Support Vector Machine

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These slides are based on slides from Andrew Zisserman, Yaser S. Abu-Mostafa, Mahdi Roozbahani
.

Outline

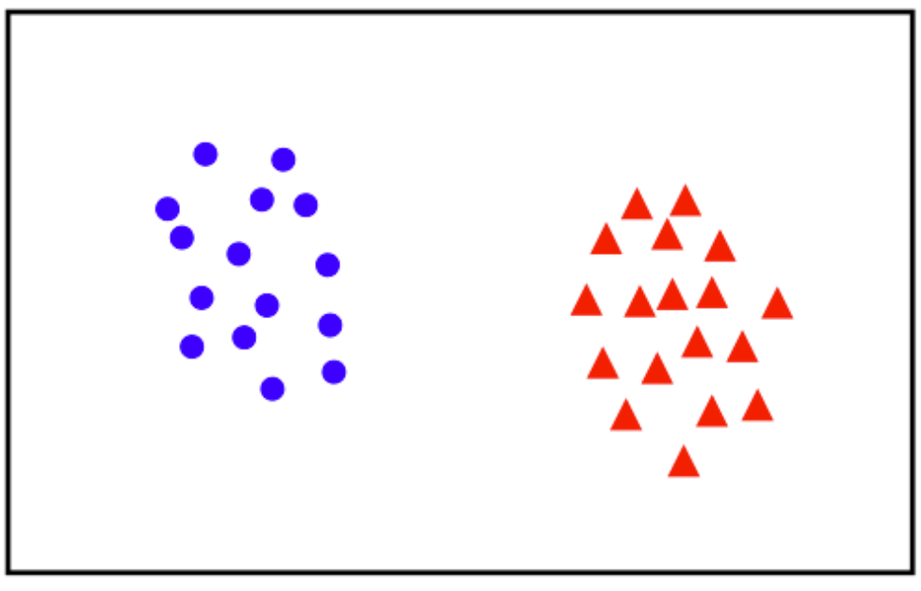
- Precursor: Linear Classifier and Perceptron
- Support Vector Machine
- Parameter Learning

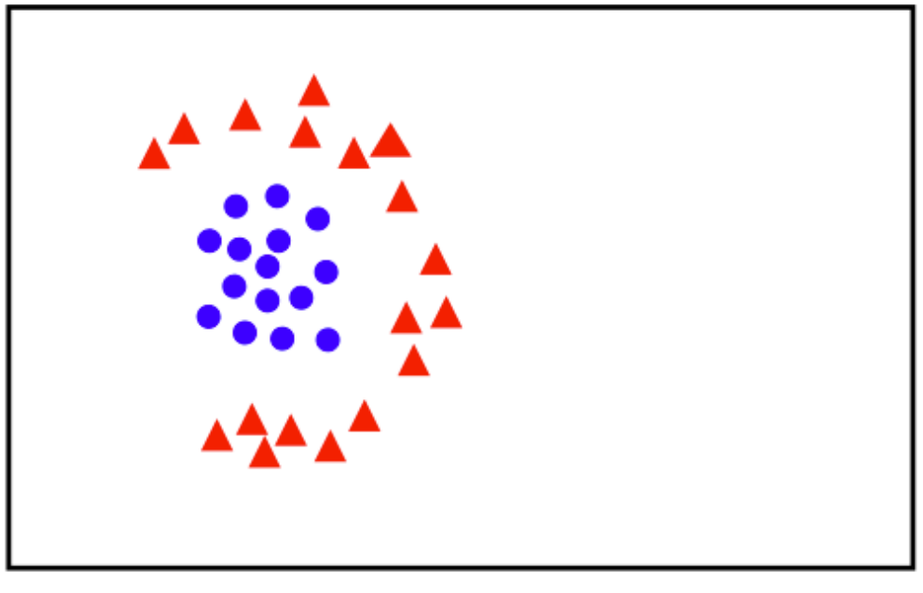
Binary Classification

Given training data $(\mathbf{x}_i, y_i)$ for $i = 1 \ldots N$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$, learn a classifier $f(\mathbf{x})$ such that

$$f(\mathbf{x}_i) \begin{cases} \geq 0 & +1 \\ < 0 & -1 \end{cases}$$

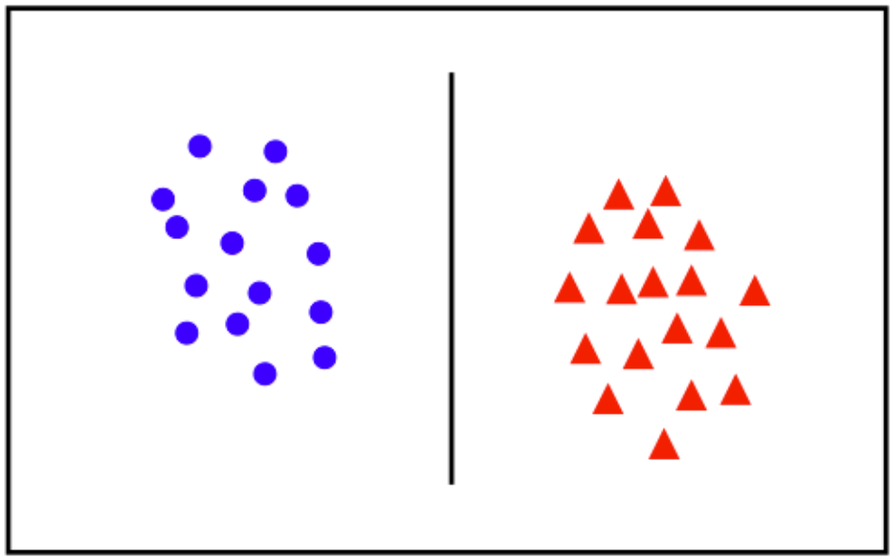
i.e. $y_i f(\mathbf{x}_i) > 0$ for a correct classification.

