

Support Vector Machines

Nipun Batra

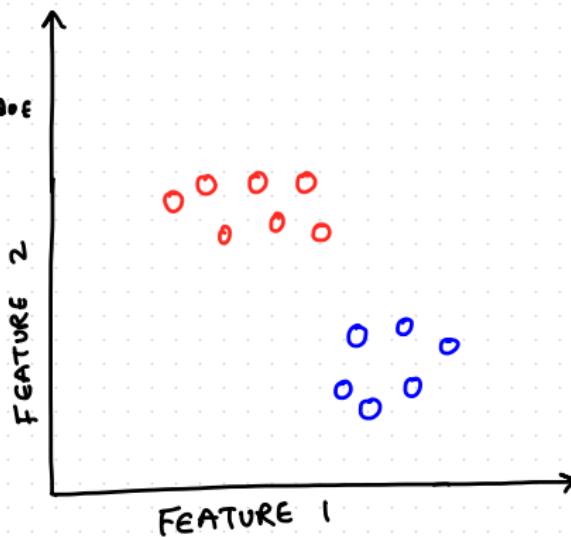
April 25, 2023

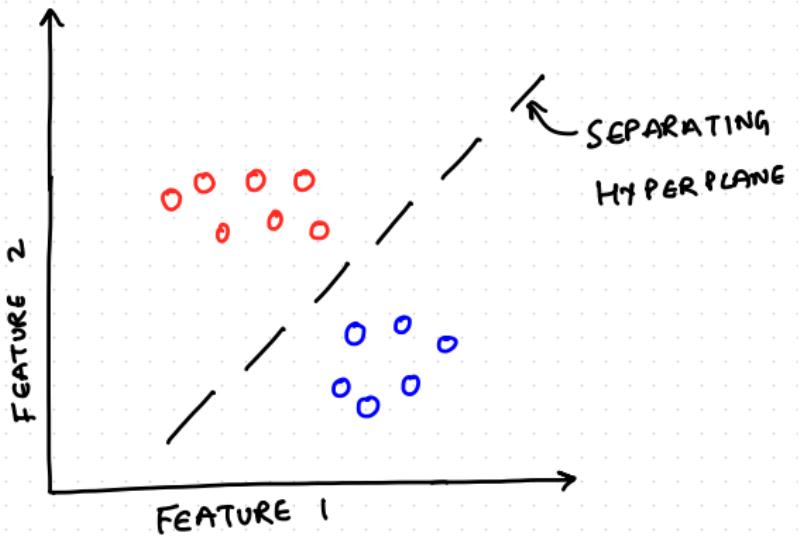
IIT Gandhinagar

SUPPORT VECTOR MACHINES

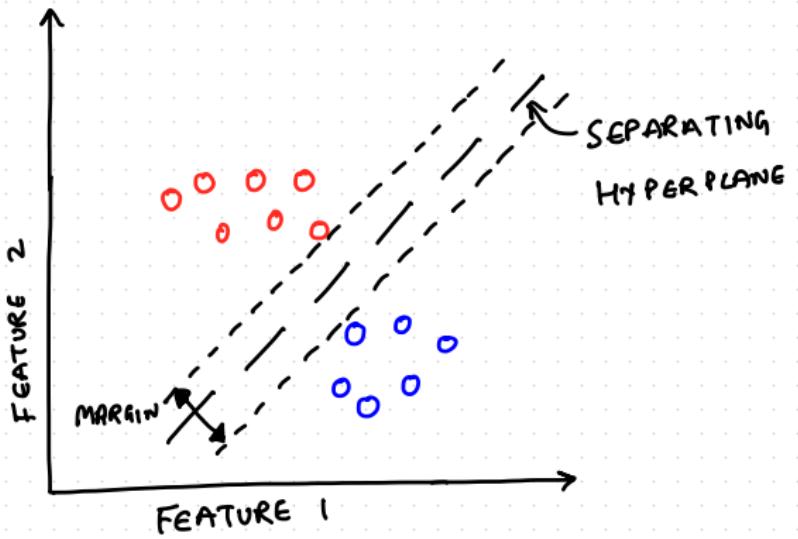
POPULAR BINARY

CLASSIFICATION TECHNIQUE

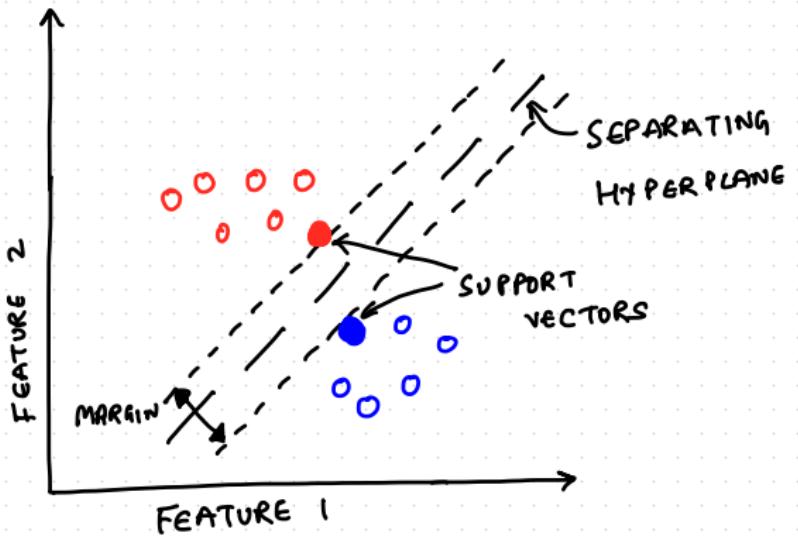




IDEA: DRAW A SEPARATING HYPERPLANE



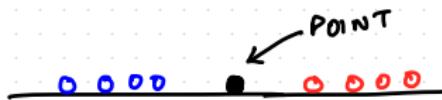
IDEA: MAXIMIZE THE MARGIN



SUPPORT VECTORS: POINTS ON BOUNDARY | MARGIN

HYPERPLANE IS # DIMENSIONS

1D

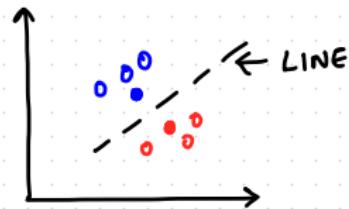


HYPERPLANE IS # DIMENSIONS

1D

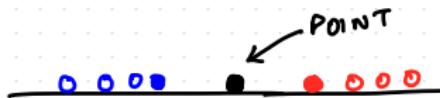


2D

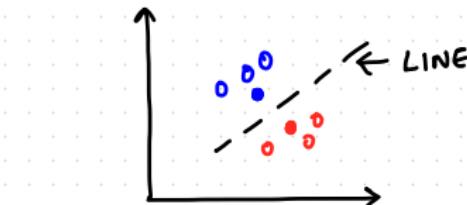


HYPERPLANE VIS # DIMENSIONS

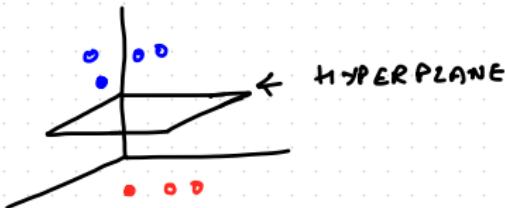
1D



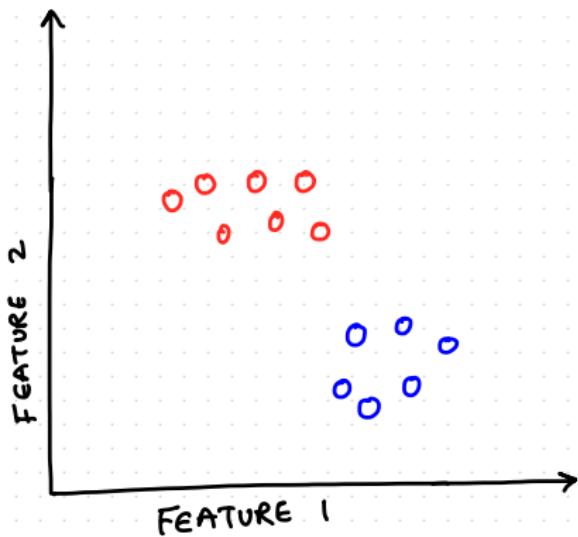
2D



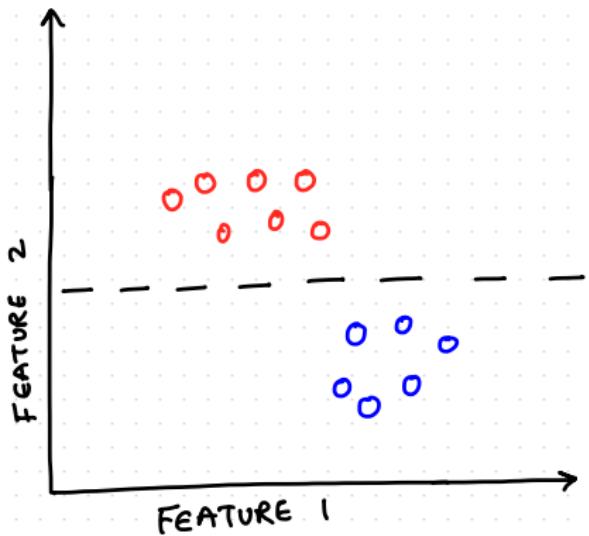
3D
(AND
MORE)



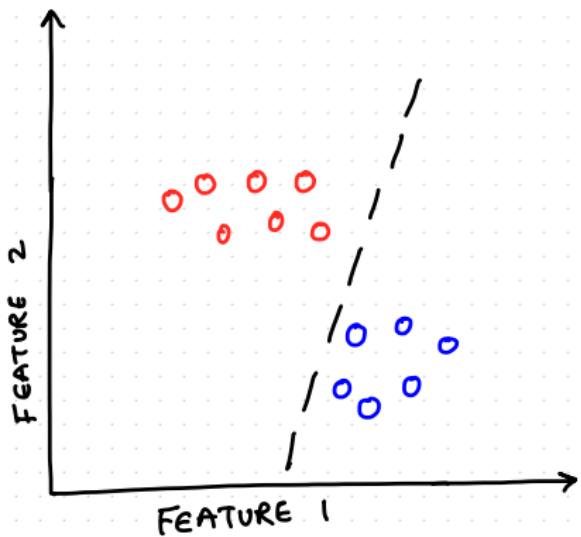
WHICH HYPERPLANE?



