CS578 Statistical Machine Learning Lecture 2

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(based on slides by Tommi Jaakkola, MIT CSAIL)

Today's topics

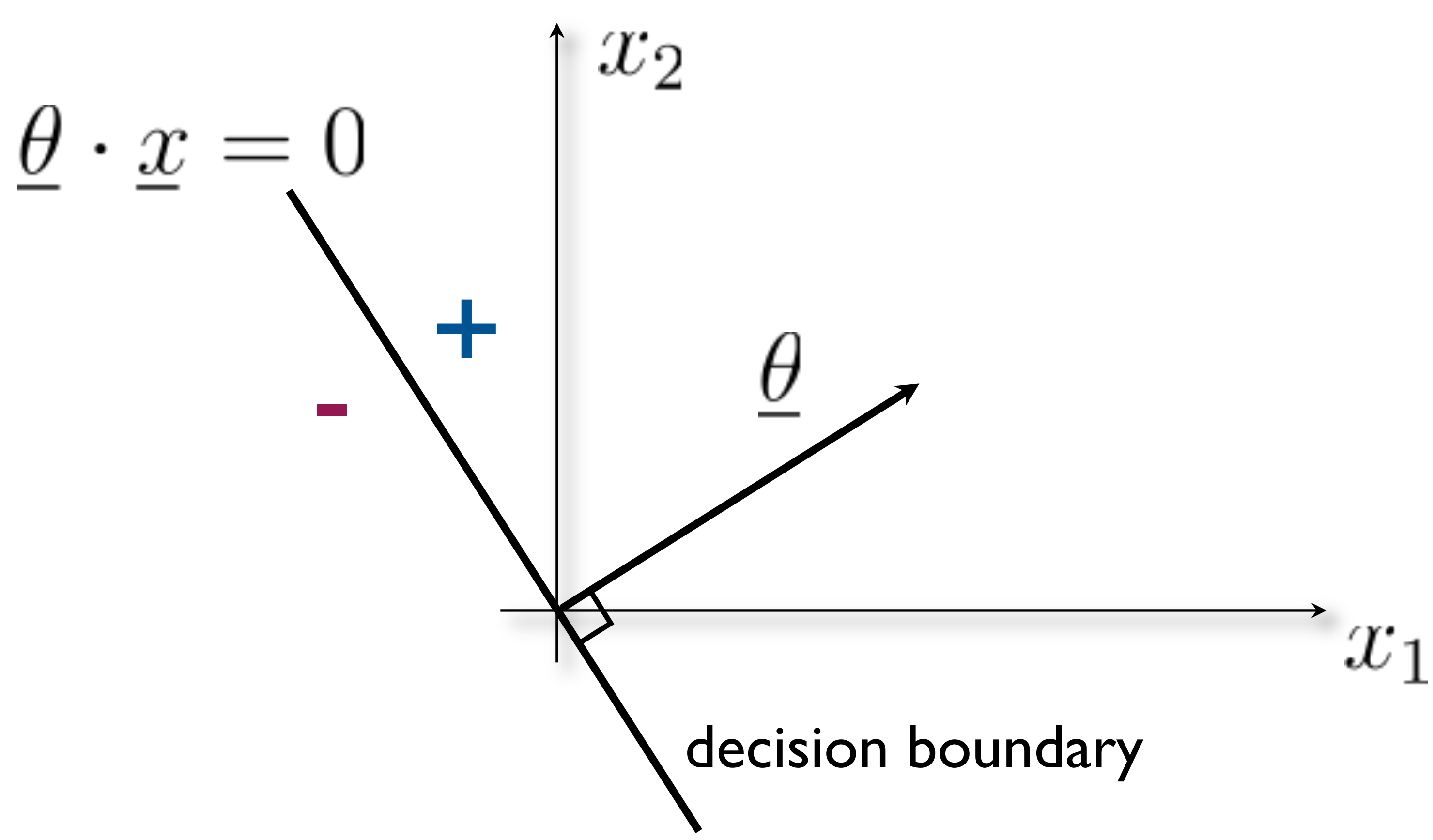
- Perceptron, convergence
  - the prediction game
  - mistakes, margin, and generalization
- Maximum margin classifier -- support vector machine
  - estimation, properties
  - allowing misclassified points

Recall: linear classifiers

- A linear classifier (through origin) with parameters $\underline{\theta}$ divides the space into positive and negative halves

$$f(\underline{x};\underline{\theta}) = \text{sign}\big(\underline{\theta}\cdot\underline{x}\big) = \text{sign}\big(\underbrace{\theta_1 x_1 + \ldots + \theta_d x_d}_{\text{discriminant function}}\big)$$

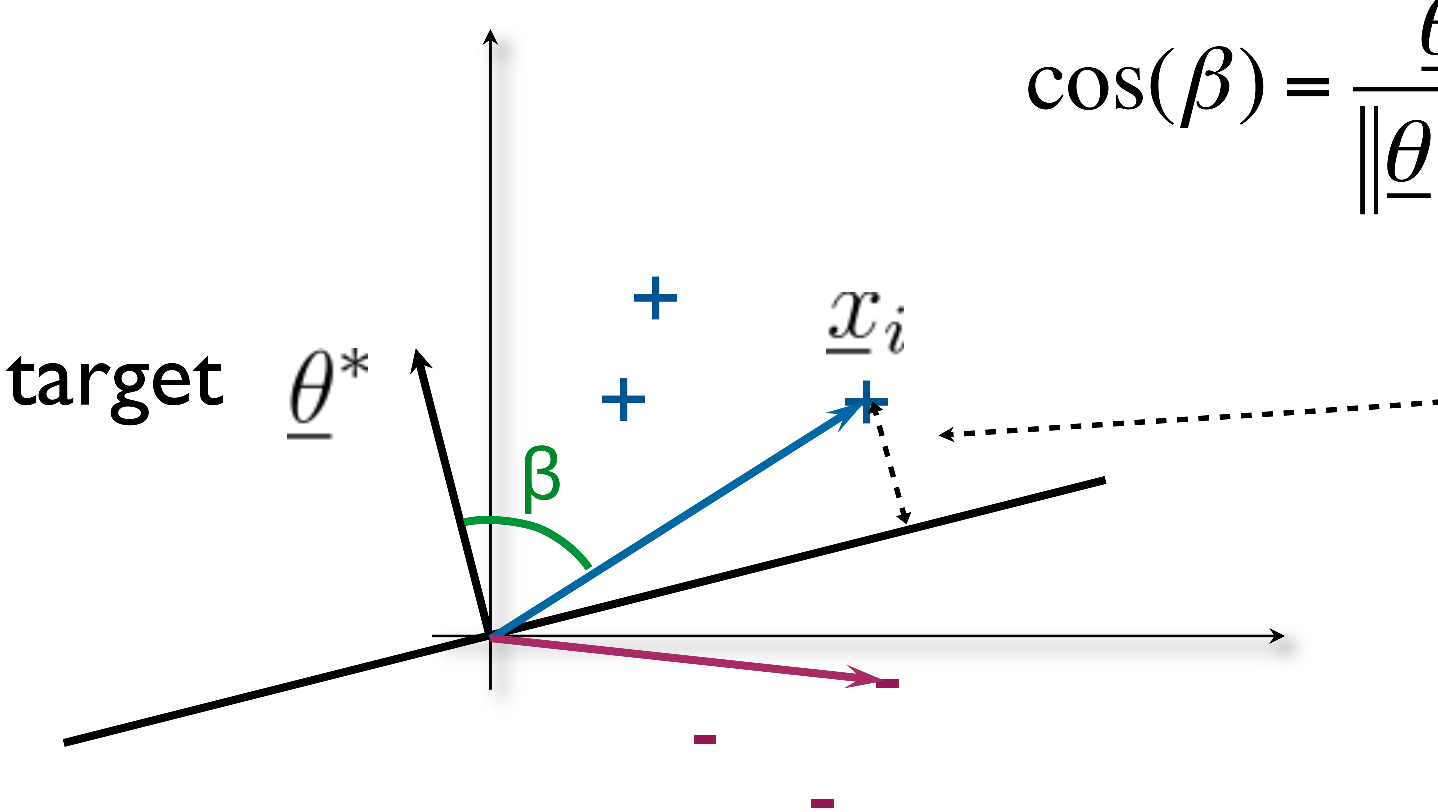
$$= \begin{cases} +1, & \text{if } \underline{\theta}\cdot\underline{x} > 0 \\ -1, & \text{if } \underline{\theta}\cdot\underline{x} \le 0 \end{cases}$$



Recall: some linear algebra

- More details about slide 1-52. Consider a positive point:

$$\cos(\beta) = \frac{\underline{\theta} \bullet \underline{x}_i}{\|\underline{\theta}\| \times \|\underline{x}_i\|} \quad , \text{ radius } r = \|\underline{x}_i\|$$



$$r\cos(\beta) = \frac{\underline{\theta} \bullet \underline{x}_i}{\|\underline{\theta}\|}$$

- Positive point: y_i=1, β<90°, cos(β)>0, $\underline{\theta} \bullet \underline{x}_i > 0$
- Negative point: y_i=-1, β>90°, cos(β)<0, $\underline{\theta} \bullet \underline{x}_i < 0$

- General formula for positive and negative points: $\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|}$

Perceptron algorithm

- The perceptron algorithm considers each training point in turn, adjusting the parameters to correct any mistakes

$$\text{Initialize: } \underline{\theta} = 0$$

$$\text{Repeat until convergence:}$$

$$\text{for } t = 1, \ldots, n$$

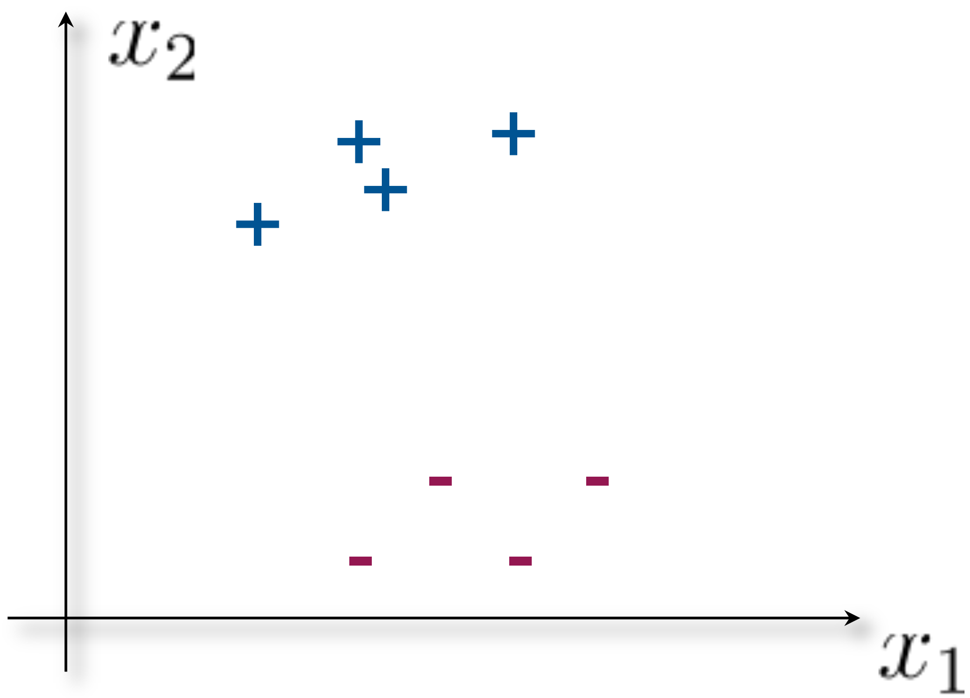
$$\text{if } y_t(\underline{\theta} \cdot \underline{x}_t) \leq 0 \text{ (mistake)}$$

$$\underline{\theta} \leftarrow \underline{\theta} + y_t \underline{x}_t$$

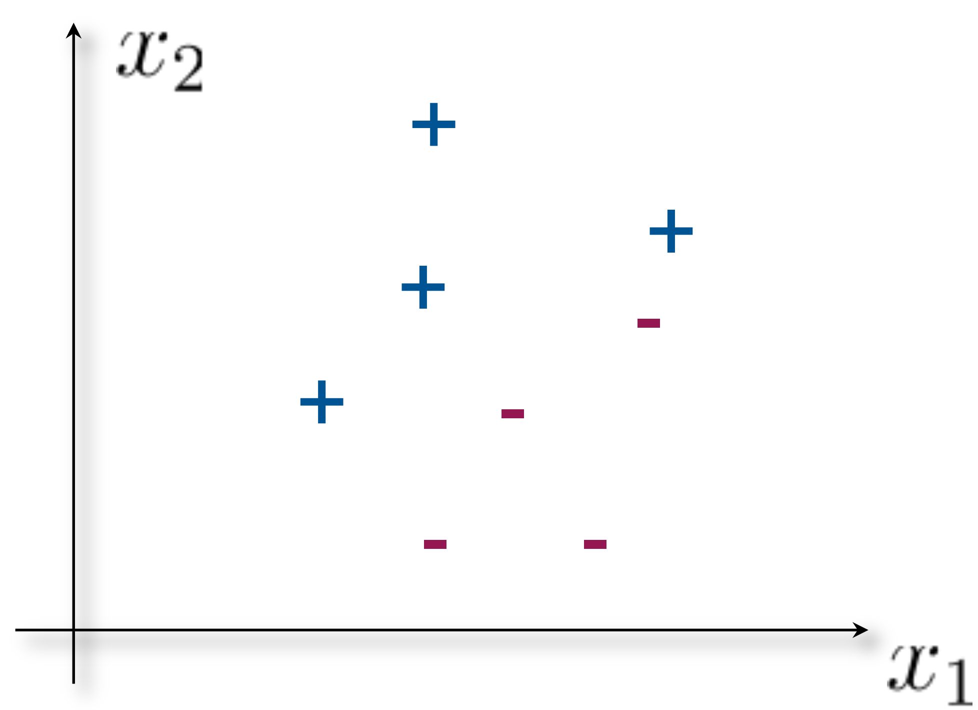
- We would like to bound the number of mistakes that the algorithm makes

