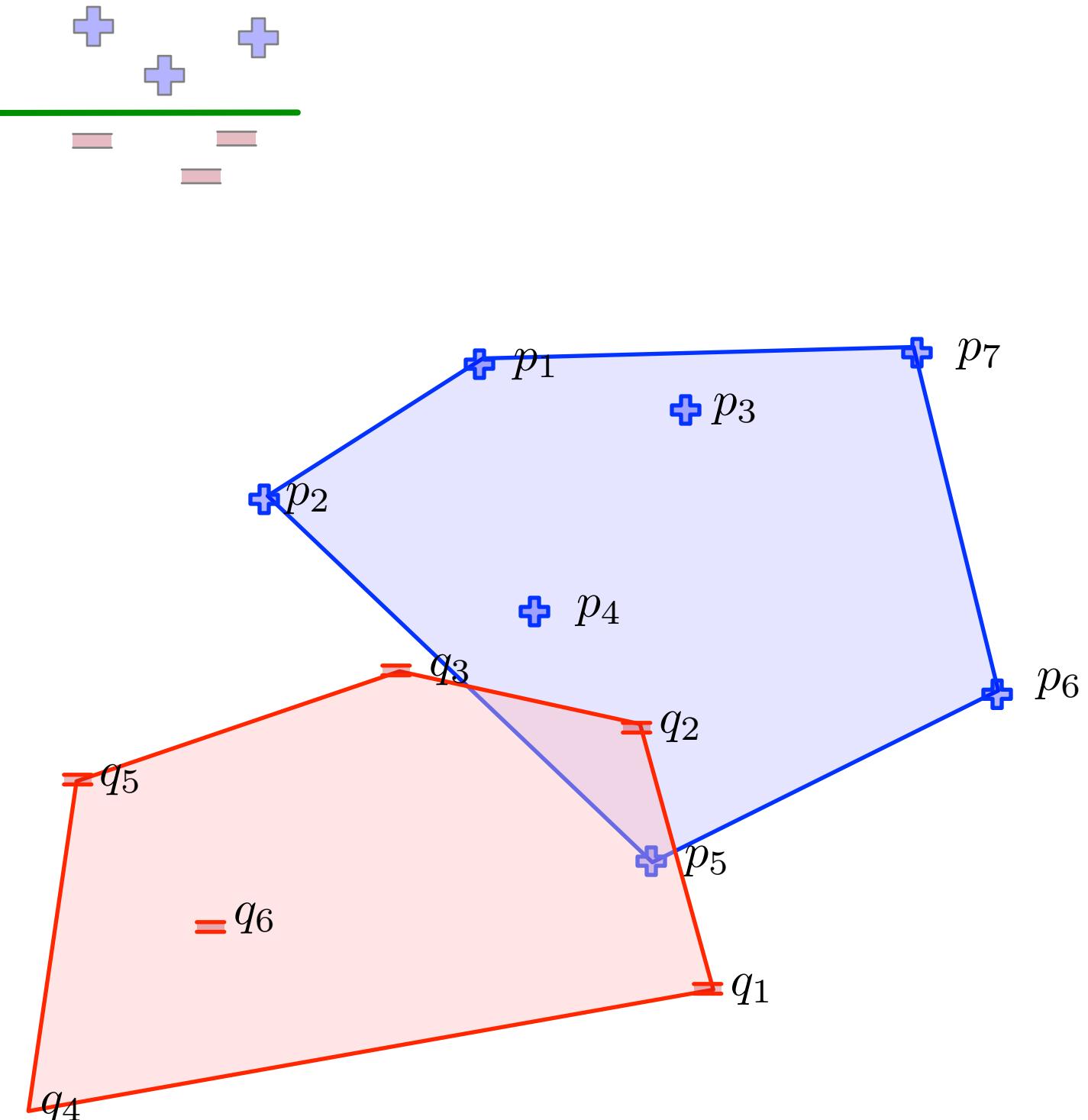
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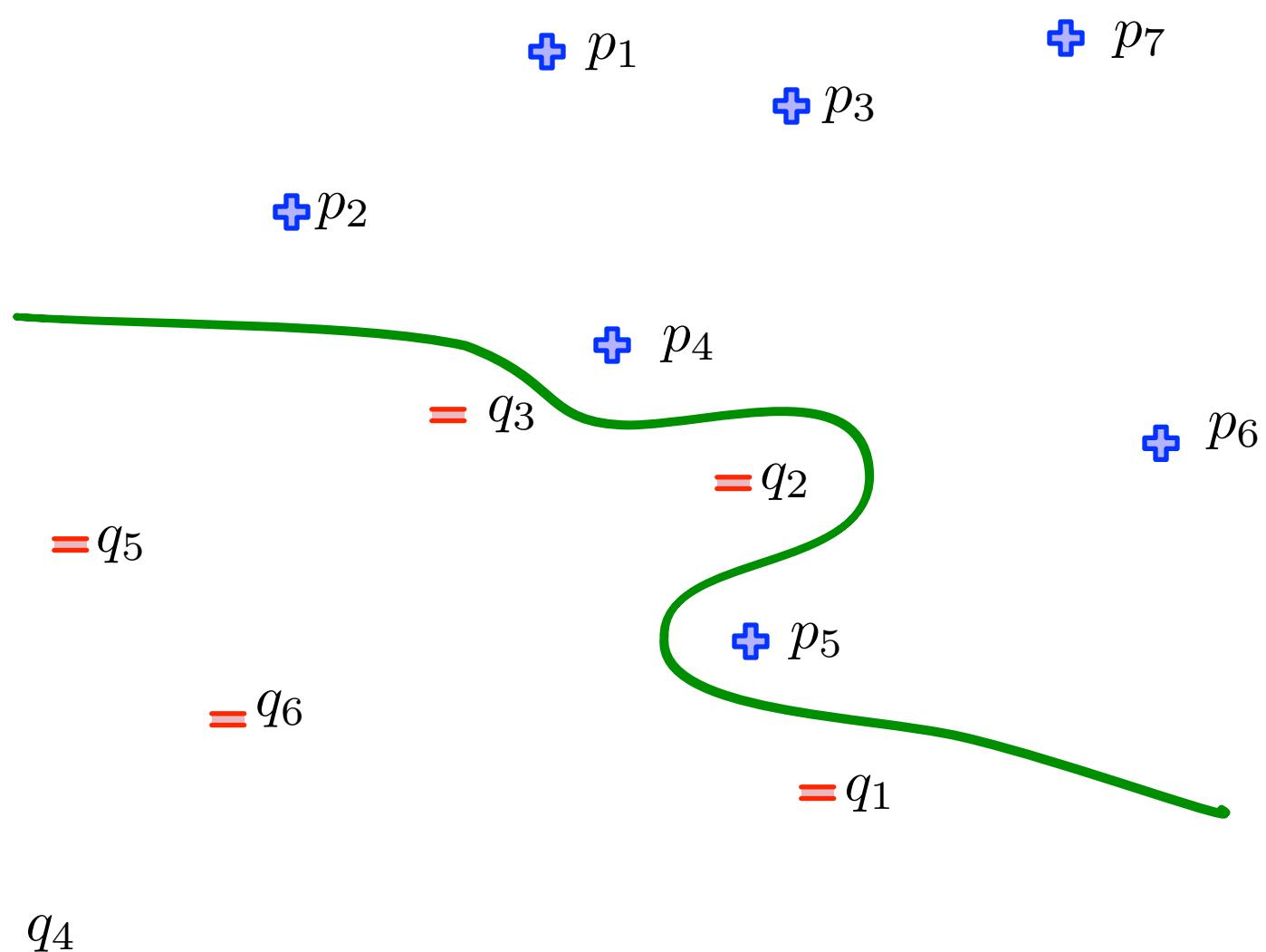
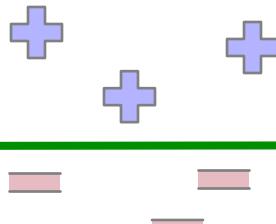
$x' = \arg \min \sigma(x)K(x, w)$

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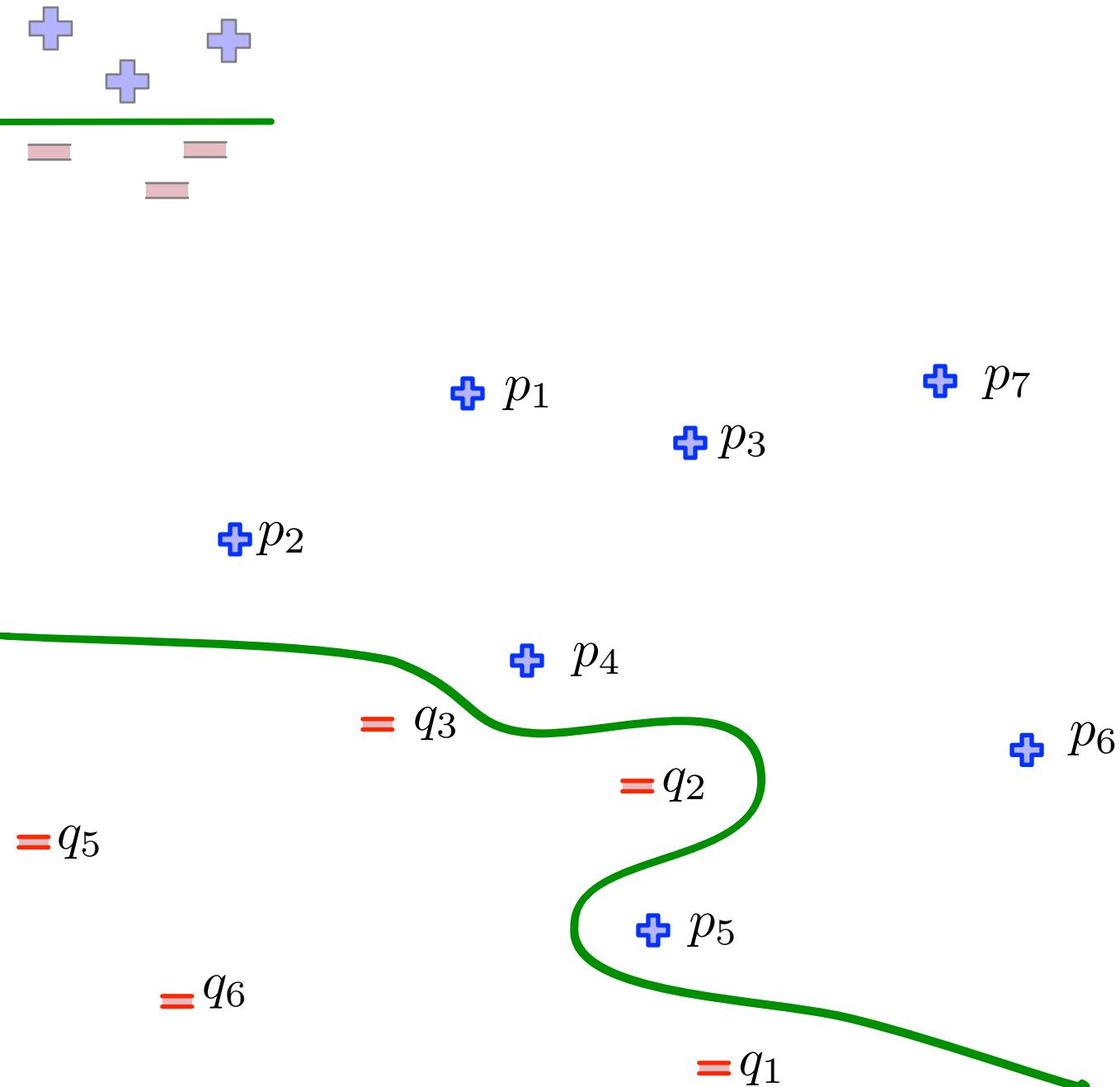
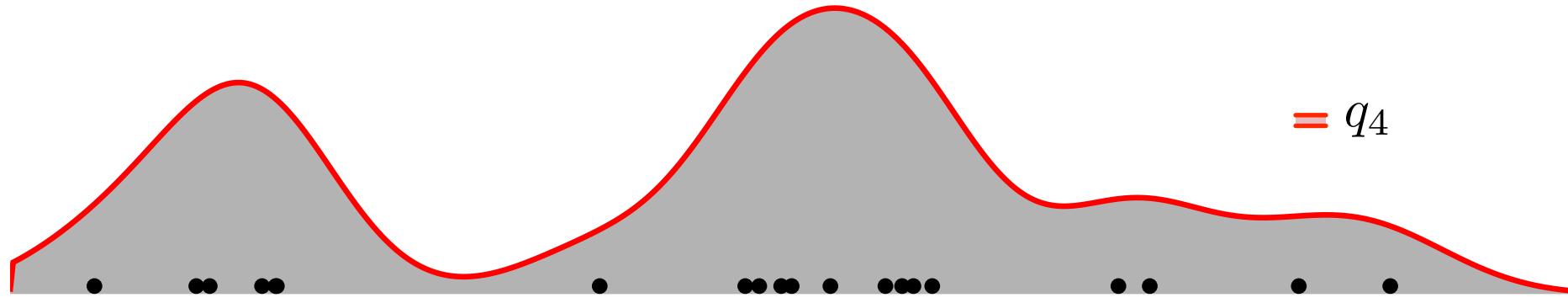
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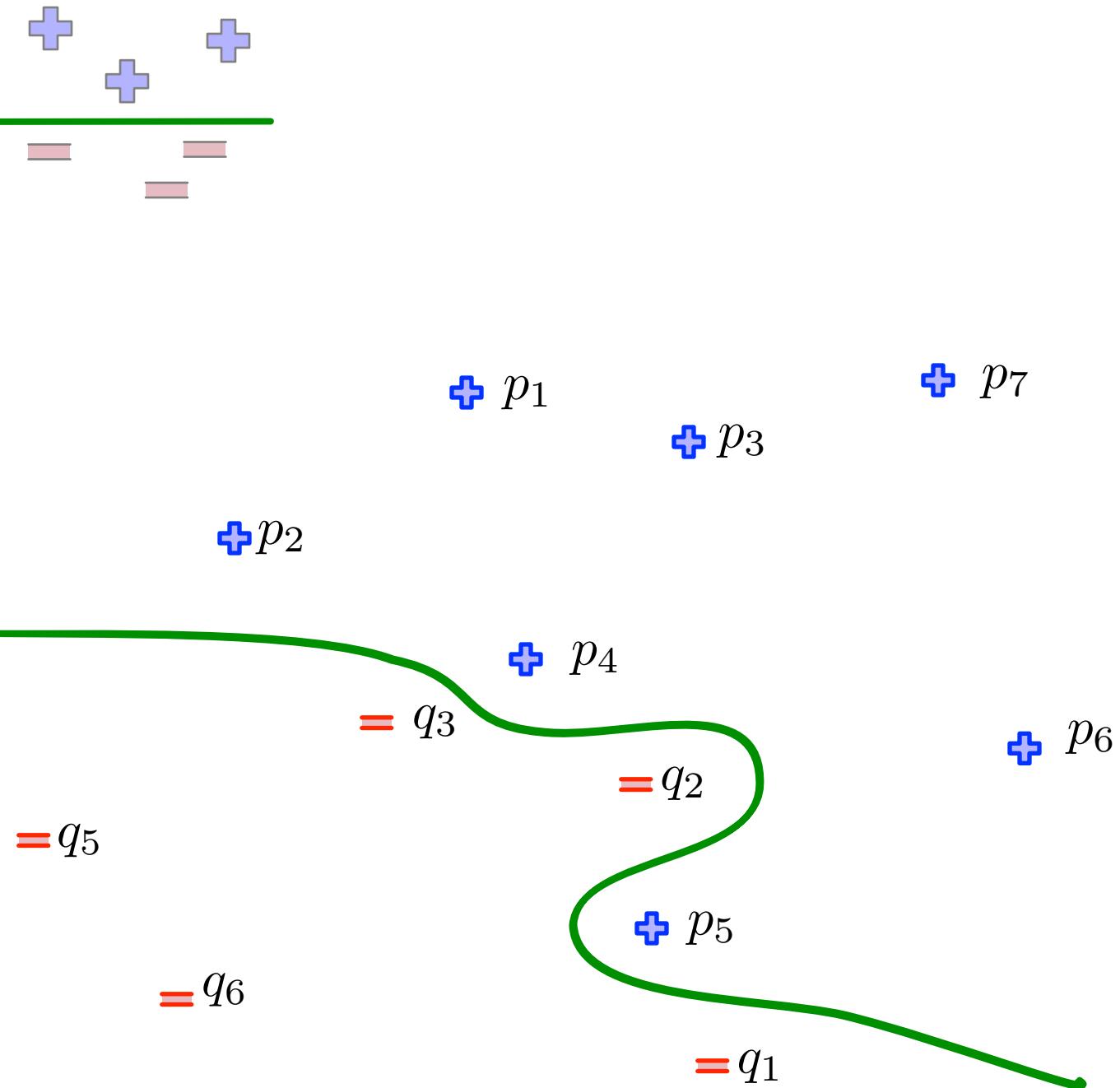
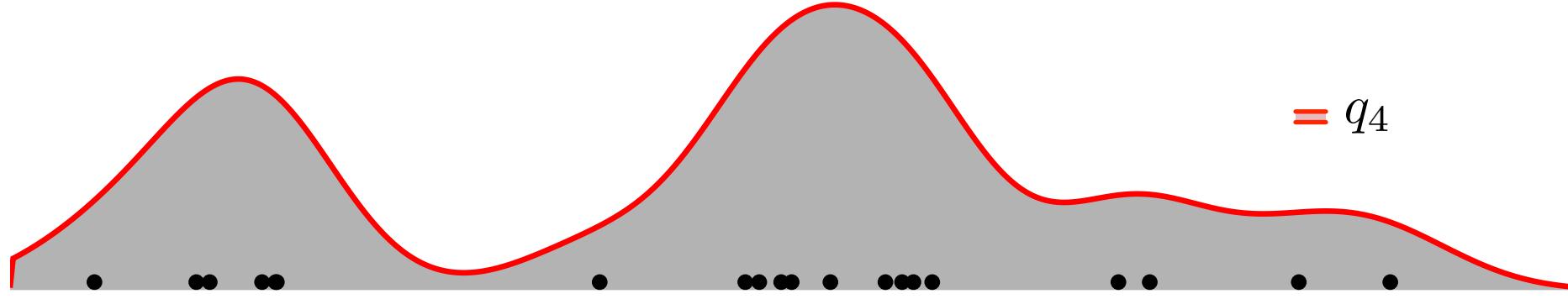
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# Sketched Kernel SVM Algorithm

