CS 360: Machine Learning

Prof. Sara Mathieson

Fall 2020

HAVERFORD COLLEGE

Outline: optional material on SVMs

- Recap Perceptron (+ Handout 13)
- Support Vector Machines (SVMs) overview
- Extensions of SVMs
- SVMs meta-optimization process (+ Handout 14)

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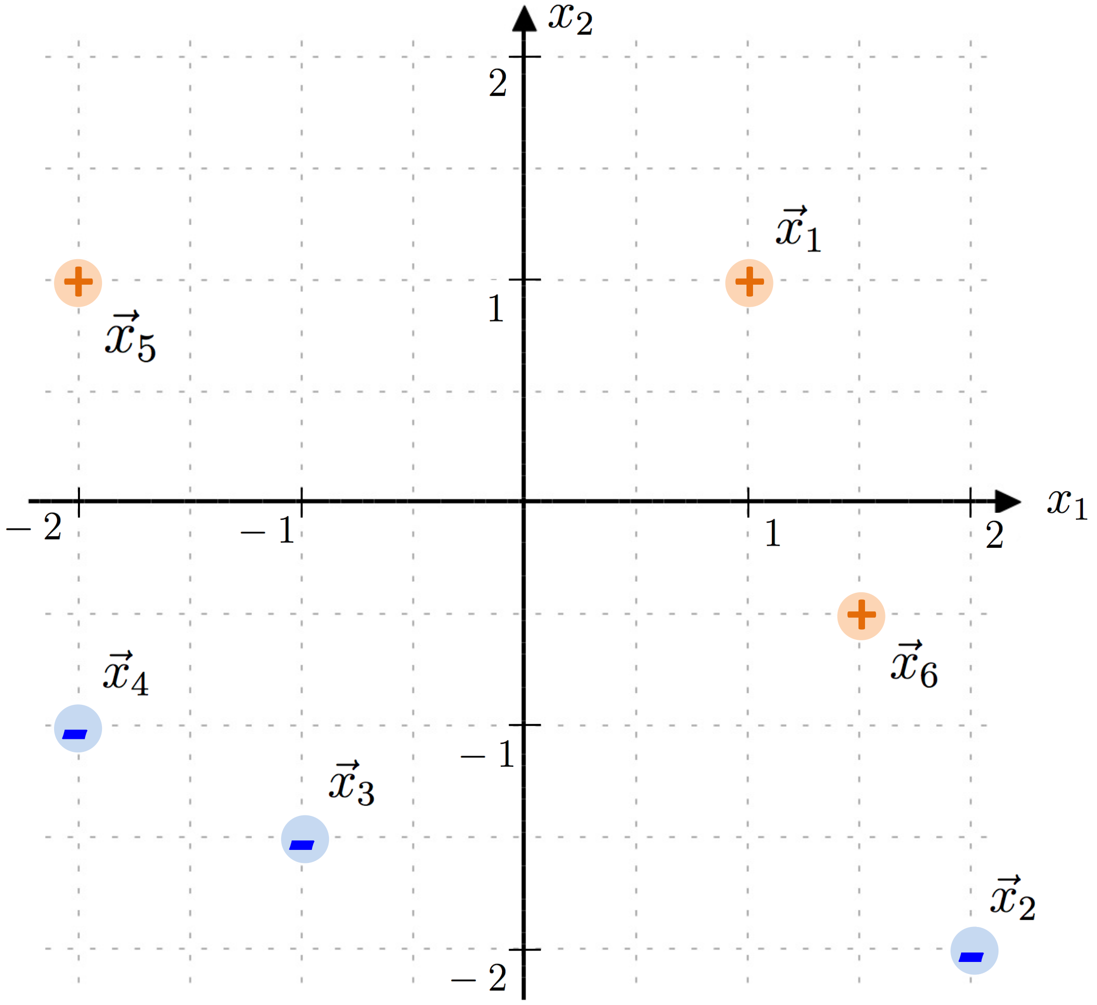
Handout 13 example

Initial values:

$$\alpha = 0.2$$

$$\vec{w} = \begin{bmatrix} 0 \\ 1 \\ 0.5 \end{bmatrix}$$



Example modified from Achim J. Lilienthal & Thorsteinn Rögnvaldsson

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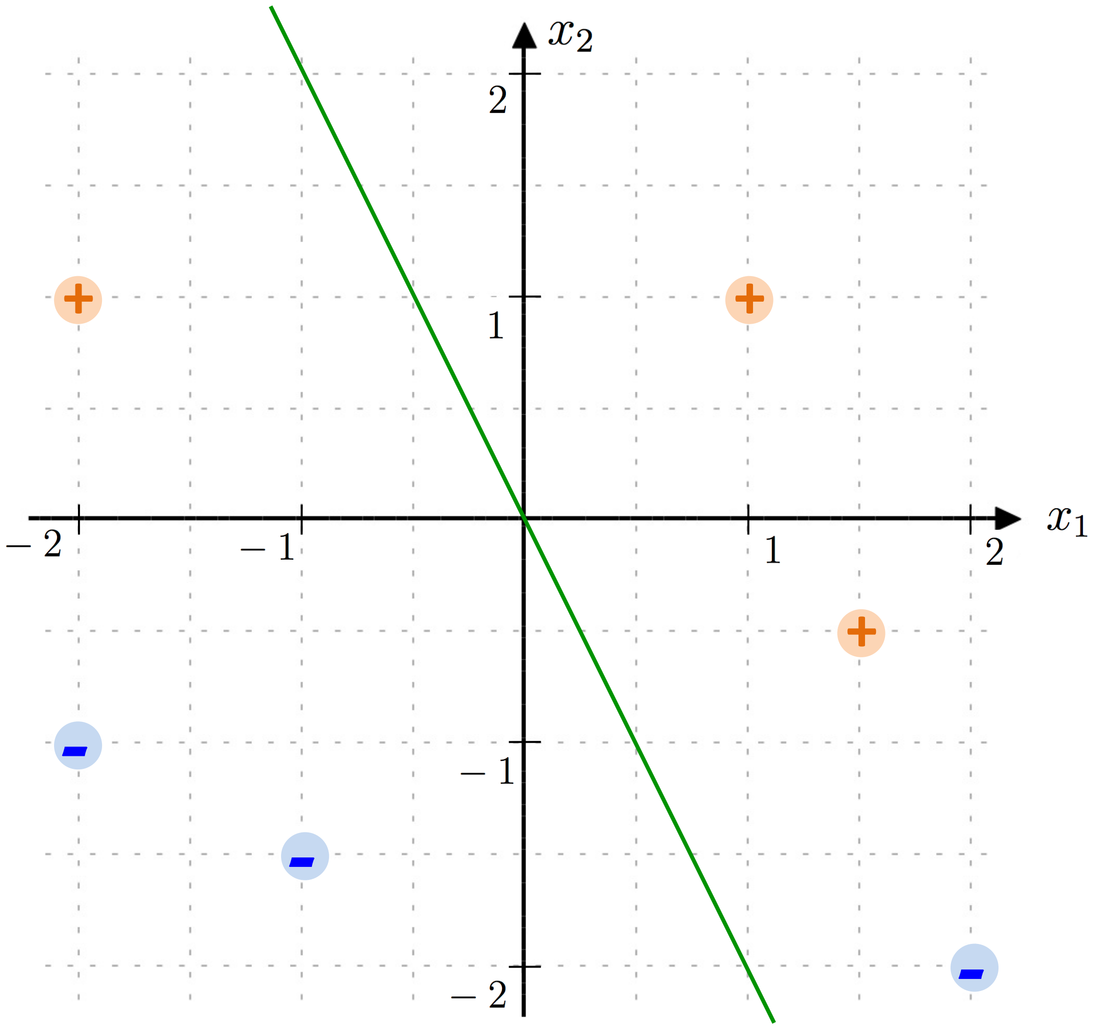

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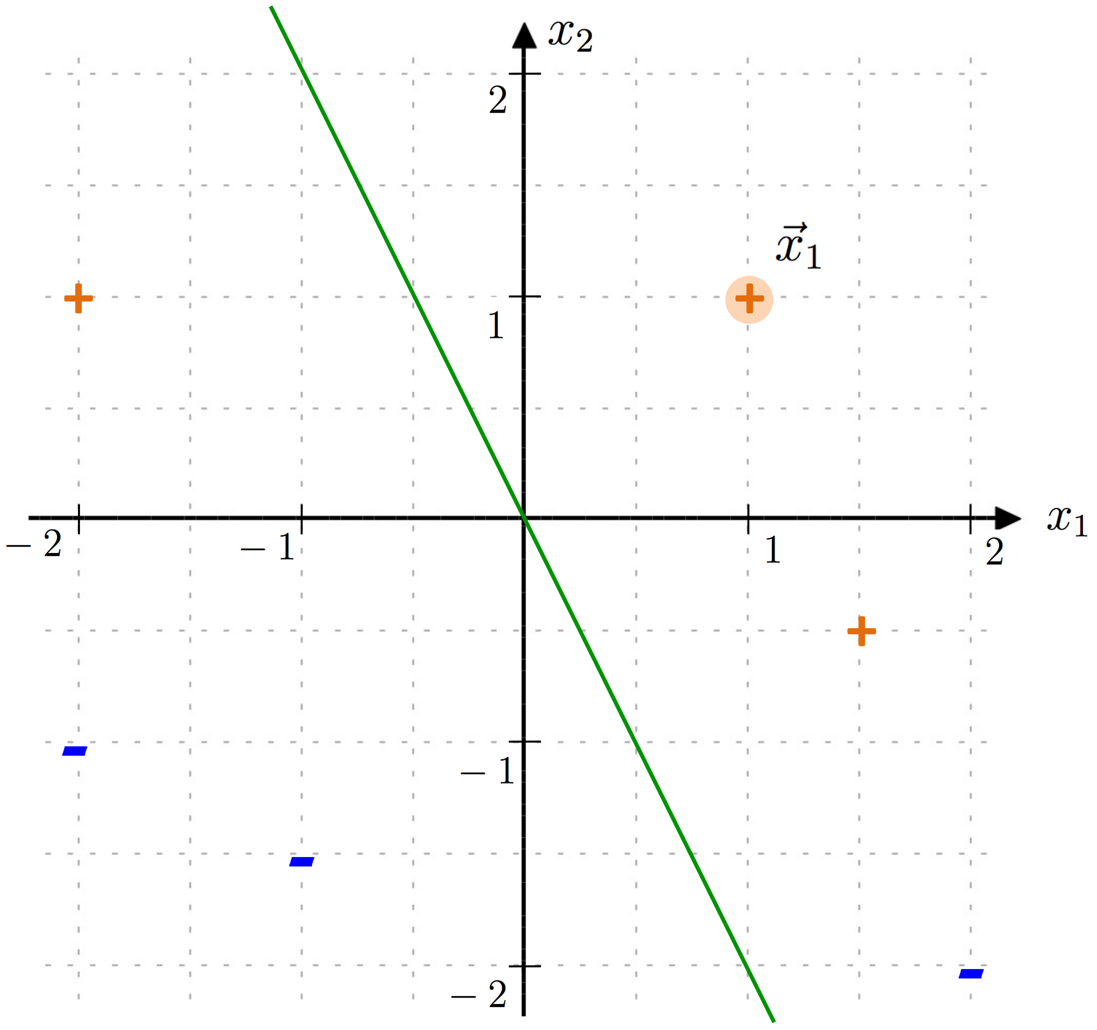
Round 1:

$$\vec{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\vec{w} \cdot \vec{x}_1 > 0$$

Correct classification, no action



Handout 13 example

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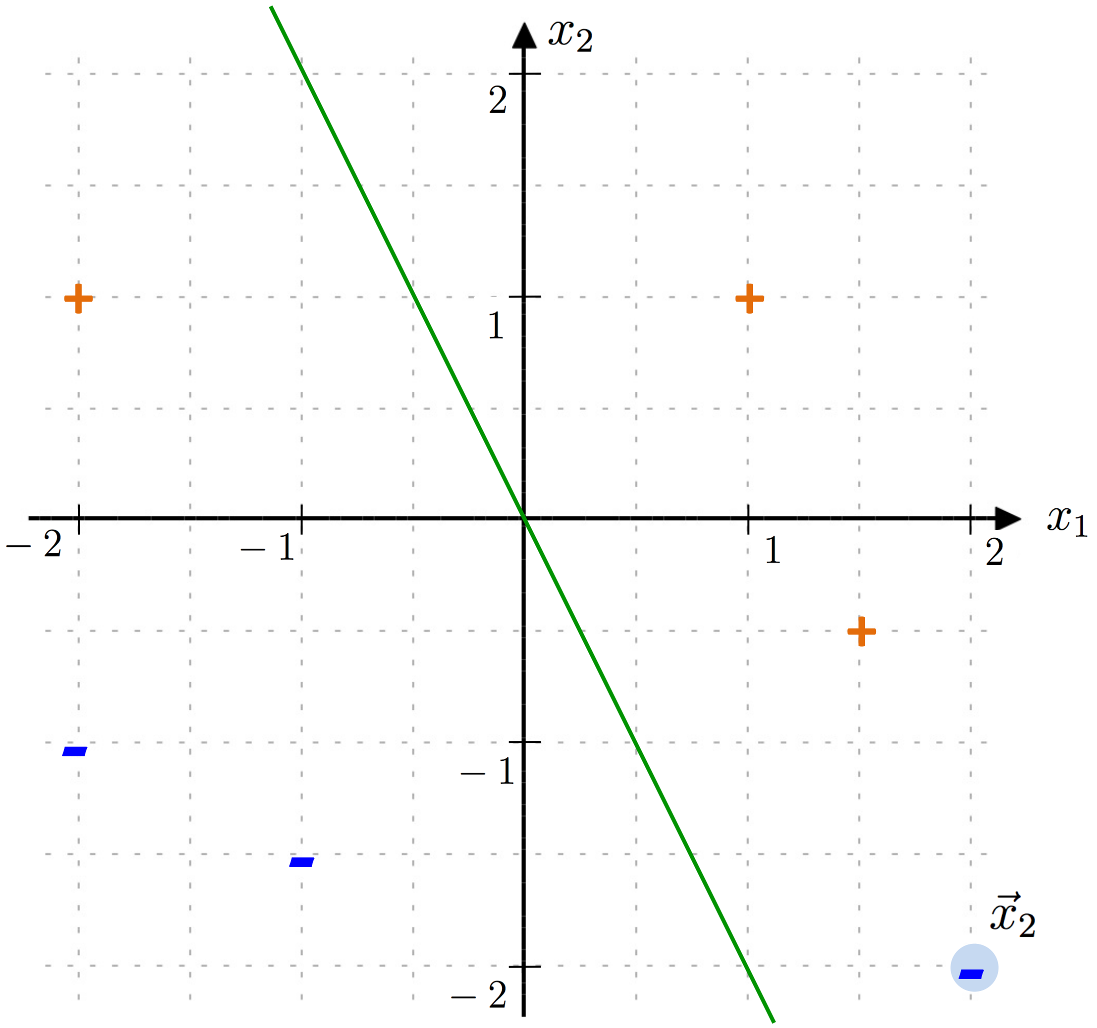
Round 2:

$$\vec{x}_2 = \begin{bmatrix} 1 \\ 2 \\ -2 \end{bmatrix}$$

$$\vec{w} \cdot \vec{x}_2 > 0$$

Incorrect classification



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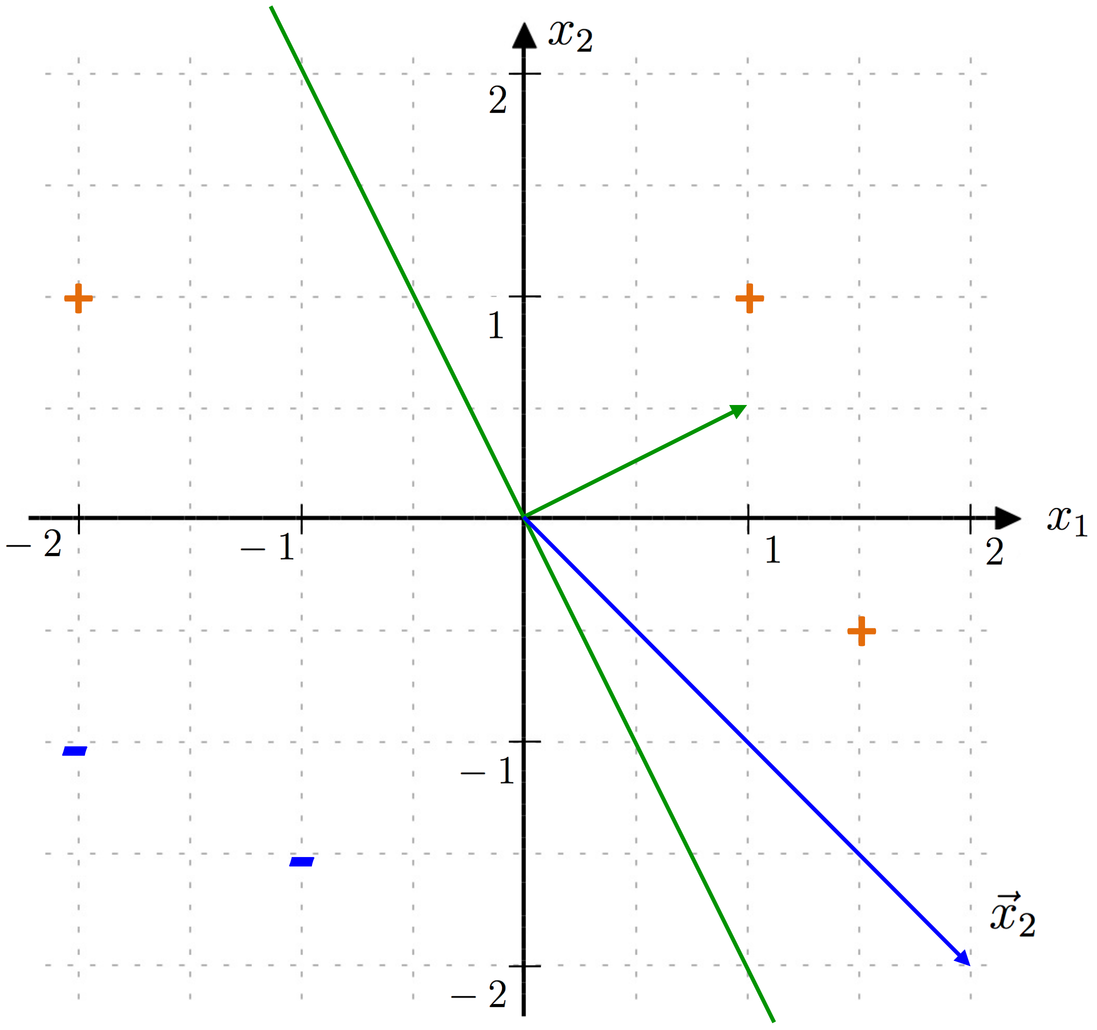

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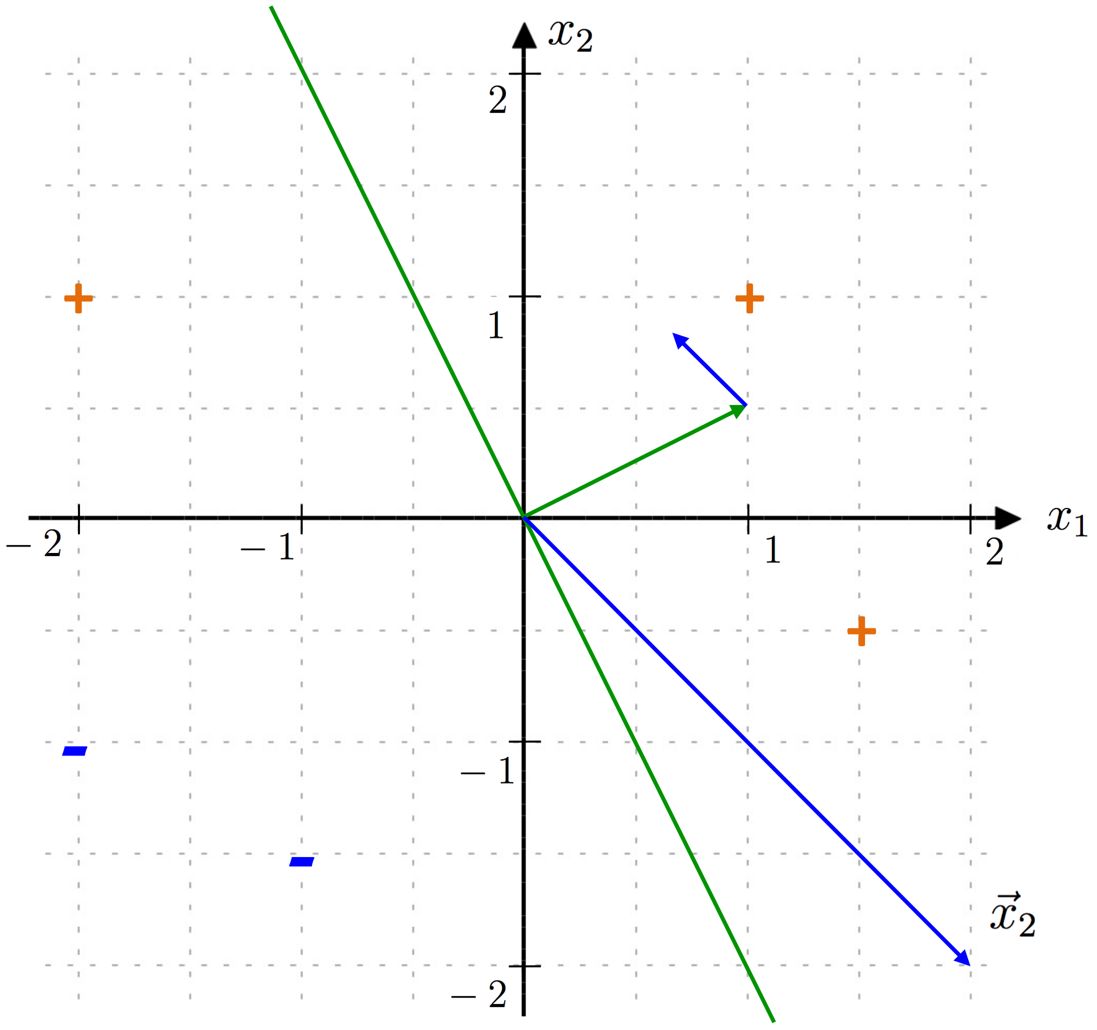
"Push" ***w*** away from negative point



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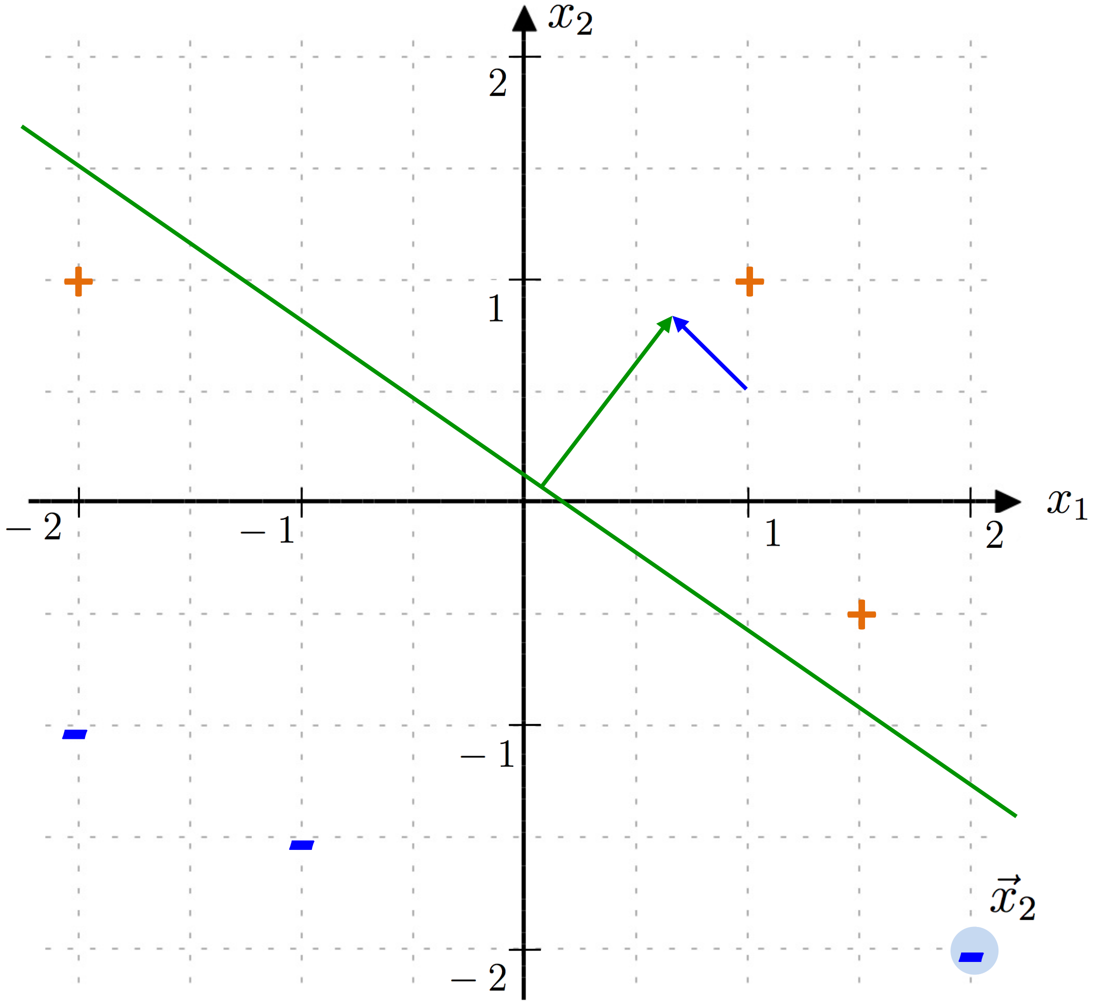

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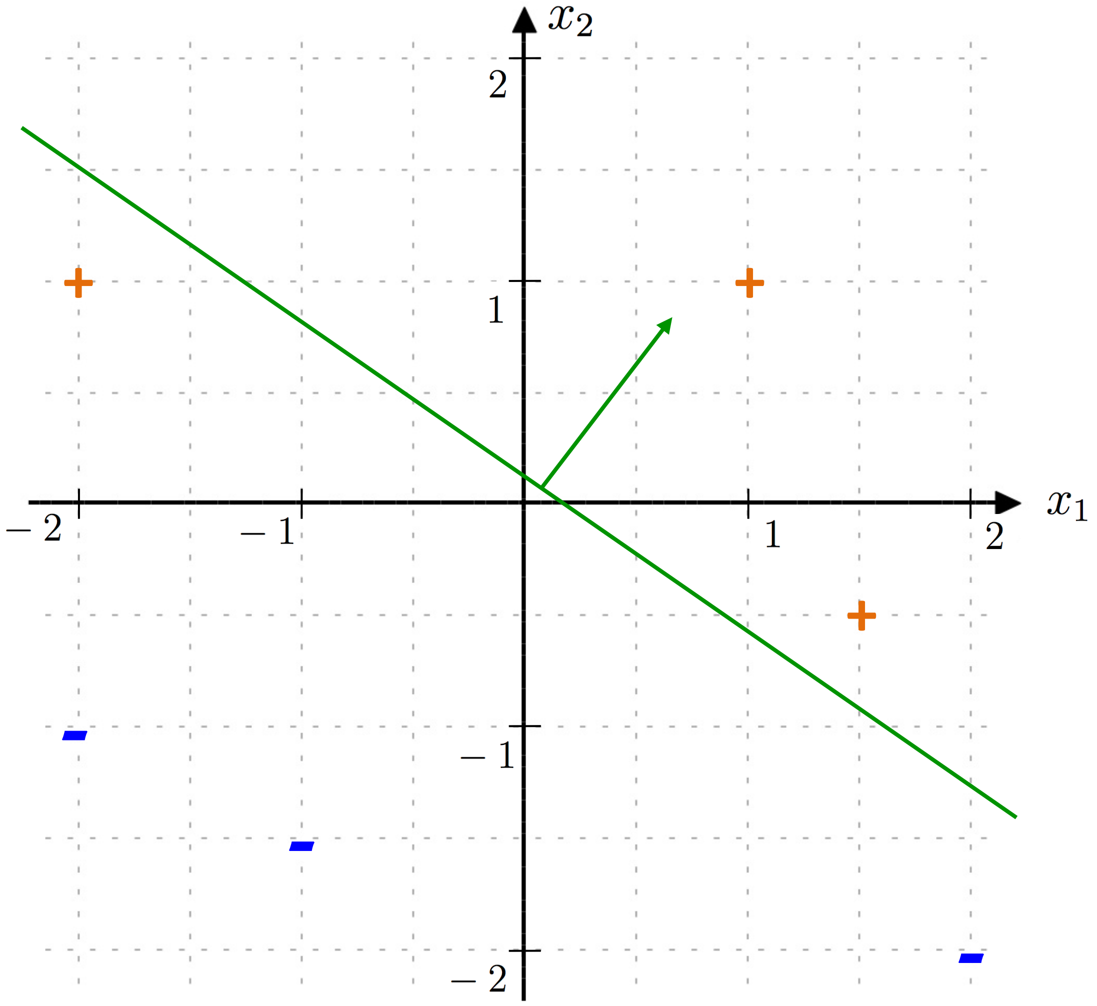
What is the new weight vector?



