Support Vector Machine

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Some of the slides are inspired based on slides from Andrew Zisserman, Yaser S. Abu-Mostafa.

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

$f(x) = X\Theta$

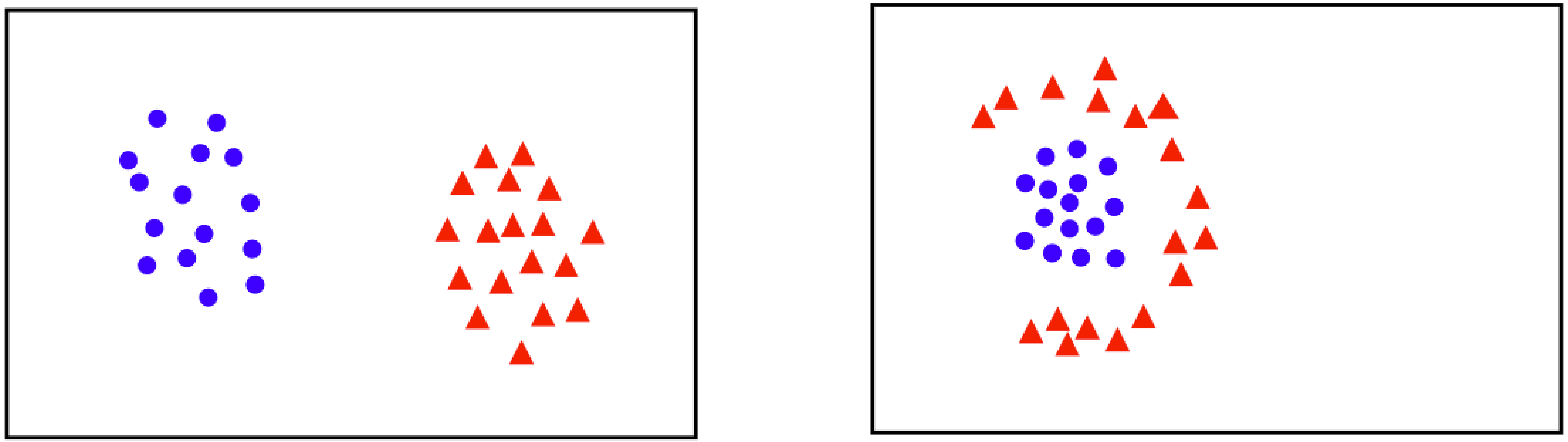
Binary Classification

$f(x_i) = \underset{\hookrightarrow 1\times d}{x_i}\,\Theta \rightsquigarrow d\times 1 \in \mathbb{R}$

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

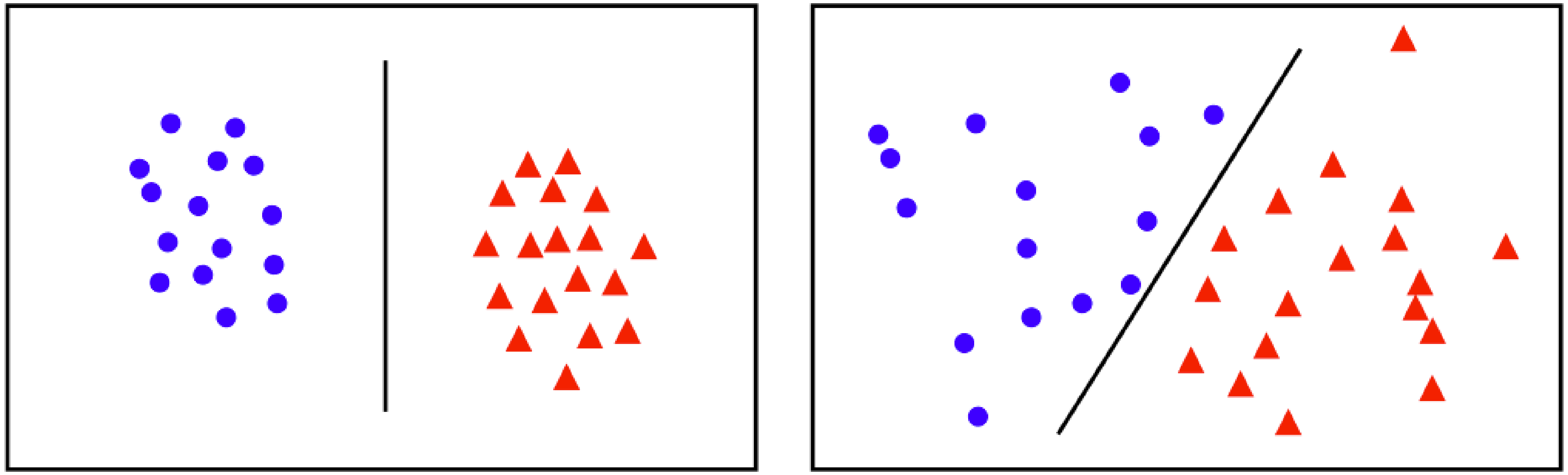
$$f(\mathbf{x}_i) \begin{cases} \geq 0 & +1 \\ < 0 & -1 \end{cases}$$

