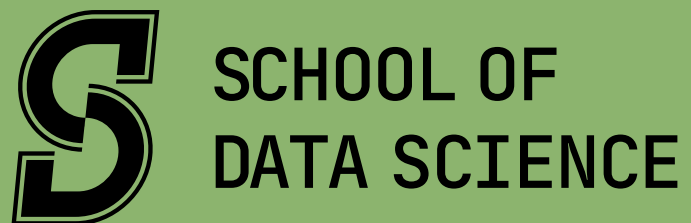


# Statistical Learning STA4042



## DECISION BOUNDARIES



## Linear and non-linear decision

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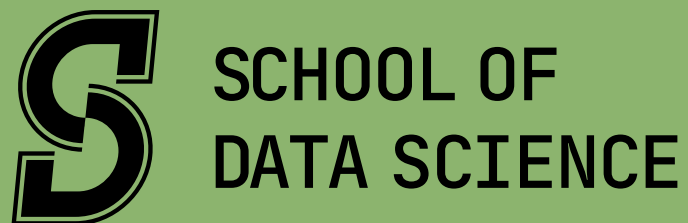
Concerns Unsupervised and Supervised learning

Although more pictural with Classification also concerns Regression

# Statistical Learning STA4042



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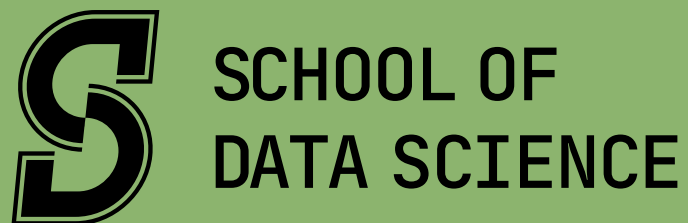
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# Statistical Learning STA4042



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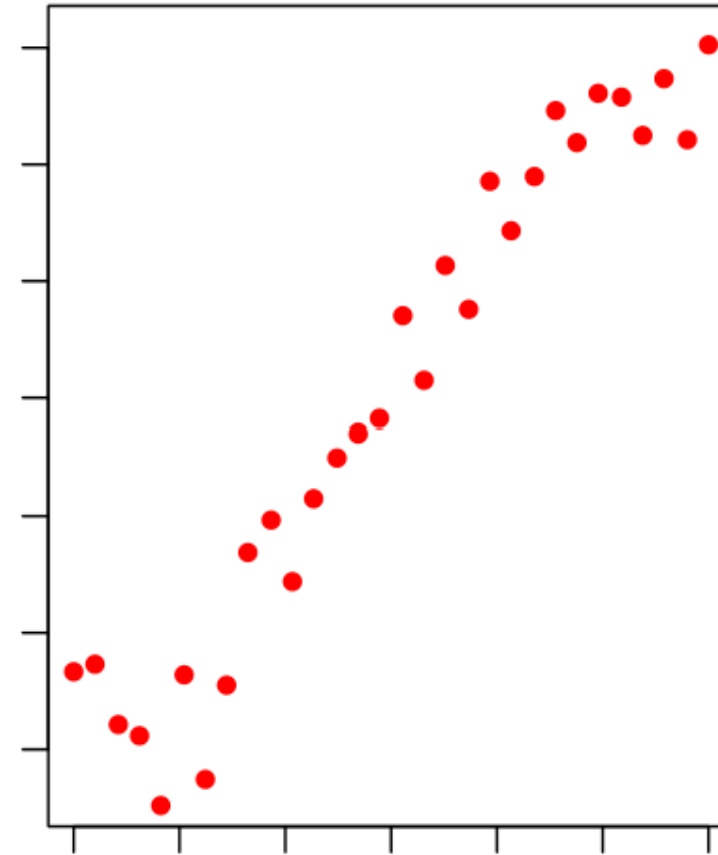
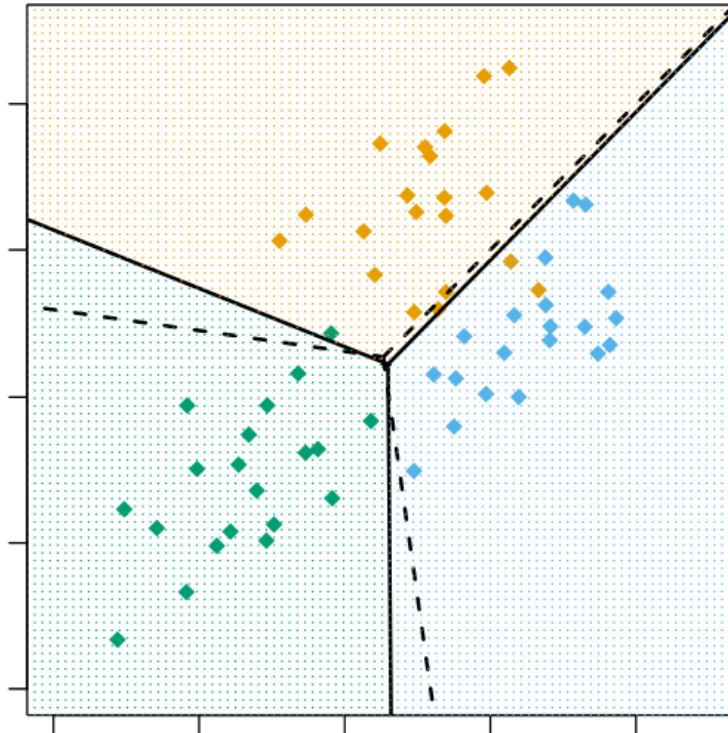
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Examples of non-linear decisions:

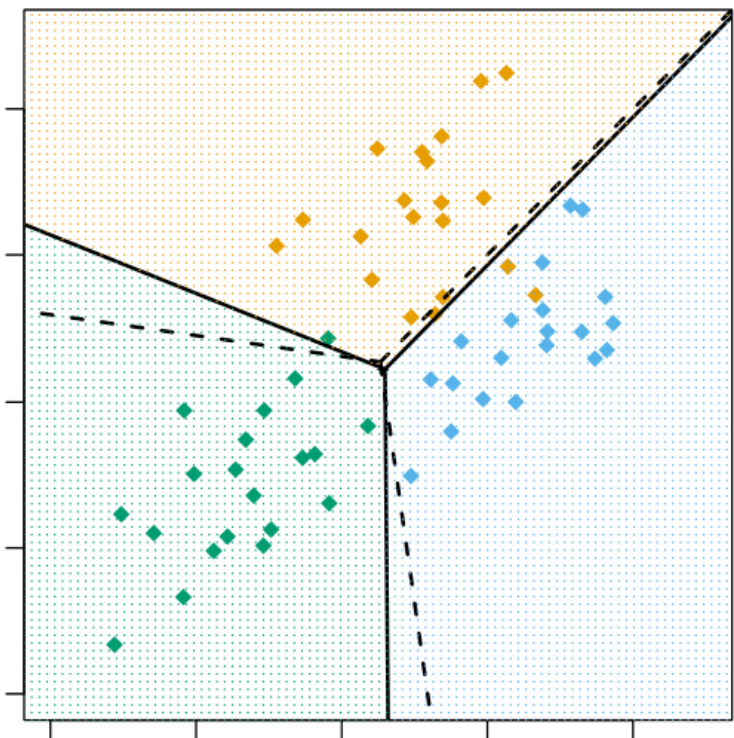
- K nearest neighbour
- QDA, Polynomial fits.
- k-means
- Kernel methods (spectral clustering, SVM)
- Neural networks

# Linear and non-linear decision

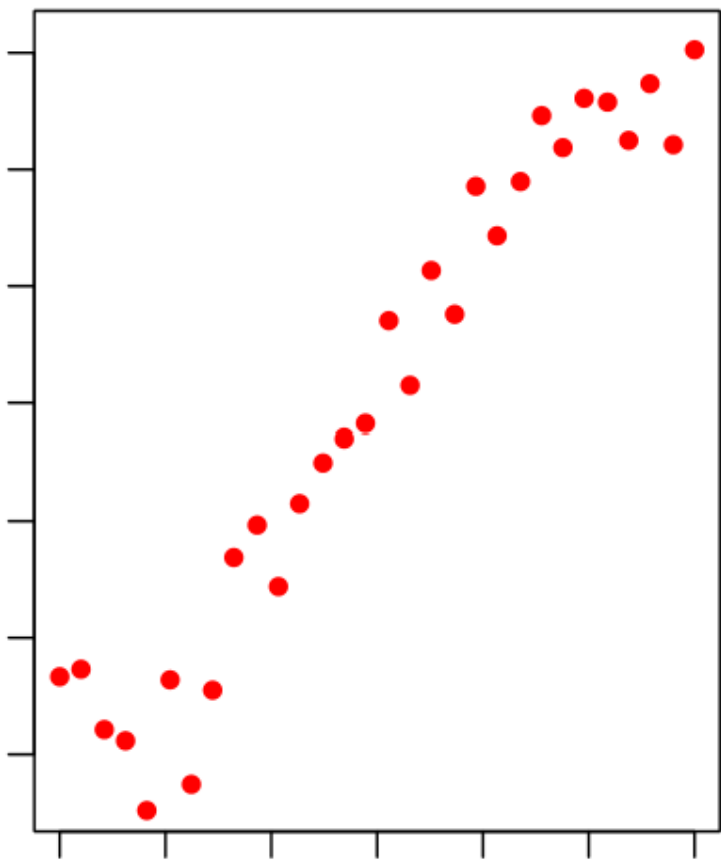


Linear Decisions

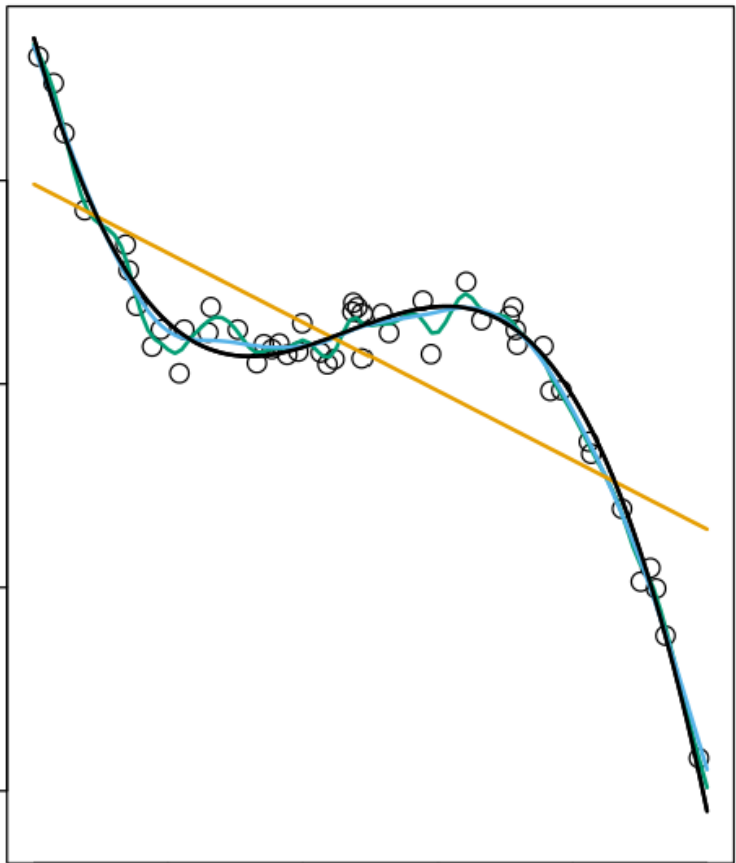
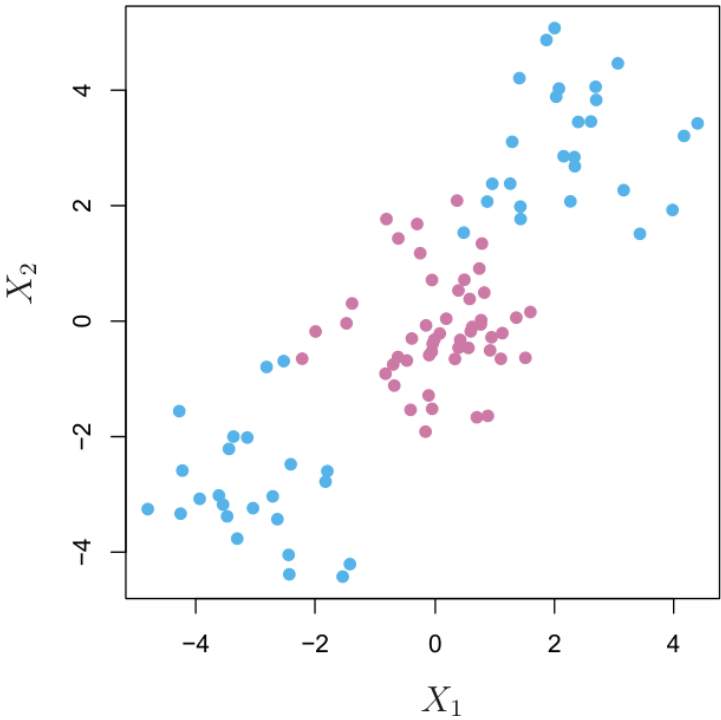
# Linear and non-linear decision