Handout 13 example

Final solution (so you can check your work):

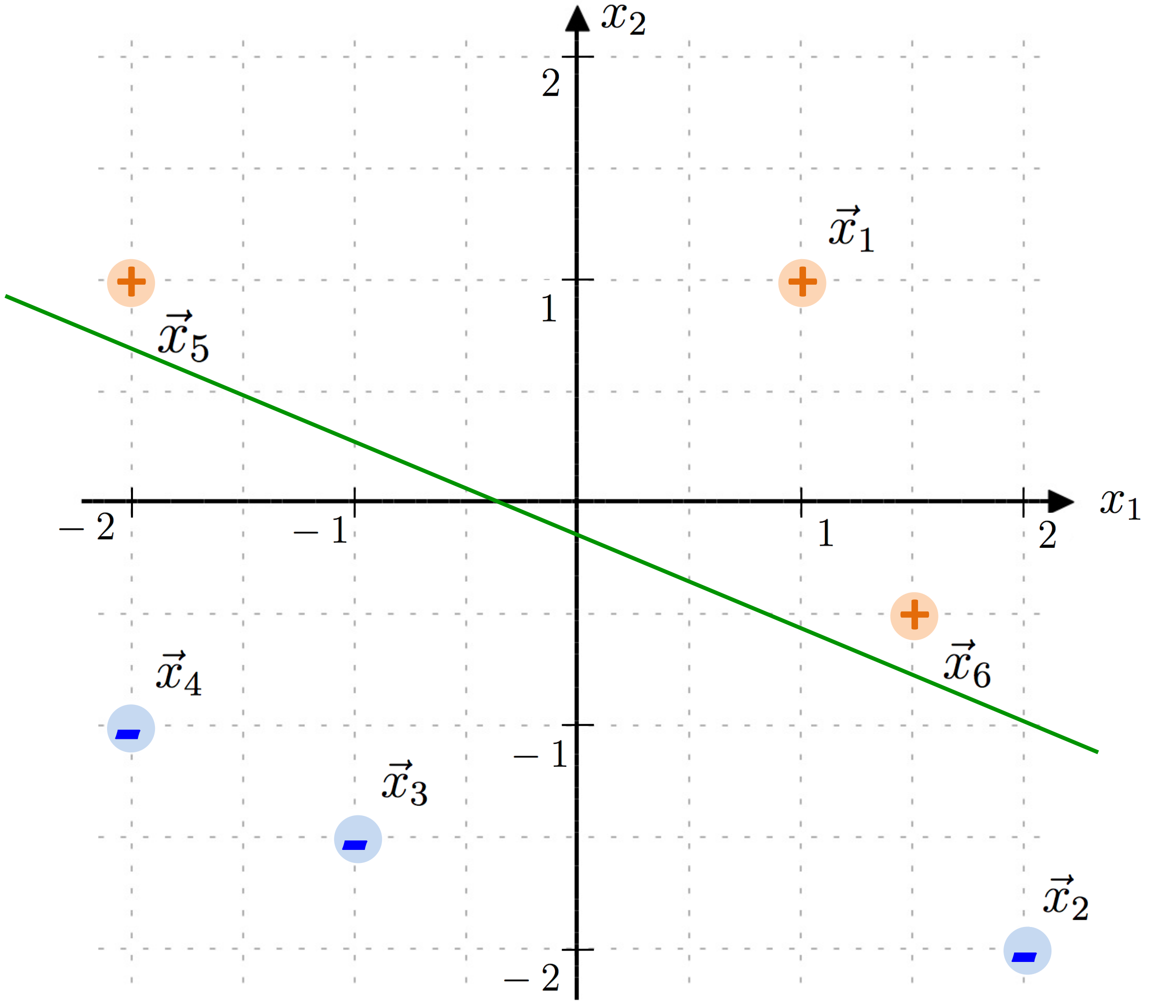
$$\vec{w}^* = \begin{bmatrix} 0.2 \\ 0.5 \\ 1 \end{bmatrix}$$

Final hyperplane:

$$0.2 + 0.5x_1 + x_2 = 0$$

$$\Rightarrow$$

$$x_2 = -0.2 - 0.5x_1$$



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Reading Quiz

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   (a) predict a continuous outcome

   (b) quantify how important each feature is for predicting the outcome

   (c) create a linear decision boundary between positives and negatives

   (d) obtain the probability of a positive label for each test example

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   No weight update!

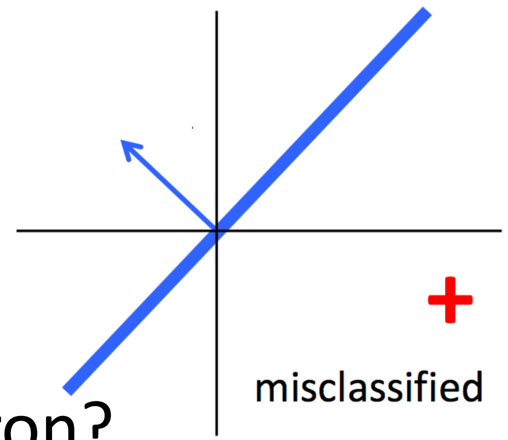
Informal discussion with a partner

1) What is the relationship between the weight vector ***w*** and the hyperplane?

2) Why is the perceptron cost function intuitive?

$$J(\vec{w}) = \sum_{i=1}^{n} \max\left(0, -y_i(\vec{w}^T\vec{x}_i)\right)$$

3) In the example to the right, how will the slope of the hyperplane change?



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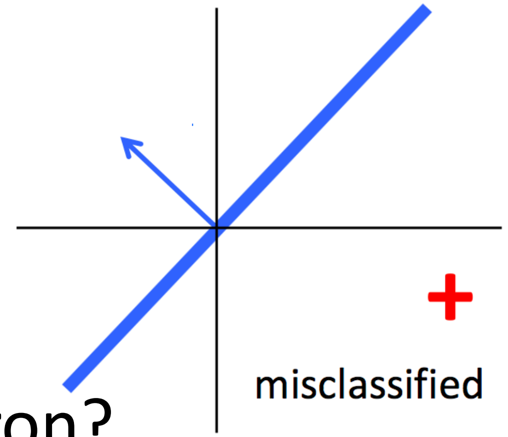

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Cost function is 0 when classification is correct, and positive when incorrect

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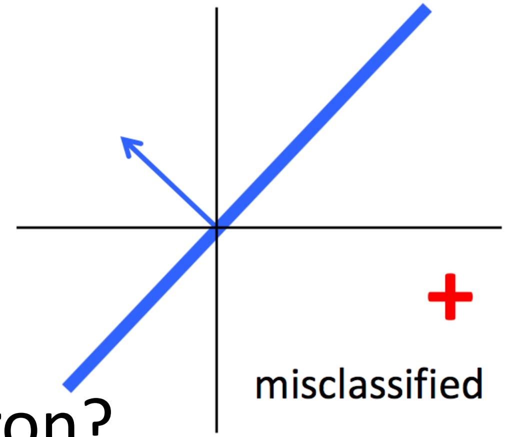

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Perceptron algorithm and intuition

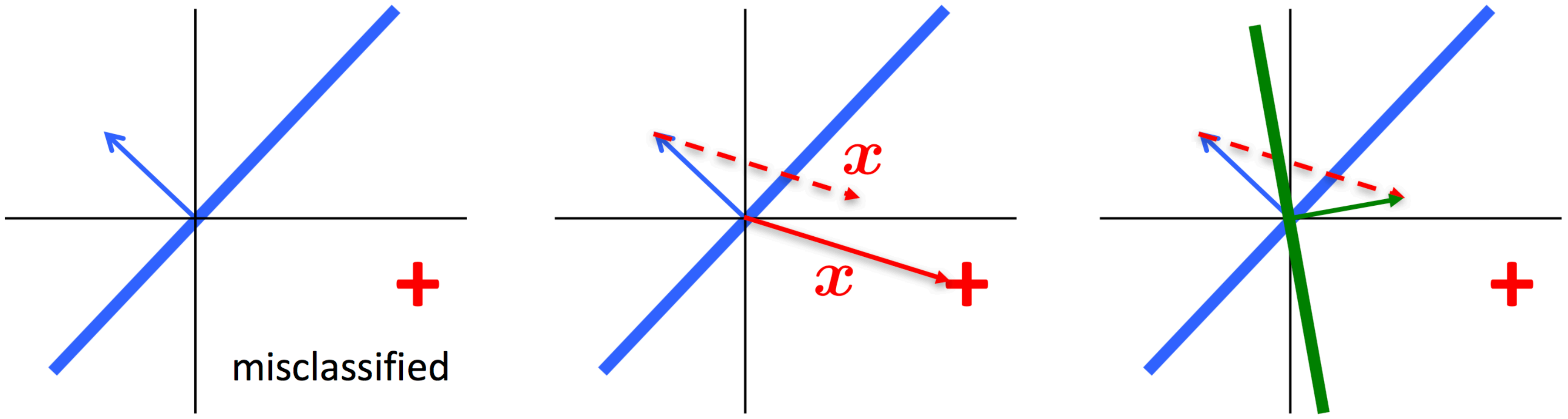
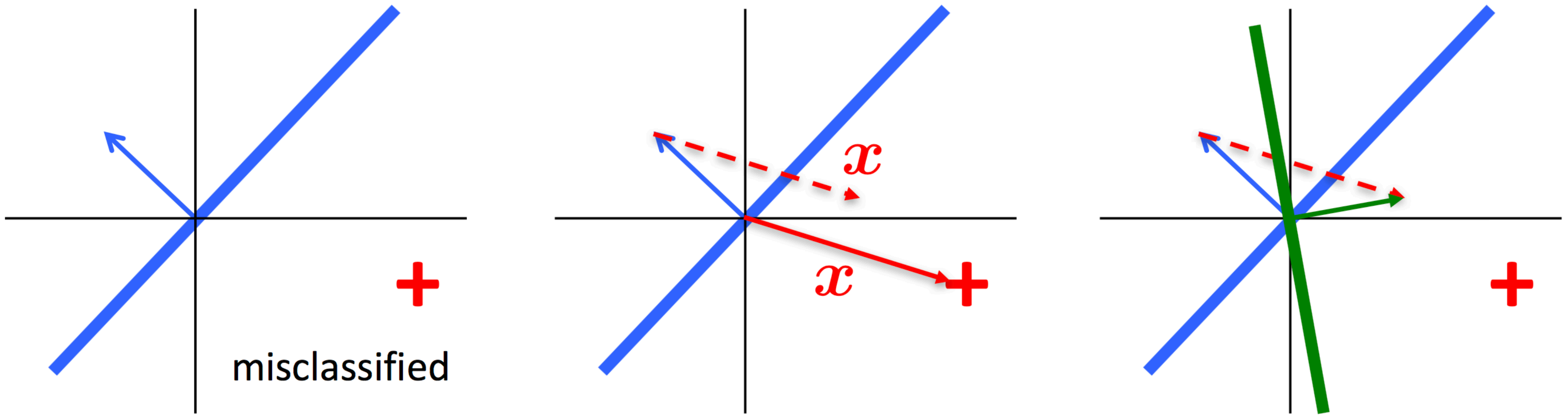


Image and Algorithm: modified from Eric Eaton

Perceptron algorithm and intuition



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Repeat until convergence:
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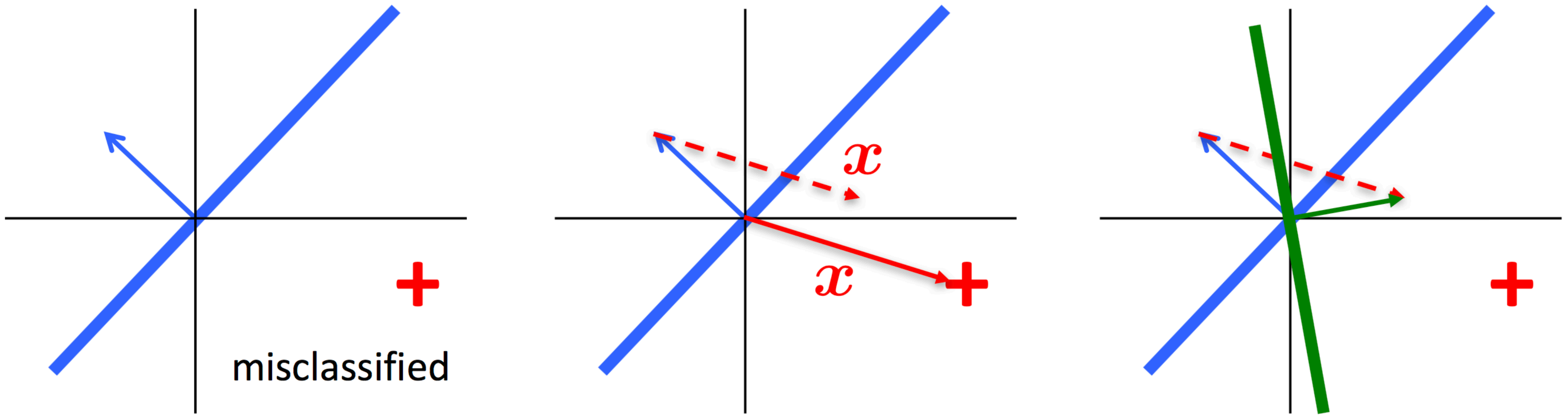