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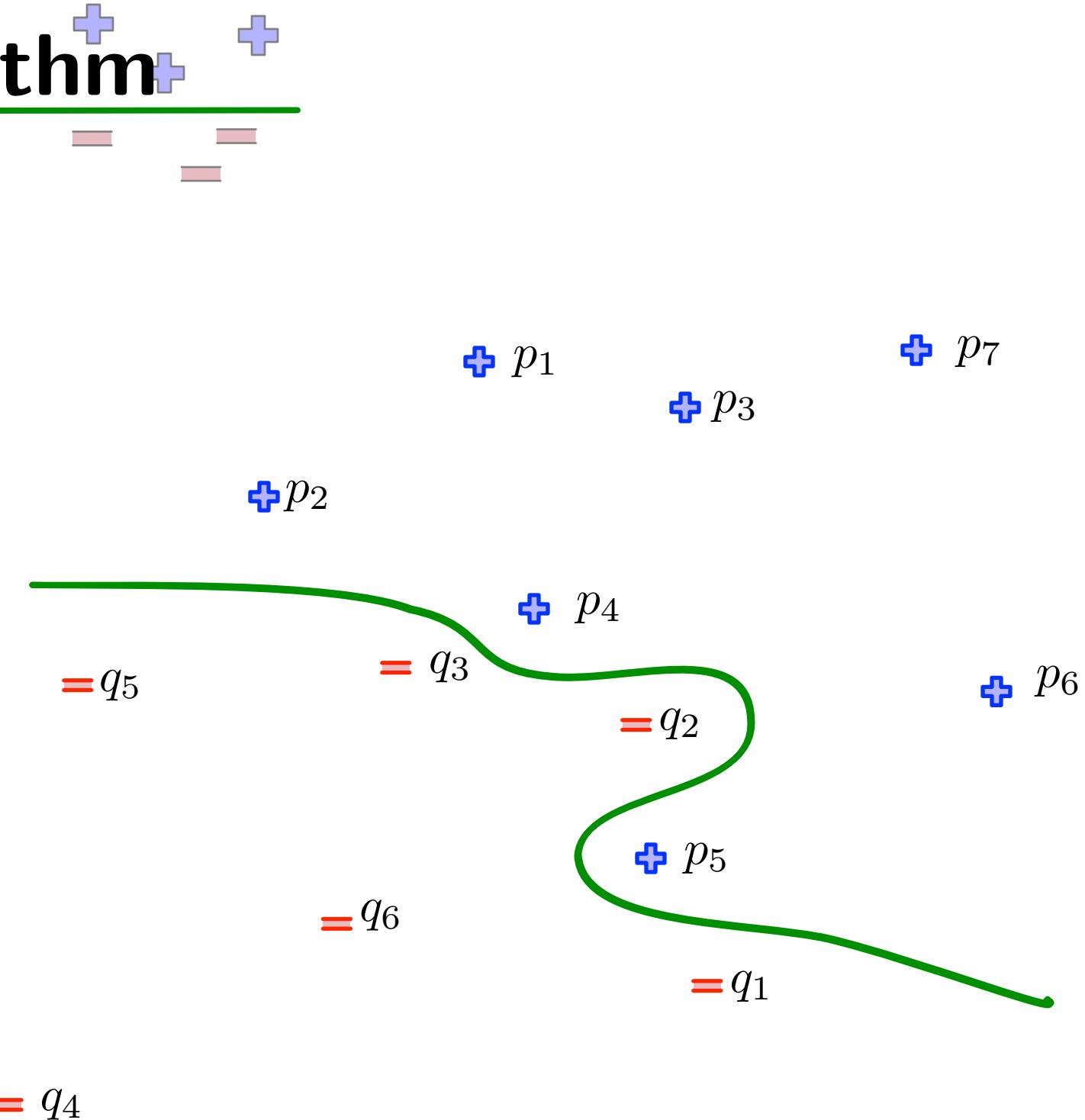
Define mapping  $\phi : X \rightarrow \mathbb{R}^\rho$

choose  $w = \sigma(x)\phi(x)$

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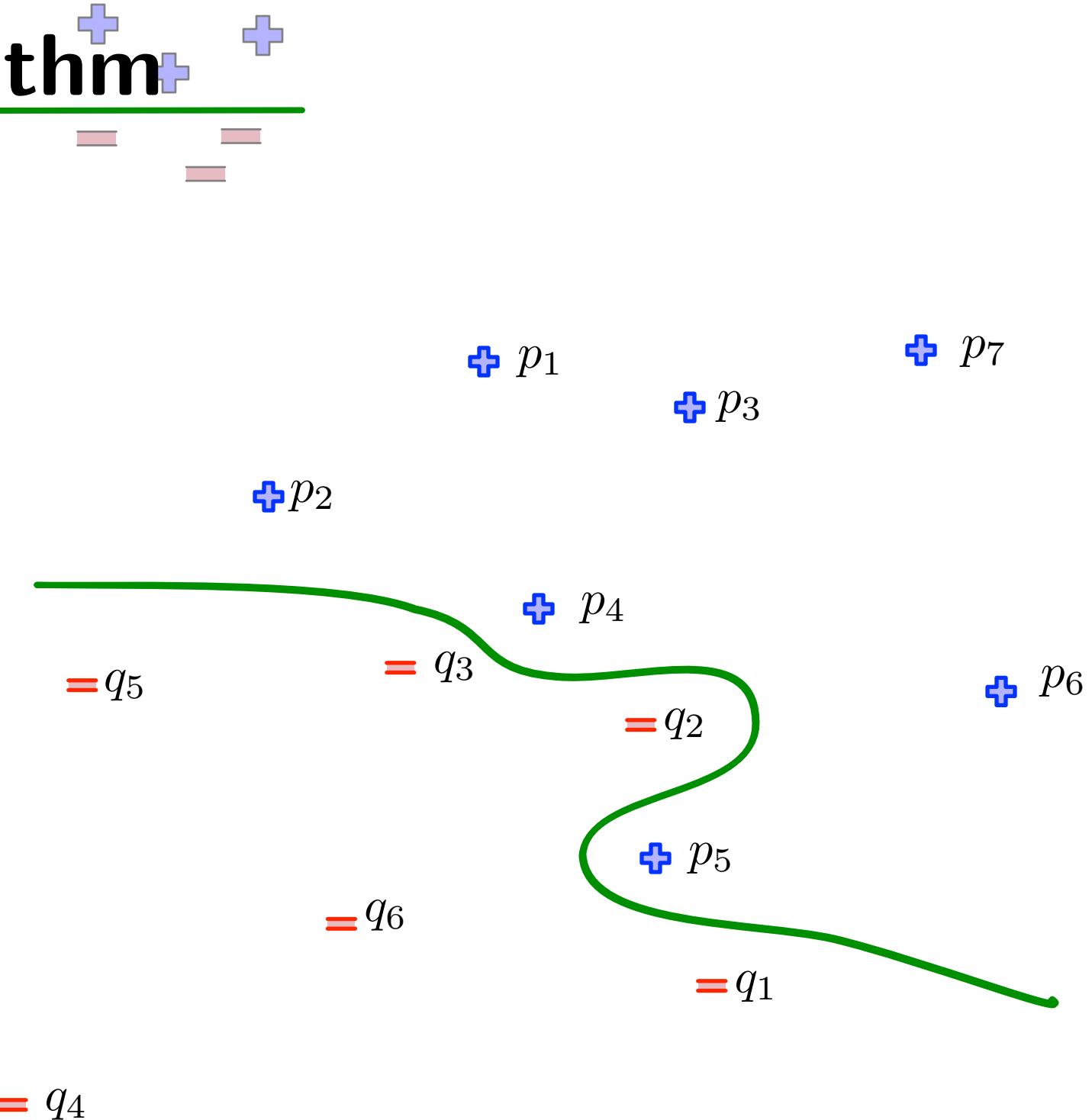
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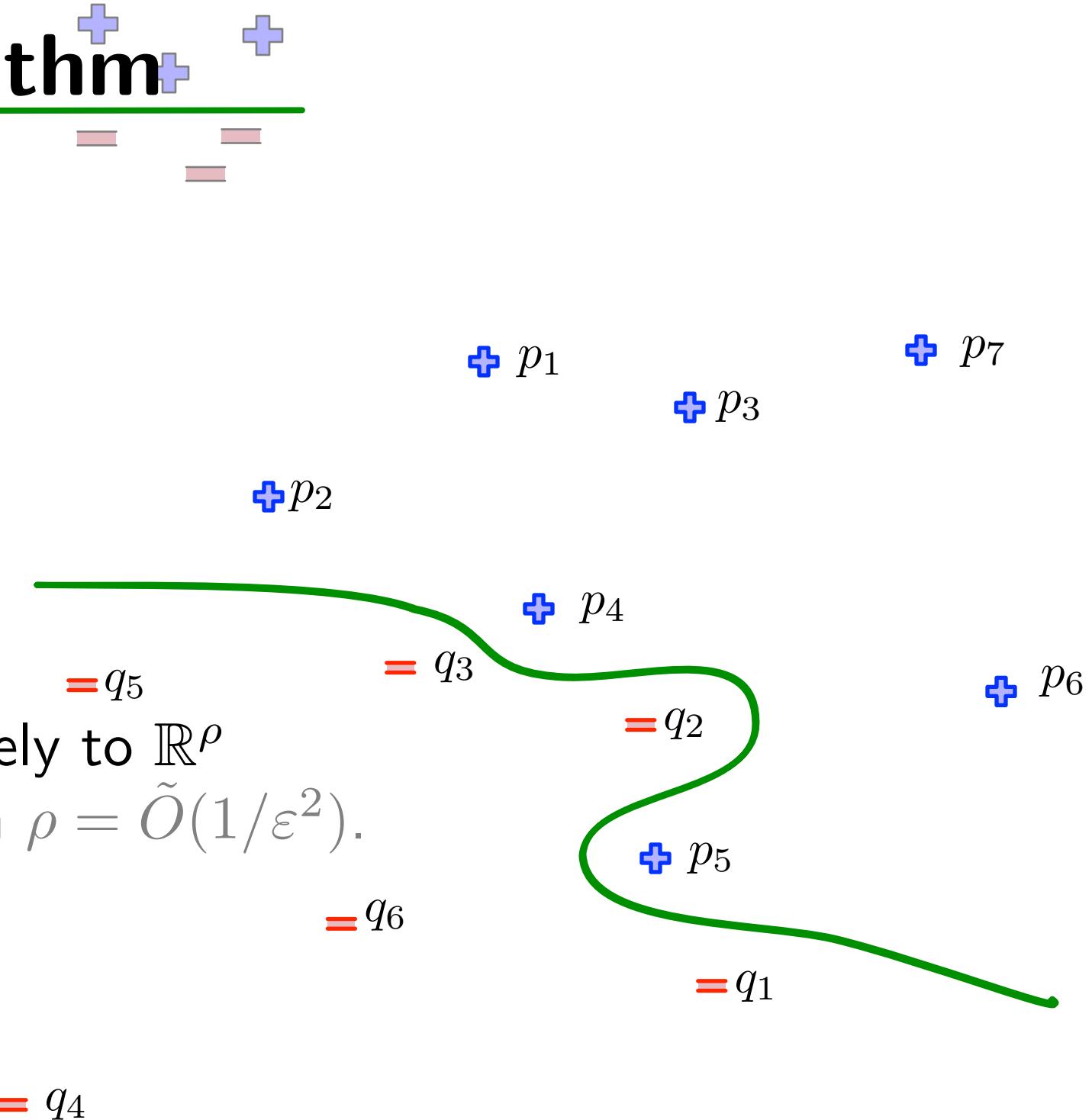
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e.g., Rahimi+Recht [NeurIPS07] additive  $\varepsilon$  in  $\rho = \tilde{O}(1/\varepsilon^2)$ .



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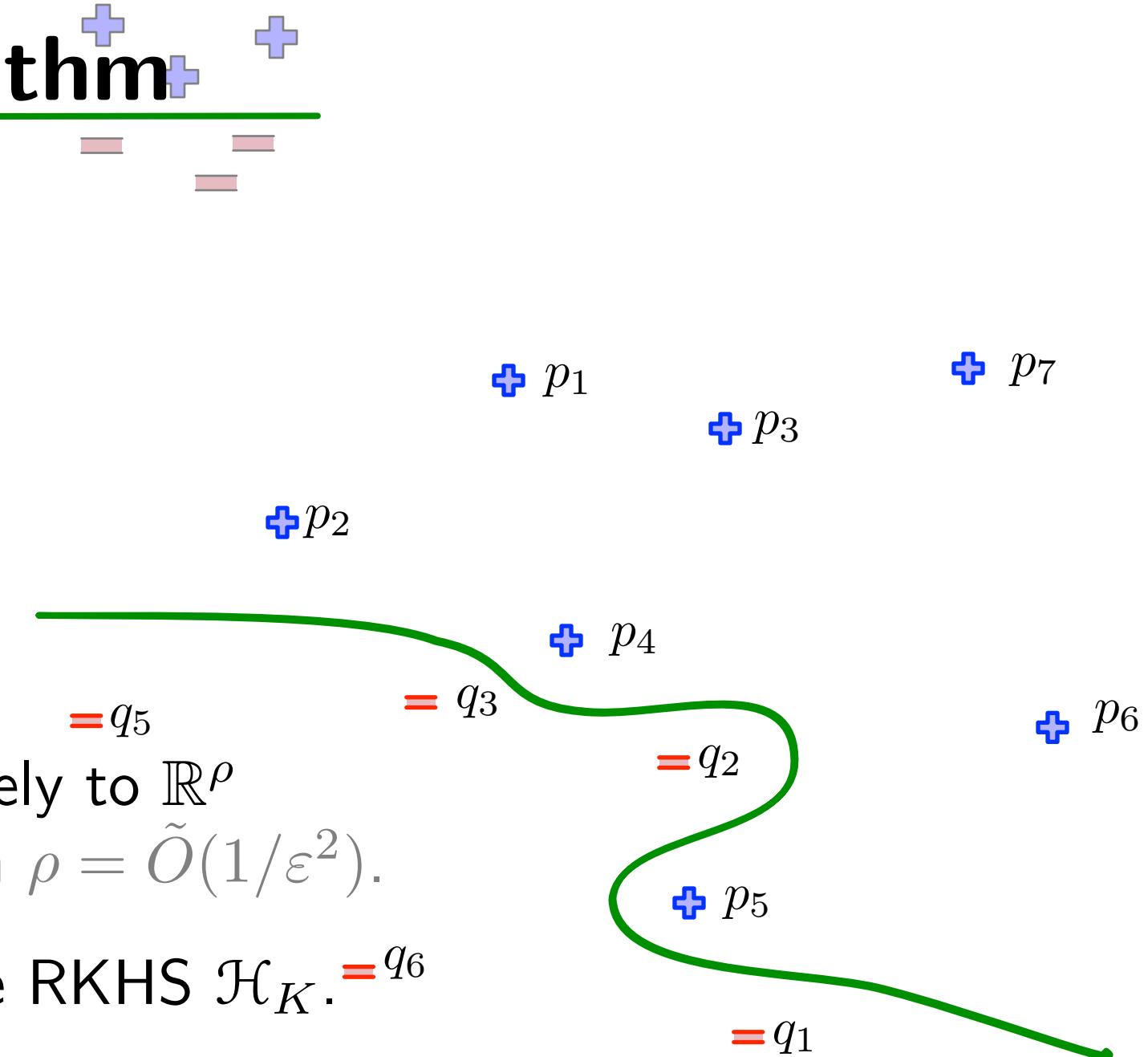
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$\phi(x) = K(x, \cdot)$  is a element of function space RKHS  $\mathcal{H}_K$ .  $= q_6$

kernel density estimate:

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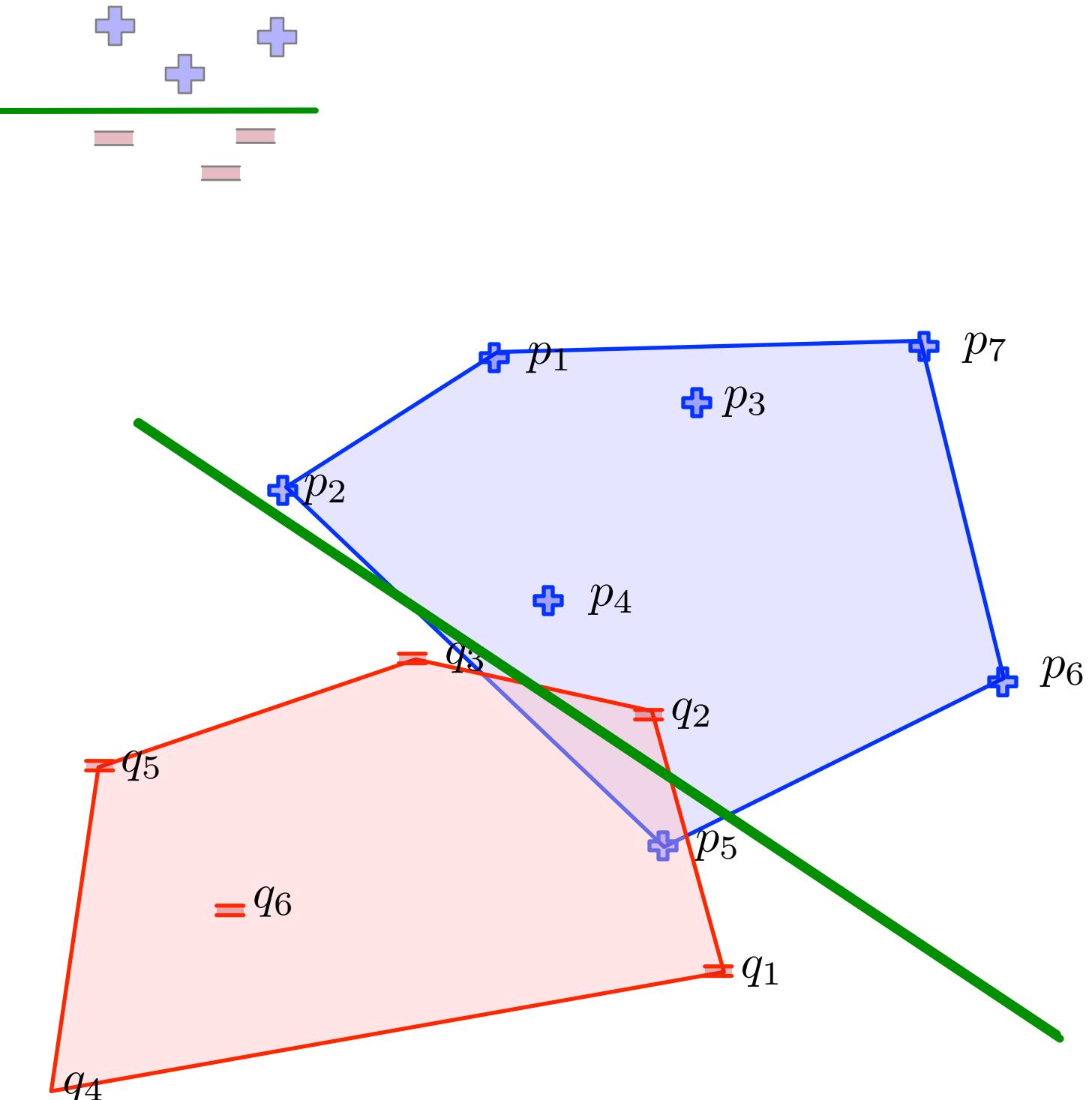
# Loss Functions