Mistakes and margin

Easy problem
- large margin
- few mistakes

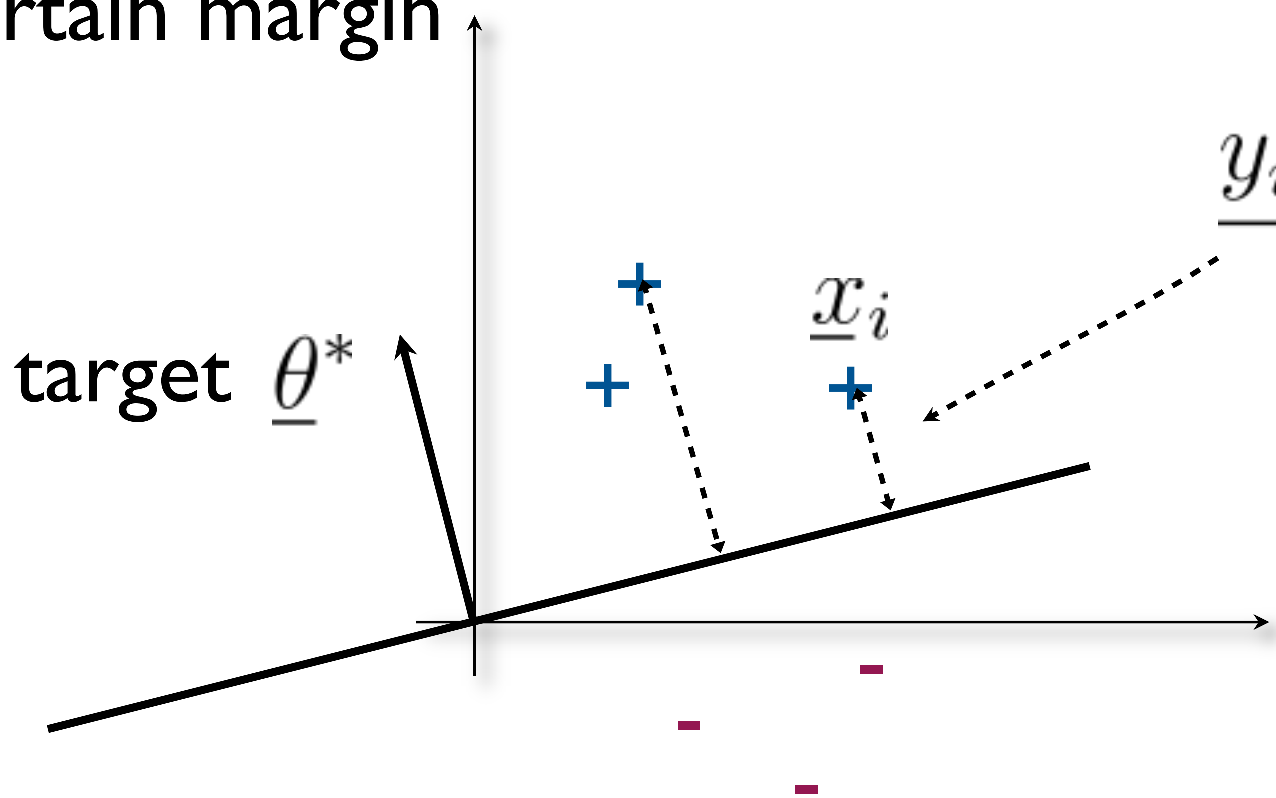


Harder problem
- small margin
- many mistakes



The target classifier

- We can quantify how hard the problem is by assuming that there exists a target classifier that achieves a certain margin



$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} = \gamma_g(i)$$

distance from the point to the separating boundary

- The geometric margin γ_g is the closest distance to the separating boundary $\gamma_g = \min_i \gamma_g(i)$

Perceptron convergence theorem

- If there exists $\underline{\theta}^*$ such that

$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g\,,\; i = 1, \ldots, n$$

and $\|\underline{x}_i\| \leq R$ then the perceptron algorithm makes at most

$$\frac{R^2}{\gamma_g^2}$$

mistakes (on the training set).

- Key points
  - large geometric margin relative to the norm of the examples implies few mistakes
  - the result does not depend on the dimension d of the examples (the number of parameters)

Mistake guarantee: proof

- We show that after k updates (mistakes),

$$\begin{aligned}\underline{\theta}^{(k)} \cdot \underline{\theta}^{*} &\geq k\gamma_g \|\underline{\theta}^{*}\| \\ \|\underline{\theta}^{(k)}\|^2 &\leq kR^2\end{aligned}$$

Mistake guarantee: proof

- We show that after k updates (mistakes),

$$\begin{aligned} \underline{\theta}^{(k)} \cdot \underline{\theta}^* &\geq k\gamma_g \|\underline{\theta}^*\| \\ \|\underline{\theta}^{(k)}\|^2 &\leq kR^2 \end{aligned}$$

- Let the kth mistake be on the ith example

$$\begin{aligned} \underline{\theta}^{(k)} \cdot \underline{\theta}^* &= [\underline{\theta}^{(k-1)} + y_i \underline{x}_i] \cdot \underline{\theta}^* \\ &= \underline{\theta}^{(k-1)} \cdot \underline{\theta}^* + y_i \underline{x}_i \cdot \underline{\theta}^* \\ &\geq \underline{\theta}^{(k-1)} \cdot \underline{\theta}^* + \gamma_g \|\underline{\theta}^*\| \end{aligned}$$

margin

Note:

Since $\underline{\theta}^{(0)} = 0$ then $\underline{\theta}^{(k)} \bullet \underline{\theta}^* \geq k\, \gamma_g\, \|\underline{\theta}^*\|$

Mistake guarantee: proof

- We show that after k updates (mistakes),

$$\begin{aligned}\underline{\theta}^{(k)} \cdot \underline{\theta}^* &\geq k\gamma_g ||\underline{\theta}^*|| \\ ||\underline{\theta}^{(k)}||^2 &\leq kR^2\end{aligned}$$

- Let the kth mistake be on the ith example

$$\begin{aligned}||\underline{\theta}^{(k)}||^2 &= ||\underline{\theta}^{(k-1)} + y_i \underline{x}_i||^2 \\ &= ||\underline{\theta}^{(k-1)}||^2 + 2y_i\underline{\theta}^{(k-1)} \cdot \underline{x}_i + ||\underline{x}_i||^2 \\ &\leq ||\underline{\theta}^{(k-1)}||^2 + ||\underline{x}_i||^2 \\ &\leq ||\underline{\theta}^{(k-1)}||^2 + R^2\end{aligned}$$

mistake: ≤ 0

Note:

For any two vectors, a and b:

$||\underline{a}+\underline{b}||^2 = (\underline{a}+\underline{b})\bullet(\underline{a}+\underline{b}) = \underline{a}\bullet\underline{a} + 2\,\underline{a}\bullet\underline{b} + \underline{b}\bullet\underline{b} = ||\underline{a}||^2 + 2\,\underline{a}\bullet\underline{b} + ||\underline{b}||^2$

Since $\underline{\theta}^{(0)} = 0$ then $||\underline{\theta}^{(k)}||^2 \leq k\,R^2$

Mistake guarantee: proof

- We have shown that after k updates (mistakes),

$$
\begin{aligned}
\underline{\theta}^{(k)} \cdot \underline{\theta}^{*} &\geq k\gamma_g \|\underline{\theta}^{*}\| \\
\|\underline{\theta}^{(k)}\|^2 &\leq kR^2
\end{aligned}
$$

- As a result,

$$
1 \geq \overbrace{\frac{\underline{\theta}^{(k)} \cdot \underline{\theta}^{*}}{\|\underline{\theta}^{(k)}\| \|\underline{\theta}^{*}\|}}^{\text{cosine}} \geq \frac{k\gamma_g}{\sqrt{k}R}
$$

$$
\Rightarrow k \leq \frac{R^2}{\gamma_g^2}
$$

Summary (perceptron)

- By analyzing the simple perceptron algorithm, we were able to relate the number of mistakes and geometric margin
- In cases where we are given a fixed set of training examples, and they are linearly separable, we can find and use the maximum margin classifier directly

Optimization

- Example problem:

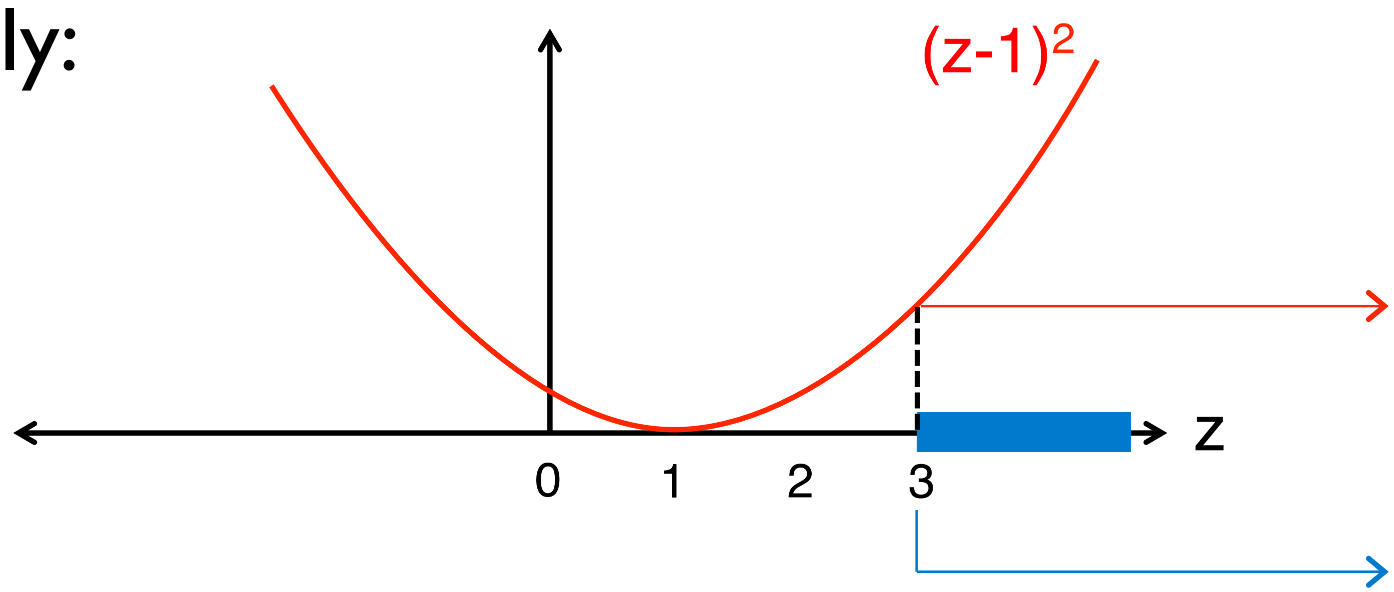
$$\begin{aligned} &\text{minimize} && (z-1)^2 \\ &\text{subject to} && z \geq 3 \end{aligned}$$

Objective function

Optimization variable z

Constraint

- Graphically:



$(z^*-1)^2 = (3-1)^2 = 4$

Optimal solution:
$z^* = 3$

- What if we have several optimization variables?

Optimization

- Example problem:

$$\text{minimize} \quad z_1^2 + z_2^2 - \frac{1}{2} z_1 z_2$$

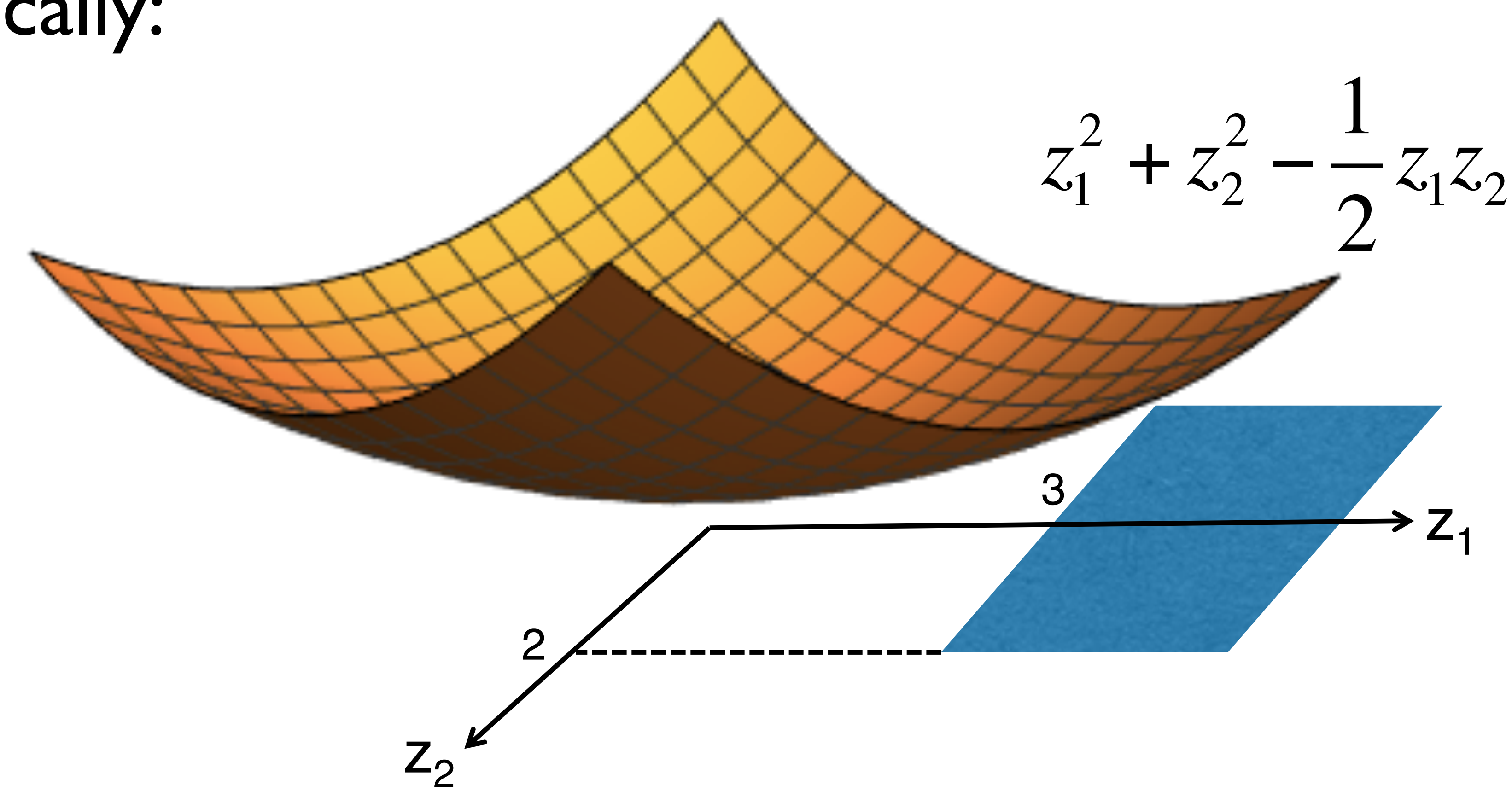
$$\text{subject to} \quad z_1 \geq 3, \quad z_2 \leq 2$$

