

Support Vector Machine

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Math moment

$$7 \times 0 = 0$$

$$3 \times 0 = 0$$


$$0 = 0$$

$$7 \times 0 = 3 \times 0$$

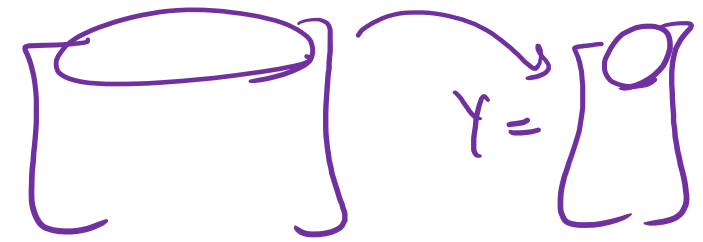
$$7 = 3$$



Outline

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

Binary Classification

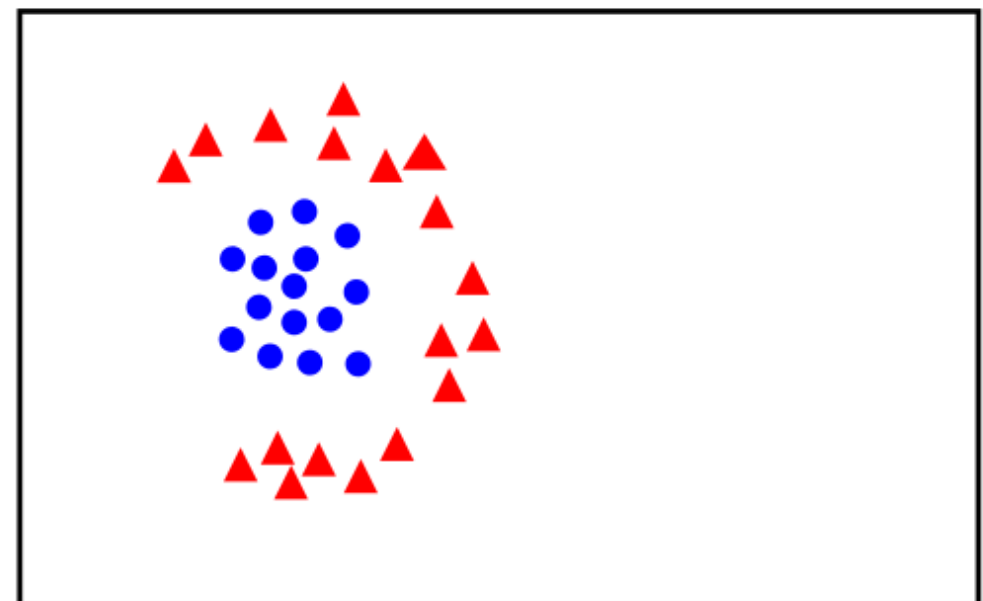
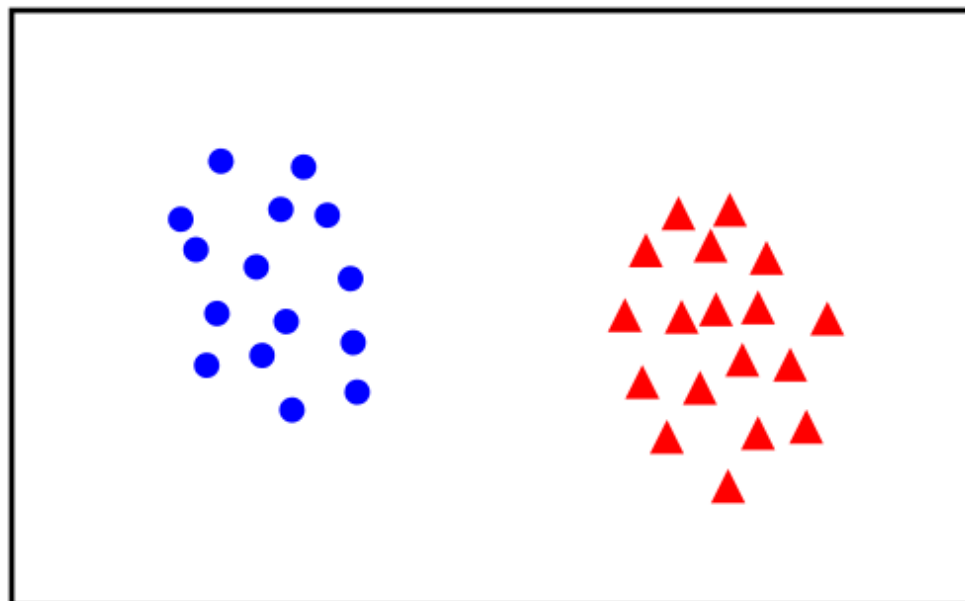


Given training data (\mathbf{x}_i, y_i) for $i = 1 \dots N$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$, learn a classifier $f(\mathbf{x})$ such that

$$f(\mathbf{x}_i) \begin{cases} \geq 0 & +1 \\ < 0 & -1 \end{cases} \quad \text{predicted linear combination of features } f(\mathbf{x}_i) = \mathbf{x}_i \boldsymbol{\theta} \in \mathbb{R}$$

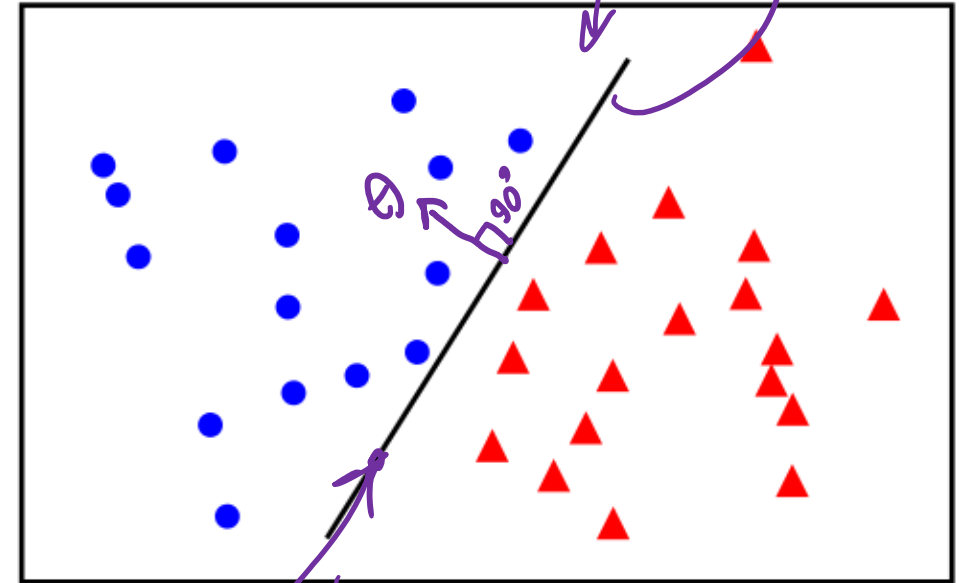
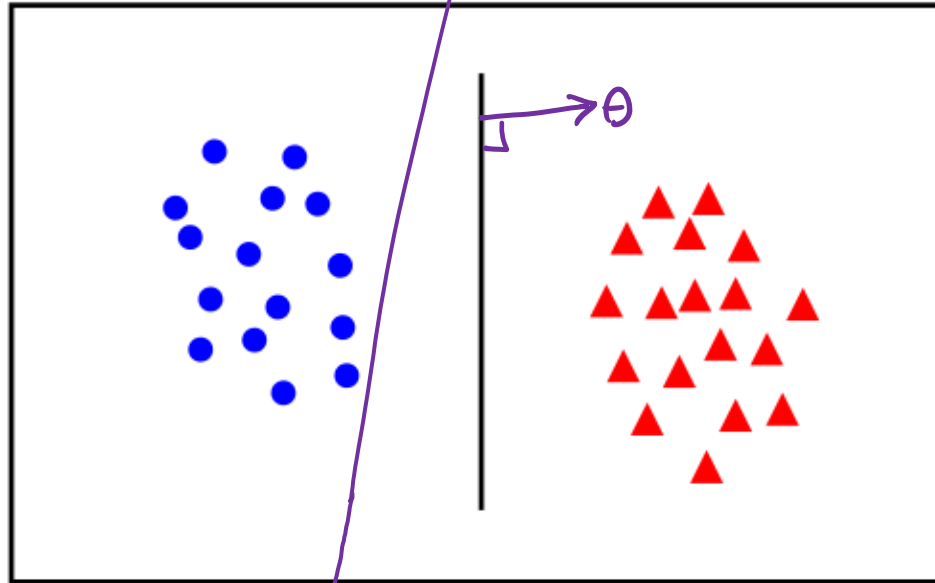
$\underbrace{\mathbf{x}_i}_{1 \times d} \underbrace{\boldsymbol{\theta}}_{d+1 \times 1} \in \mathbb{R}$
 $f(\mathbf{x}_i) = \mathbf{x}_i \boldsymbol{\theta} = 0$

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

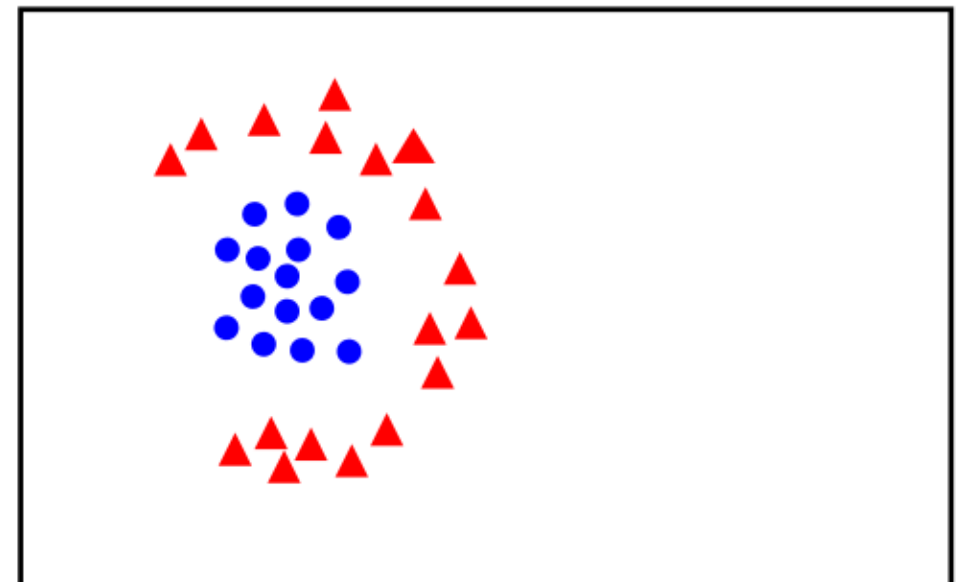
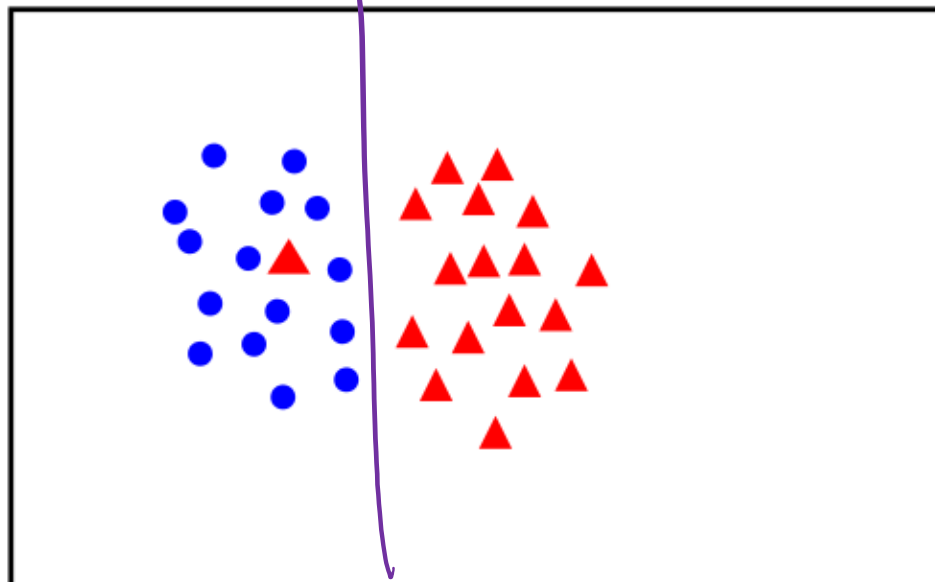