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

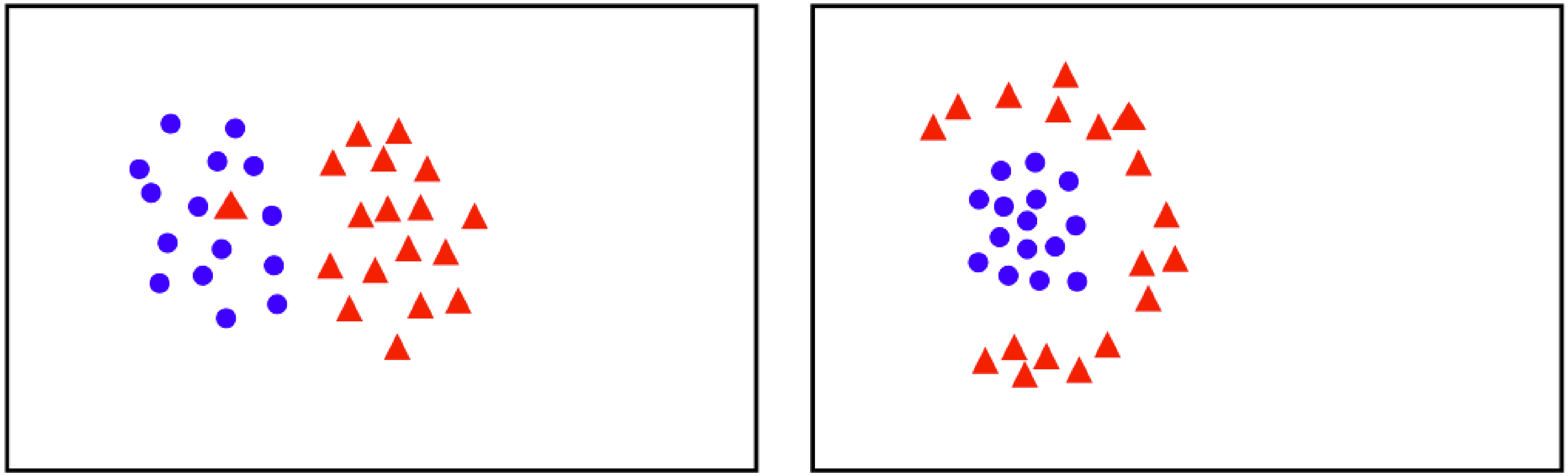


Linear Separability

linearly separable



not linearly separable



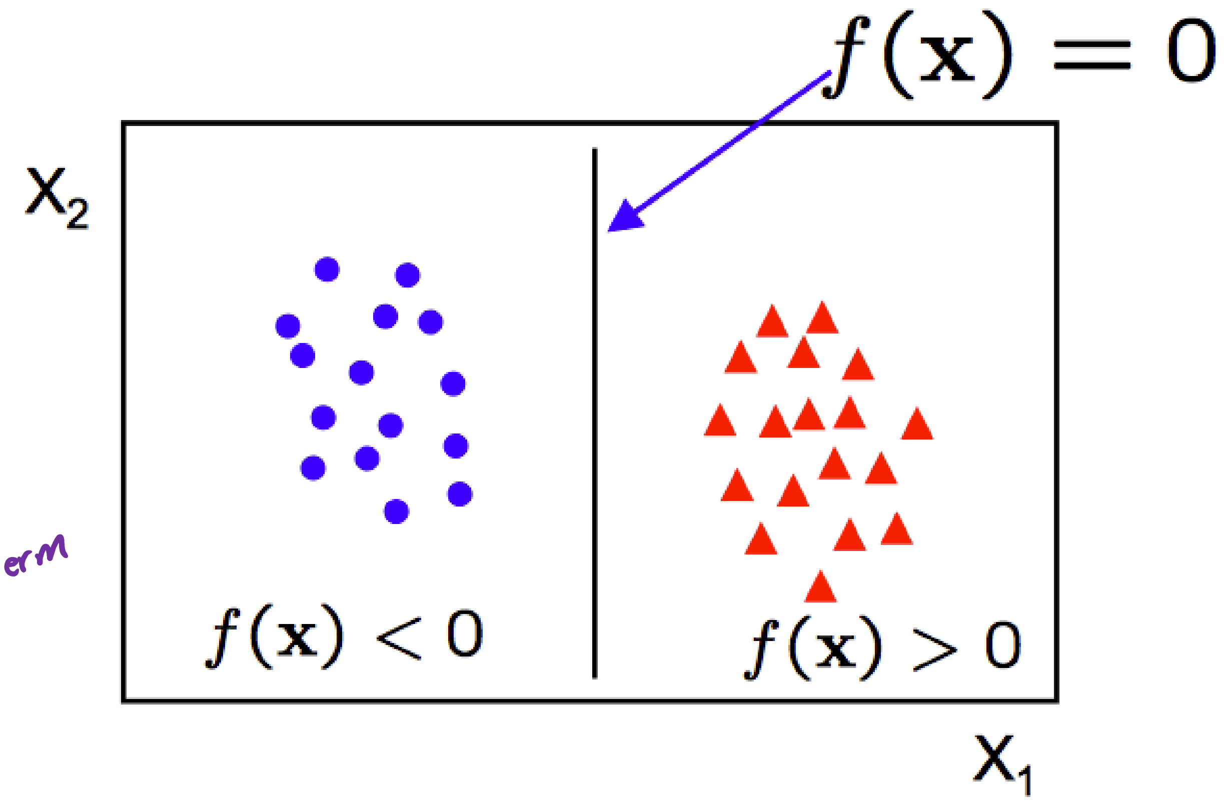
Linear Classifier

A linear classifier has the form

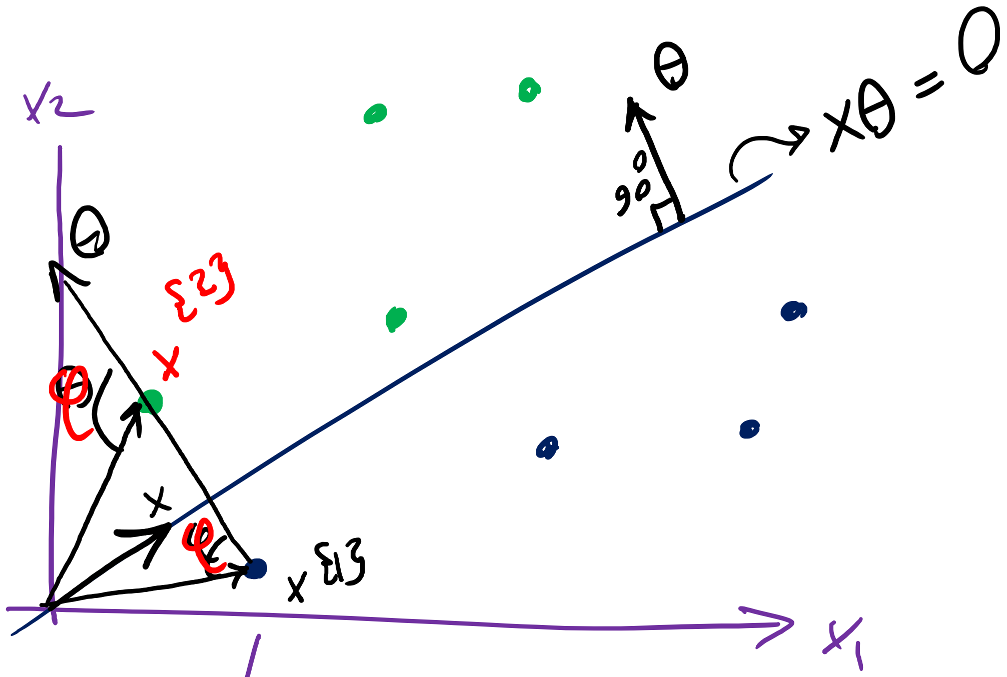
$$f(x) = x\theta + \theta_0$$

bias term

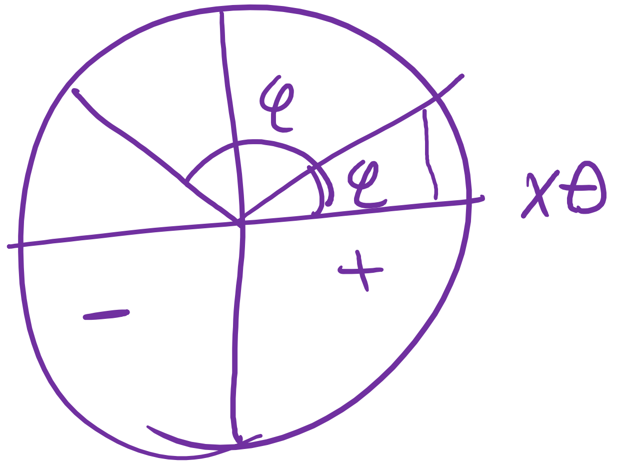
$X\theta = 0$



- 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



$X^{\{1\}}_{1\times d}$



$$X^{\{1\}} \cdot \theta = |X^{\{1\}}|\,|\theta| \cos \boxed{\varphi} > 0 \qquad \text{sign}(>0) = +1$$

$$\varphi < 90$$

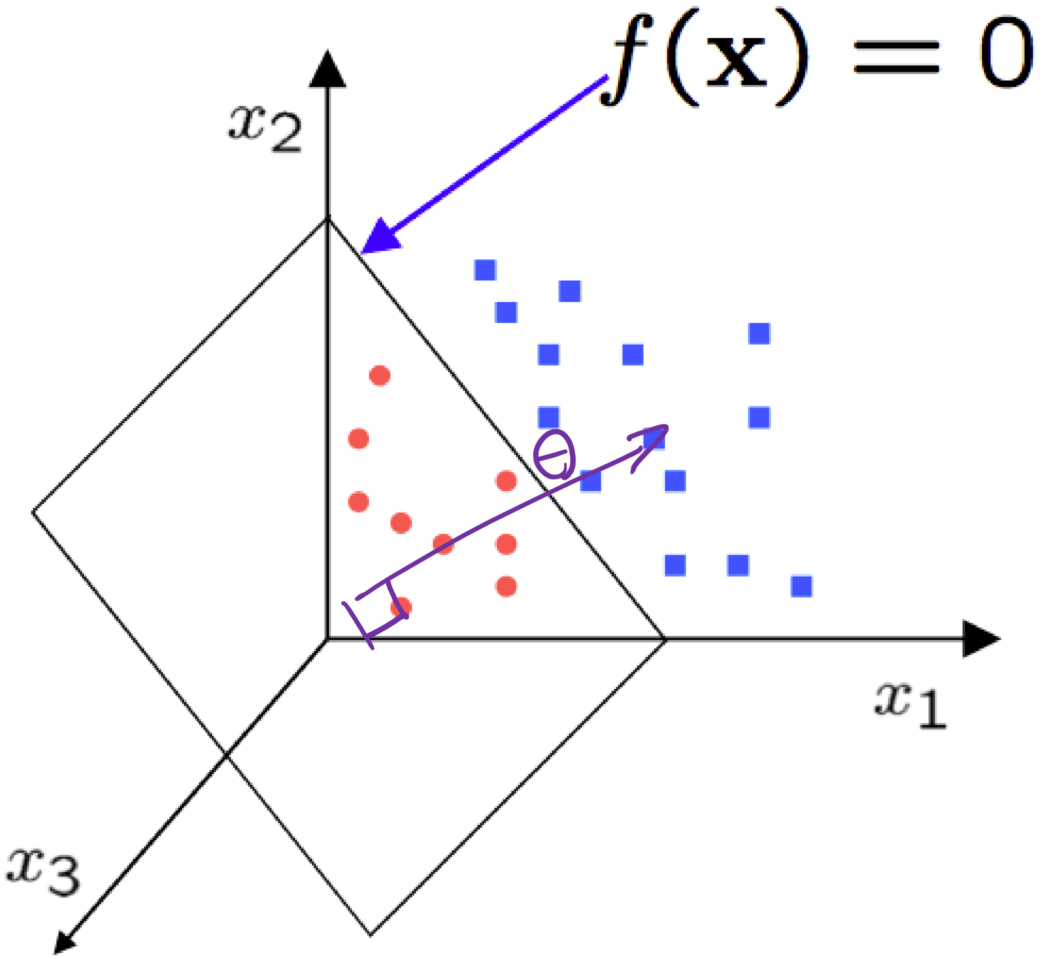
$$X^{\{2\}} \cdot \theta = |X^{\{2\}}|\,|\theta| \cos \varphi < 0 \qquad \text{sign}(<0) = -1$$

$$\varphi > 90$$

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

$$f(x_i) = x_i\theta$$

Bias is inside θ now

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

$y_i f(x_i) < 0$

$\underset{1x1}{\boxed{y_i}}\ \underset{1x1}{\underset{1xd}{x_i}\overset{xdx1}{\theta}} \in \mathbb{R}$

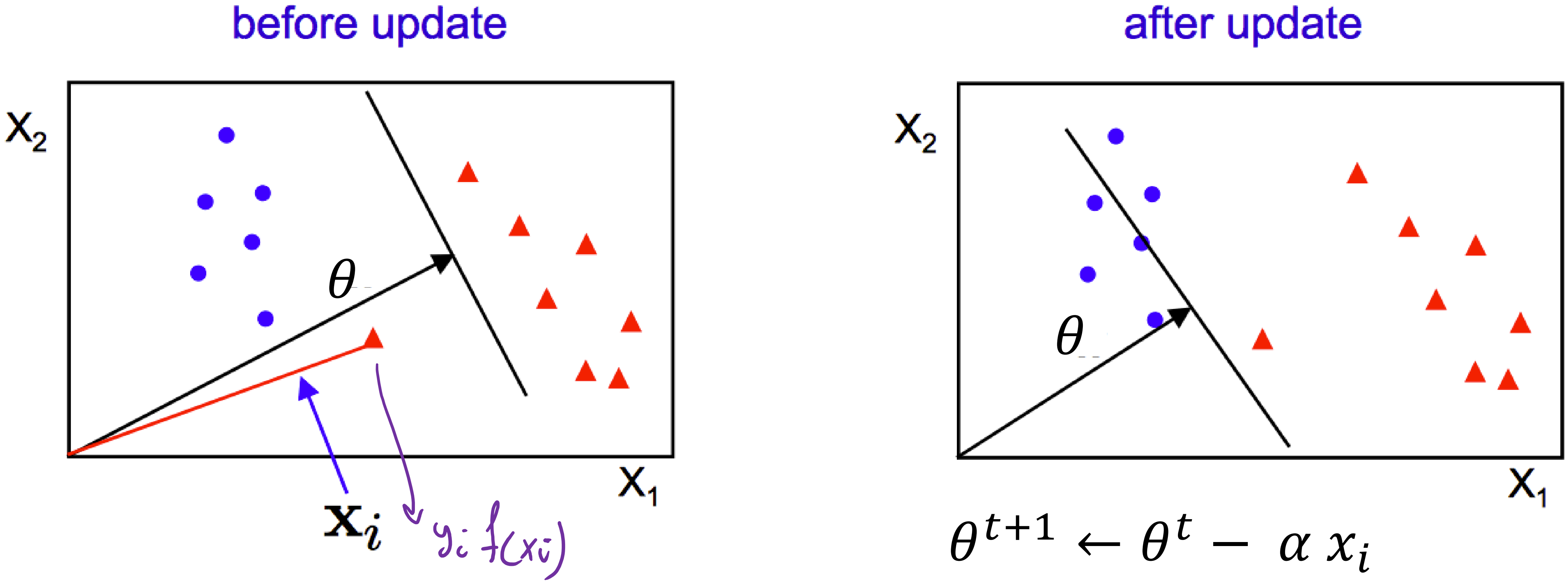
Misclassified

Ex. $\underset{\text{actual}}{y_i}\underset{\text{predicted}}{f(x_i)} < 0$

Perceptron Algorithm:

- Initialize θ =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

- Initialize θ =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


before update

after update

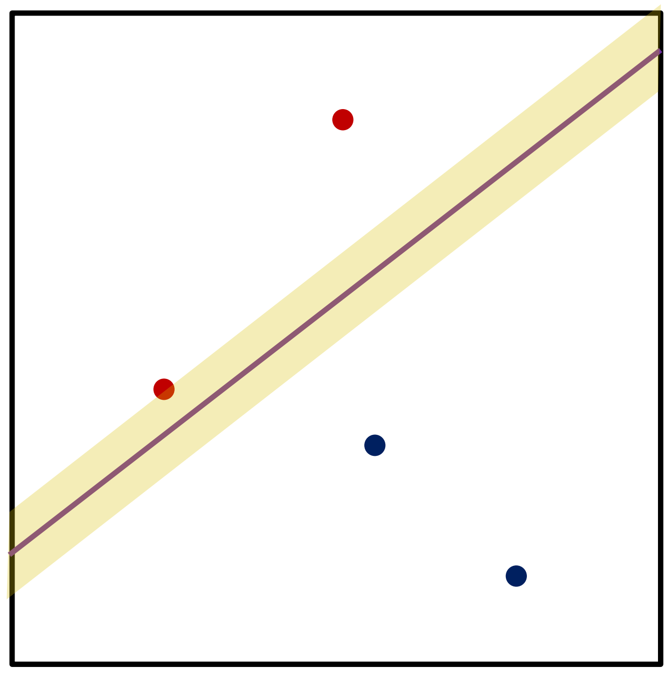
$$\theta^{t+1} \leftarrow \theta^t - \alpha\, x_i$$

Linear separation

We can have different separating lines

$\theta = [\theta_0 \ \theta_1 \cdots \ \theta_d]$

1



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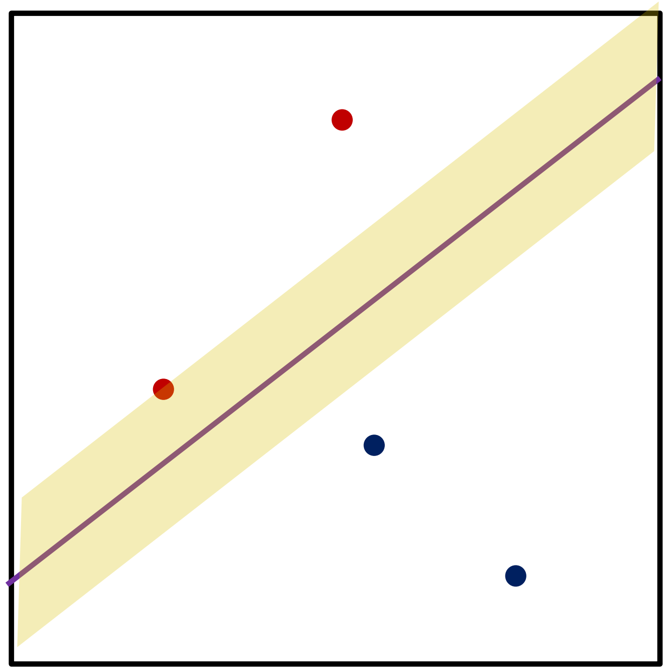
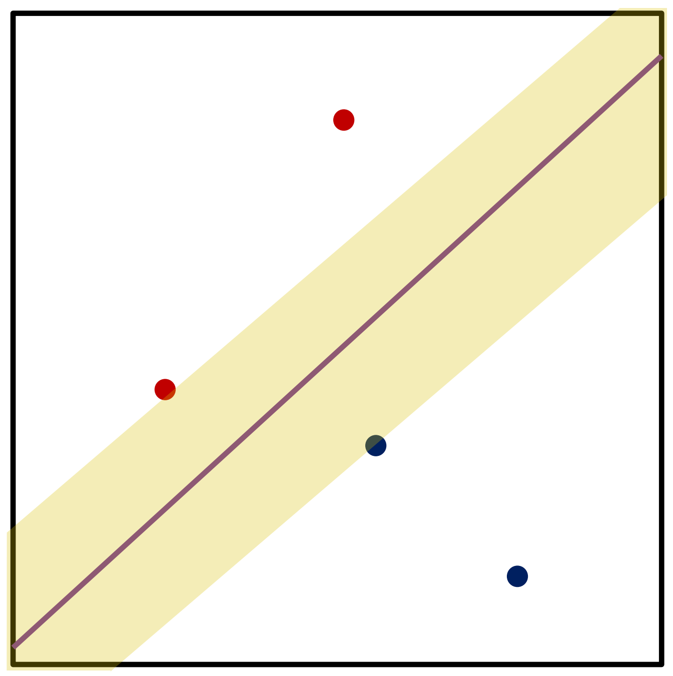


3



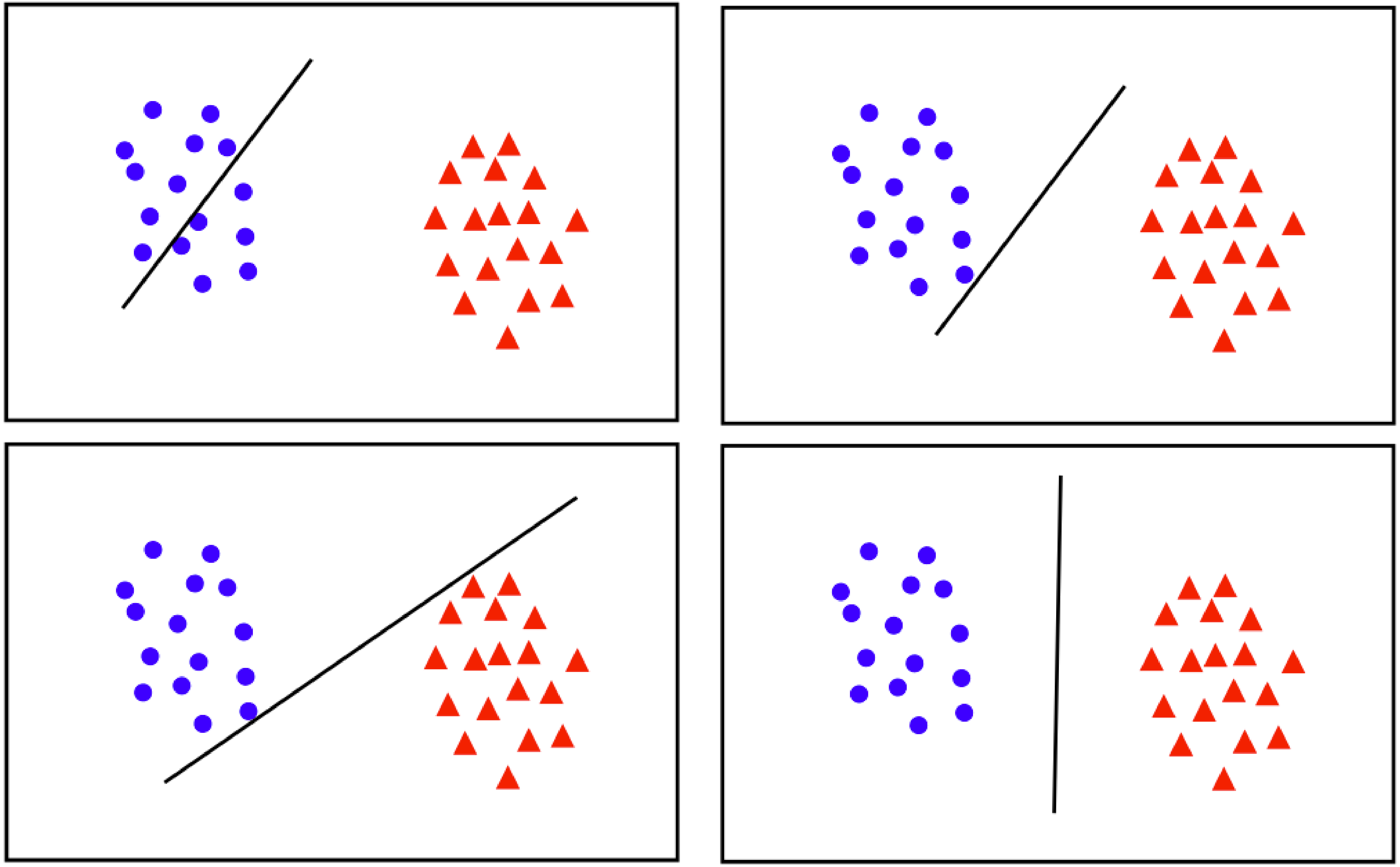
Which line is the best?

Why is the bigger margin better?

What $\boldsymbol{\theta}$ maximizes the margin?