Objective function

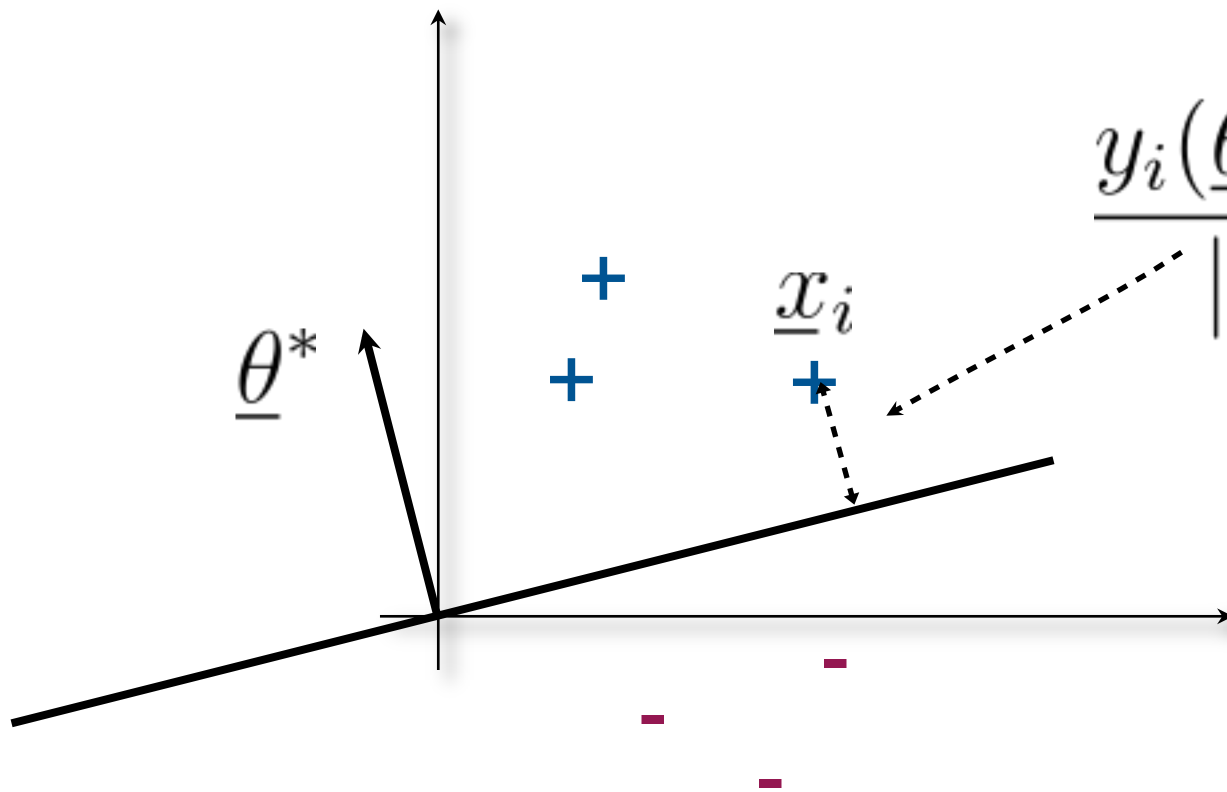
Constraints

Optimization variable $\underline{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$

- Graphically:



Maximum margin classifier

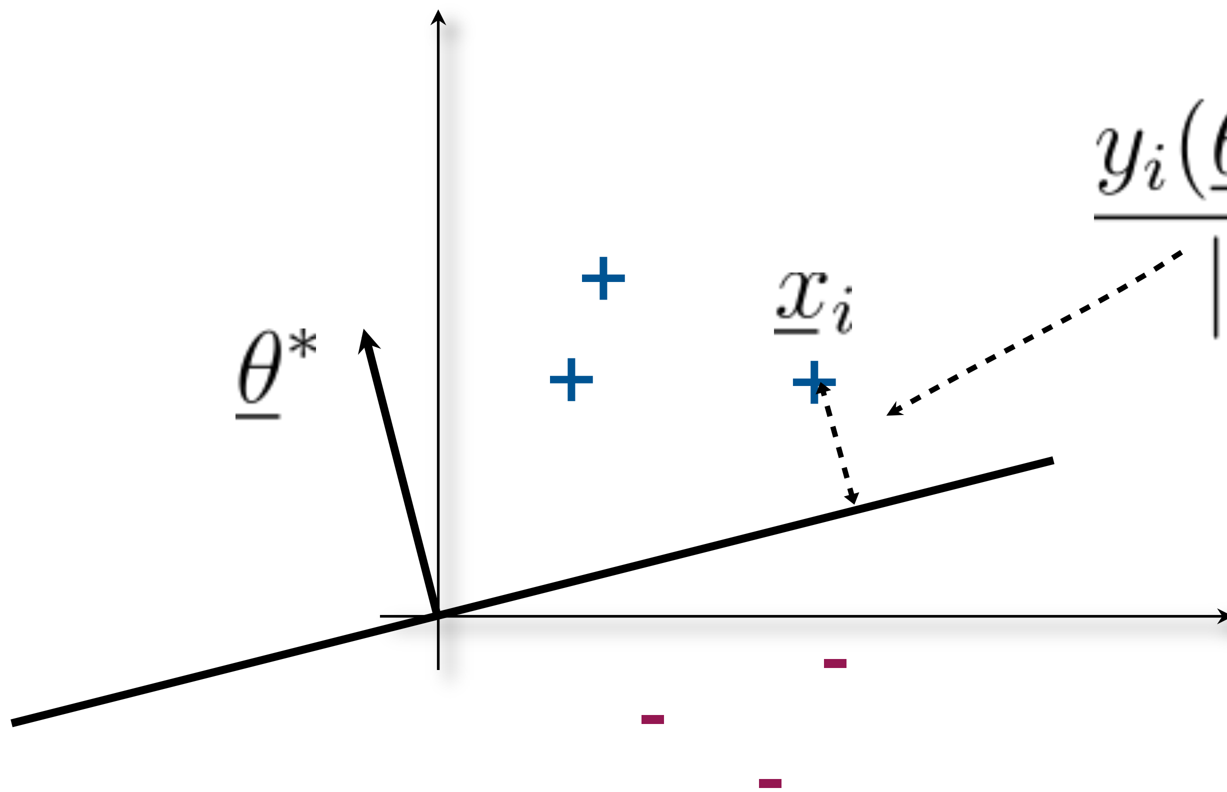


$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

- Lets maximize the margin γ_g directly

Maximum margin classifier



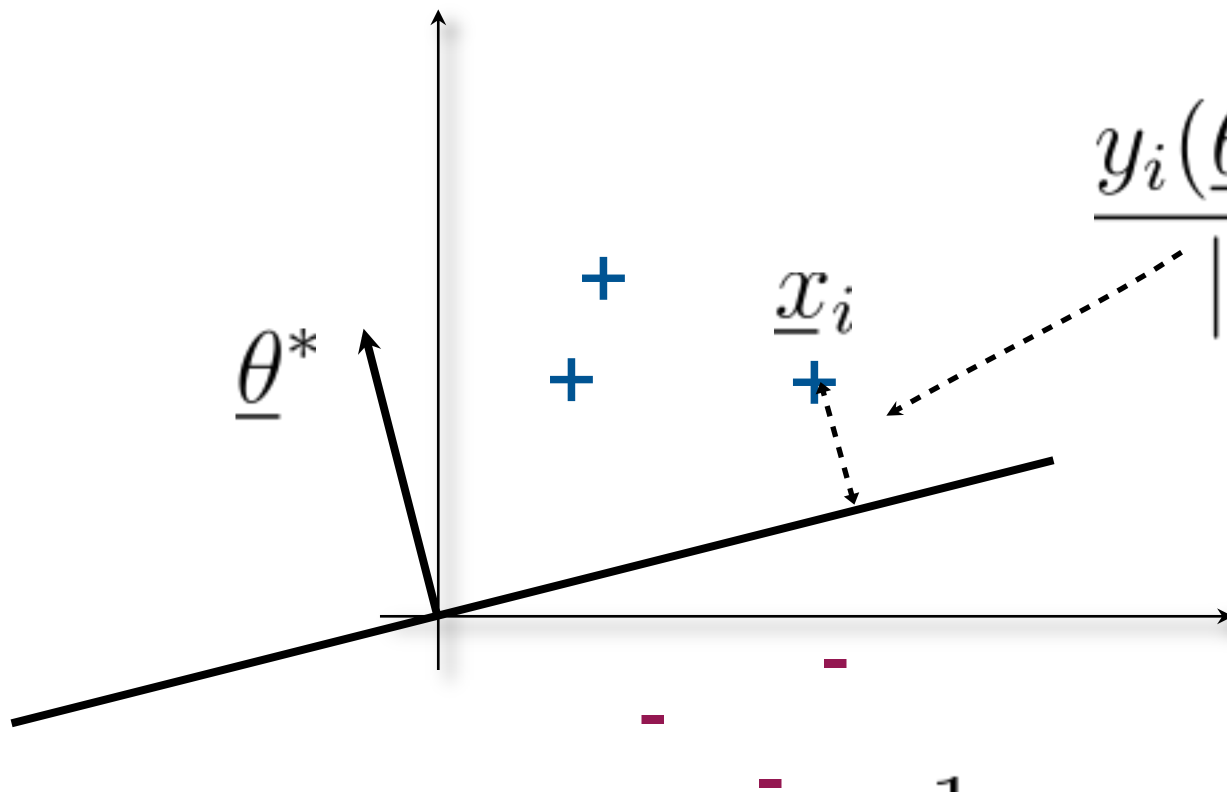
$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

$$\text{maximize } \gamma_g \text{ subject to}$$

$$\text{To find } \underline{\theta}^* : \quad \frac{y_i(\underline{\theta} \cdot \underline{x}_i)}{\|\underline{\theta}\|} \geq \gamma_g, \quad i = 1, \ldots, n$$

Maximum margin classifier



$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

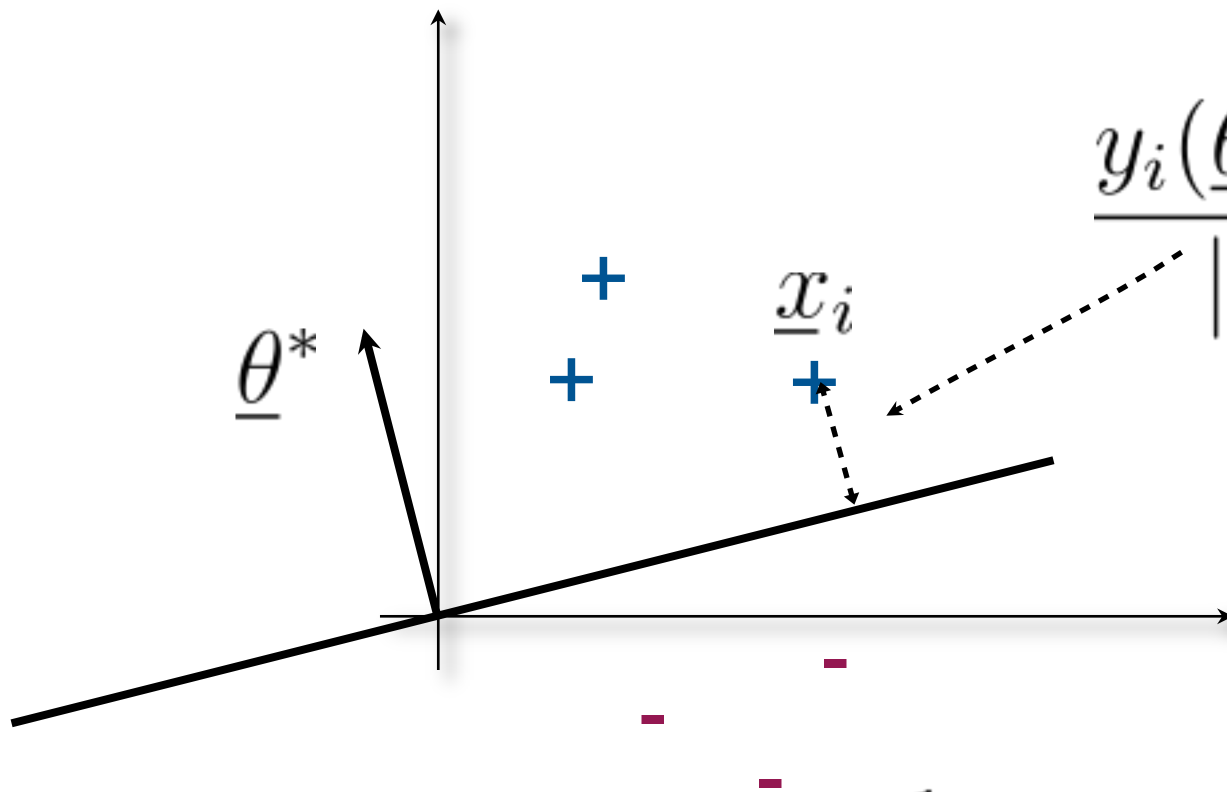
Assume: $\gamma_g = \dfrac{1}{\|\underline{\theta}^*\|}$

To find $\underline{\theta}^*$:

$$\text{maximize } \frac{1}{\|\underline{\theta}\|} \text{ subject to}$$

$$\frac{y_i(\underline{\theta} \cdot \underline{x}_i)}{\|\underline{\theta}\|} \geq \frac{1}{\|\underline{\theta}\|}, \quad i = 1, \ldots, n$$