Set up penalty for misclassified points

$$f_X(w) = \sum_{x \in X} \ell(w, x) + \text{prior}(w)$$

loss  $\ell_i = \ell(w, x_i) = \ell(z_i)$

with  $z_i = \sigma(x_i) \langle w, x_i \rangle$



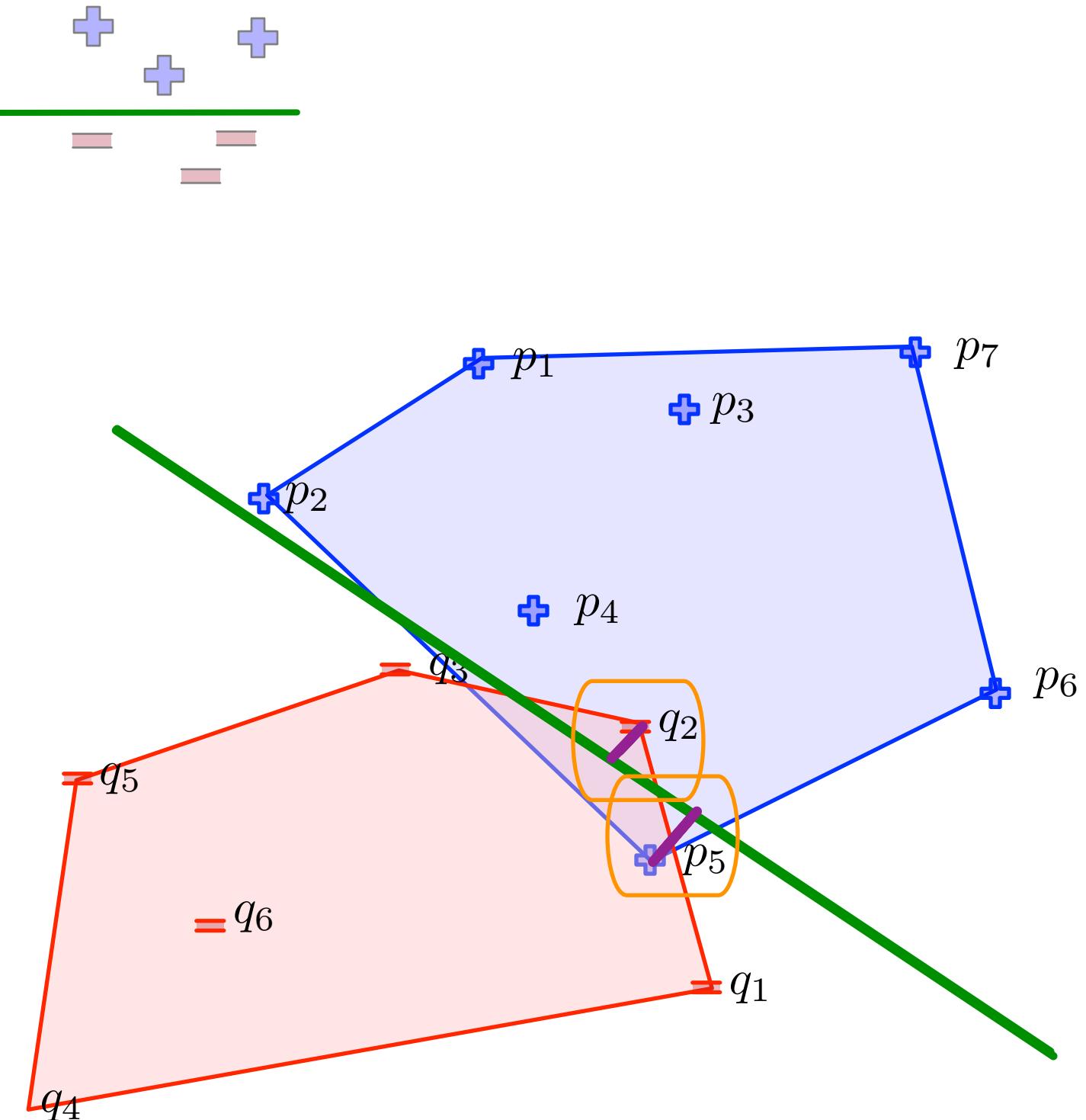
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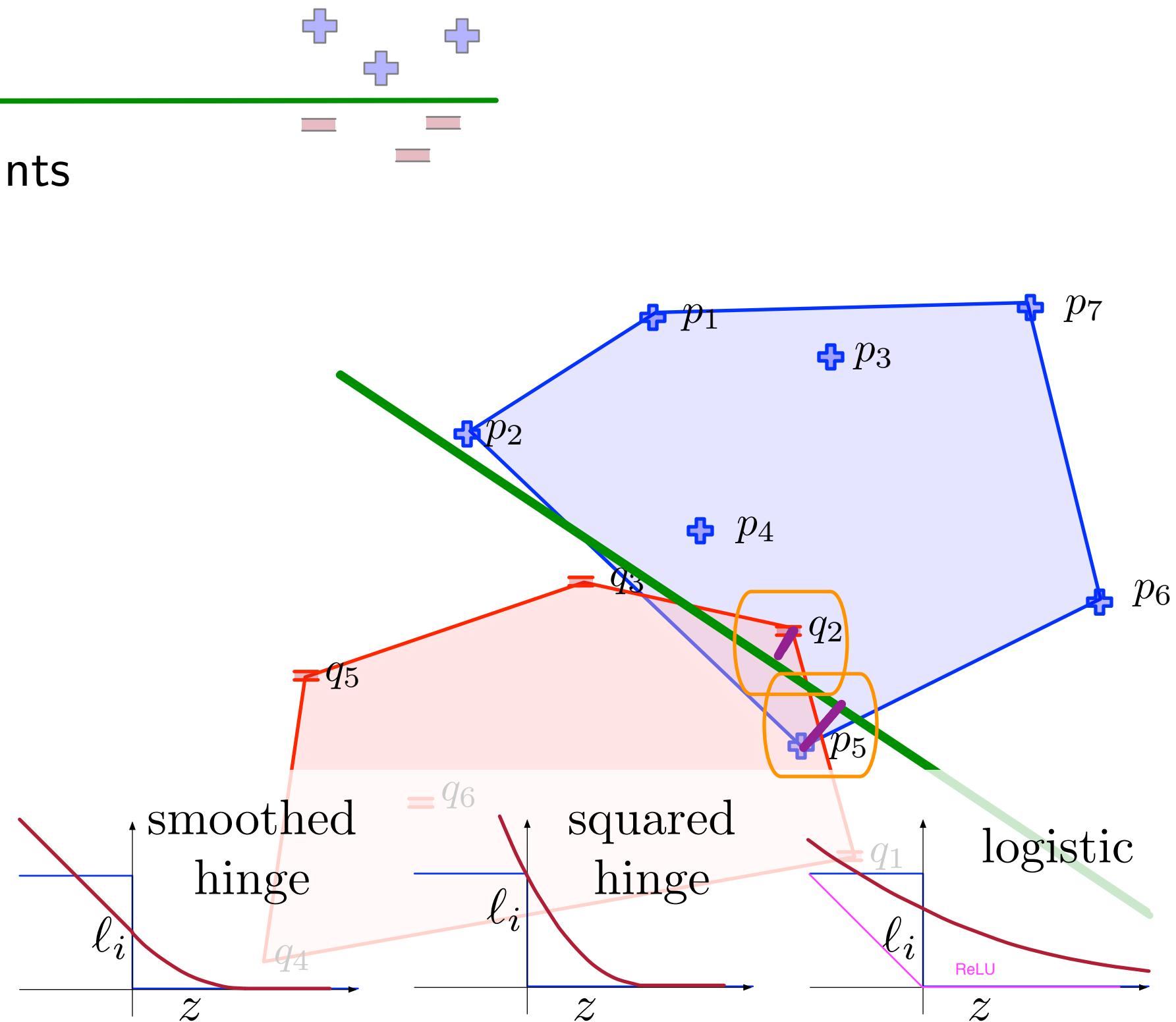
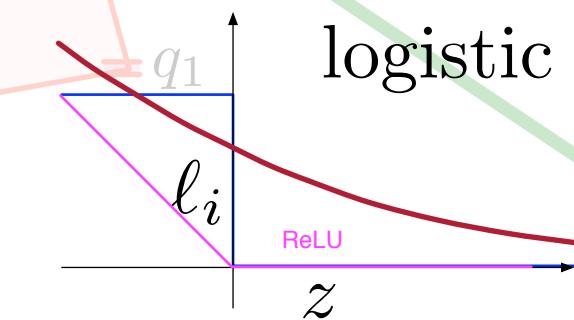
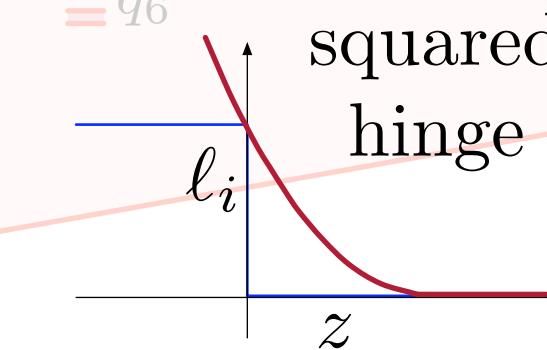
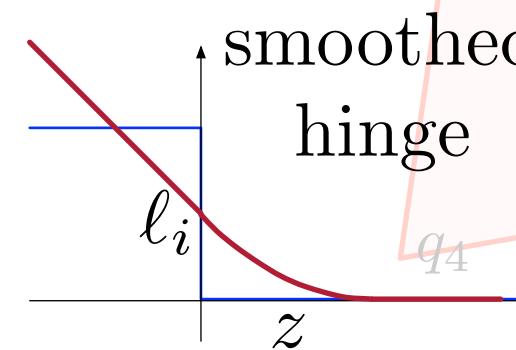
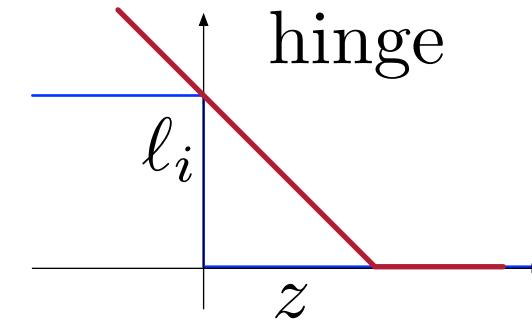
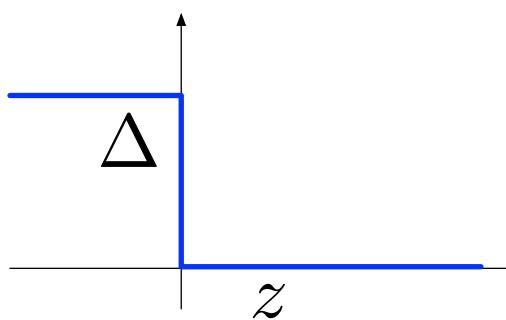
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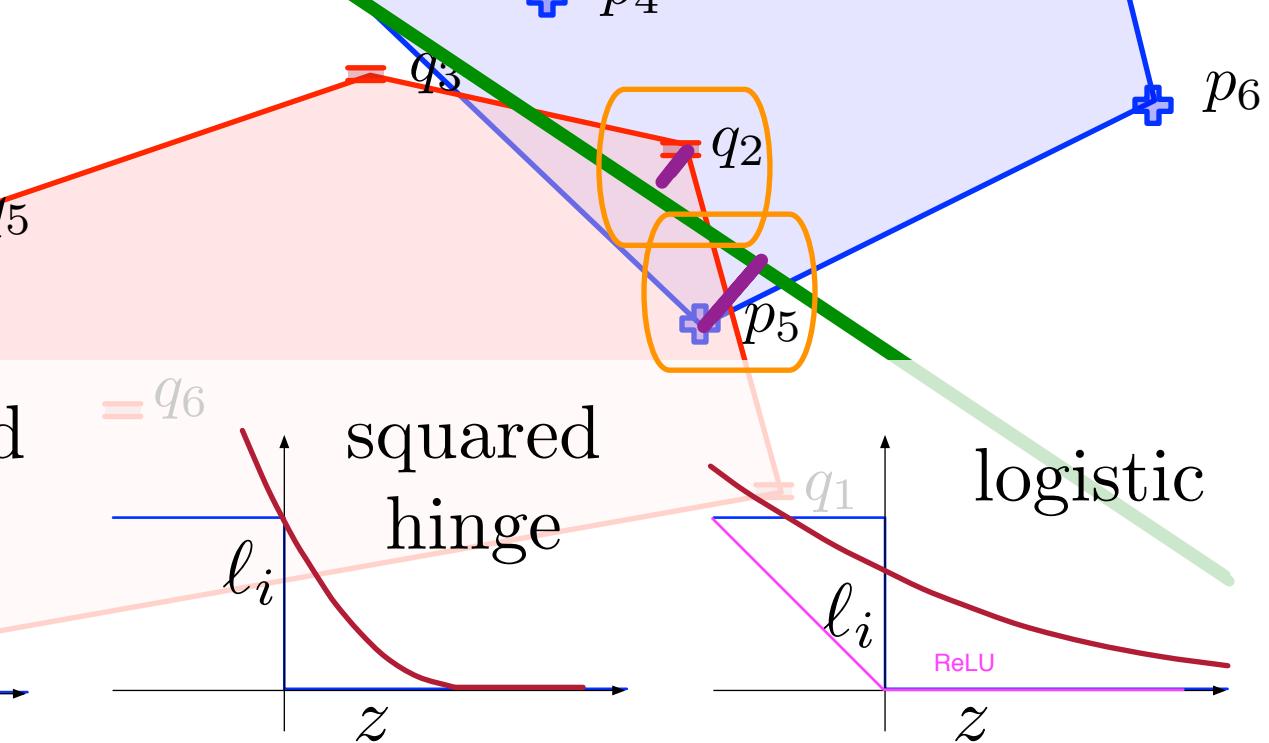
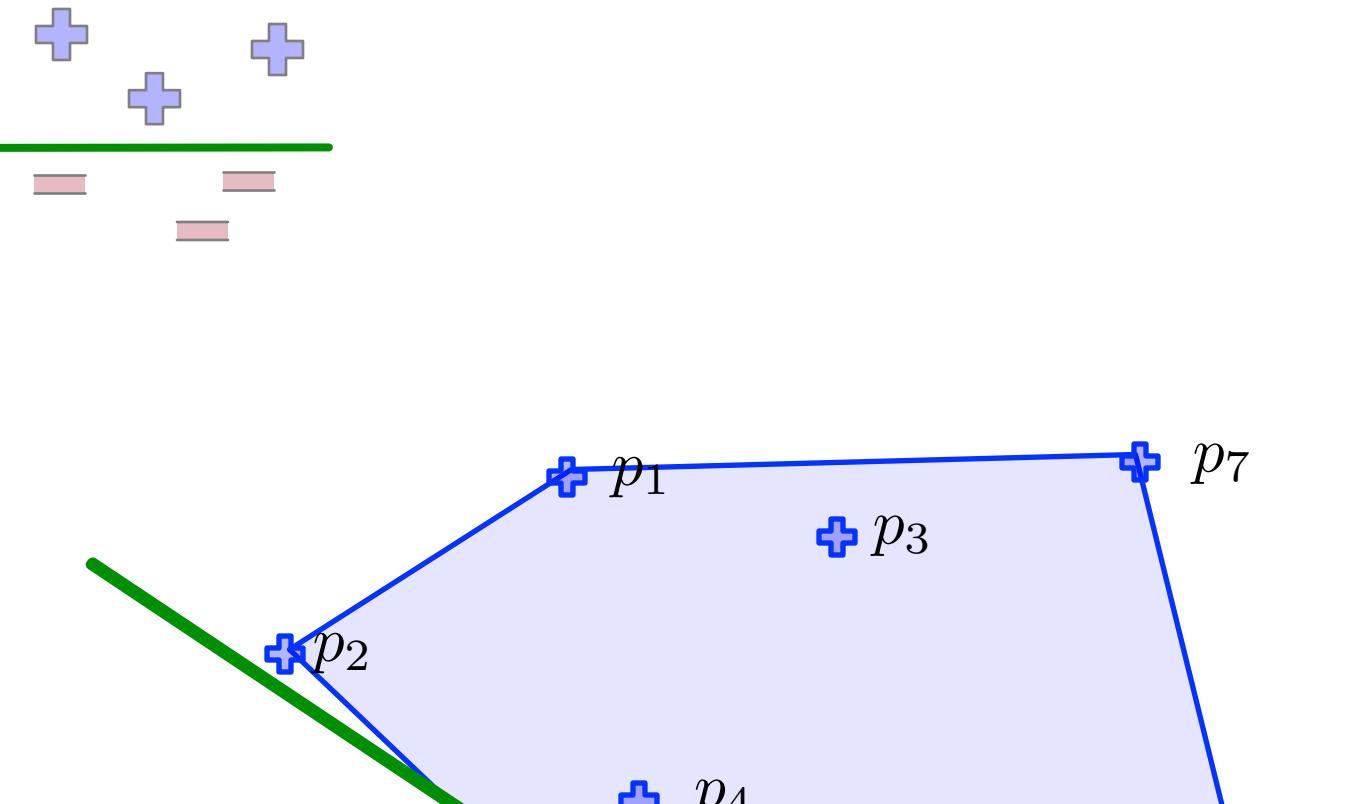
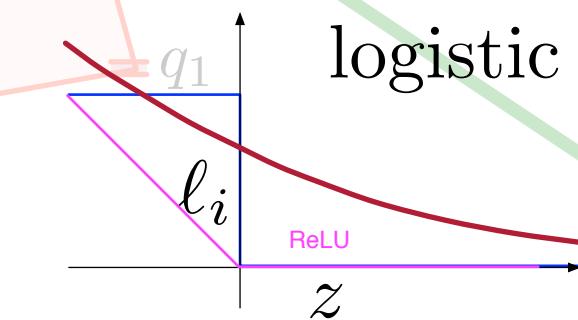
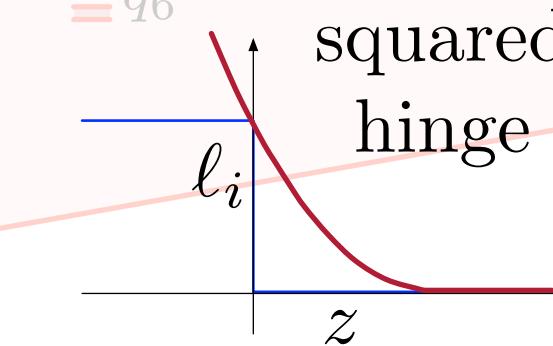
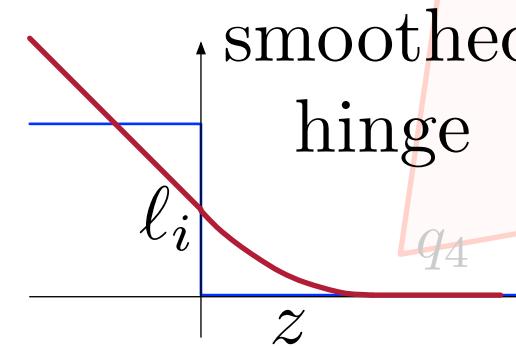
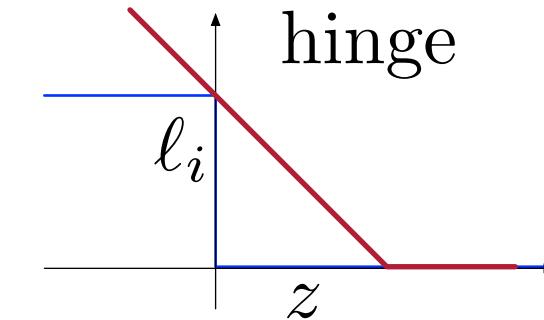
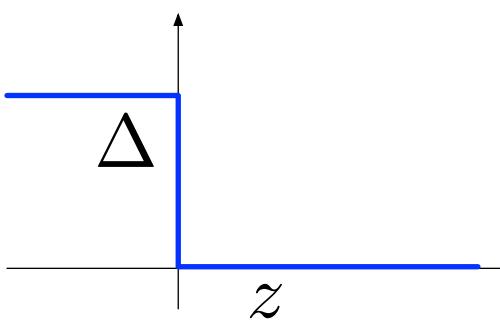
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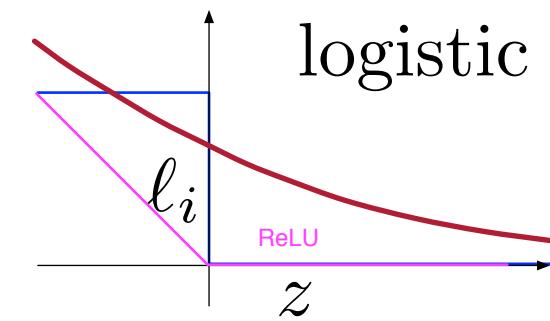
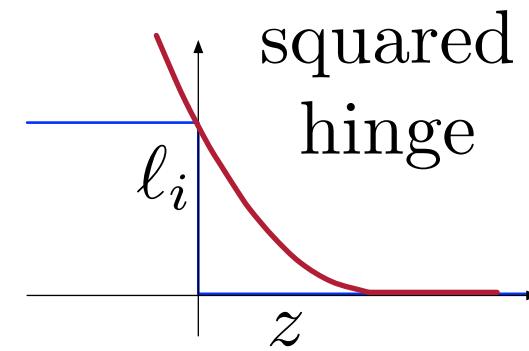
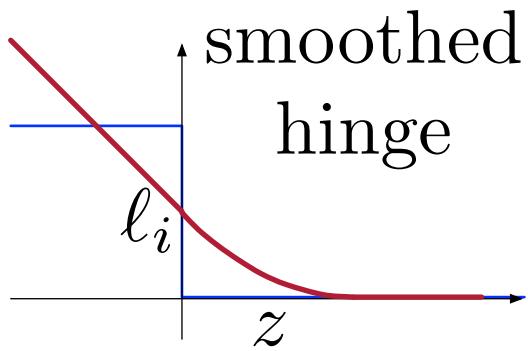
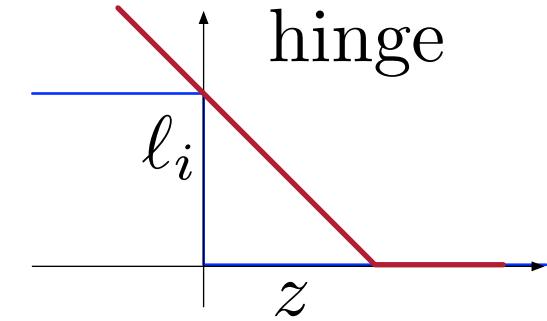
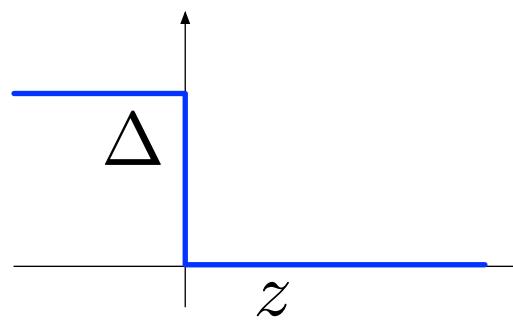
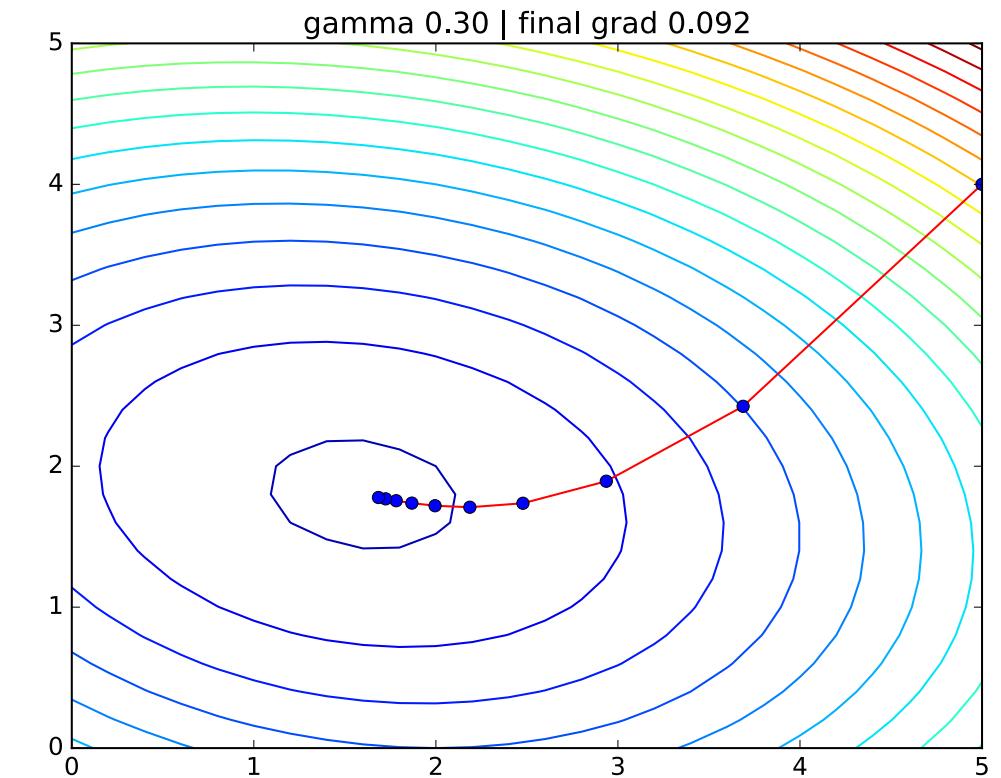
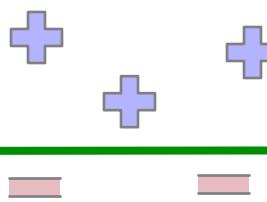
with  $z_i = \sigma(x_i) \langle w, x_i \rangle$

If linear or  $K$  is pd  
then  $f_X$  is **convex**

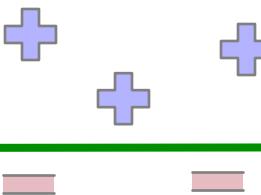


# Coresets for Optimization

Solve for  $w^* = \arg \min_w f_X(w)$  ... gradient descent



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Subgradient Descent  $\approx$  Frank-Wolfe