Linear Separability

linearly
separable



not
linearly
separable



Linear Classifier

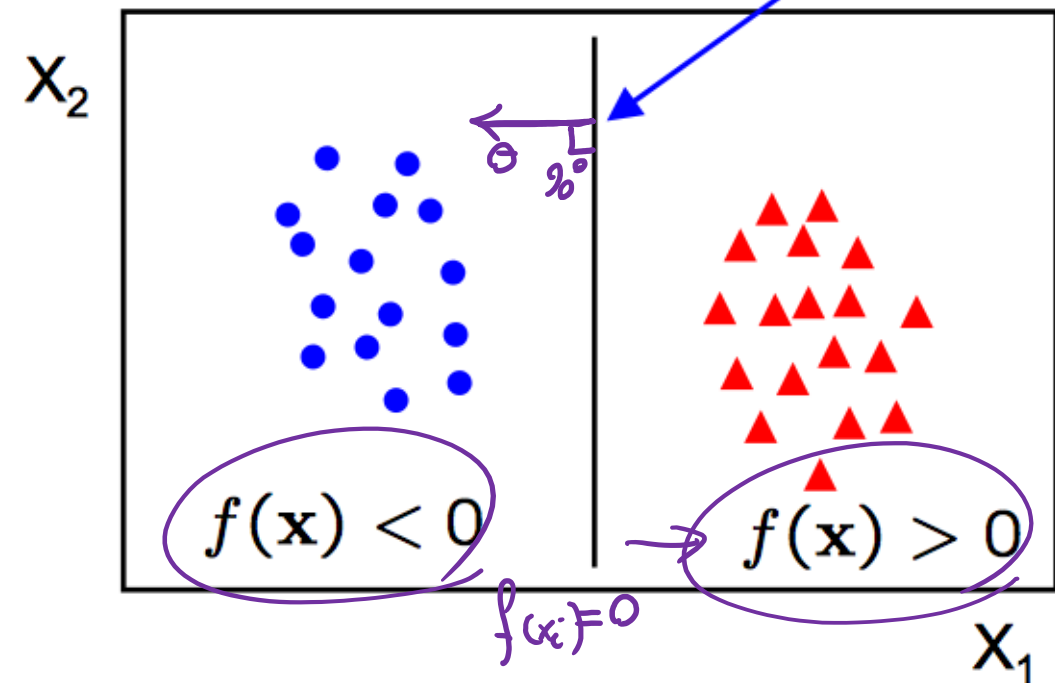
$$x\theta = 0$$

$$f(x_i) = \underbrace{x_i}_{1 \times d+1} \underbrace{\theta}_{d+1 \times 1} \rightarrow \in \mathbb{R}$$

A linear classifier has the form

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

$$f(\mathbf{x}) = 0$$

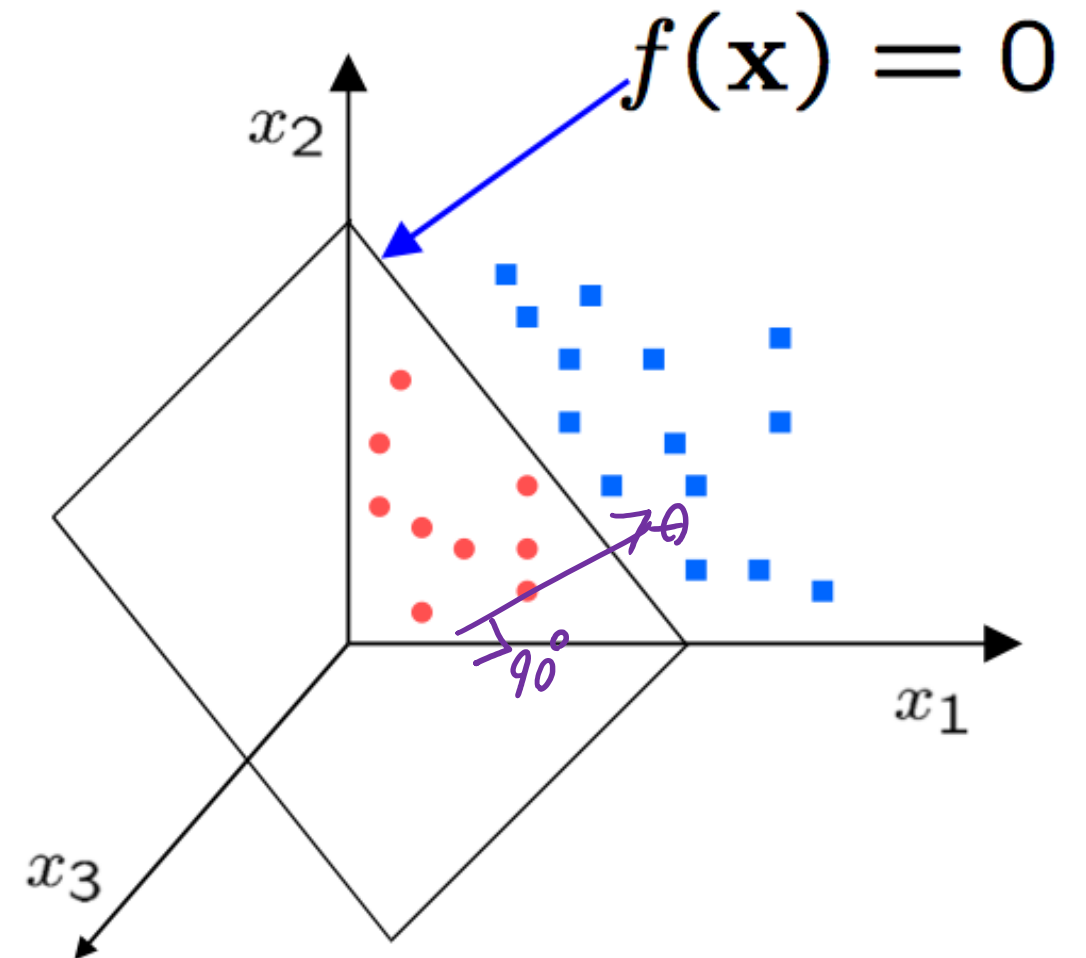


- in 2D the discriminant is a line
- θ is the **normal** to the line, and θ_0 the **bias term**
- θ is known as the **weight vector**

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

The Perceptron Classifier

Considering \mathbf{x} is linearly separable and \mathbf{y} has two labels of $\{-1, 1\}$

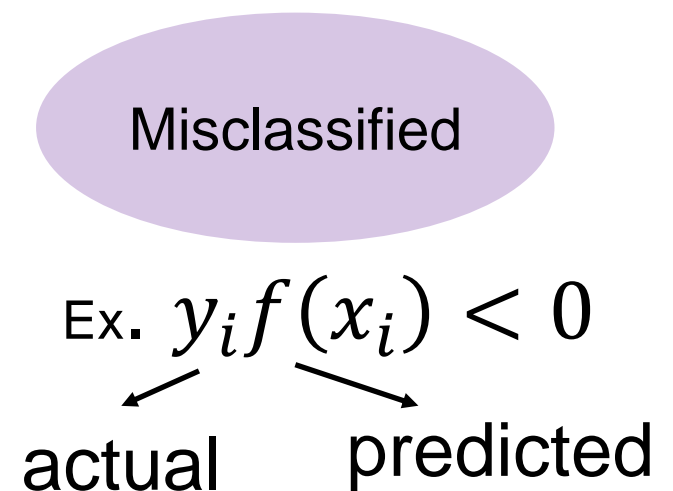
$$f(x_i) = x_i \theta \quad \text{Bias is inside } \theta \text{ now}$$

How can we separate datapoints with label 1 from datapoints with label -1 using a line?

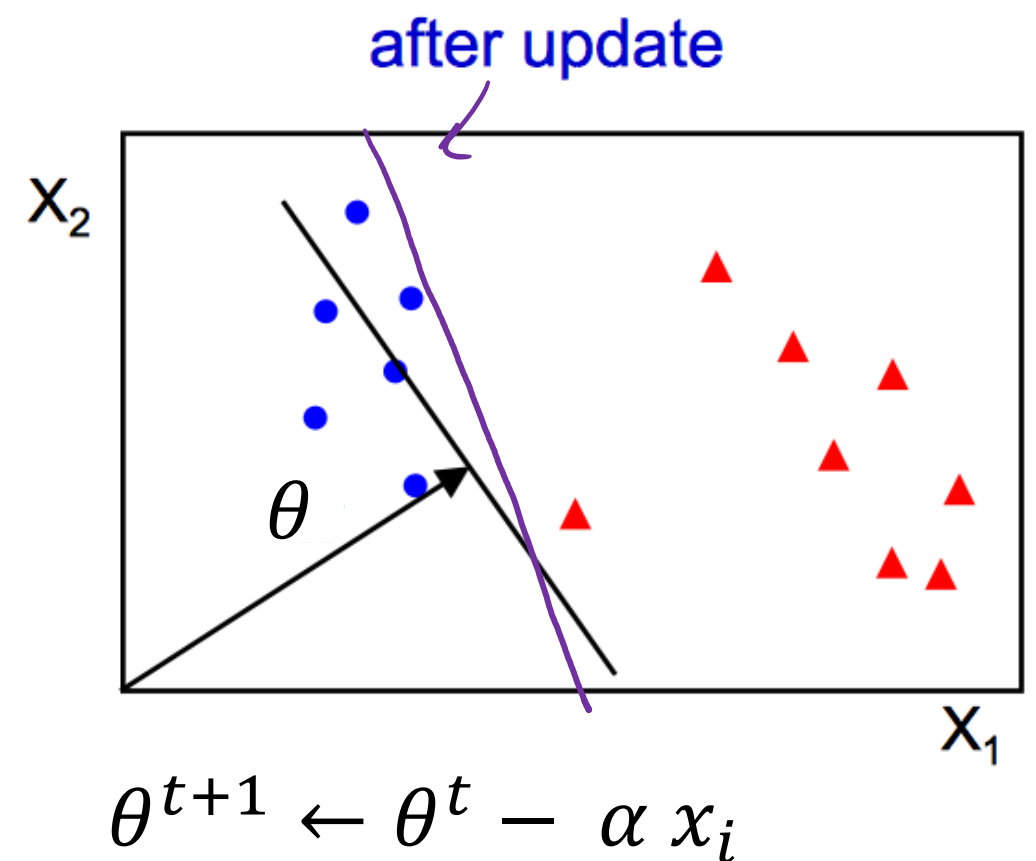
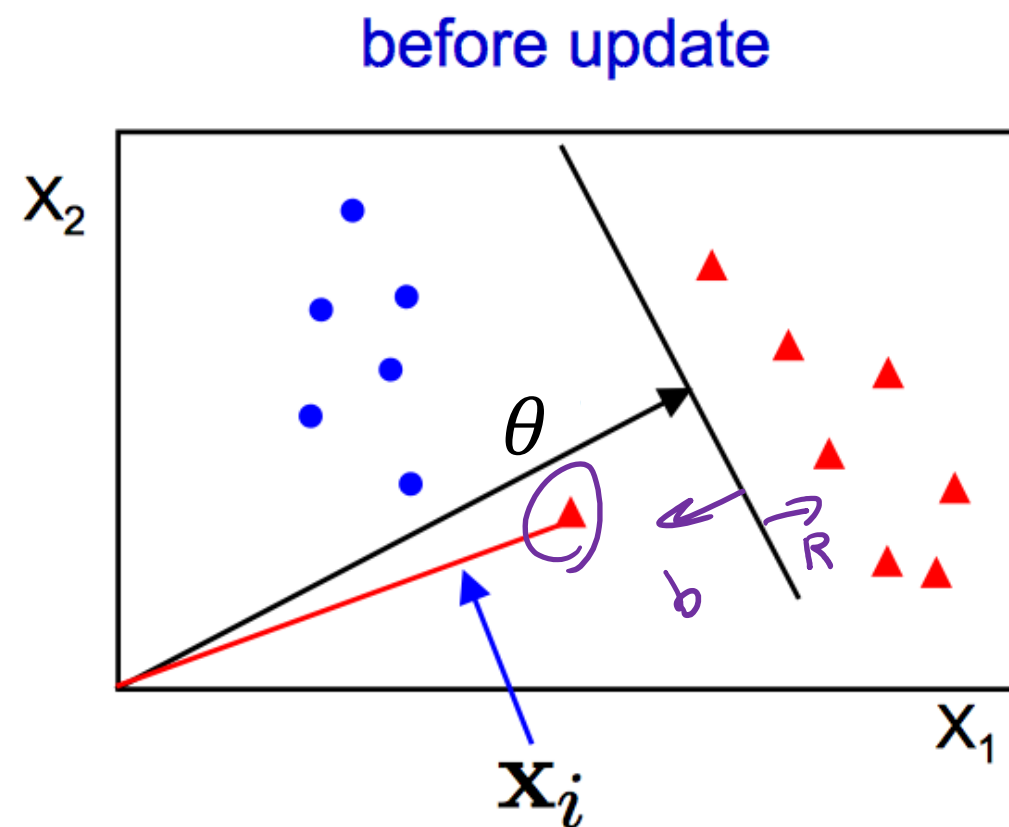
Perceptron Algorithm:

- Initialize $\theta = 0$
- Go through each datapoint $\{x_i, y_i\}$
 - If x_i is misclassified then $\theta^{t+1} \leftarrow \theta^t + \alpha y_i x_i$
- Until all datapoints are correctly classified

$$y_i \frac{f(x_i)}{x_i \theta} < 0$$



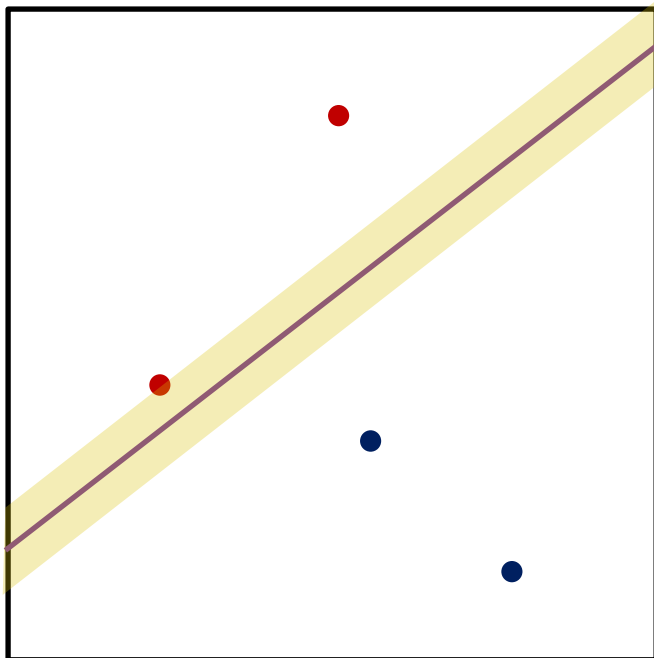
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- Until all datapoints are correctly classified