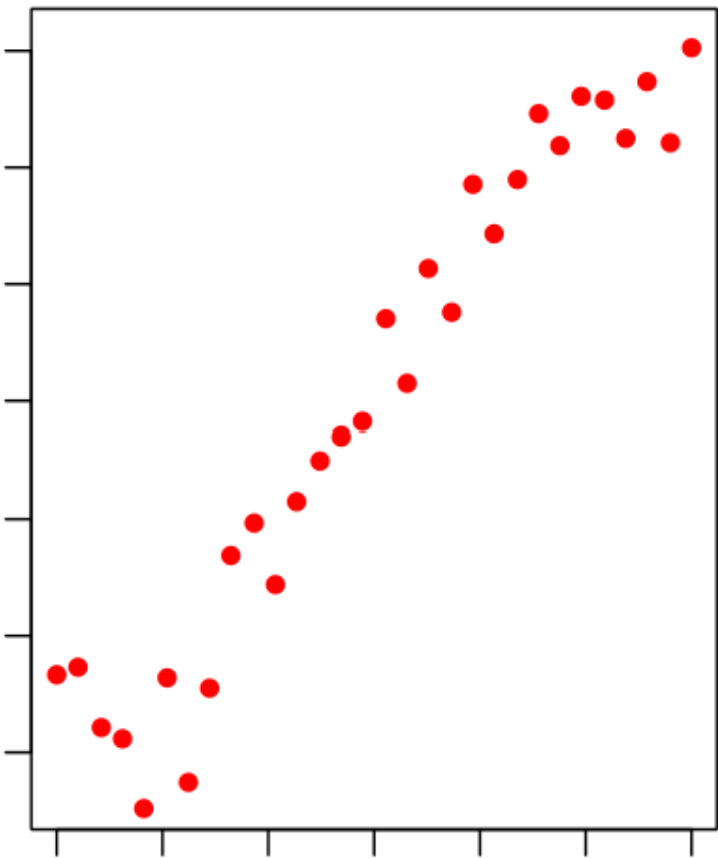
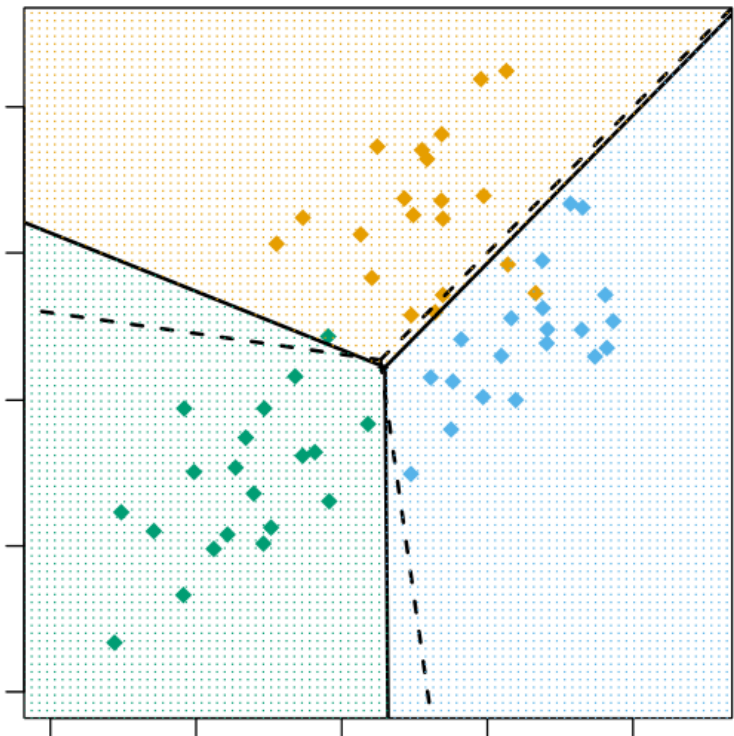
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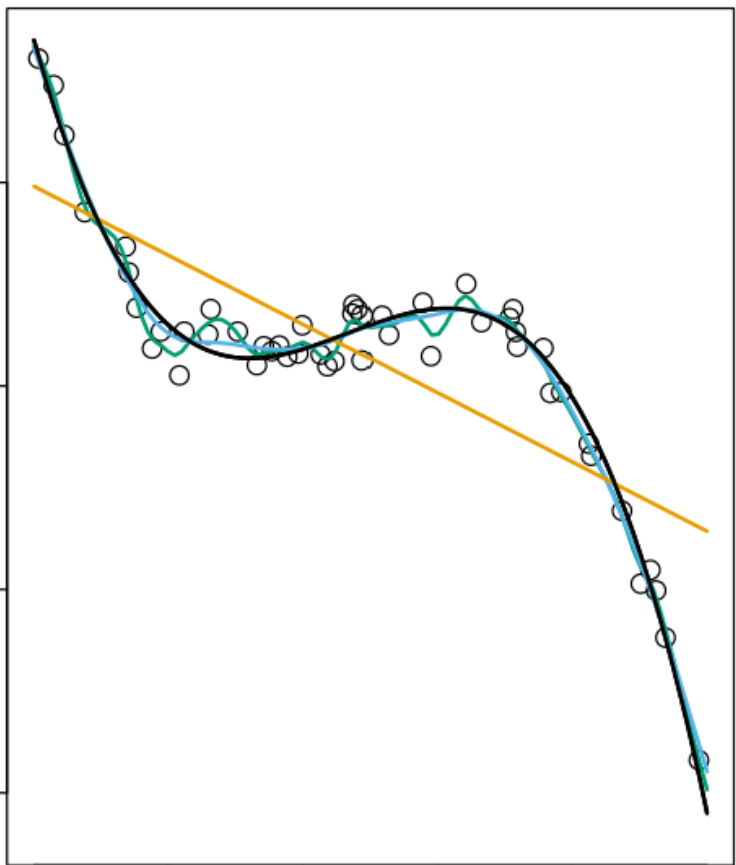
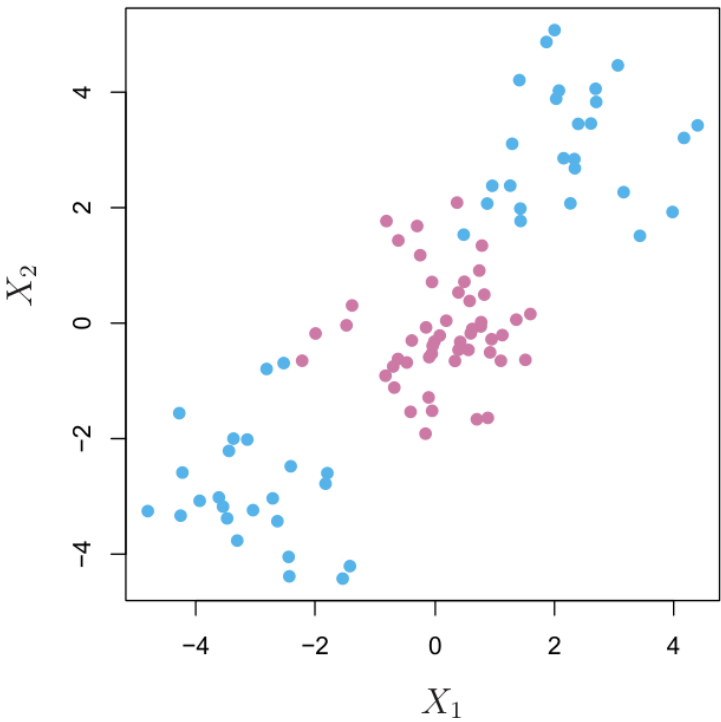
Non-linear decisions