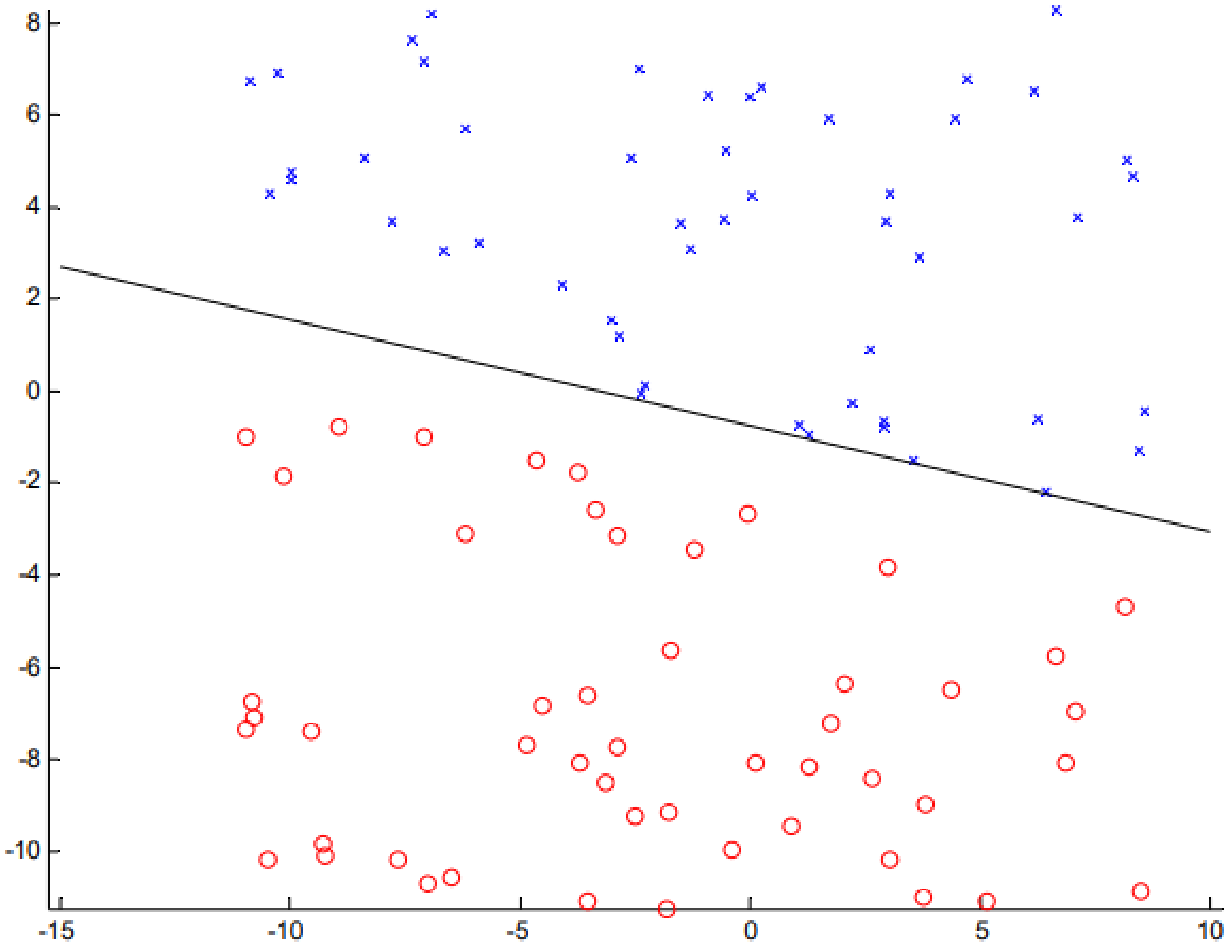
All cases, error is zero and they are linear, so they are all good for generalization.

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)

Outline

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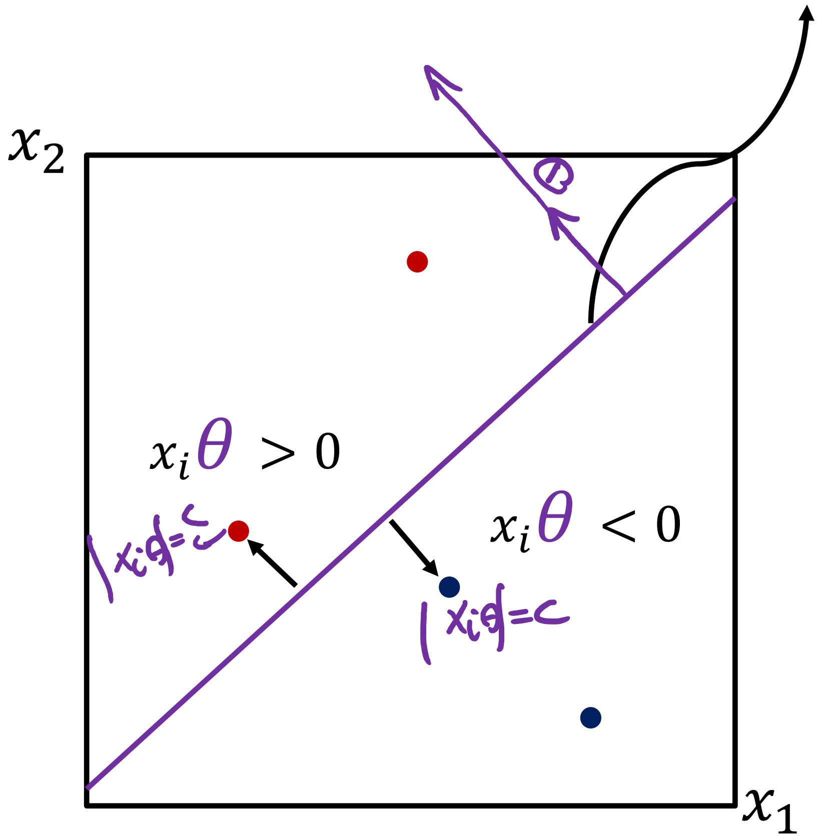
Finding θ with a **fat** margin

on decision line

$f(x) = x\theta = 0$

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



$\downarrow\uparrow$

$x_i\theta = c$ $\quad |x_i\theta| = 1$

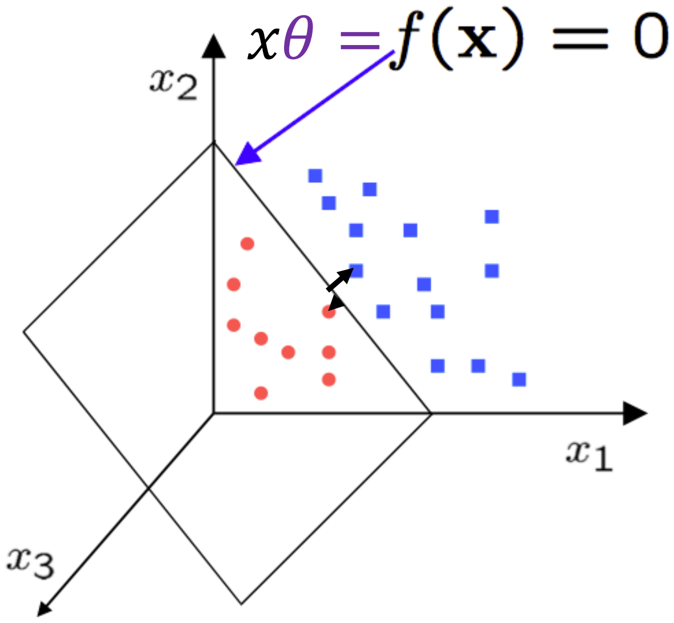
Let x_i to be the nearest data point to the line (plane):

$$|x_i\theta| > 0$$

Our line solution is $x\theta = 0$

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

$|x_i\theta| = 1$ → normalization



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

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

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.

You should ask me why?