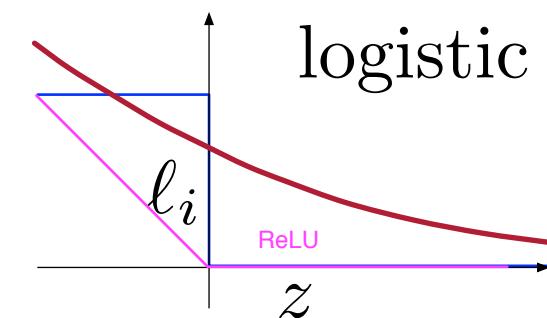
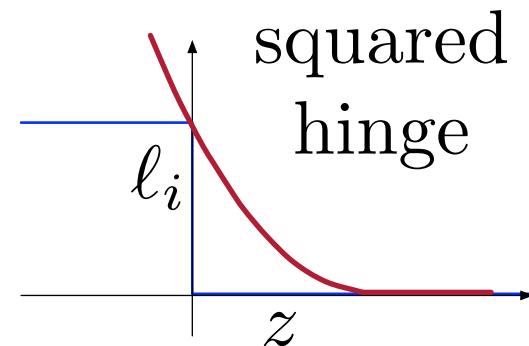
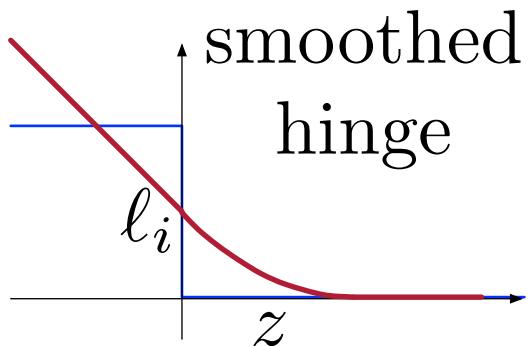
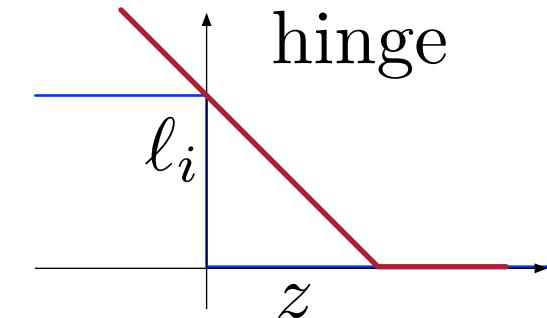
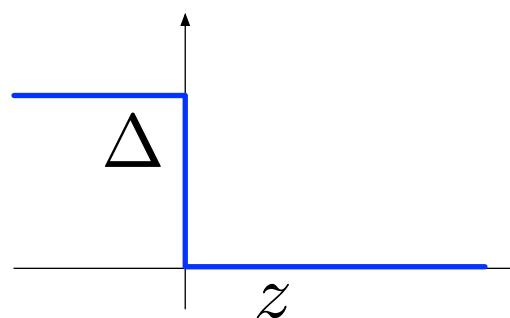
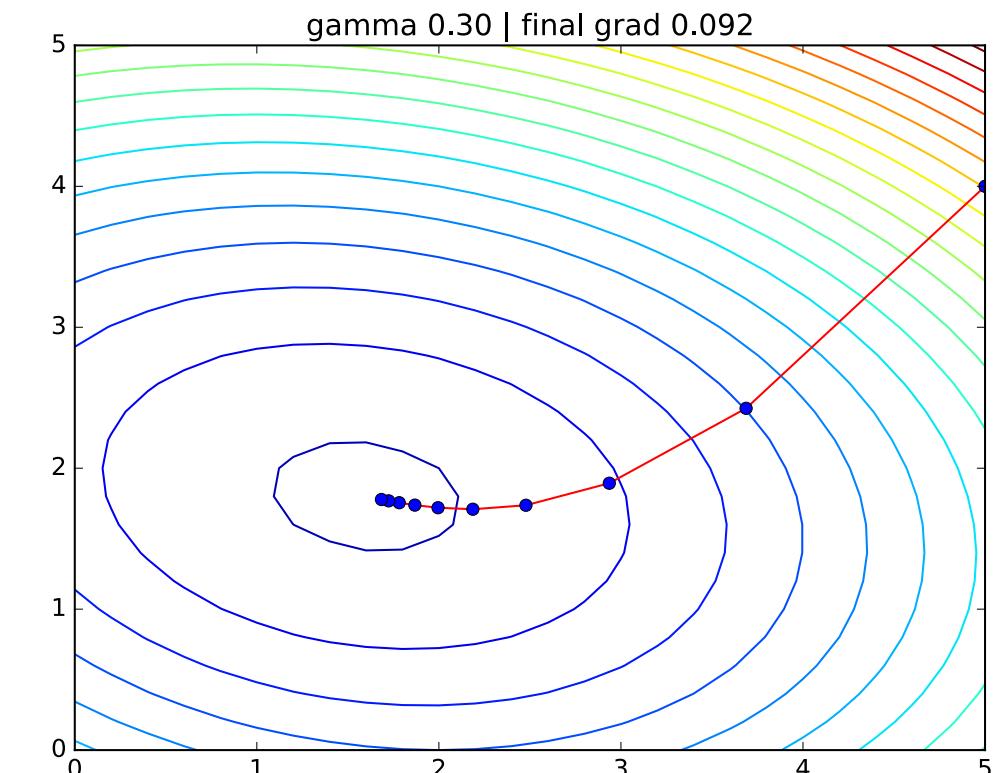
Move towards most helpful point

$O(C/\varepsilon^2)$  steps to  $\pm\varepsilon$  mean for  $\|x\| \leq 1$ .

Stochastic gradient descent (SGD)

For large  $X$ , most common

Randomly chooses  $x \in X$ , and step towards  $-\nabla f_x(w)$ .



# VC-dimension and Sample Complexity

Assume: *data  $X$  is drawn iid from  $\mu$ .*

Build: classifier  $g : \mathbb{R}^d \rightarrow \{-1, +1\}$  so  $\mathbf{E}_{x \sim \mu}[\mathbf{1}(g(x) = \sigma(x))]$ .

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*how much accuracy is preserved under random sampling?*

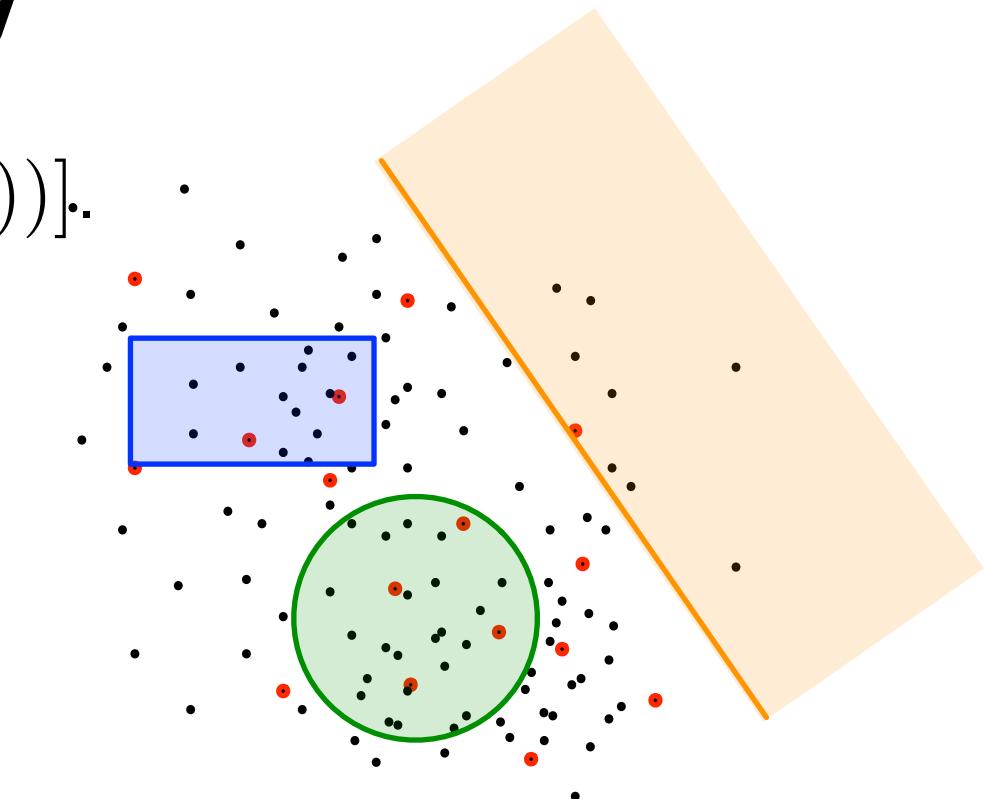
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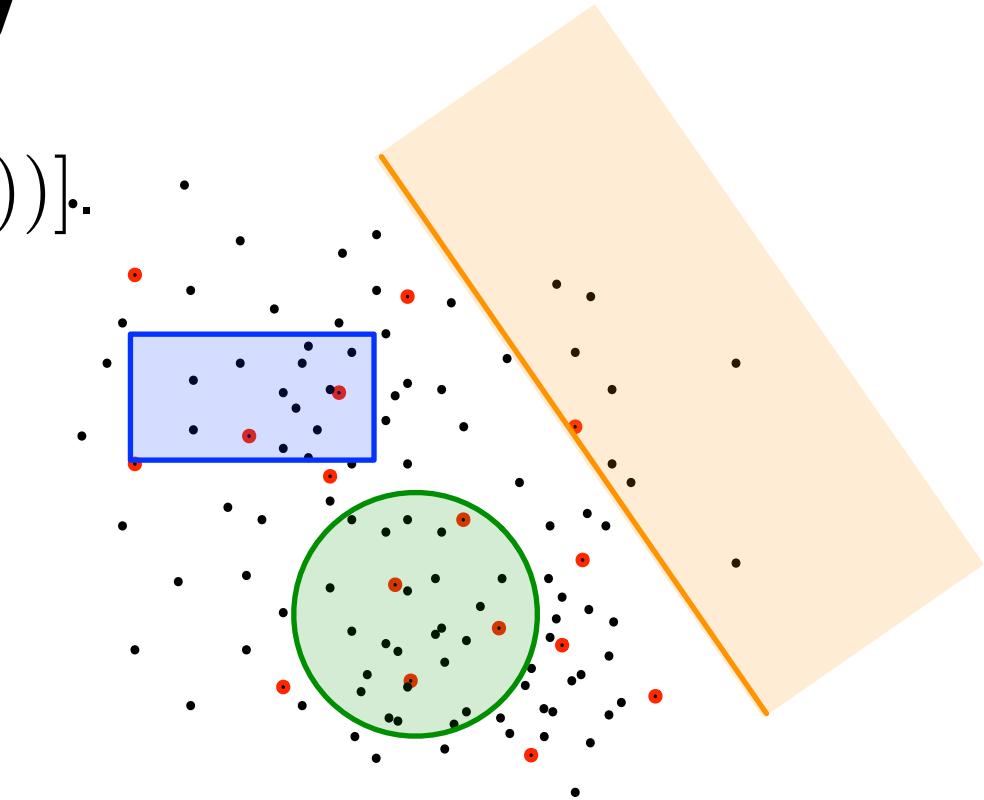
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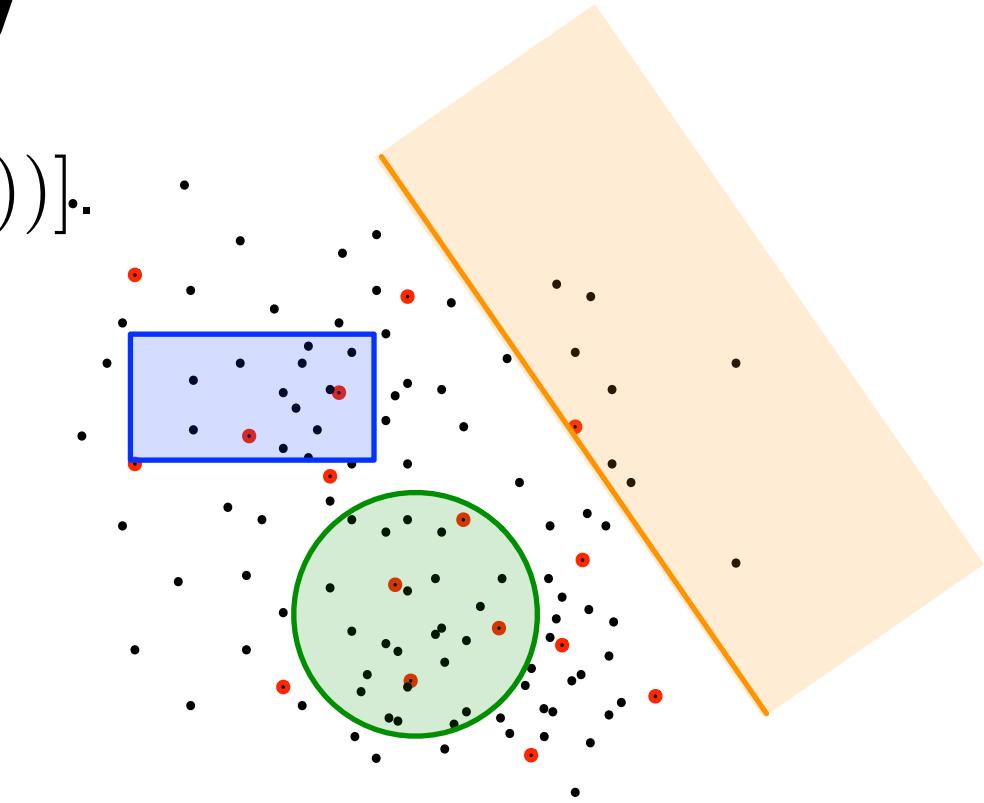
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An  $\varepsilon$ -**sample** is a subset  $S \subset X$  so  $|S| = O(1/\varepsilon^{2-2/(\nu+1)})$

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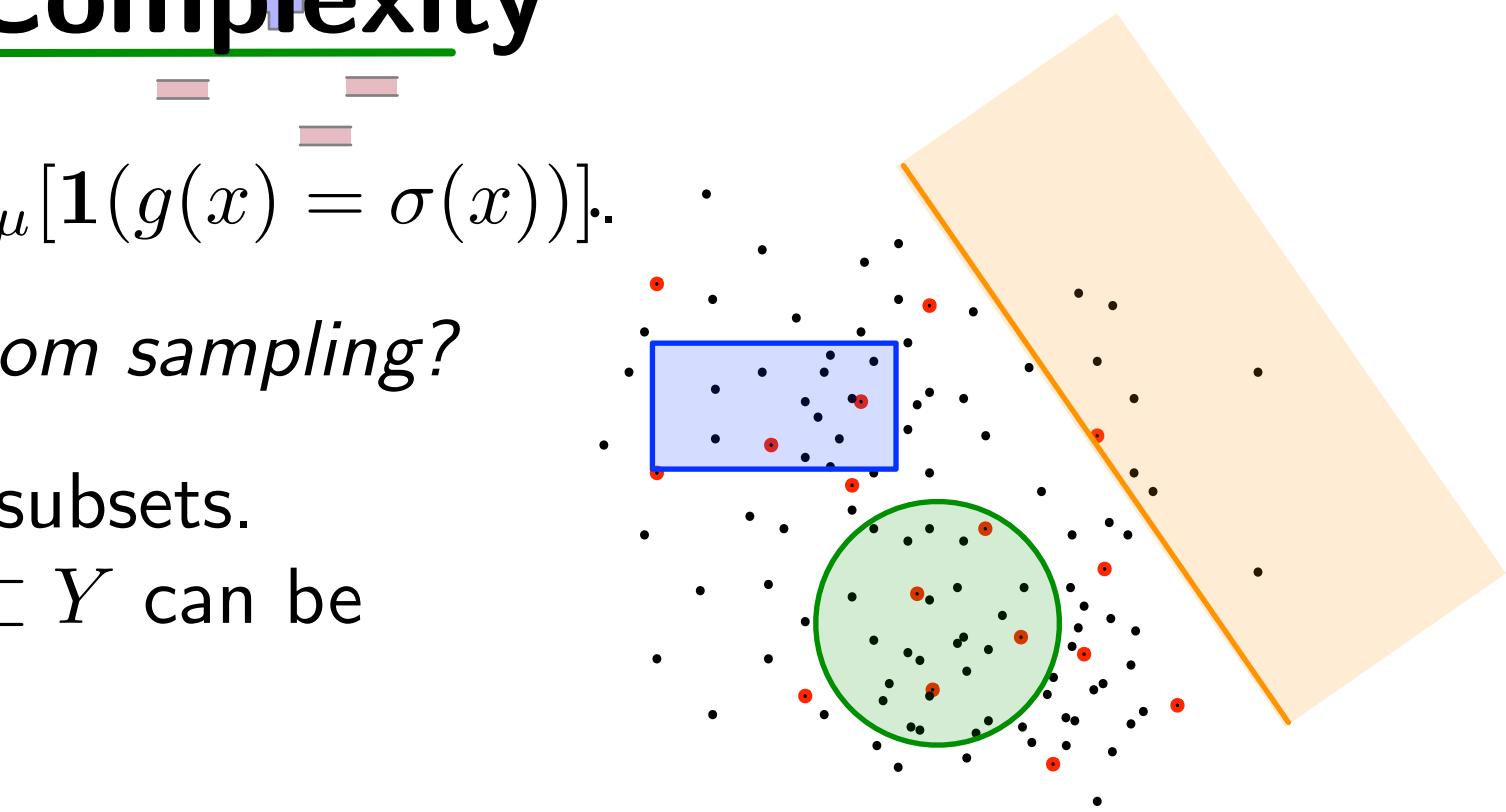
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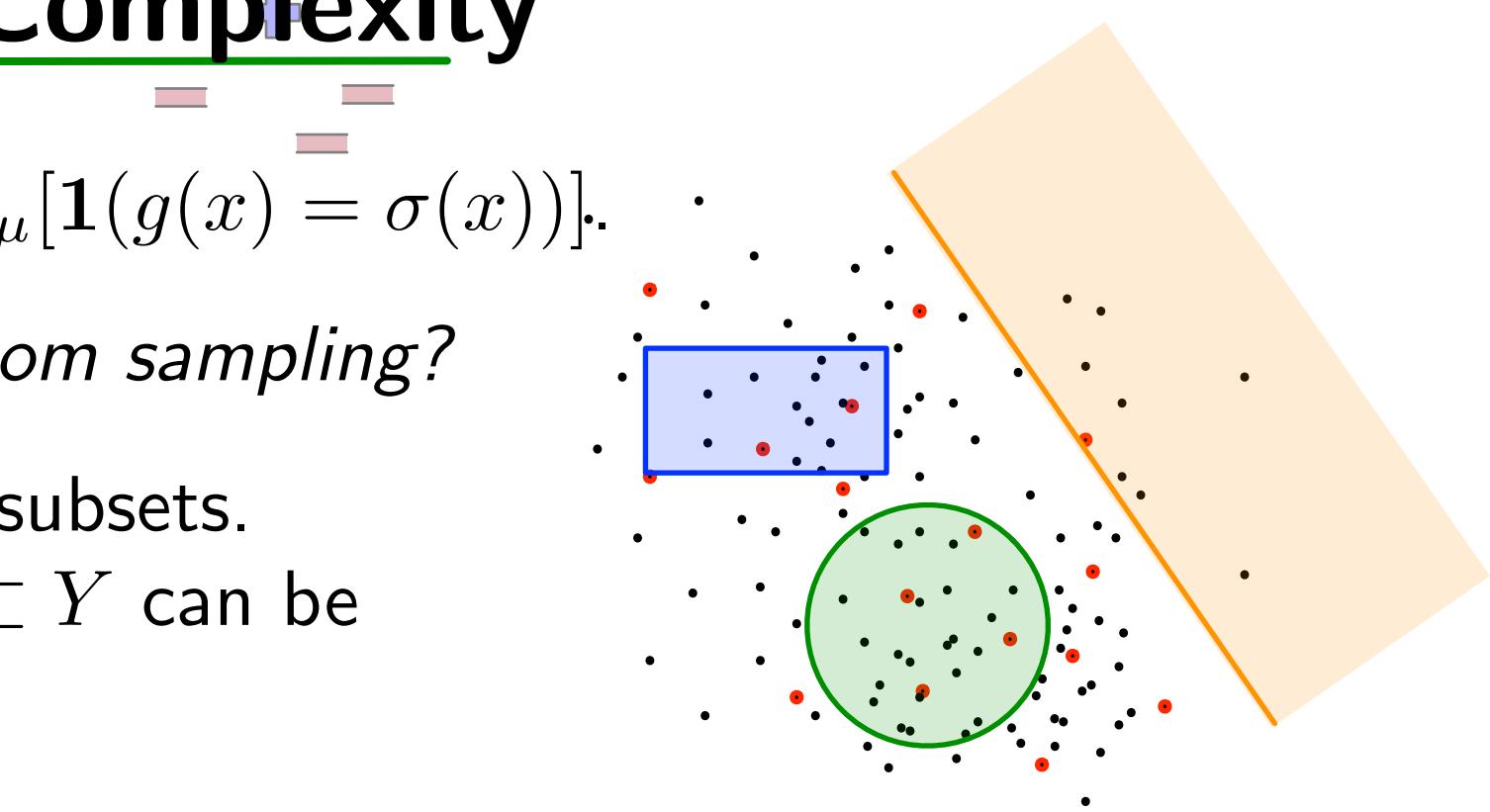
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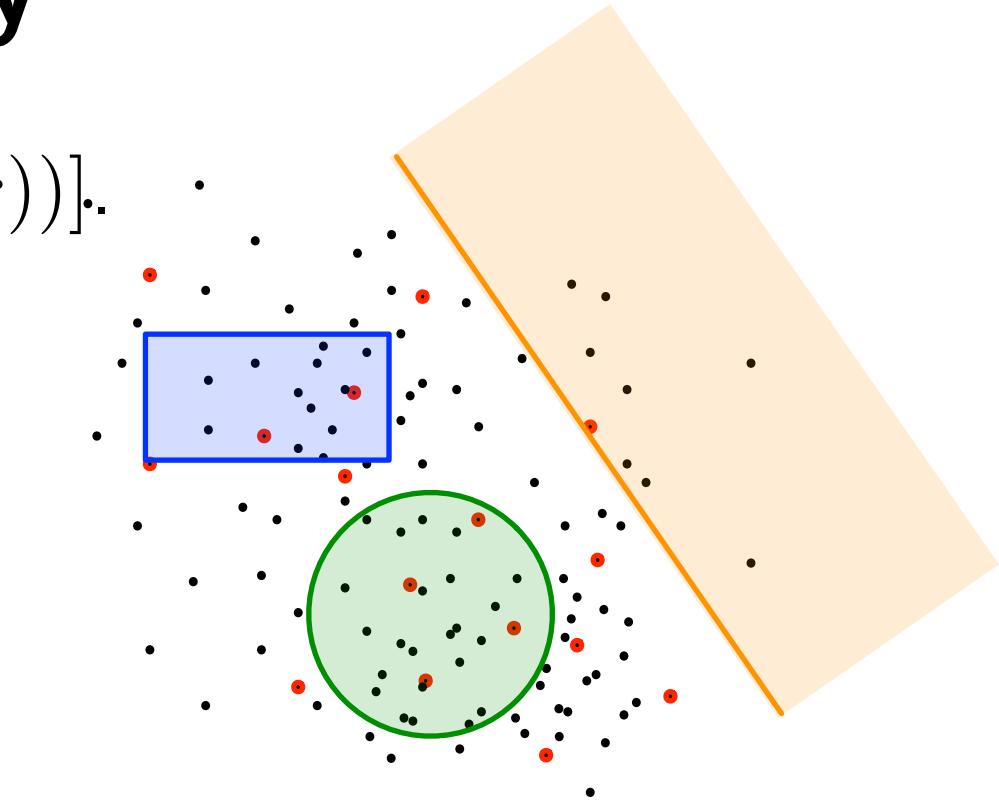
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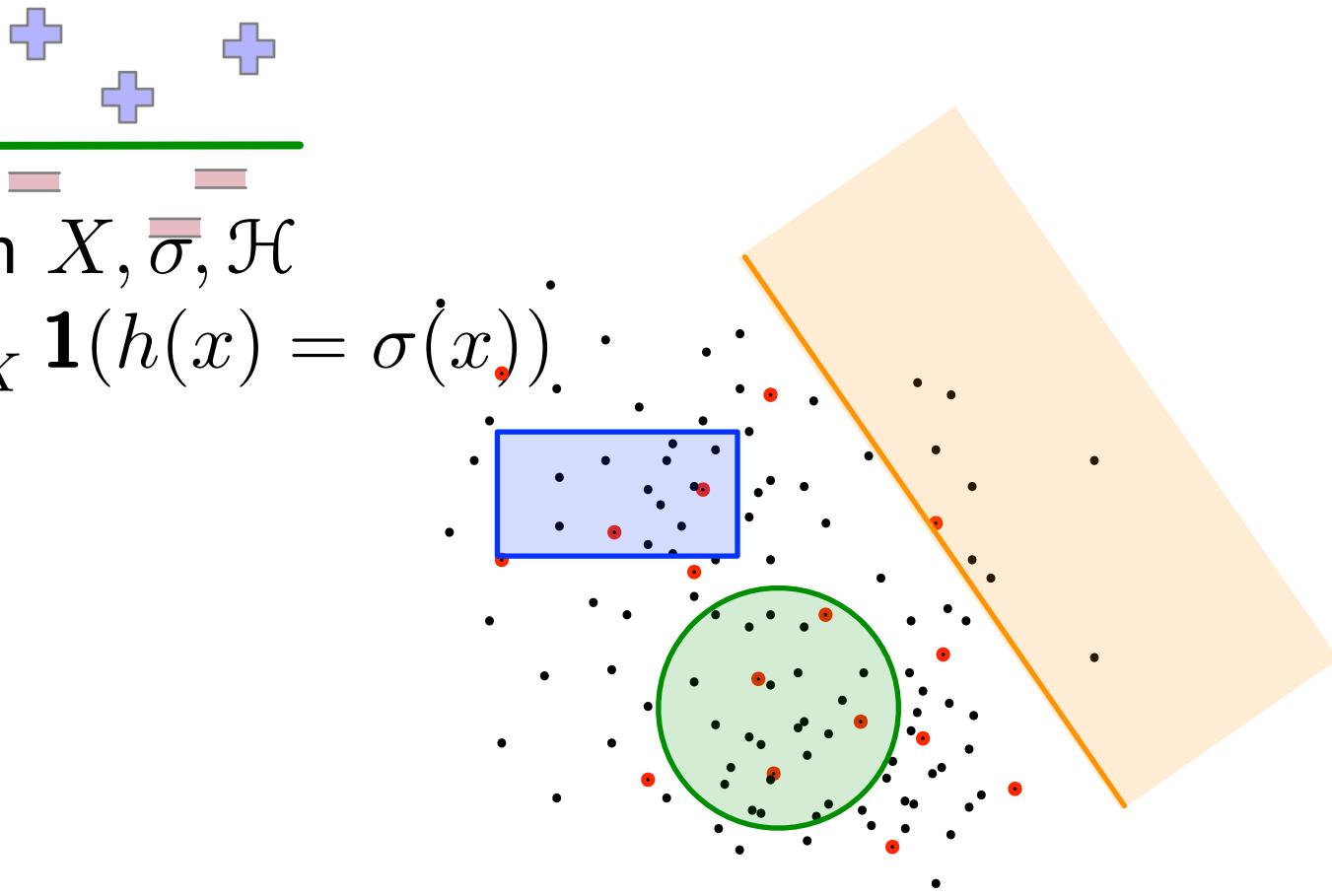