# Linear and non-linear decision



Non-linear decisions

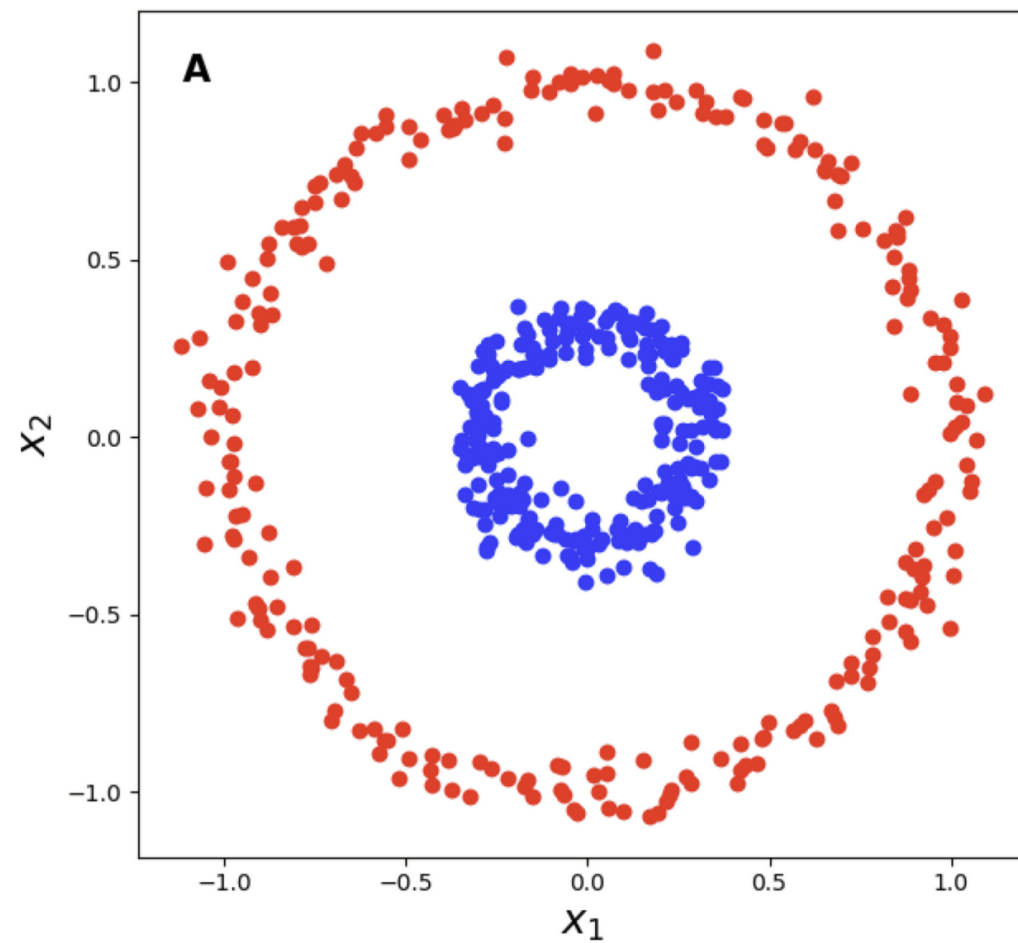


Linear Decisions

Question even more important with bigger dimension

# How to deal with non linear boundaries ? (*Classification or regression*)

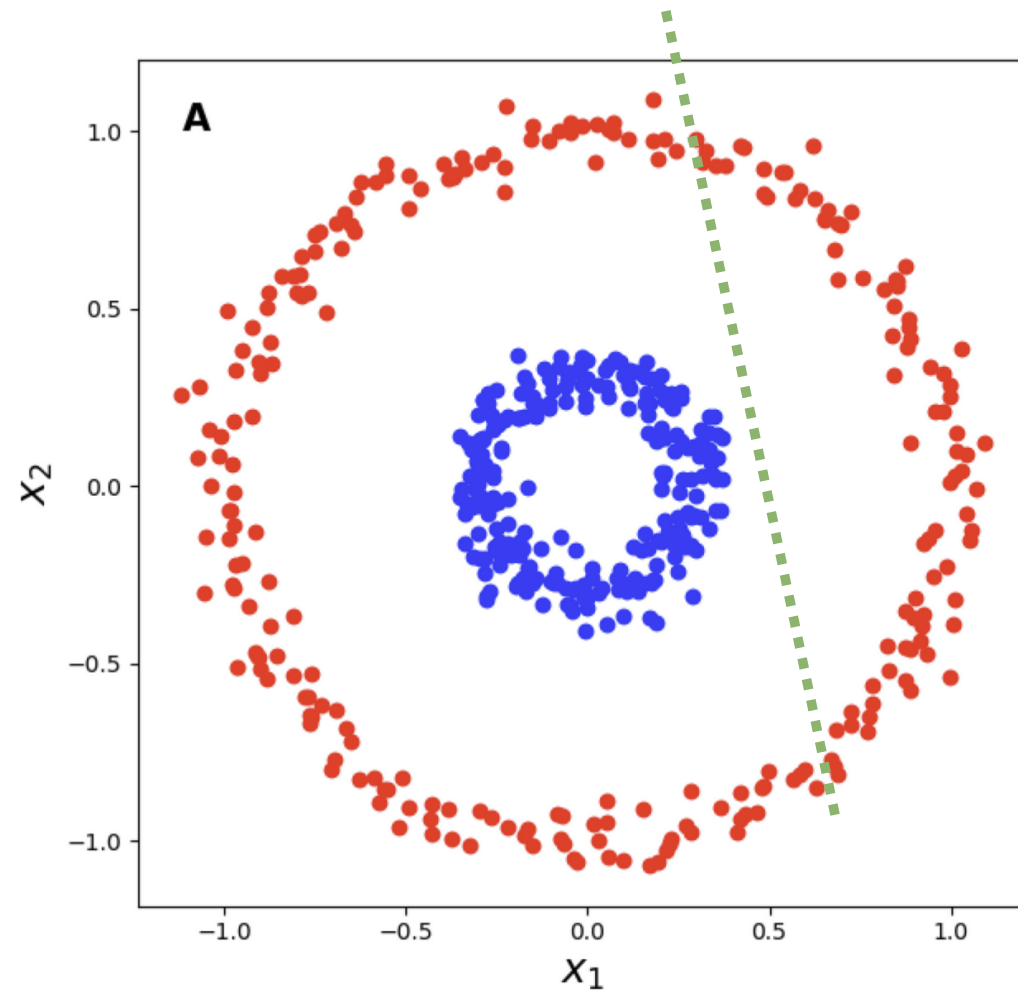
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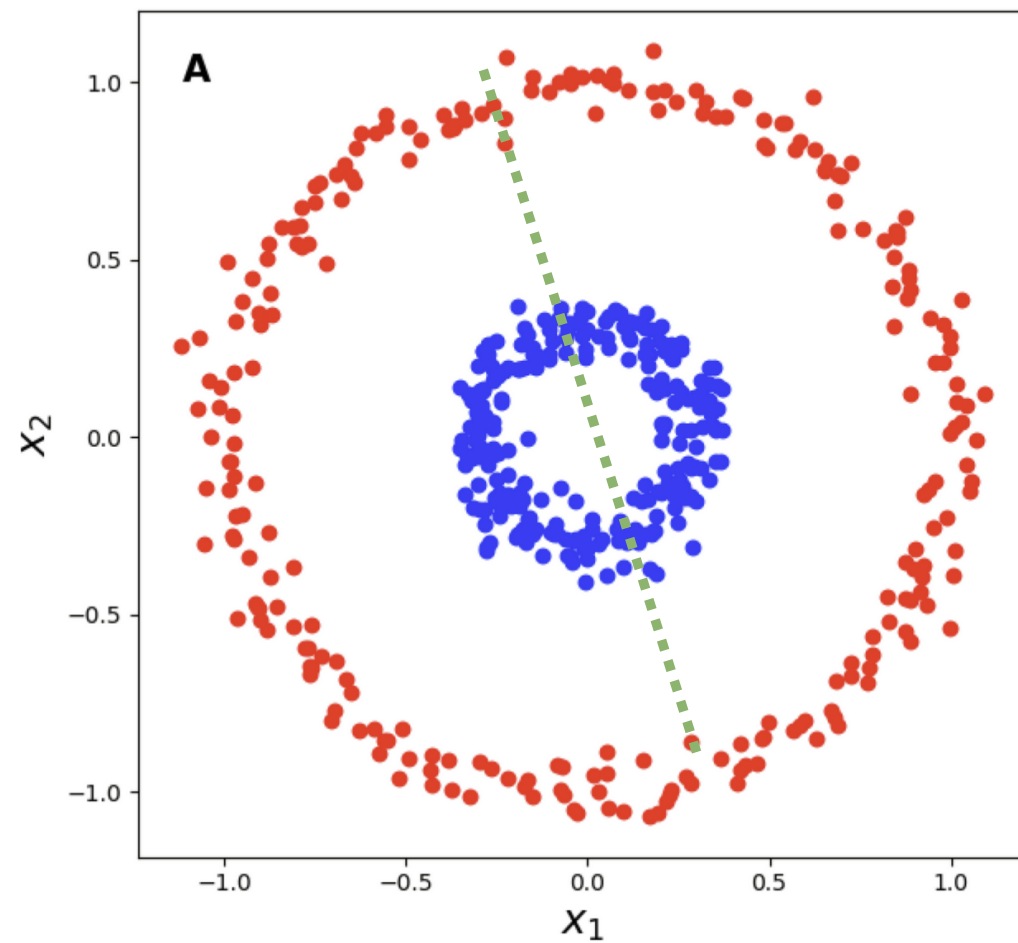
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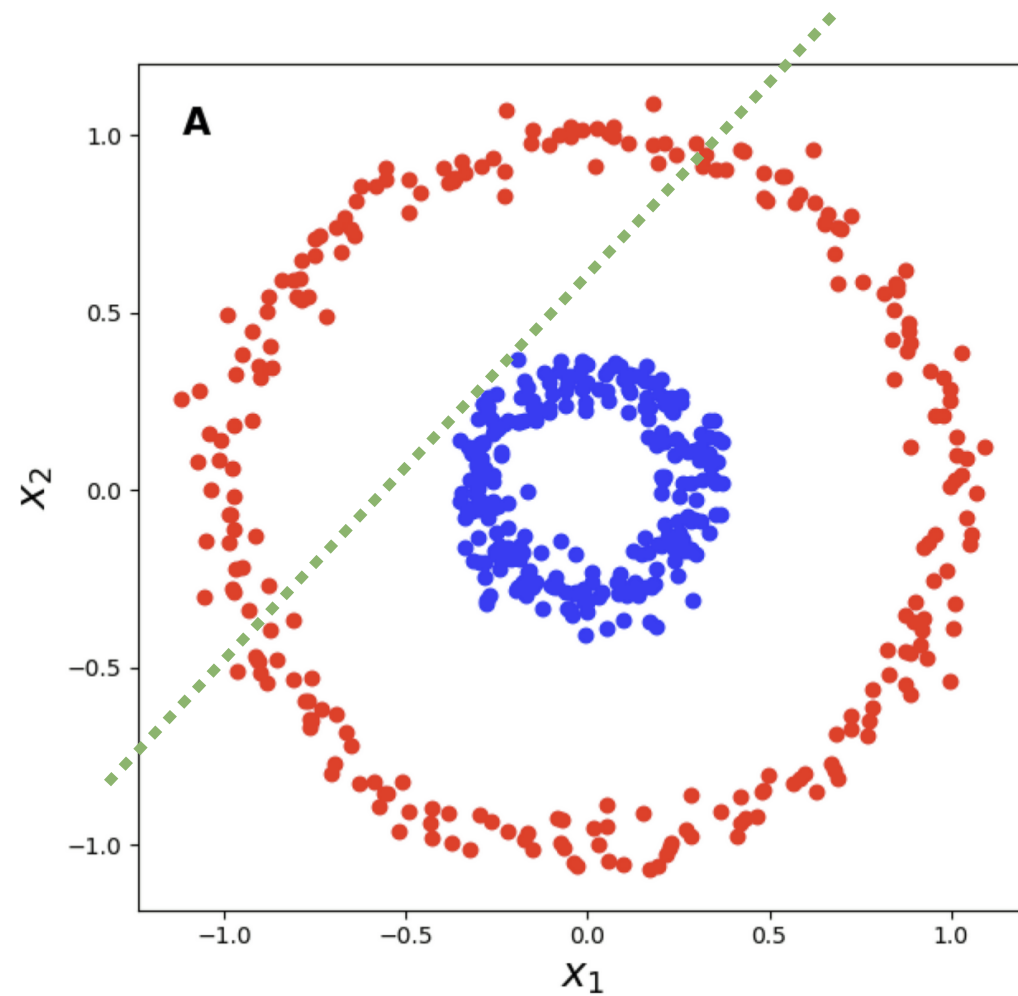
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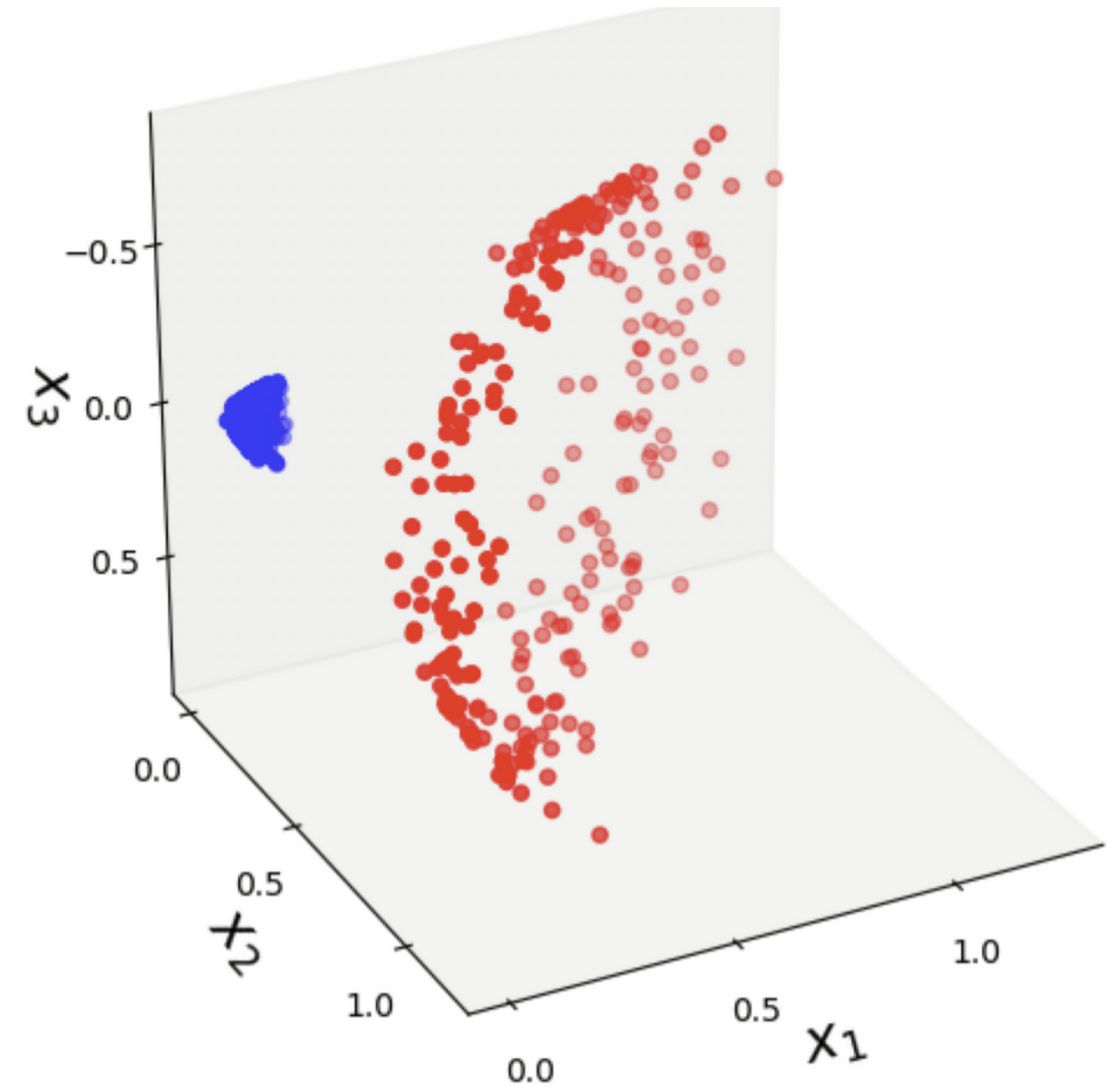
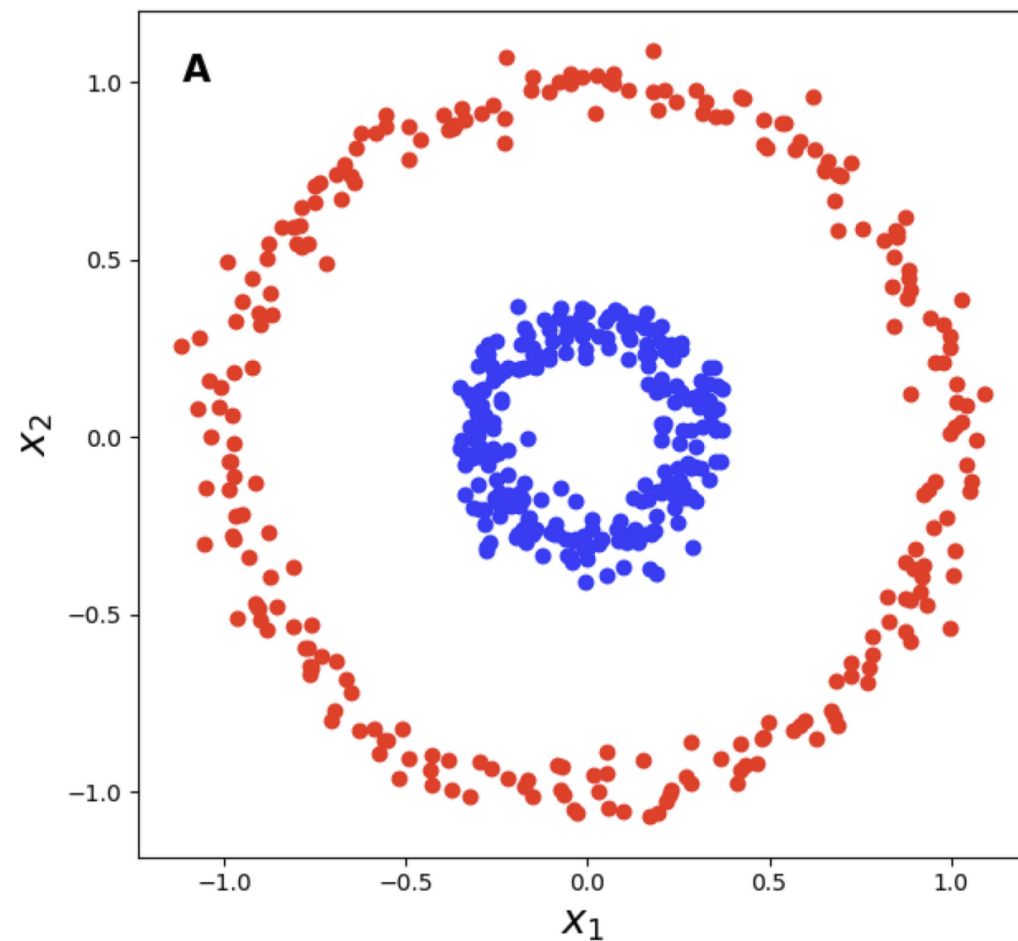
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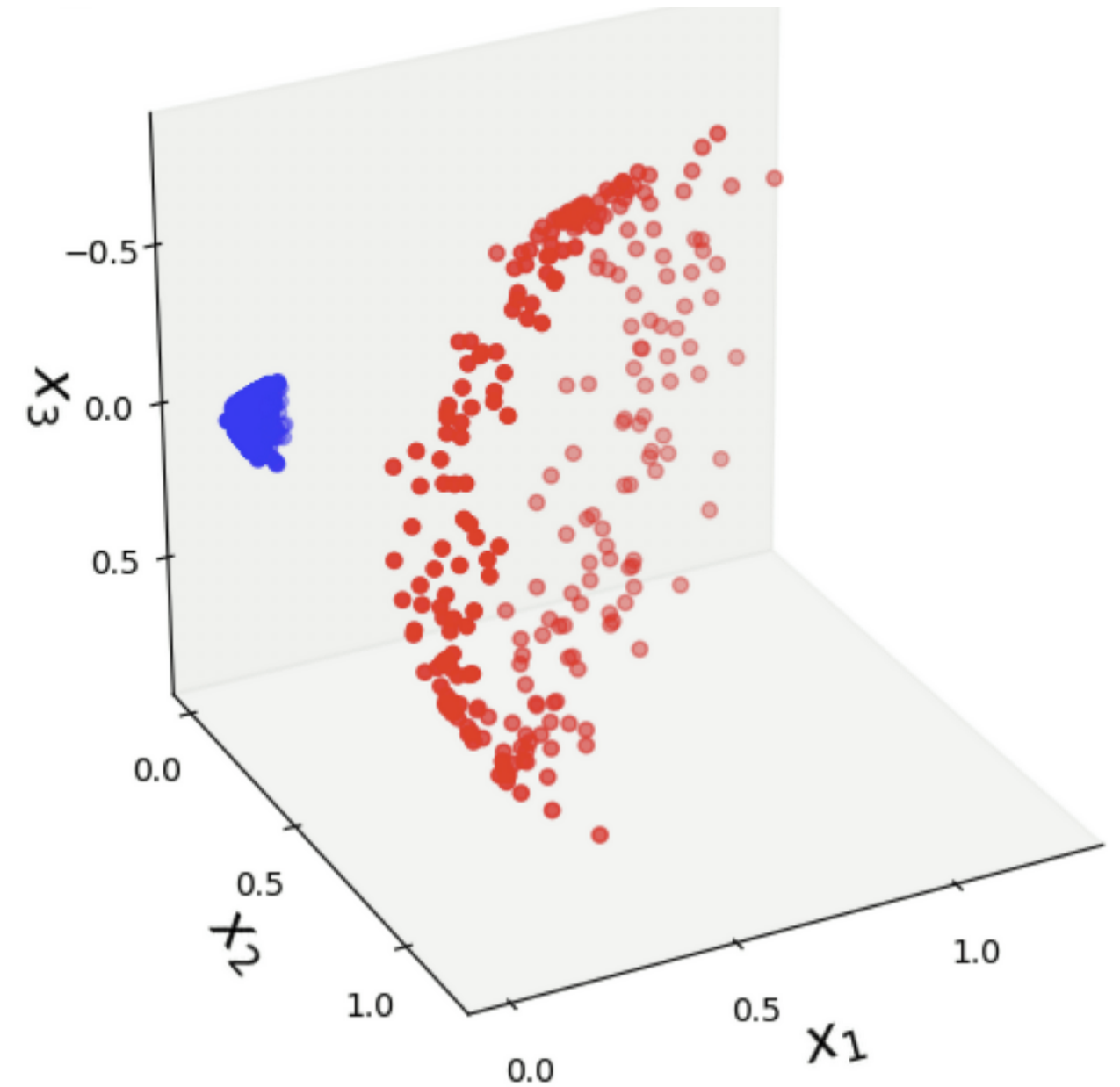
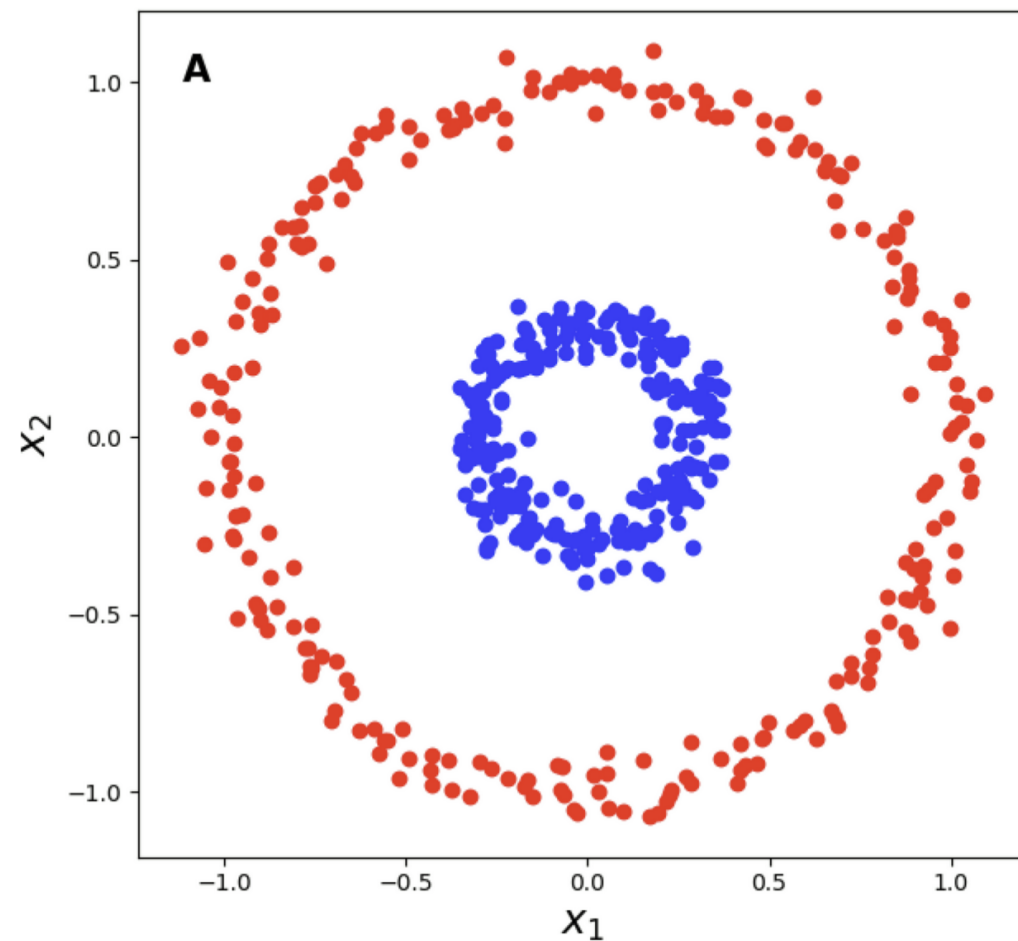
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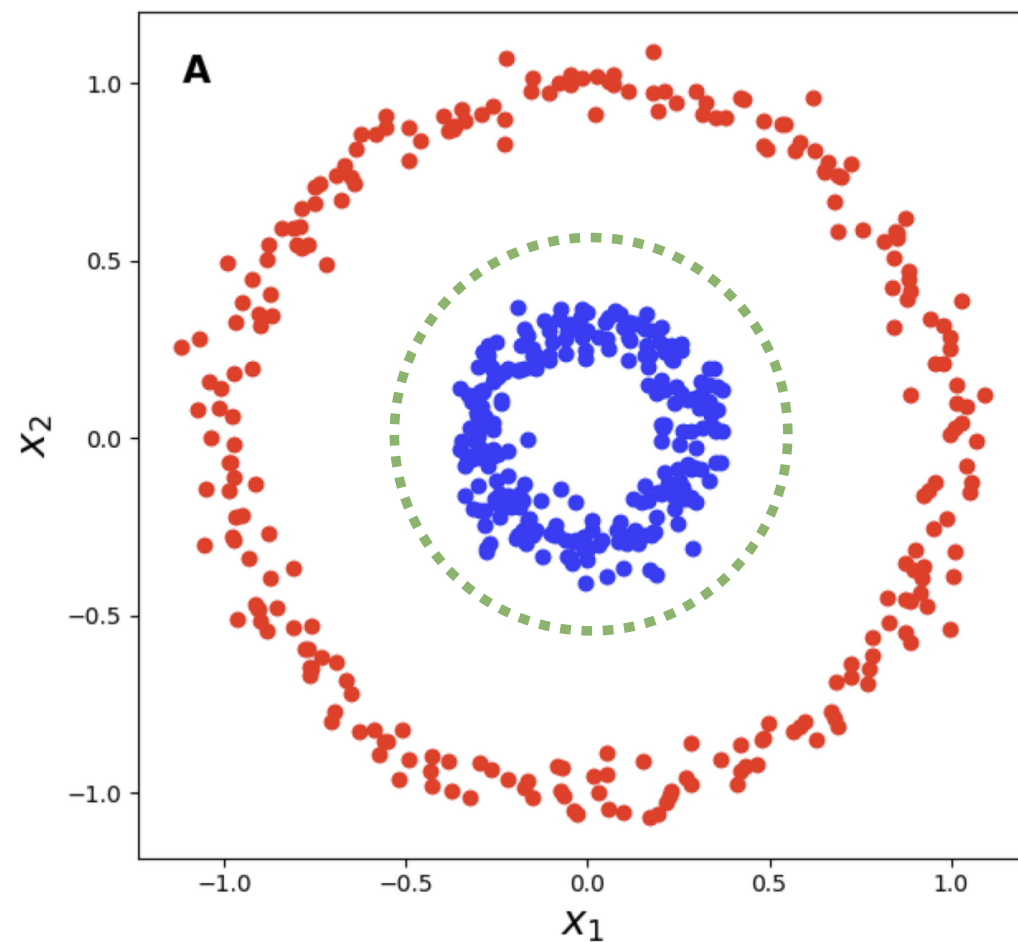
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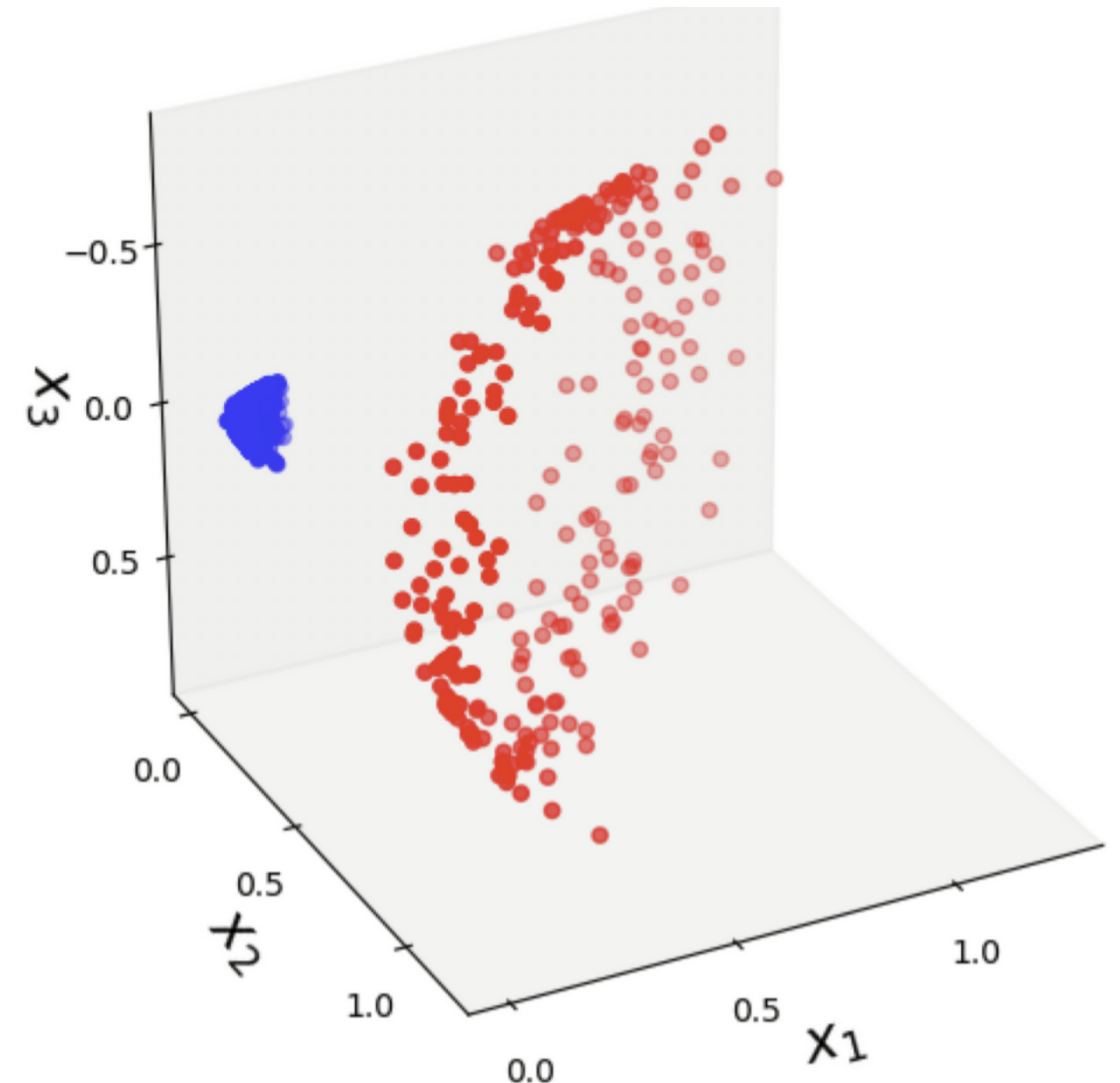
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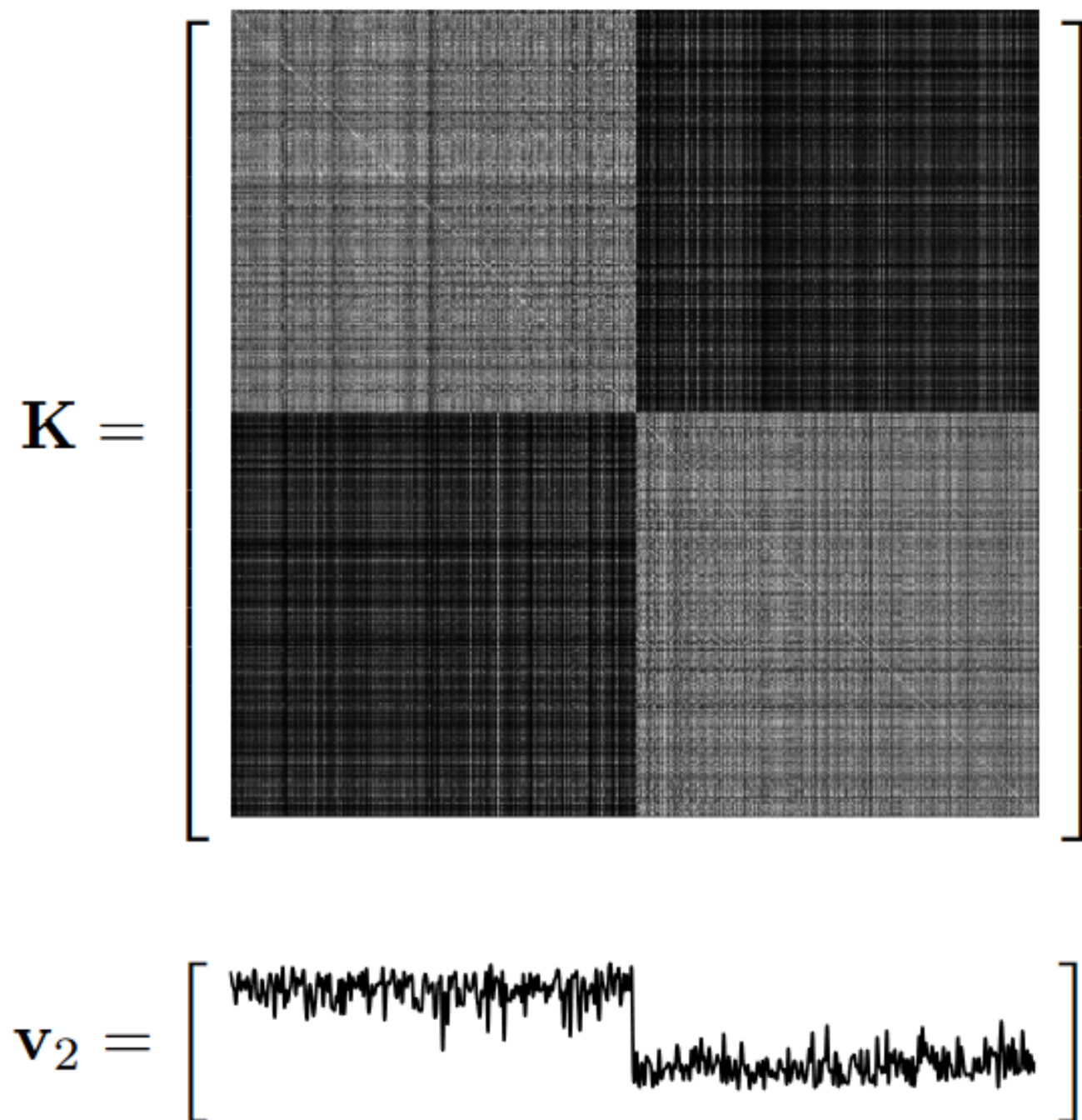