Maximum margin classifier



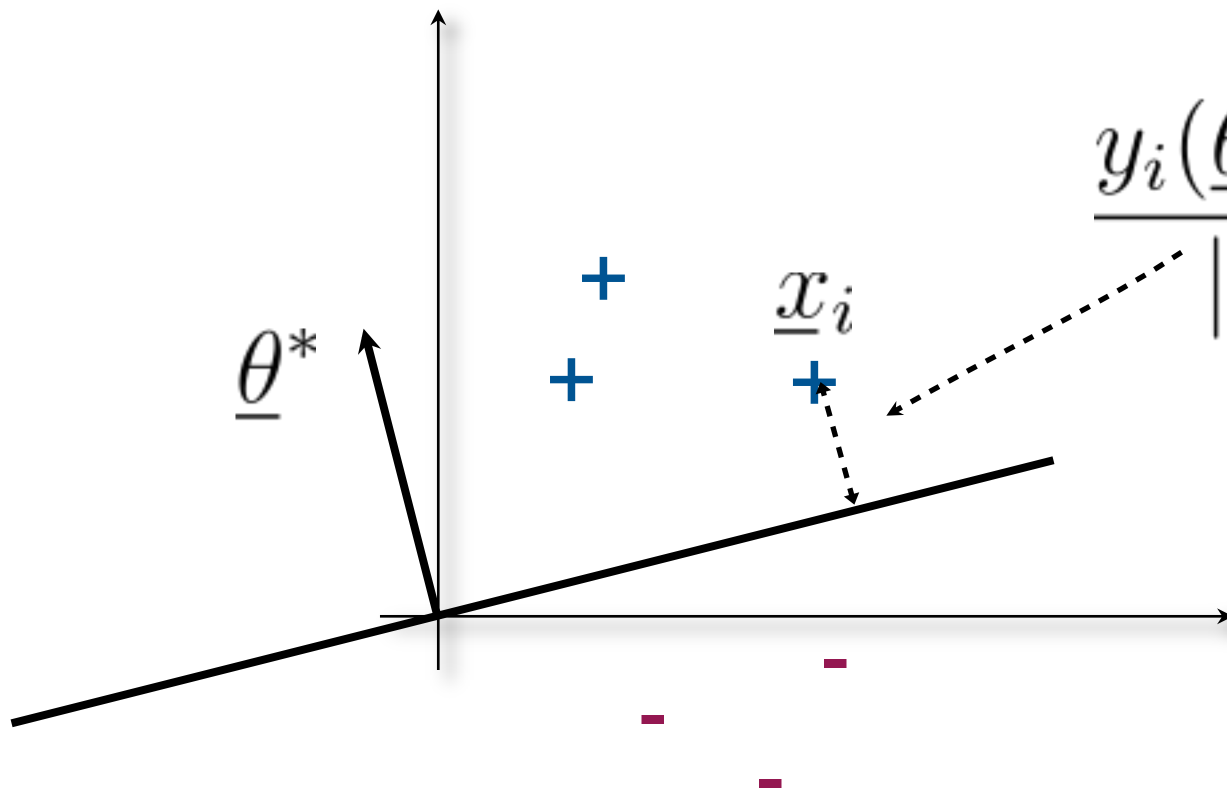
$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

Assume: $\gamma_g = \dfrac{1}{\|\underline{\theta}^*\|}$

To find $\underline{\theta}^*$: $$\text{maximize } \frac{1}{\|\underline{\theta}\|} \text{ subject to}$$
$$y_i(\underline{\theta} \cdot \underline{x}_i) \geq 1, \quad i = 1, \ldots, n$$

Maximum margin classifier



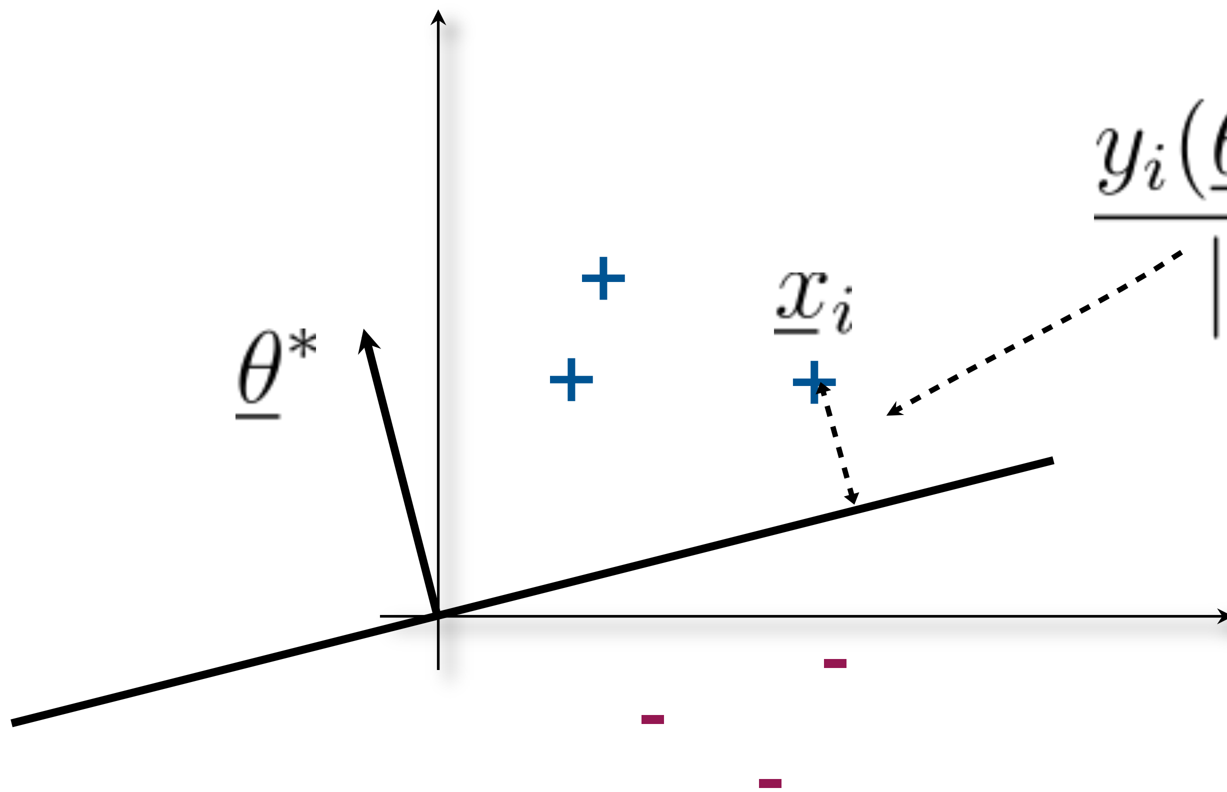
$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

Assume: $\gamma_g = \dfrac{1}{\|\underline{\theta}^*\|}$

To find $\underline{\theta}^*$:
$$\text{minimize } \|\underline{\theta}\| \text{ subject to}$$
$$y_i(\underline{\theta} \cdot \underline{x}_i) \geq 1, \quad i = 1, \ldots, n$$

Support vector machine



$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

Assume: $\gamma_g = \dfrac{1}{\|\underline{\theta}^*\|}$

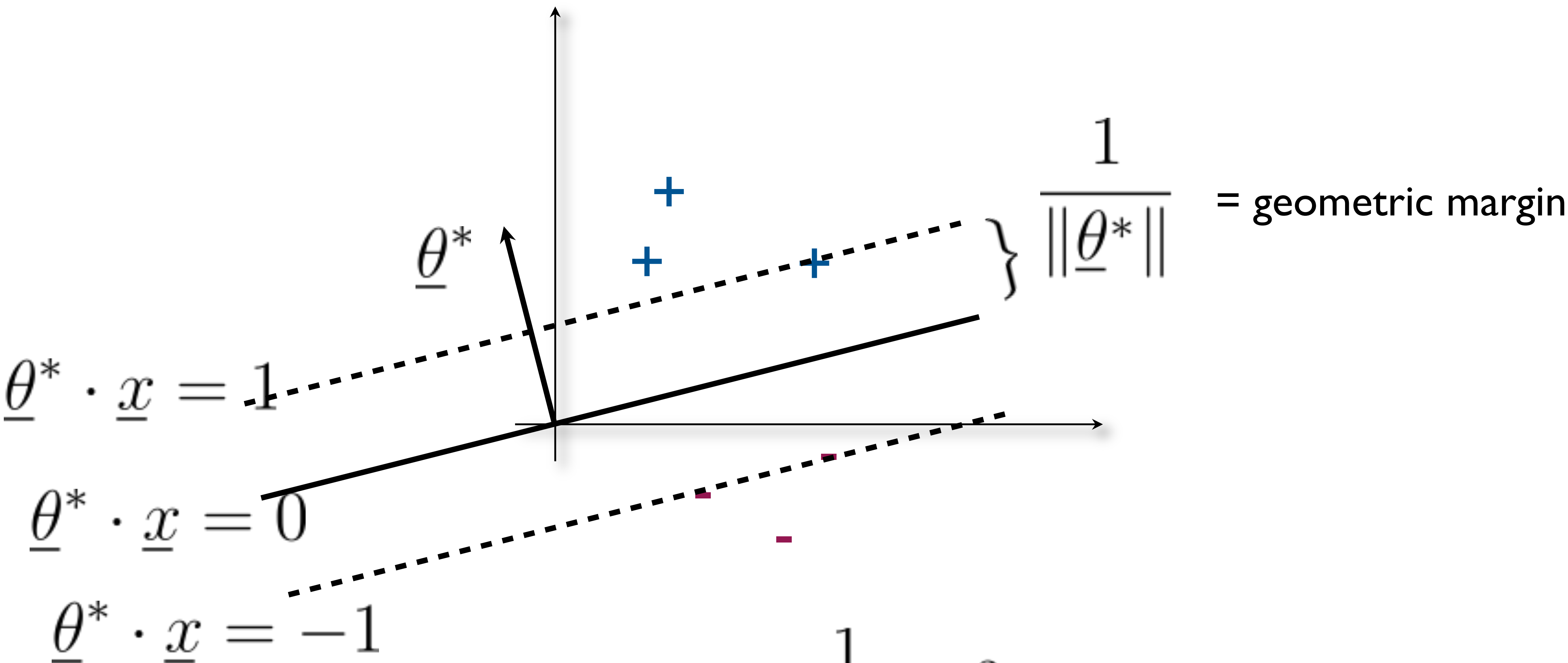
To find $\underline{\theta}^*$:

$$\text{minimize } \frac{1}{2}\|\underline{\theta}\|^2 \text{ subject to}$$

$$y_i(\underline{\theta} \cdot \underline{x}_i) \geq 1, \quad i = 1, \ldots, n$$

- This is a quadratic programming problem (quadratic objective, linear constraints)

Support vector machine



To find $\underline{\theta}^*$:

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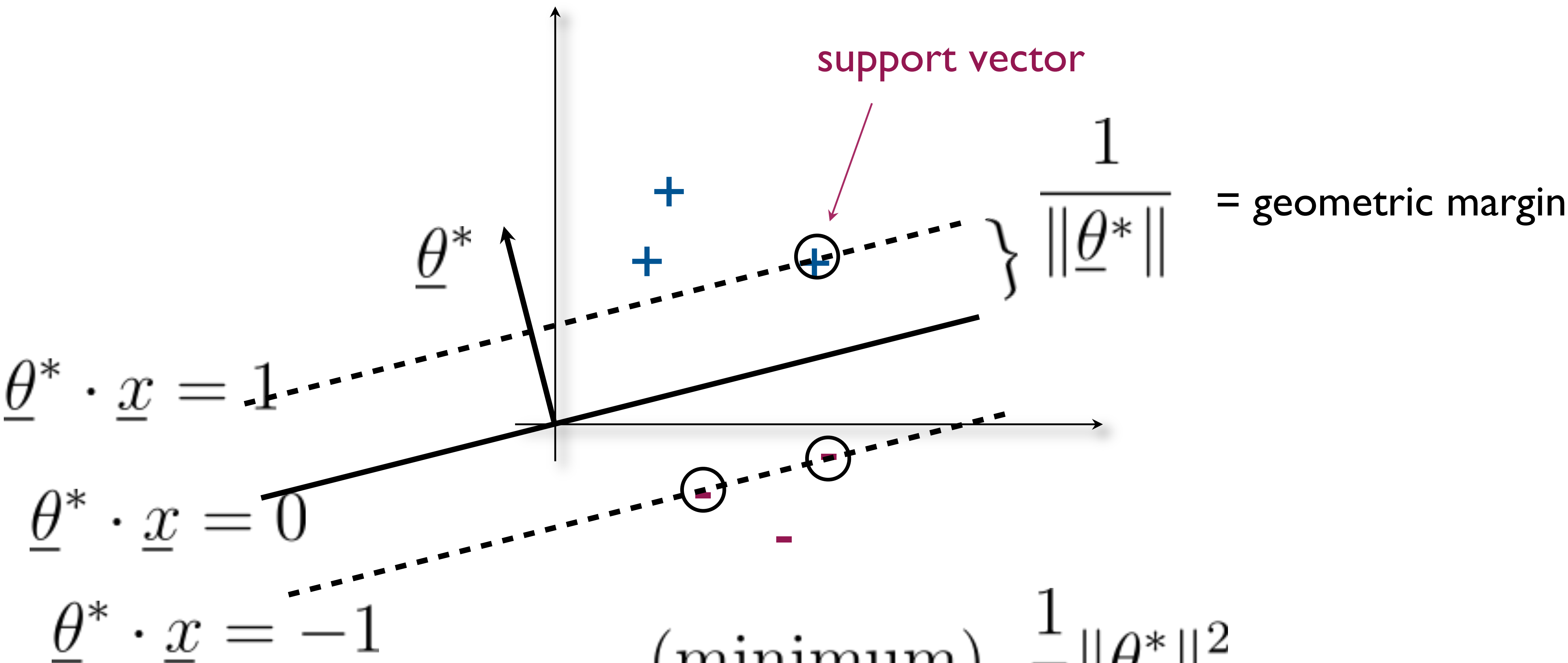
Support vector machine