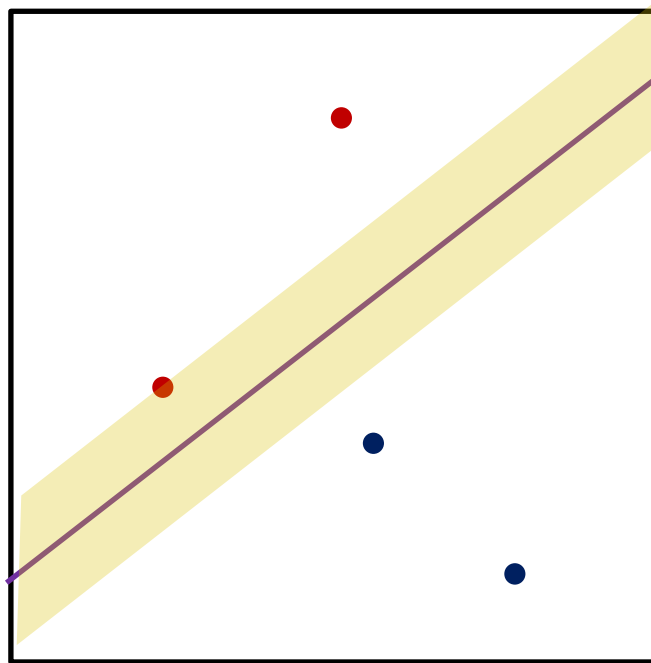
Linear separation

We can have different separating lines

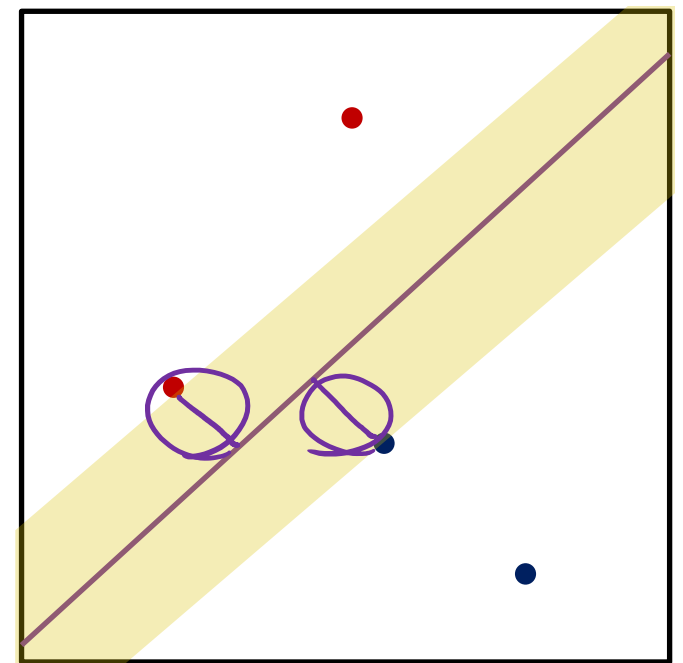
①



②



③



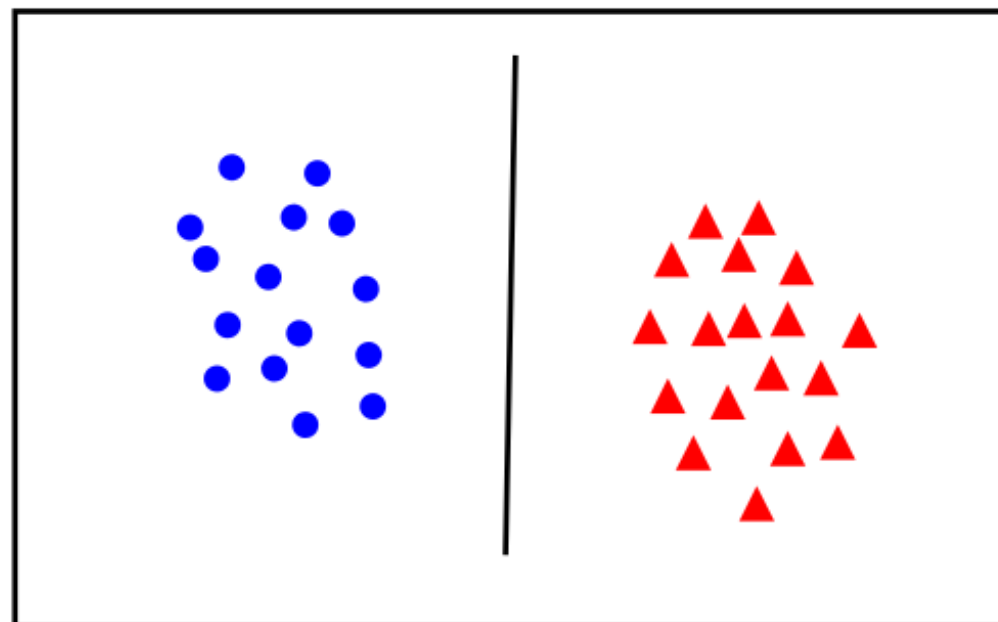
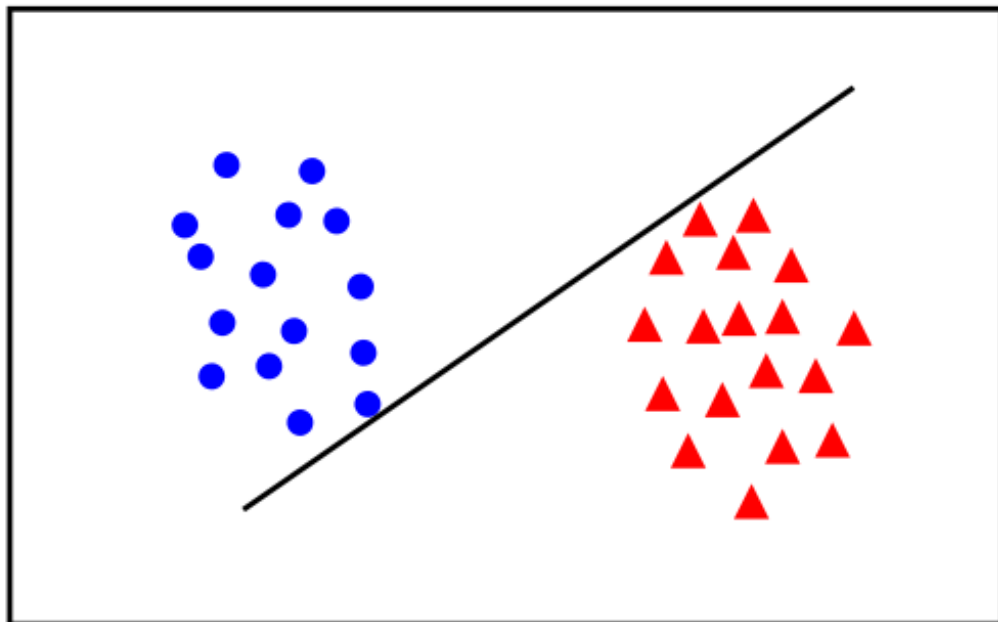
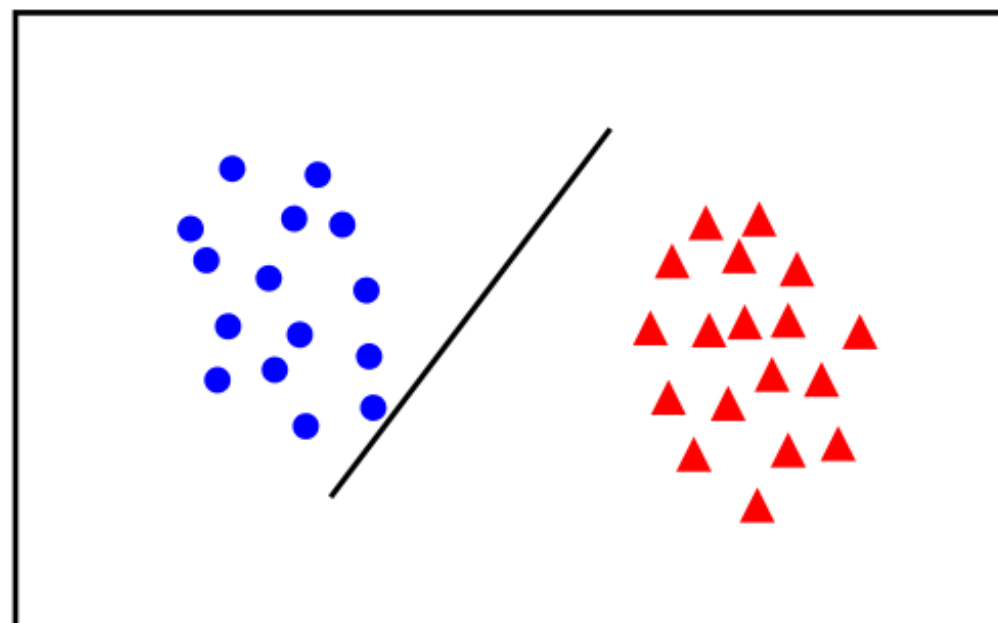
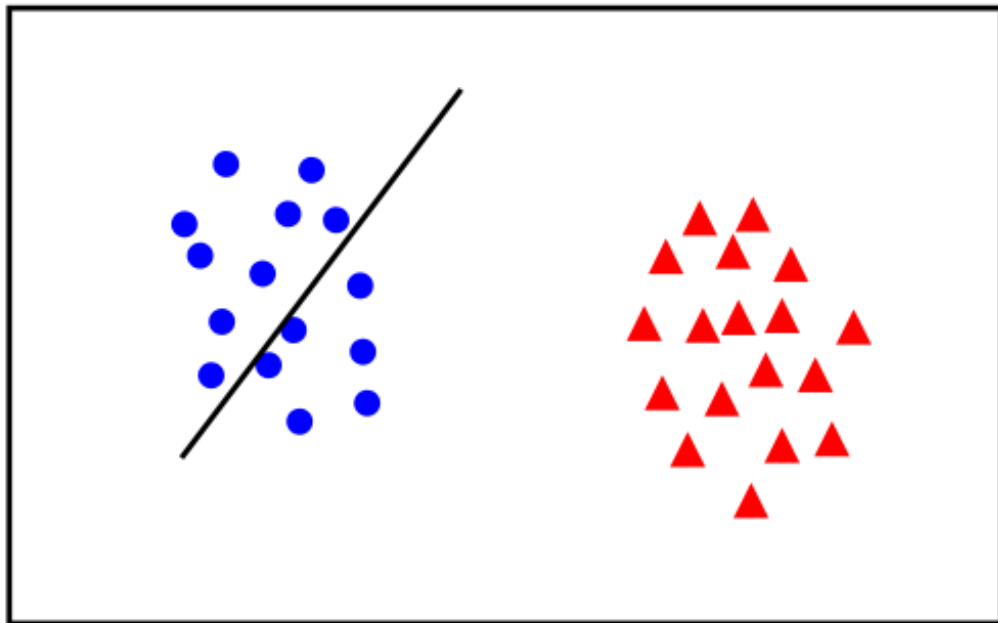
Which line is the best?

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

Why is the bigger margin better?

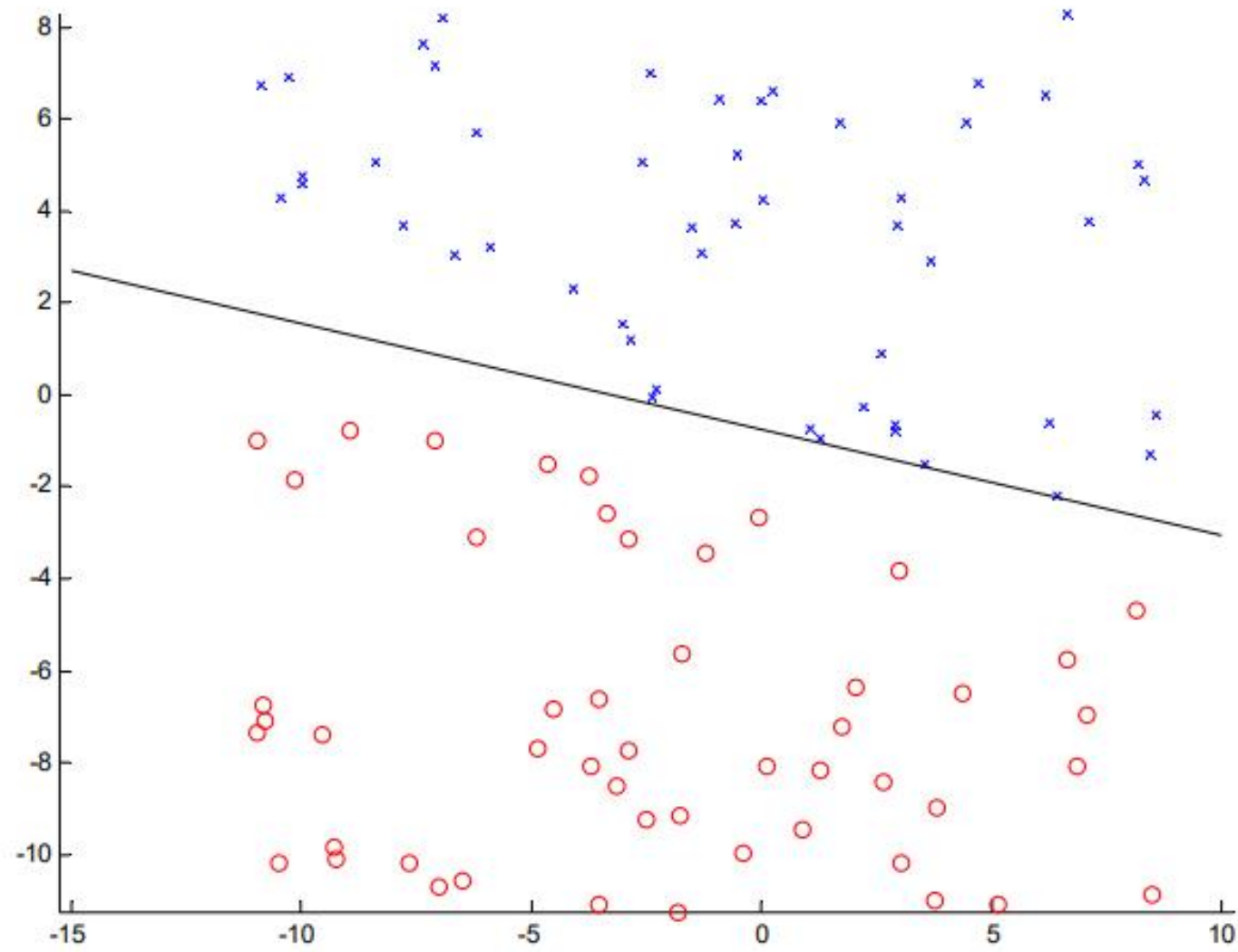
What θ maximizes the margin?

What is the Best θ ?





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Perceptron example



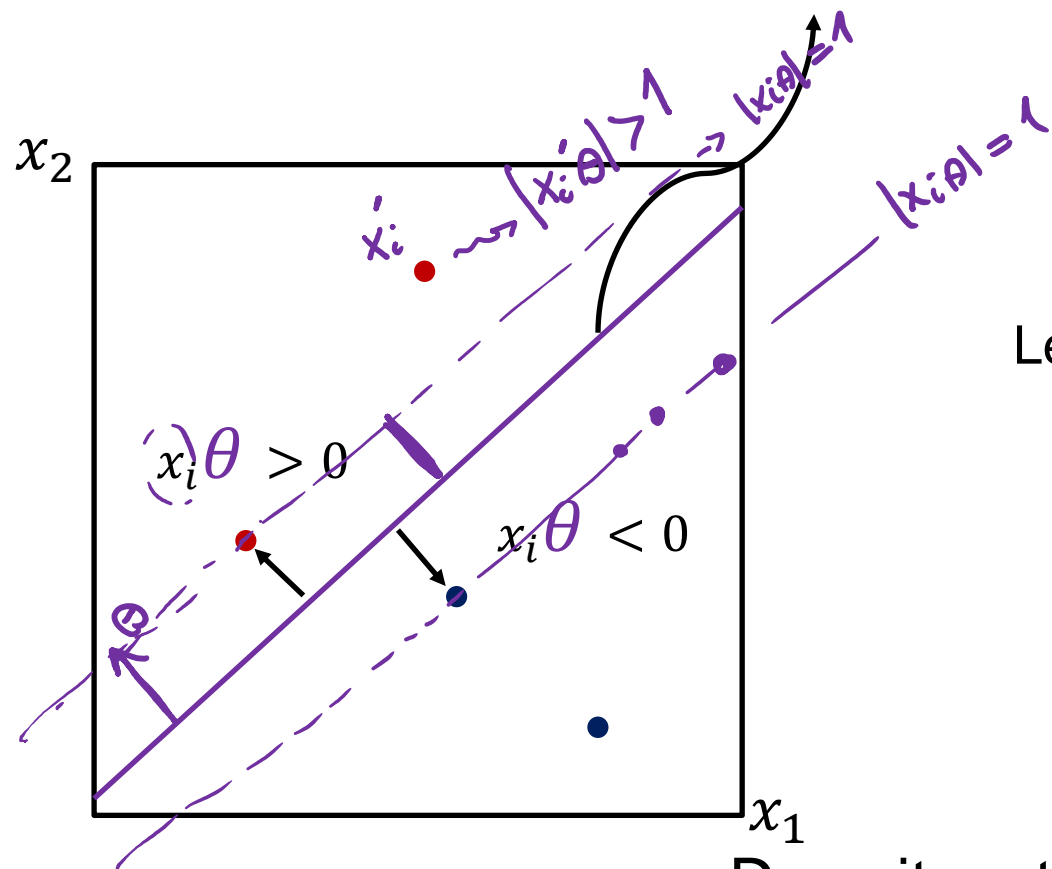
- if the data is linearly separable, then the algorithm will converge
- convergence can be slow ...
- separating line close to training data
- we would prefer a larger margin for generalization (better generalization)

Outline

- Precursor: Linear Classifier and Perceptron
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Finding θ with a **fat** margin

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



$$x\theta = 0$$

$$|x_i\theta| = 1$$

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

$$|x_i\theta| > 0$$

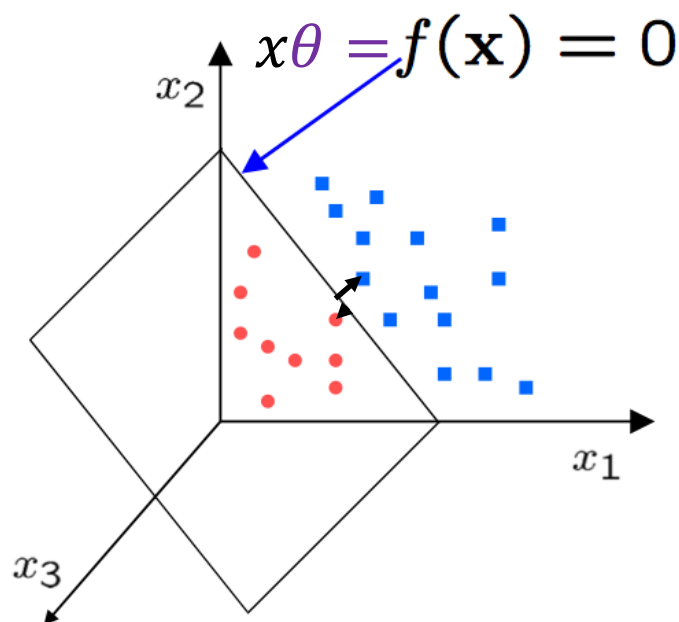
Our line solution is $x\theta = 0$

Does it matter if I scale up or down θ for the decision boundary?

$$|x_i\theta| = 1 \rightarrow \text{normalization}$$

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

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



Computing the distance

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

The vector θ is perpendicular to the decision line.