- Use flexible method (NN, KNN, k-means, kernel-based methods..)





# Recall: Spectral clustering



Two classes:

- $x_1, \dots, x_{n/2} \sim \mathcal{N}(\mu, I_p)$
- $x_{n/2+1}, \dots, x_n \sim \mathcal{N}(-\mu, I_p)$

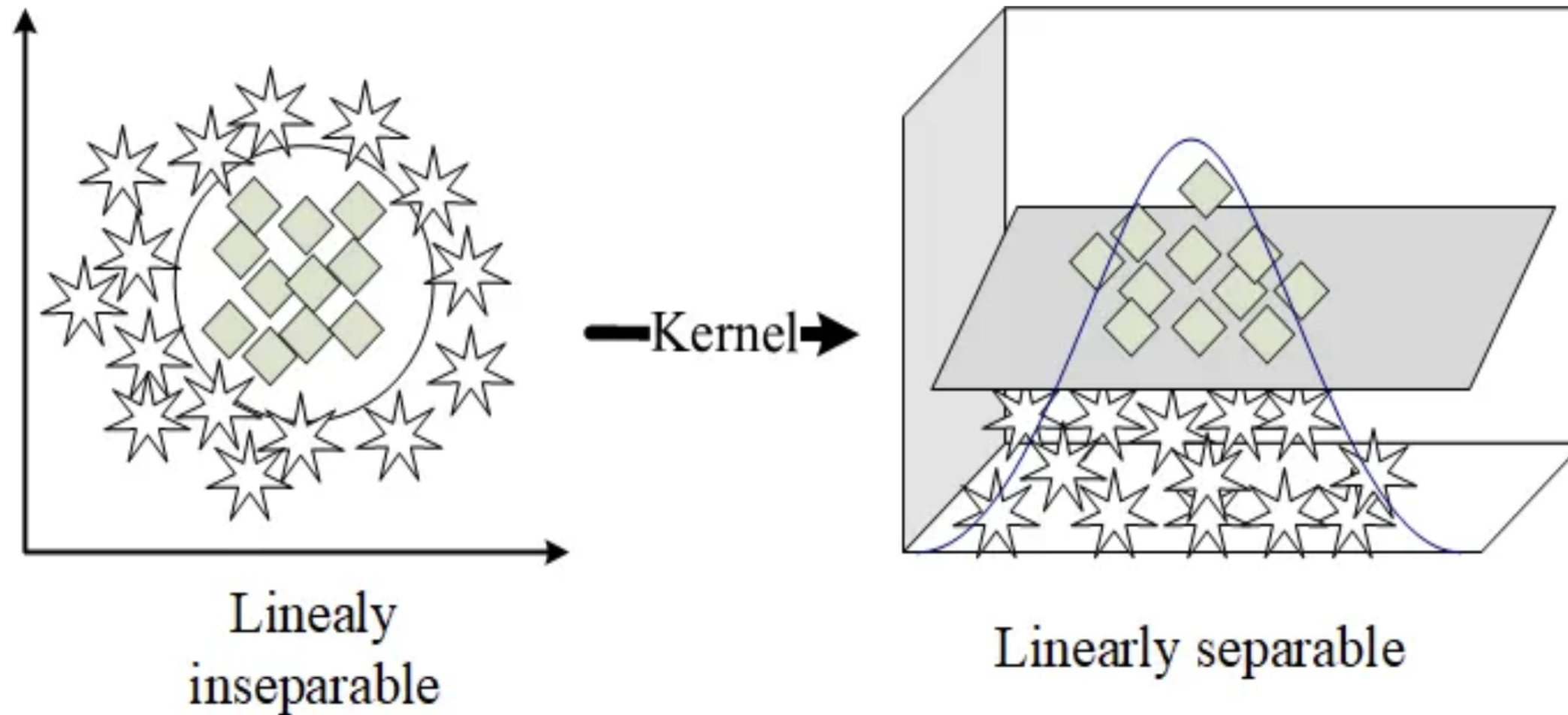
with  $\mu = (2, 0, \dots, 0) \in \mathbb{R}^p$ ,  $n = 500$ ,  $p = 5$ .

$$= (K(x_i, x_j))_{i,j \in [n]} \in \mathbb{R}^{n \times n}$$

with for ex.  $K(x, y) = e^{-\frac{\|x-y\|^2}{2p}}$  (“Heat kernel”)

$\implies$  Look for first eigenvectors of  $K$  should capture class information