$$(\text{minimum}) \quad \frac{1}{2}\|\underline{\theta}^*\|^2$$

$$y_1(\underline{\theta}^* \cdot \underline{x}_1) = 1$$

$$y_2(\underline{\theta}^* \cdot \underline{x}_2) > 1$$

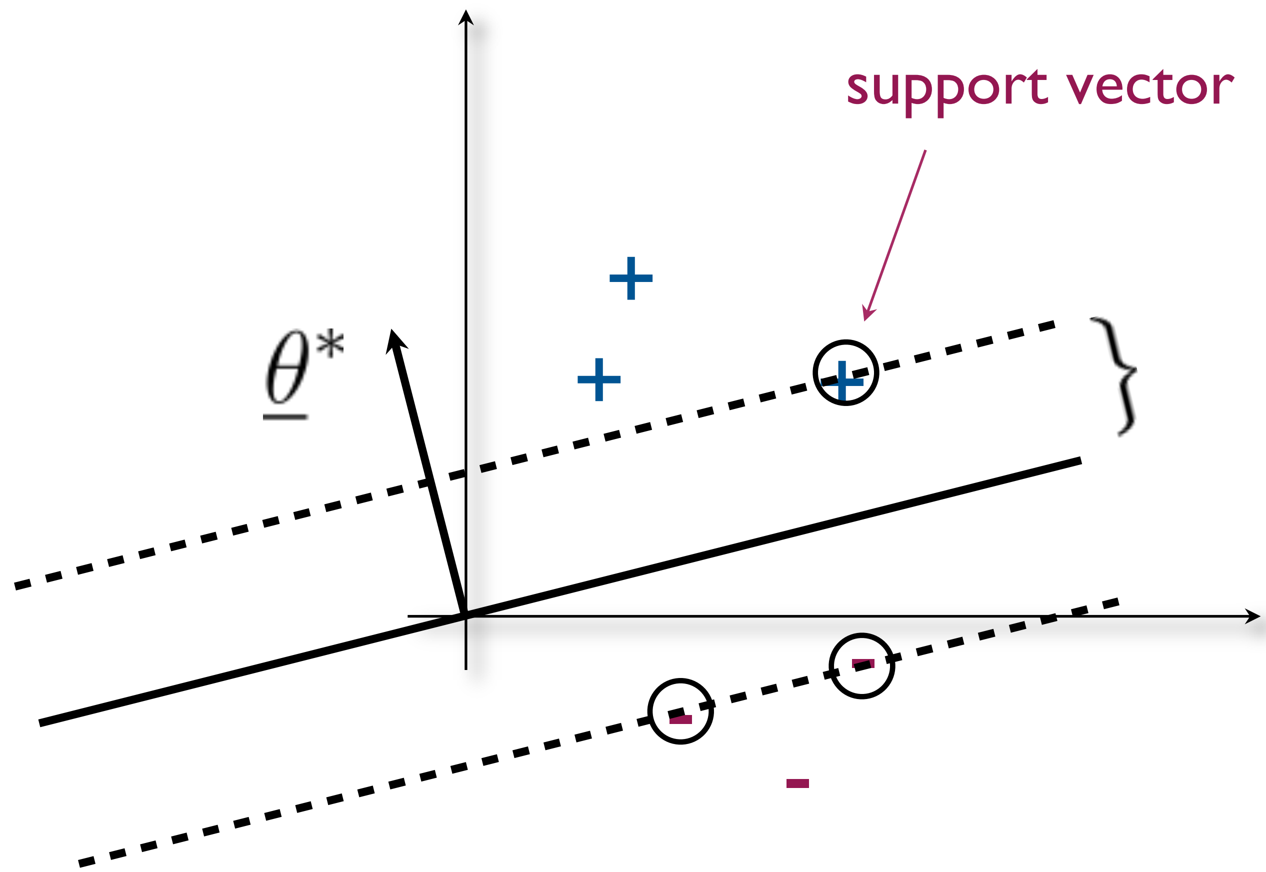
$$y_3(\underline{\theta}^* \cdot \underline{x}_3) = 1$$

$$\ldots$$

active constraints
= support vectors

The solution is **sparse**

Is sparse solution good?



- We can simulate test performance by evaluating Leave-One-Out Cross-Validation error

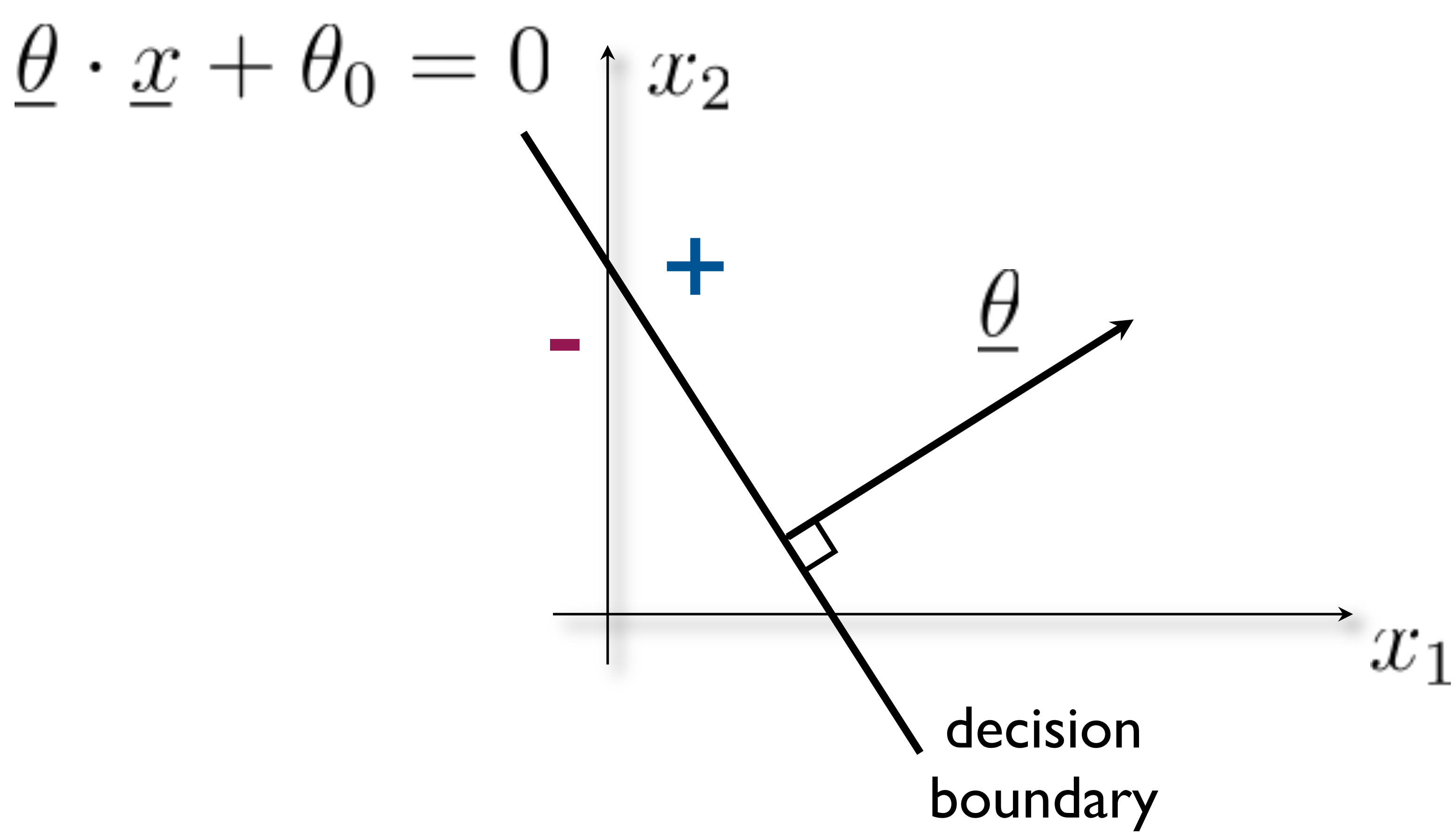
$$\mathrm{LOOCV}(\underline{\theta}^*) \leq \frac{\#\text{ of support vectors}}{n}$$

Intuitively:
if you remove the support vector from the training set, and you receive the support vector as a test point, then you would make a mistake

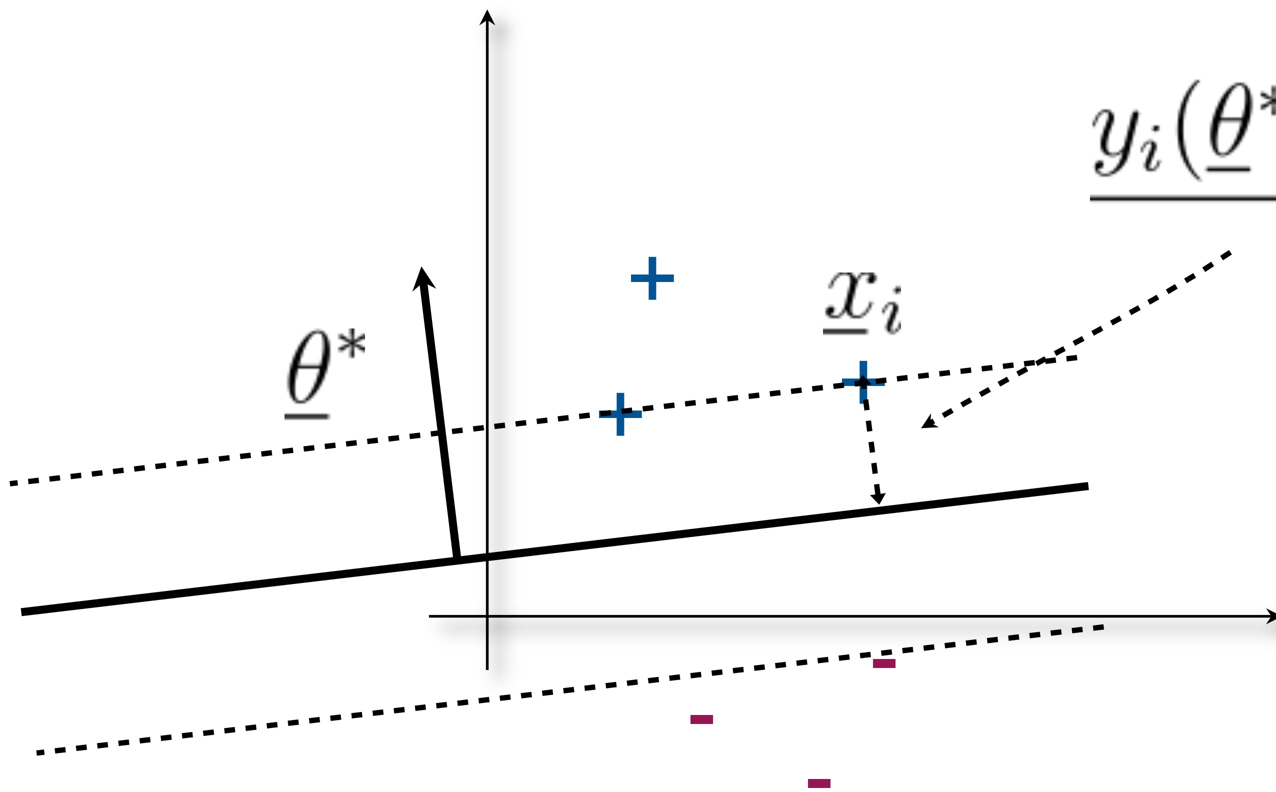
Linear classifiers (with offset)

- A linear classifier with parameters $(\underline{\theta}, \theta_0)$

$$
\begin{aligned}
f(\underline{x}; \underline{\theta}, \theta_0) &= \operatorname{sign}\big(\underline{\theta} \cdot \underline{x} + \theta_0\big) \\
&= \begin{cases} +1, & \text{if } \underline{\theta} \cdot \underline{x} + \theta_0 > 0 \\ -1, & \text{if } \underline{\theta} \cdot \underline{x} + \theta_0 \leq 0 \end{cases}
\end{aligned}
$$



Support vector machine



$$\frac{y_i(\underline{\theta}^* \cdot \underline{x}_i + \theta_0^*)}{\|\underline{\theta}^*\|} \geq \gamma_g$$

geometric margin

$$\gamma_g = \frac{1}{\|\underline{\theta}^*\|}$$

To find $\underline{\theta}^*, \theta_0^*$:

$$\text{minimize } \frac{1}{2}\|\underline{\theta}\|^2 \text{ subject to}$$

$$y_i(\underline{\theta} \cdot \underline{x}_i + \theta_0) \geq 1, \quad i = 1, \ldots, n$$

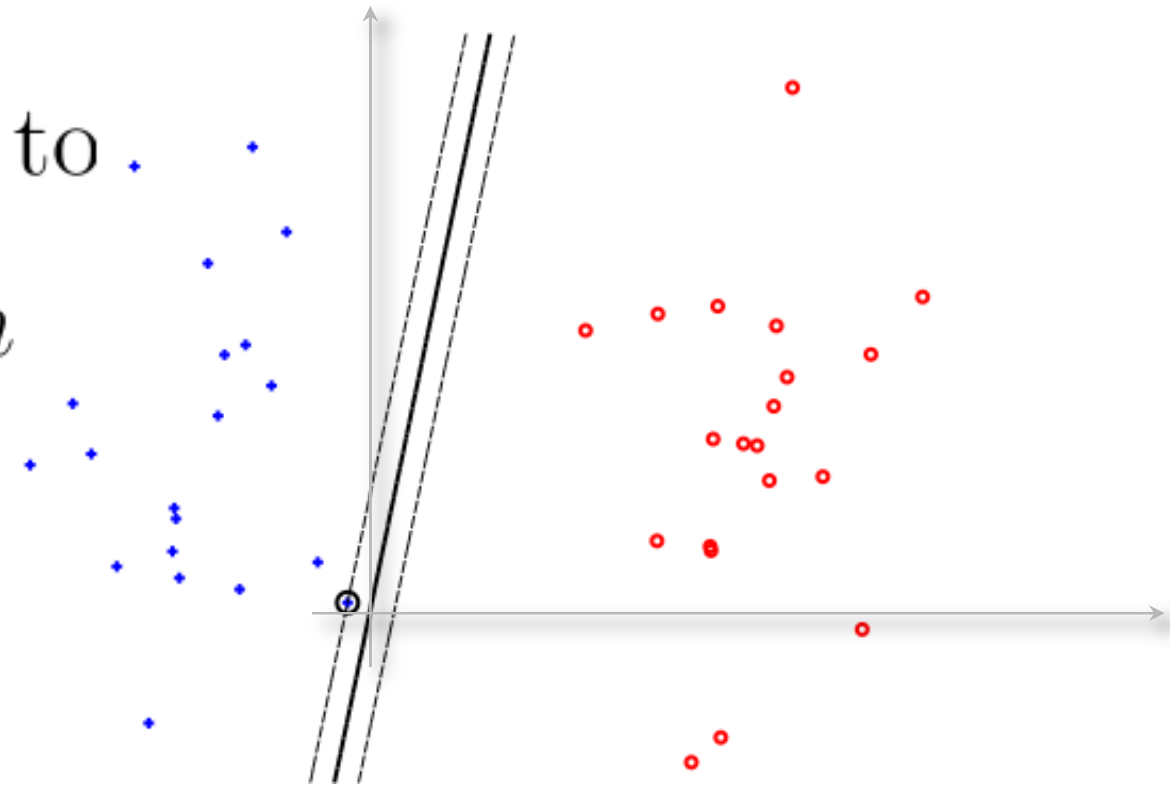
- Still a quadratic programming problem (quadratic objective, linear constraints)