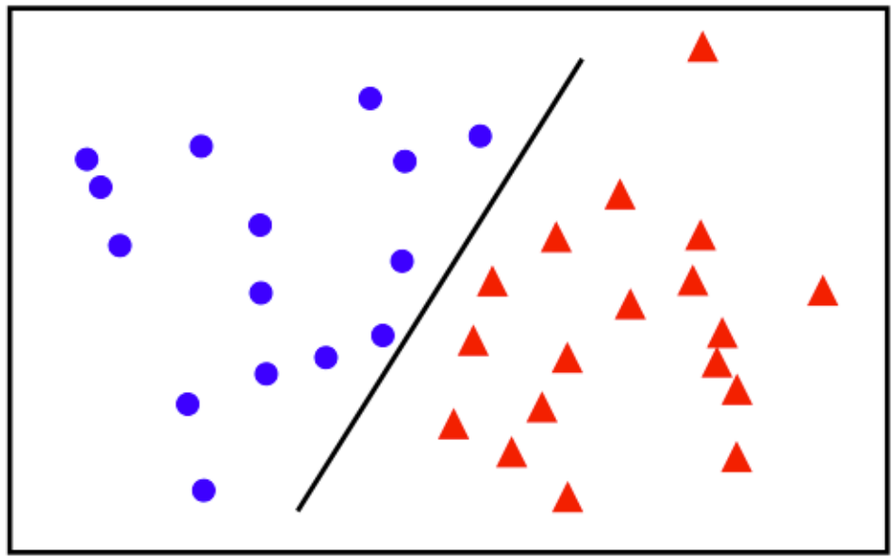




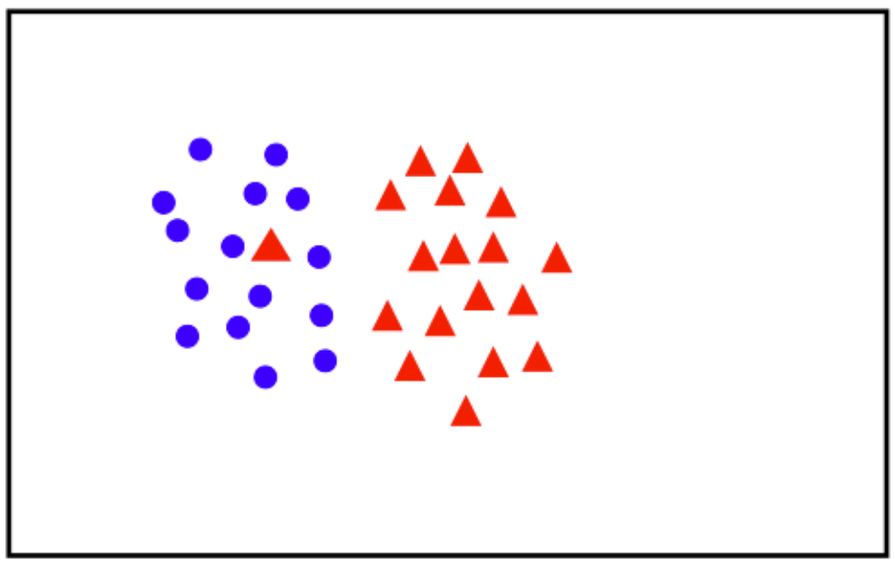
Linear Separability

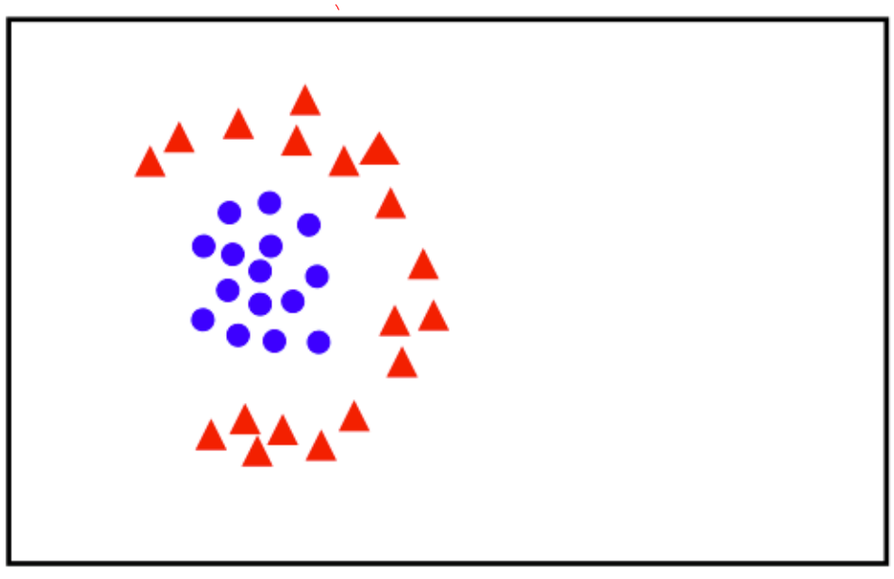
linearly separable





not linearly separable





Linear Classifier

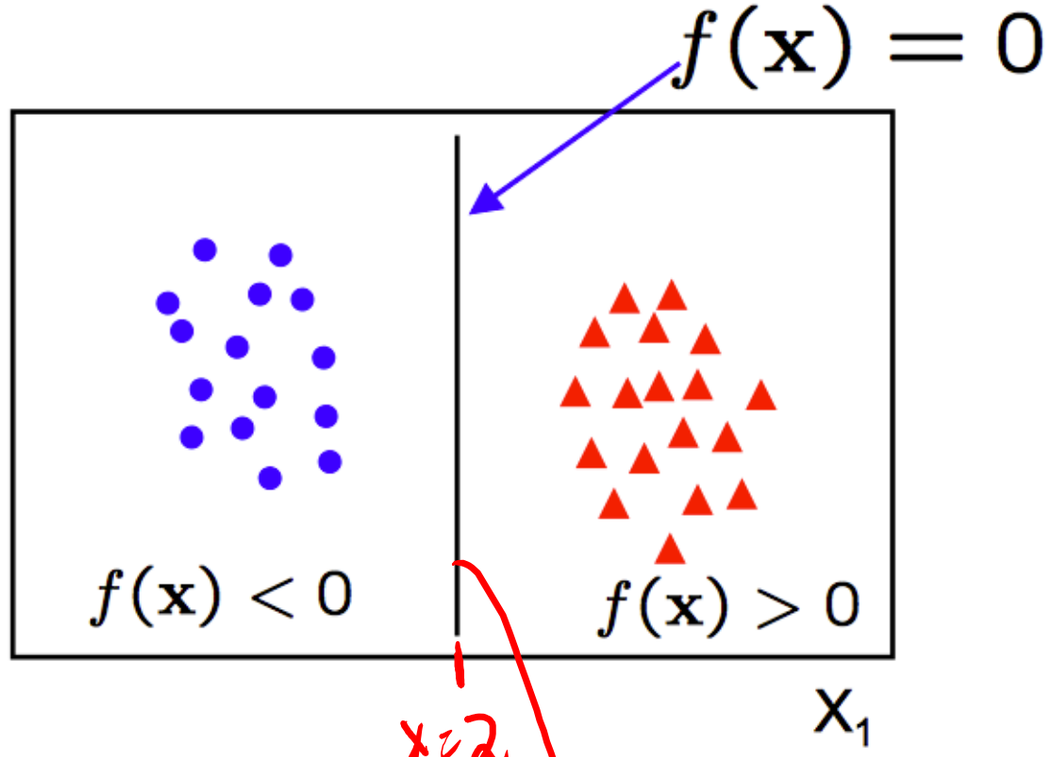
A linear classifier has the form

$y = mx + c$

$y = wx + b$ → bias

weight vector / Slope ← Unknowns

θ_0 / c / b

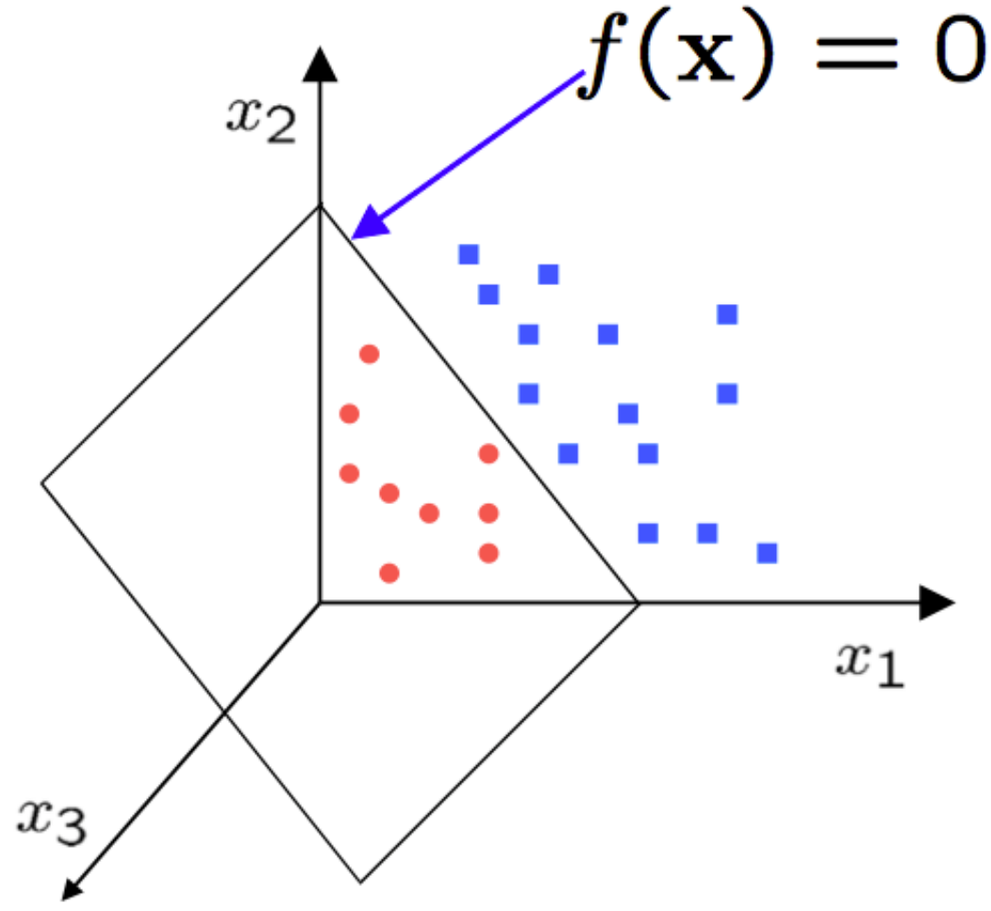


- in 2D the discriminant is a line
- θ is the normal to the line, and θ_0 the bias
- θ is known as the weight vector

Linear Classifier (higher dimension)

A linear classifier has the form

$$f(x) = x\theta + \theta_0$$



- in 3D the discriminant is a plane, and in nD it is a hyperplane

Perceptron Algorithm

Input: A sequence of training examples $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots$

where all $x_i \in \Re^n$, $y_i \in \{-1,1\}$

- Initialize $\mathbf{w}_0 = 0 \in \Re^n$
- For each training example $(\mathbf{x}_i, y_i)$:
  - Predict $y' = \text{sgn}(\mathbf{w}_t^T \mathbf{x}_i)$
  - If $y_i \neq y'$:
    - Update $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + r\,(y_i\,\mathbf{x}_i)$
- Return final weight vector

Mistake on positive: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + r\,\mathbf{x}_i$
Mistake on negative: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - r\,\mathbf{x}_i$

r is the learning rate, a small positive number less than 1

Update only on error. A mistake-driven algorithm

This is the simplest version. We will see more robust versions at the end

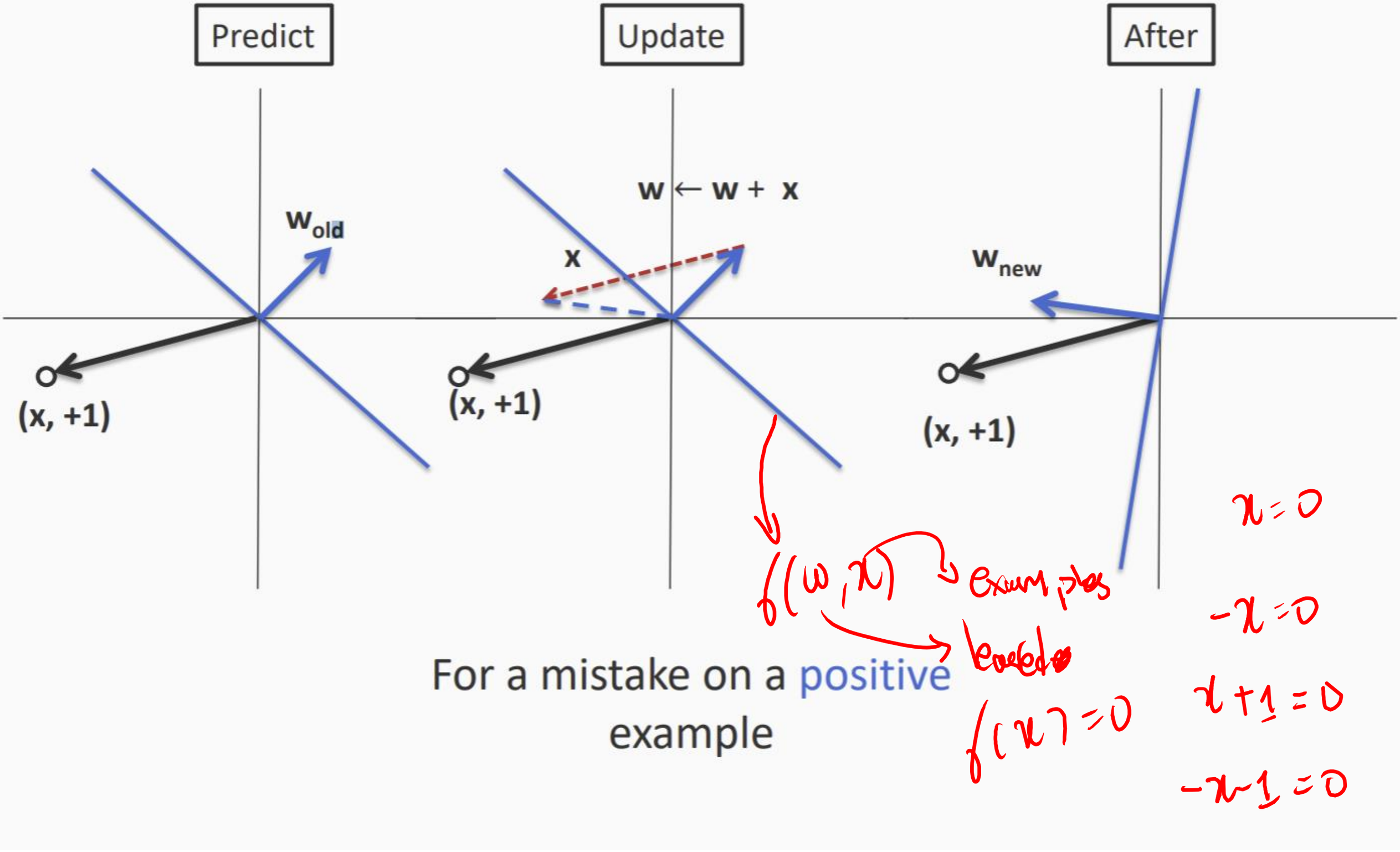
Mistake can be written as $y_i \mathbf{w}_t^T \mathbf{x}_i \leq 0$

These slides are from Vivek Srikumar

Mistake on positive: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + r\,\mathbf{x}_i$

Mistake on negative: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - r\,\mathbf{x}_i$

Geometry of the perceptron update



For a mistake on a positive example

f(w, x) examples
correct
f(x) = 0

x = 0

-x = 0

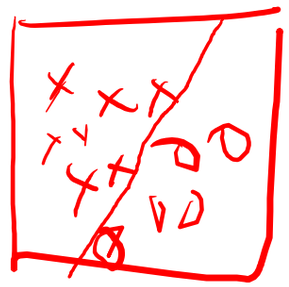
x + 1 = 0

-x - 1 = 0

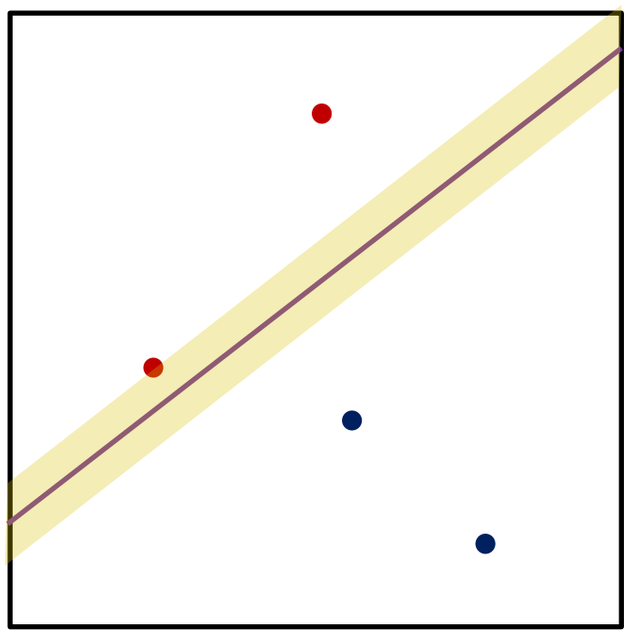
These slides are from Vivek Srikumar

Linear separation

We can have different separating lines



1.



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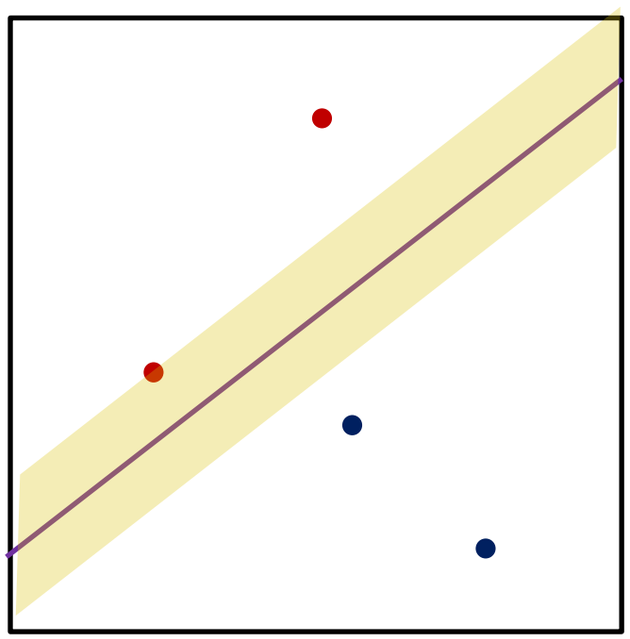