# Kernels

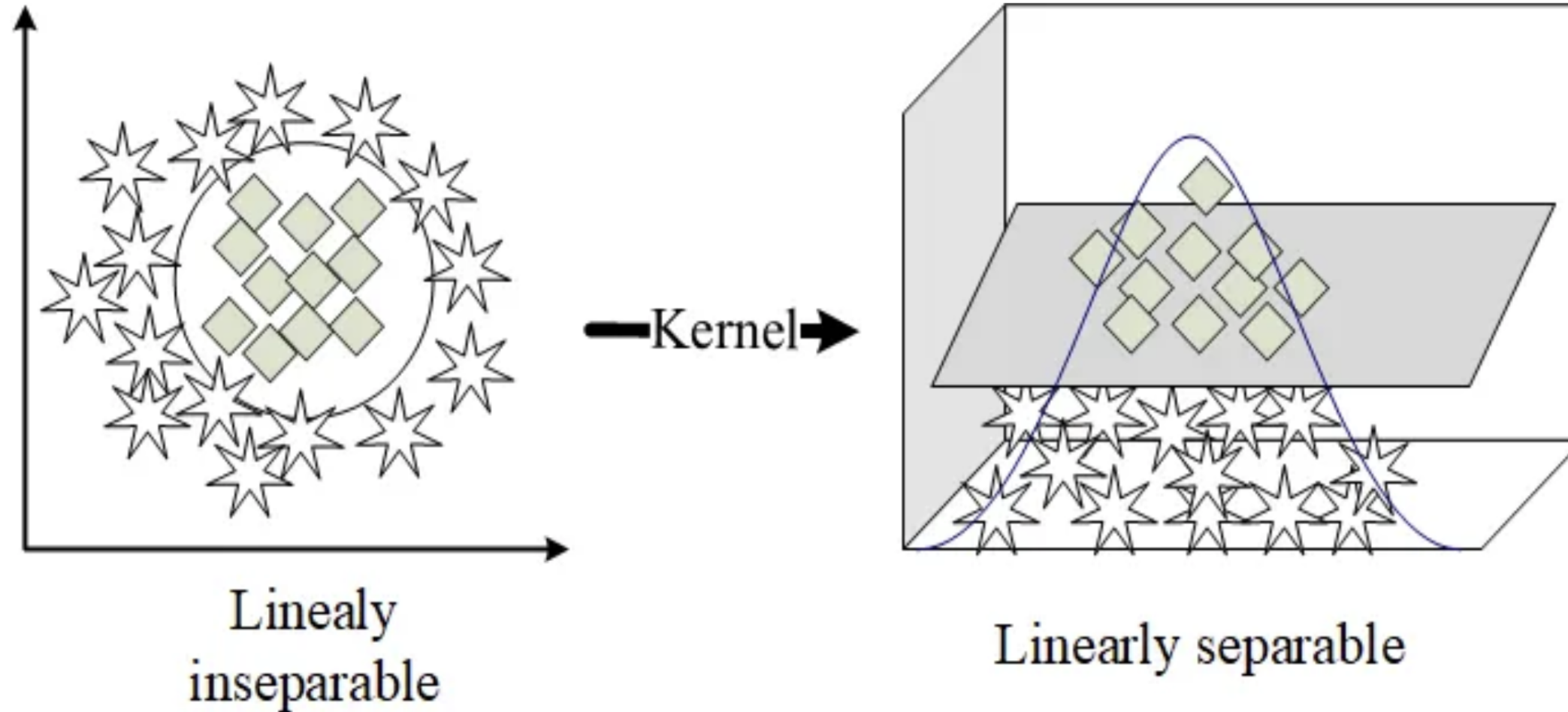


**Definition:**  $K : E^2 \rightarrow \mathbb{R}$  is a *Mercer Kernel* or a *Positive semi-definite kernel* iif:

$$\forall x_1, \dots, x_n \in E, \forall c = (c_1, \dots, c_n) \in \mathbb{R}^n : \quad \sum_{i,j=1}^n c_i c_j K(x_i, x_j) \geq 0$$



# Kernels



**Theorem:** Given a Mercer Kernel  $K : E^2 \rightarrow \mathbb{R}$  there exists:

- a Hilbert space  $(H, \langle \cdot | \cdot \rangle)$
  - a mapping  $\phi : E \rightarrow H$
- such that:

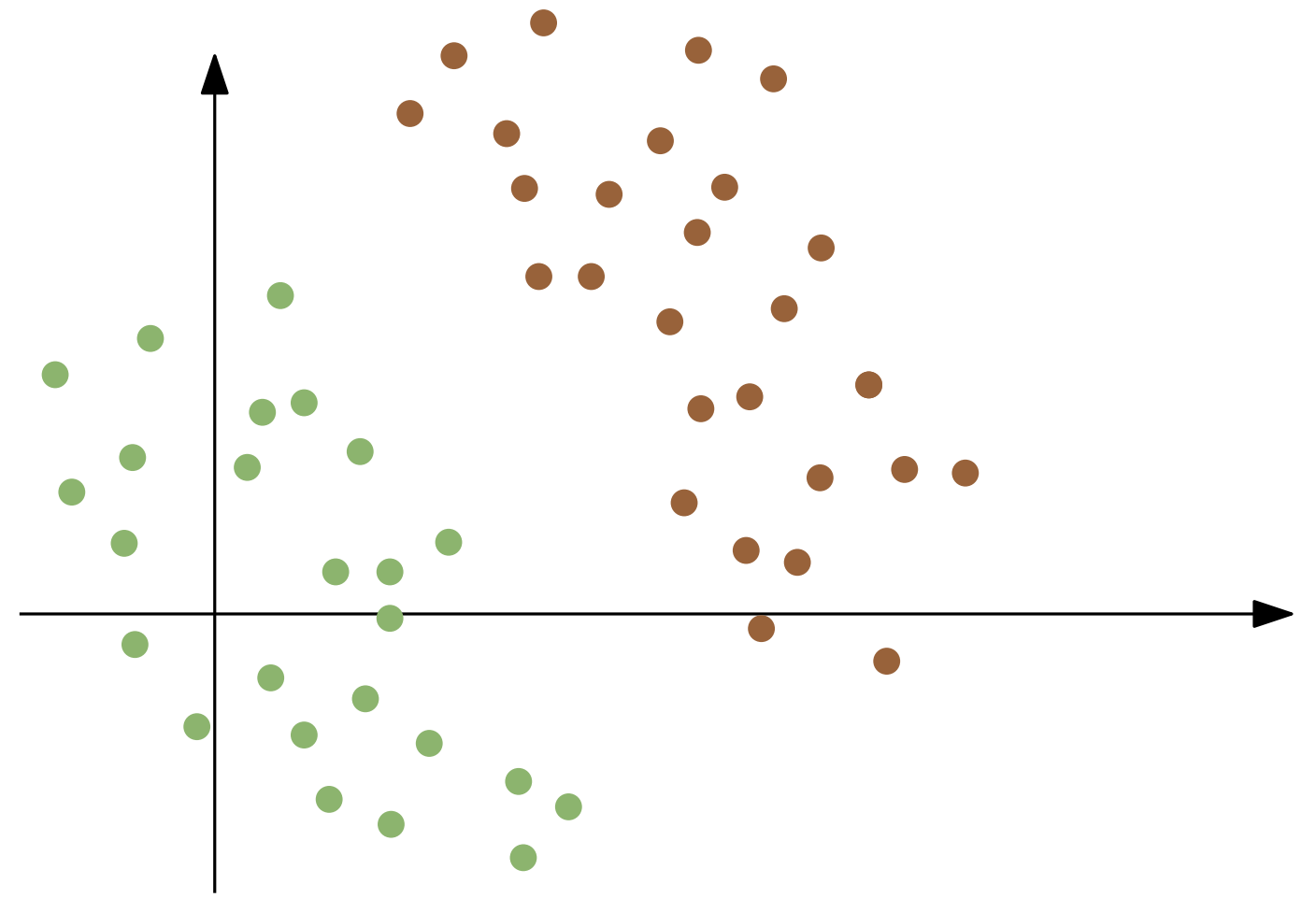
$$\forall x, y \in E :$$

$$K(x, y) = \langle \phi(x), \phi(y) \rangle$$

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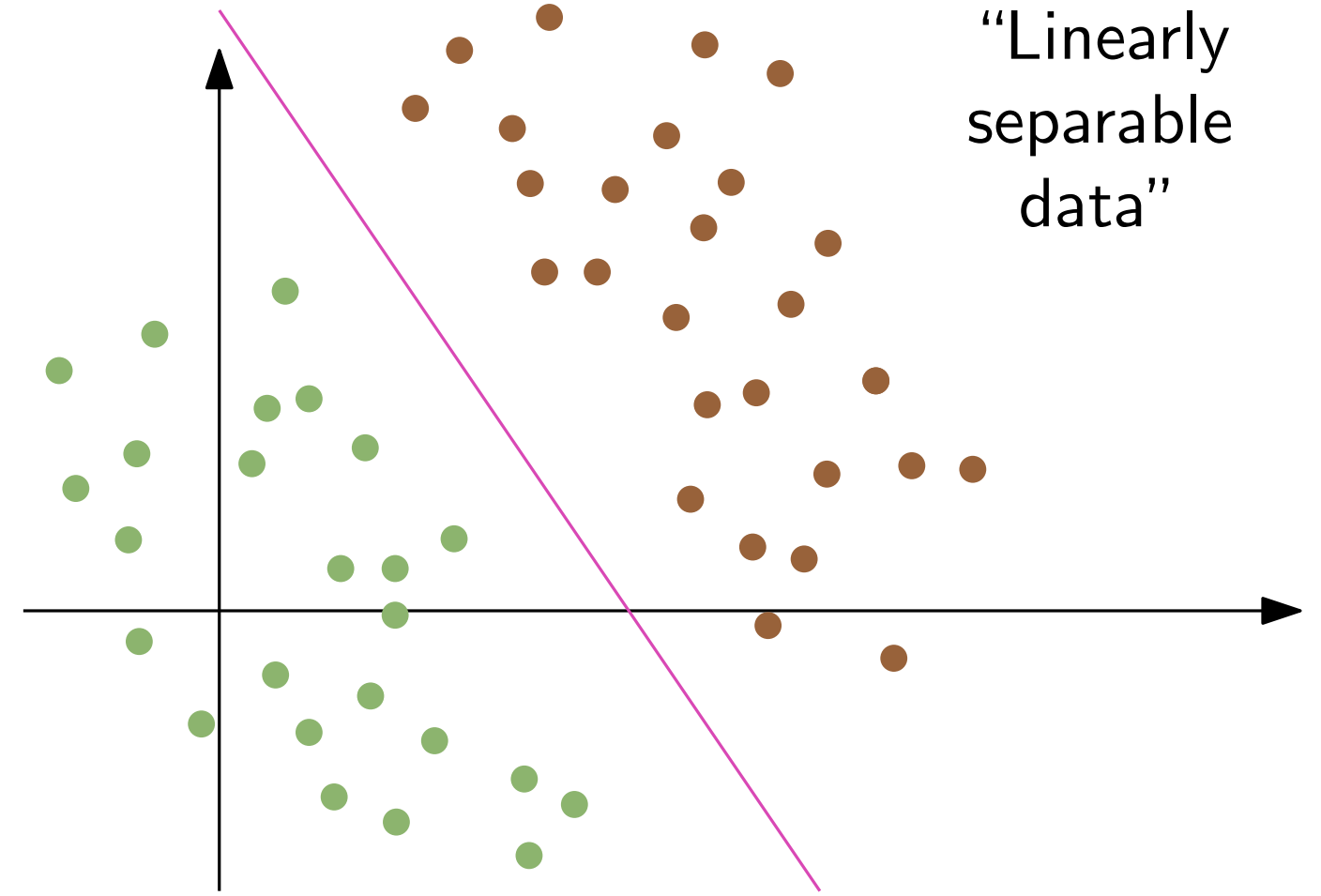
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# Example of Support vector machines



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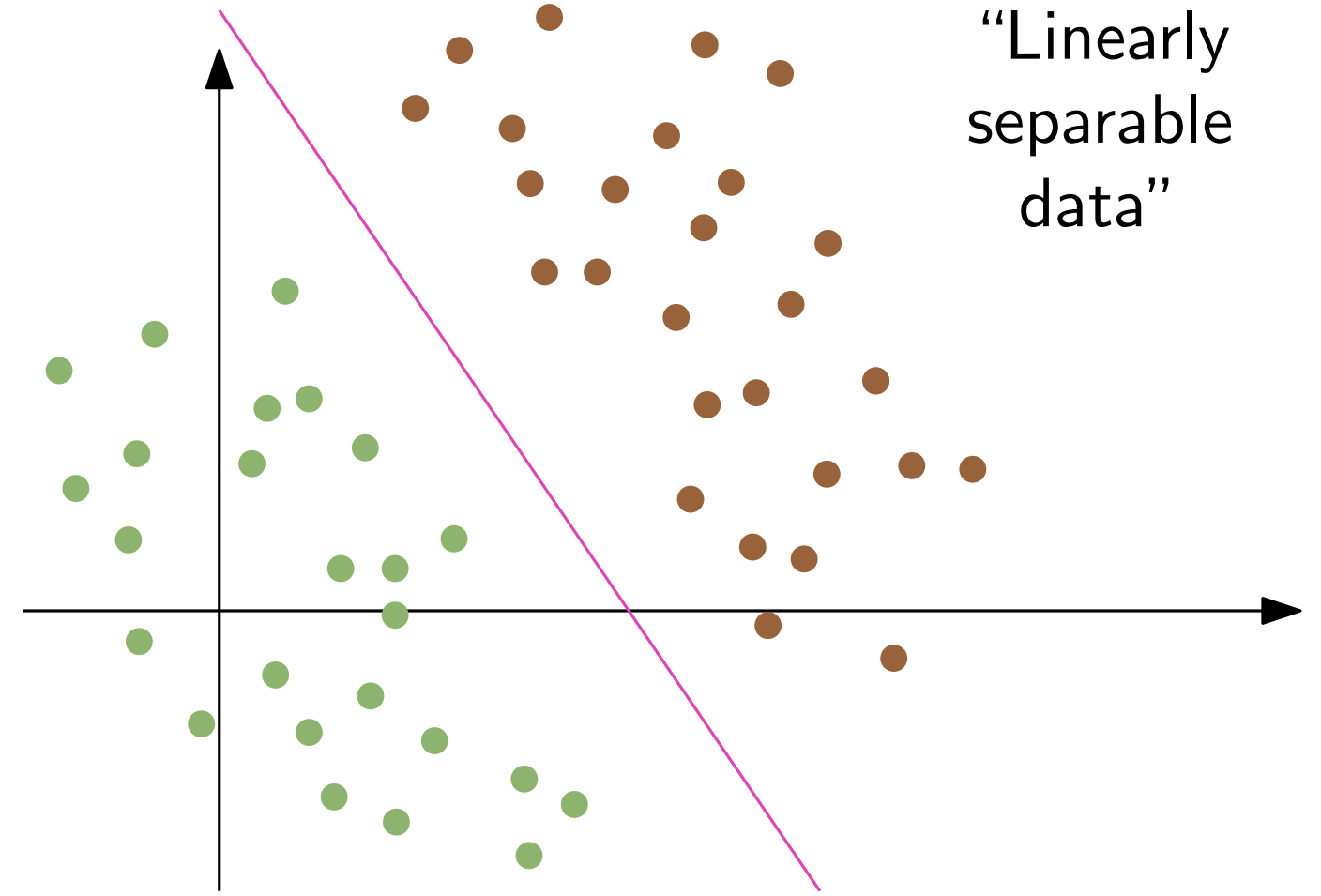
## 1 - Large (or hard) margin SVM