You should ask me why?

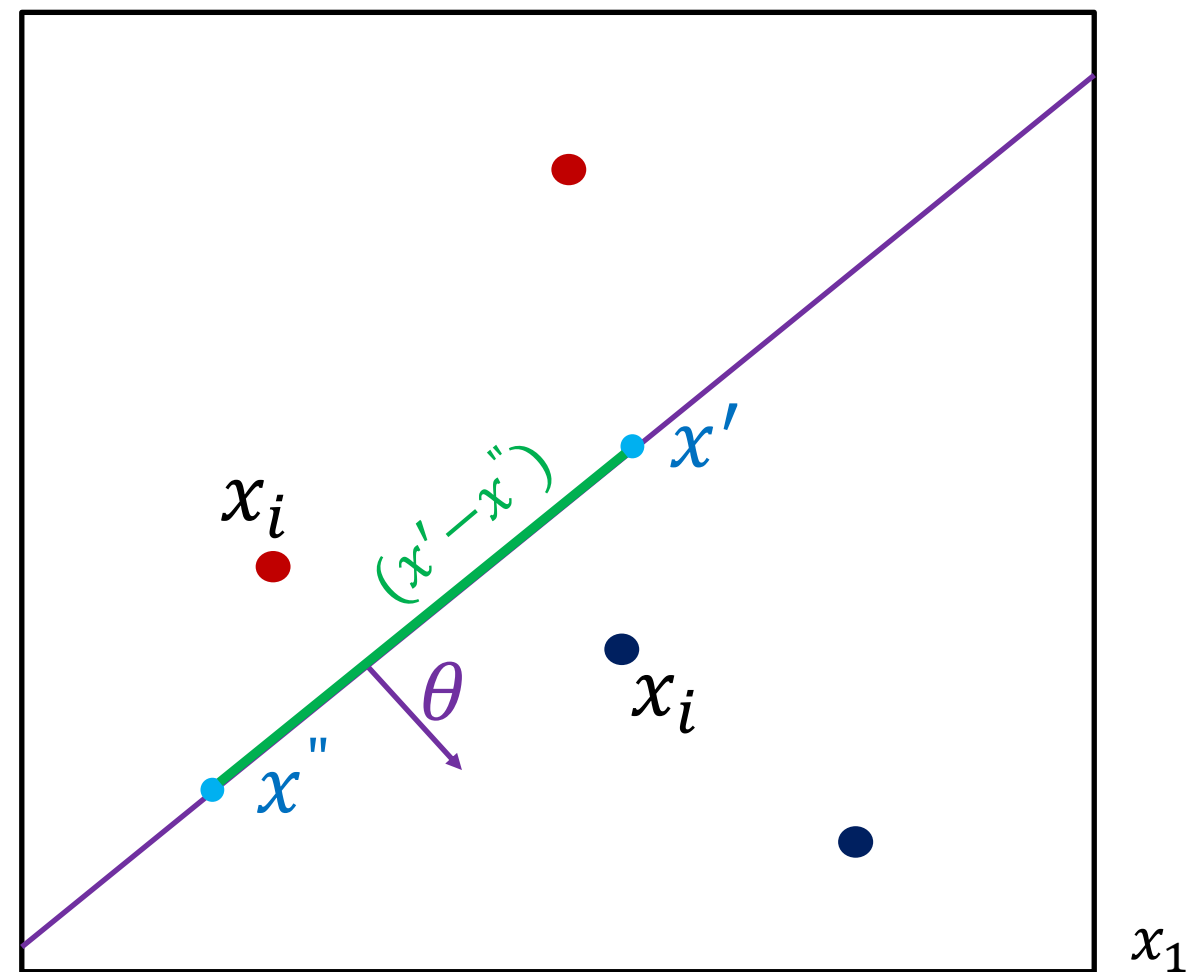
Consider x' and x'' on the plane

$$x'\theta + b = 0 \quad \text{and} \quad x''\theta + b = 0$$

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

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

x_2



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.

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

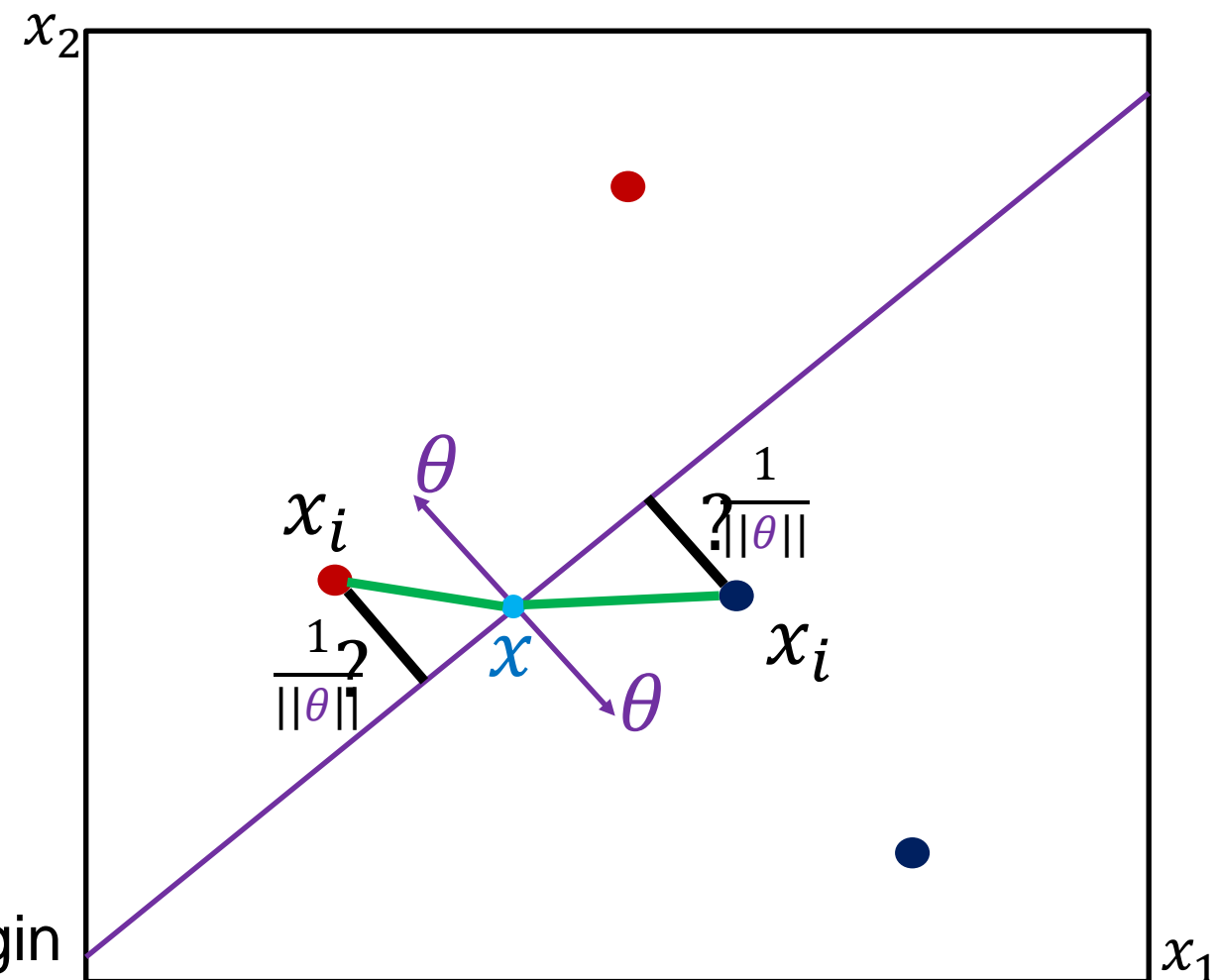
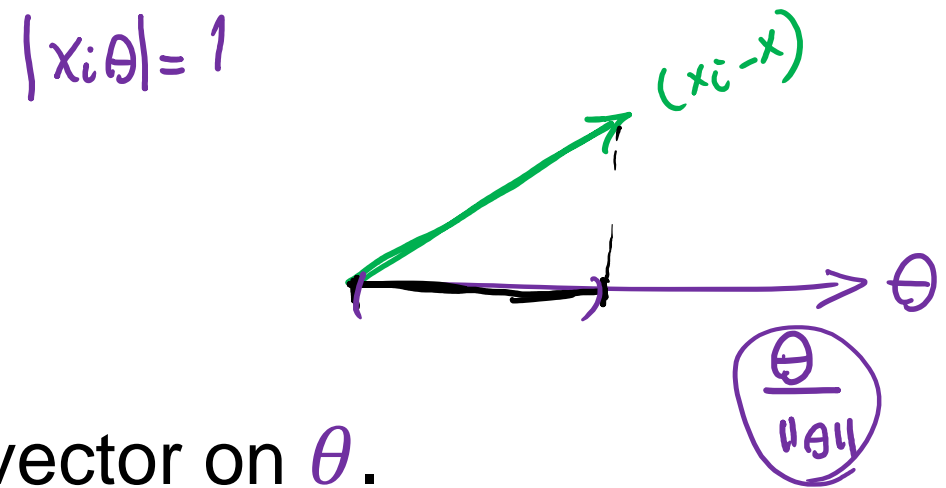
$$\text{distance} = \frac{1}{\|\theta\|} |(x_i \theta - x \theta)|$$