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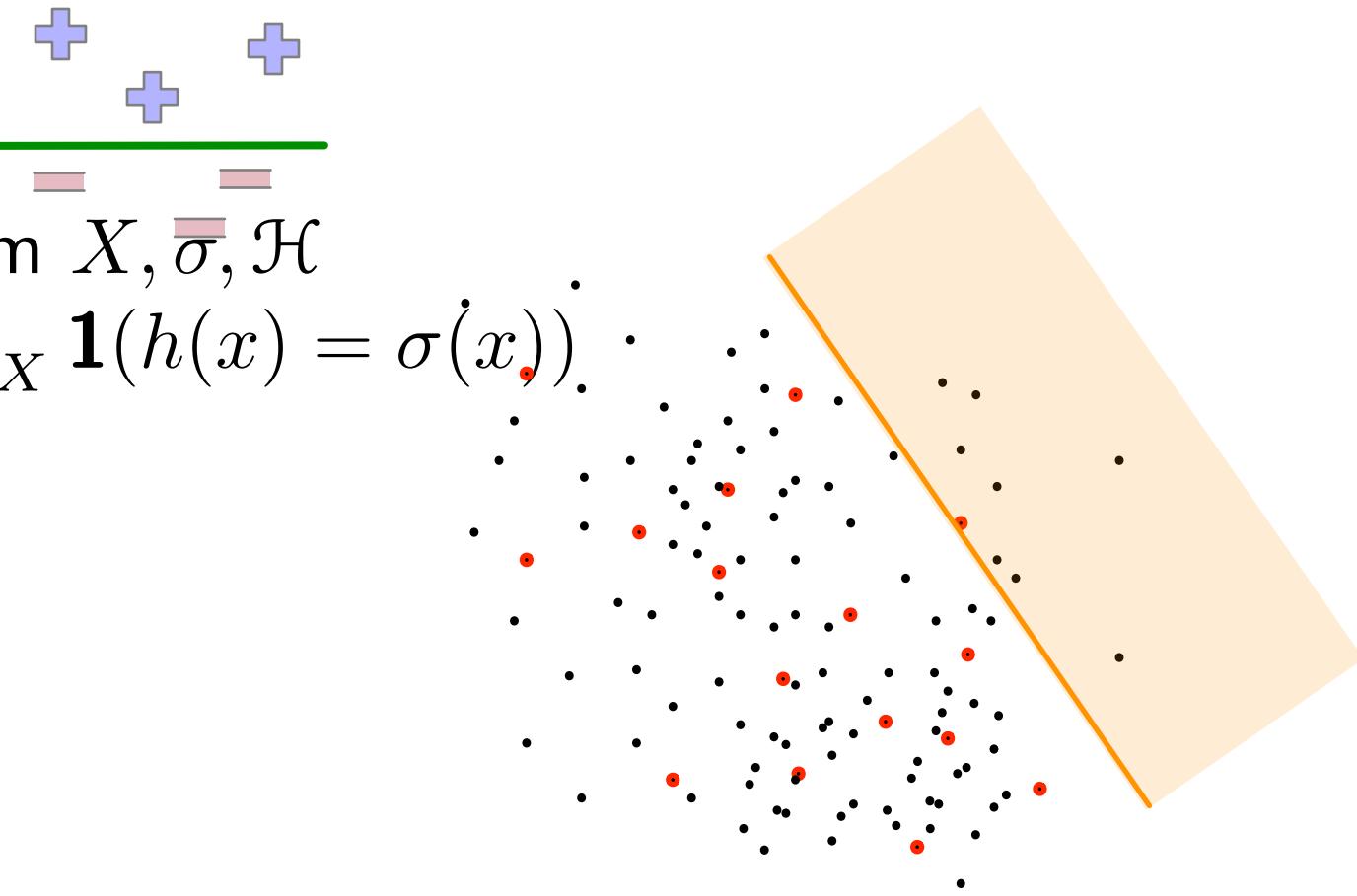