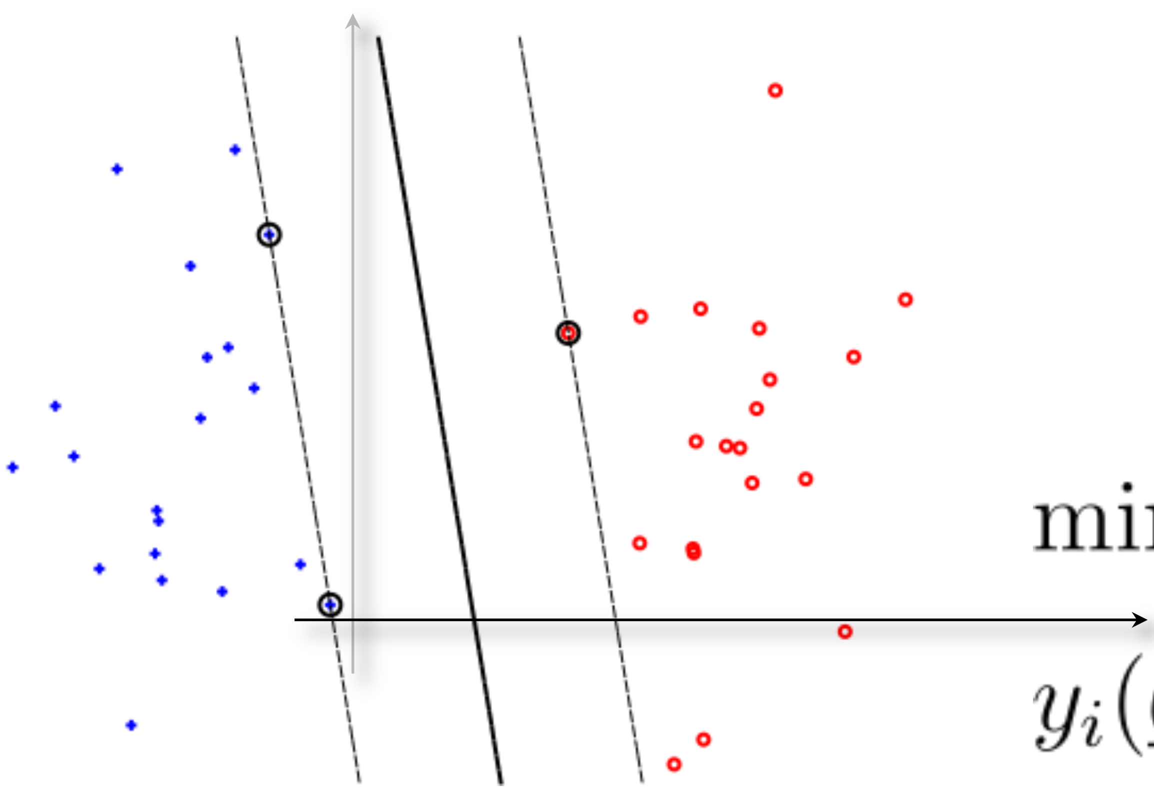
The impact of offset

- Adding the offset parameter to the linear classifier can substantially increase the margin

$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad \text{subject to}$$

$$y_i(\underline{\theta} \cdot \underline{x}_i) \geq 1, \quad i = 1, \ldots, n$$





$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad \text{subject to}$$

$$y_i(\underline{\theta} \cdot \underline{x}_i + \theta_0) \geq 1, \quad i = 1, \ldots, n$$

Support vector machine

- A desirable property
  - maximizes the margin on the training set ($\approx$ good generalization, since it will still predict correctly for points between the decision boundary and the dotted line)
- But...
  - the solution is sensitive to outliers, labeling errors, as they may drastically change the resulting max-margin boundary
  - if the training set is not linearly separable, there's no solution!

Support vector machine

- Relaxed quadratic optimization problem

penalty for constraint violation

$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad + \quad \overbrace{C\sum_{i=1}^{n}\xi_i} \quad \text{subject to}$$

$$\begin{aligned} y_i(\underline{\theta} \cdot \underline{x}_i + \theta_0) \quad &\geq \quad 1 - \xi_i, \quad i = 1, \ldots, n \\ \xi_i \quad &\geq \quad 0, \quad i = 1, \ldots, n \end{aligned}$$

slack variables permit us to violate some of the margin constraints

Support vector machine

- Relaxed quadratic optimization problem

penalty for constraint violation

$$\text{minimize } \frac{1}{2}\|\underline{\theta}\|^2 + \overbrace{C\sum_{i=1}^{n}\xi_i} \text{ subject to}$$

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slack variables permit us to violate some of the margin constraints

$$\text{large } C \Rightarrow \text{few (if any) violations}$$

$$\text{small } C \Rightarrow \text{many violations}$$

Support vector machine

- Relaxed quadratic optimization problem

penalty for constraint violation

$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad + \quad \overline{C\sum_{i=1}^{n} \xi_i} \quad \text{subject to}$$

$$\begin{aligned} y_i(\underline{\theta} \cdot \underline{x}_i + \theta_0) &\geq 1 - \xi_i, \quad i = 1, \ldots, n \\ \xi_i &\geq 0, \quad i = 1, \ldots, n \end{aligned}$$

slack variables permit us to violate some of the margin constraints

$$\text{large } C \Rightarrow \text{few (if any) violations}$$

$$\text{small } C \Rightarrow \text{many violations}$$

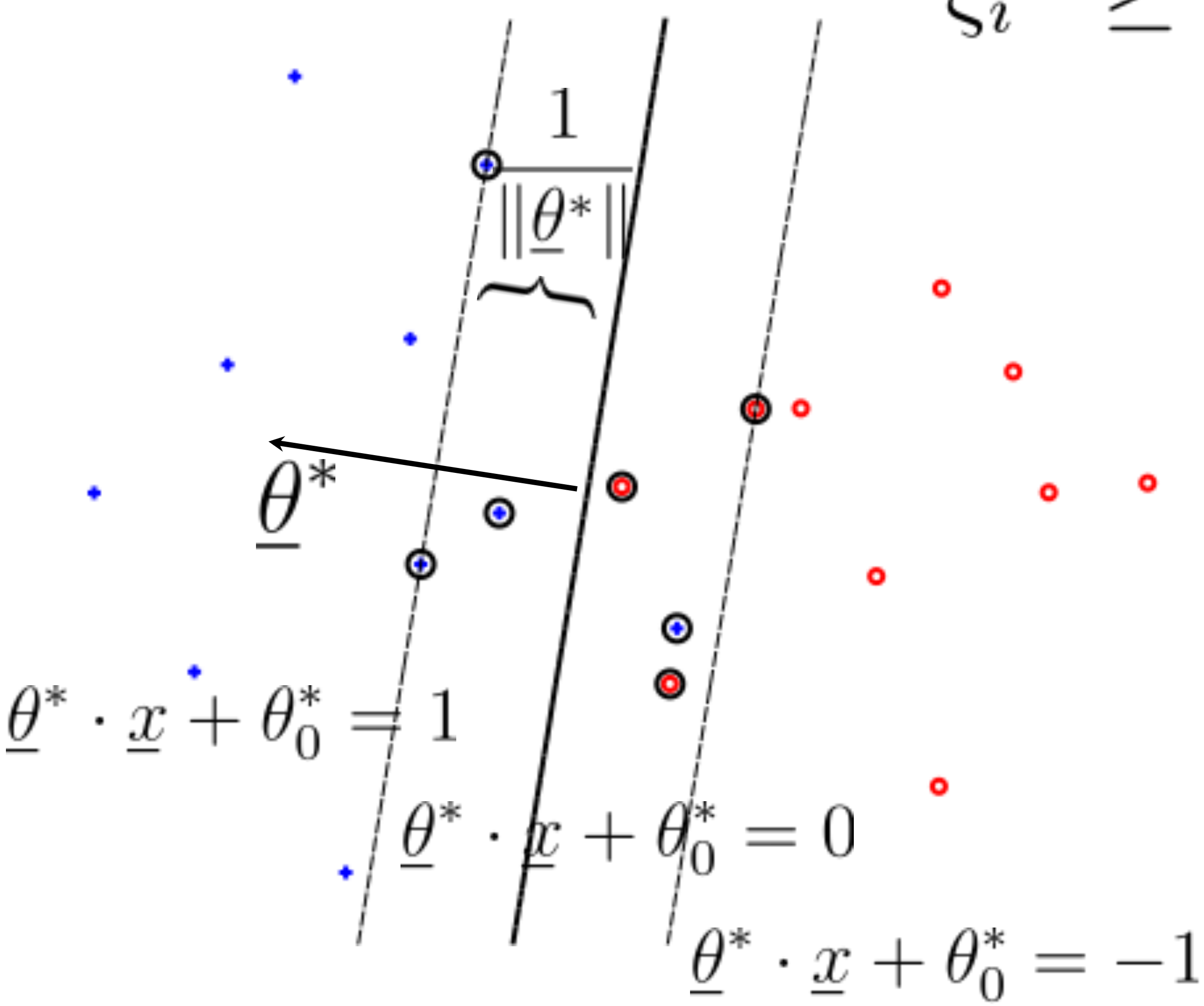
$$\text{we can still interpret the margin as } 1/\|\underline{\theta}^*\|$$

Support vector machine

- Relaxed quadratic optimization problem

$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad + \quad C\sum_{i=1}^{n}\xi_i \quad \text{subject to}$$

$$\begin{aligned} y_i(\underline{\theta}\cdot\underline{x}_i+\theta_0) &\geq 1-\xi_i, \quad i=1,\ldots,n \\ \xi_i &\geq 0, \quad i=1,\ldots,n \end{aligned}$$

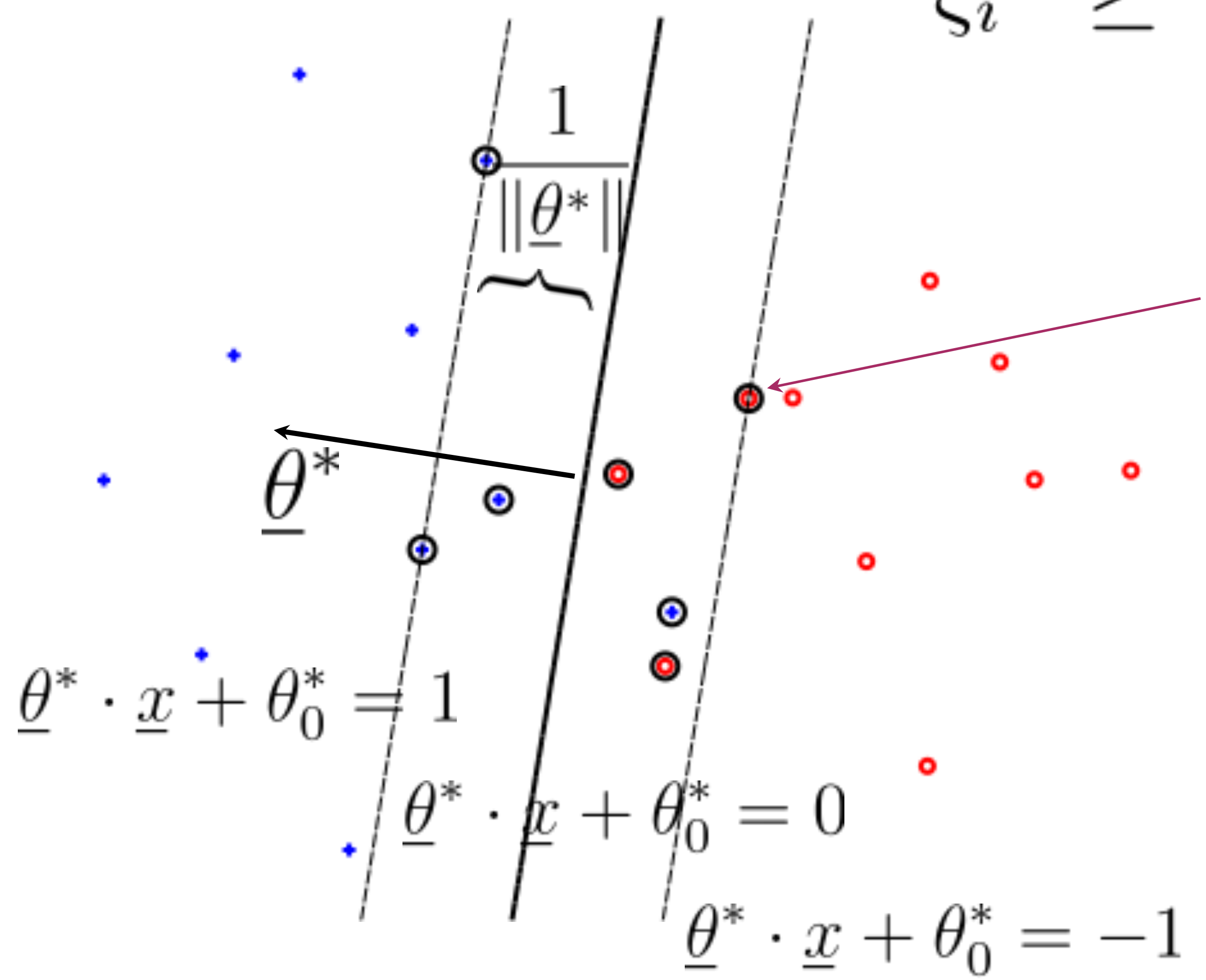


Support vectors and slack

- The solution now has three types of support vectors

$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad + \quad C\sum_{i=1}^{n}\xi_i \quad \text{subject to}$$

$$\begin{aligned} y_i(\underline{\theta}\cdot\underline{x}_i+\theta_0) &\geq 1-\xi_i, \quad i=1,\ldots,n \\ \xi_i &\geq 0, \quad i=1,\ldots,n \end{aligned}$$