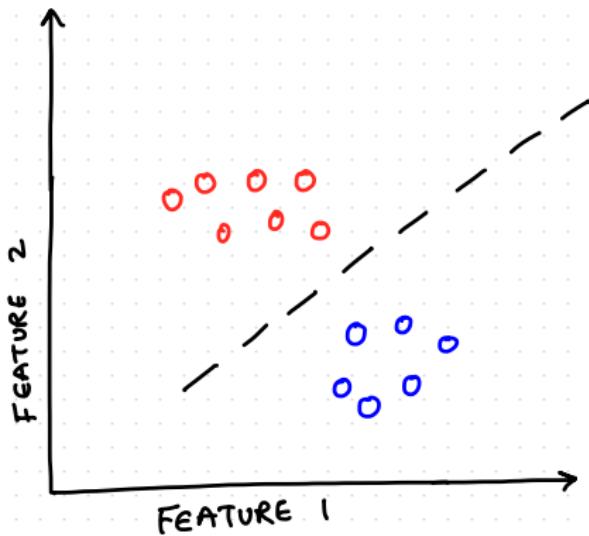
WHICH HYPERPLANE?



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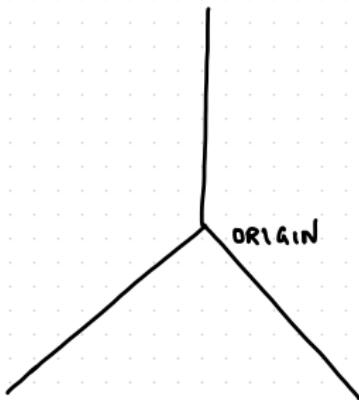


WHICH HYPERPLANE?

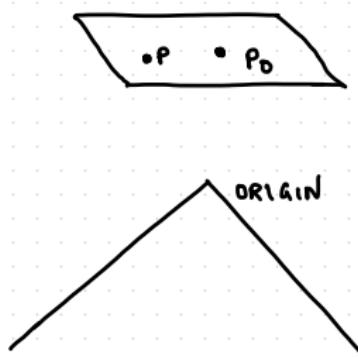


EQUATION OF HYPERPLANE

HOW TO DEFINE?



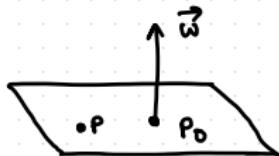
EQUATION OF HYPERPLANE



P: Any point on plane

P₀: One point on plane

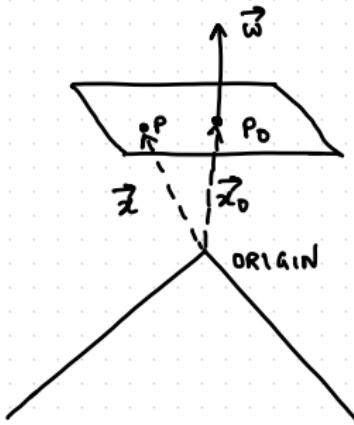
EQUATION OF HYPERPLANE



\vec{w} : \perp vector to
plane at P_0

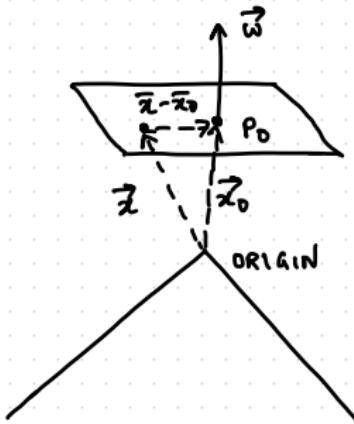


EQUATION OF HYPERPLANE



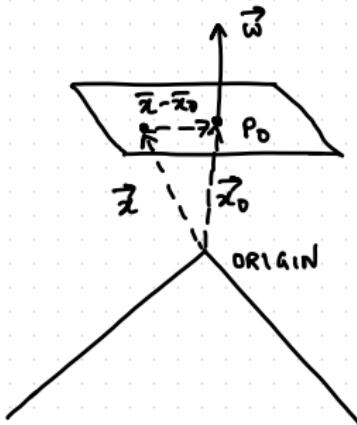
P and P_0 lie on
plane

EQUATION OF HYPERPLANE



$\vec{P} P_0 = \vec{x} - \vec{x}_0$ lies on
plane

EQUATION OF HYPERPLANE



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plane

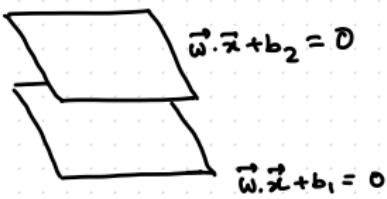
$$\Rightarrow \vec{w} \perp (\vec{x} - \vec{x}_0)$$

$$\text{or, } \vec{w} \cdot (\vec{x} - \vec{x}_0) = 0$$

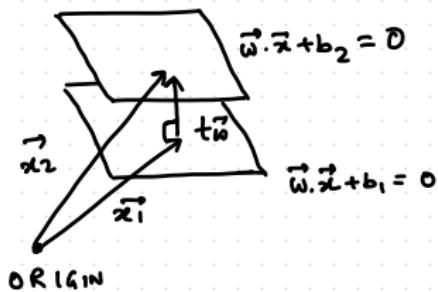
$$\text{or, } \vec{w} \cdot \vec{x} - \vec{w} \cdot \vec{x}_0 = 0$$

$$\boxed{\vec{w} \cdot \vec{x} + b = 0}$$

DISTANCE B/W II HYPERPLANES



DISTANCE B/W II HYPERPLANES



Distance between 2 parallel hyperplanes

Equation of two planes is:

$$\vec{w} \cdot \vec{x} + b_1 = 0$$

$$\vec{w} \cdot \vec{x} + b_2 = 0$$

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For a point \vec{x}_1 on plane 1 and \vec{x}_2 on plane 2, we have:

$$\vec{x}_2 = \vec{x}_1 + t\vec{w}$$

$$D = |t\vec{w}| = |t| |\vec{w}|$$

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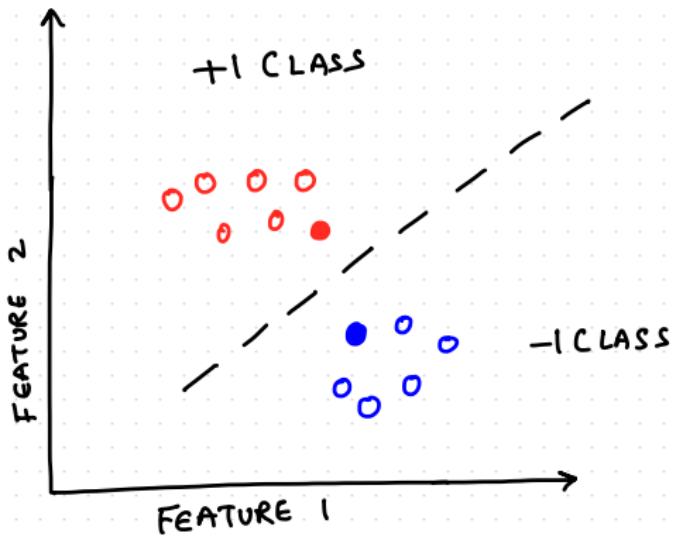
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$$\vec{w} \cdot \vec{x}_2 + b_2 = 0$$