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

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

$$y_i f(x_i) > 0$$

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

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

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

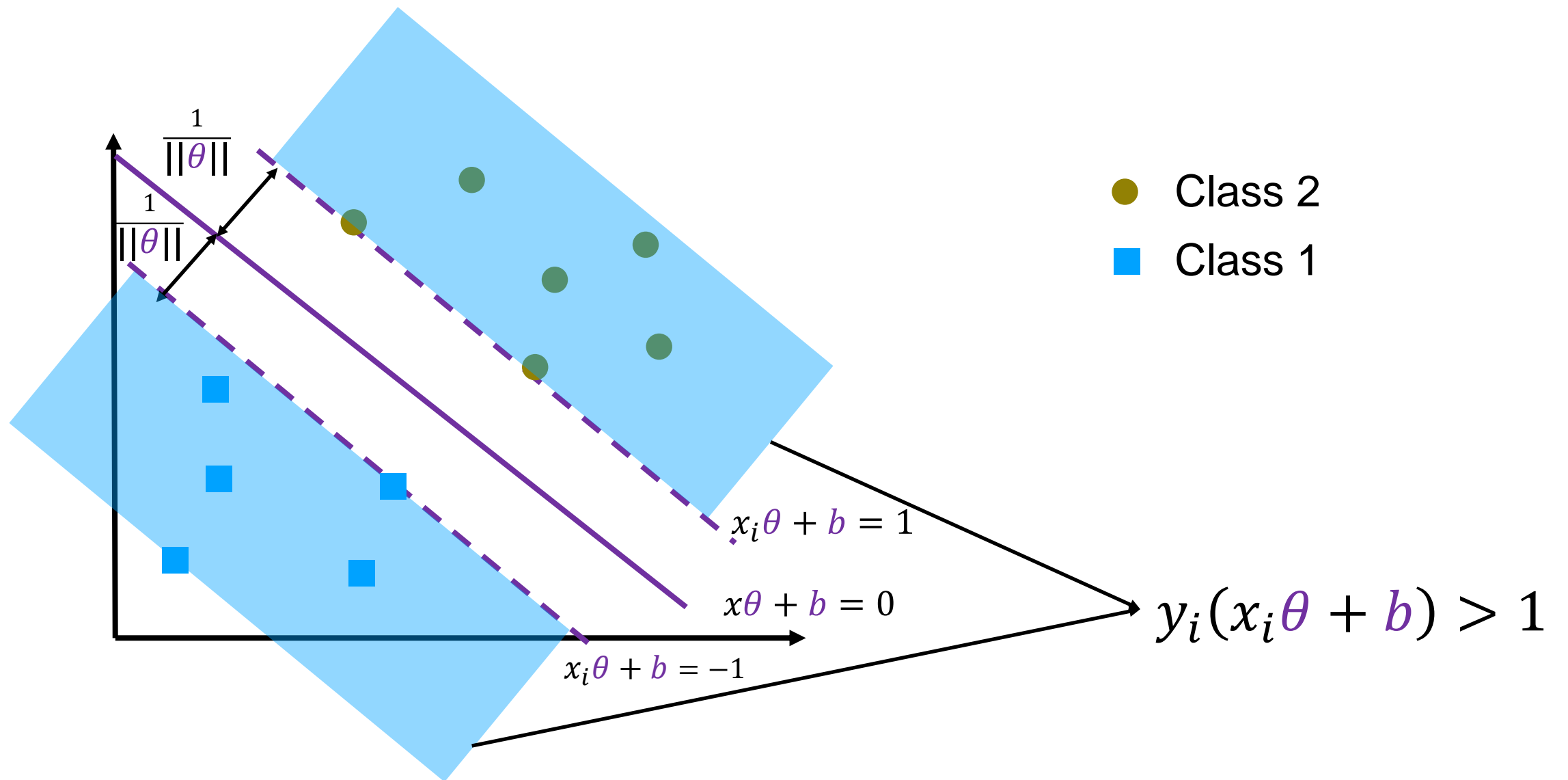
Can I write the following term to get rid of absolute value?

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

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

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

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



Maximize $\frac{2}{\|\theta\|}$

$\|\theta\| = \theta\theta^T$

If $\theta \neq 0$, there exists a max value

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 $i = 1, 2, \dots, N$

Constrained optimization

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

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

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

$$g(x) = y_i(x_i \theta + b) - 1 \geq 0$$

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

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

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

We need to optimize

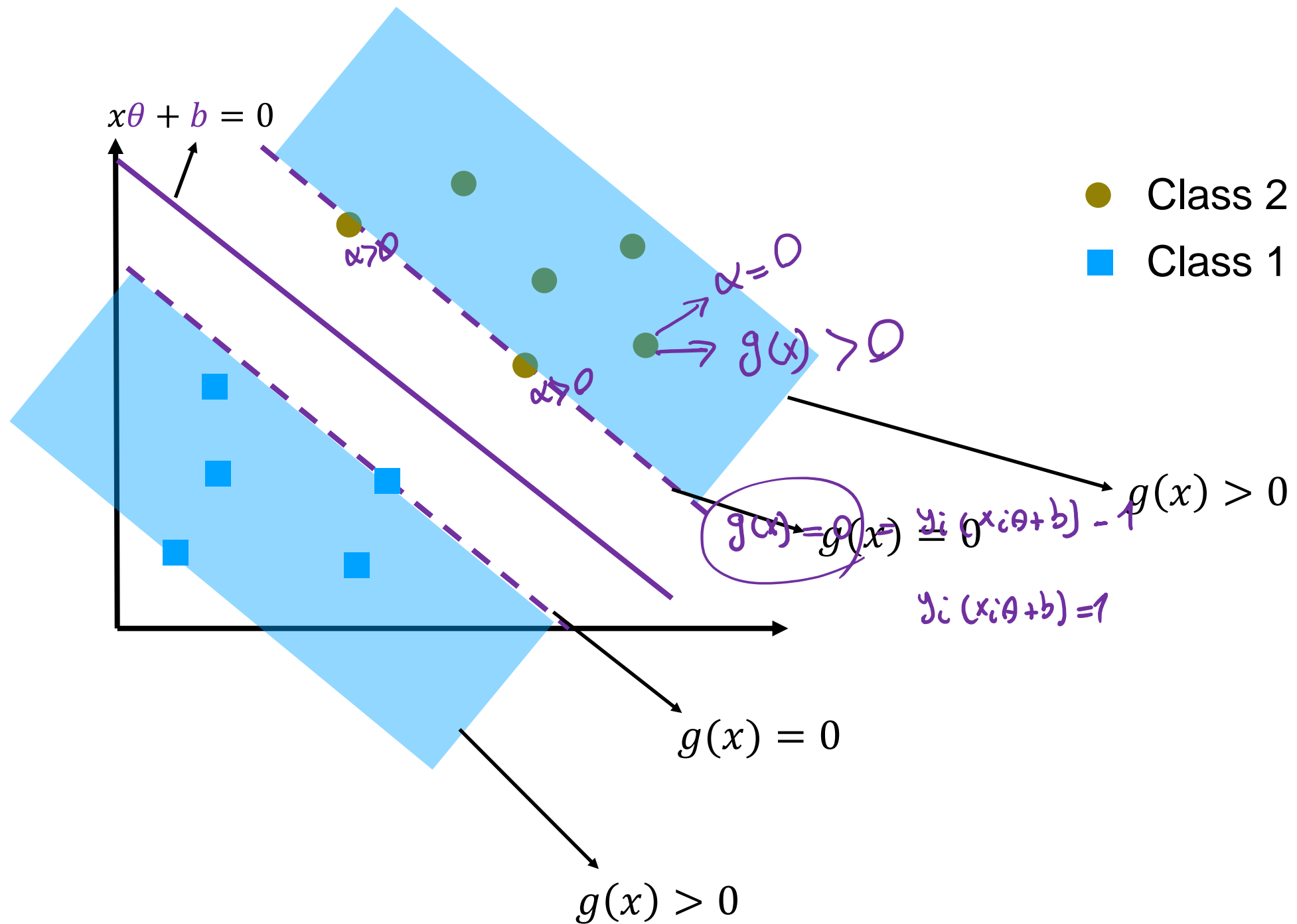
1) Stationary

θ, b , and α

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

3) $\alpha \geq 0$ Dual feasibility

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



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

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

Lagrange formulation

$$\begin{aligned} & f(x) \\ \text{s.t. } & g(x) \\ \mathcal{L}(\lambda, x) &= f(x) - \lambda g(x) \end{aligned}$$

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

Primal form

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

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

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

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

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

Minimize w.r b

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

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

Let's substitute these in the Lagrangian:

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

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

$\sum \alpha_i y_i x_i \theta + b \sum \alpha_i y_i$

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

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

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

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

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

→ Dual form

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

and

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

The solution – quadratic programming

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

Quadratic programming packages usually use “min”

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

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

$n \times n$

Handwritten annotations:

- A purple oval encircles the top-left 1×1 element of the matrix, with an arrow pointing to it labeled 1×1 .
- A purple oval encircles the top-right $1 \times d$ element of the matrix, with an arrow pointing to it labeled $1 \times d$.
- A purple oval encircles the bottom-left $d \times 1$ element of the matrix, with an arrow pointing to it labeled $d \times 1$.

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

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

$\alpha \geq 0$

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

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

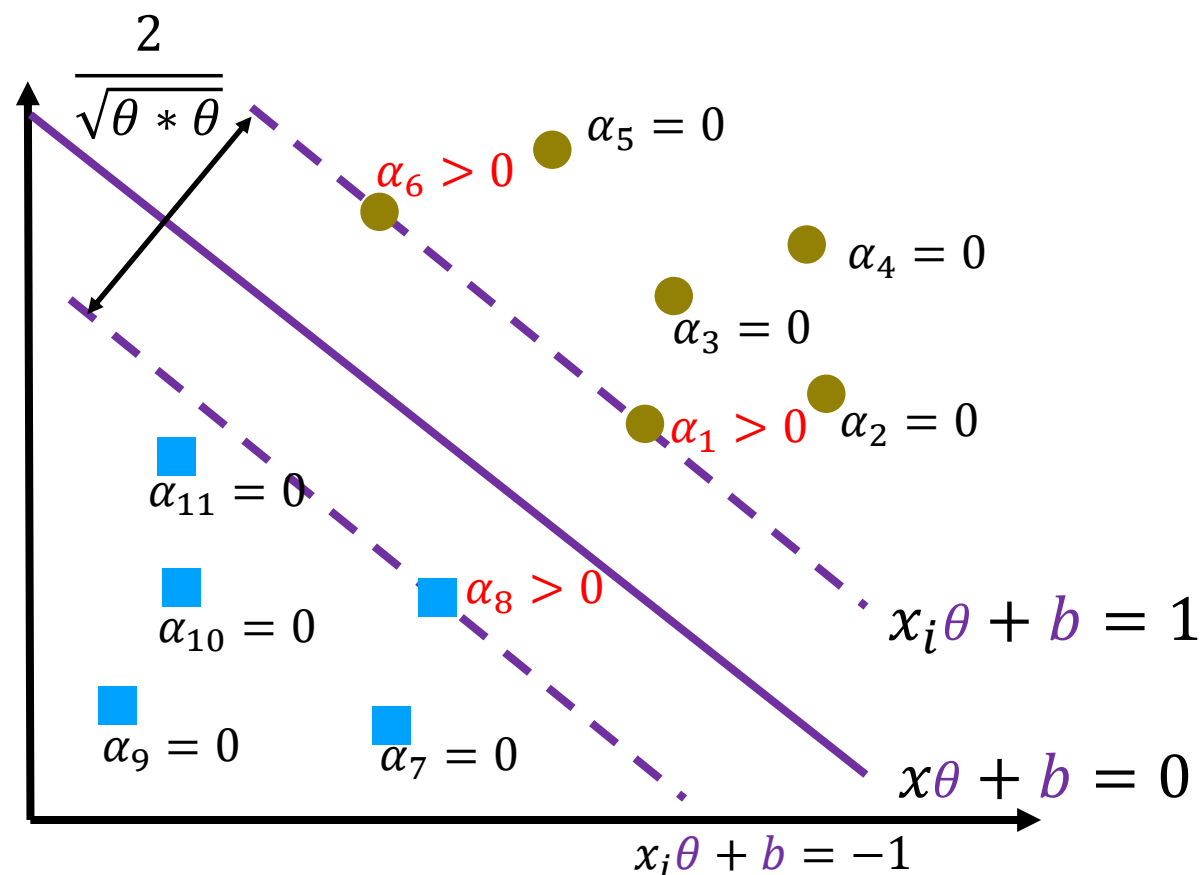
Quadratic programming will give us α

$\alpha g(x) = 0$ Solution: $\alpha = \alpha_1, \dots, \alpha_N$

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

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

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



- Class 2
- Class 1

Training

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

No need to go over all datapoints

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

and for b pick any support vector and calculate: $y_i(x_i \theta + b) = 1$

Testing

For a new test point s ^{$1 \times d$}

Compute:

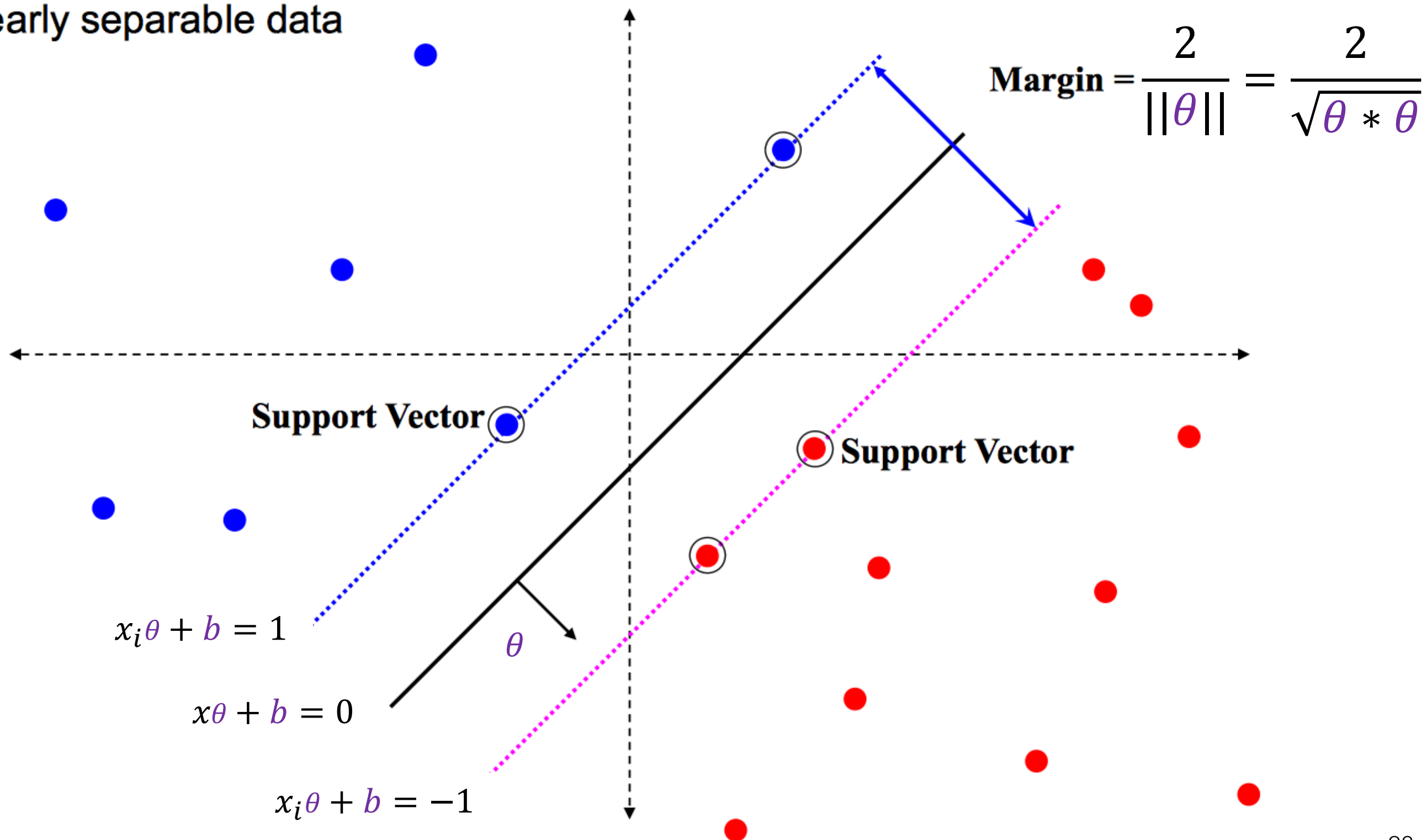
$$s\theta + b = \sum_{x_i \text{ in } SV} \alpha_i y_i \underline{x_i} \underline{s}^T + b$$

+1
↑
> 0
↓
0
-1

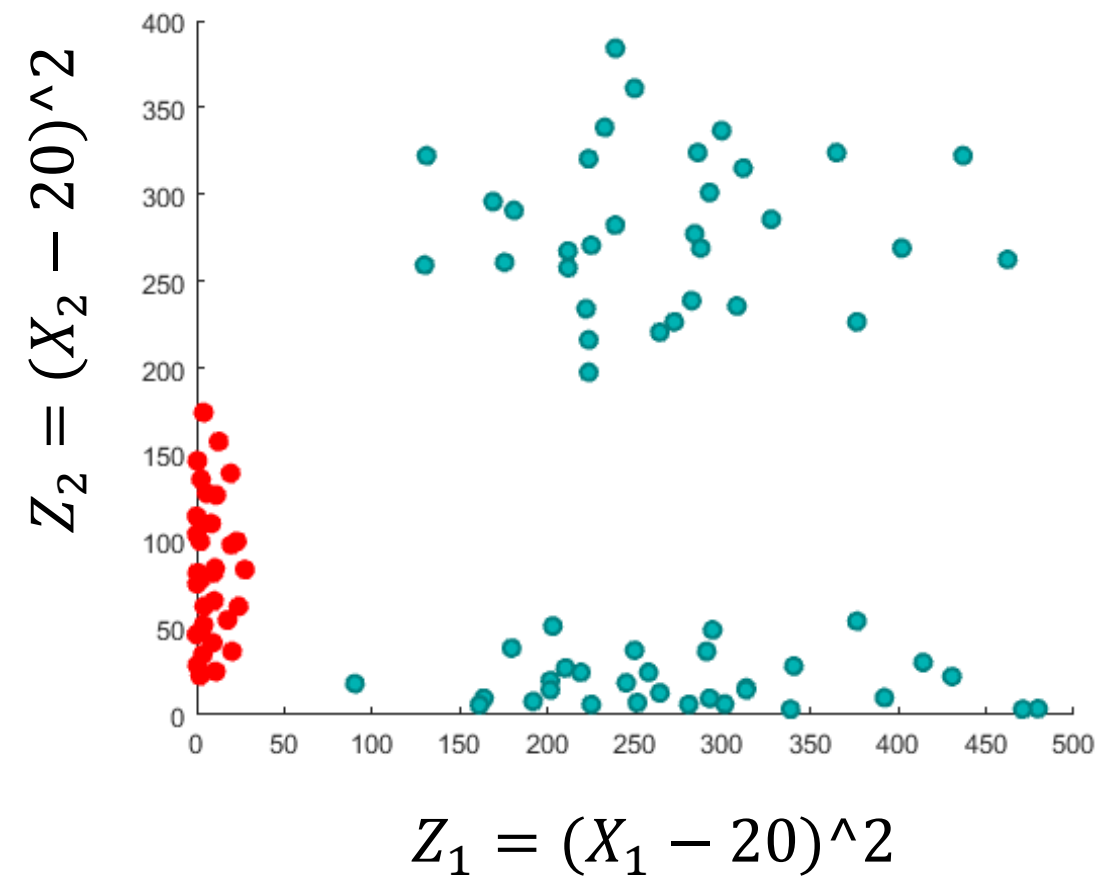
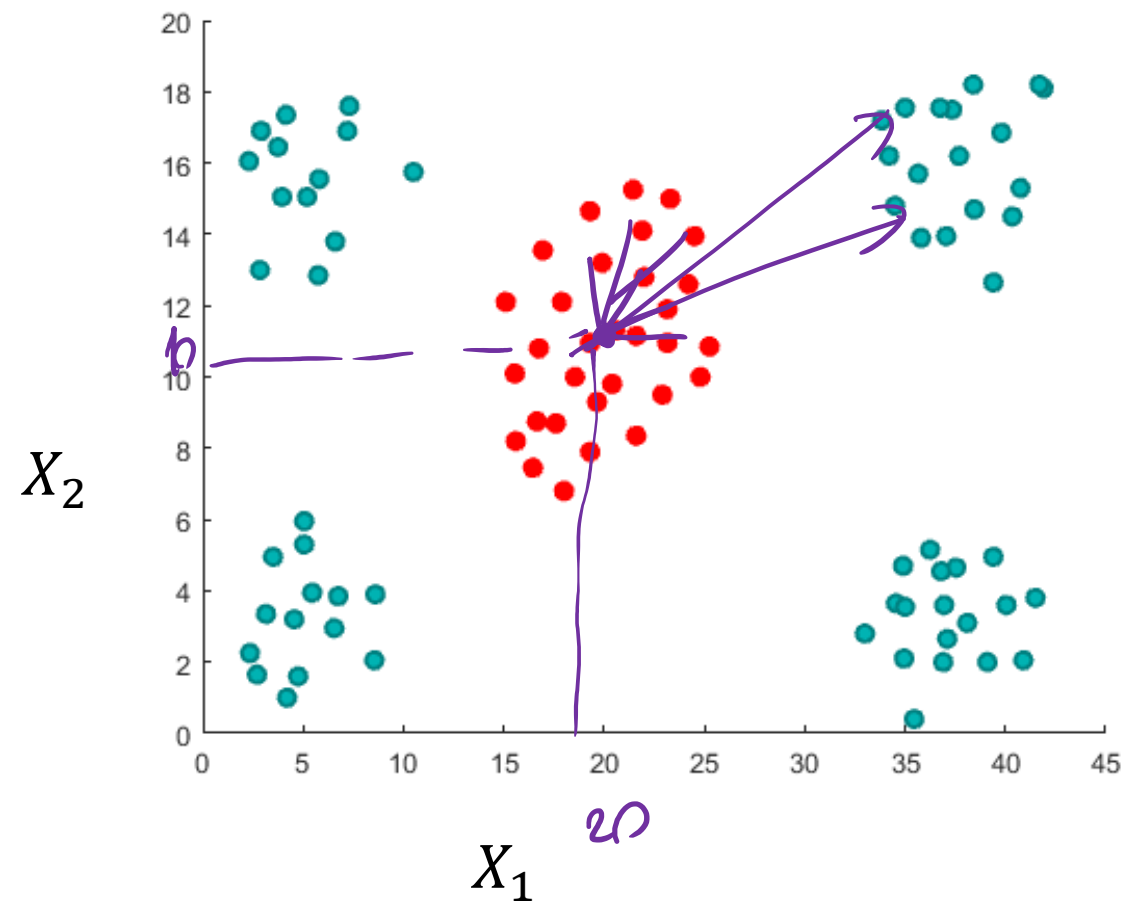
Classify s as class 1 if the result is positive, and class 2 otherwise