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```

Convergence:

- All data points correctly classified
- Fixed number of iterations passed

Often: alpha = 1 (only changes magnitude of weight vector)

Image and Algorithm: modified from Eric Eaton

Binary classifier wishlist

- If data is linearly separable, want a “good” hyperplane (idea: far from points close to the boundary)

- If data is not linearly separable, want something reasonable (not just give up or fail to converge)

- Might not want to constrain ourselves to linear separators

Outline: optional material on SVMs

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Support Vector Machines (SVMs)

- Will give us everything on our wishlist!
- Often considered the best “off the shelf” binary classifier
- Widely used in many fields

Brief history

- 1963: Initial idea by Vladimir Vapnik and Alexey Chervonenkis
- 1992: nonlinear SVMs by Bernhard Boser, Isabelle Guyon and Vladimir Vapnik
- 1993: “soft-margin” by Corinna Cortes and Vladimir Vapnik

Idea: “best” hyperplane has a large margin

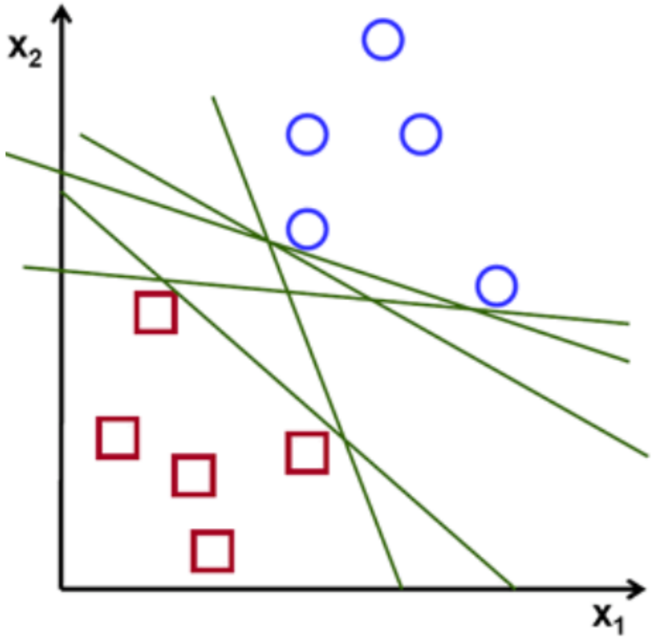

Image: “Towards Data Science”

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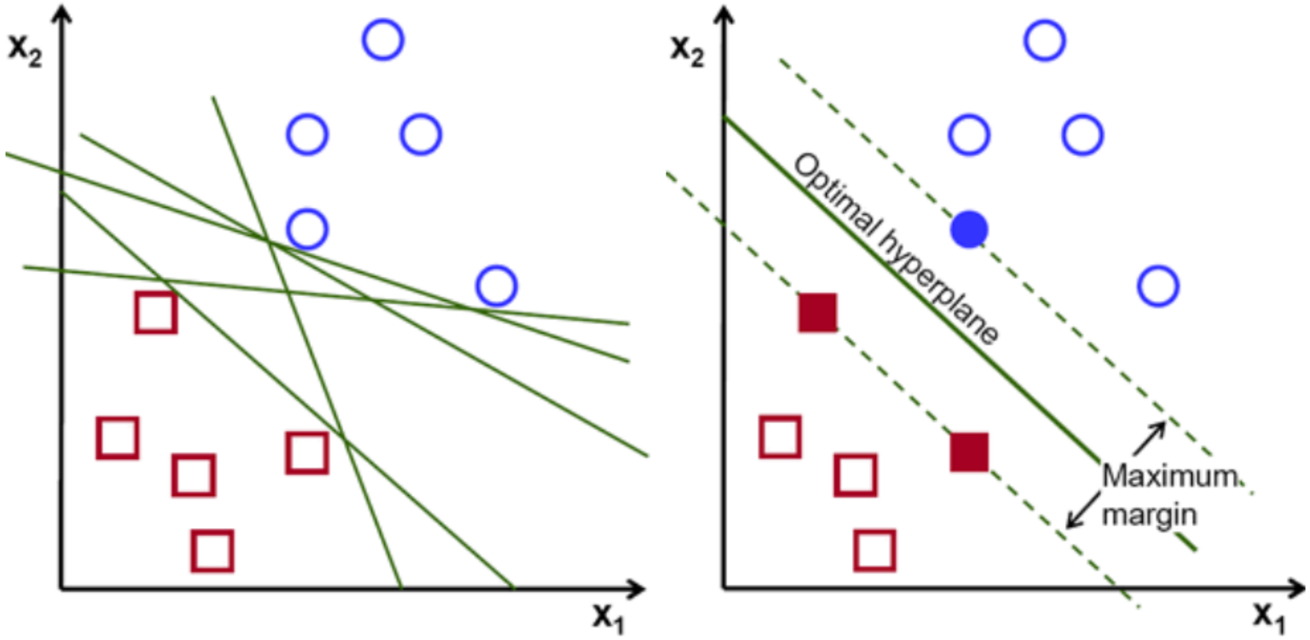

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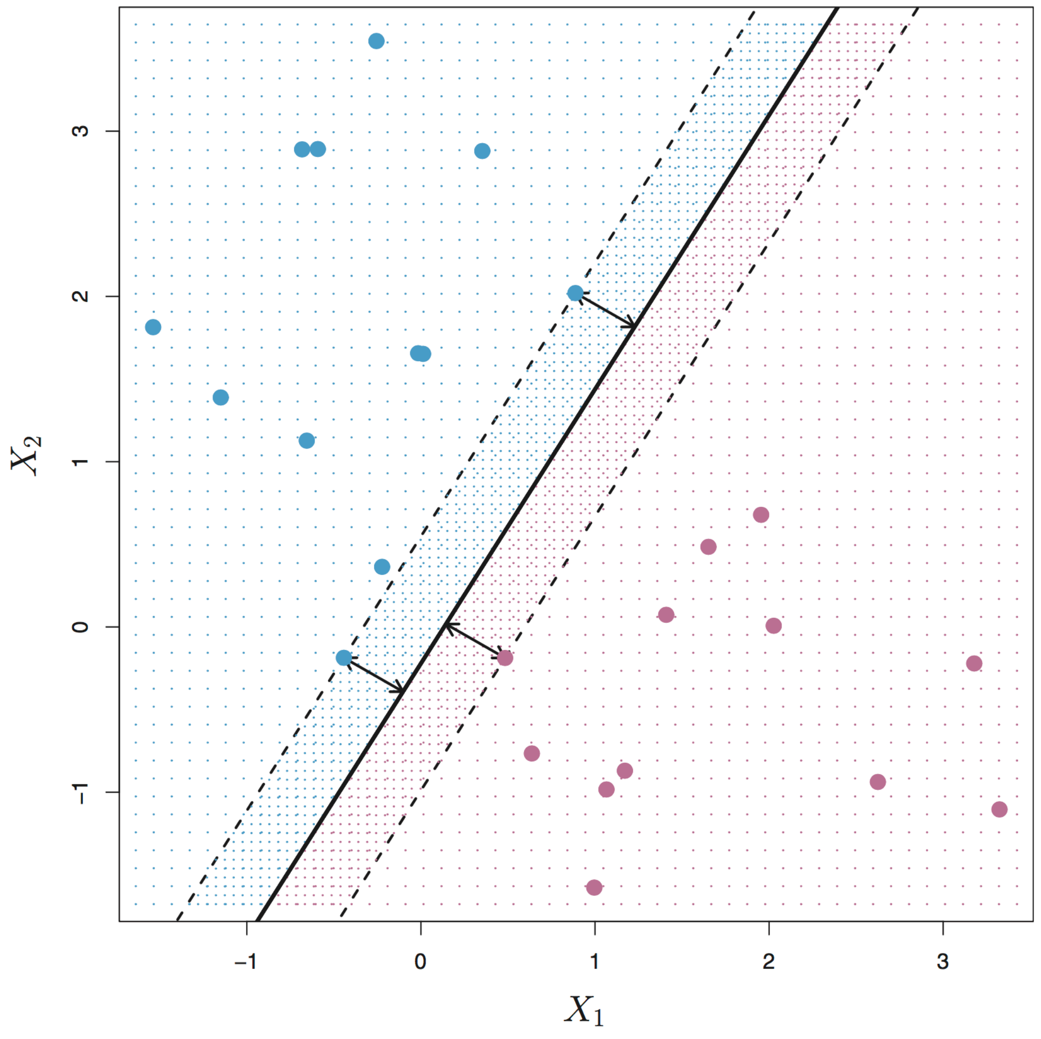
Datapoints that lie on the margin are called "support vectors"



Modified from ISL: Figure 9.3

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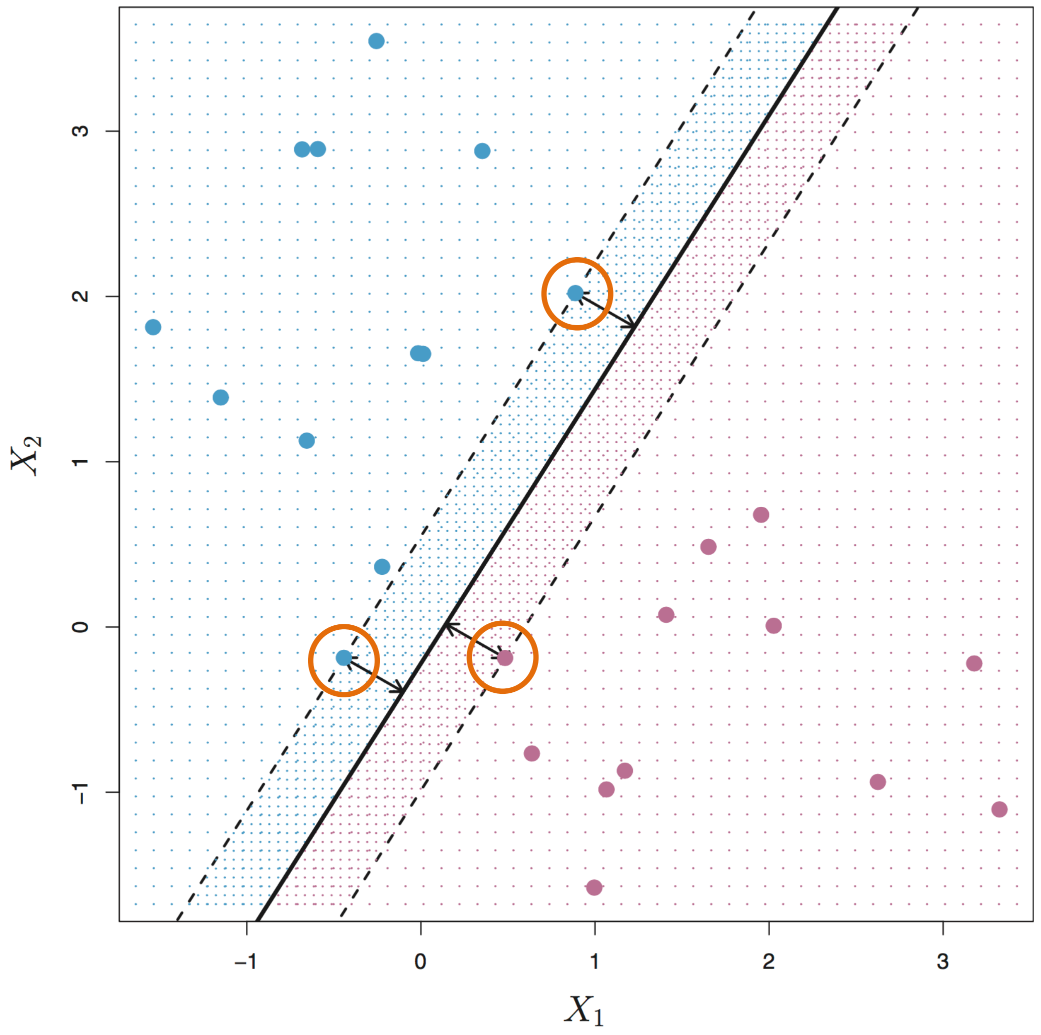

Support vectors

Modified from ISL: Figure 9.3

Functional and Geometric Margins

SVM classifier:
(same as perceptron)

$$h(\vec{x}) = \text{sign}\left(\vec{w} \cdot \vec{x} + b\right)$$

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Geometric Margin:
(distance between
example and hyperplane)

$$\gamma_i = y_i \left(\frac{\vec{w}}{||\vec{w}||} \cdot \vec{x}_i + \frac{b}{||\vec{w}||} \right)$$

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Note:

$$\boxed{\gamma_i = \frac{\hat{\gamma}_i}{||\vec{w}||}}$$

Optimization Problem: try 1

Goal: maximize the minimum distance between example and hyperplane

$$\gamma = \min_{i=1,\cdots,n} \gamma_i$$

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Formulation: optimize a function with respect to a constraint

$$\begin{aligned} \max_{\gamma,\vec{w},b} \quad & \gamma \\ \text{s.t.} \quad & y_i(\vec{w}\cdot\vec{x}_i + b) \geq \gamma, \quad i = 1,\cdots,n \\ \text{and} \quad & \|\vec{w}\| = 1 \end{aligned}$$

(force functional and geometric margin to be equal)

Optimization Problem: try 2

Idea: substitute functional margin divided by magnitude of weight vector

$$\max_{\hat{\gamma},\vec{w},b} \quad \frac{\hat{\gamma}}{\|\vec{w}\|}$$

$$\text{s.t.} \quad y_i(\vec{w}\cdot\vec{x}_i + b) \geq \hat{\gamma}, \quad i = 1,\cdots,n$$

(gets rid of non-convex constraint)

Optimization Problem: try 3

Idea: put arbitrary constraint on functional margin

$$\boxed{\hat{\gamma} = 1}$$

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

$$\text{s.t.} \quad y_i(\vec{w}\cdot\vec{x}_i + b) \geq 1, \quad i = 1, \cdots, n$$