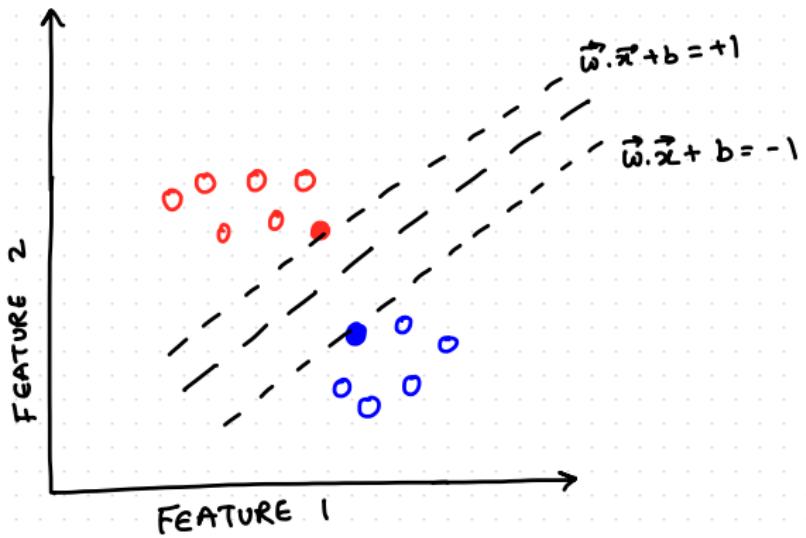
$$\Rightarrow \vec{w} \cdot (\vec{x}_1 + t\vec{w}) + b_2 = 0$$

$$\Rightarrow \vec{w} \cdot \vec{x}_1 + t\|\vec{w}\|^2 + b_1 - b_1 + b_2 = 0 \Rightarrow t = \frac{b_1 - b_2}{\|\vec{w}\|^2} \Rightarrow D = t\|\vec{w}\| = \frac{b_1 - b_2}{\|\vec{w}\|}$$

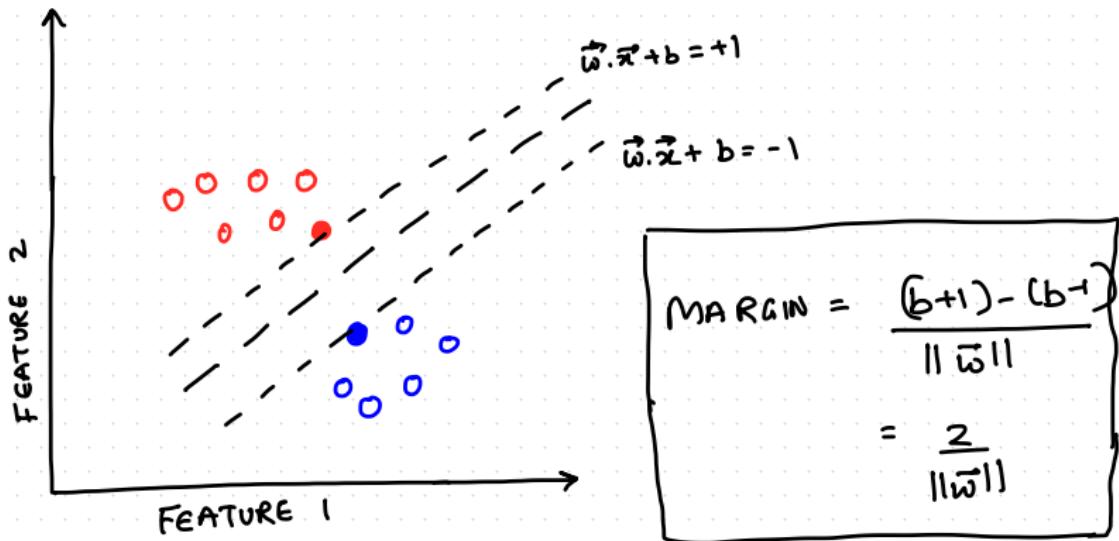
FORMULATION



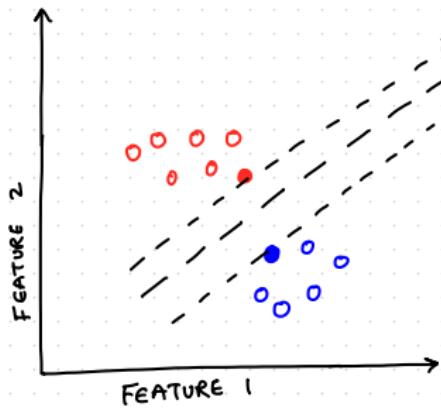
FORMULATION



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FORMULATION



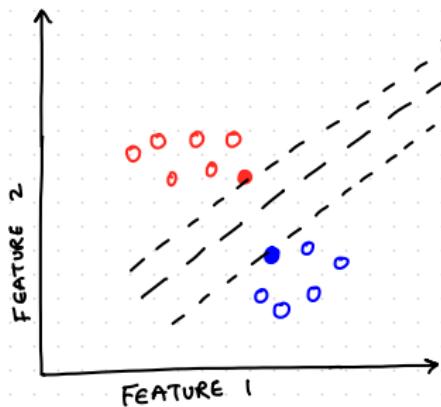
GOAL: MAXIMIZE MARGIN

$$\Rightarrow \text{MAXIMIZE } \frac{2}{\|\vec{w}\|}$$

$$\Rightarrow \text{MINIMIZE } \|\vec{w}\|$$

S.T. Correctly label points

FORMULATION



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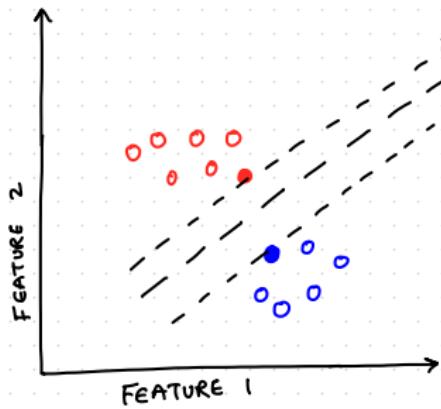
$$\Rightarrow \text{MINIMIZE } \|\vec{w}\|$$

S.T. correctly label points

i.e. if $y_i = -1$
 $\vec{w} \cdot \vec{x}_i + b \leq -1$

if $y_i = +1$
 $\vec{w} \cdot \vec{x}_i + b \geq +1$

FORMULATION



GOAL: MAXIMIZE MARGIN

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$$\boxed{y_i (\vec{w} \cdot \vec{x}_i + b) \geq 1}$$

Primal Formulation

Objective

$$\begin{aligned} & \text{Minimize } \frac{1}{2} ||w||^2 \\ & \text{s.t. } y_i(w \cdot x_i + b) \geq 1 \quad \forall i \end{aligned}$$

Primal Formulation

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Q) What is $||w||$?

Primal Formulation

Objective

$$\text{Minimize } \frac{1}{2} \|w\|^2$$

$$\text{s.t. } y_i(w \cdot x_i + b) \geq 1 \quad \forall i$$

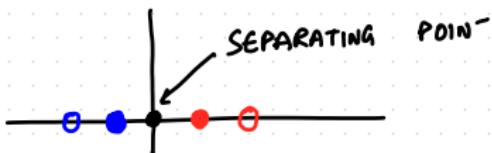
Q) What is $\|w\|$?

$$w = \begin{bmatrix} w_1 \\ w_2 \\ \dots \\ w_n \end{bmatrix}$$

$$\|w\| = \sqrt{w^T w}$$

$$= \sqrt{\begin{bmatrix} w_1, w_2, \dots, w_n \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \dots \\ w_n \end{bmatrix}^T}$$

EXAMPLE (IN 1D)



Simple Exercise

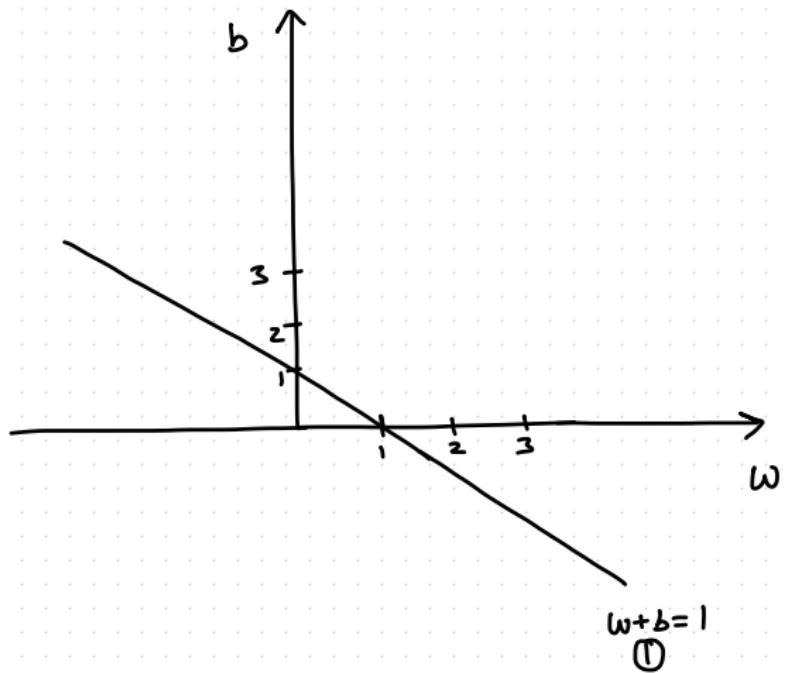
$$\begin{bmatrix} x & y \\ 1 & 1 \\ 2 & 1 \\ -1 & -1 \\ -2 & -1 \end{bmatrix}$$