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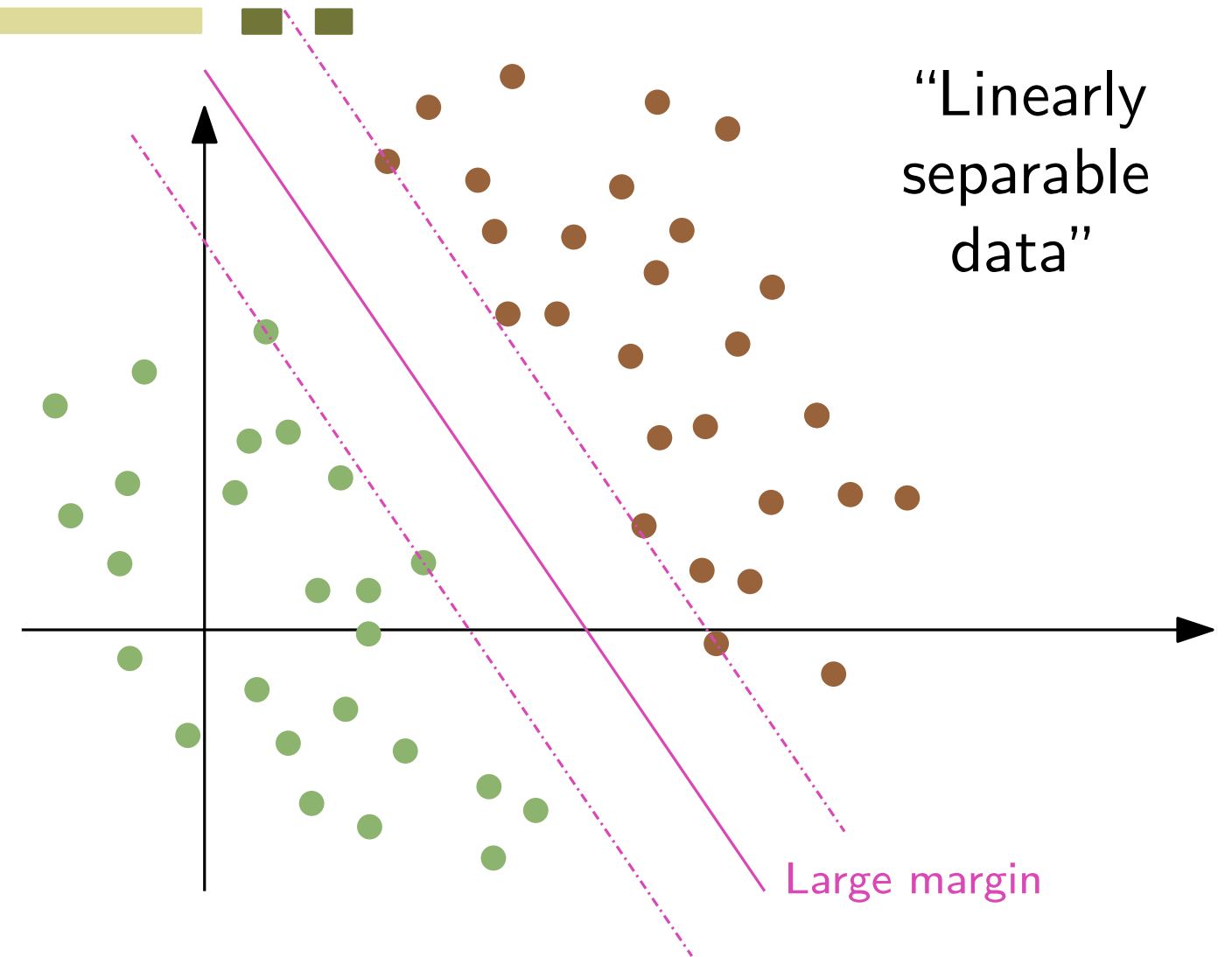
**Idea:** Look for a linear boundary with largest margin



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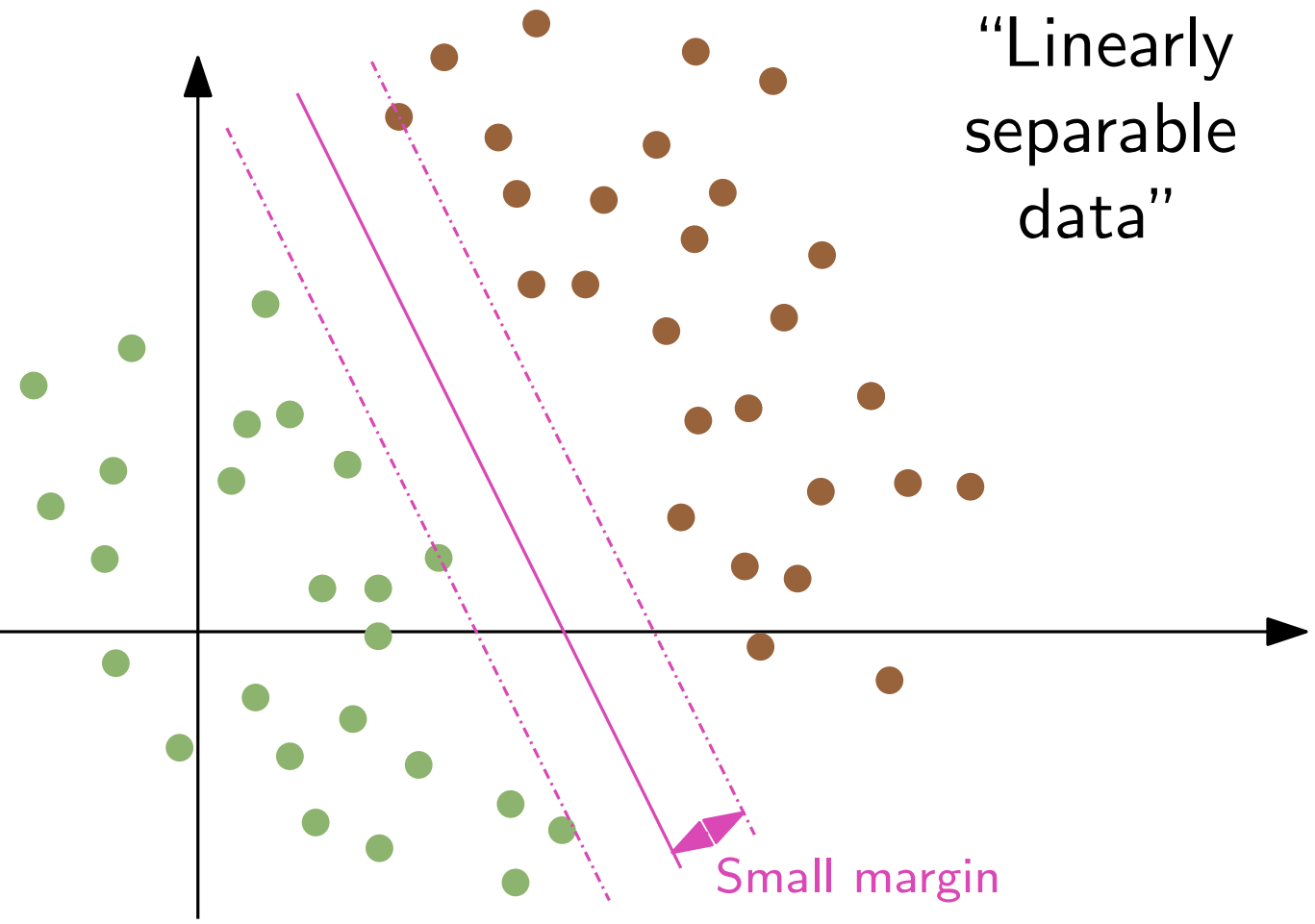
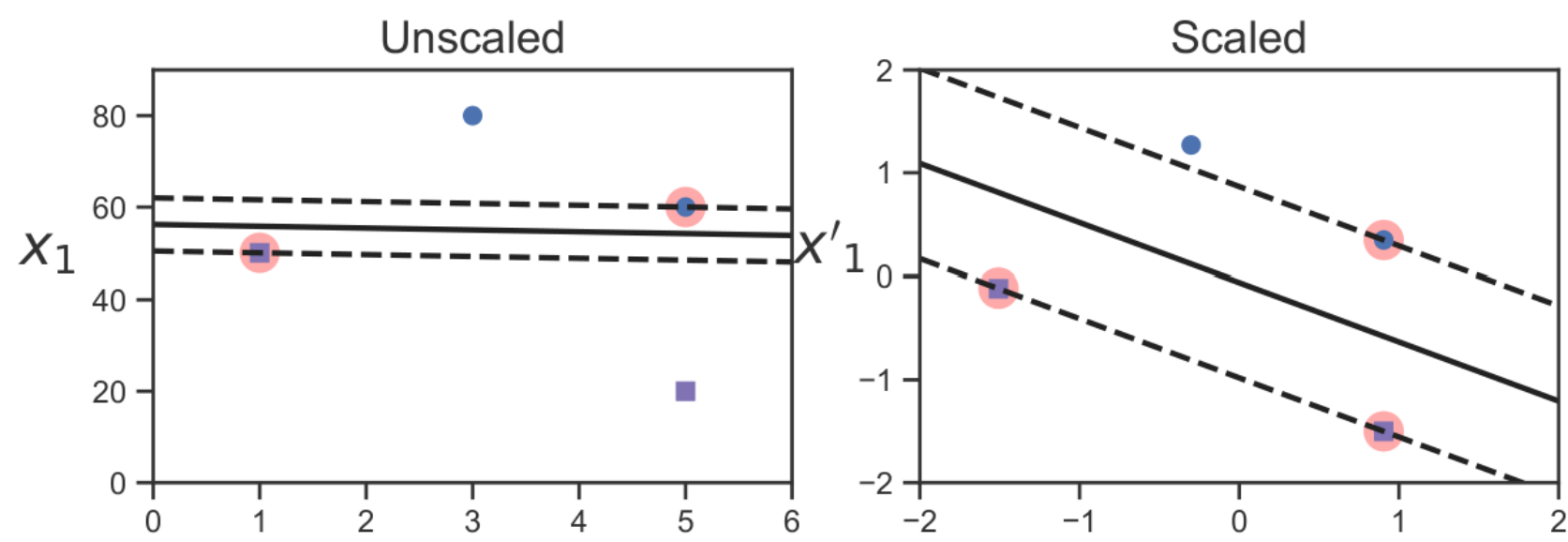
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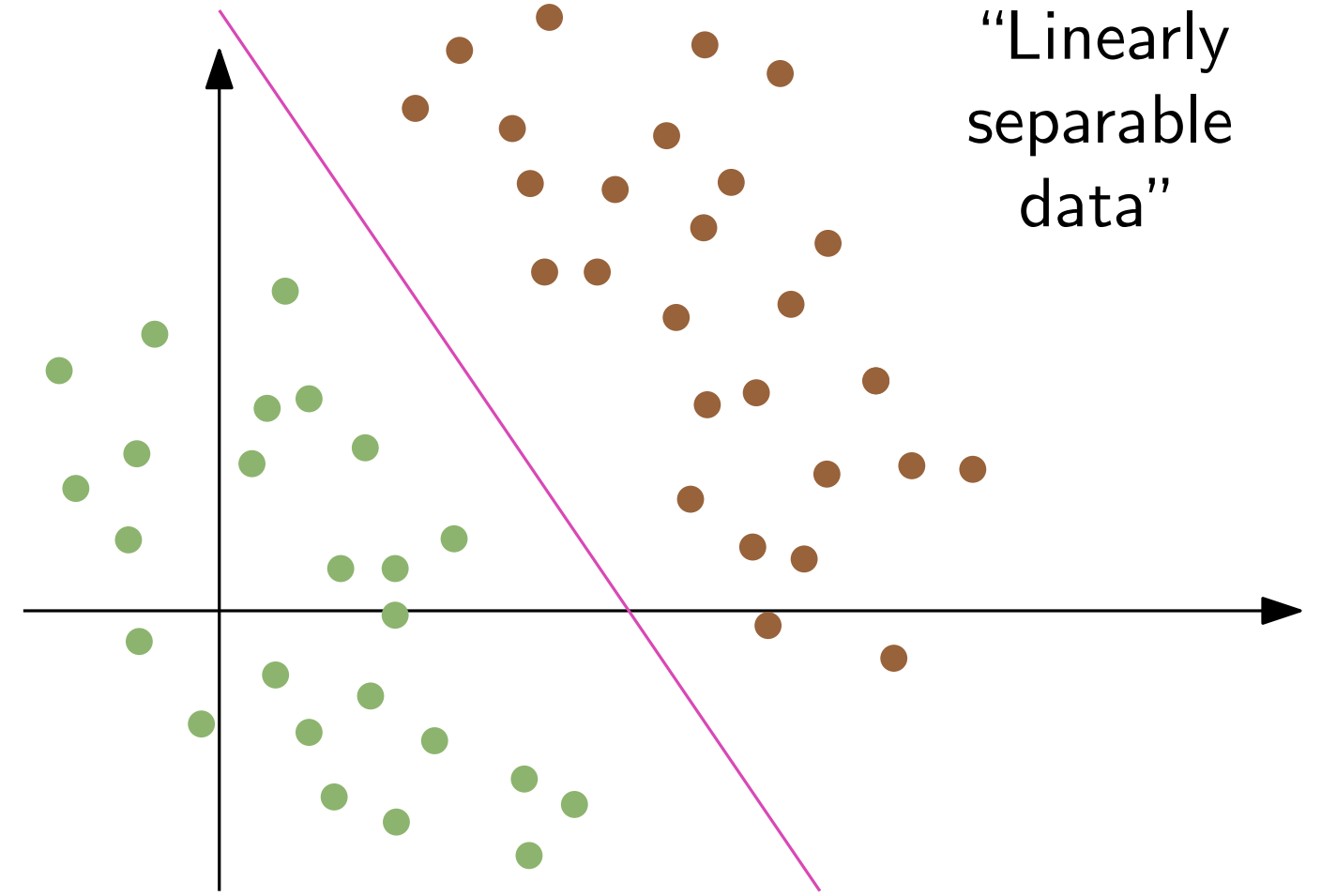
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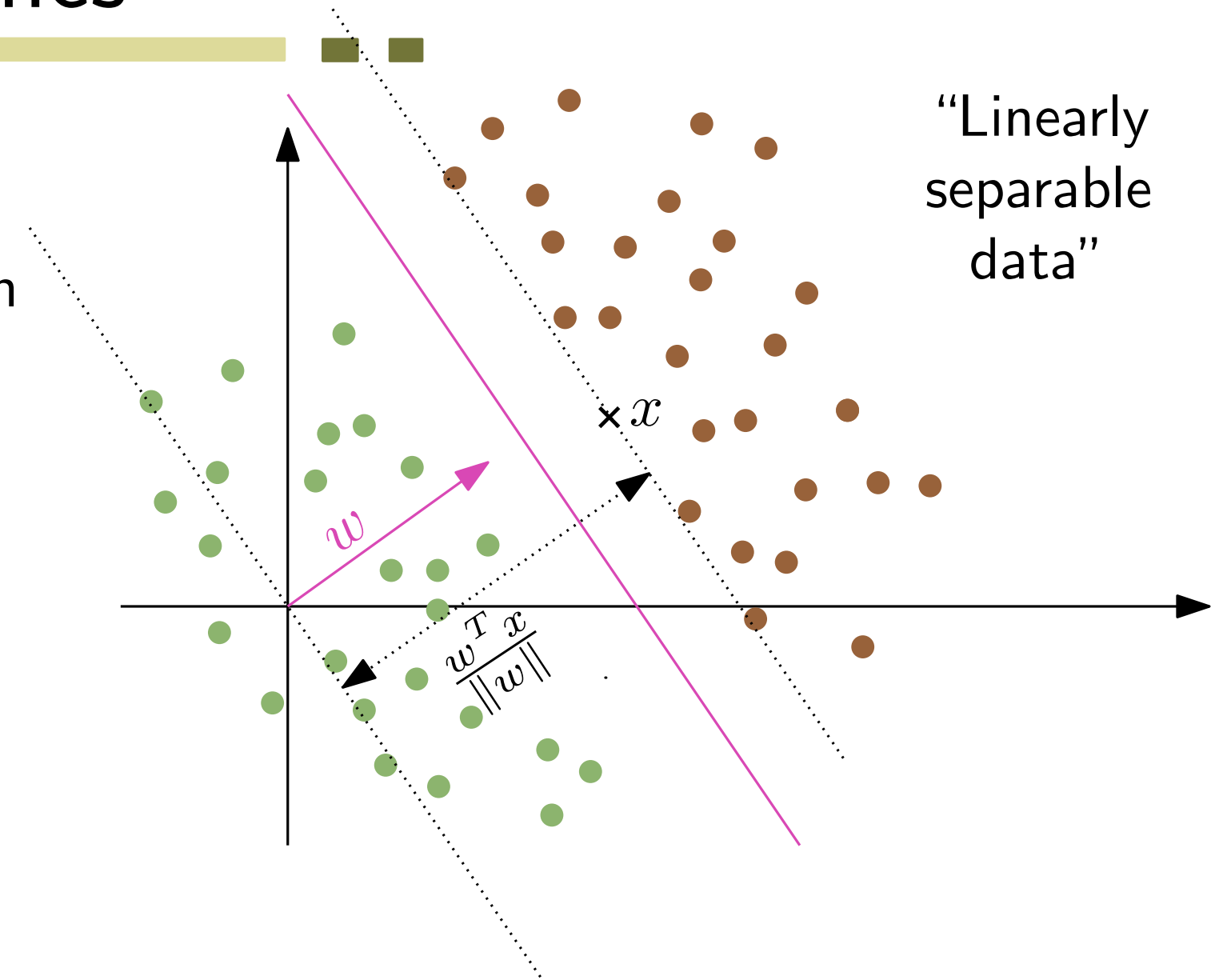