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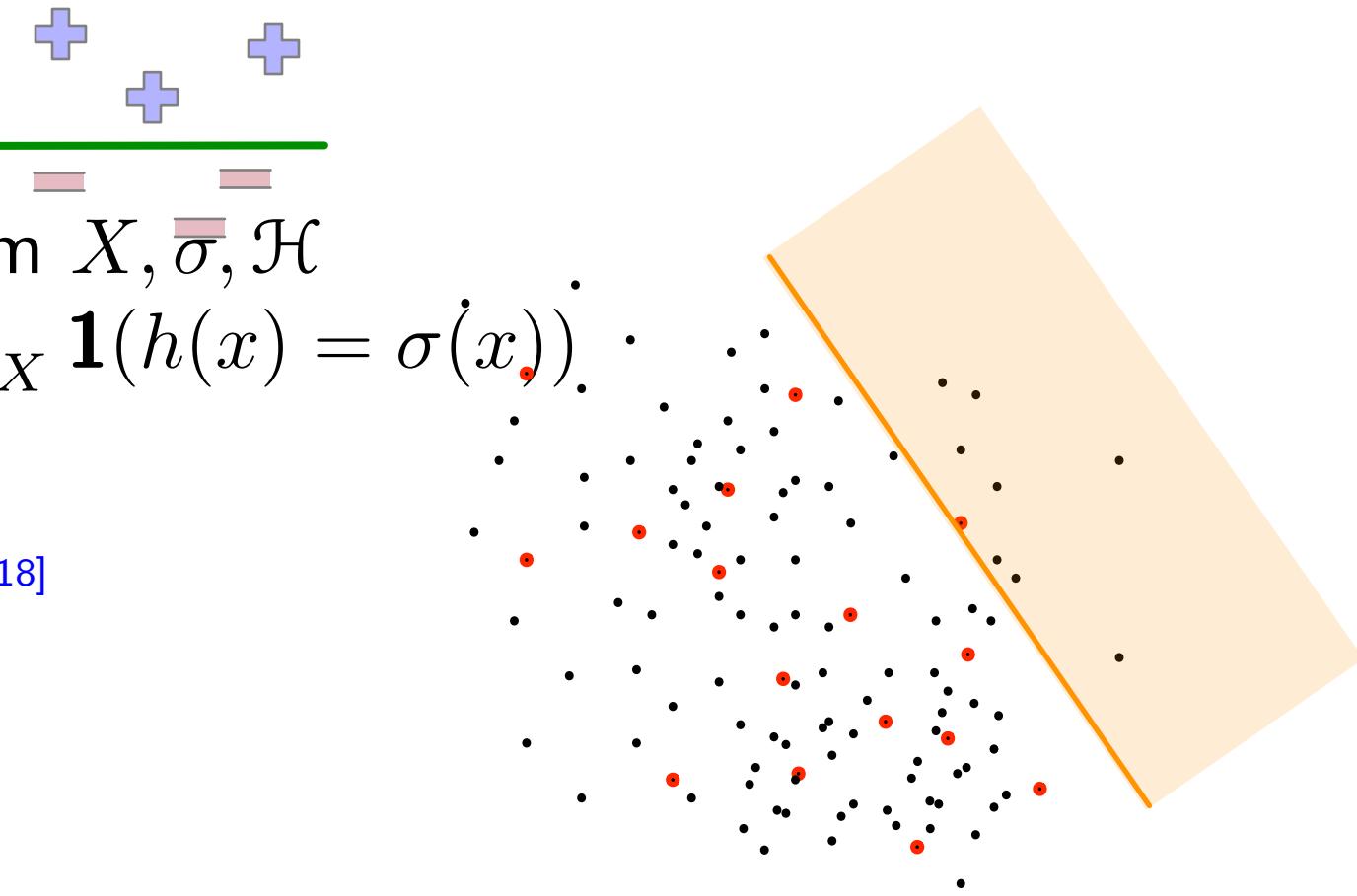
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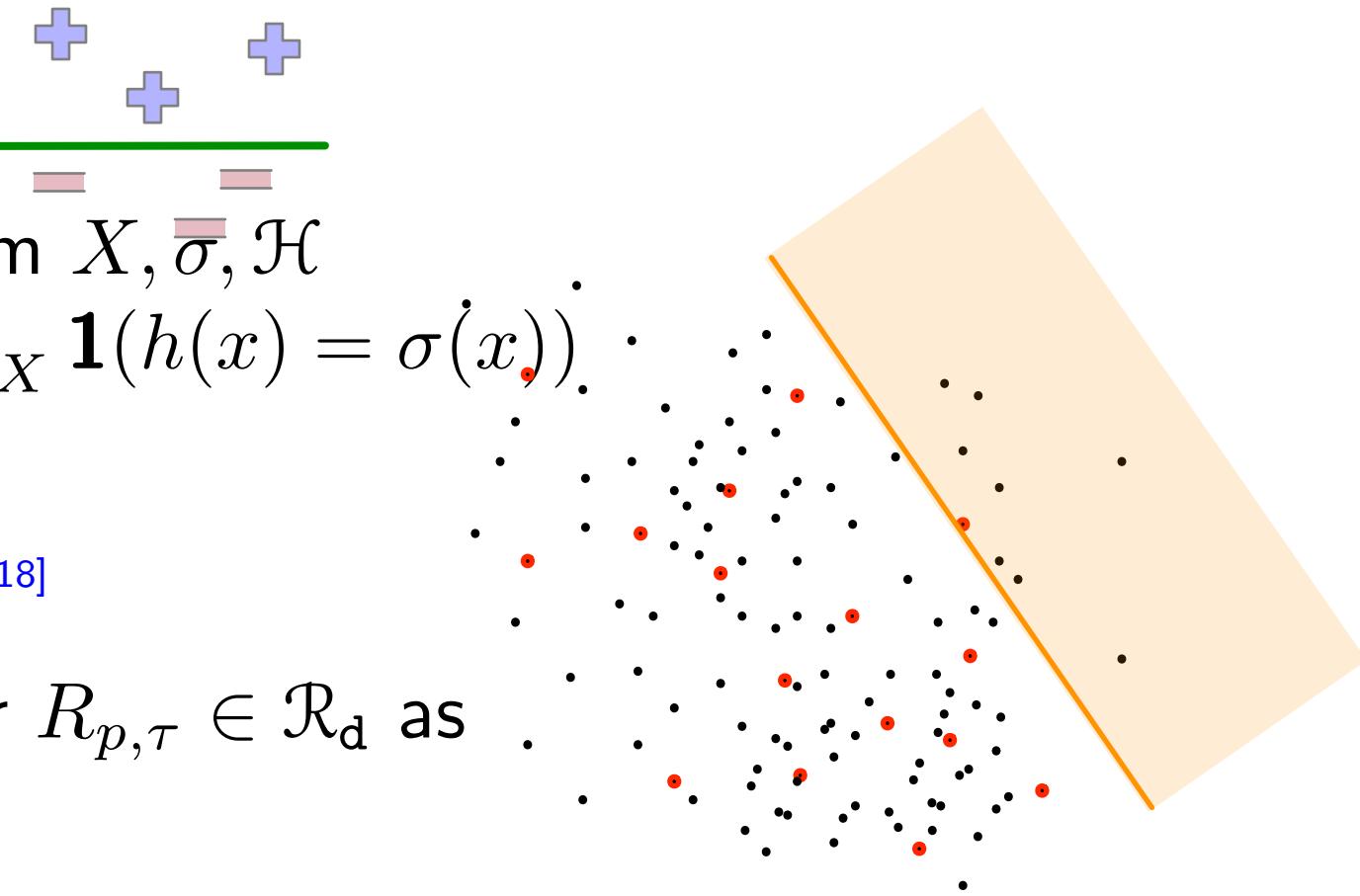
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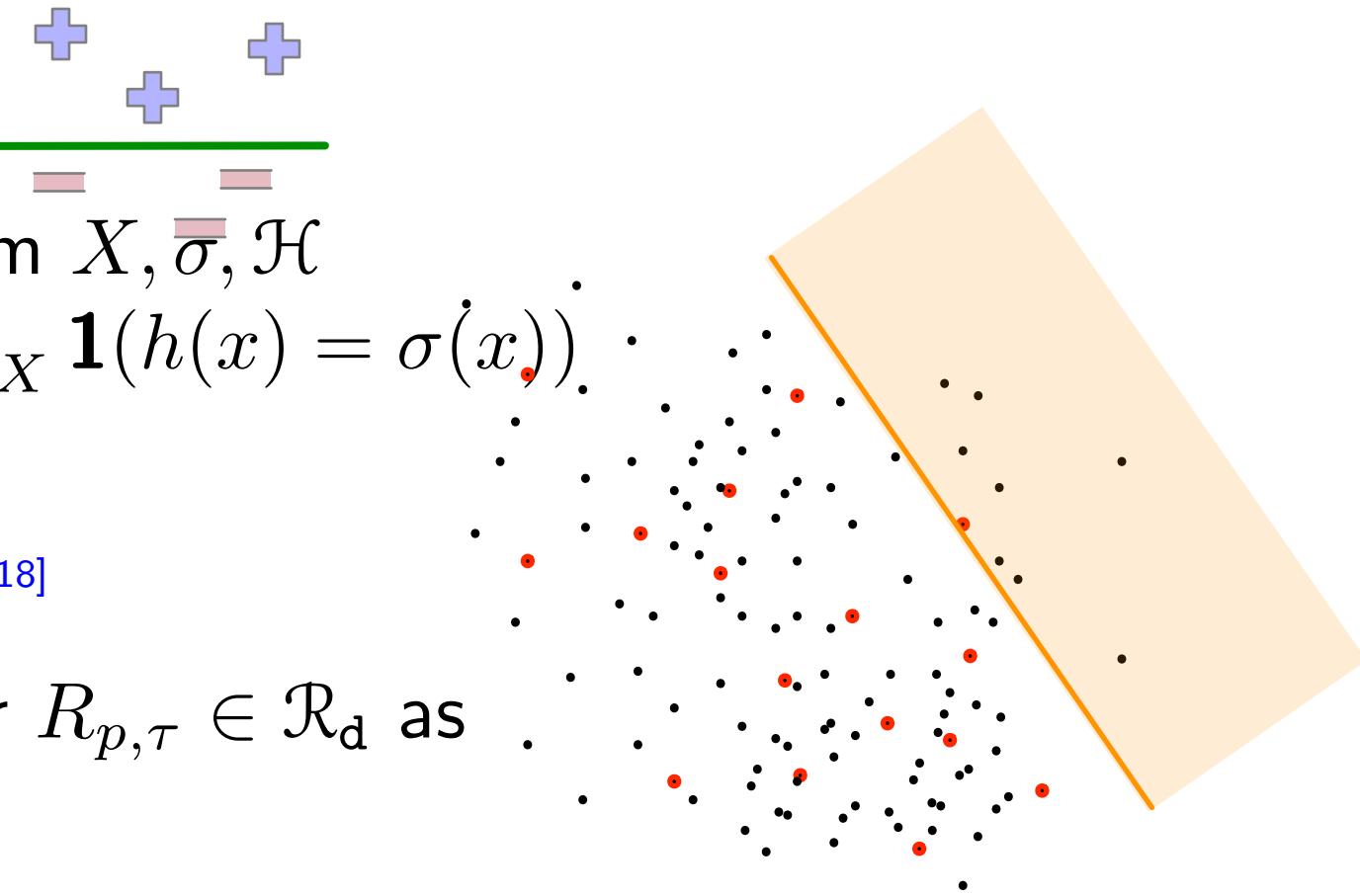
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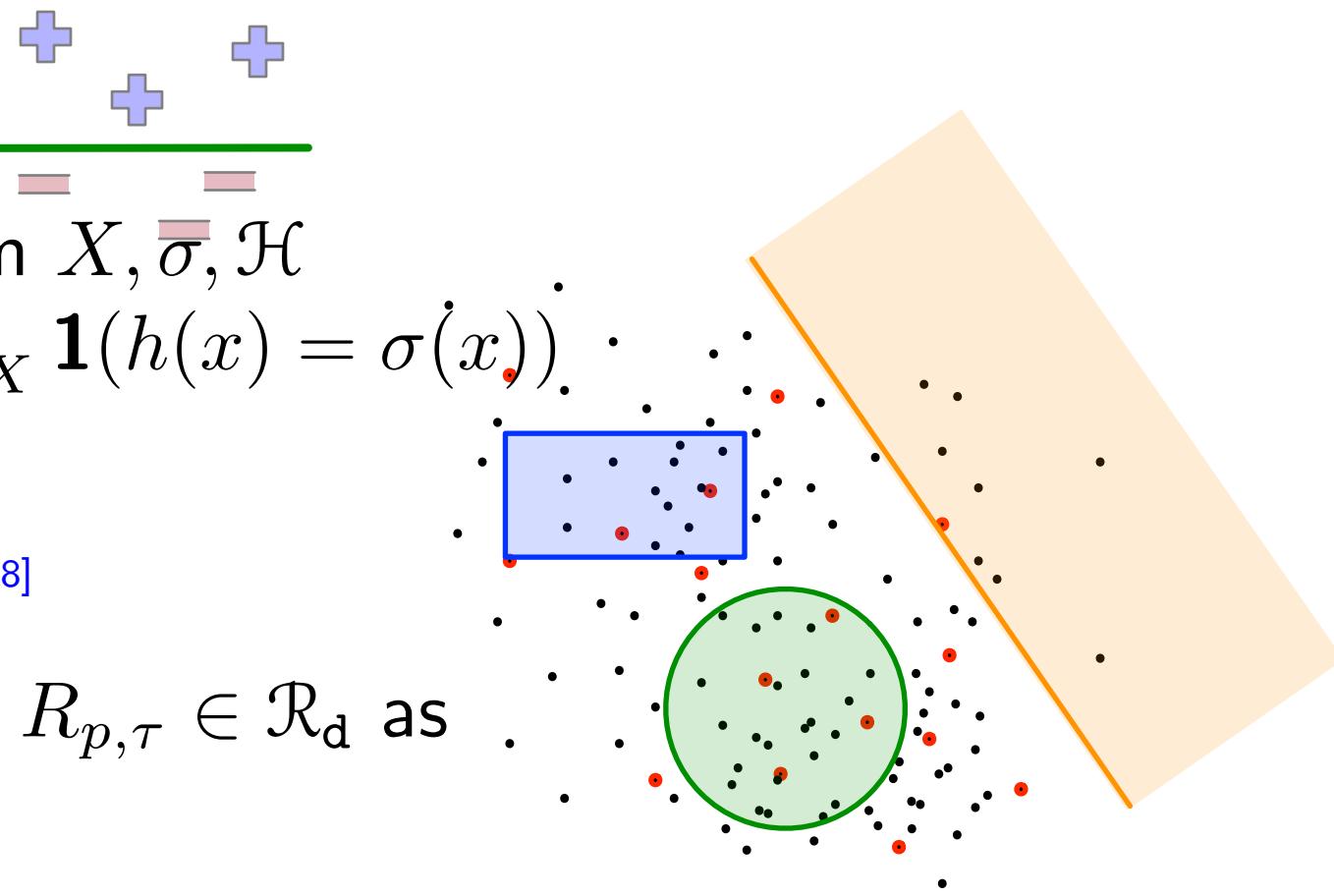
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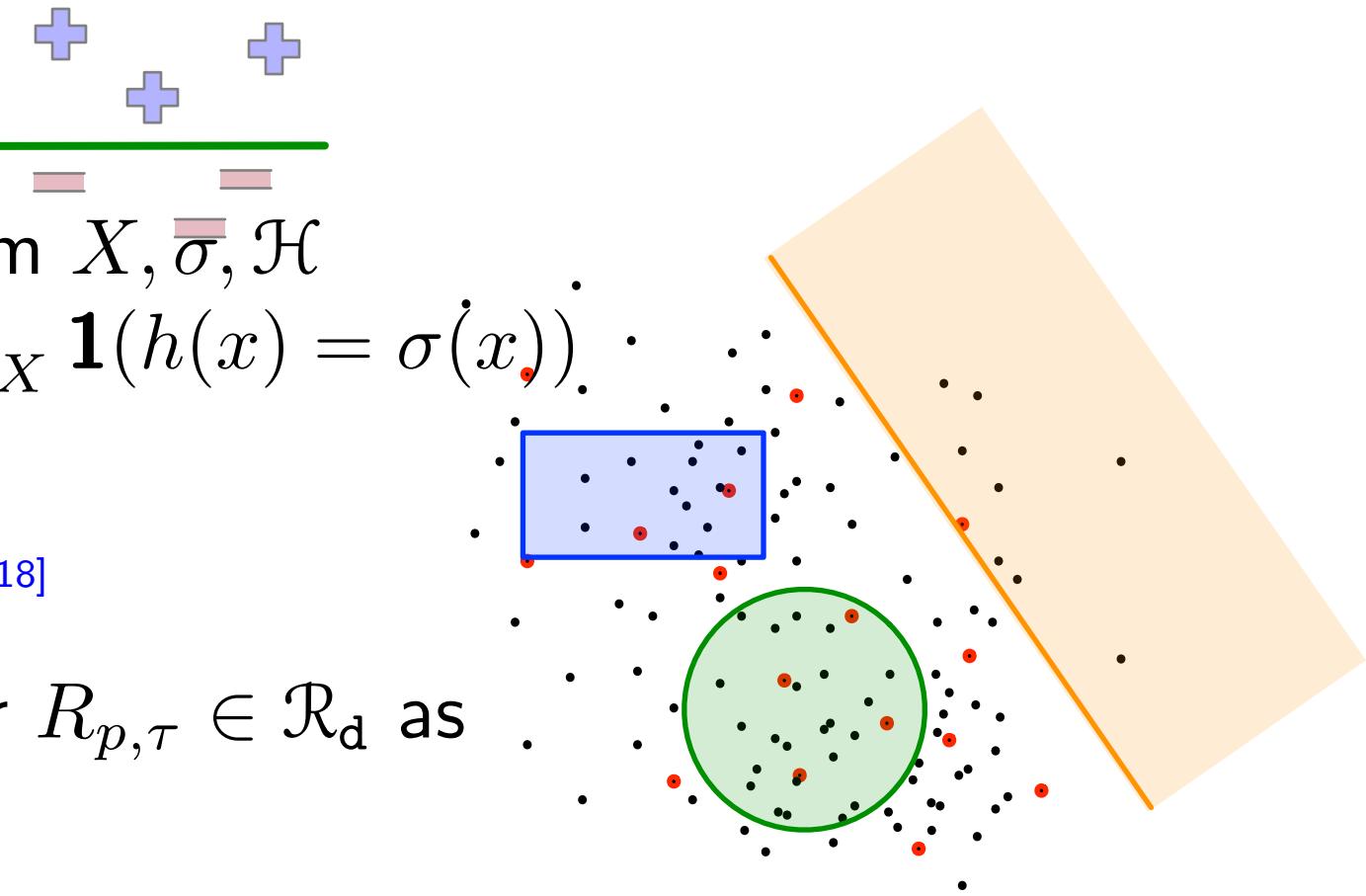
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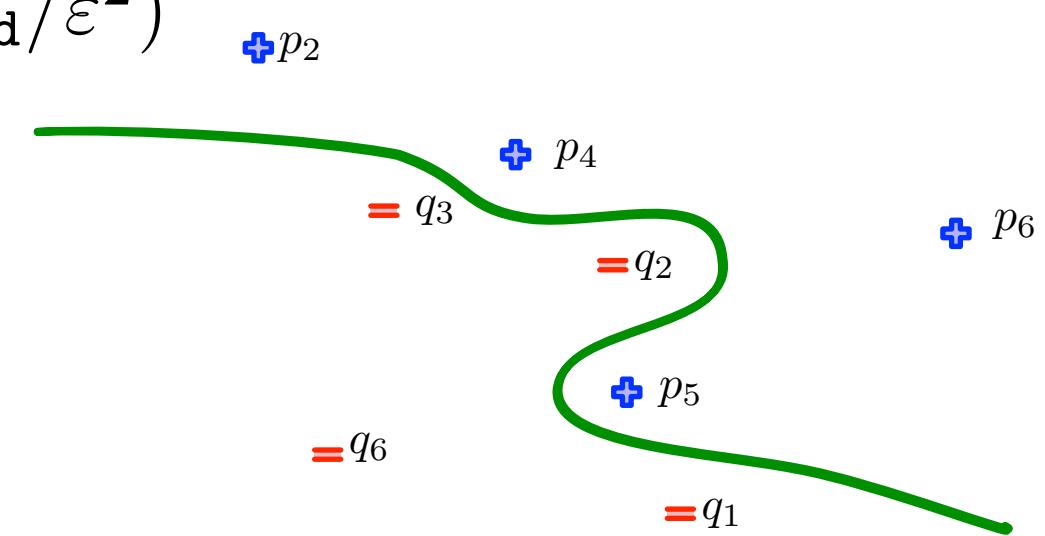
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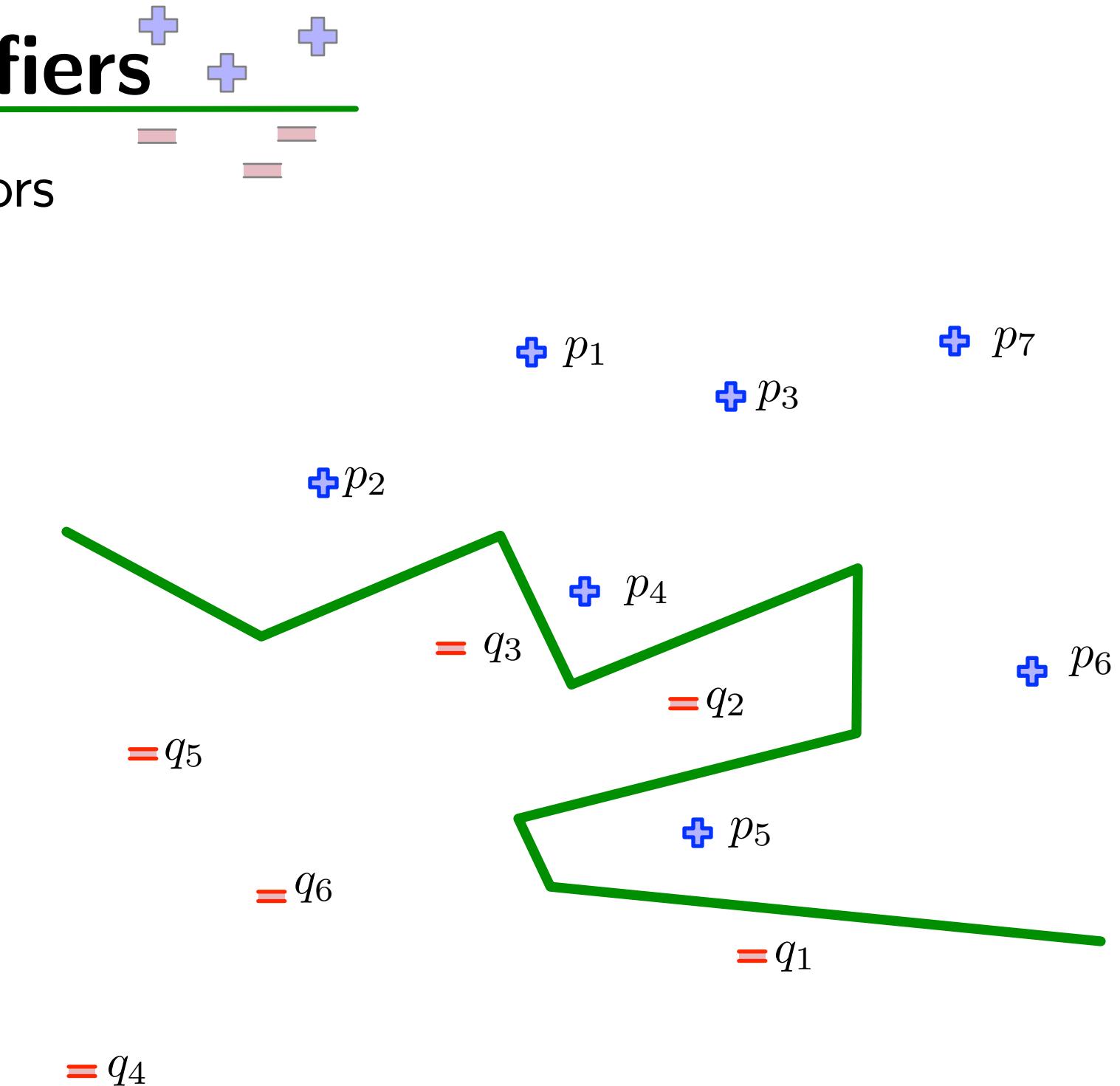
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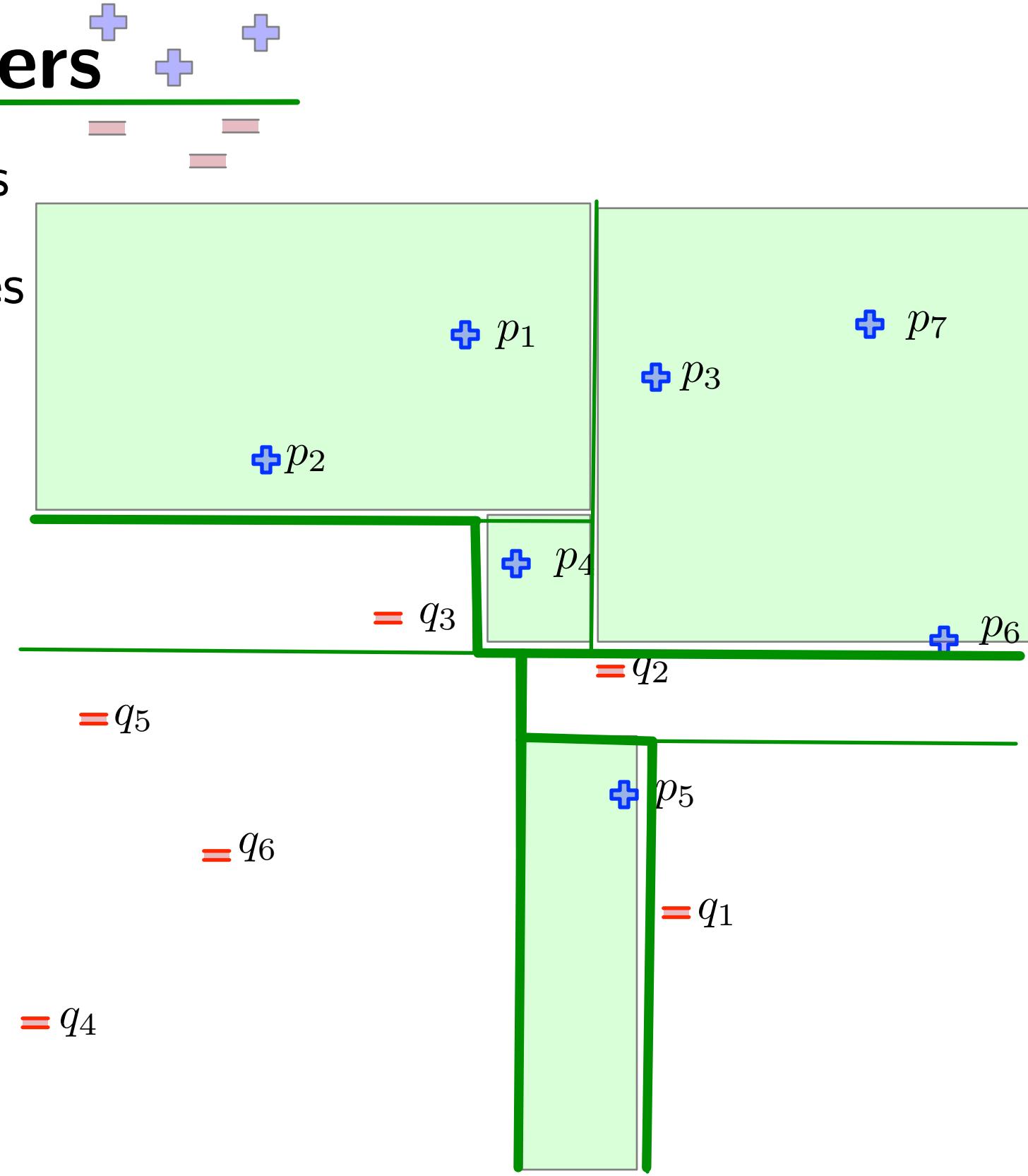
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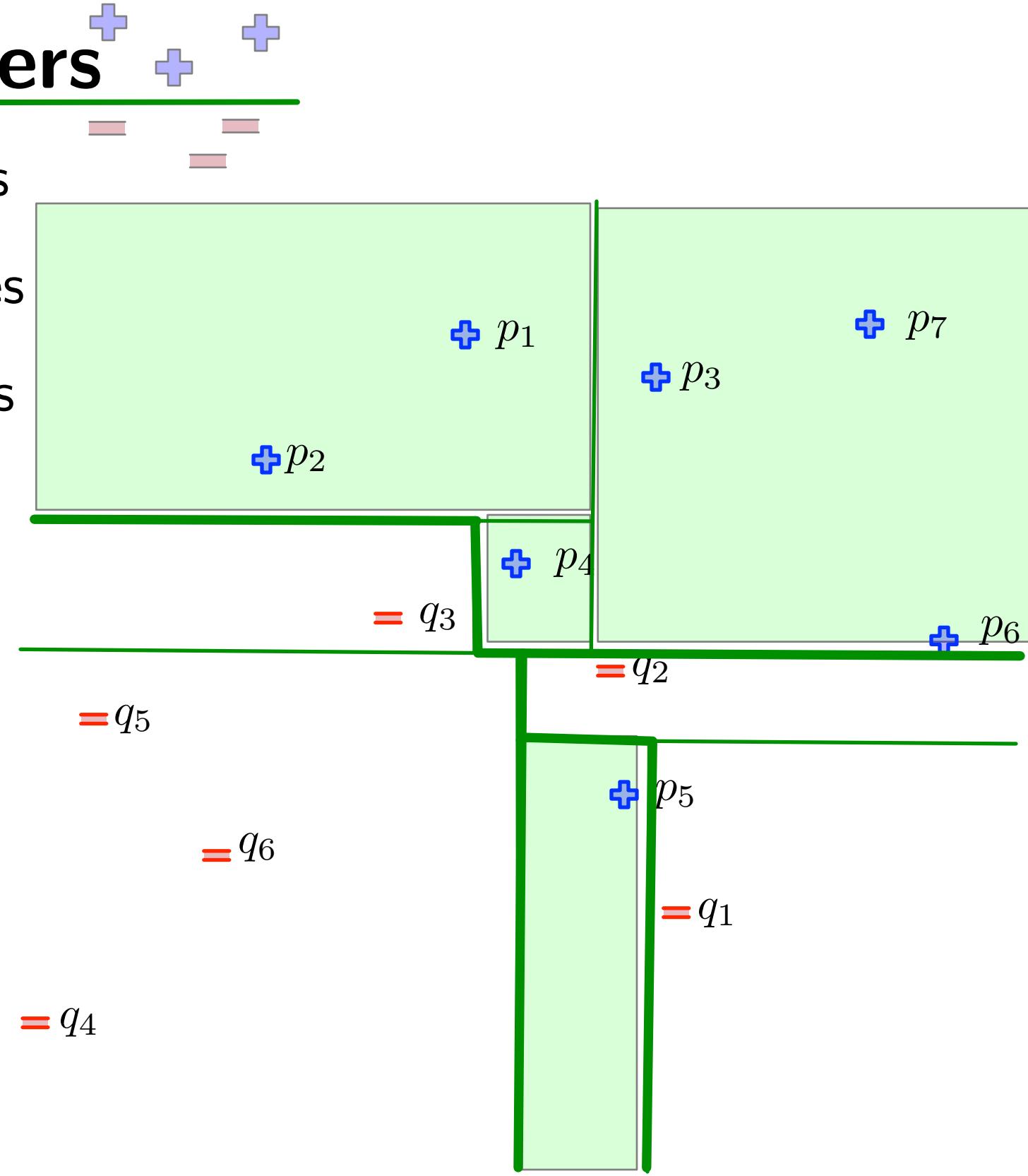
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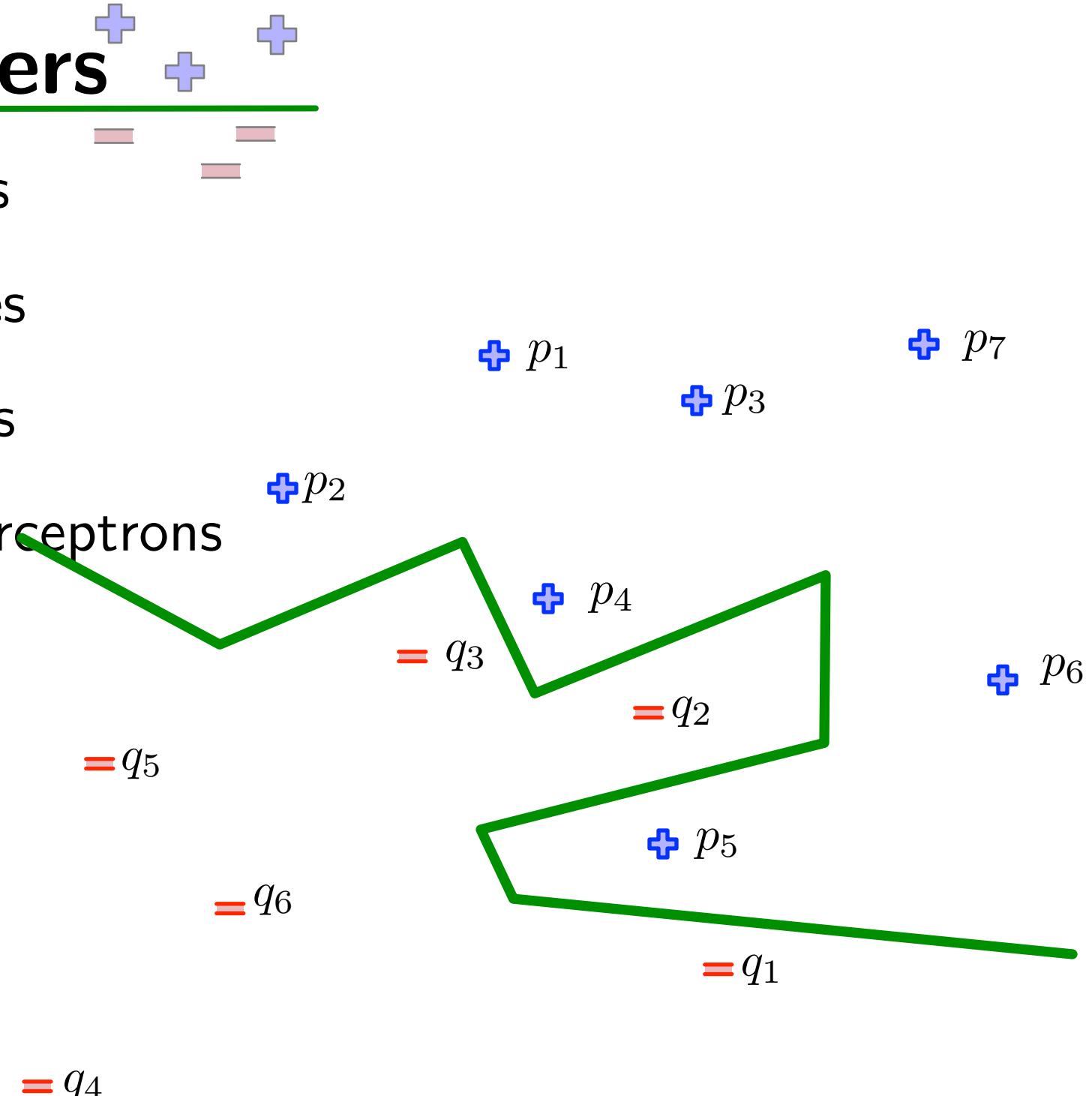
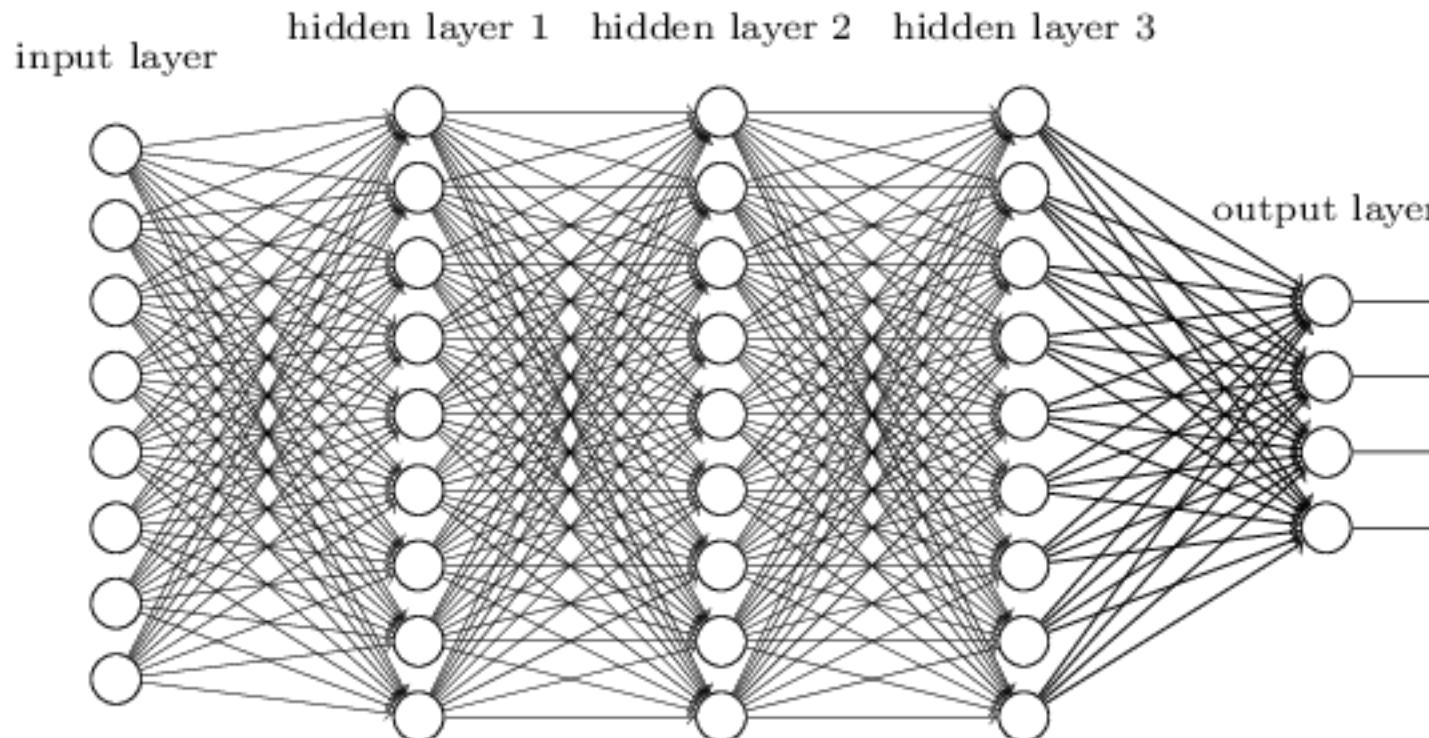
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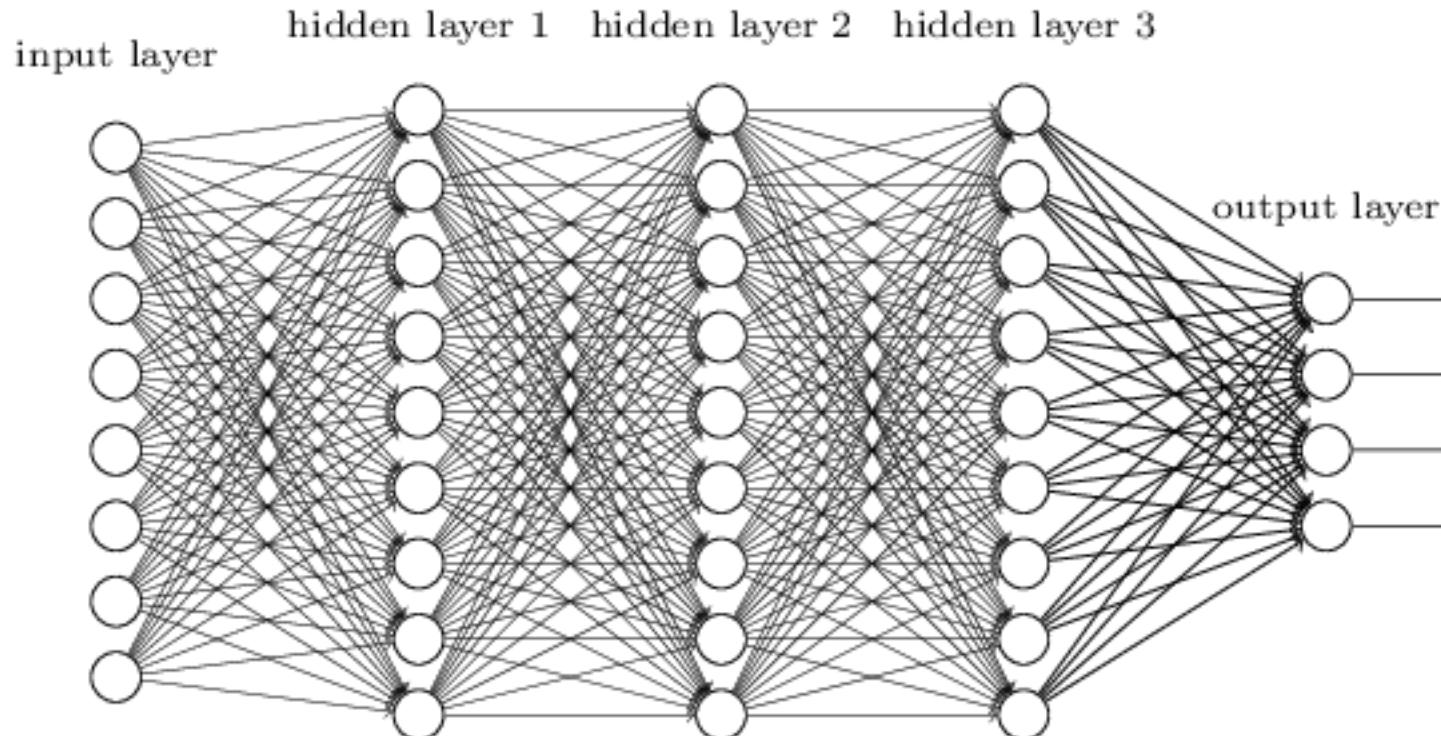
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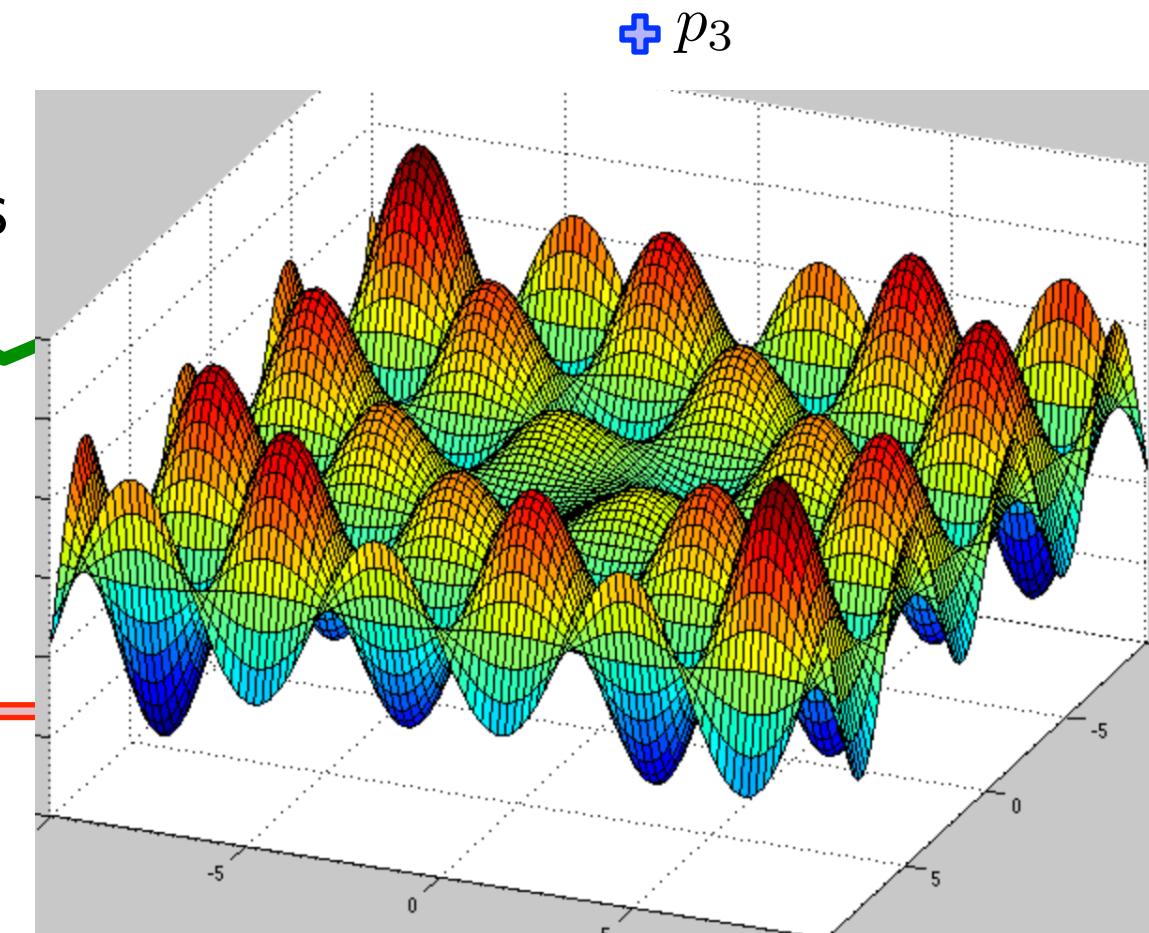