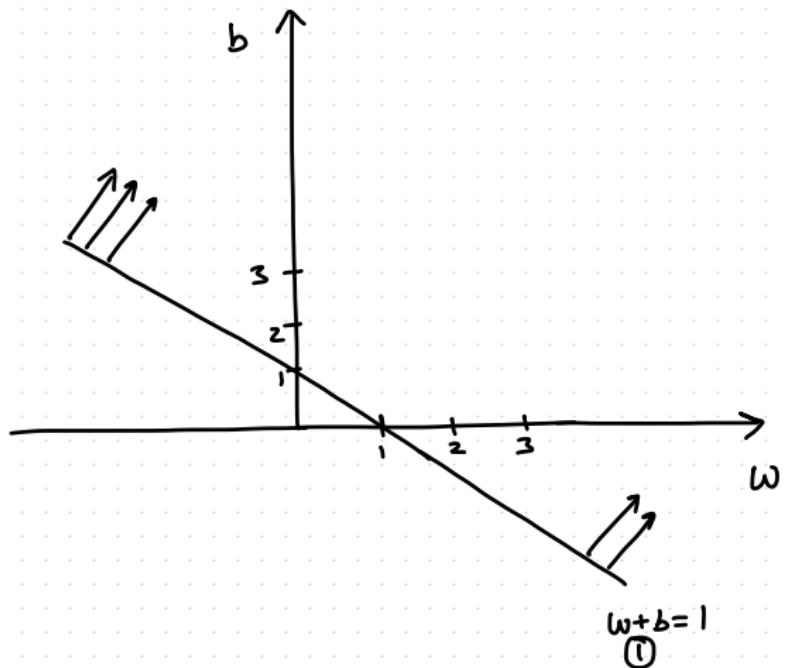
Separating Hyperplane: $wx + b = 0$

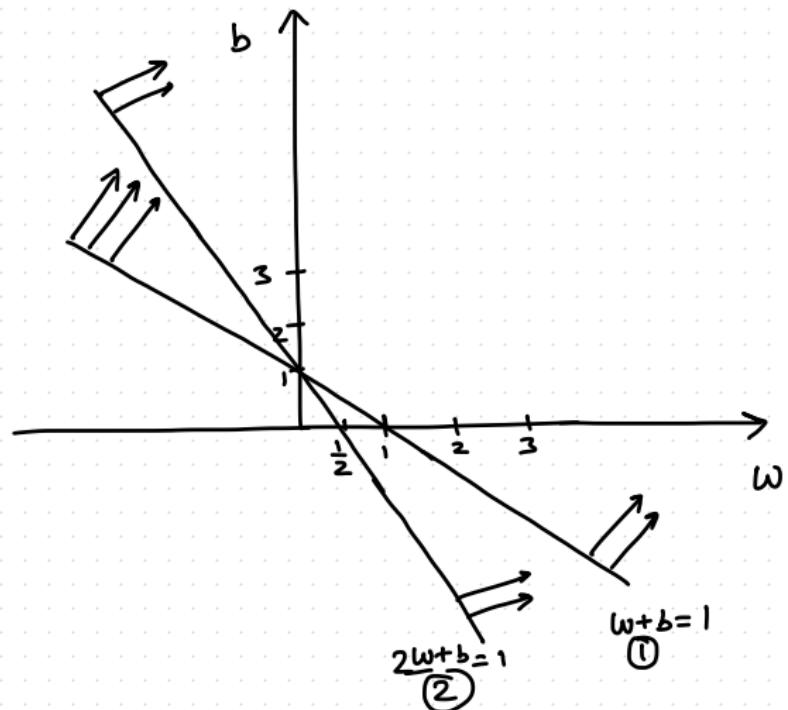
Simple Exercise

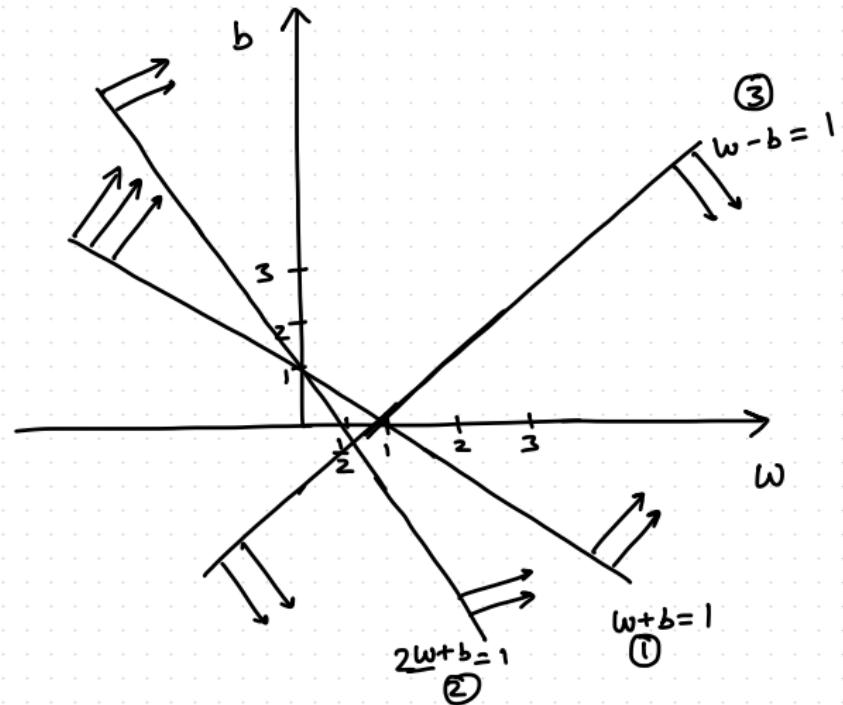
$$y_i(w_i x_i + b) \geq 1$$

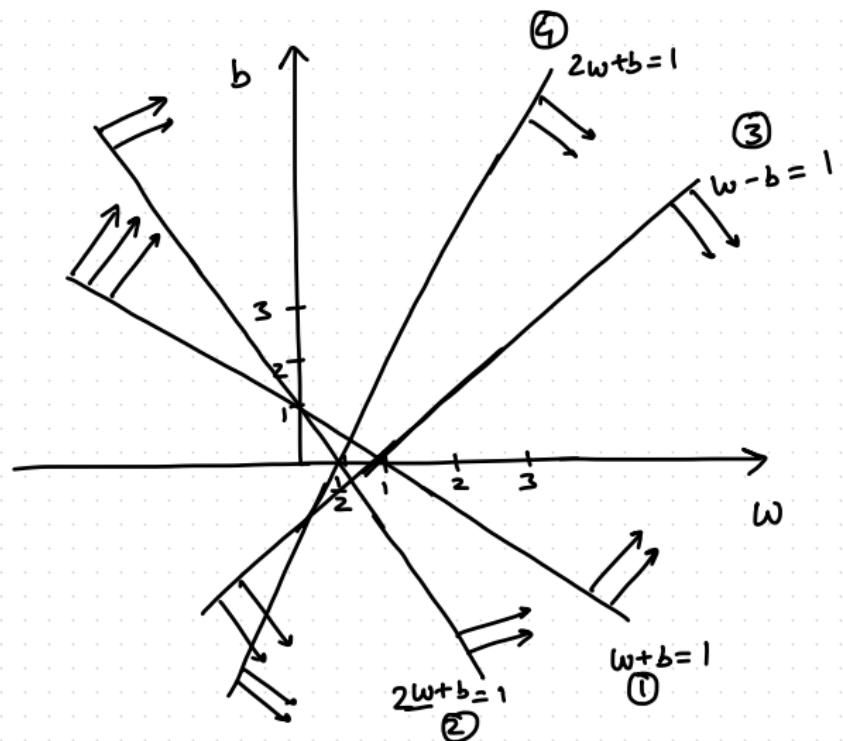
$$\begin{bmatrix} x_1 & y \\ 1 & 1 \\ 2 & 1 \\ -1 & -1 \\ -2 & -1 \end{bmatrix} \Rightarrow y_i(w_i x_i + b) \geq 1$$
$$\Rightarrow 1(w_1 + b) \geq 1$$
$$\Rightarrow 1(2w_1 + b) \geq 1$$
$$\Rightarrow -1(-w_1 + b) \geq 1$$
$$\Rightarrow -1(-2w_1 + b) \geq 1$$