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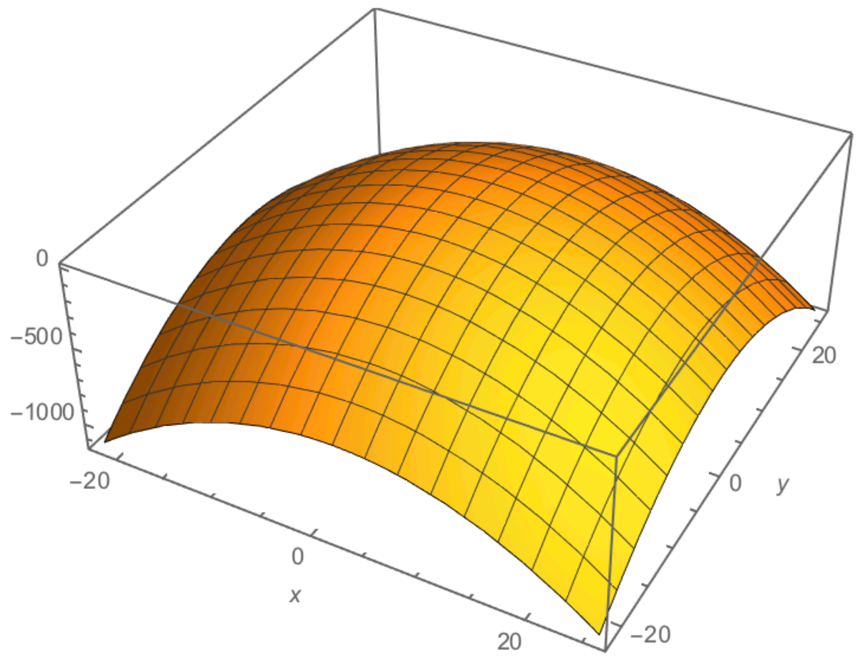
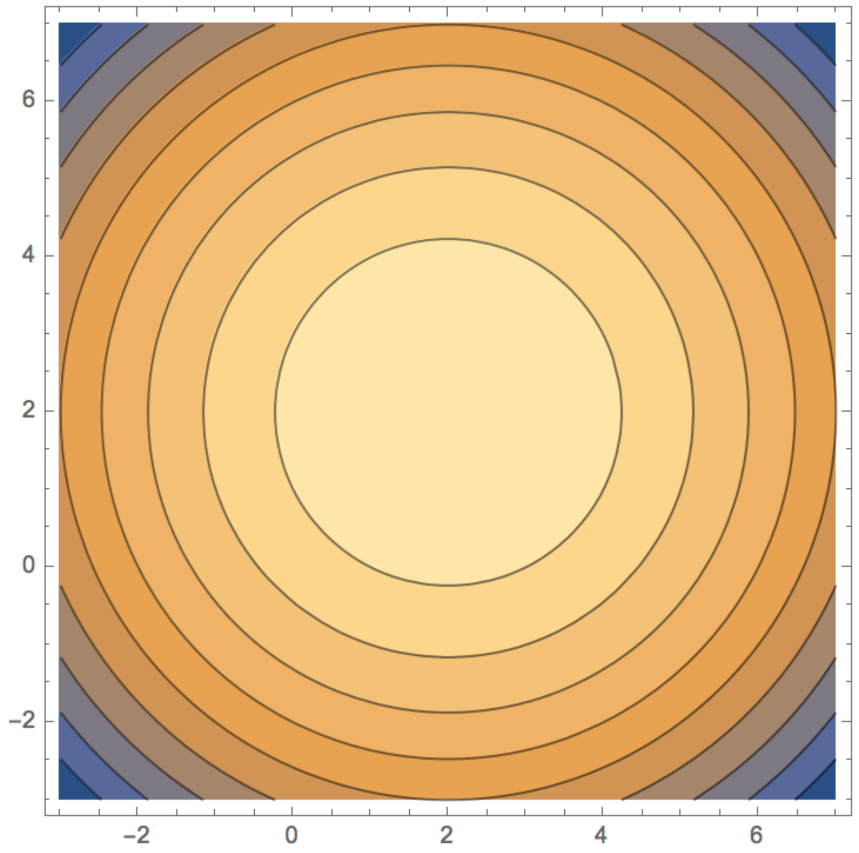
Lagrange multipliers example

$$f(x,y) = 5 - (x-2)^2 - (y-2)^2$$



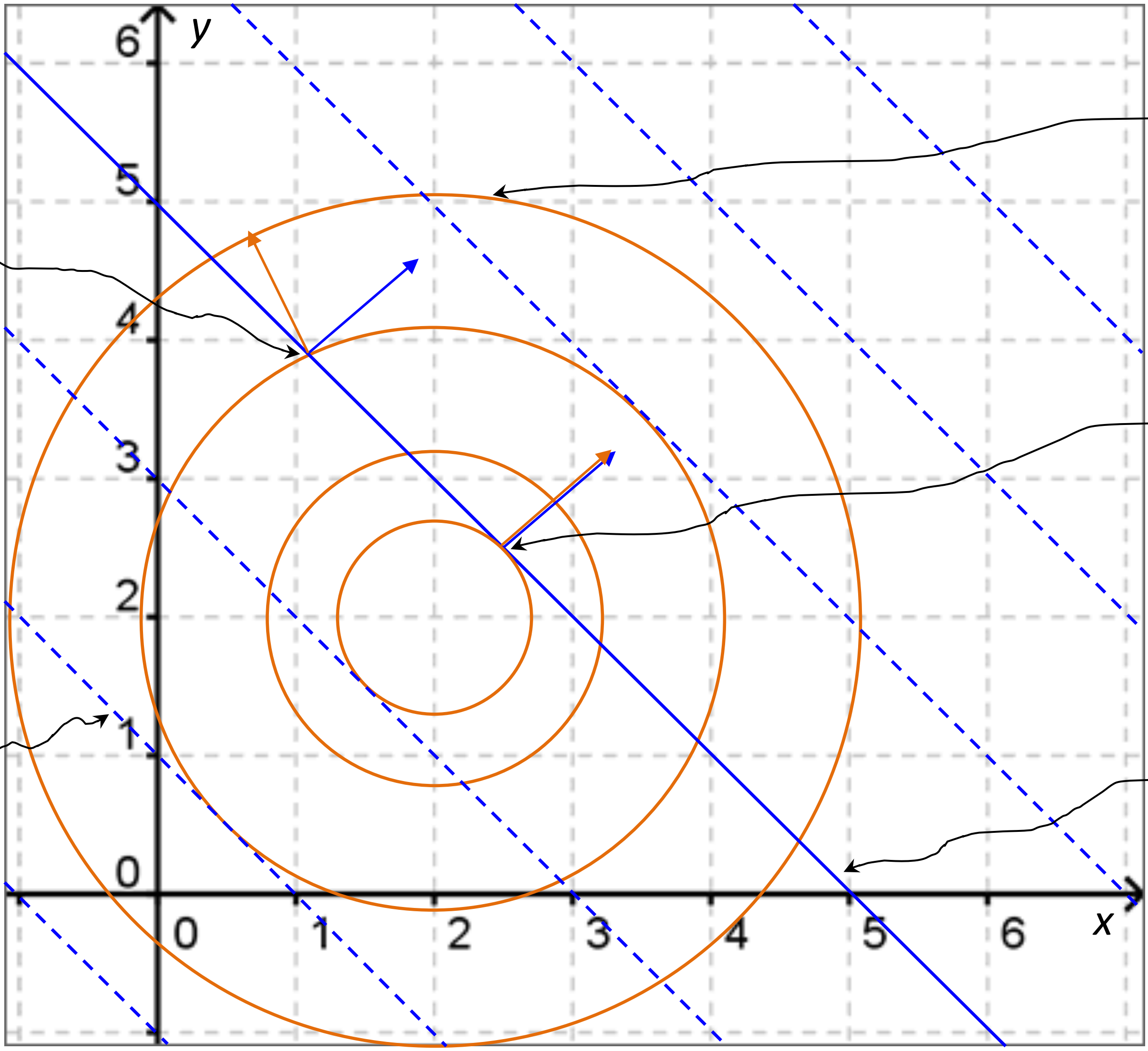


Contour plot of *f*(*x*,*y*)

$$\begin{aligned} &\text{maximize}_{x,y} \quad f(x,y) \\ &s.t. \quad g(x,y) = 0 \end{aligned}$$

$$g(x,y) = -5 + x + y$$

Lagrange multipliers example



Normals (and derivatives) **not** parallel

level curves of $f(x,y)$

<u>SOLUTION</u>: Normals (and derivatives) parallel

x = 2.5

y = 2.5

level curves of $g(x,y)$

$g(x,y) = 0$

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Kernel Idea

- By solving the dual form of the problem, we have seen how all computations can be done in terms of inner products between examples

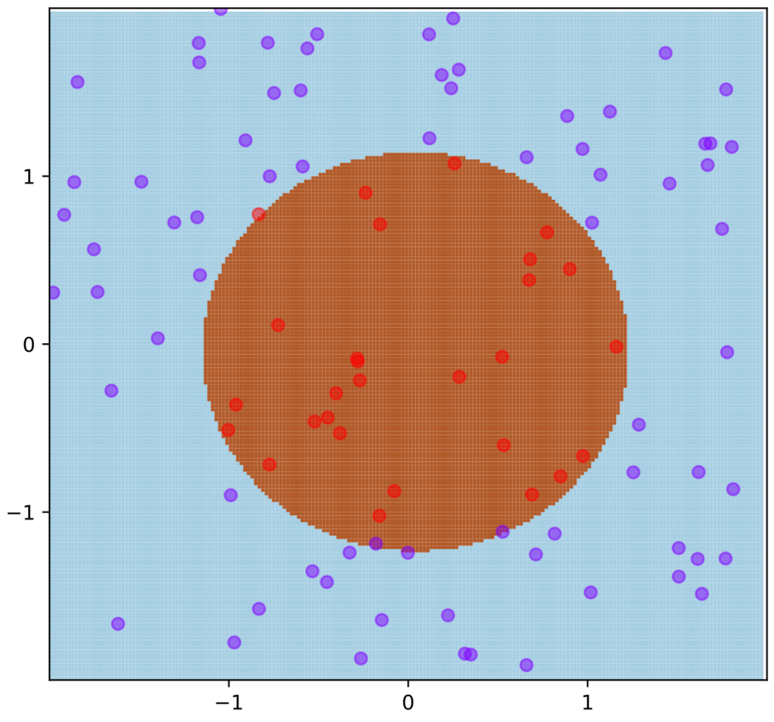
- One example of an inner product is the dot product, which is the linear version of SVMs

- But there are many others!

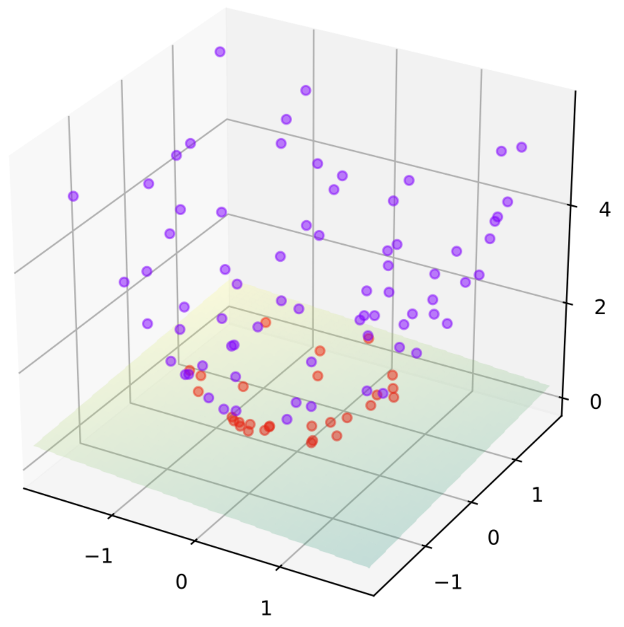
- Intuition: if points are close together, their kernel function will have a large value (measure of similarity)

Kernel Trick example

Feature mapping: $\varphi(\boldsymbol{x}) = (x_1,\ x_2,\ x_1^2 + x_2^2)$



Original feature space



Mapping after applying kernel
(can now find a hyperplane)

Kernel function: $K(\boldsymbol{x},\ \boldsymbol{z}) = \boldsymbol{x}\bullet\boldsymbol{z} + \|\boldsymbol{x}\|^2\,\|\boldsymbol{z}\|^2$

Image: Shiyu Ji (wikipedia)

Gaussian Kernel

- Gaussian kernel is near 0 when points are far apart and near 1 when they are similar
- Also called Radial Basis Function (RBF) kernel

$$K(\vec{x}, \vec{z}) = \exp\left(-\frac{\|\vec{x} - \vec{z}\|^2}{2\sigma^2}\right)$$

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$$K(\vec{x}, \vec{z}) = \exp\left(-\frac{\|\vec{x} - \vec{z}\|^2}{2\sigma^2}\right)$$

Often re-parametrized by gamma (different gamma!)