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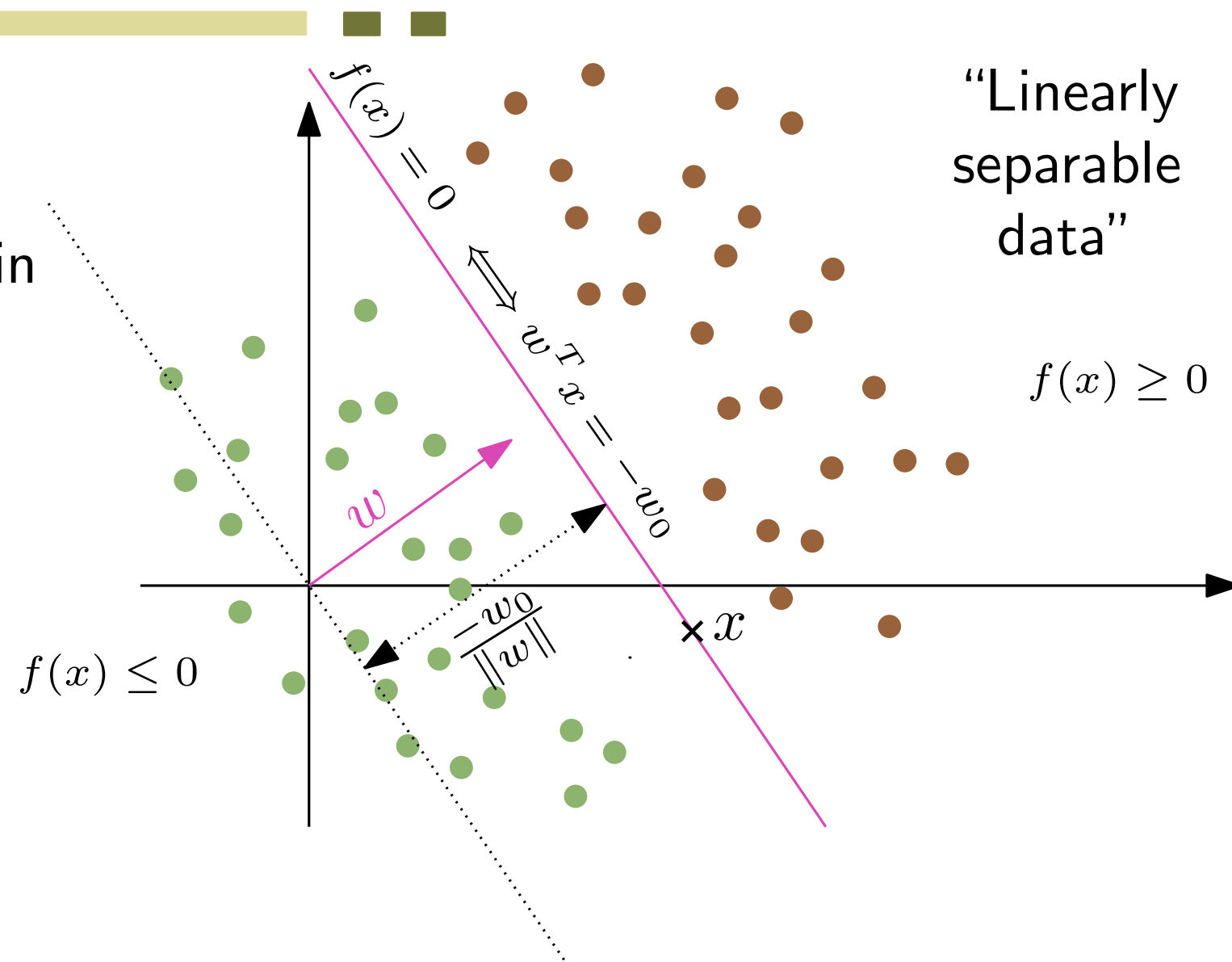
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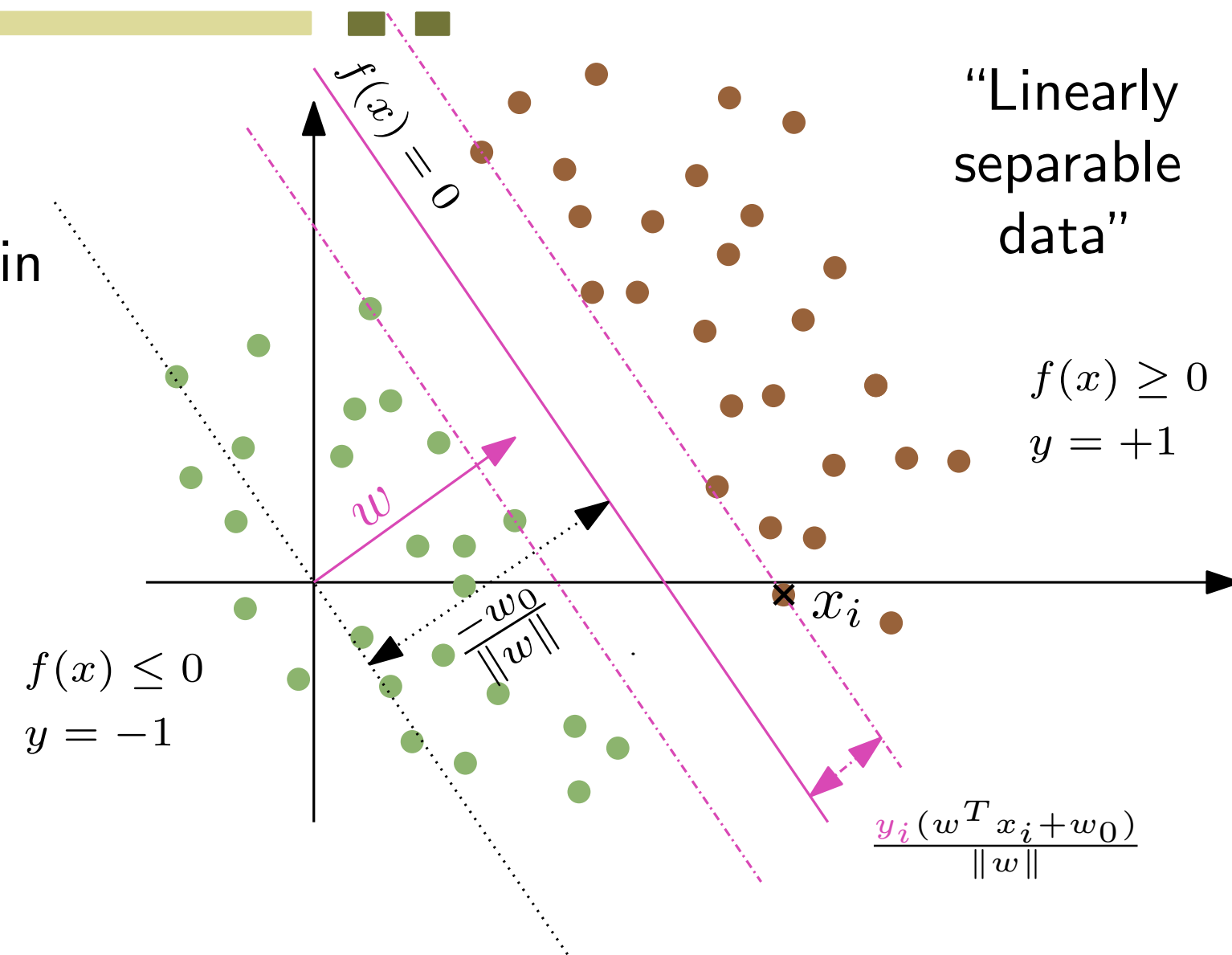
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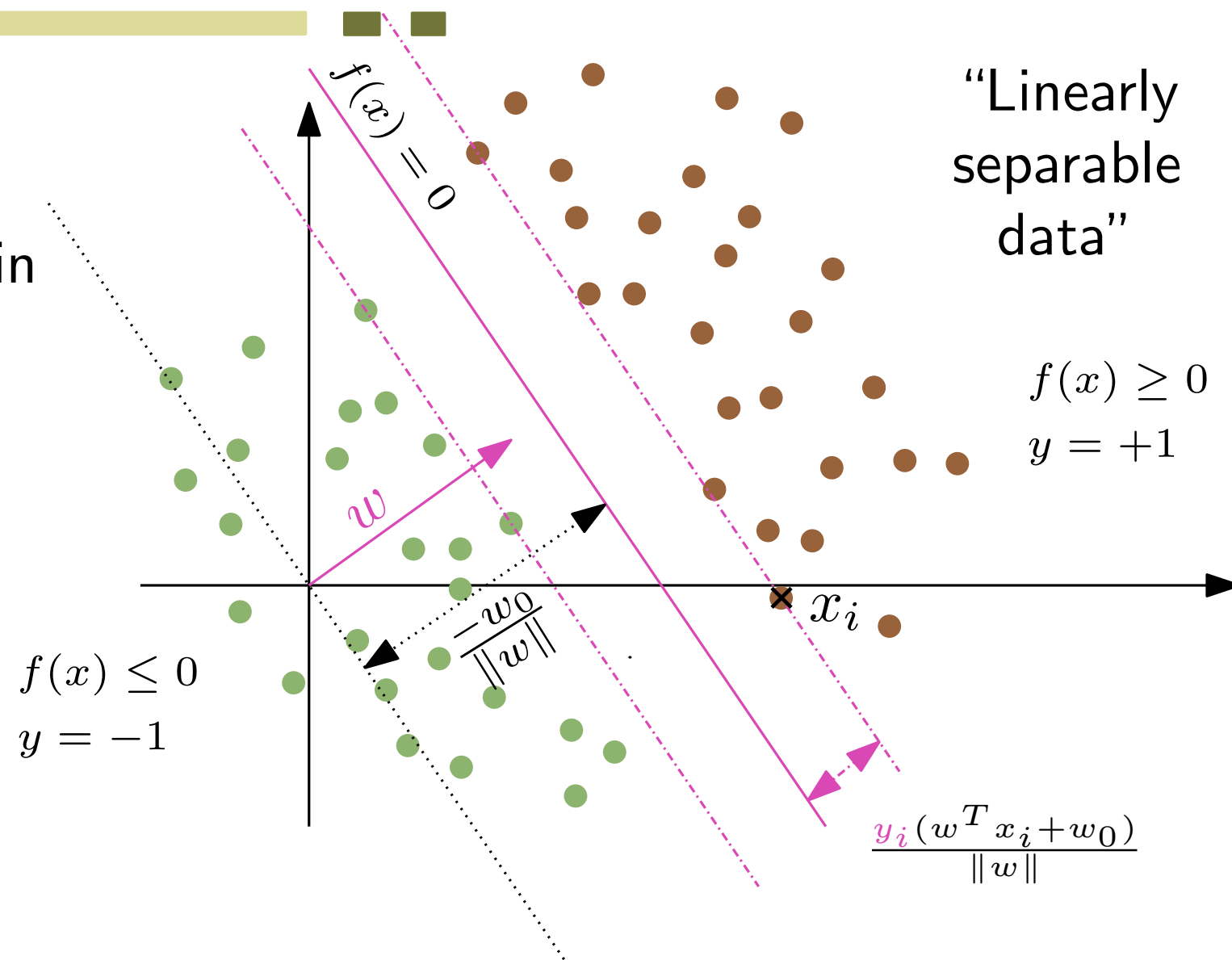
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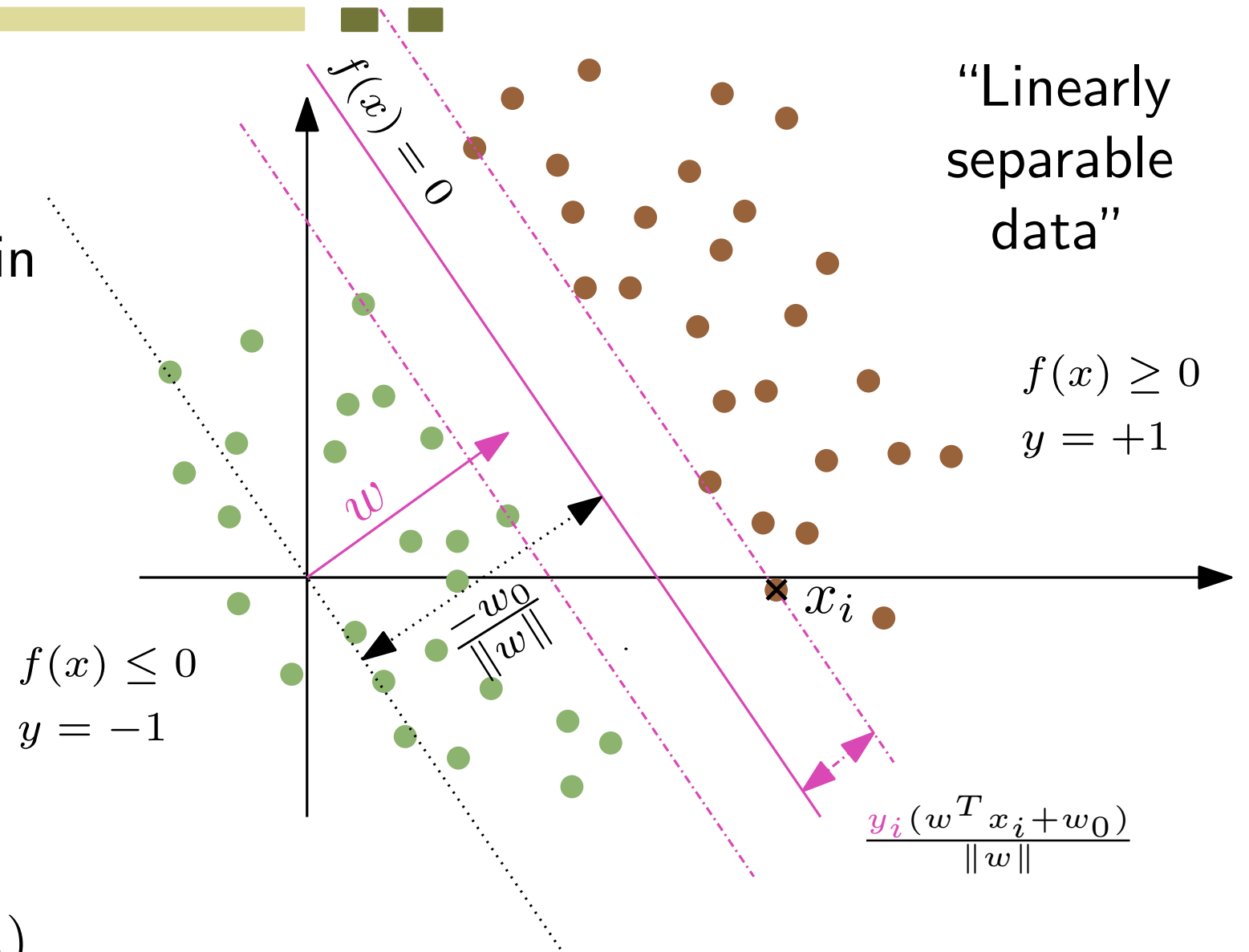
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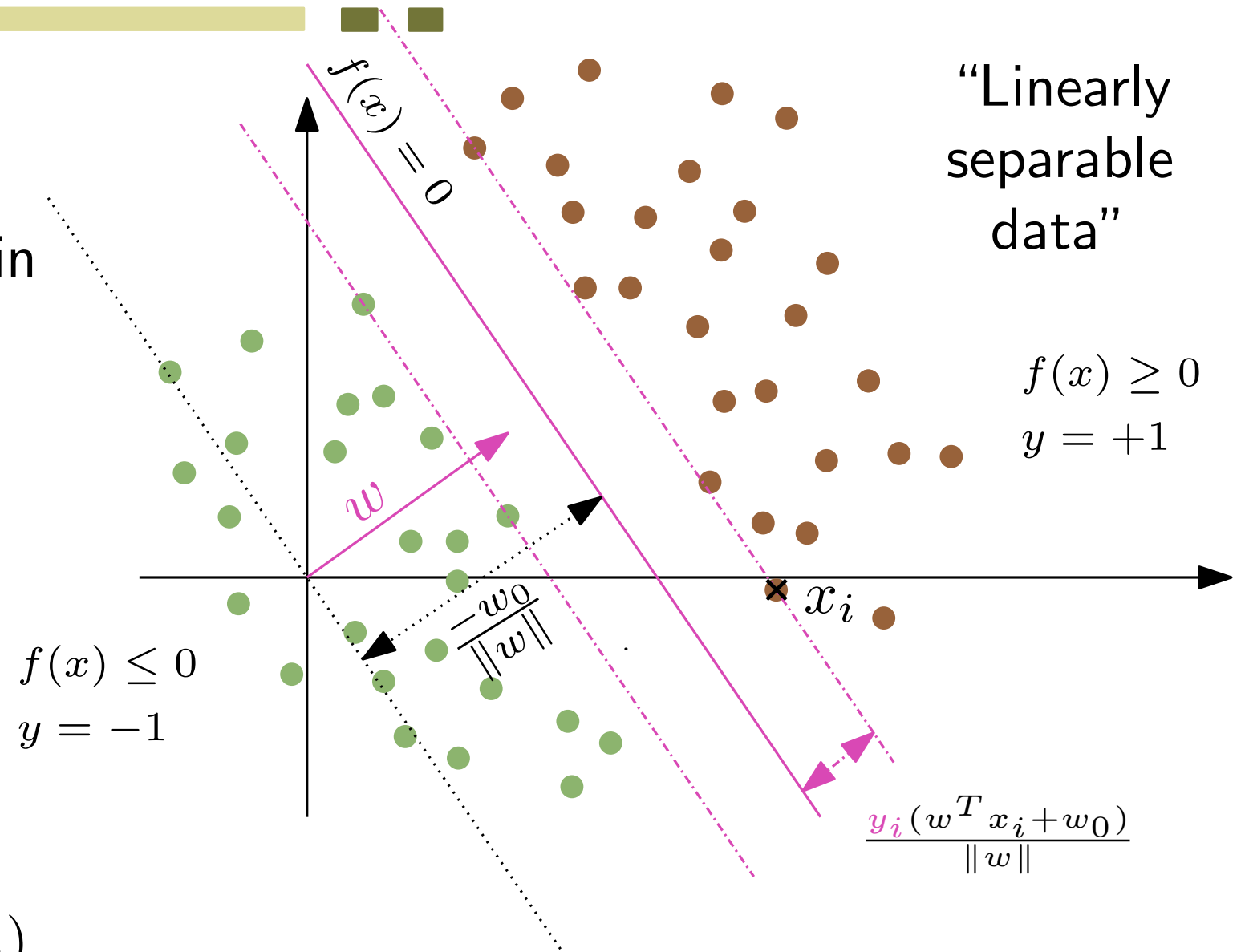
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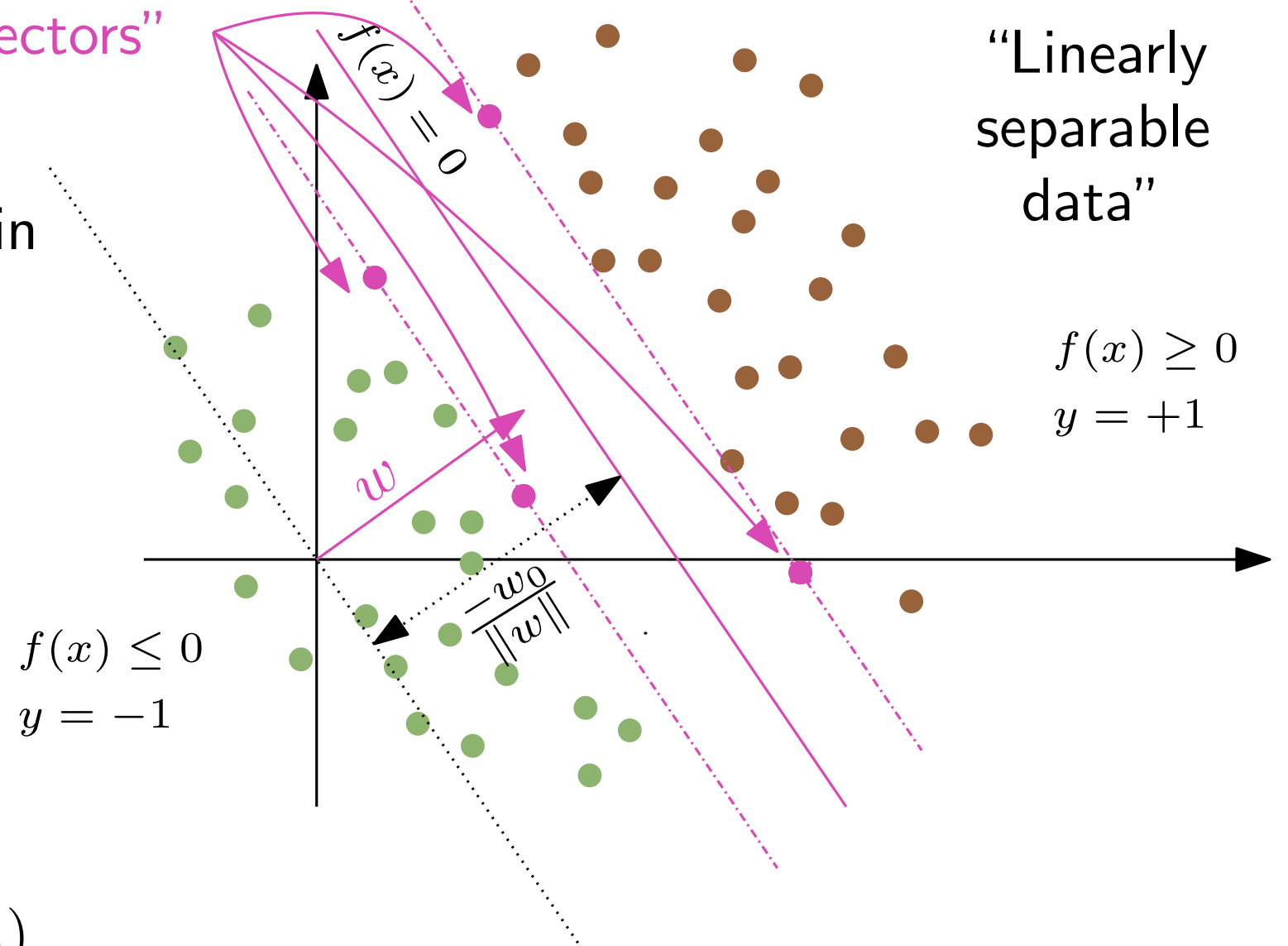
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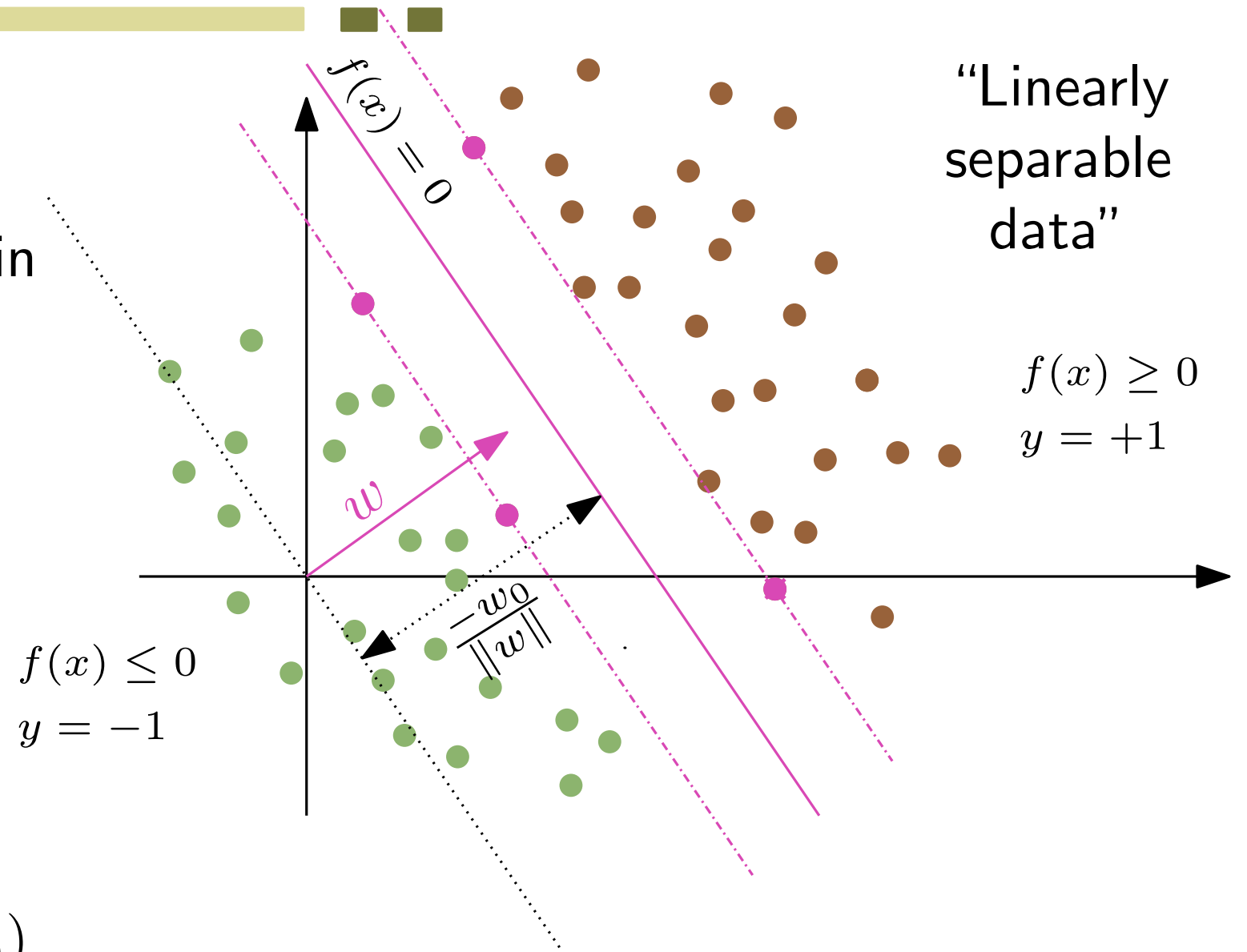
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Lagrangian:  $L(w, w_0, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i(w^T x_i + w_0) - 1), \quad w \in \mathbb{R}^p, w_0 \in \mathbb{R}, \alpha \in \mathbb{R}_+^p$