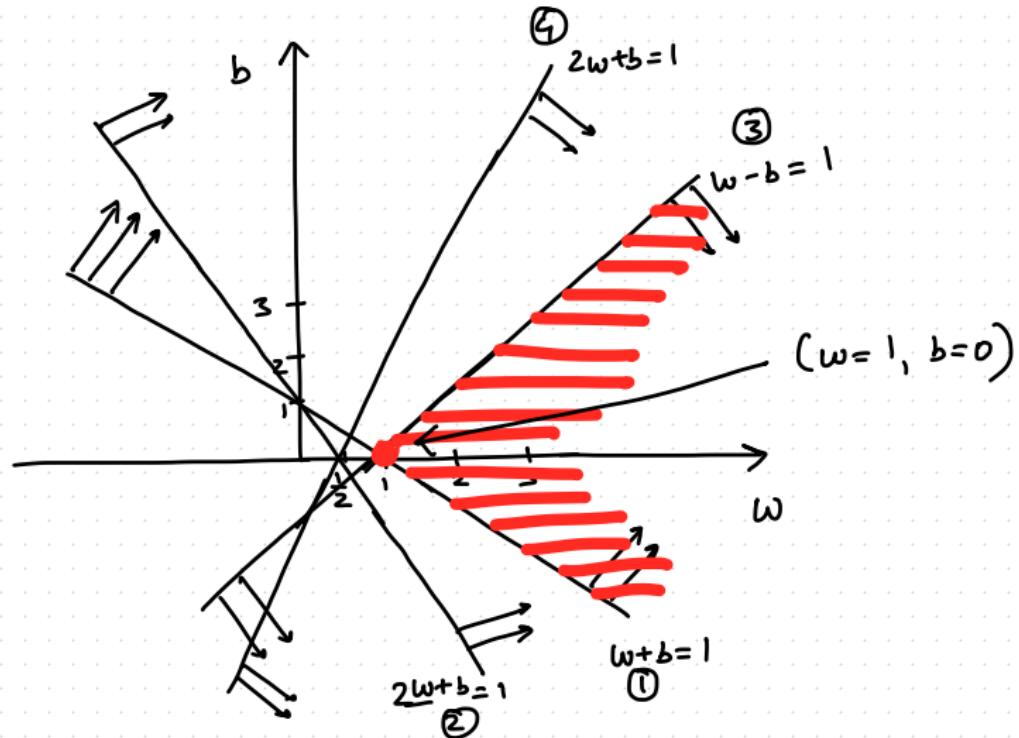












Simple Exercise

$$w_{min} = 1, b = 0$$

$$w.x + b = 0$$

$$x = 0$$

Simple Exercise

Minimum values satisfying constraints $\Rightarrow w = 1$ and $b = 0$
 \therefore Max margin classifier $\Rightarrow x = 0$

Primal Formulation is a Quadratic Program

Generally;

⇒ Minimize Quadratic(x)

⇒ such that, Linear(x)

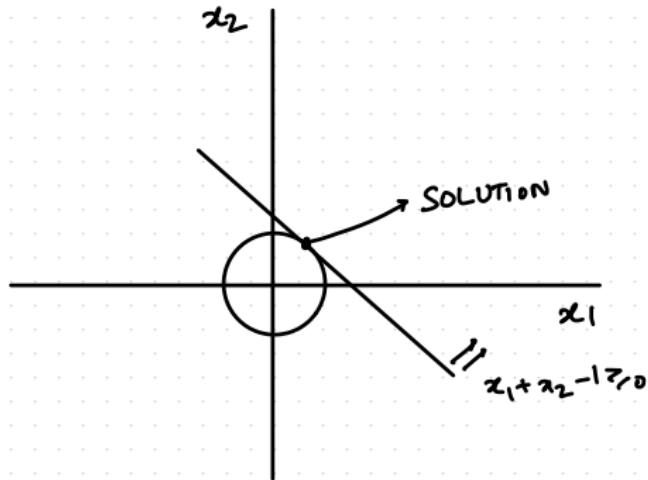
Question

$$x = (x_1, x_2)$$

$$\text{minimize } \frac{1}{2} ||x||^2$$

$$: x_1 + x_2 - 1 \geq 0$$

MINIMIZE QUADRATIC
S.T. LINEAR



Converting to Dual Problem

Primal \Rightarrow Dual Conversion using Lagrangian multipliers

$$\begin{aligned} & \text{Minimize } \frac{1}{2} \|\bar{w}\|^2 \\ & \text{s.t. } y_i(\bar{w} \cdot x_i + b) \geq 1 \\ & \quad \forall i \end{aligned}$$

$$L(\bar{w}, b, \alpha_1, \alpha_2, \dots, \alpha_n) = \frac{1}{2} \sum_{i=1}^d w_i^2 - \sum_{i=1}^N \alpha_i (y_i(\bar{w} \cdot \bar{x}_i + b) - 1) \quad \forall \alpha_i \geq 0$$

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^n \alpha_i y_i = 0$$

Converting to Dual Problem

$$\frac{\partial L}{\partial w} = 0 \Rightarrow \bar{w} - \sum_{i=1}^n \alpha_i y_i \bar{x}_i = 0$$

$$\bar{w} = \sum_{i=1}^N \alpha_i y_i \bar{x}_i$$

$$\begin{aligned} L(\bar{w}, b, \alpha_1, \alpha_2, \dots, \alpha_n) &= \frac{1}{2} \sum_{i=1}^d w_i^2 - \sum_{i=1}^N \alpha_i (y_i (\bar{w} \cdot \bar{x}_i + b) - 1) \\ &= \frac{1}{2} \|\bar{w}\|^2 - \sum_{i=1}^N \alpha_i y_i \bar{w} \cdot \bar{x}_i - \sum_{i=1}^N \alpha_i y_i b + \sum_{i=1}^N \alpha_i \\ &= \sum_{i=1}^N \alpha_i + \frac{(\sum_i \alpha_i y_i \bar{x}_i) (\sum_j \alpha_j y_j \bar{x}_j)}{2} - \sum_i \alpha_i y_i \left(\sum_j \alpha_j y_j \bar{x}_j \right) \bar{x}_i \end{aligned}$$

Converting to Dual Problem

$$L(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \bar{x}_i \cdot \bar{x}_j$$

Minimize $\|\bar{w}\|^2 \Rightarrow \text{Maximize } L(\alpha)$

s.t

$$y_i (\bar{w}, x_i + b) \geq 1 \quad \sum_{i=1}^N \alpha_i y_i = 0 \quad \forall \alpha_i \geq 0$$

Question

Question:

$$\alpha_i (y_i (\bar{w} \cdot \bar{x}_i + b) - 1) = 0 \quad \forall i \text{ as per KKT slackness}$$

What is α_i for support vector points?

Answer: For support vectors,

$$\bar{w} \cdot \bar{x}_i + b = -1 \text{ (+ve class)}$$

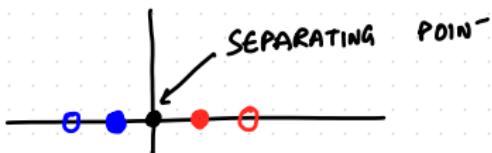
$$\bar{w} \cdot \bar{x}_i + b = +1 \text{ (+ve class)}$$

$$y_i (\bar{w} \cdot \bar{x}_i + b) - 1 = 0 \quad \text{for } i = \{\text{support vector points}\}$$

$$\therefore \alpha_i \text{ where } i \in \{\text{support vector points}\} \neq 0$$

For all non-support vector points $\alpha_i = 0$

EXAMPLE (IN 1D)



Revisiting the Simple Example

$$\begin{bmatrix} x_1 & y \\ 1 & 1 \\ 2 & 1 \\ -1 & -1 \\ -2 & -1 \end{bmatrix}$$

$$L(\alpha) = \sum_{i=1}^4 \alpha_i - \frac{1}{2} \sum_{i=1}^4 \sum_{j=1}^4 \alpha_i \alpha_j y_i y_j \bar{x}_i \bar{x}_j \quad \alpha_i \geq 0$$
$$\sum \alpha_i y_i = 0 \quad \alpha_i (y_i (\bar{w} \cdot \bar{x}_i + b) - 1) = 0$$

Revisiting the Simple Example

$$\begin{aligned} L(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = & \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 \\ & - \frac{1}{2} \{ \alpha_1 \alpha_1 \times (1 * 1) \times (1 * 1) \\ & + \\ & \alpha_1 \alpha_2 \times (1 * 1) \times (1 * 2) \\ & + \\ & \alpha_1 \alpha_3 \times (1 * -1) \times (1 * 1) \\ & \dots \\ & \alpha_4 \alpha_4 \times (-1 * -1) \times (-2 * -2) \} \end{aligned}$$

How to Solve? \Rightarrow Use the QP Solver!!

Revisiting the Simple Example

For the trivial example,

We know that only $x = \pm 1$ will take part in the constraint actively.

Thus, $\alpha_2, \alpha_4 = 0$

By symmetry, $\alpha_1 = \alpha_3 = \alpha$ (say)

$$\& \sum y_i \alpha_i = 0$$

$$L(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = 2\alpha$$

$$- \frac{1}{2} \{ \alpha^2(1)(-1)(1)(-1)$$

$$+ \alpha^2(-1)(1)(-1)(1)$$

$$+ \alpha^2(1)(1)(1)(1) + \alpha^2(-1)(-1)(-1)(-1)$$

}

$$\underset{\alpha}{\text{Maximize}} \quad 2\alpha - \frac{1}{2}(4\alpha^2)$$

Revisiting the Simple Example

$$\frac{\partial}{\partial \alpha} (2\alpha - 2\alpha^2) = 0 \Rightarrow 2 - 4\alpha = 0$$
$$\Rightarrow \alpha = 1/2$$

$$\therefore \alpha_1 = 1/2 \quad \alpha_2 = 0; \quad \alpha_3 = 1/2 \quad \alpha_4 = 0$$

$$\vec{w} = \sum_{i=1}^N \alpha_i y_i \bar{x}_i = 1/2 \times 1 \times 1 + 0 \times 1 \times 2$$
$$+ 1/2 \times -1 \times -1 + 0 \times -1 \times -2$$
$$= 1/2 + 1/2 = 1$$

Revisiting the Simple Example

Finding b:

For the support vectors we have,

$$y_i(\vec{w} \cdot \vec{x}_i + b) - 1 = 0$$

or, $y_i (\bar{w} \cdot \bar{x}_i + b) = 1$

or, $y_i^2 (\bar{w} \cdot \bar{x}_i + b) = y_i$

or, $\bar{w} \cdot \bar{x}_i + b = y_i \quad (\because y_i^2 = 1)$

or, $b = y_i - w \cdot x_i$

In practice, $b = \frac{1}{N_{SV}} \sum_{i=1}^{N_{SV}} (y_i - \bar{w} \cdot \bar{x}_i)$

Obtaining the Solution

$$\begin{aligned} b &= \frac{1}{2} \{(1 - (1)(1)) + (-1 - (1)(-1)) \\ &= \frac{1}{2} \{0 + 0\} = 0 \\ &= 0 \\ \therefore w &= 1 \quad \& \quad b = 0 \end{aligned}$$

Making Predictions

Making Predictions

$$\hat{y}(x_i) = \text{SIGN}(w \cdot x_i + b)$$

For $x_{test} = 3$; $\hat{y}(3) = \text{SIGN}(1 \times 3 + 0) = +ve$ class

Making Predictions

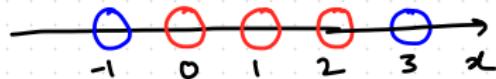
Alternatively,

$$\begin{aligned}\hat{y}(x_{TEST}) &= \text{SIGN}(\bar{w} \cdot \bar{x}_{TEST} + b) \\ &= \text{SIGN}\left(\sum_{i=1}^{N_S} \alpha_j y_j x_j \cdot x_{test} + b\right)\end{aligned}$$

In our example,

$$\alpha_1 = 1/2; \alpha_2 = 0; \alpha_3 = 1/2; \alpha_4 = 0$$

$$\begin{aligned}\hat{y}(3) &= \text{SIGN}\left(\frac{1}{2} \times 1 \times (1 \times 3) + 0 + \frac{1}{2} \times (-1) \times (-1 \times 3) + 0\right) \\ &= \text{SIGN}\left(\frac{6}{2}\right) = \text{SIGN}(3) = +1\end{aligned}$$



ORIGINAL DATA
IN R

Non-Linearly Separable Data

Non-Linearly Separable Data

Data not separable in \mathbb{R}

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Can we still use SVM?

Non-Linearly Separable Data

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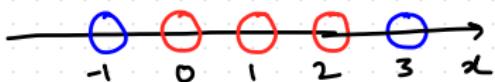
Non-Linearly Separable Data

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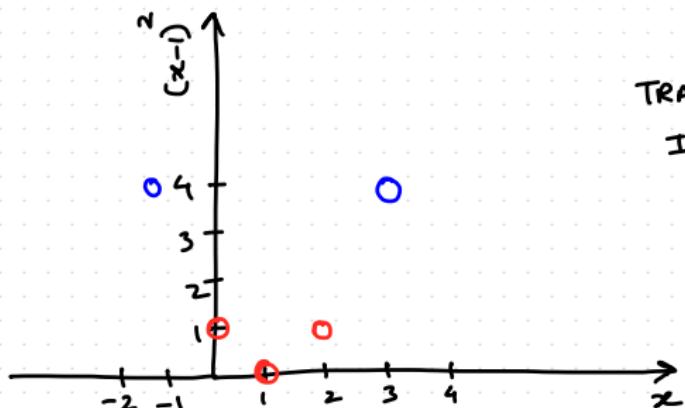
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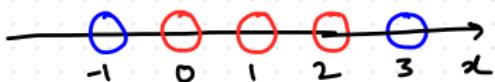
How? Project data to a higher dimensional space.



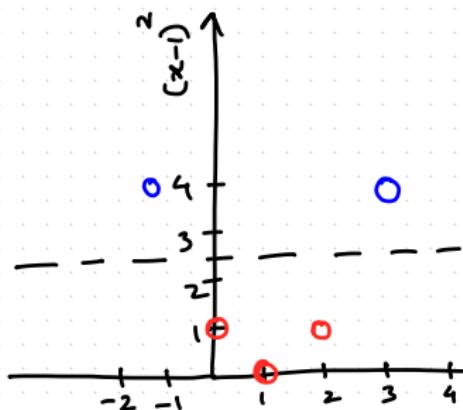
ORIGINAL DATA
IN \mathbb{R}



TRANSFORMED DATA
IN \mathbb{R}^2

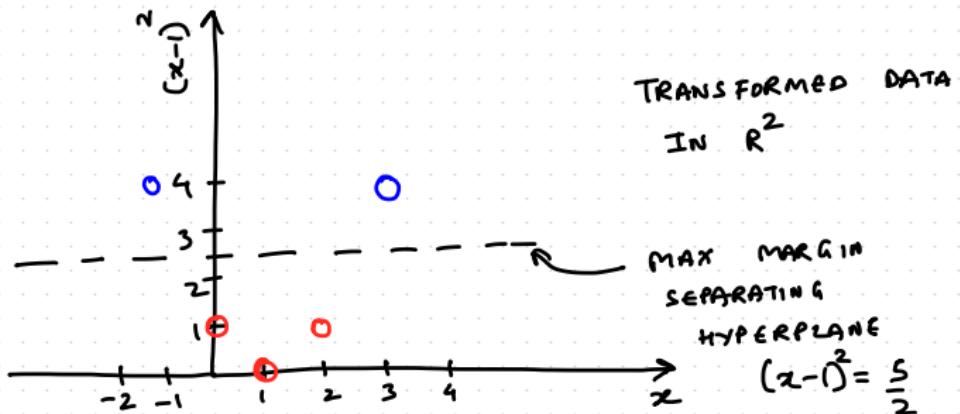
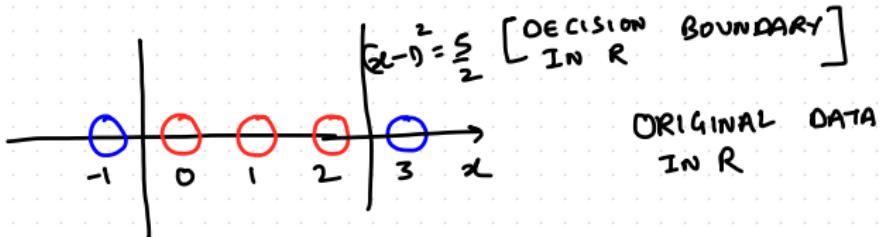


ORIGINAL DATA
IN \mathbb{R}

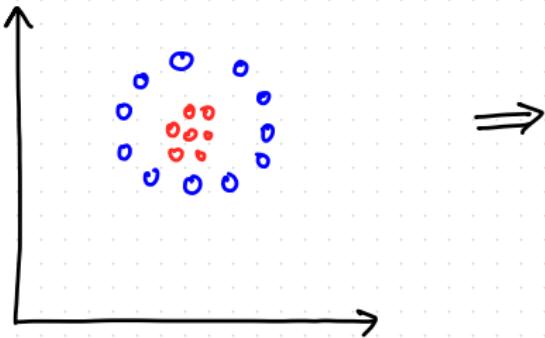


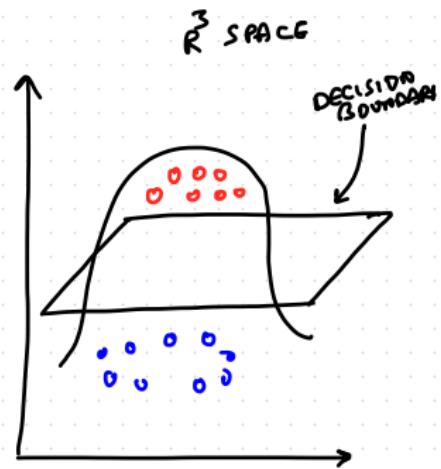
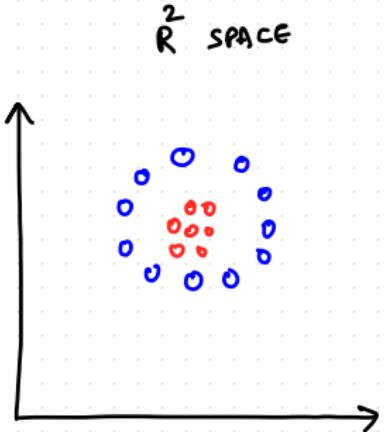
TRANSFORMED DATA
IN \mathbb{R}^2