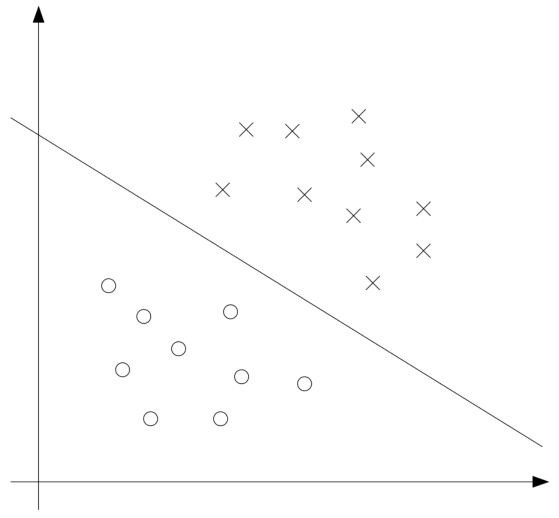
$$\boxed{\gamma = \frac{1}{2\sigma^2}}$$

$$K(\vec{x}, \vec{z}) = \exp\left(-\gamma\|\vec{x} - \vec{z}\|^2\right)$$

Soft-margin SVMs (non-separable case)

- Idea: we will use regularization to add a cost for each point being incorrectly classified by the hyperplane

- Hopefully many costs will be 0, but we can accommodate a few outliers



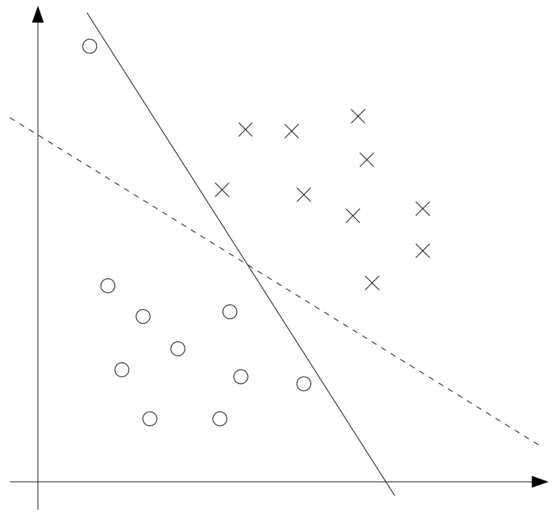


Figure: Andrew Ng

Soft-margin SVMs (non-separable case)

- New optimization problem with regularization

$$\min_{\xi,\vec{w},b} \quad \frac{1}{2}\|\vec{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

"flexible margin"

$$\text{s.t.} \quad y_i(\vec{w}\cdot\vec{x}_i + b) \geq 1 - \xi_i, \quad i = 1,\cdots,n$$

$$\text{and} \quad \xi_i \geq 0, \quad i = 1,\cdots,n$$

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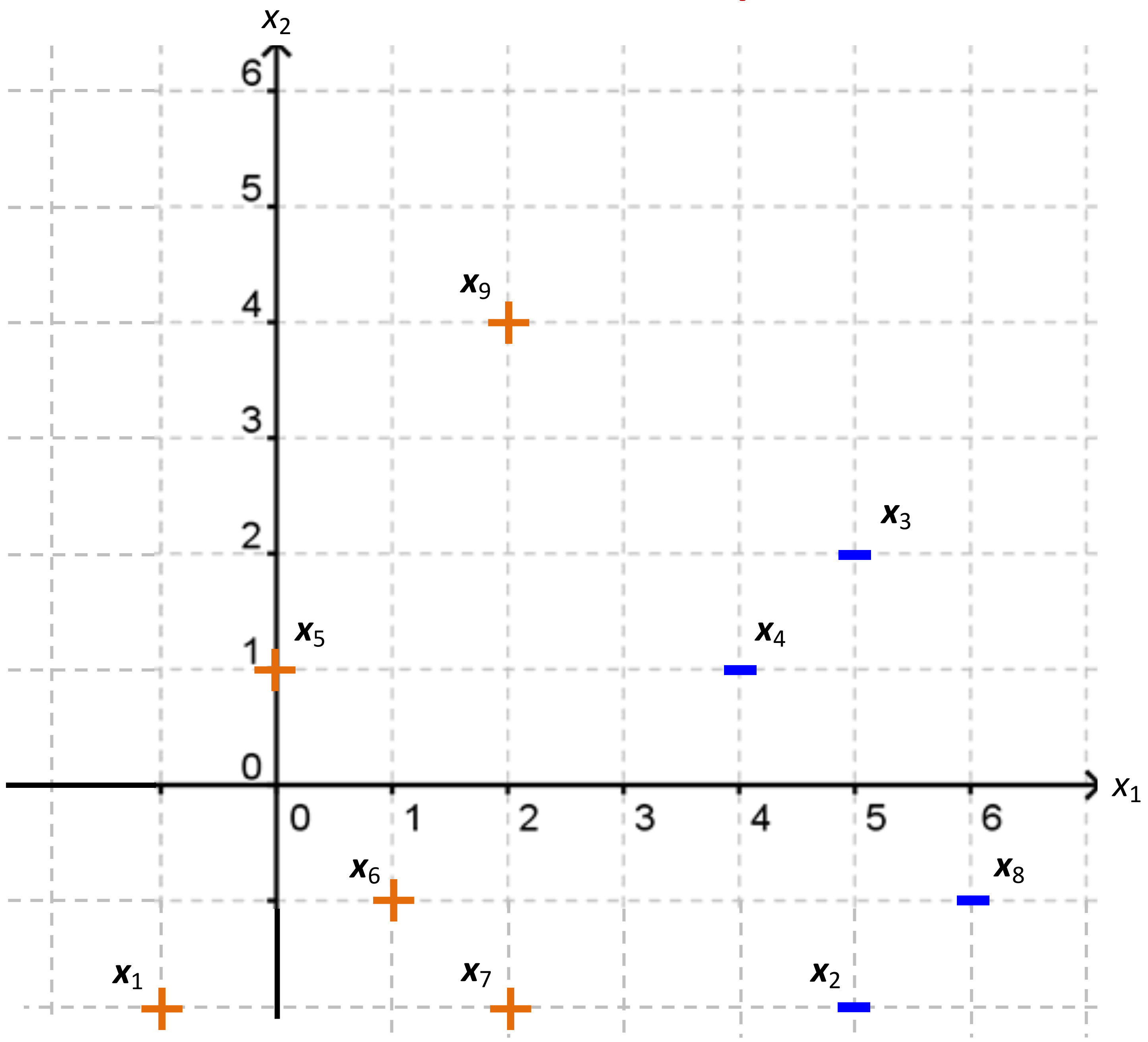
- Incremental SVM optimization algorithm
- Choose a subset S of examples and run optimization to get alpha values
- Identify which alpha values are 0 => these cannot be support vectors in final solution!
- Discard these points and add new ones; repeat

Meta-optimization: example



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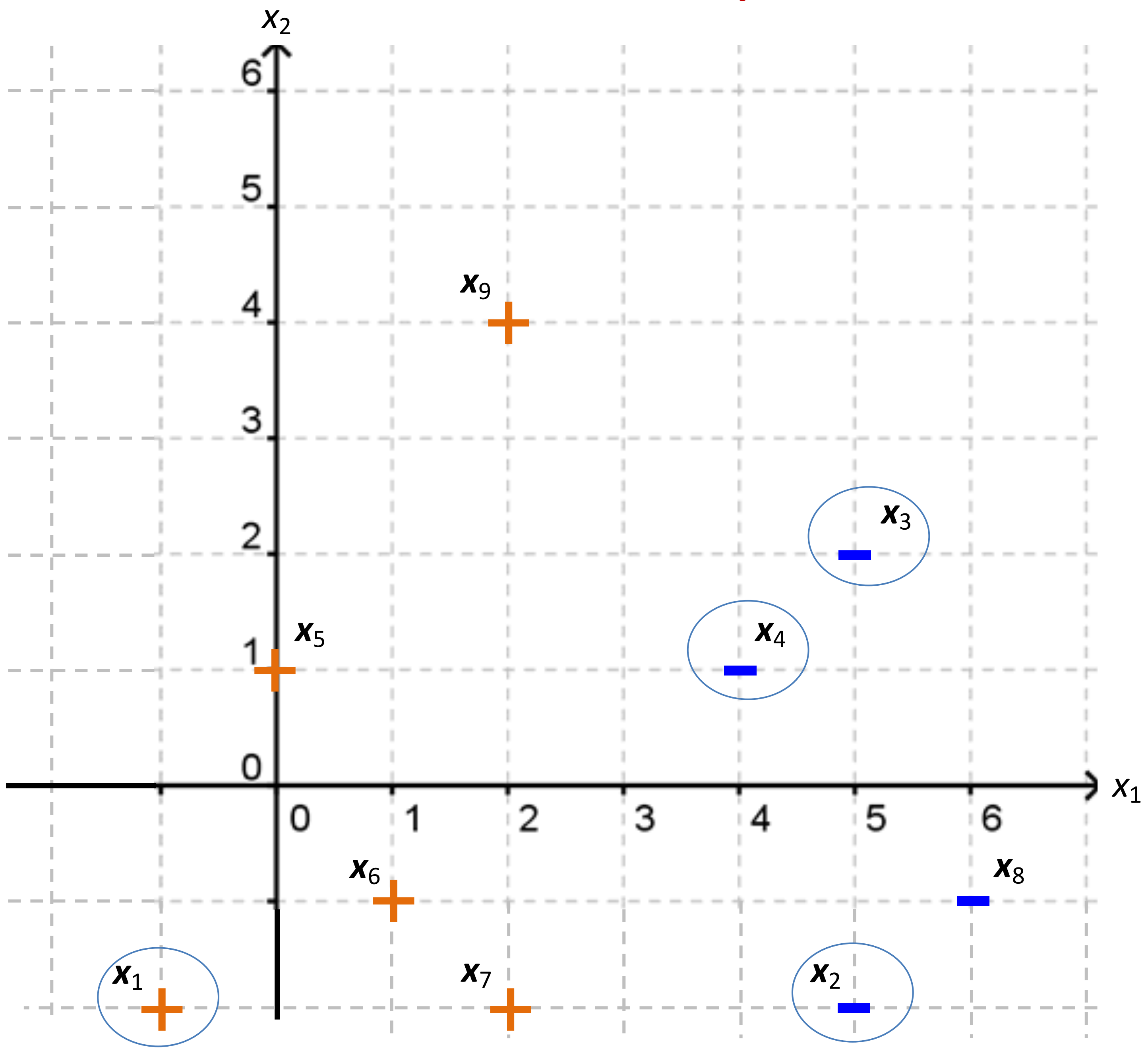
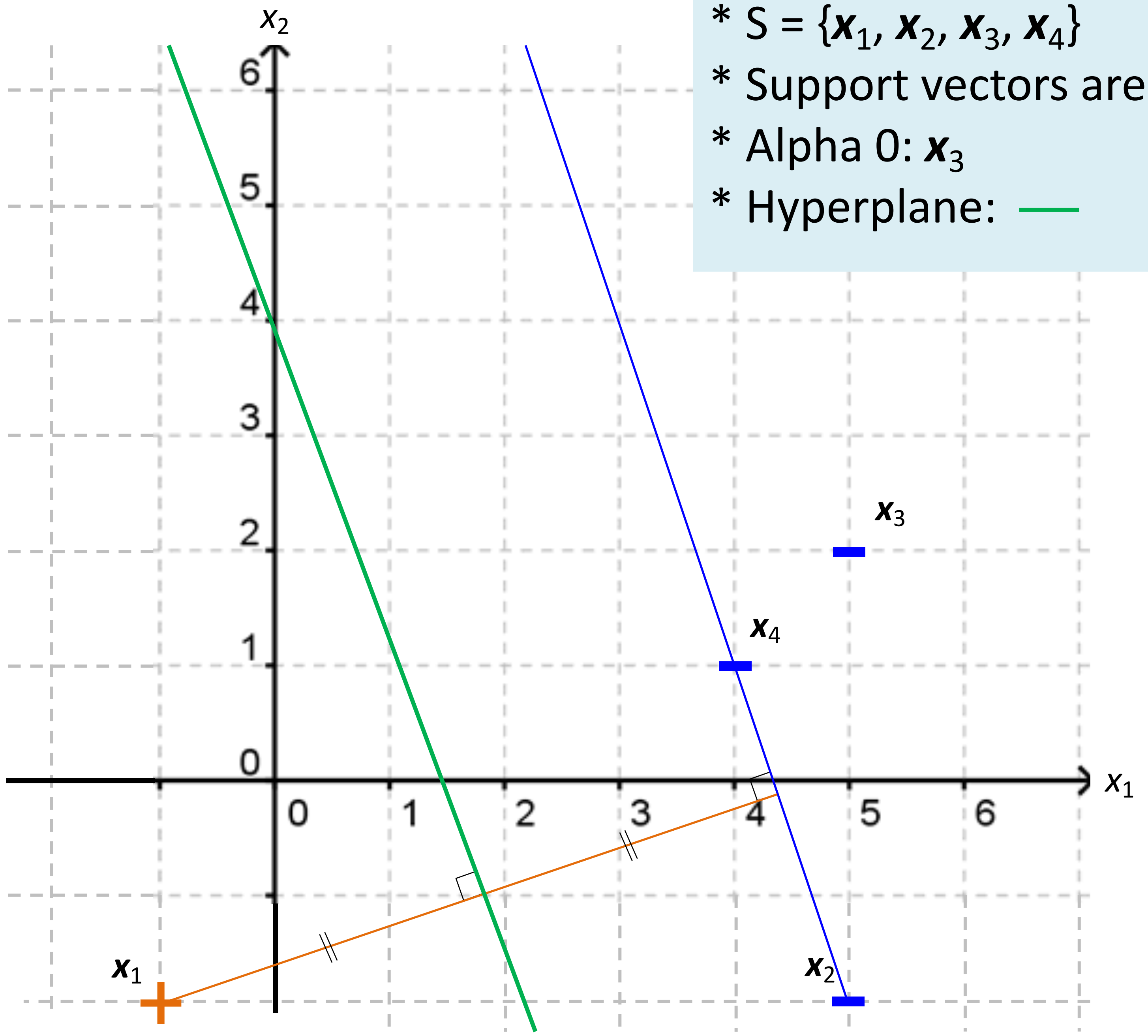
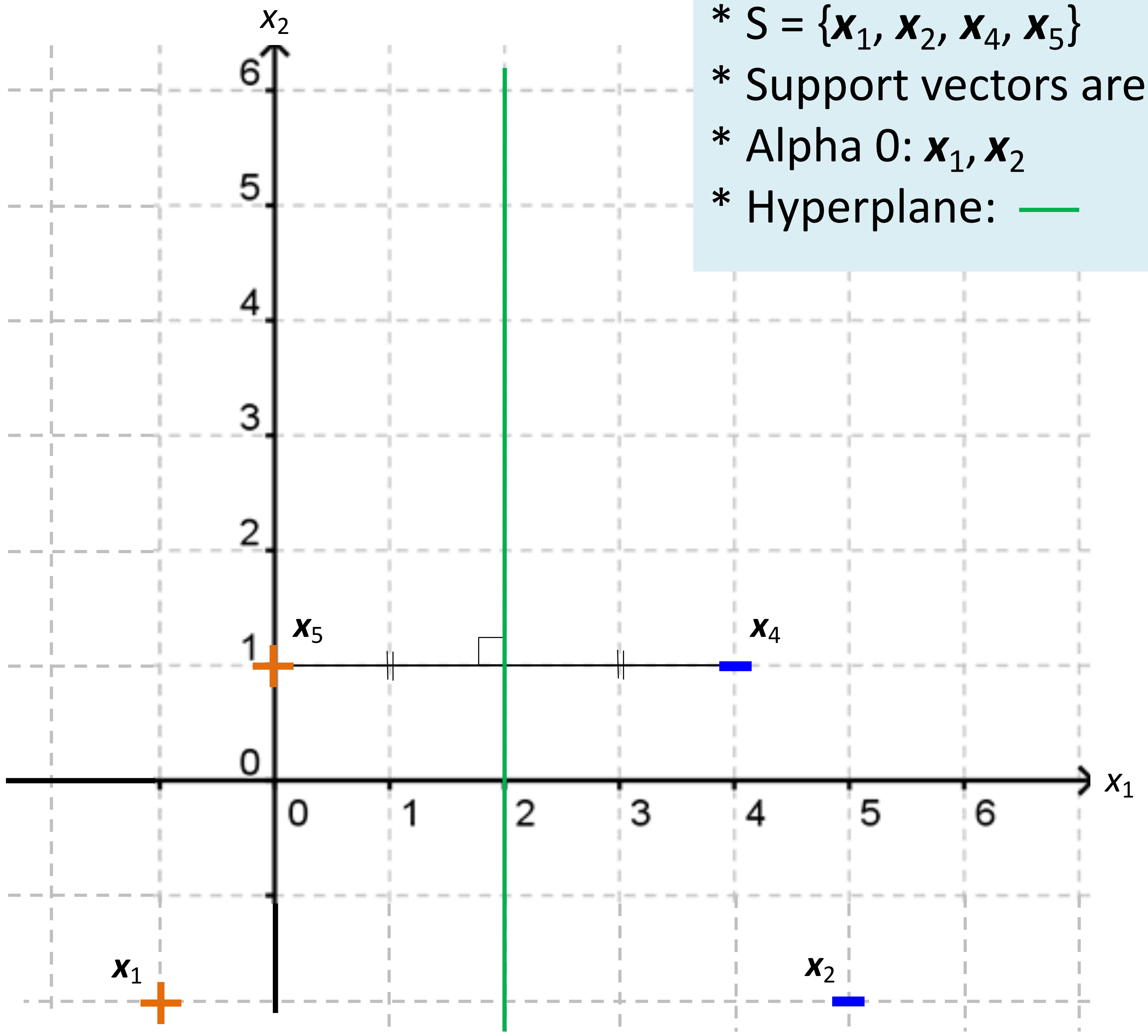