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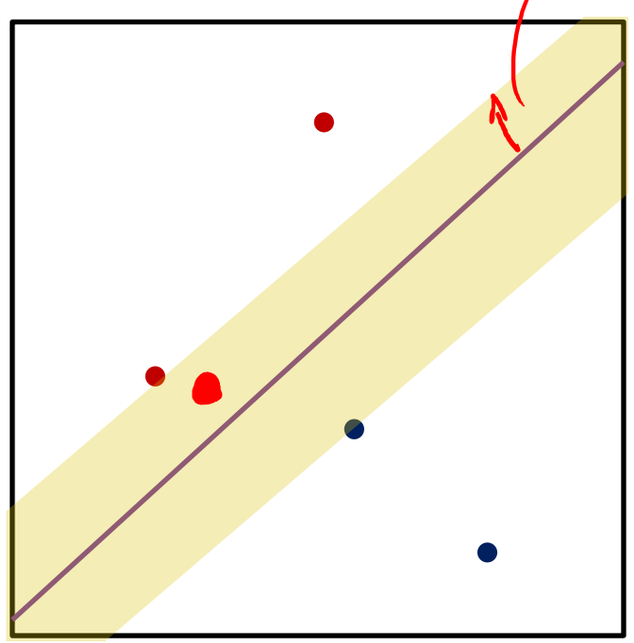
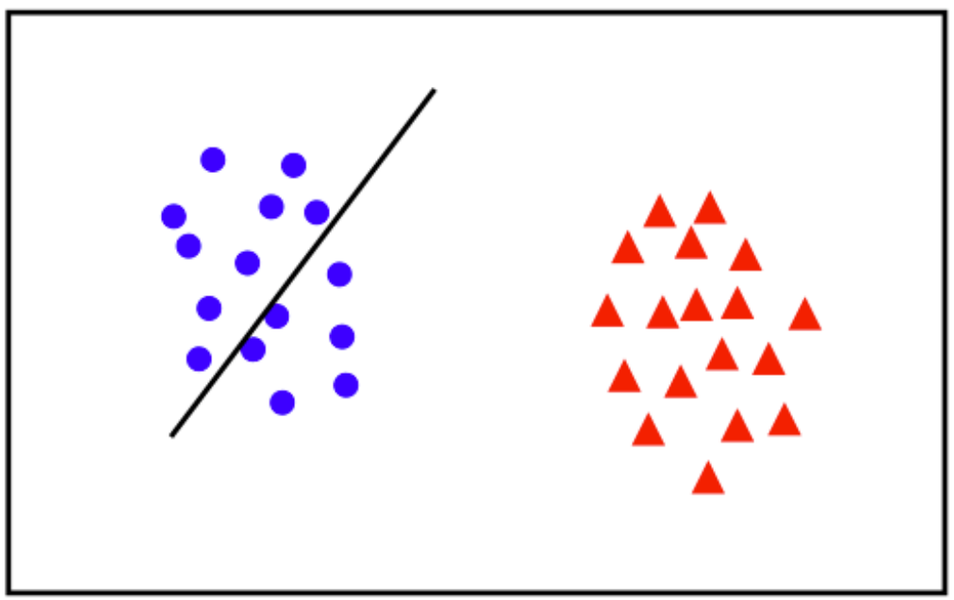


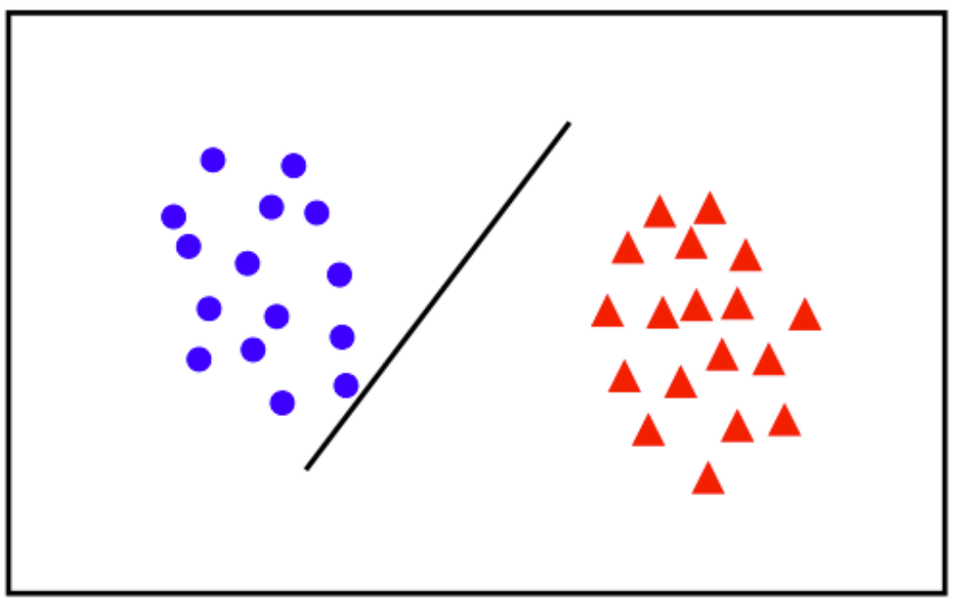
Which line is the best?

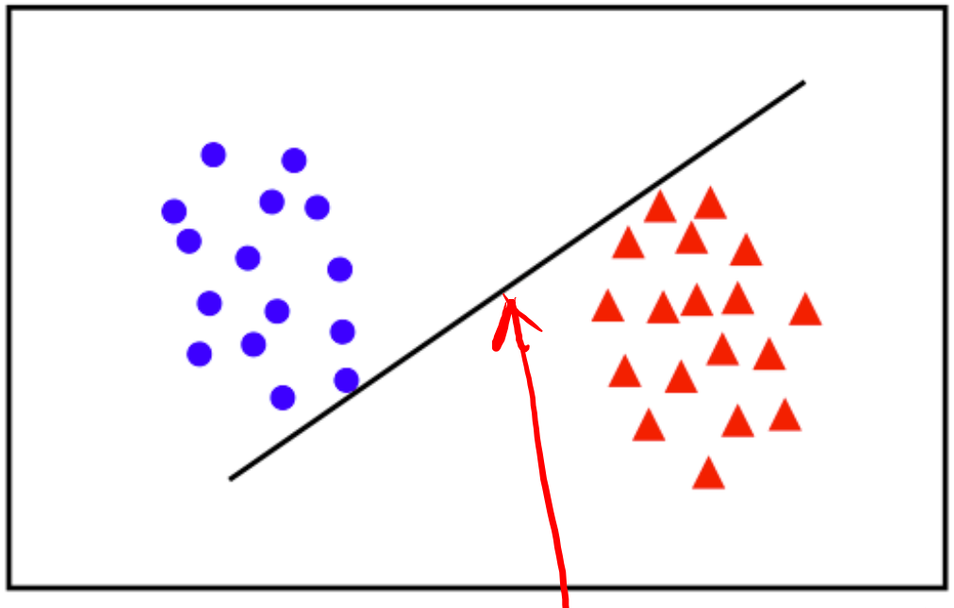
- Why is the bigger margin better?
- What $\boldsymbol{\theta}$ maximizes the margin?

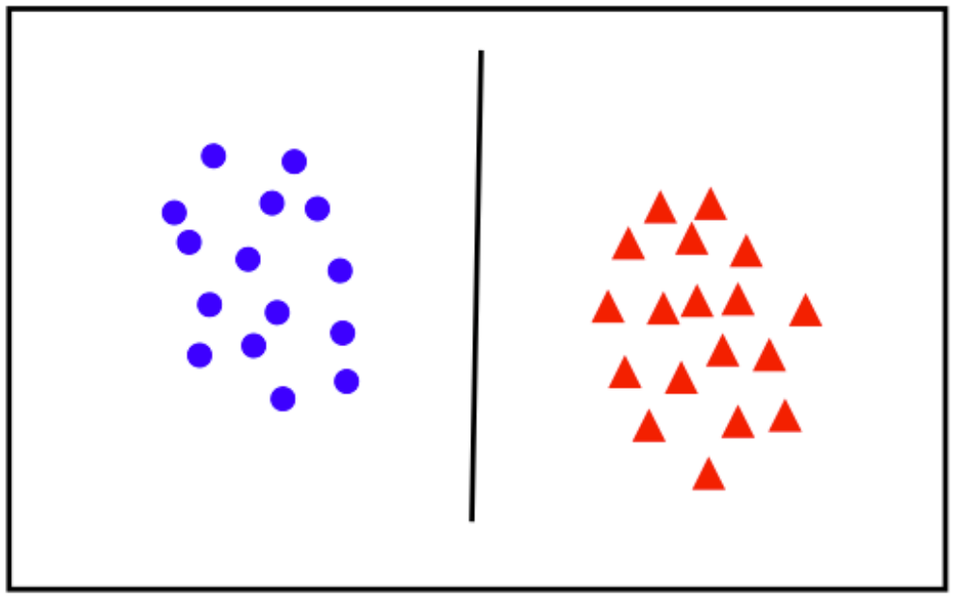
All cases, error is zero and they are linear, so they are all good for generalization.

What is the Best θ?



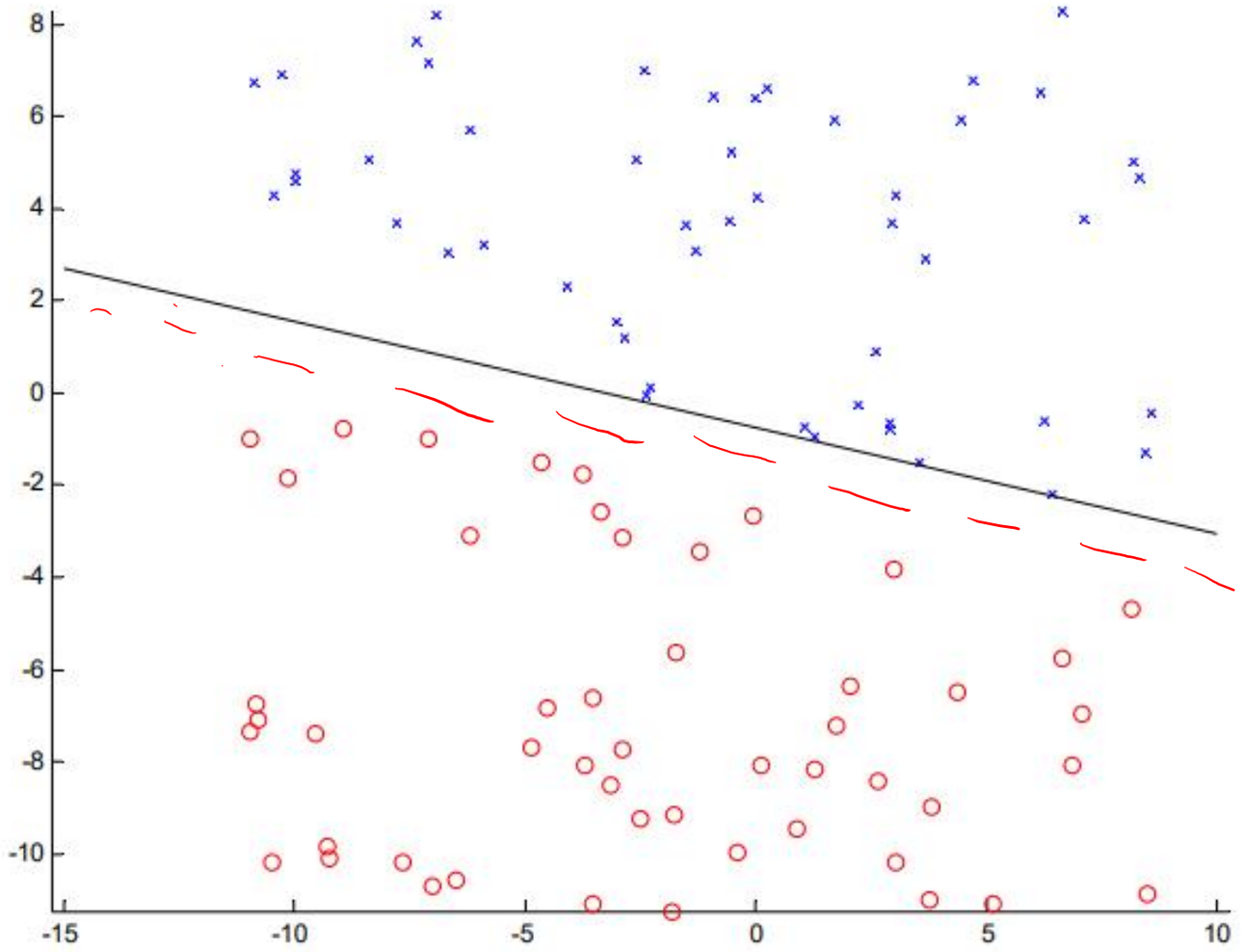






- maximum margin solution: most stable under perturbations of the inputs

Perceptron example



- if the data is linearly separable, then the algorithm will converge
- convergence can be slow …
- separating line close to training data
- we would prefer a larger margin for generalization (better generalization)

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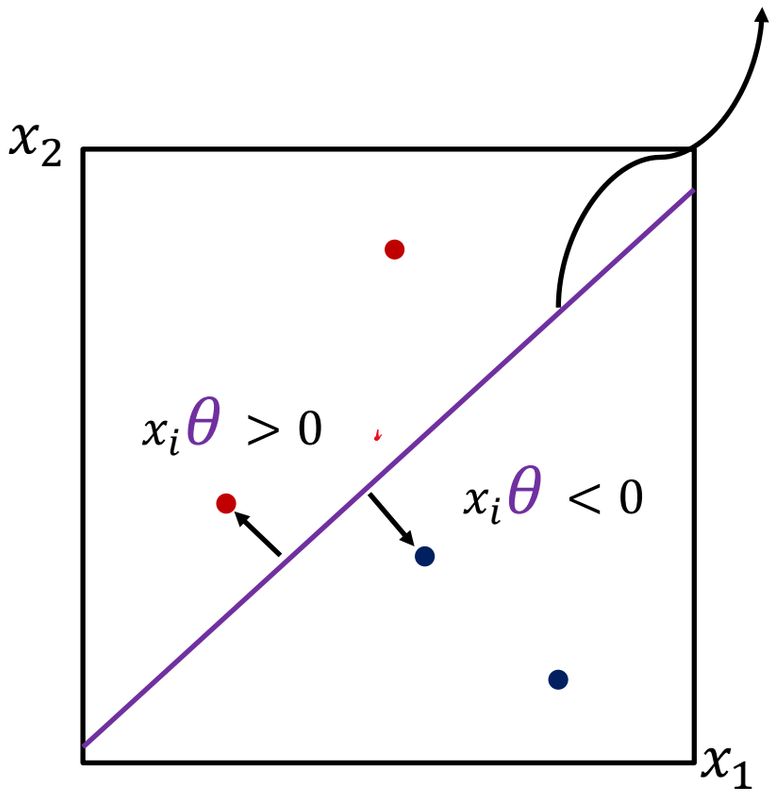
Finding θ with a **fat** margin