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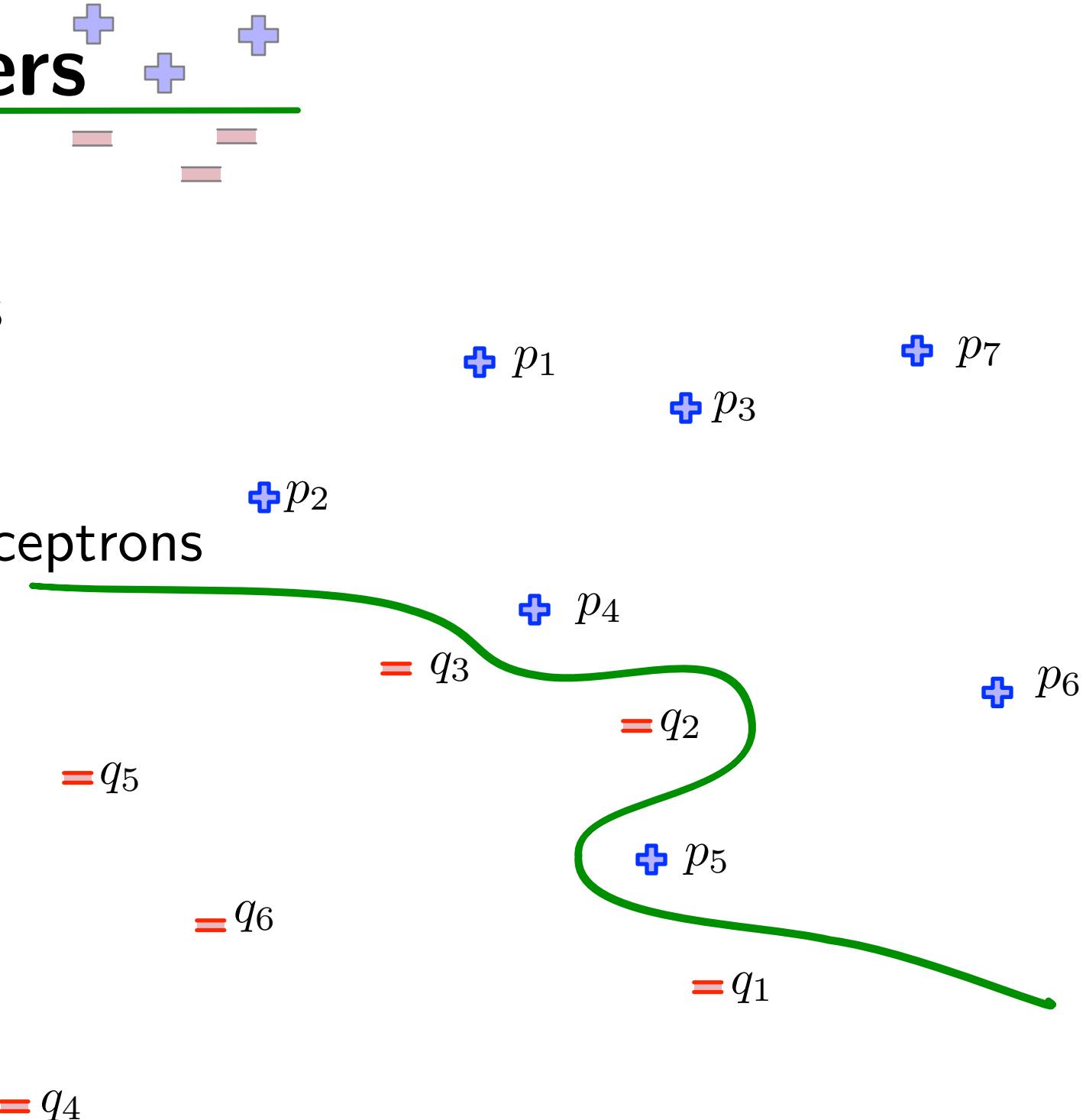
$$= q_4 \\ = q_5$$