$K = 4$

Round 1:

* S = {$\boldsymbol{x}_1$, $\boldsymbol{x}_2$, $\boldsymbol{x}_3$, $\boldsymbol{x}_4$}
* Support vectors are: $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, $\boldsymbol{x}_4$
* Alpha 0: $\boldsymbol{x}_3$
* Hyperplane: 🟩



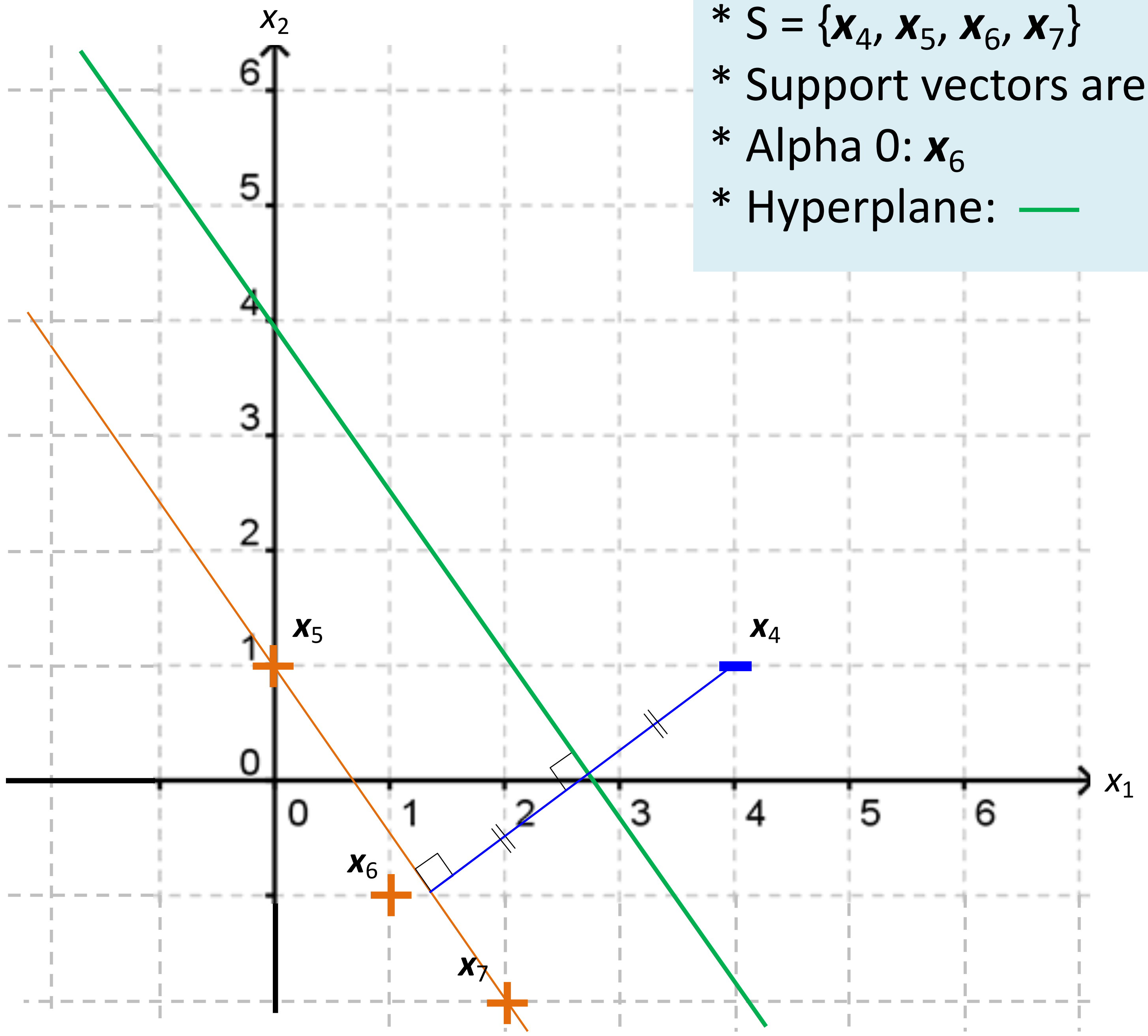


Round 1:

* S = $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_4, \boldsymbol{x}_5\}$
* Support vectors are: $\boldsymbol{x}_4$, $\boldsymbol{x}_5$
* Alpha 0: $\boldsymbol{x}_1$, $\boldsymbol{x}_2$
* Hyperplane: 🟩

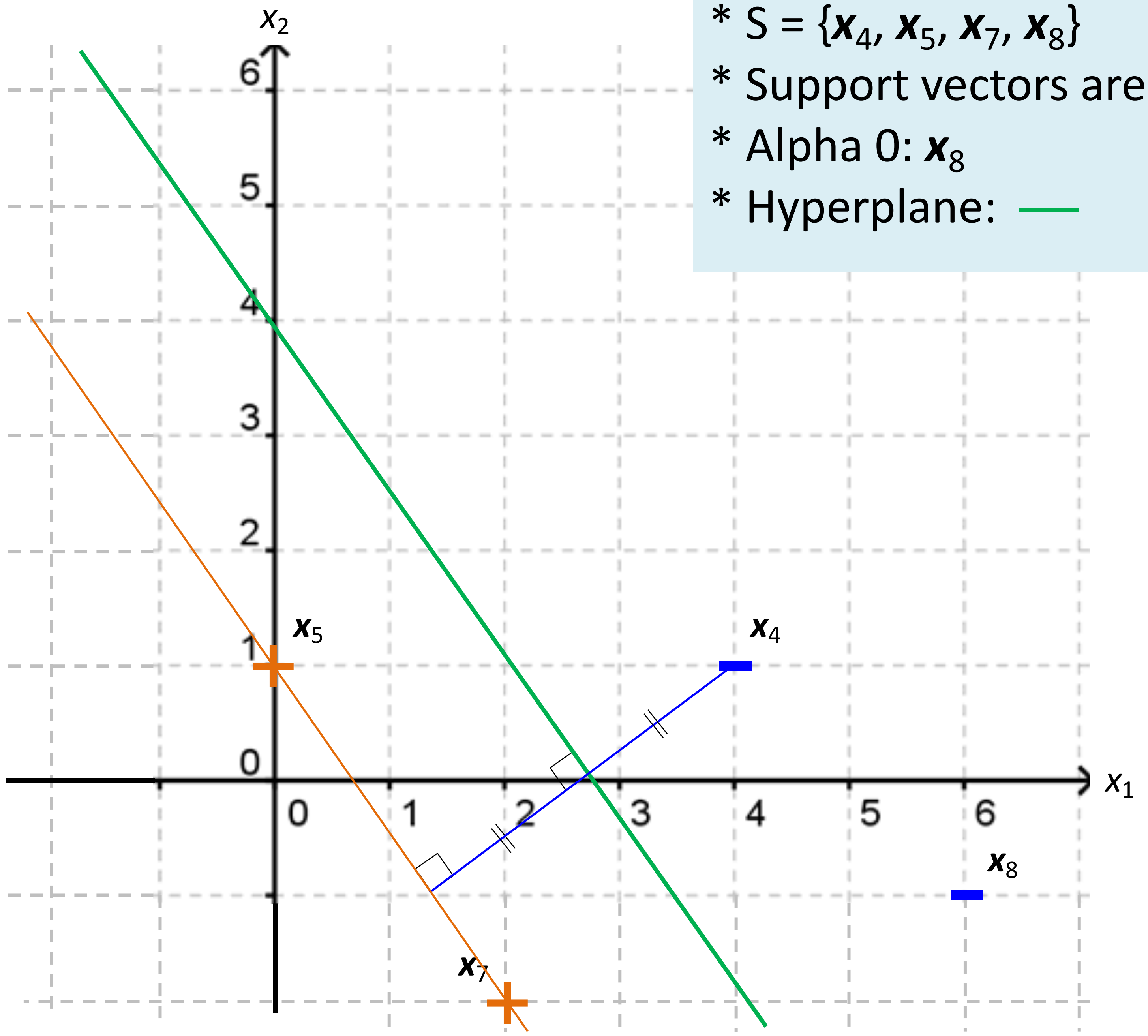
Round 3:

* S = {$\boldsymbol{x}_4$, $\boldsymbol{x}_5$, $\boldsymbol{x}_6$, $\boldsymbol{x}_7$}
* Support vectors are: $\boldsymbol{x}_4$, $\boldsymbol{x}_5$, $\boldsymbol{x}_7$
* Alpha 0: $\boldsymbol{x}_6$
* Hyperplane: —



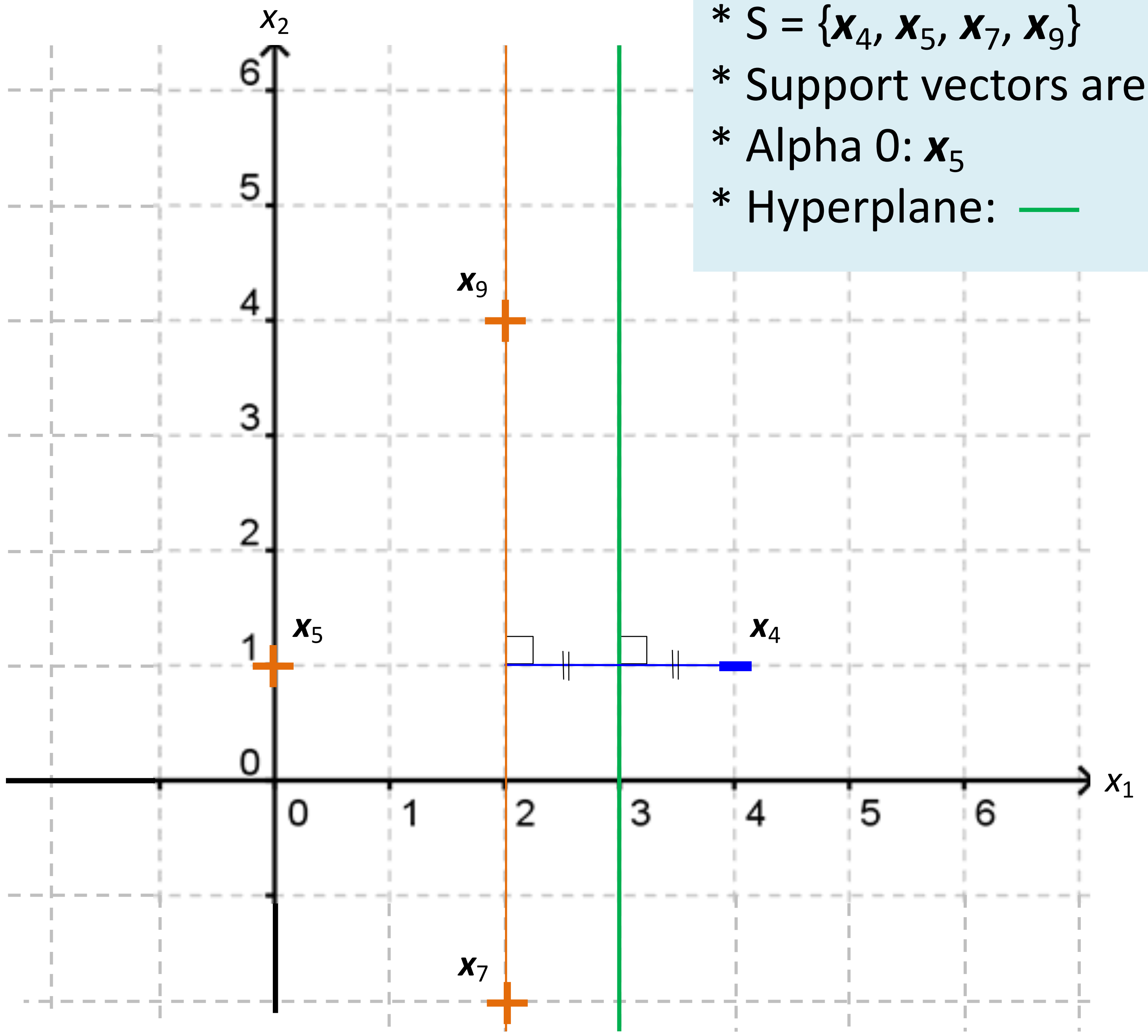
Round 4:

* S = {$\boldsymbol{x}_4$, $\boldsymbol{x}_5$, $\boldsymbol{x}_7$, $\boldsymbol{x}_8$}
* Support vectors are: $\boldsymbol{x}_4$, $\boldsymbol{x}_5$, $\boldsymbol{x}_7$
* Alpha 0: $\boldsymbol{x}_8$
* Hyperplane: 🟩

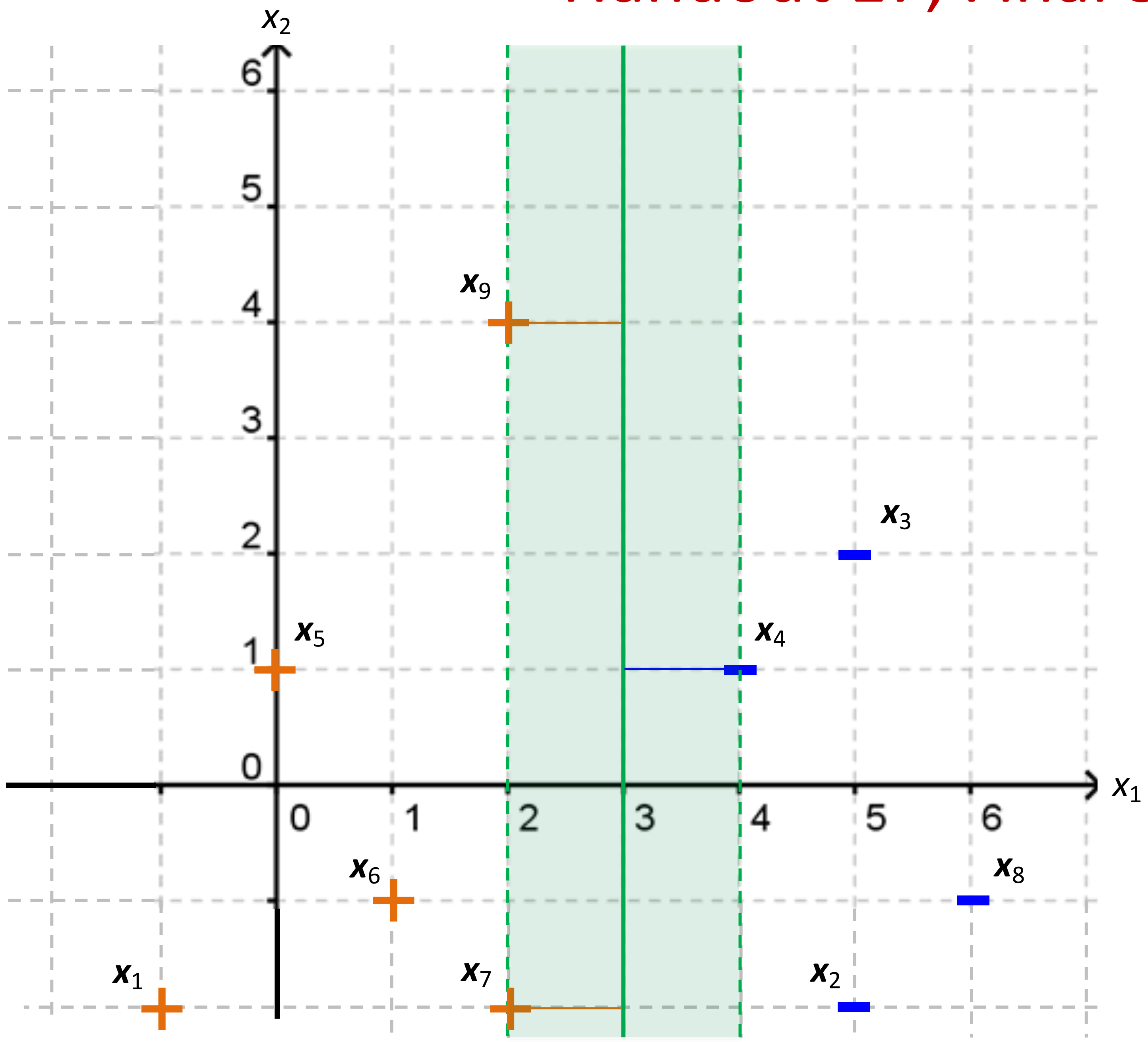


Round 5:

* S = {$\boldsymbol{x}_4$, $\boldsymbol{x}_5$, $\boldsymbol{x}_7$, $\boldsymbol{x}_9$}
* Support vectors are: $\boldsymbol{x}_4$, $\boldsymbol{x}_7$, $\boldsymbol{x}_9$
* Alpha 0: $\boldsymbol{x}_5$
* Hyperplane: 🟩



Handout 17, Final Solution



Reading Quiz #8

1. If $\vec{x}_i$ is a support vector, what can we say about it? Circle all that apply:

   (a) its Lagrange multiplier $\alpha_i > 0$

   (b) its Lagrange multiplier $\alpha_i = 0$

   (c) $y_i(\vec{w} \cdot \vec{x}_i + b) = 0$

   (d) $y_i(\vec{w} \cdot \vec{x}_i + b) = 1$

   (e) $\vec{x}_i$ lies on the margin

Reading Quiz #8

1. If $\vec{x}_i$ is a support vector, what can we say about it? Circle all that apply:

   [✓ (a) its Lagrange multiplier $\alpha_i > 0$]

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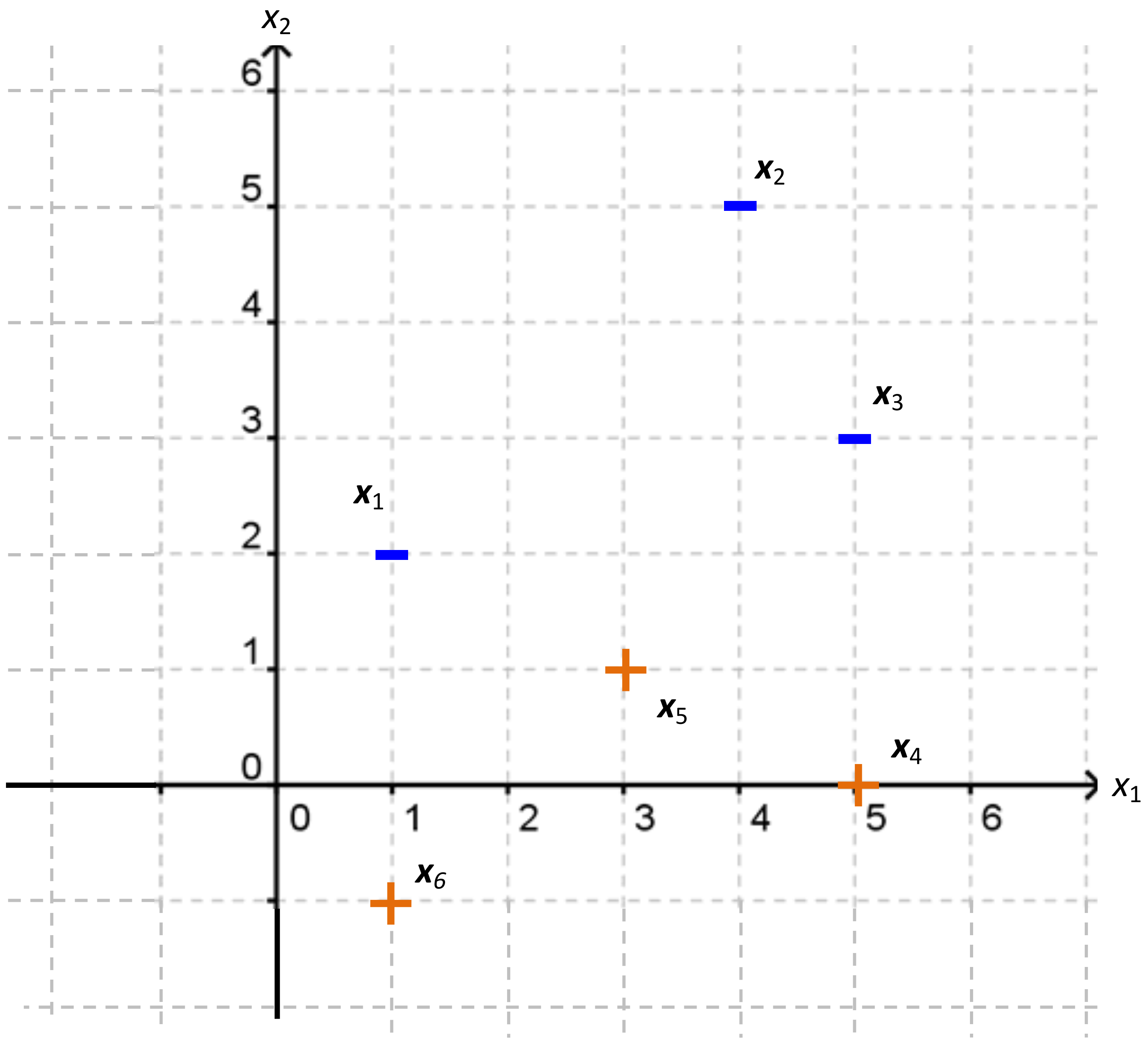
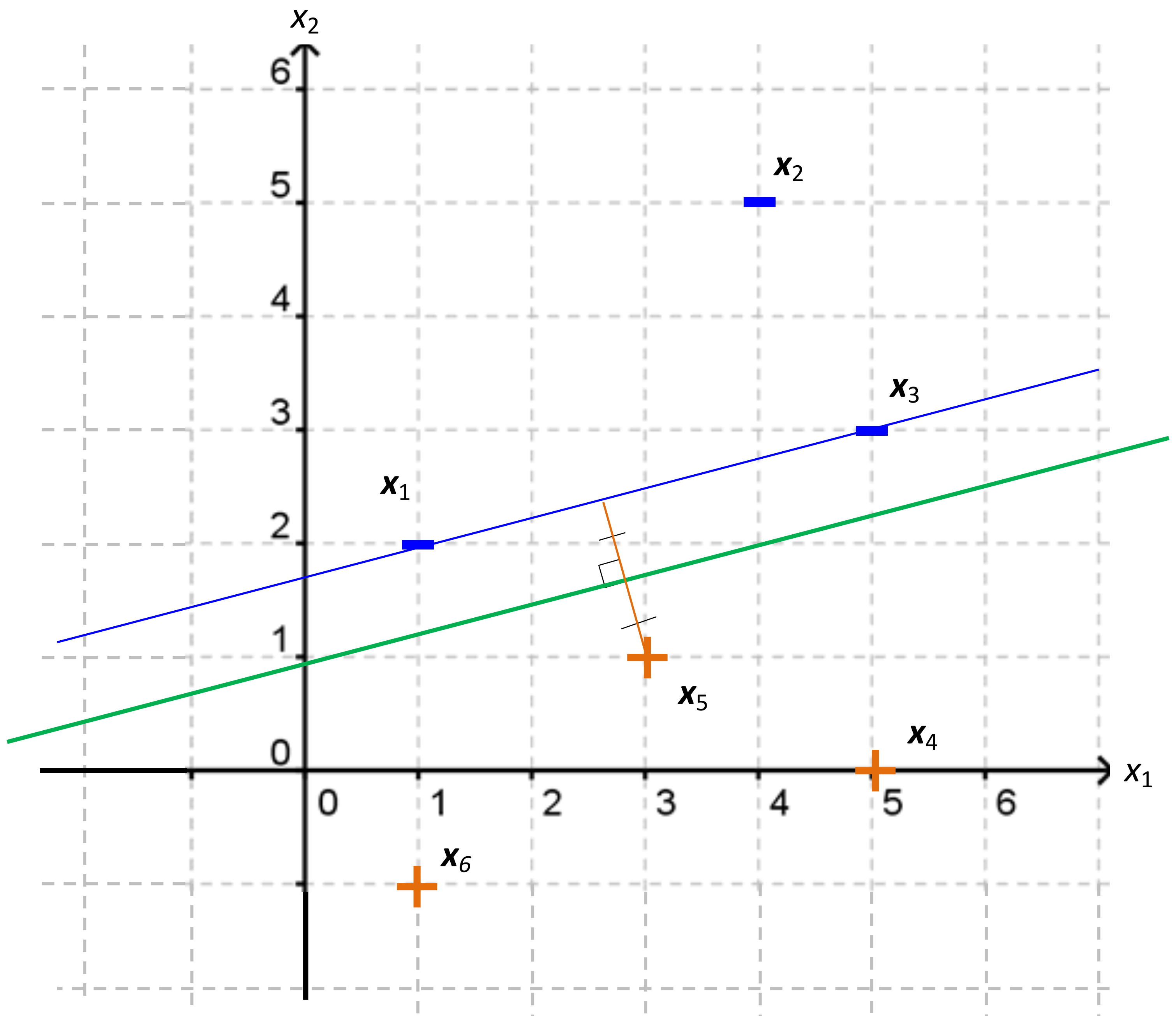
   (c) $y_i(\vec{w} \cdot \vec{x}_i + b) = 0$

   [✓ (d) $y_i(\vec{w} \cdot \vec{x}_i + b) = 1$]

   [✓ (e) $\vec{x}_i$ lies on the margin]



x_2
x_1
$\boldsymbol{x}_1$
$\boldsymbol{x}_2$
$\boldsymbol{x}_3$
$\boldsymbol{x}_4$
$\boldsymbol{x}_5$
$\boldsymbol{x}_6$
0 1 2 3 4 5 6



x_2
x_1
6
5
4
3
2
1
0
0
1
2
3
4
5
6
$\boldsymbol{x}_1$
$\boldsymbol{x}_2$
$\boldsymbol{x}_3$
$\boldsymbol{x}_4$
$\boldsymbol{x}_5$
$\boldsymbol{x}_6$

Reading Quiz #8

3. After training an SVM and obtaining the α values for each training example, I can use this formula to find the optimal weight vector:

$$\vec{w}^* = \sum_{i=1}^{n} \alpha_i y_i \vec{x}_i$$

Then when I predict a label for a test example $\vec{x}$, I can use:

$$\hat{y} = h(\vec{x}) = \text{sign}\left(\sum_{i=1}^{n} \alpha_i y_i (\vec{x}_i \cdot \vec{x}) + b\right)$$

Explain why it does not take $O(n)$ work to predict a label for each test point.

Reading Quiz #8

3. After training an SVM and obtaining the α values for each training example, I can use this formula to find the optimal weight vector:

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Explain why it does not take $O(n)$ work to predict a label for each test point.

Most of the alpha values are 0, so we only need to consider the support vectors!