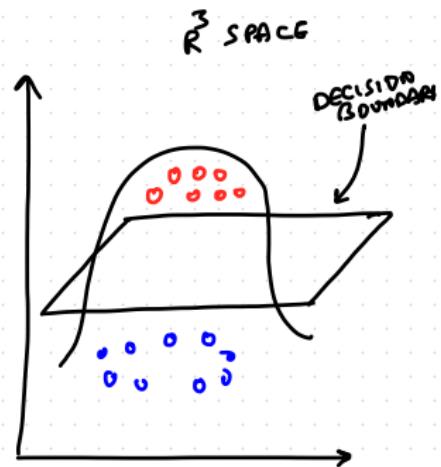
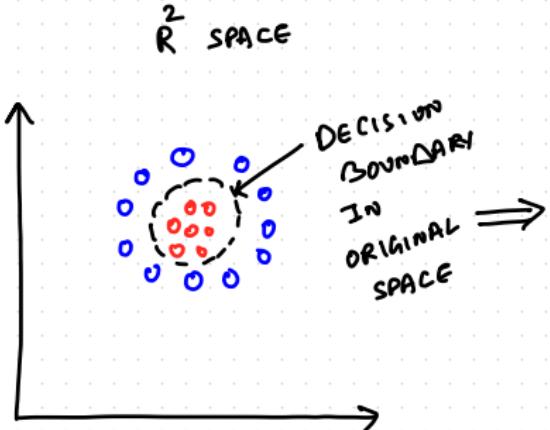
MAX MARGIN
SEPARATING
HYPERPLANE
 $(x-1)^2 = \frac{5}{2}$

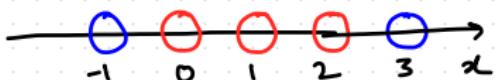


\mathbb{R}^2 SPACE

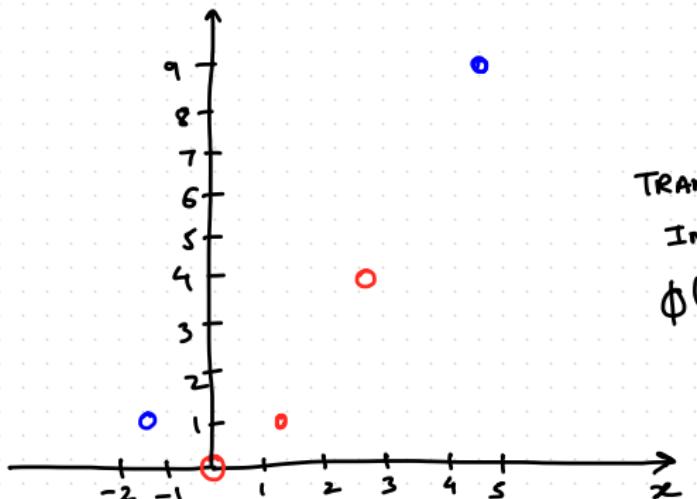






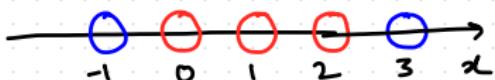


ORIGINAL DATA
IN \mathbb{R}

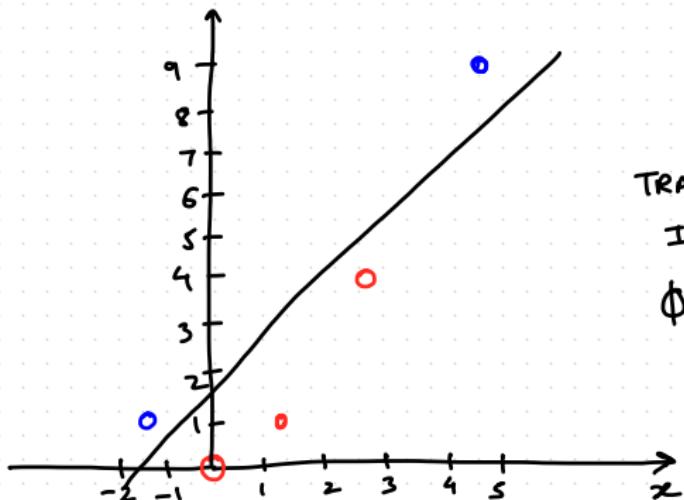


TRANSFORMED DATA
IN \mathbb{R}^2

$$\phi(x) = \begin{bmatrix} \sqrt{2}x \\ x^2 \end{bmatrix}$$

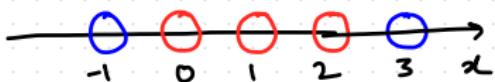


ORIGINAL DATA
IN \mathbb{R}

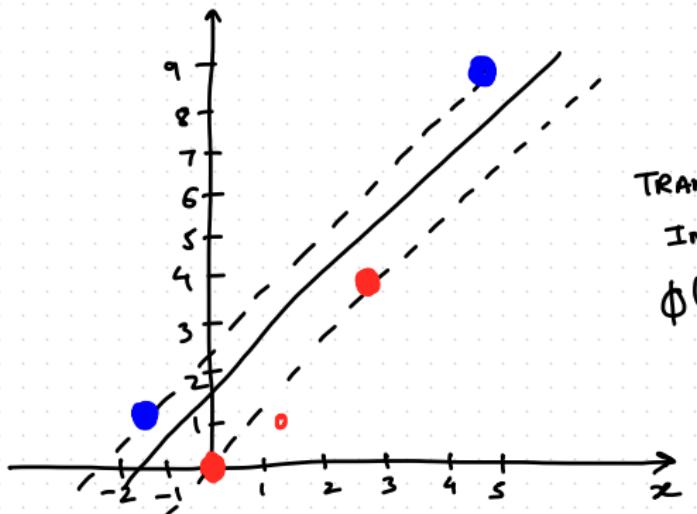


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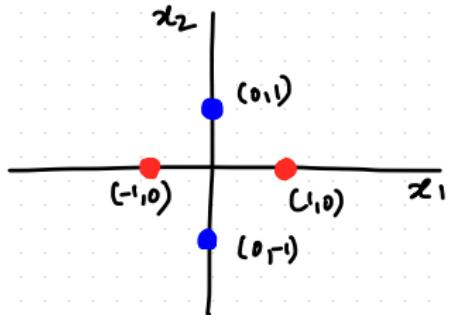


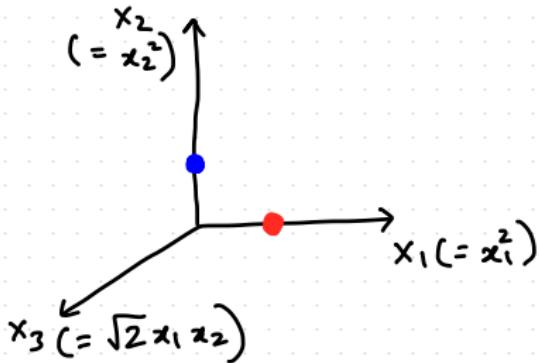
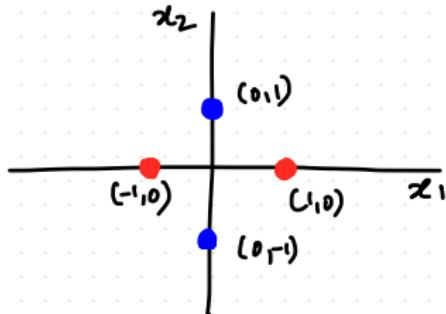
ORIGINAL DATA
IN R

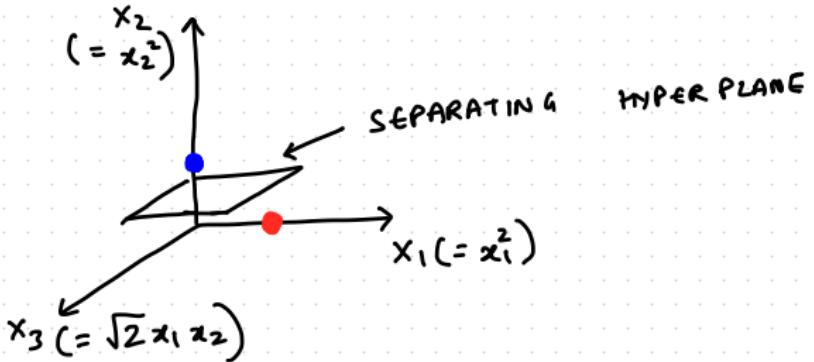
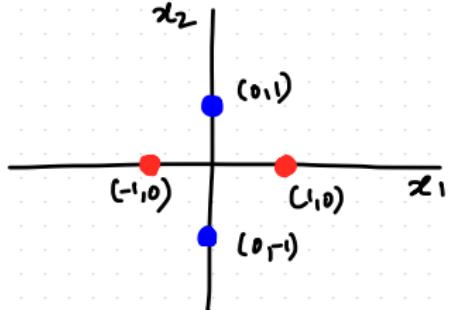


TRANSFORMED DATA
IN R^2

$$\phi(x) = \begin{bmatrix} \sqrt{2}x \\ x^2 \end{bmatrix}$$







Linear SVMs in higher dimensions

Linear SVM:

Maximize

$$L(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \bar{x}_i \cdot \bar{x}_j$$

such that constraints are satisfied.



Transformation (ϕ)



$$L(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \phi(\bar{x}_i) \cdot \phi(\bar{x}_j)$$

Linear SVMs in higher dimensions: Steps

1. Compute $\phi(x)$ for each point

$$\phi : \mathbb{R}^d \rightarrow \mathbb{R}^D$$

2. Compute dot products over \mathbb{R}^D space

Q. If $D \gg d$

Both steps are expensive!