- non-convex function  $f_X(w)$
- lots of data!
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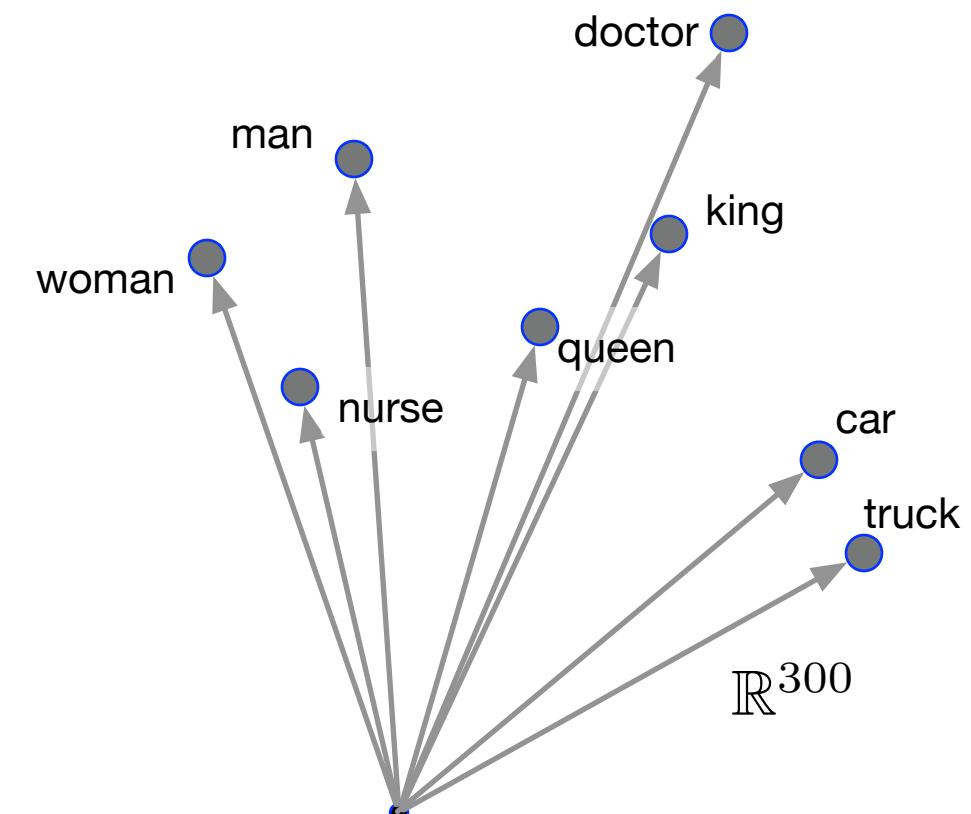
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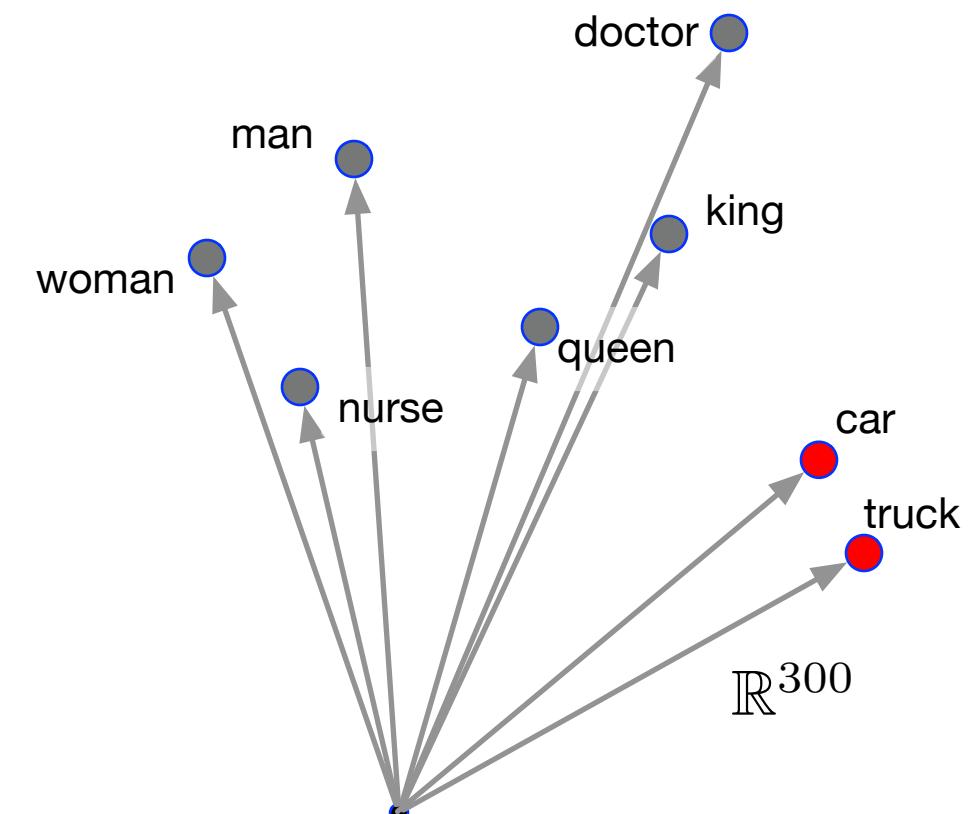
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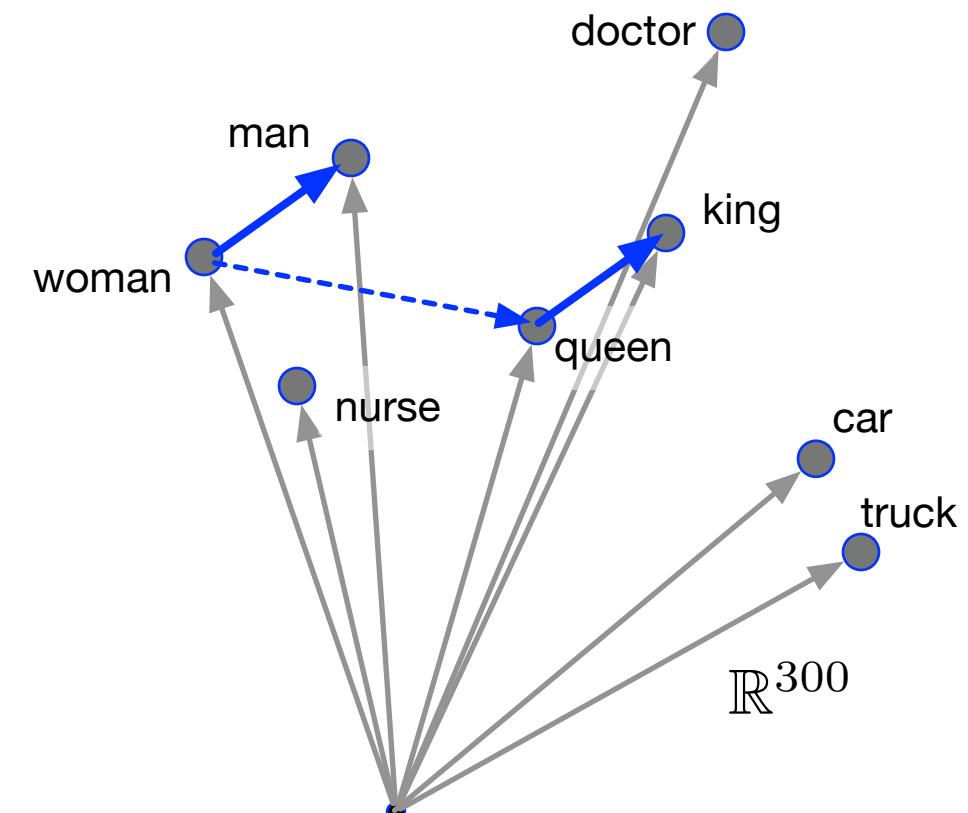
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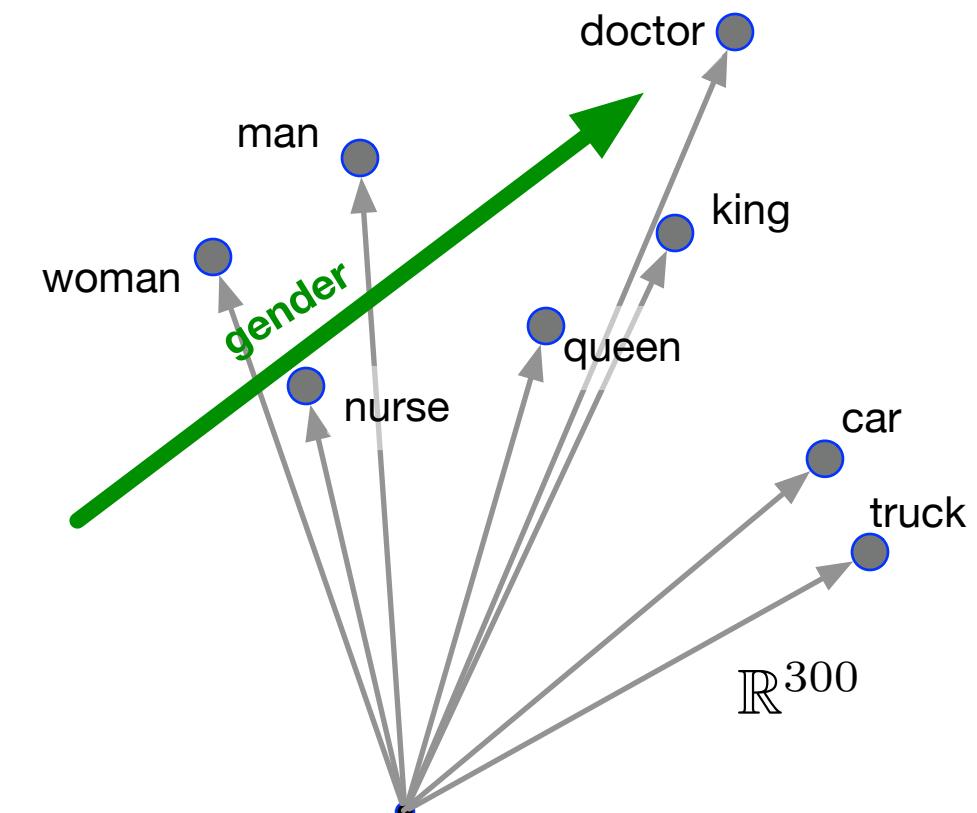
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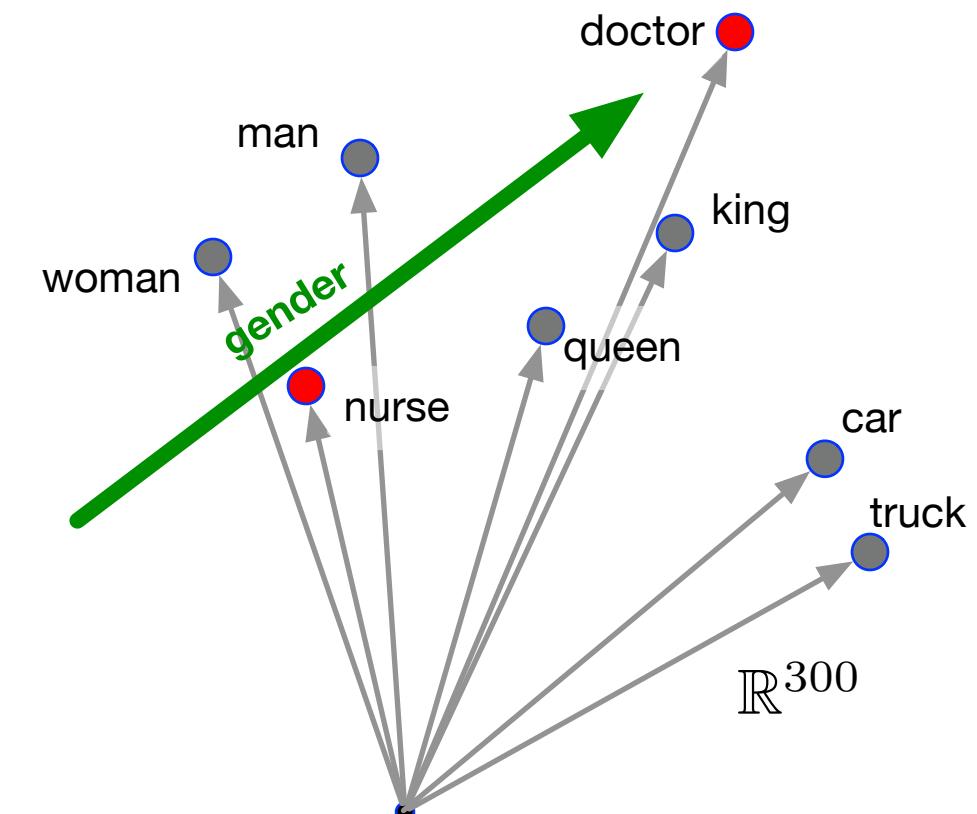
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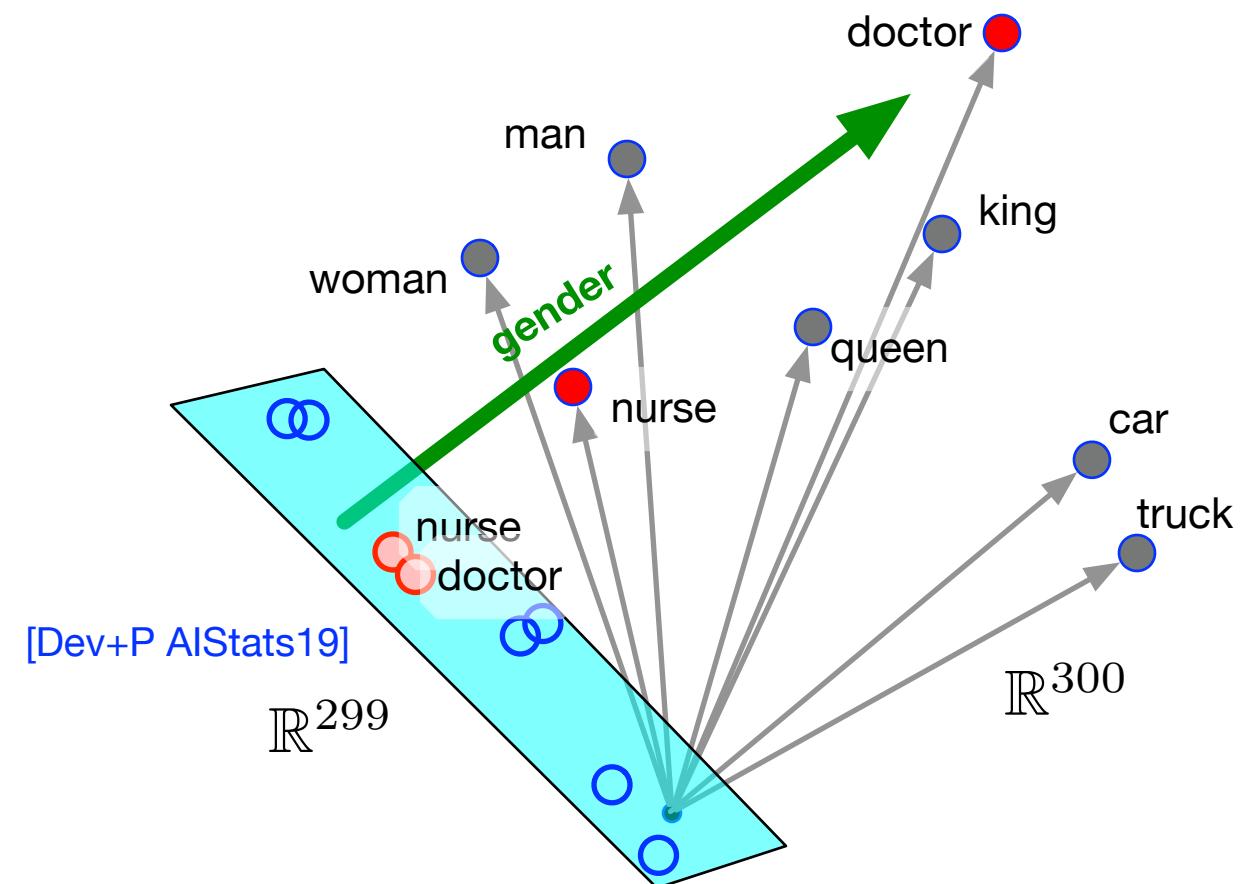
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# MATHEMATICAL FOUNDATIONS FOR DATA ANALYSIS

## Implementation Hints:

To implement the Perceptron algorithm, inside the inner loop we need to find some misclassified point  $(x_i, y_i)$ , if one exists. This can require another implicit loop. A common approach would be to, for some ordering of points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  keep an iterator index  $i$  that is maintained outside the **repeat-until** loop. It is modularly incremented every step: it loops around to  $i = 1$  after  $i = n$ . That is, the algorithm keeps cycling through the data set, and updating  $w$  for each misclassified point it observes.

## Algorithm: Perceptron( $X, y$ )

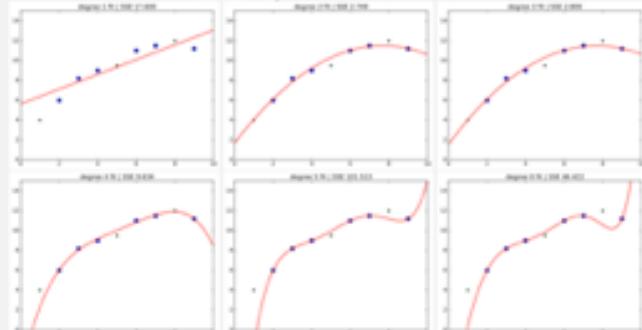
```
Initialize  $w = y_0 x_0$  for any  $(x_0, y_0) \in (X, y)$ ; Set  $i = 1; t = 0; \text{LAST-UPDATE} = 1$ 
repeat
    If  $y_i \langle x_i, w \rangle < 0$ 
         $w \leftarrow w + y_i x_i$ 
         $t = t + 1; \text{LAST-UPDATE} = i$ 
         $i = i + 1 \bmod n$ 
    until ( $t = T$  or  $\text{LAST-UPDATE} = i$ )
return  $w \leftarrow w/\|w\|$ 
```

## Example: Simple polynomial example with Cross Validation

Now split our data sets into a train set and a test set:

train:	$x$	2	3	4	6	7	8	test:	$x$	1	5	9
	$y$	6	8.2	9	11	11.5	12		$y$	4	9.5	11.2

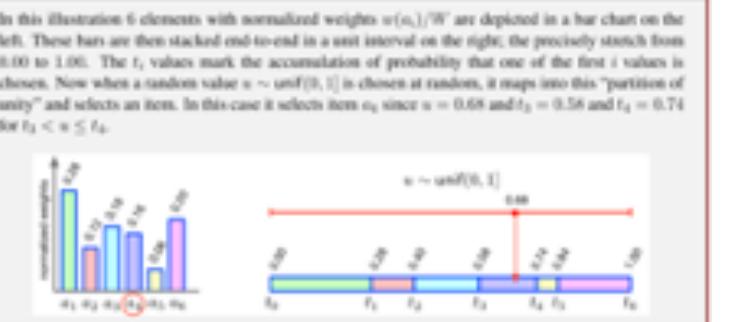
With the following polynomial fits for  $p = \{1, 2, 3, 4, 5, 8\}$  generating model  $M_{\text{opt}}$  on the test data. We then calculate the  $\text{SSE}(x_{\text{test}}, M_{\text{opt}})$  score for each (as shown):



And the polynomial model with degree  $p = 2$  has the lowest SSE score of 2.719. It is also the simplest model that does a very good job by the "eye-ball" test. So we would choose this as our model.

# JEFF M. PHILLIPS

<http://www.cs.utah.edu/~jeffp/M4D/M4D.html>



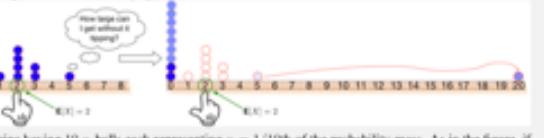
In this illustration 6 elements with normalized weights  $w(a_i)/W$  are depicted in a bar chart on the left. These bars are then stacked end-to-end in a unit interval on the right, the precisely stretch from 0.00 to 1.00. The  $t_i$  values mark the accumulation of probability that one of the first  $i$  values is chosen. Now when a random value  $u \sim \text{unif}[0, 1]$  is chosen at random, it maps into this "partition of unity" and selects an item. In this case it selects item  $a_1$  since  $u = 0.68$  and  $t_1 = 0.58$  and  $t_2 = 0.74$  for  $t_1 < u \leq t_2$ .

## Geometry of the Markov Inequality

Consider balancing the pdf of some random variable  $X$  on your finger at  $\mathbb{E}[X]$ , like a waitress balances a tray. If your finger is not under a value  $\mu$  so  $\mathbb{E}[X] = \mu$ , then the pdf (and the waitress's tray) will tip, and fall in the direction of  $\mu$  – the "center of mass". Now for some amount of probability  $\alpha$ , how large can we increase its location so we retain  $\mathbb{E}[X] = \mu$ . For each part of the pdf we increase, we must decrease some in proportion. However, by the assumption  $X \geq 0$ , the pdf must not be positive below 0. In the limit of this, we can set  $\Pr[X = 0] = 1 - \alpha$ , and then move the remaining  $\alpha$  probability as large as possible, to a location  $\delta$  so  $\mathbb{E}[X] = \mu$ . That is

$$\mathbb{E}[X] = 0 \cdot \Pr[X = 0] + \delta \cdot \Pr[X = \delta] = 0 \cdot (1 - \alpha) + \delta \cdot \alpha = \delta \cdot \alpha.$$

Solving for  $\delta$  we find  $\delta = \mathbb{E}[X]/\alpha$ .



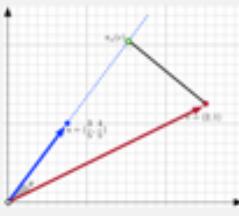
Imagine having 10  $\alpha$ -balls each representing  $\alpha = 1/10$ th of the probability mass. As in the figure, if these represent a distribution with  $\mathbb{E}[X] = 2$  and this must stay fixed, how far can one ball increase if all others balls must take a value at least 0? One ball can move to 20.

## Geometry of the Dot Product

A dot product is one of my favorite mathematical operations! It encodes a lot of geometry. Consider two vectors  $u = (\|u\|, \langle u, v \rangle)$  and  $v = (\|v\|, \langle u, v \rangle)$ , with an angle  $\theta$  between them. Then it holds

$$\langle u, v \rangle = \text{length}(u) \cdot \text{length}(v) \cdot \cos(\theta).$$

Here  $\text{length}(\cdot)$  measures the distance from the origin. We'll see how to measure length with a "norm"  $\|\cdot\|$  soon.



Moreover, since  $\|u\| = \text{length}(u) = 1$ , then we can also interpret  $\langle u, v \rangle$  as the length of  $v$  projected onto the line through  $u$ . That is, let  $v_\perp(u)$  be the closest point to  $v$  to the line through  $u$  (the line through  $u$  and the line segment from  $v$  to  $v_\perp(u)$  make a right angle). Then

$$\langle u, v \rangle = \text{length}(v_\perp(u)) = \|v_\perp(u)\|.$$

## Geometry of Why Perceptron Works

Here we will show that after at most  $T = (1/\gamma^*)^2$  steps (where  $\gamma^*$  is the margin of the maximum margin classifier), then there can be no more misclassified points.

To show this we will bound two terms as a function of  $t$ , the number of mistakes found. The term any  $\langle w, w^* \rangle$  and  $\|w\|^2 = \langle w, w \rangle$ ; this is before we ultimately normalize  $w$  in the return step.

First we can argue that  $\|w\|^2 \leq t$ , since each step increases  $\|w\|^2$  by at most 1:

$$\langle w + y_i x_i, w + y_i x_i \rangle = \langle w, w \rangle + \langle y_i \rangle^2 \langle x_i, x_i \rangle + 2y_i \langle w, x_i \rangle \leq \langle w, w \rangle + 1 + 0.$$

This is true since each  $\|x_i\| \leq 1$ , and if  $x_i$  is mis-classified, then  $y_i \langle w, x_i \rangle$  is negative.

Second, we can argue that  $\langle w, w^* \rangle \geq \gamma^*$  since each step increases it by at least  $\gamma^*$ . Recall that  $\|w^*\| = 1$

$$\langle w + y_i x_i, w^* \rangle = \langle w, w^* \rangle + \langle y_i \rangle \langle x_i, w^* \rangle \geq \langle w, w^* \rangle + \gamma^*.$$

The inequality follows from the margin of each point being at least  $\gamma^*$  with respect to the max-margin classifier  $w^*$ .

Combining these facts ( $\langle w, w^* \rangle \geq \gamma^*$  and  $\|w\|^2 \leq t$ ) together we obtain

$$\gamma^* \leq \langle w, w^* \rangle \leq \langle w, \frac{w}{\|w\|} \rangle = \|w\| \leq \sqrt{t}.$$

Solving for  $t$  yields  $t \leq (1/\gamma^*)^2$  as desired.