$\xi_i = 0$ constraint is tight but there's no slack

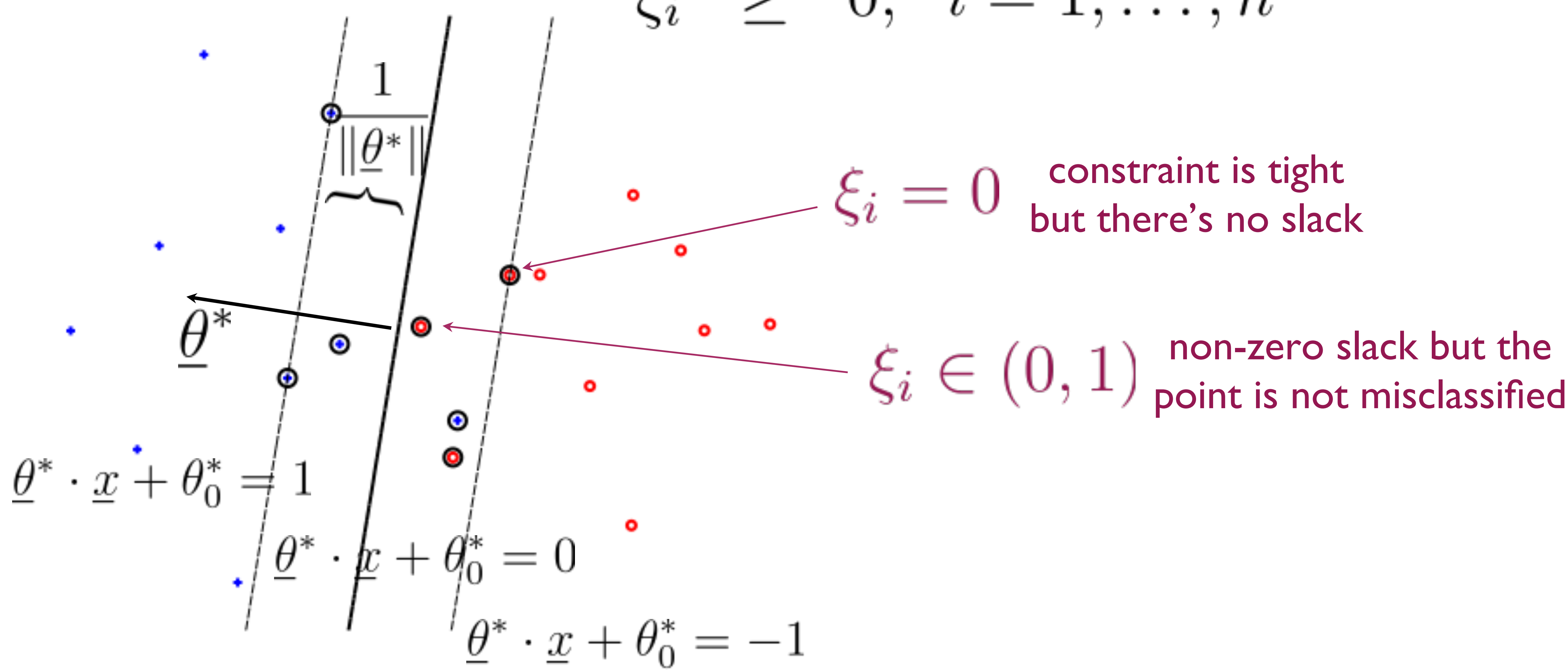
Support vectors and slack

- The solution now has three types of support vectors

$$\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad + \quad C\sum_{i=1}^{n}\xi_i \quad \text{subject to}$$

$$y_i(\underline{\theta}\cdot\underline{x}_i + \theta_0) \quad \geq \quad 1 - \xi_i, \quad i = 1, \ldots, n$$

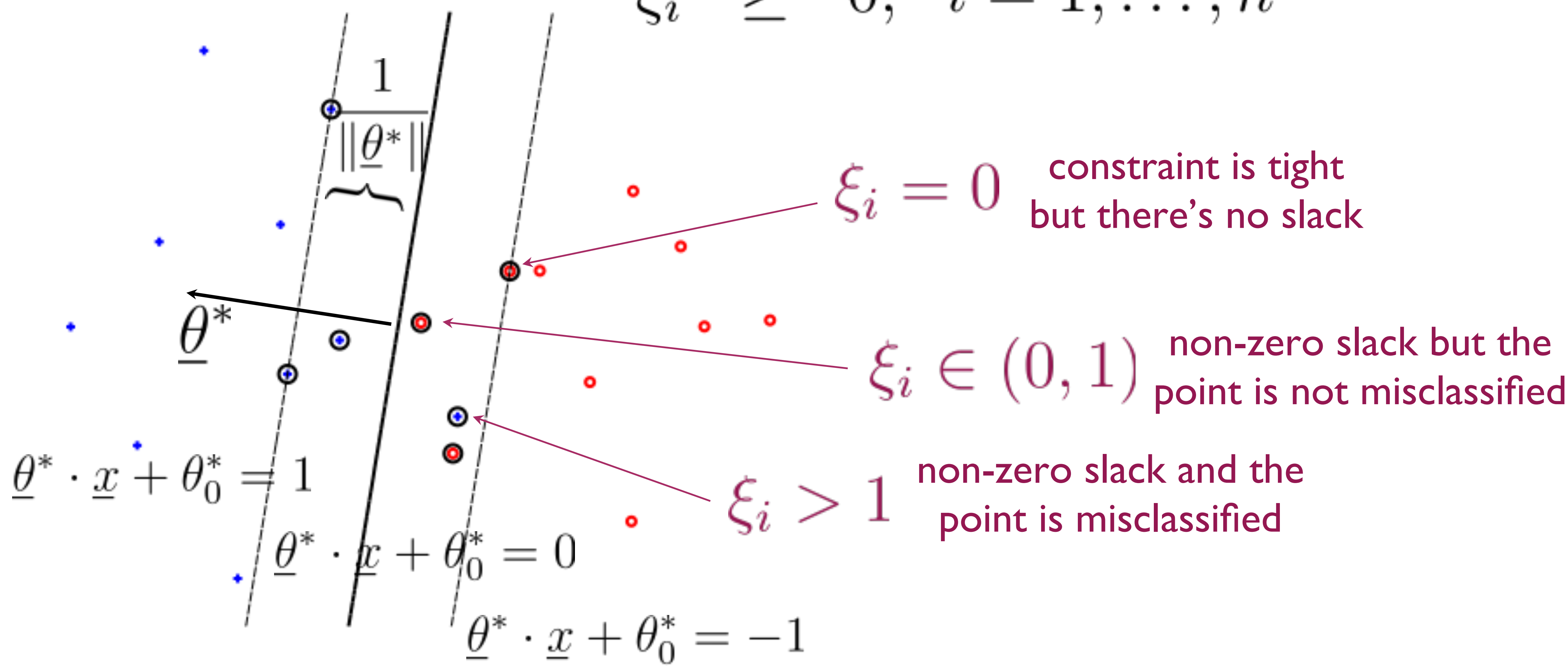
$$\xi_i \quad \geq \quad 0, \quad i = 1, \ldots, n$$



Support vectors and slack

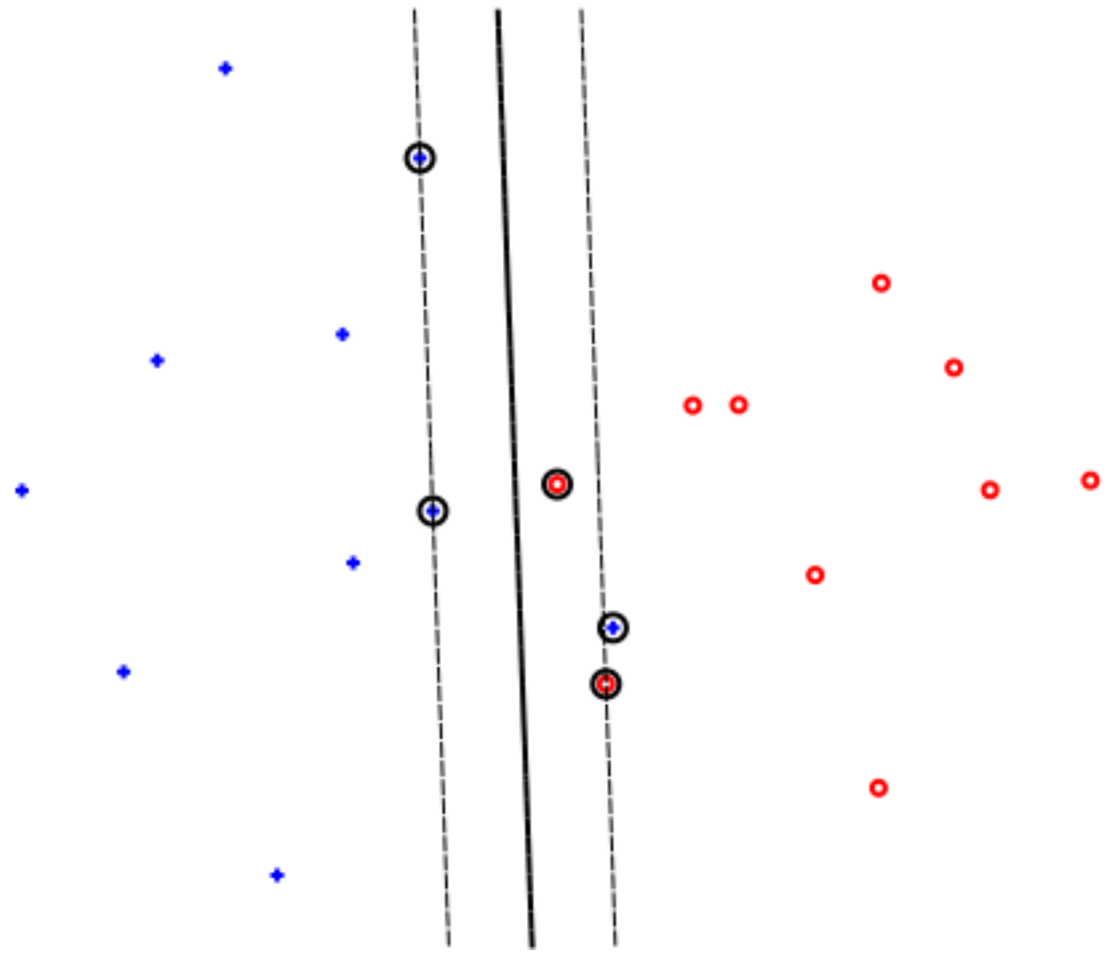
- The solution now has three types of support vectors

$$
\begin{aligned}
\text{minimize} \quad \frac{1}{2}\|\underline{\theta}\|^2 \quad + \quad C\sum_{i=1}^{n}\xi_i \quad & \text{subject to} \\
y_i(\underline{\theta}\cdot\underline{x}_i+\theta_0) \quad \geq \quad & 1-\xi_i, \quad i=1,\ldots,n \\
\xi_i \quad \geq \quad & 0, \quad i=1,\ldots,n
\end{aligned}
$$