Geometric Interpretation

linearly separable data



From x to z space

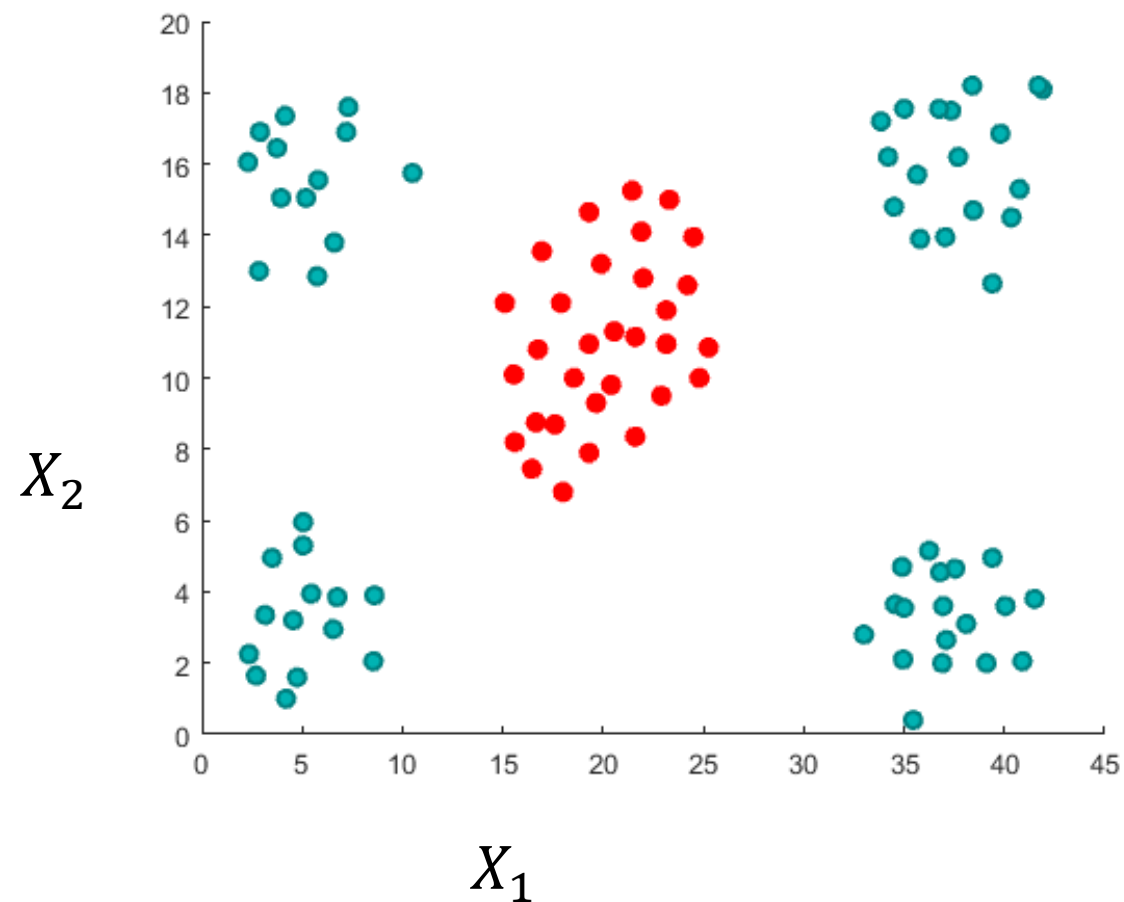


$$X \xrightarrow{(X_1^2, X_2^2)} Z$$

In x space

$$\underbrace{XX^T}_{n \times n} \quad X_{n \times d}$$

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

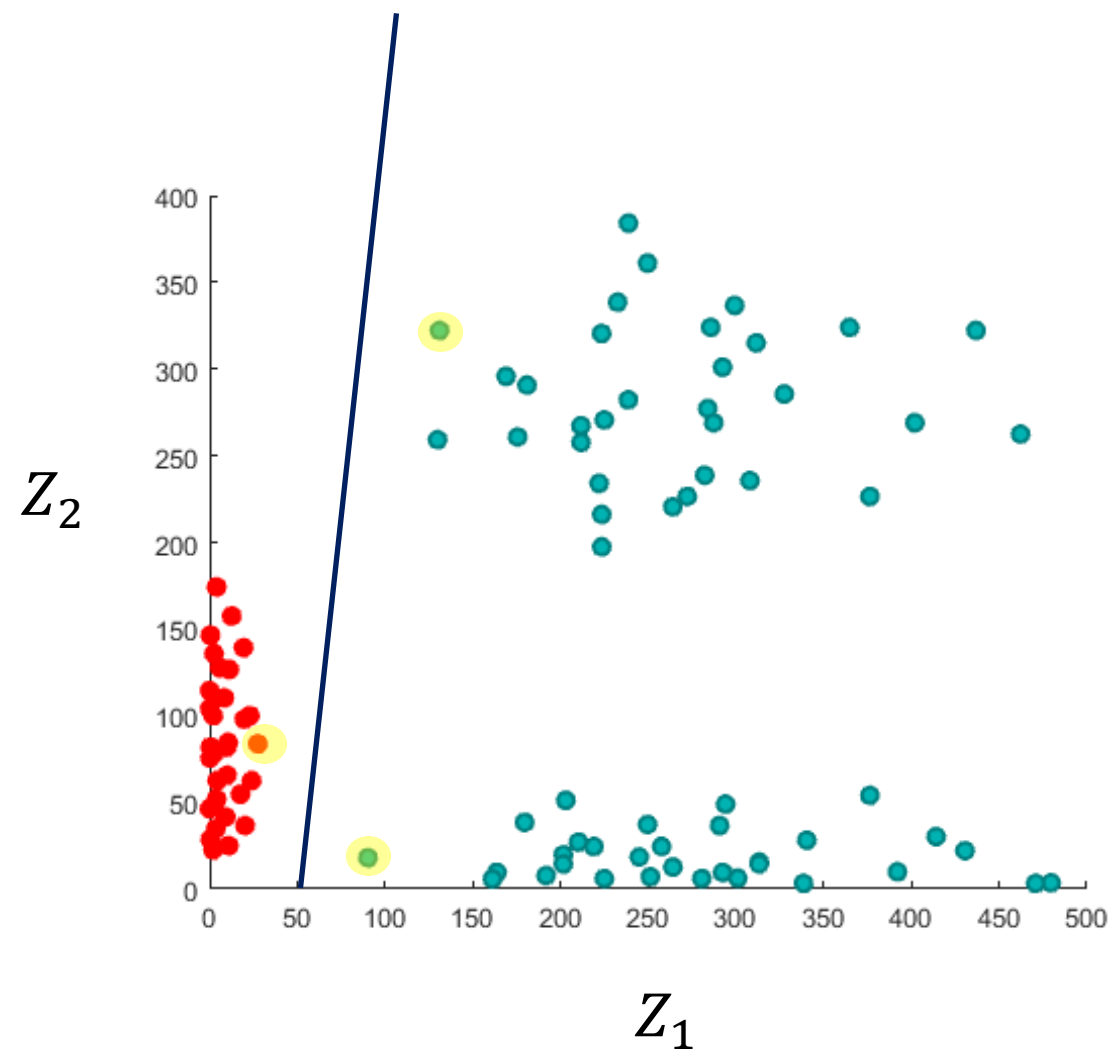


let's say x is $n \times d$
 xx^T will be $n \times n$

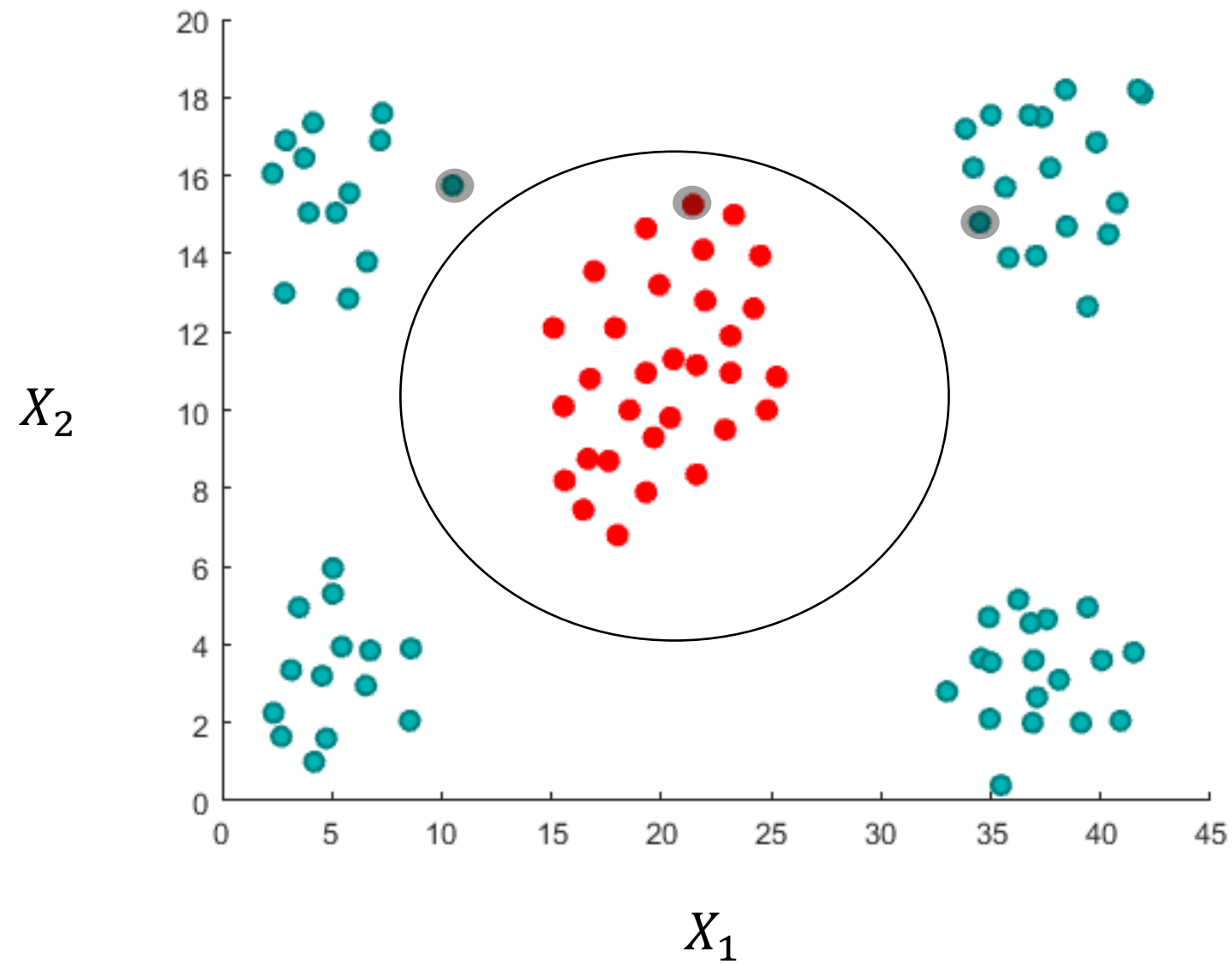
If I add millions of
 dimensions to x , would
 it affect the final size of
 xx^T ?

In z space

$$\max_{\alpha} \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \mathbf{z}_i \mathbf{z}_j^T$$



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



Take-Home Messages

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