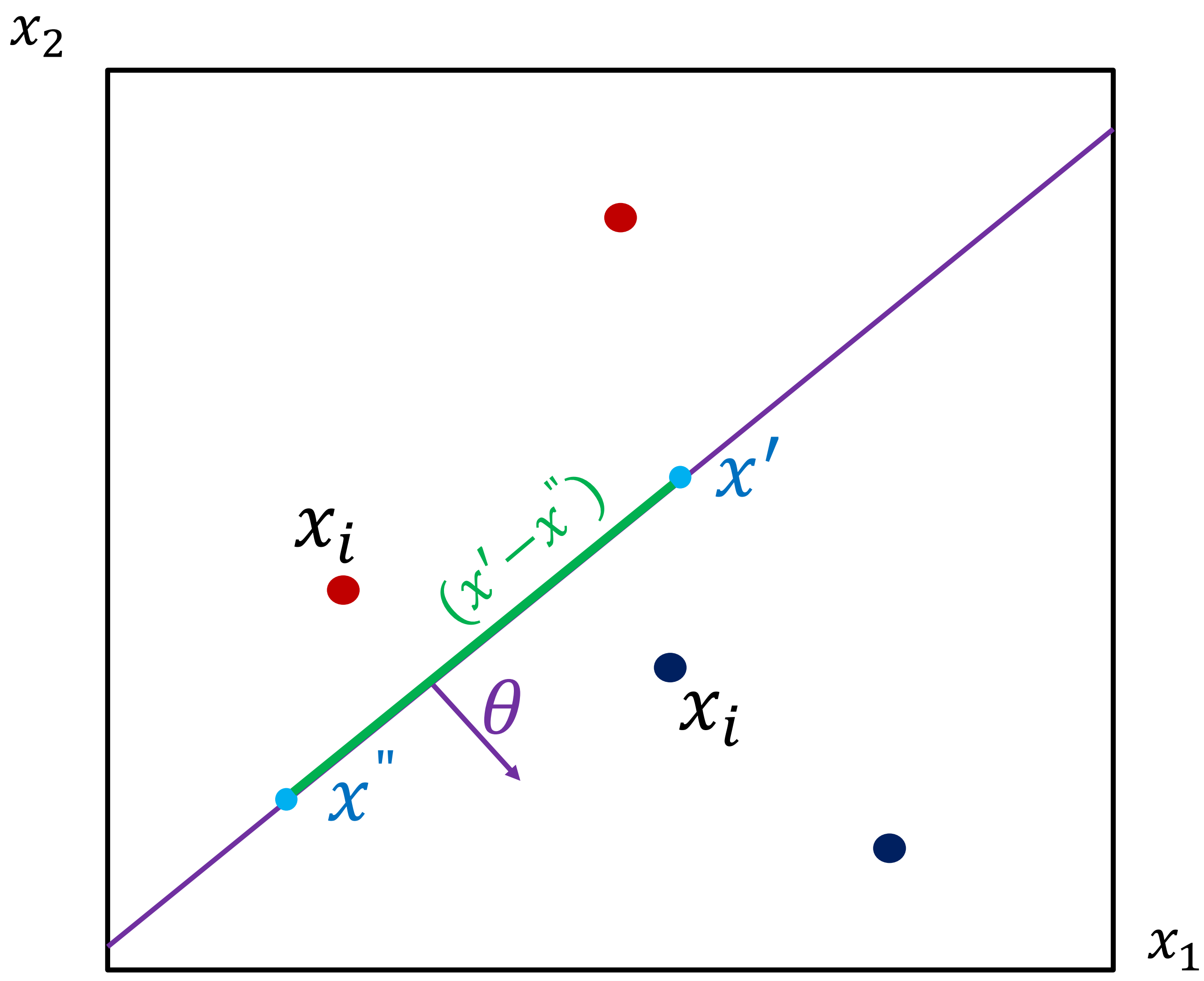
Consider x' and x'' on the plane

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

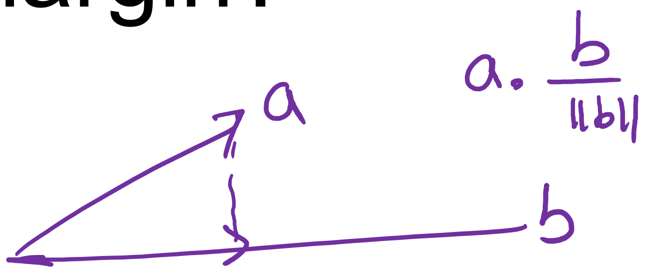
$$\Downarrow$$

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

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



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

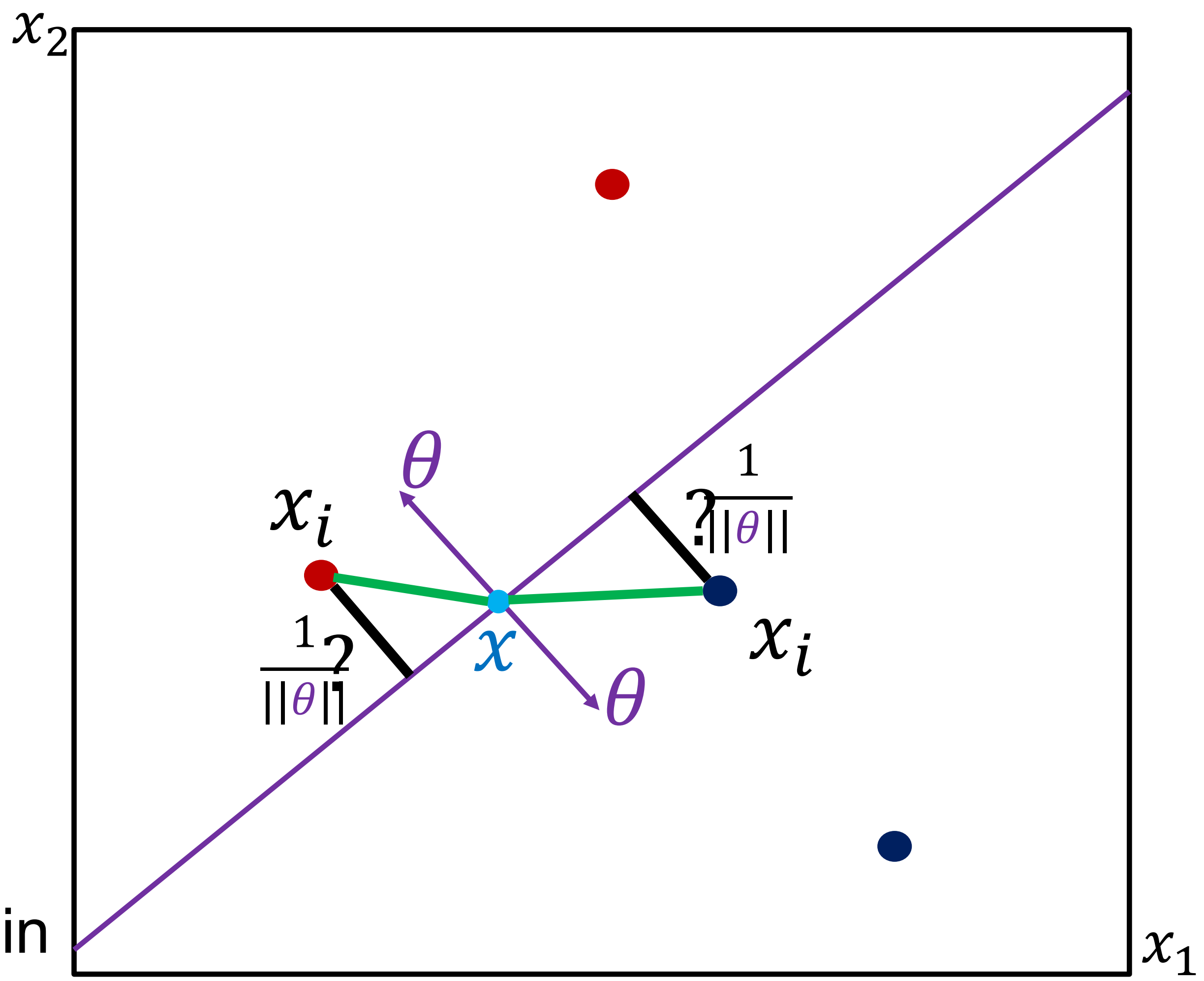
$$\text{distance} = \frac{1}{||\theta||}|(x_i\theta - x\theta)|$$

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

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

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)

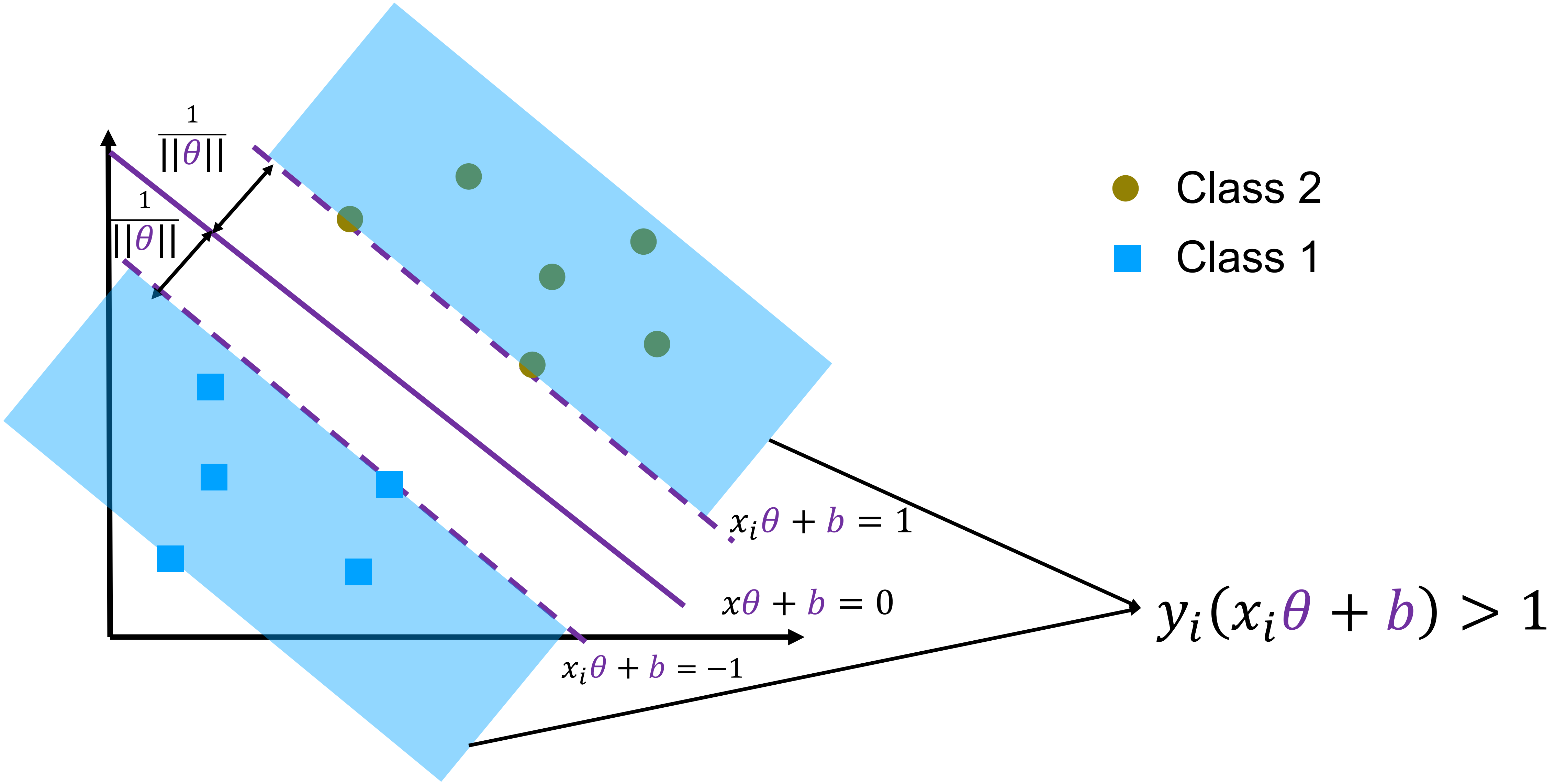
Can I write the following term to get rid of absolute value?

$|x_i\theta + b| = y_i(x_i\theta + b) \Rightarrow$ 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 $\frac{2}{||\theta||_2^2}$