Kernel Trick

Kernel Trick

- Can we compute $K(\bar{x}_i, \bar{x}_j)$, such that

Kernel Trick

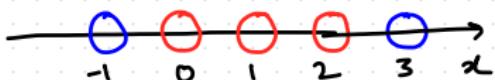
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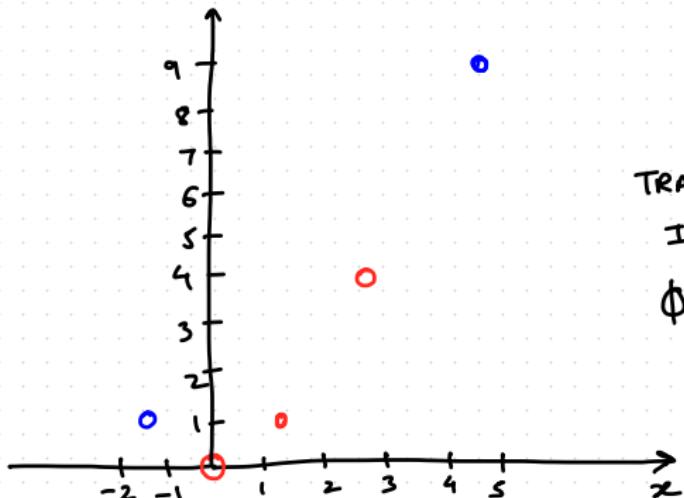
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- $K(\bar{x}_i, \bar{x}_j)$ is some function of dot product in original dimension
- $\phi(\bar{x}_i).\phi(\bar{x}_j)$ is dot product in high dimensions (after transformation)



ORIGINAL DATA
IN R

KERNEL
TRICK



TRANSFORMED DATA
IN R^2

$$\phi(x) = \begin{bmatrix} \sqrt{2}x \\ x^2 \end{bmatrix}$$

KERNEL TRICK

$$\phi(x) = \begin{bmatrix} \sqrt{2}x \\ x^2 \end{bmatrix}$$

$$K(x_i, x_j) = ?$$

KERNEL TRICK

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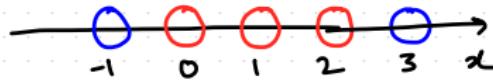
$$K(x_i, x_j) = (1 + x_i \cdot x_j)^2 - 1$$

KERNEL TRICK

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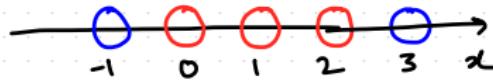
$$K(x_i, x_j) = (1 + x_i \cdot x_j)^2 - 1$$

$$\begin{aligned}(1 + x_i \cdot x_j)^2 - 1 &= 1 + 2x_i \cdot x_j + x_i^2 x_j^2 - 1 \\&= 2x_i \cdot x_j + x_i^2 x_j^2 \\&= (\sqrt{2}x_i \cdot \sqrt{2}x_j + x_i^2 \cdot x_j^2) \\&= \langle \sqrt{2}x_i, x_i^2 \rangle \cdot \langle \sqrt{2}x_j, x_j^2 \rangle \\&= \phi(x_i) \cdot \phi(x_j)\end{aligned}$$



ORIGINAL DATASET

x	y
-1	-1
0	1
1	1
2	1
3	-1

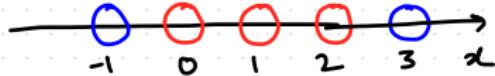


ORIGINAL DATASET

x	y
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TRANSFORMED DATASET

x	$\sqrt{2}x$	x^2	y
-1	$-\sqrt{2}$	1	-1
0	0	0	1
1	$\sqrt{2}$	1	1
2	$2\sqrt{2}$	4	1
3	$3\sqrt{2}$	9	-1



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Calculation w/o Kernel Trick

$$\phi(x_1) = \langle \sqrt{2}x, x^2 \rangle : 2$$

$$\phi(x_2) = \langle \sqrt{2}x, x^2 \rangle : 2$$

$$\phi(x_1) \cdot \phi(x_2) = 2 \text{ MULTPLICATION} + 1 \text{ ADDITION}$$

7



ORIGINAL DATASET

x	y
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TRANSFORMED DATASET

x	$\sqrt{2}x$	x^2	y
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Calculation with Kernel Trick

$$K(x_1, x_2) = (1 + x_1 \cdot x_2)^2 - 1$$

$$x_1 \cdot x_2 \rightarrow 1$$

$$1 + x_1 \cdot x_2 \rightarrow 1$$

$$\begin{aligned} (1 + x_1 \cdot x_2)^2 &\rightarrow 1 \\ (1 + x_1 \cdot x_2) - 1 &\rightarrow 1 \end{aligned}$$

} 4

Kernel Trick

Q) Why did we use dual form?

Kernel Trick

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Kernels again!!

Kernel Trick

Q) Why did we use dual form?

Kernels again!!

Primal form doesn't allow for the kernel trick $K(\bar{x}_1, \bar{x}_2)$ in dual and compute $\phi(x)$ and then dot product in D dimensions

Some Kernels

1. Linear: $K(\bar{x}_1, \bar{x}_2) = \bar{x}_1 \bar{x}_2$
2. Polynomial: $K(\bar{x}_1, \bar{x}_2) = (p + \bar{x}_1 \bar{x}_2)^q$
3. Gaussian: $K(\bar{x}_1, \bar{x}_2) = e^{-\gamma ||\bar{x}_1 - \bar{x}_2||^2}$ where $\gamma = \frac{1}{2\sigma^2}$ - Also called Radial Basis Function (RBF)

Kernels

Q) For $\bar{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ what space does kernel $K(\bar{x}, \bar{x}') = (1 + \bar{x}\bar{x}')^3$ belong to?

$$\bar{x} \in \mathbb{R}^2$$

$$\phi(\bar{x}) \in \mathbb{R}^?$$

$$K(x, z) = (1 + x_1 z_1 + x_2 z_2)^3$$

$$= \dots$$

$$= <1, x_1, x_2, x_1^2, x_2^2, x_1^2 x_2, x_1 x_2^2, x_1^3, x_2^3, x_1 x_2>$$

10 dimensional?

Does RBF involve dot product in lower-dimensional space?

Assuming x is a one-dimensional vector, we can rewrite the RBF kernel as:

$$K(x, z) = e^{-\gamma \|x-z\|^2} = e^{-\gamma(x-z)^2}$$

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Notice that the term $e^{2\gamma xz}$ is a dot product of the original data points x and z in the one-dimensional feature space.

What space does the RBF kernel lie in?

Q) For $\bar{x} = x$; what space does RBF kernel lie in?

$$\begin{aligned} K(x, z) &= e^{-\gamma||x-z||^2} \\ &= e^{-\gamma(x-z)^2} \end{aligned}$$

Now:

$$e^\alpha = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}$$

$\therefore e^{-\gamma(x-z)^2}$ is ∞ dimensional!!

Interpretation of RBF

- $\hat{y}(x) = \text{sign}(\sum_{i=1}^n \alpha_i y_i K(x, x_i) + b)$

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- $-\|x - x_i\|^2$ corresponds to radial term

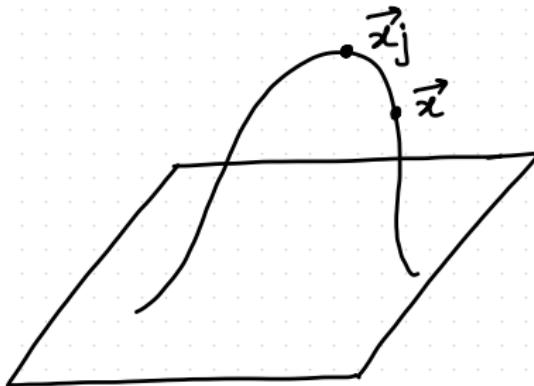
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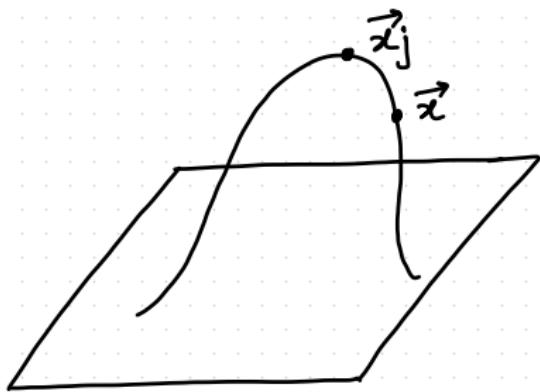
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- $-\|x - x_i\|^2$ corresponds to radial term
- $\sum \alpha_i y_i$ is the activation component
- $e^{-\|x - x_i\|^2}$ is the basis component

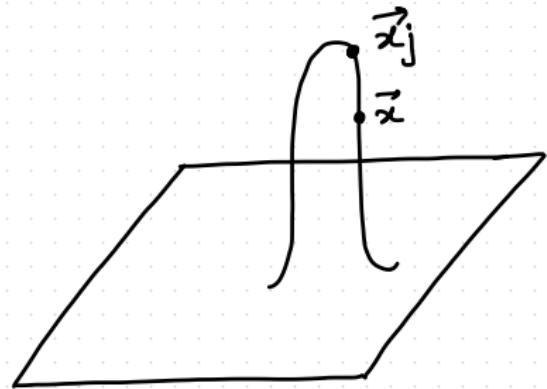
RBF INTERPRETATION



RBF INTERPRETATION



LOW γ
HIGH INFLUENCE OF \vec{x}_j



HIGH γ
LOW INFLUENCE OF \vec{x}_j