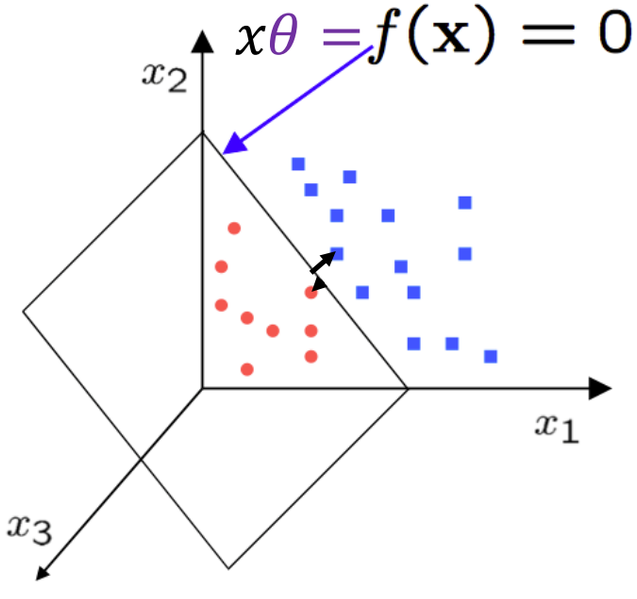
Solution (decision boundary) of the line: $x\theta = 0$



Let x_i to be the nearest data point to the line (plane):

$$|x_i\theta| > 0$$

Our line solution is $x\theta = 0$



Does it matter if θ is scaled up or down for the decision boundary?

Finding θ with a **fat** margin

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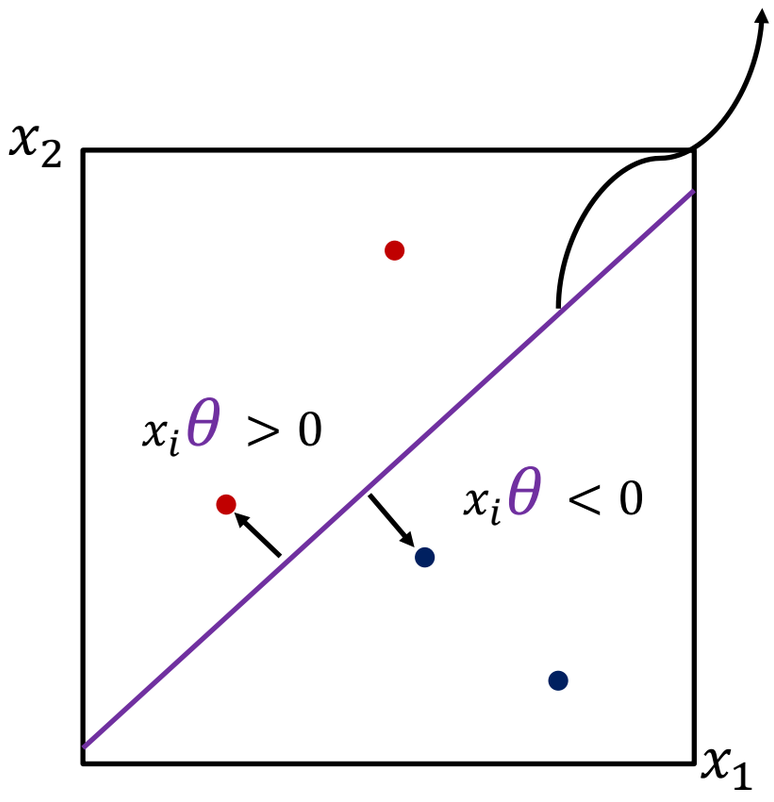

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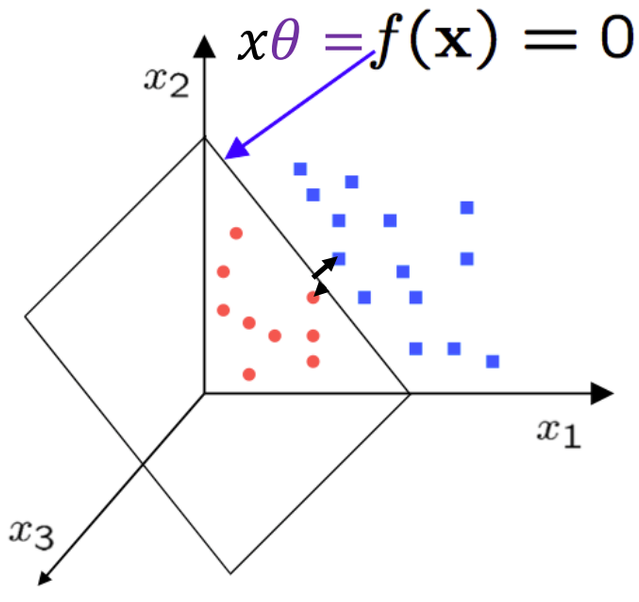


$|x_i\theta| = 1$ → normalization

Let's pull out θ_0 from $\theta = (\theta_1, \ldots, \theta_d)$ and call it be b

Decision boundary would be: $x\theta + b = 0$

Computing the distance

The distance between $\boldsymbol{x_i}$ and the line $x\theta + b = 0$ where $|x_i\theta + b| = 1$

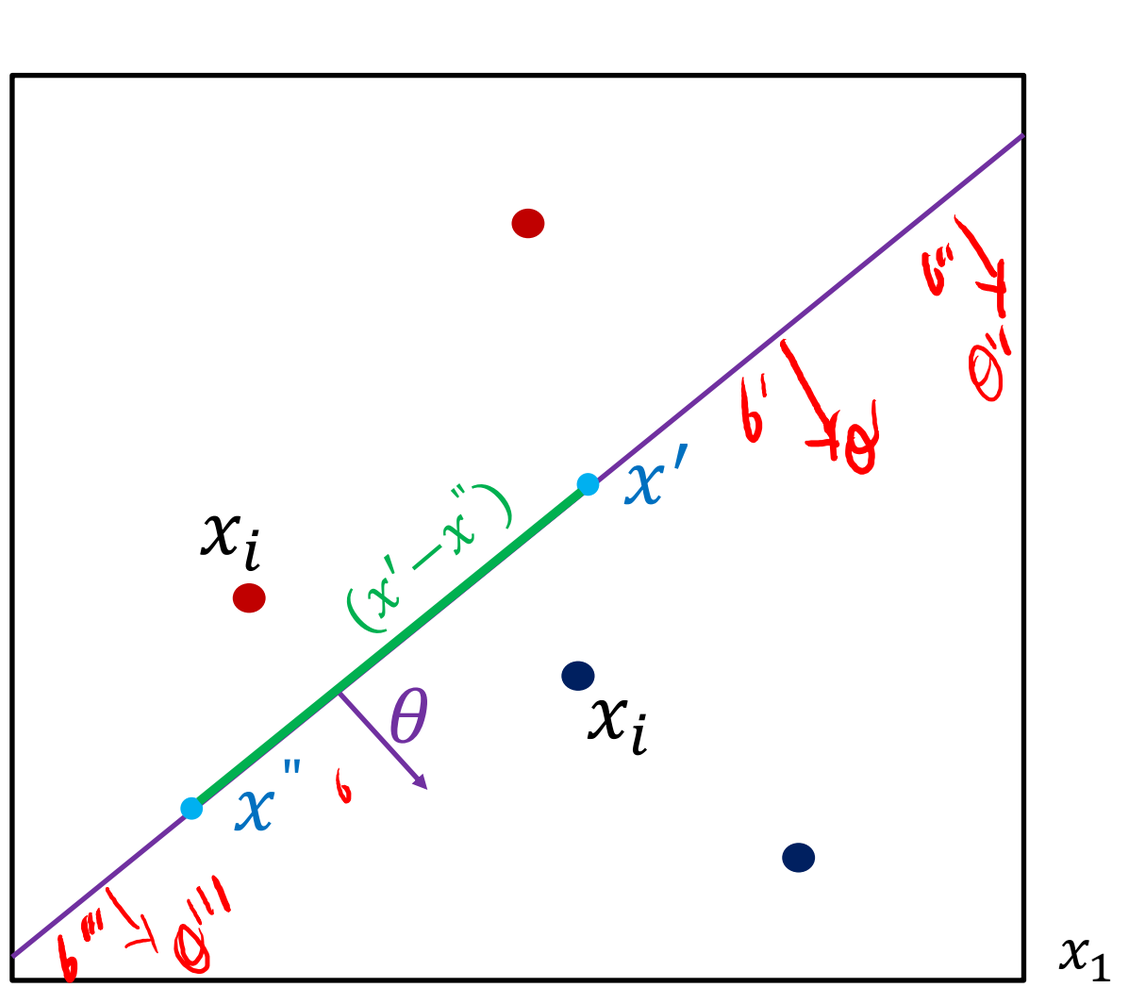
The vector θ is perpendicular to the decision line.

Consider x' and x'' on the plane

$x'\theta + b = 0$ and $x''\theta + b = 0$

$$x'\theta + b = x''\theta + b$$

$$(x' - x'')\theta = 0$$



What is the distance of my fat margin?

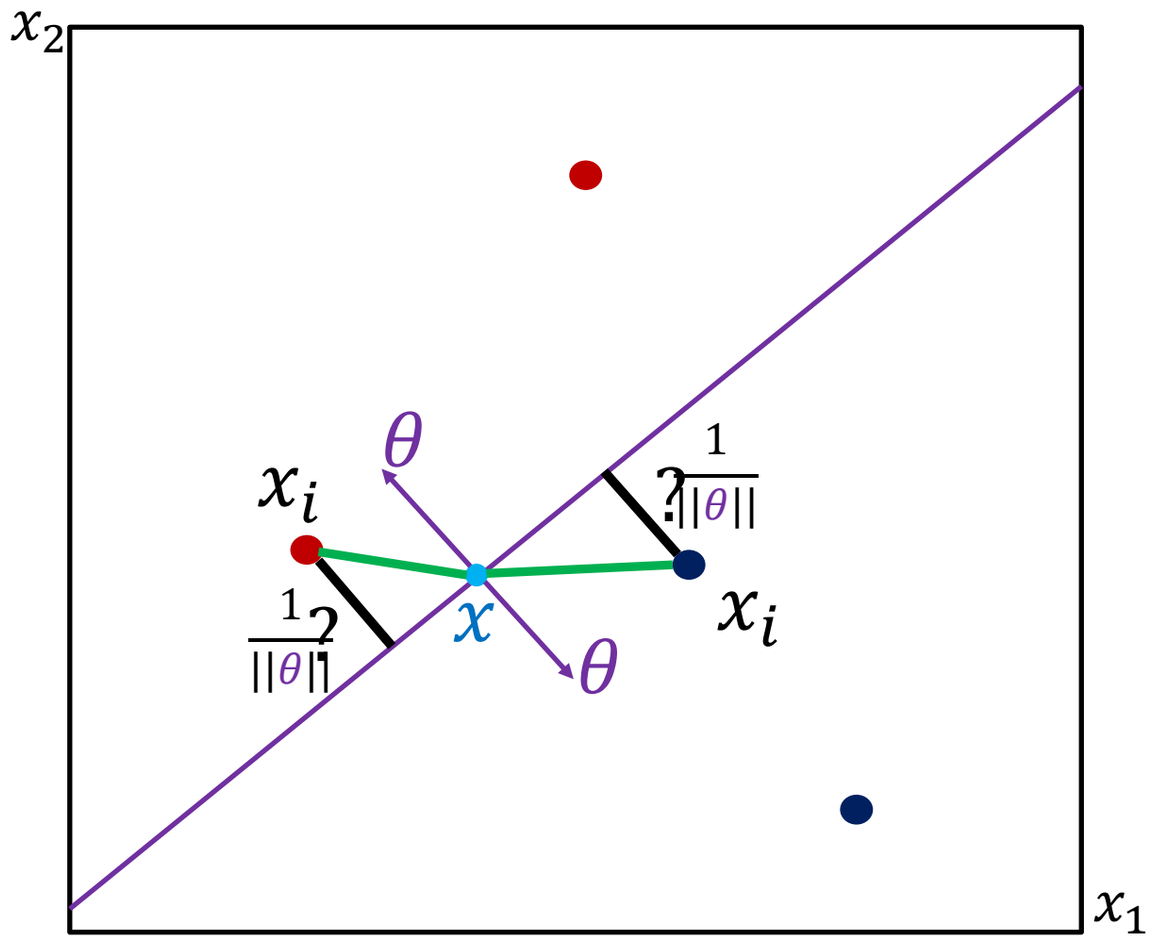
What is the distance between x_i and the plane?