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

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

$||\theta||_2^2 = \theta\theta^T$

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

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

Minimize

$L(\theta, \alpha) = \frac{1}{2}\theta\theta^T - \alpha g(x)$

α

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

$g(x) \geq 0$

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

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

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

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

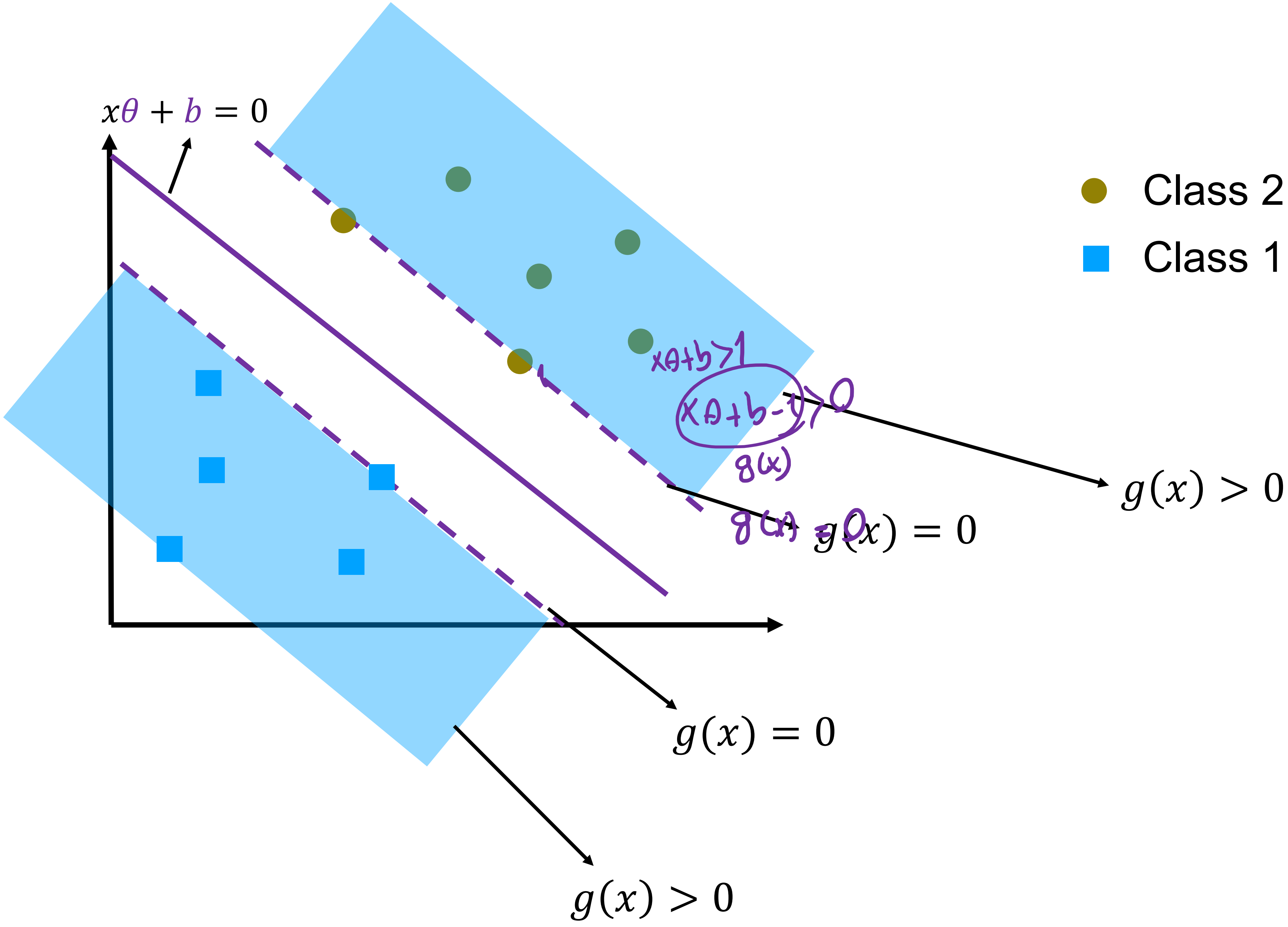
We need to optimize $\theta, b, and\ \alpha$

1) Stationary

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

3) $\alpha \geq 0$ Dual feasibility

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



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

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

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. $y_i(x_i\theta + b) - 1 \geq 0$

Primal form

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

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

$$\boxed{\theta_{1\times d} = \sum \alpha_i y_i x_i}$$

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

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

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

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

Let's substitute these in the Lagrangian:

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

$$-\left[\overset{\theta^T}{\boxed{\sum \alpha_i y_i x_i}}\theta + b\overset{0}{\cancel{\sum \alpha_i y_i}}\right]$$

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

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

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

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

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

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

Dual form

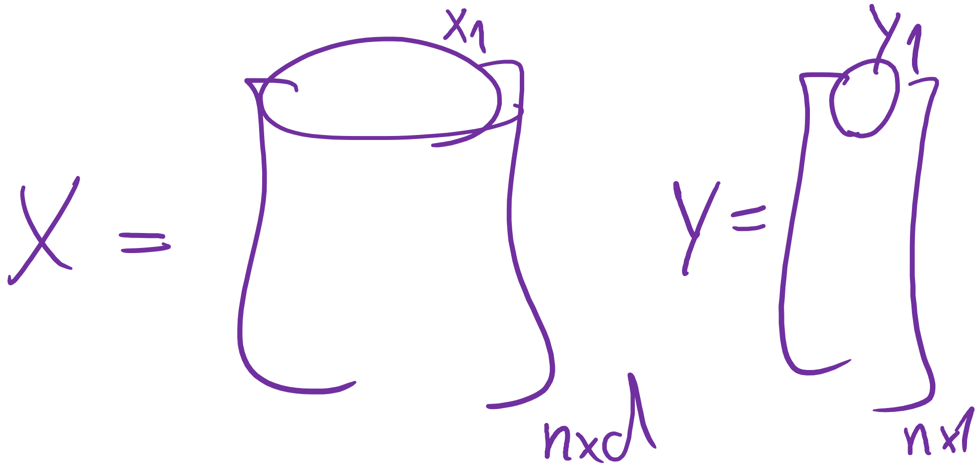
$$\boxed{\mathcal{L}(\theta, b, \alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j x_i x_j^T}$$

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”

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

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

$$\min_{\alpha} \frac{1}{2}\alpha^T \underbrace{\begin{bmatrix} y_1y_1x_1x_1^T & y_1y_1x_1x_2^T & \dots & y_1y_Nx_1x_N^T \\ y_2y_1x_2x_1^T & y_2y_2x_2x_2^T & \cdots & y_2y_Nx_2x_N^T \\ \dots & \dots & \cdots & \dots \\ y_Ny_1x_Nx_1^T & y_Ny_2x_nx_2^T & \cdots & y_Ny_Nx_Nx_N^T \end{bmatrix}}_{\text{Quadratic coefficients}} \alpha + \underbrace{(-I^T)}_{\text{Linear term}}\alpha$$

Pass these to a quadratic programming package

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

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

$\alpha \geqslant 0$

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

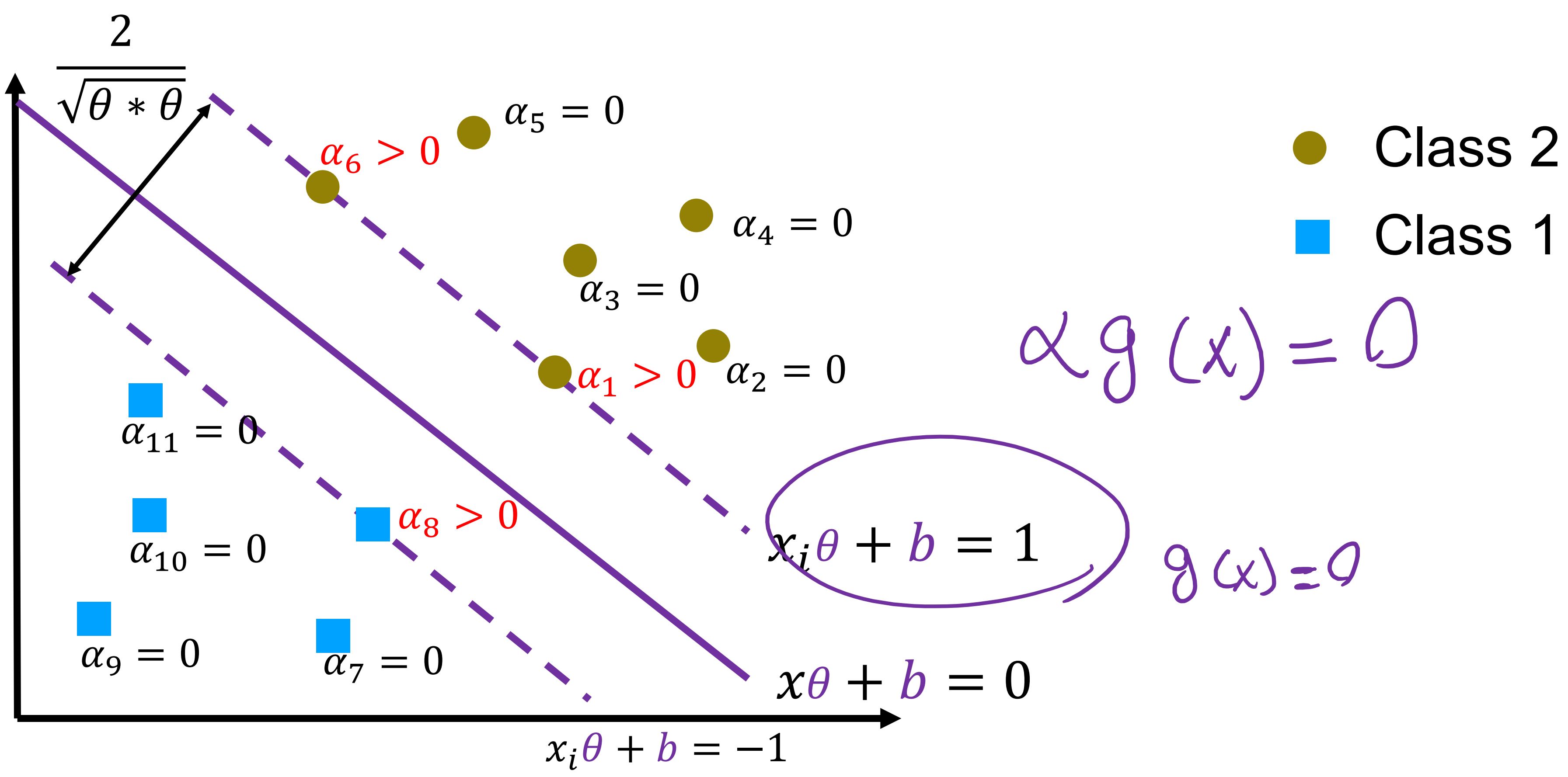
Quadratic programming will give us α

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

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

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

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



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:

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

Testing

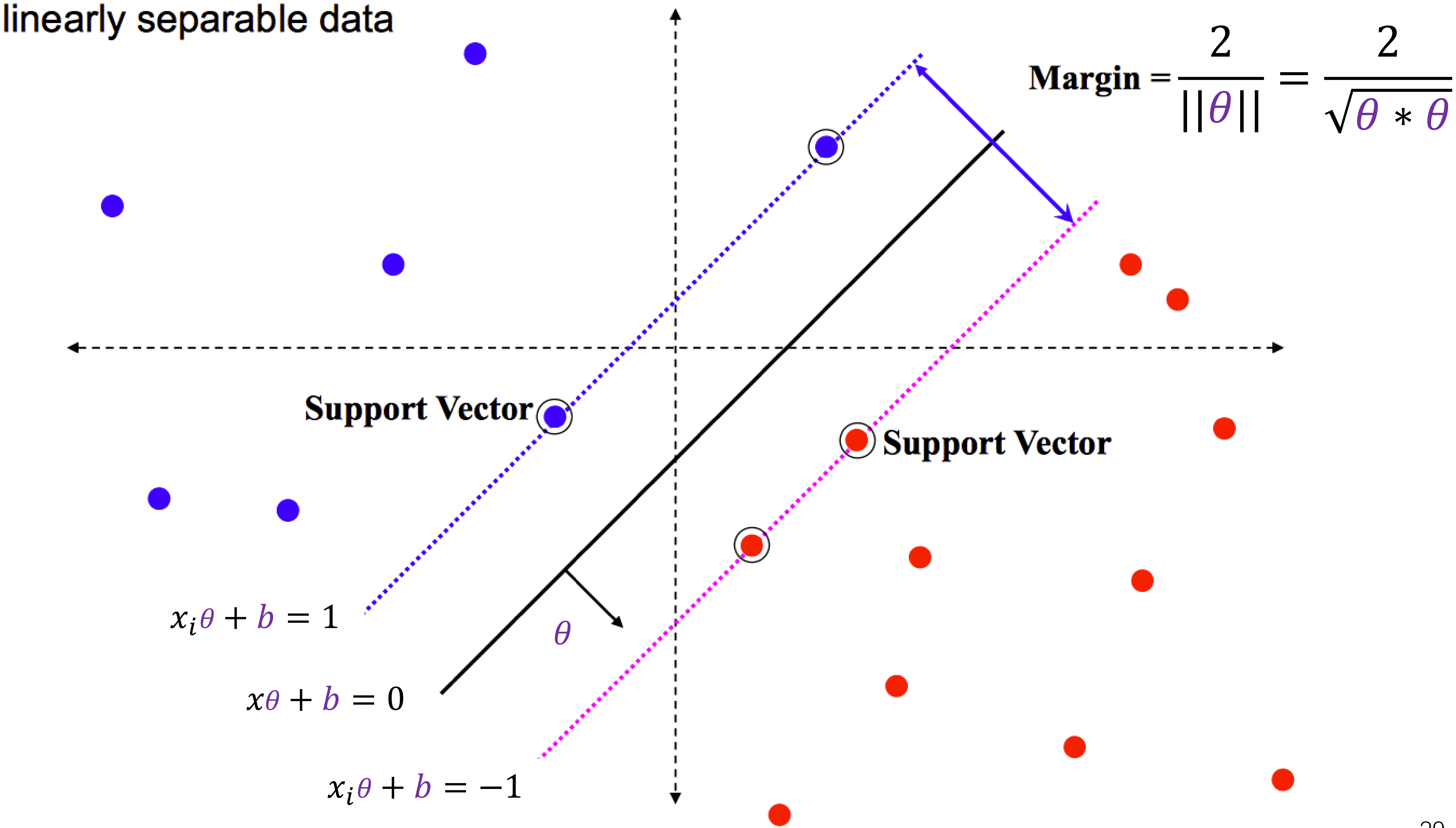
For a new test point s

Compute:

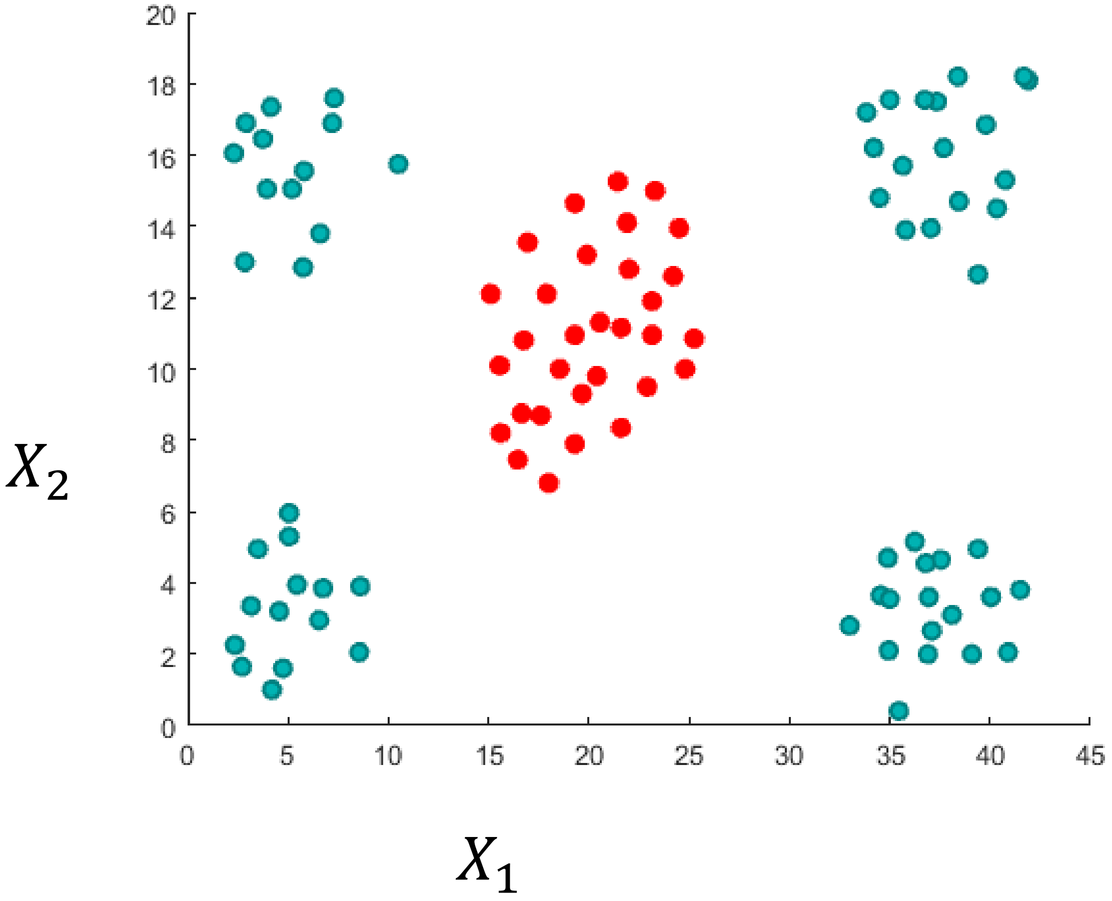
$$\overbrace{s\theta + b}^{\text{Primal form}} = \overbrace{\boxed{\sum_{x_i \, in \, SV} \alpha_i y_i x_i s^T + b}}^{\text{Dual form}}$$

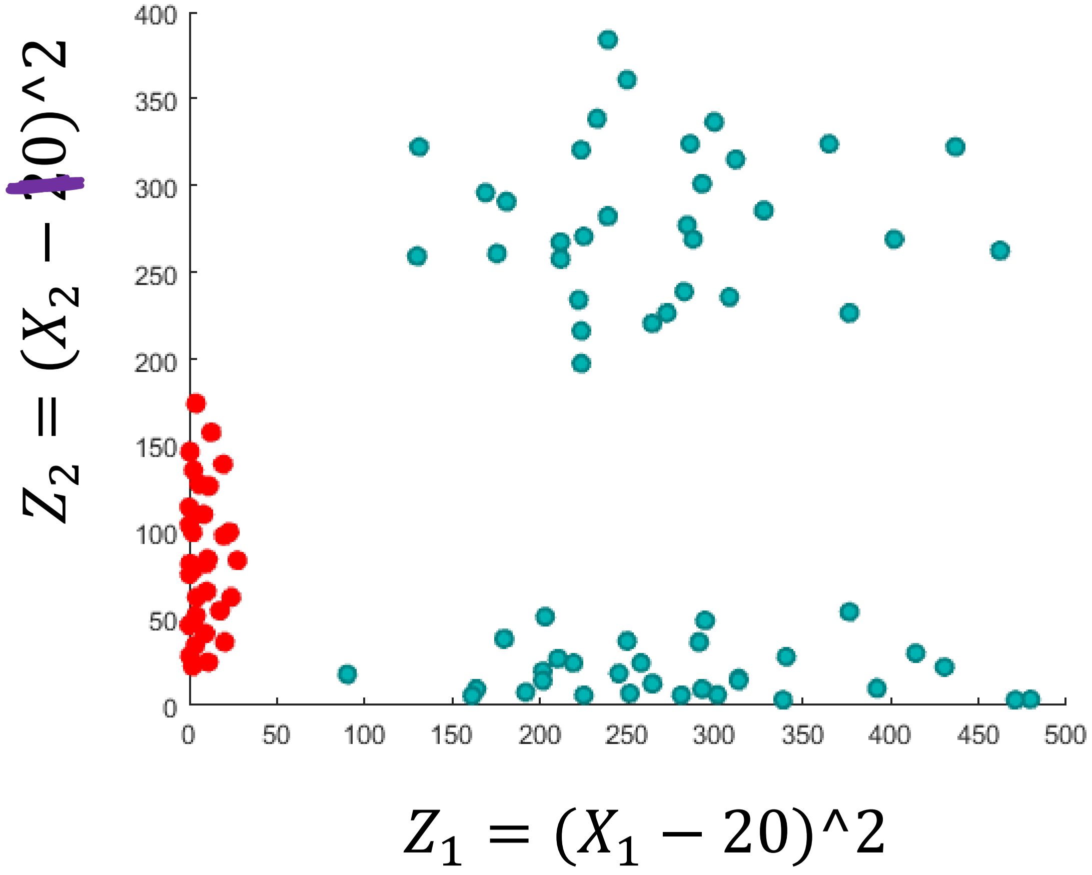
Classify s as class 1 if the result is positive, and class 2 otherwise