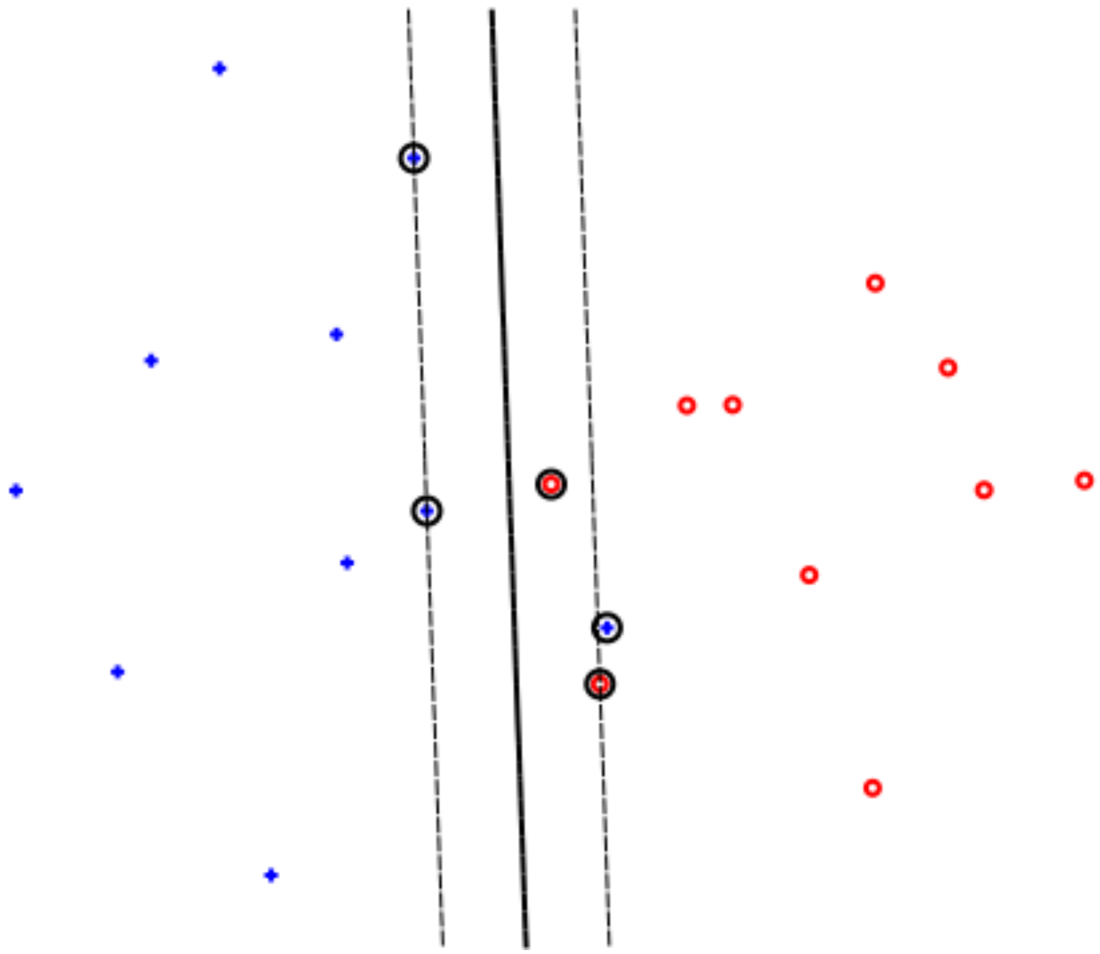
Examples

- C=100



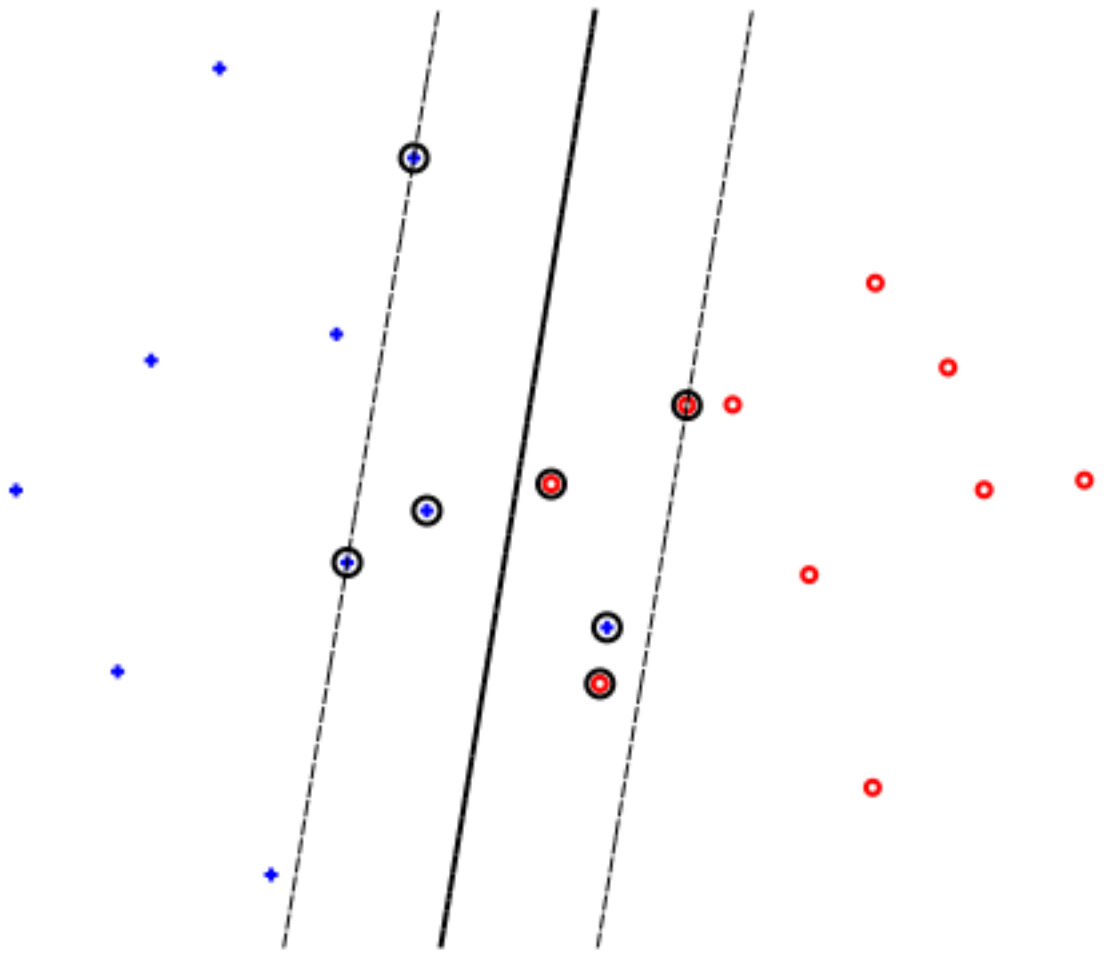
Examples

- C=10



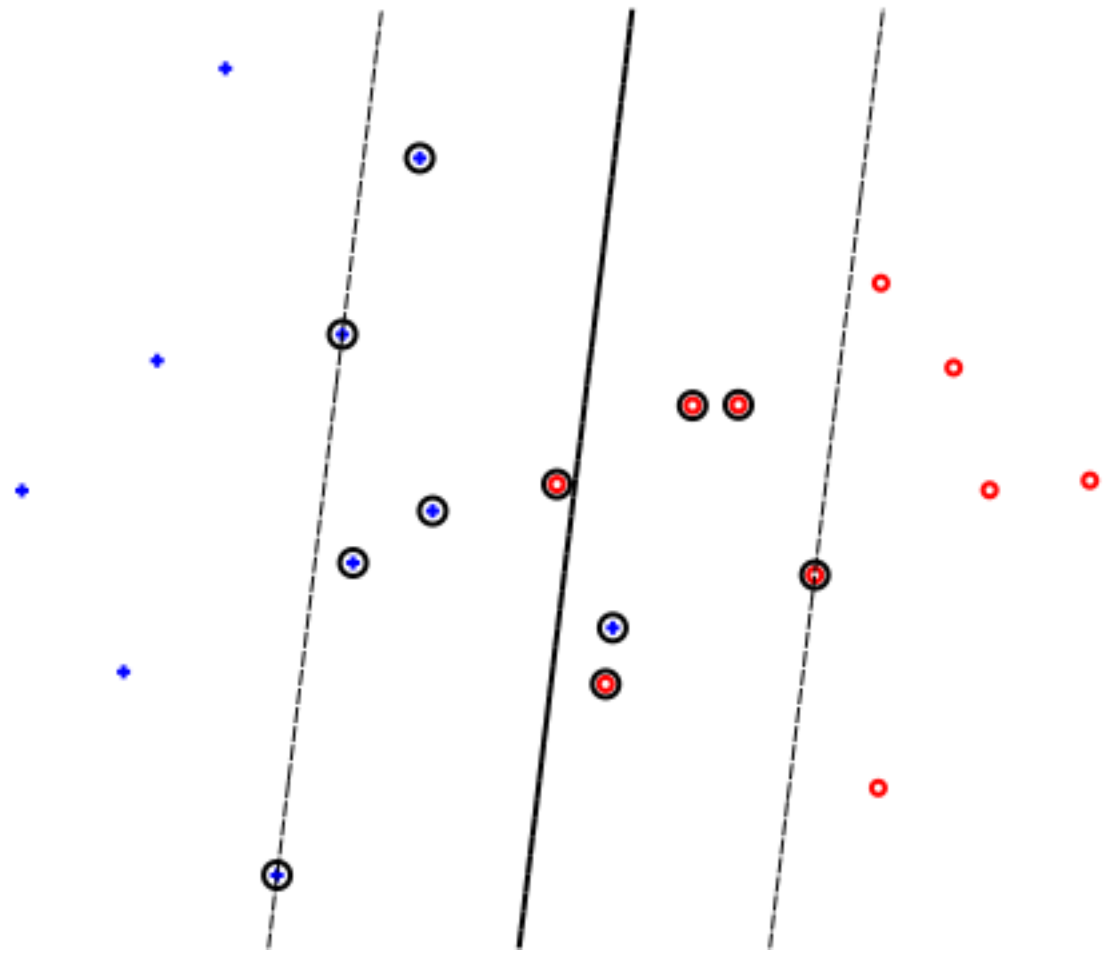
Examples

- C=1



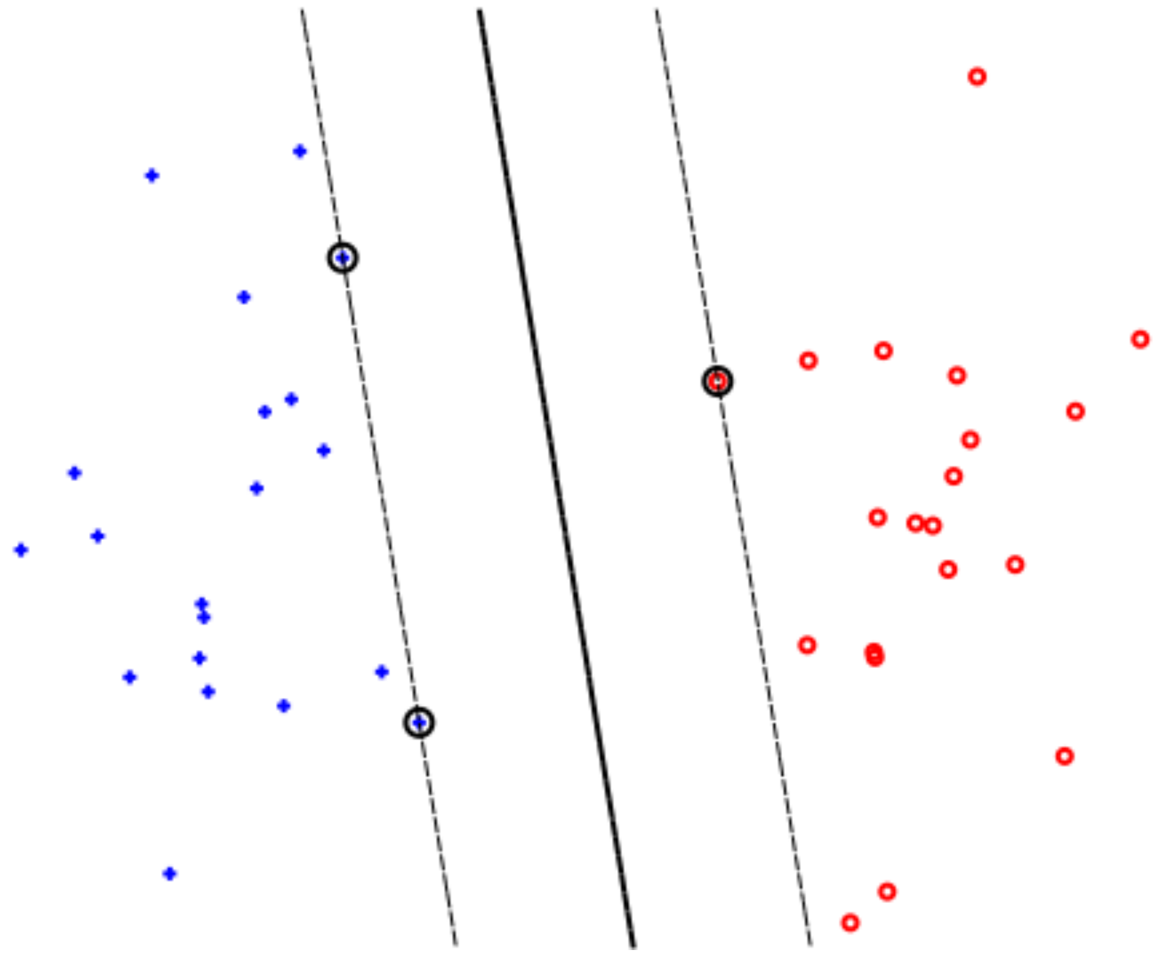
Examples

- C=0.1



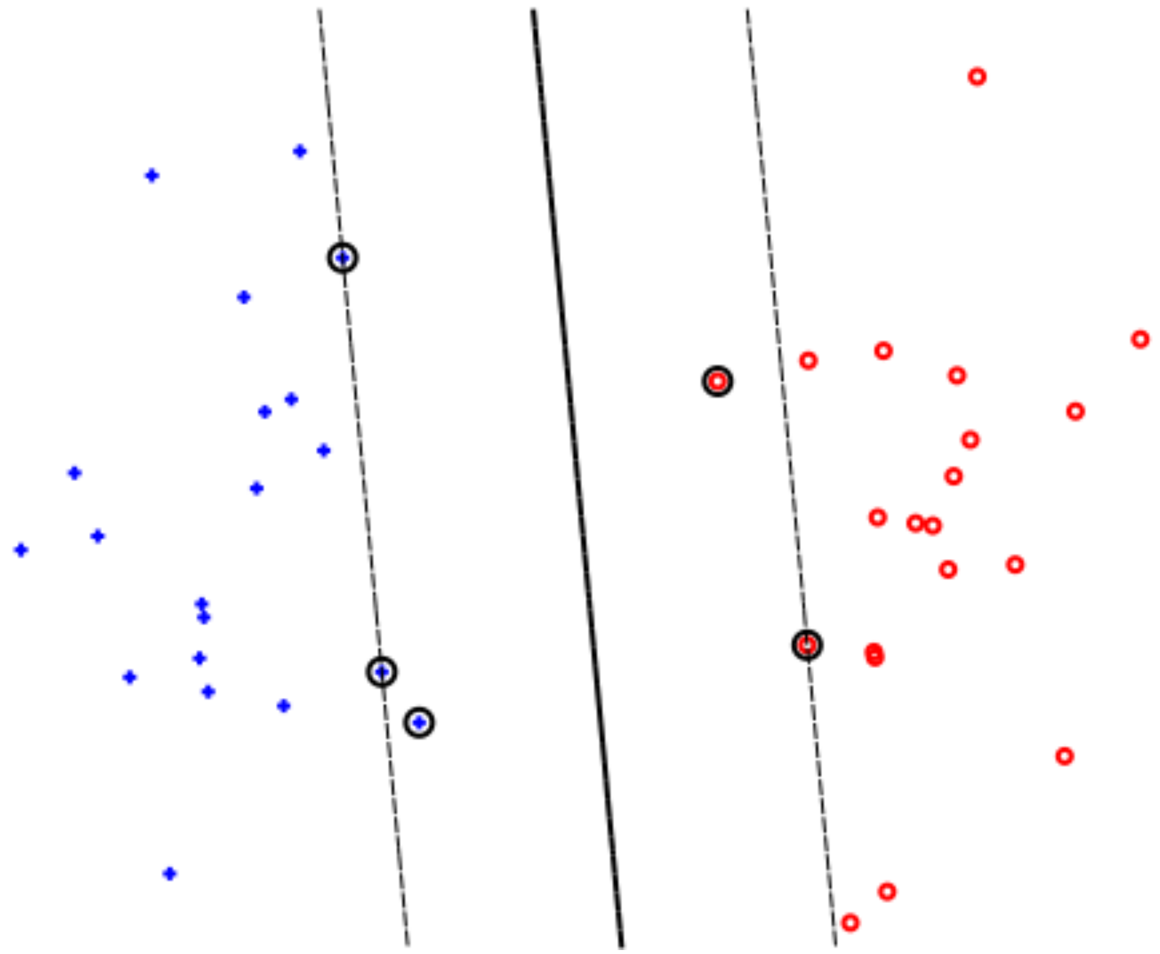
Examples

- C potentially affects the solution even in the separable case
- C = 1



Examples

- C potentially affects the solution even in the separable case
- C = 0.1



Examples

- C potentially affects the solution even in the separable case
- C = 0.01