Let's take any point x on the line:

Distance would be projection of $(x_i - x)$ vector on θ.

To project the vector, we need to normalize θ to get the unit vector.

$\hat{\theta} = \frac{\theta}{||\theta||} \Rightarrow \text{distance} = \left| (x_i - x)\hat{\theta} \right|$ which is the dot product



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$(x_i - x) \cdot \hat{\theta}$

To project the vector, we need to normalize θ to get the unit vector.

$$\hat{\theta} = \frac{\theta}{||\theta||} \Rightarrow \text{distance} = \left| (x_i - x)\hat{\theta} \right|$$ which is the dot product

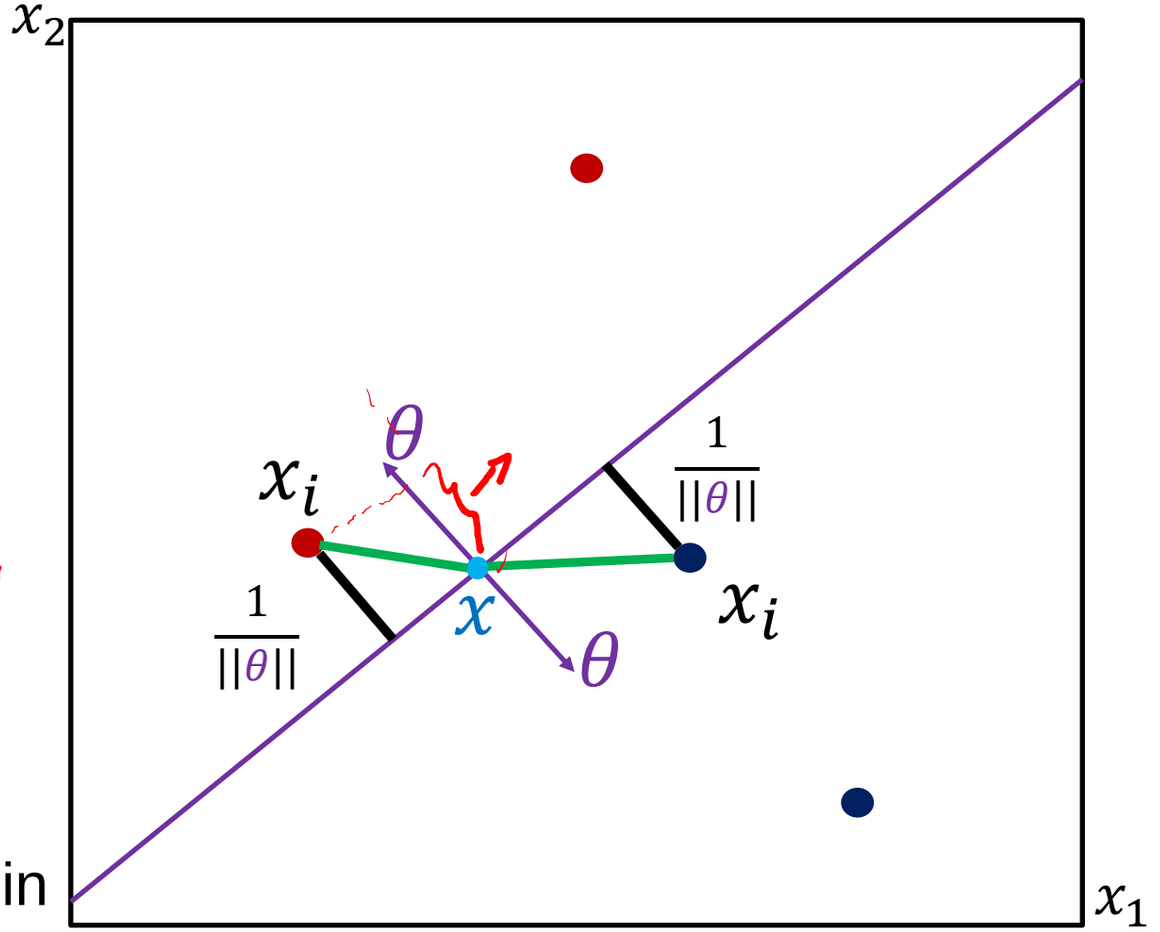
$$\text{distance} = \frac{1}{||\theta||} |(x_i\theta - x\theta)|$$

$$= \frac{1}{||\theta||} |(\underbrace{x_i\theta + b}_{\text{My constraint}} \underbrace{- x\theta - b}_{\text{A point on the decision line}})| = \frac{1}{||\theta||}$$

My constraint: $|x_i\theta + b| = 1$

A point on the decision line: $x\theta + b = 0$

The margin



Now we need to maximize the margin

Maximize $\frac{1}{||\theta||}$

we hate min & absolute in constraints

Subject to Min value of $|x_i\theta + b| = 1 \Rightarrow nearest\ neighbour$
$i = 1,2, \dots, N$

There is a “min” in our constraining; it can be hard to optimize this problem(non-convex form)

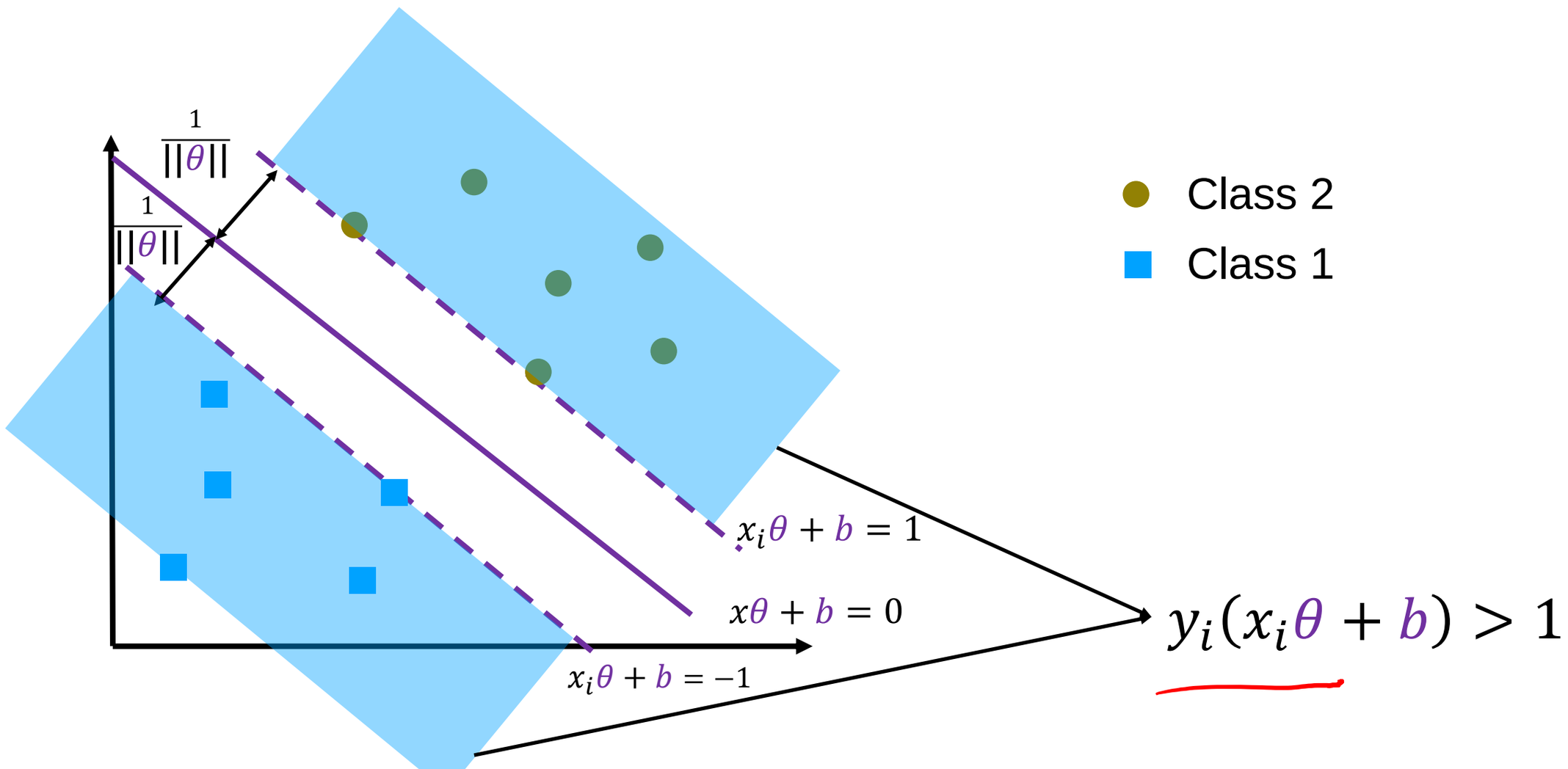
Can I write the following term to get rid of absolute value?

$$|x_i\theta + b| = y_i(x_i\theta + b) \Rightarrow \text{for a correct classification}$$

If min $|x_i\theta + b| = 1 \Rightarrow so\ it\ can\ be\ at\ least\ 1$

Maximize $\frac{1}{||\theta||}$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2, \dots, N$

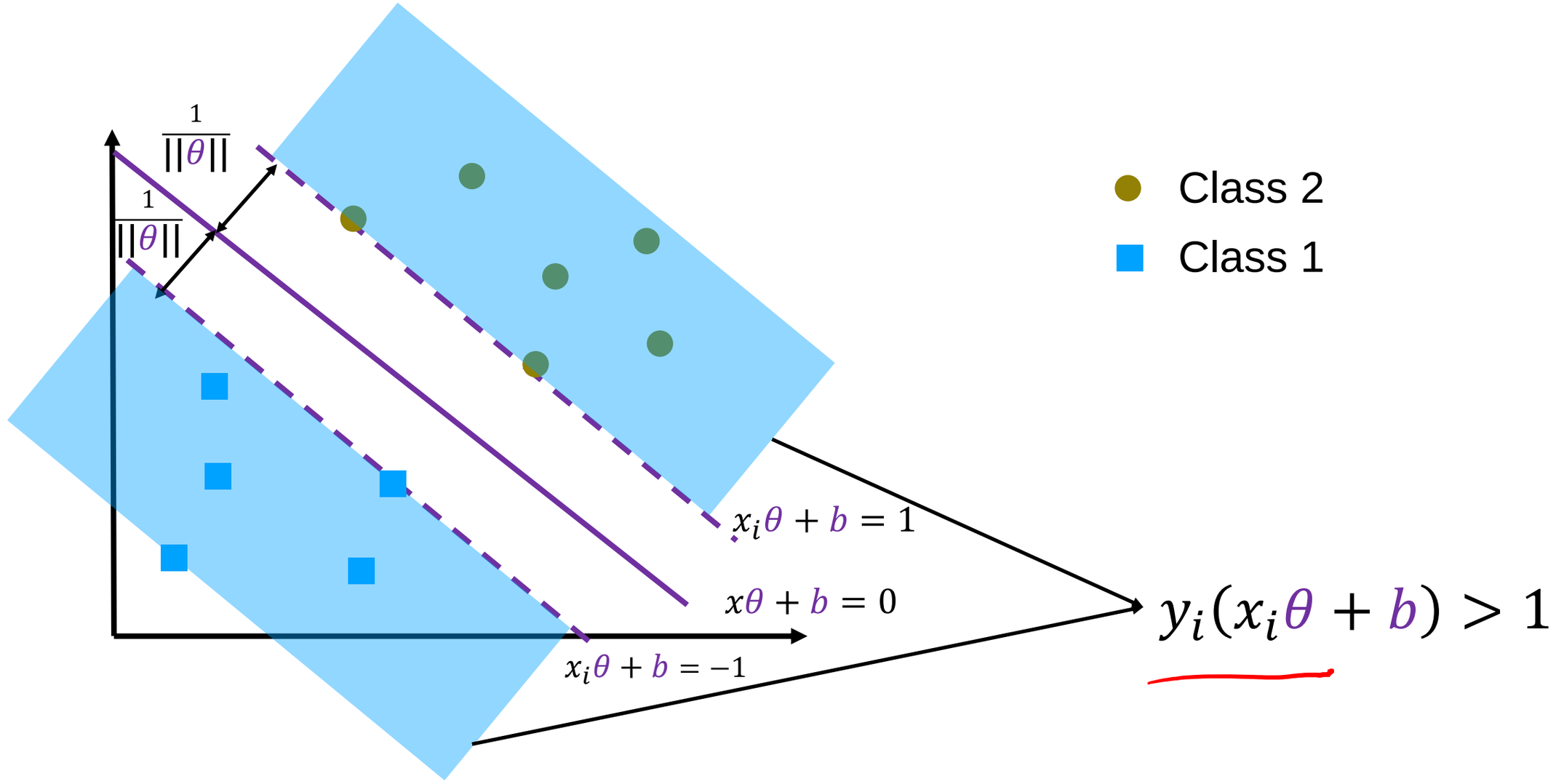


Maximize $\frac{1}{||\theta||}$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\dots,N$