Geometric Interpretation



From x to z space



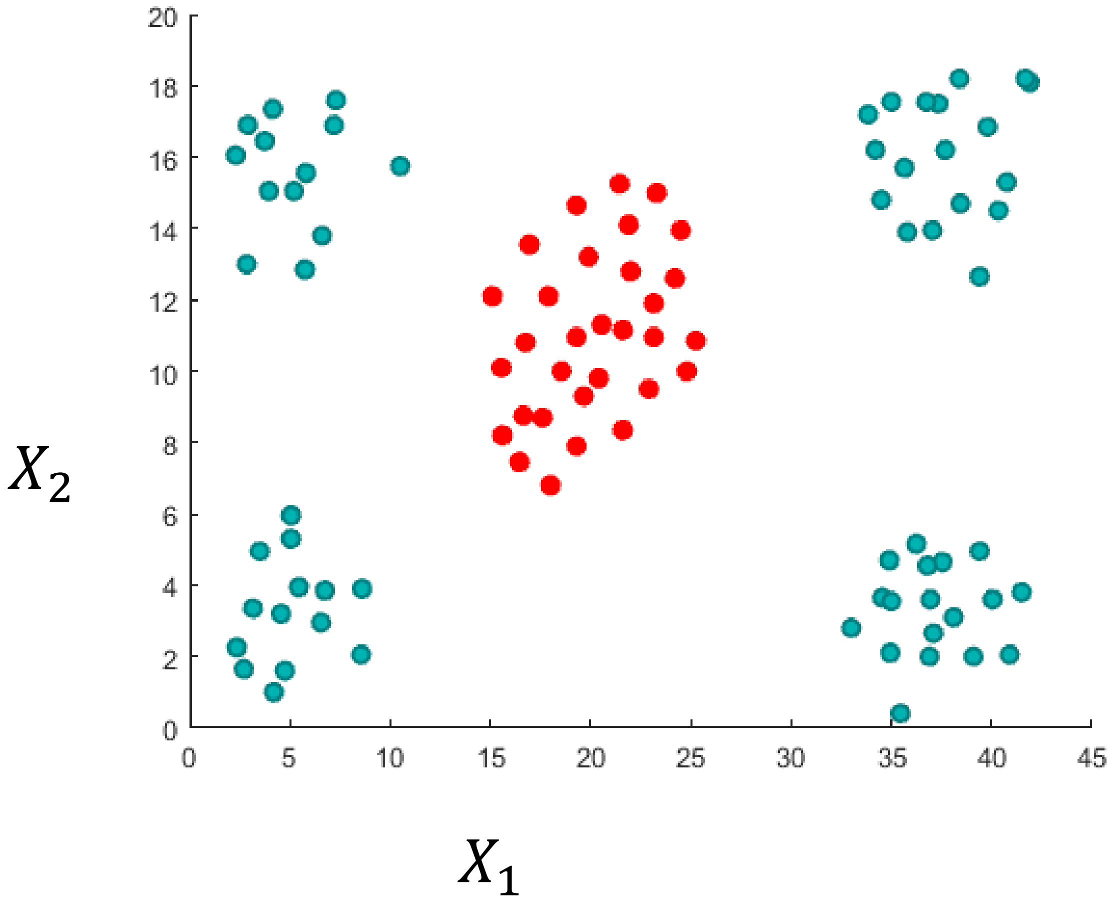


$$X \xrightarrow[(X_1^2, X_2^2)]{} Z$$

In x space

$X_{n \times d}$ $(XX^T)_{n \times n}$

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



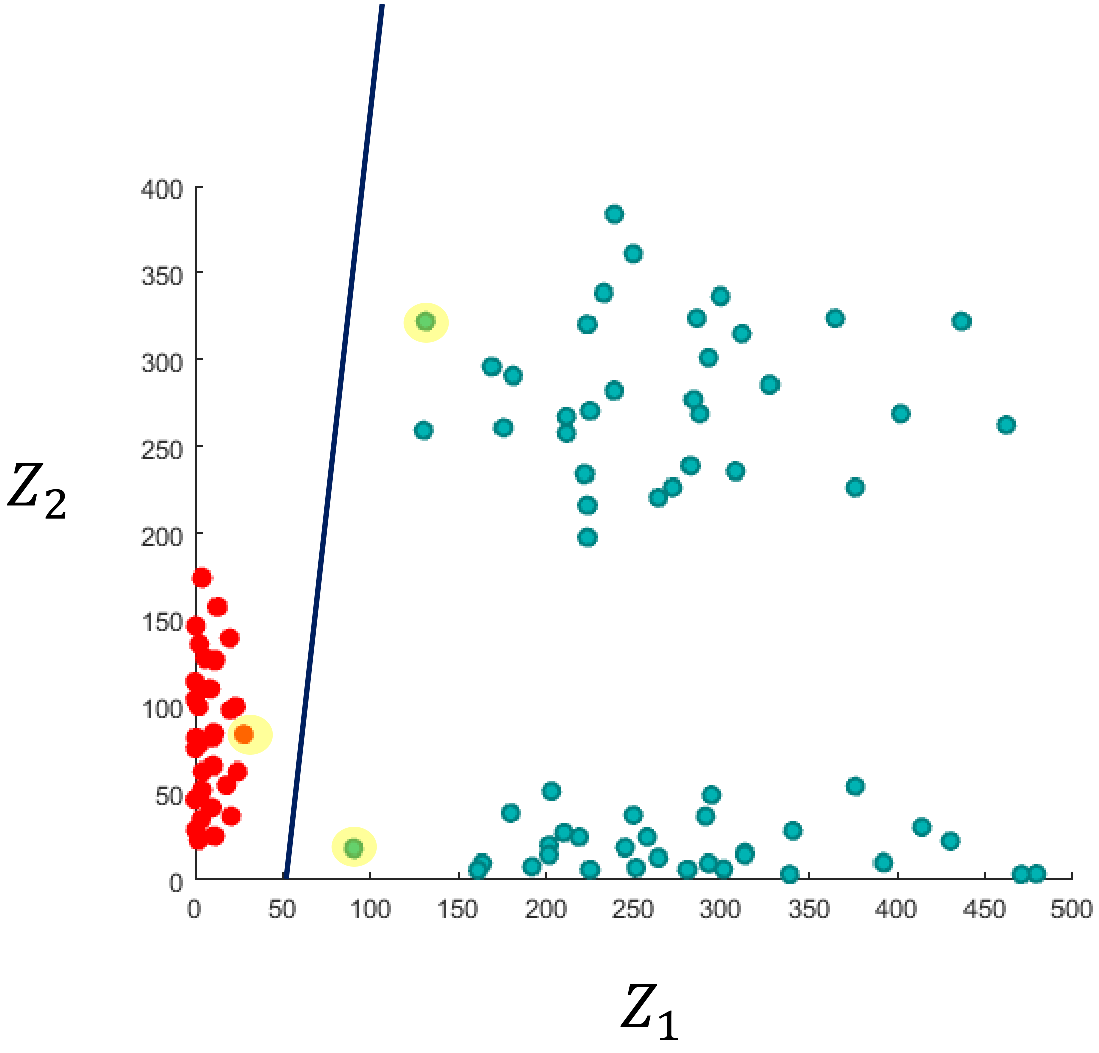
$let's\ say\ x\ is\ n \times d$

$x\mathrm{x}^{\mathrm{T}}$ will be n × n

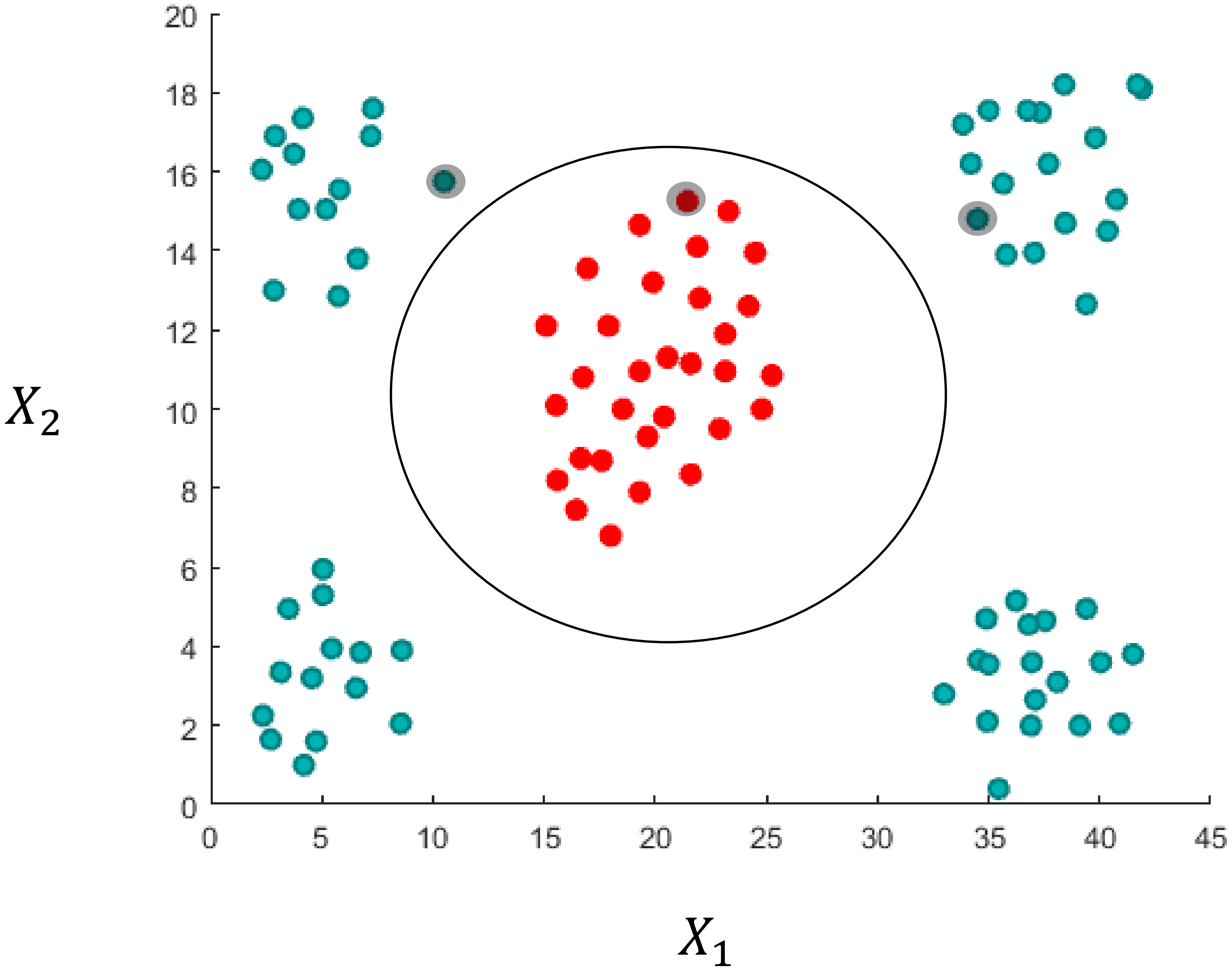
If I add millions of dimensions to x, would it affect the final size of $x\mathrm{x}^{\mathrm{T}}$?

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



Take-Home Messages

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