Minimize $\frac{1}{2}\theta\theta^T$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\dots,N$



Minimize $\frac{1}{2}\theta\theta^T$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\ldots,N$

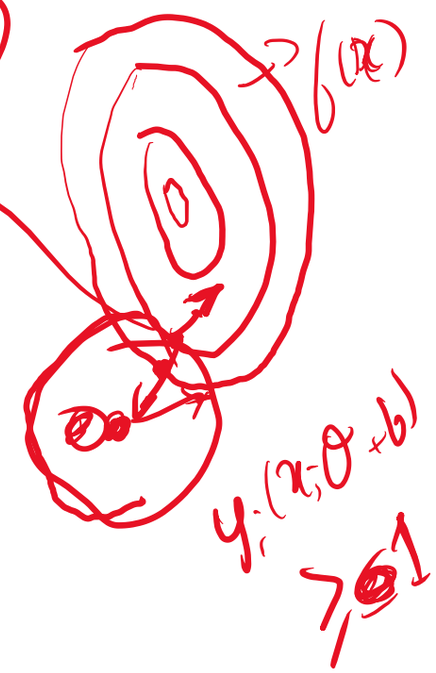
Def(1):

$$\min f(x)$$
$$\text{s.t.} \quad g(x) \le 0$$
$$h(x) = 0$$

Lagrange multipliers

$$L(x, \alpha, \beta) = f(x) + \alpha g(x) + \beta(h(x))$$

$\nabla f(x) = \alpha \nabla g(x)$ ← integrate



$$\min \frac{1}{2}\theta\theta^T$$
$$\text{s.t.} \quad y_i(x_i\theta + b) \ge 1$$

negative sign ⇒ constraint in the opposite direction

$$L(\theta, b, \alpha) = \frac{1}{2}\theta\theta^T - \sum_i^N \alpha_i (y_i(x_i\theta + b) - 1)$$
$$= \frac{1}{2}\theta\theta^T - \sum_i^N \alpha_i g(x_i) \quad \leftarrow \text{notation from def. (1)}$$

Primal problem:

$$p^* = \min_{\theta} \max_{\alpha_i, \lambda_i \geq 0} \frac{1}{2}\theta\theta^T - \sum_{i}^{N} \alpha_i g(x_i)$$

optimal sol

Dual problem:

$$d^* = \max_{\alpha_i, \lambda_i \geq 0} \min_{\theta} \frac{1}{2}\theta\theta^T - \sum_{i}^{N} \alpha_i g(x_i)$$

$$L(\theta, b, \alpha) = \frac{1}{2}\theta\theta^T - \sum_{i}^{N} a_i(y_i(b\theta + b) - 1)$$

Constrained optimization

Minimize $\frac{1}{2}\theta\theta^T$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\dots,N$

$\theta \in \mathbb{R}^d, b \in \mathbb{R}$

Using Lagrange method: But wait, there is an **inequality** in our constraints

We use **Karush-Kuhn-Tucker (KKT)** condition to deal with this problem

Constrained optimization

Minimize $\frac{1}{2}\theta\theta^T$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\dots,N$

$\theta \in \mathbb{R}^d, b \in \mathbb{R}$

Using Lagrange method: But wait, there is an **inequality** in our constraints

We use **Karush-Kuhn-Tucker (KKT)** condition to deal with this problem

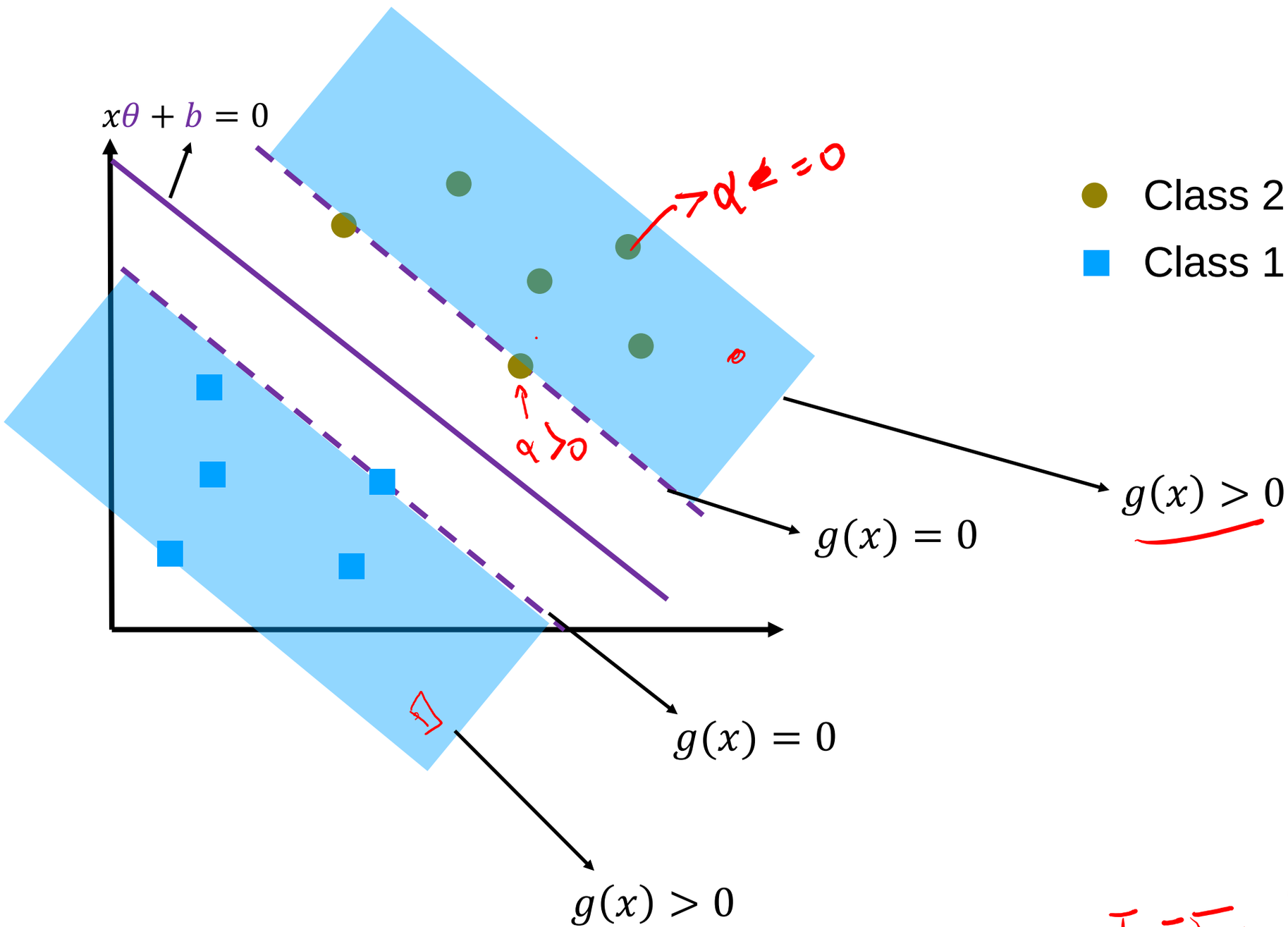
$g(x) = y_i(x_i\theta + b) - 1$ $\alpha = lagrange\ multiplier$

We need to optimize
$\theta, b, and\ \alpha$

1) $g(x) \geq 0$ Primal feasibility

2) $\alpha \geq 0$ Dual feasibility

3) $g(x)\alpha = 0$ Complementary slackness $\Rightarrow \begin{cases} g(x) > 0, & \alpha = 0 \\ \alpha > 0, & g(x) = 0 \end{cases}$



$$L(\theta, b, \alpha) = \frac{1}{2}\theta\theta^T - \sum_i \alpha_i \left(y_i(x_i\theta + b) - 1\right)$$

$$= \frac{1}{2}\theta\theta^T - \sum_i \alpha_i g(x_i)$$

$$g(x) = y_i(x_i\theta + b) - 1$$

3) $g(x)\alpha = 0$ Complementary slackness $\Rightarrow$ $\begin{cases} g(x) > 0, & \alpha = 0 \\ \alpha > 0, & g(x) = 0 \end{cases}$

Lagrange formulation

Minimize $\frac{1}{2}\theta\theta^T$ s.t. $y_i(x_i\theta + b) - 1 \geq 0$

$$\mathcal{L}(\theta, b, \alpha) = \frac{1}{2}\theta\theta^T - \sum_{i=1}^{N} \alpha_i (y_i(x_i\theta + b) - 1)$$

Minimize w.r.t θ and b and maximize *w.r.t* each $\alpha_i \geq 0$

$$\nabla_\theta \mathcal{L}(\theta, b, \alpha) = \theta - \sum_{i=1}^{N} \alpha_i y_i x_i = 0$$

$$\nabla_b \mathcal{L}(\theta, b, \alpha) = -\sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\theta = \sum_{i=1}^{N} \alpha_i y_i x_i$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

Let's substitute these in the Lagrangian:

$$\mathcal{L}(\theta, b, \alpha) = \frac{1}{2}\theta\theta^T - \sum_{i=1}^{N} \alpha_i (y_i(x_i\theta + b) - 1)$$

$$\mathcal{L}(\theta, b, \alpha) = \sum_{i=1}^{N} \alpha_i + \frac{1}{2}\theta\theta^T - \sum_{i=1}^{N} \alpha_i (y_i(x_i\theta + b))$$

$$\mathcal{L}(\theta, b, \alpha) = \sum_{i=1}^{N} \alpha_i + \frac{1}{2}\theta\theta^T - \sum_{i=1}^{N} \alpha_i (y_i(x_i\theta)) = \sum_{i=1}^{N} \alpha_i + \frac{1}{2}\theta\theta^T - \theta\theta^T =$$

$$= \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\theta\theta^T$$

$$\theta = \sum_{i=1}^{N} \alpha_i y_i x_i$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\mathcal{L}(\theta, b, \alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \theta \theta^T$$

$$\mathcal{L}(\theta, b, \alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j x_i x_j^T$$

Dual

maximize *w.r.t* each $\alpha_i \geq 0$ for $i = 1, \ldots, N$

and

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

The solution – quadratic programming

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j x_i x_j^T \qquad (1)$$

Quadratic programming packages usually use “min”

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j x_i x_j^T - \sum_{i=1}^{N} \alpha_i \qquad (2)$$

$-1 \times (1) = (2)$

$$\min_{\alpha} \frac{1}{2} \alpha^T \begin{bmatrix} y_1 y_1 x_1 x_1^T & y_1 y_2 x_1 x_2^T & \cdots & y_1 y_N x_1 x_N^T \\ y_2 y_1 x_2 x_1^T & y_2 y_2 x_2 x_2^T & \cdots & y_2 y_N x_2 x_N^T \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 x_N x_1^T & y_N y_2 x_N x_2^T & \cdots & y_N y_N x_N x_N^T \end{bmatrix} \alpha + (-I^T) \alpha$$

$$\min_{\alpha} \frac{1}{2} \alpha^T \underbrace{\begin{bmatrix} y_1 y_1 x_1 x_1^T & y_1 y_1 x_1 x_2^T & \cdots & y_1 y_N x_1 x_N^T \\ y_2 y_1 x_2 x_1^T & y_2 y_2 x_2 x_2^T & \cdots & y_2 y_N x_2 x_N^T \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 x_N x_1^T & y_N y_2 x_n x_2^T & \cdots & y_N y_N x_N x_N^T \end{bmatrix}}_{\text{Quadratic coefficients}} \alpha + \underbrace{(-I^T)}_{\text{Linear term}} \alpha$$

Subject to $\underbrace{\sum_{i=1}^{N} \alpha_i y_i = y^T \alpha = 0}_{\text{Linear equality constraint}}$

Pass these to a quadratic programming package

$$lower\ bound(0) \leq \alpha \leq \text{upper bound}(\infty)$$

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - 1^T\alpha \quad \text{subject to} \quad y^T\alpha = 0; \alpha \geq 0$$

Quadratic programming will give us α

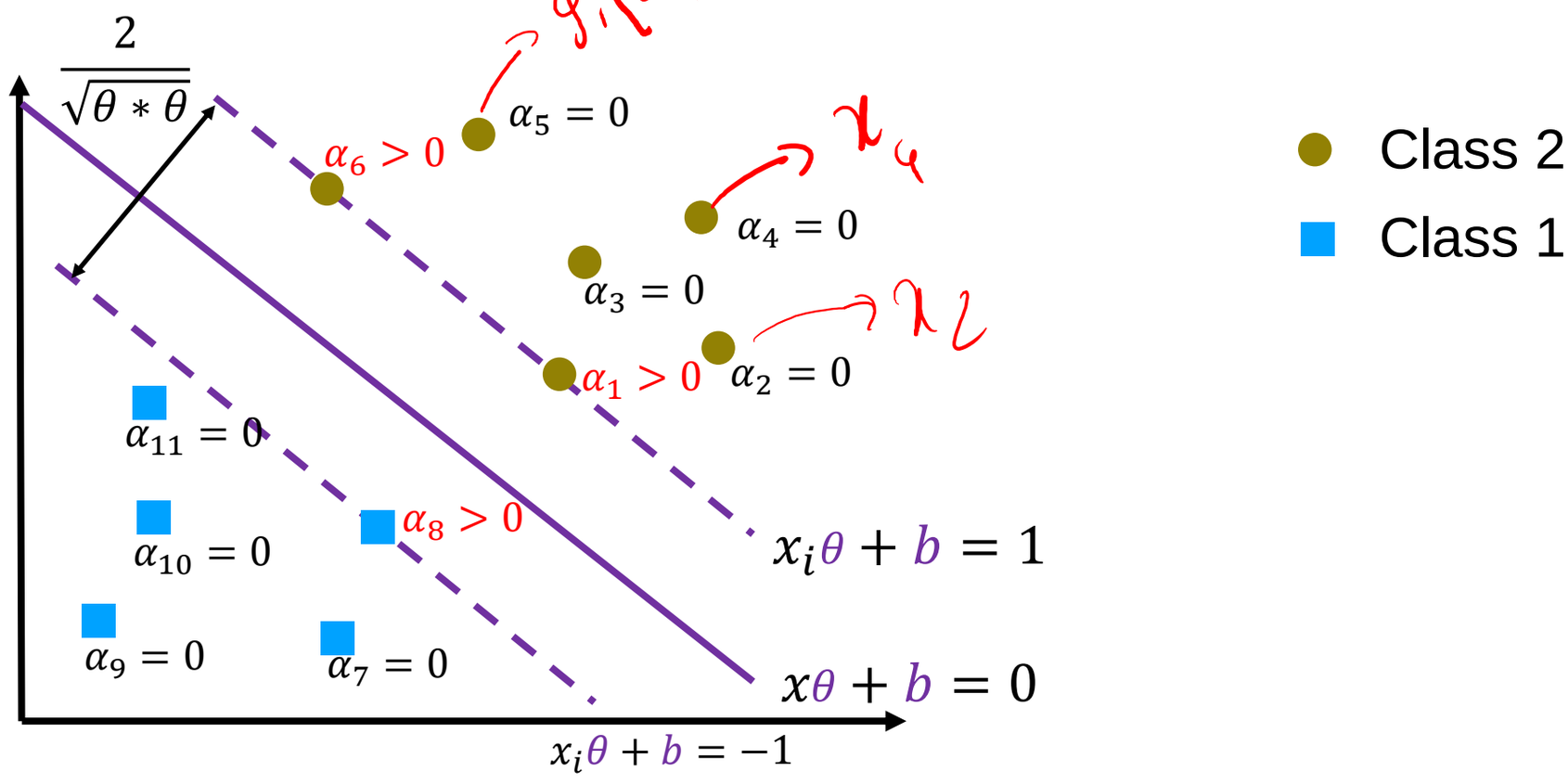
Solved

Solution: $\alpha = \alpha_1, \ldots, \alpha_N$

KKT condition ($\alpha_i g_i(\theta) = 0$): $\alpha_i(y_i(x_i\theta + b) - 1) = 0$

$(y_i(x_i\theta + b) - 1) > 0 \quad \Rightarrow \quad \alpha_i = 0$

$(y_i(x_i\theta + b) - 1) = 0 \quad \Rightarrow \quad \alpha_i > 0 \Rightarrow x_i \text{ is a support vector}$



Training

$$\theta = \sum_{i=1}^{N} \alpha_i y_i x_i$$

No need to go over all datapoints

$$\rightarrow \theta = \sum_{x_i in\ SV} \alpha_i y_i x_i$$

and for b pick any support vector and calculate:

$$y_i(x_i\theta + b) = 1$$

Training

$$\theta = \sum_{i=1}^{N} \alpha_i y_i x_i$$

No need to go over all datapoints

$$\rightarrow \theta = \sum_{x_i in\ SV} \alpha_i y_i x_i$$

and for b pick any support vector and calculate:

$$y_i(x_i\theta + b) = 1$$

Testing

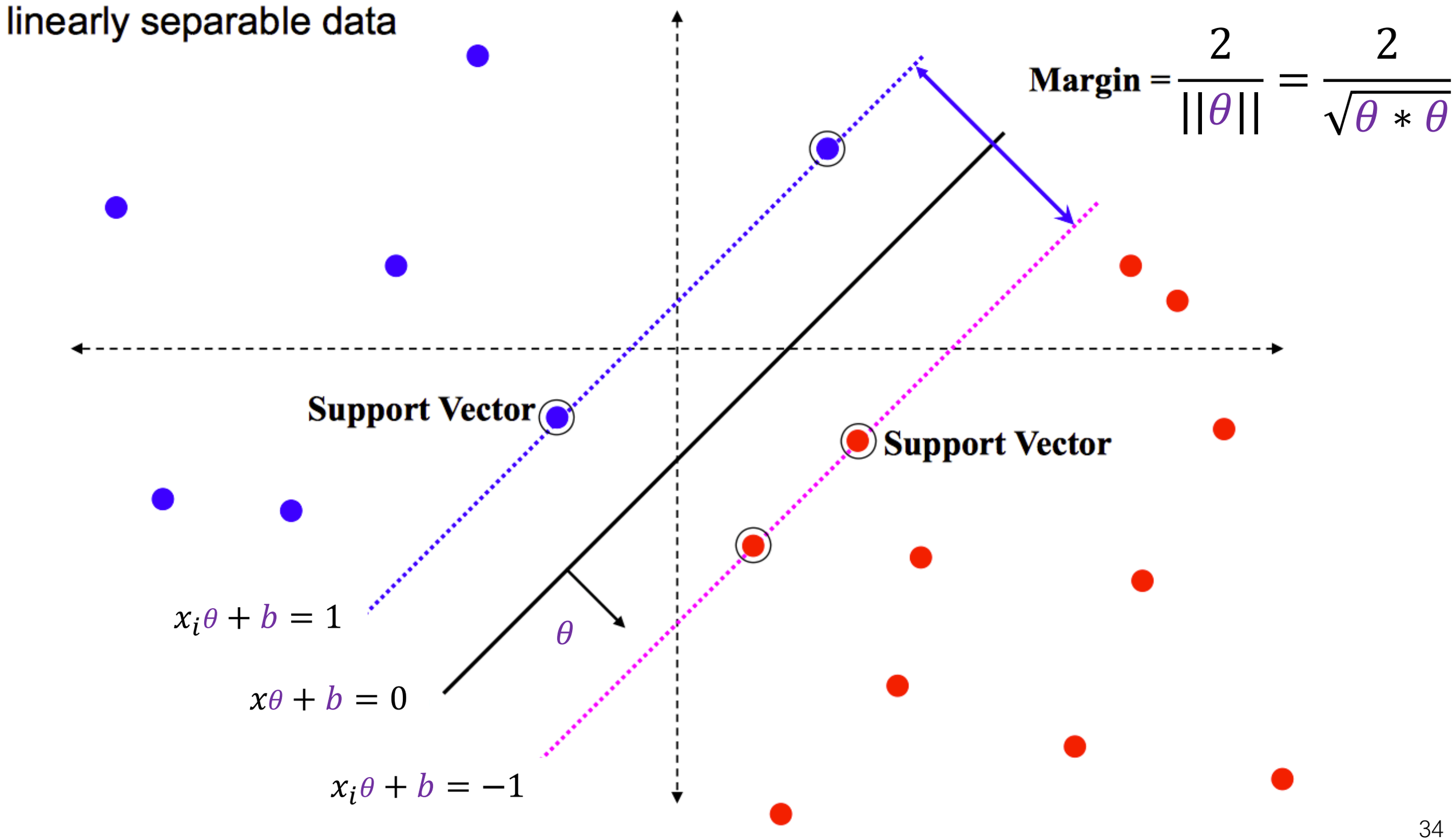
For a new test point s

Compute:

$$s\theta + b = \sum_{x_i in\ SV} \alpha_i y_i x_i s^T + b$$

Classify s as class 1 if the result is positive, and class 2 otherwise

Geometric Interpretation



Recap

Regularization lecture

$$\theta = argmin_\theta E(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2 \rightarrow MSE$$

$$Minimize\ \frac{1}{N}(z\theta - y)^T(z\theta - y)$$

Subject to $\theta^t\theta \leq C$

↳ weight constraint

For simplicity let's call θ_{lin} as weights' solution for non constrained one and θ for the constrained model.

Constrained optimization

Minimize $\frac{1}{2}\theta\theta^T$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\dots,N$

$\theta \in \mathbb{R}^d, b \in \mathbb{R}$

Using Lagrange method: But wait, there is an **inequality** in our constraints

We use **Karush-Kuhn-Tucker (KKT)** condition to deal with this problem

Regularization vs SVMs

- Regularization:

$$Minimize\ \frac{1}{N}(z\theta - y)^T(z\theta - y)$$

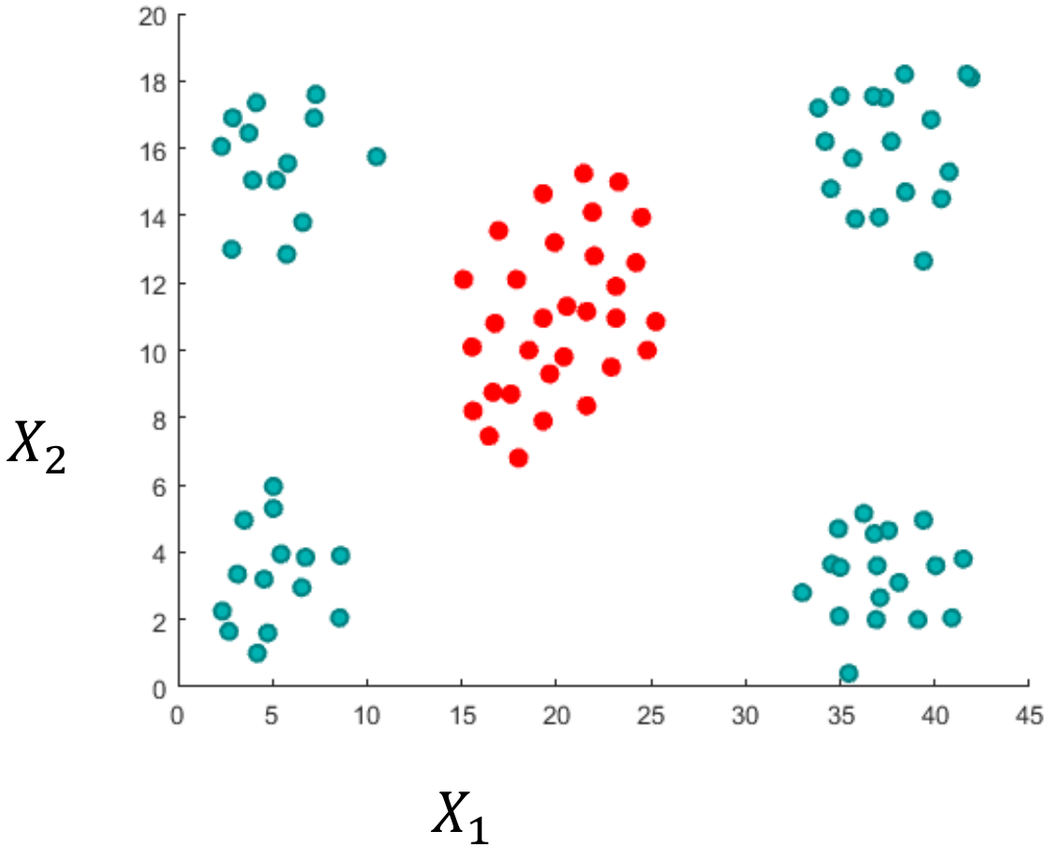
Subject to $\theta^t\theta \leq C$

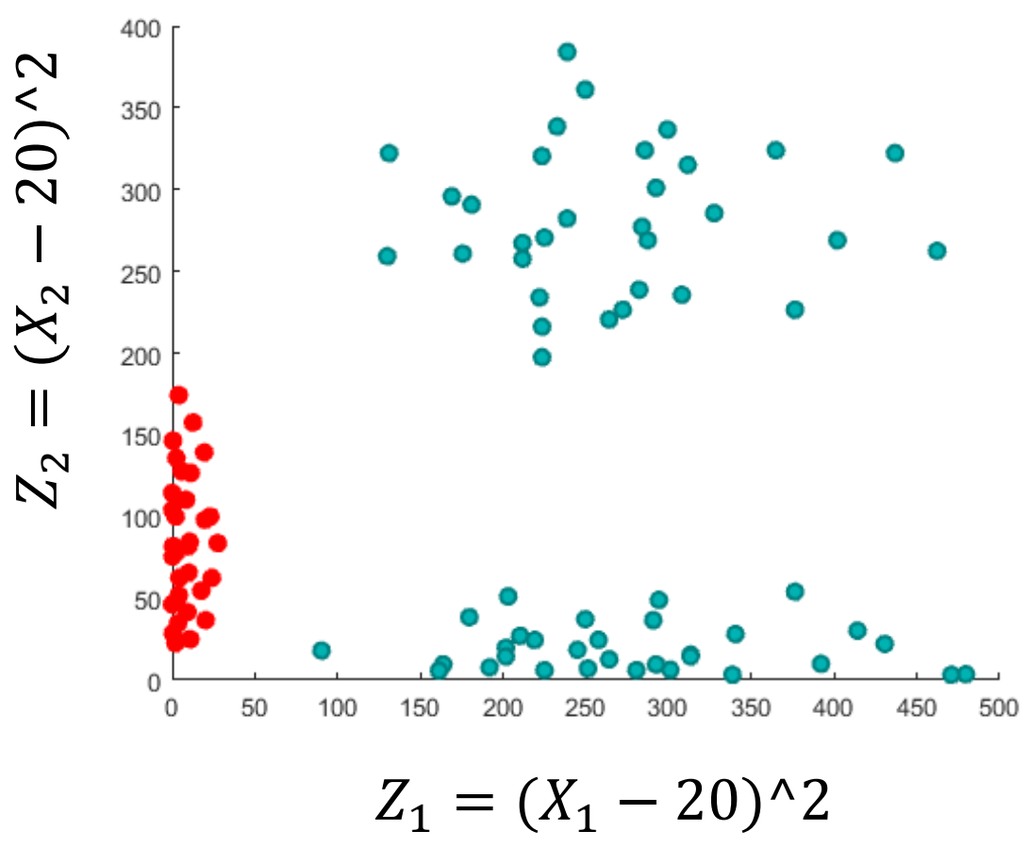
- SVM:

Minimize $\frac{1}{2}\theta\theta^T$

Subject to $y_i(x_i\theta + b) \geq 1$ for $i = 1,2,\dots,N$

From x to z space



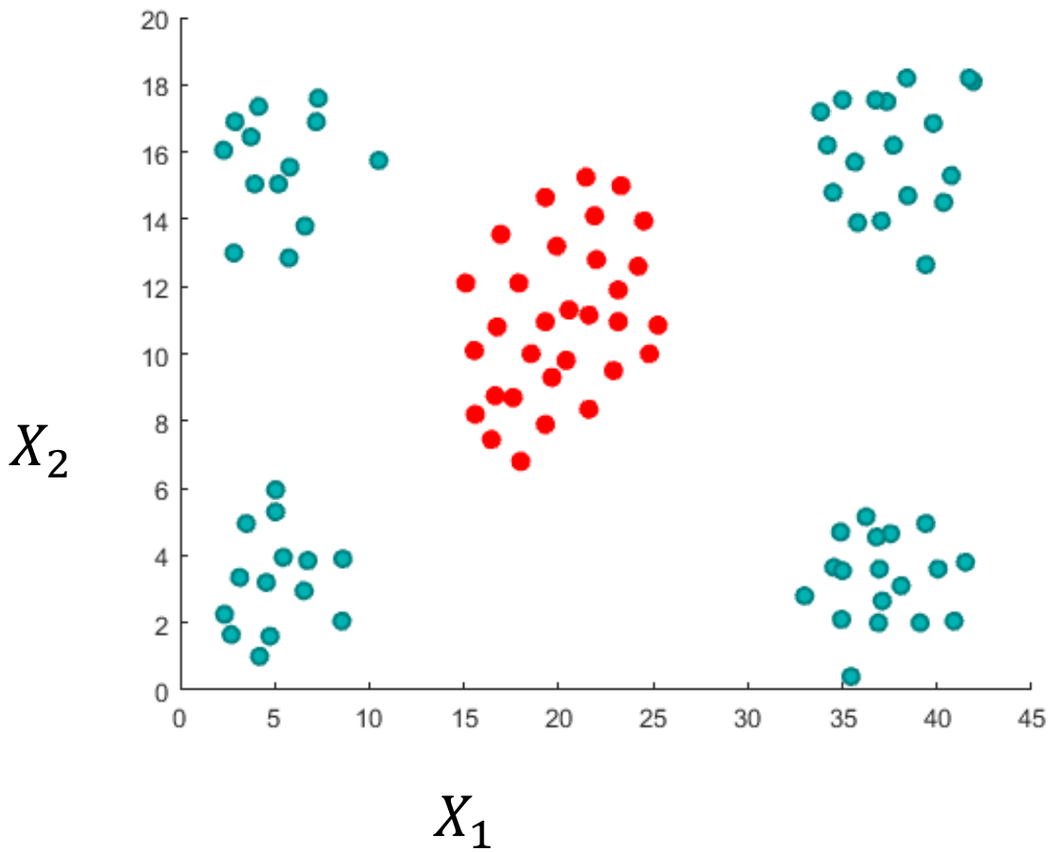


$$X \xrightarrow[(X_1^2, X_2^2)]{} Z$$

In x space

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j x_i x_j^T$$

$1 \times d \cdot d \times 1$



No. of points

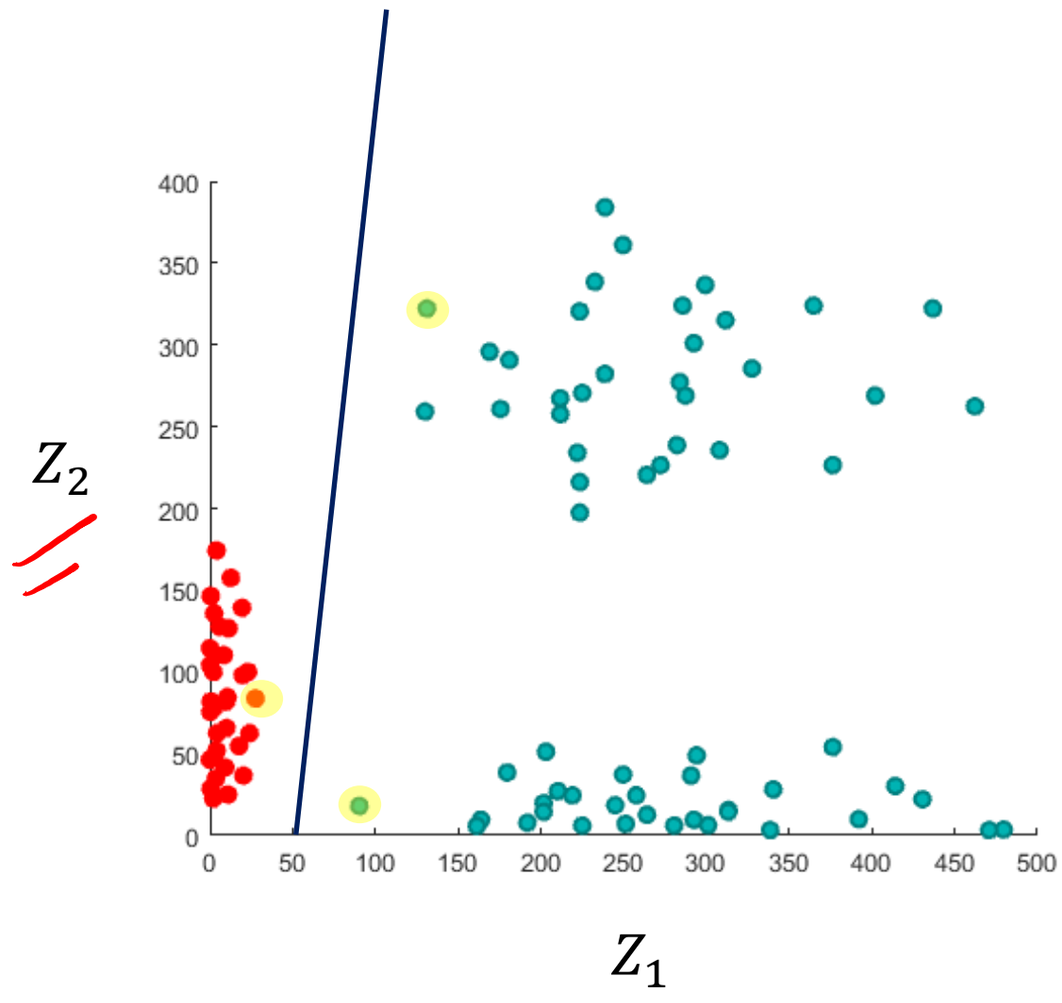
$let's\ say\ x\ is\ n \times d$

xx^T will be $n \times n$

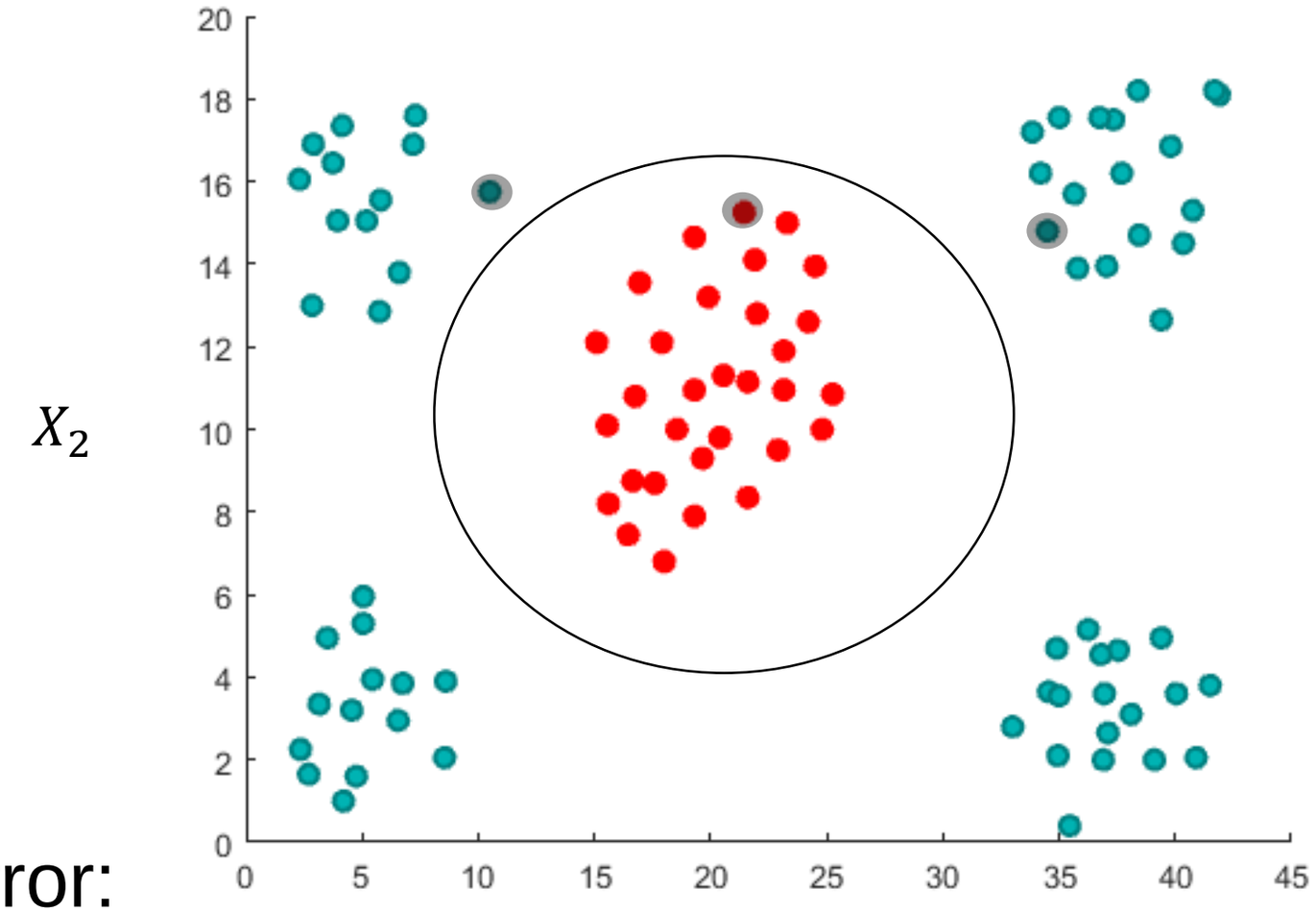
If I add millions of dimensions to x, would it affect the final size of xx^T?

In z space

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j z_i z_j^T$$



In x space, they are called pre-images of support vectors



Out of sample error:

$$\mathrm{E}[E_{out}] \leq \frac{\mathrm{E}[\#\ SV]}{N-1}$$

Take-Home Messages

- Linear Separability
- Perceptron
- SVM: Geometric Intuition and Formulation