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$$(\text{ Because if } \exists i \in [n] \text{ s.t. } y_i(w^T x_i + w_0) < 1 \text{ then } \max_{\alpha_i \geq 0} -\alpha_i (y_i(w^T x_i + w_0) - 1) = +\infty)$$

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**Optimization theory Theorem:** There exist  $\hat{w}, \hat{w}_0, \hat{\alpha}$  s.t. (denoting  $f : x \mapsto \hat{w}^T x + \hat{w}_0$ ):

$$\bullet \min_{w \in \mathbb{R}^p, w_0 \in \mathbb{R}} \max_{\alpha \in \mathbb{R}_+^n} L(w, w_0, \alpha) = L(\hat{w}, \hat{w}_0, \hat{\alpha}) = \max_{\alpha \in \mathbb{R}_+^n} \min_{w \in \mathbb{R}^p, w_0 \in \mathbb{R}} L(w, w_0, \alpha)$$



# Large Margin SVM

## Primal Problem:

$$\text{Minimize } \frac{1}{2} \|w\|^2 \text{ subject to } \forall i \in [n] : y_i(w^T x_i + w_0) \geq 1, \quad w \in \mathbb{R}^p, w_0 \in \mathbb{R} \quad (P)$$

$$\text{Lagrangian: } L(w, w_0, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i(w^T x_i + w_0) - 1), \quad w \in \mathbb{R}^p, w_0 \in \mathbb{R}, \alpha \in \mathbb{R}_+^n$$

$$\hat{w}, \hat{w}_0 \text{ solve } (P) \iff \frac{1}{2} \|\hat{w}\|^2 = \max_{\alpha \in \mathbb{R}_+^n} L(\hat{w}, \hat{w}_0, \alpha)$$

$$\text{Thus: } \hat{w}, \hat{w}_0 \text{ solve } (P) \iff \hat{w}, \hat{w}_0 = \underset{w \in \mathbb{R}^p, w_0 \in \mathbb{R}}{\text{Argmin}} \max_{\alpha \in \mathbb{R}_+^n} L(w, w_0, \alpha)$$

**Optimization theory Theorem:** There exist  $\hat{w}, \hat{w}_0, \hat{\alpha}$  s.t. (denoting  $f : x \mapsto \hat{w}^T x + \hat{w}_0$ ):

$$\bullet \min_{w \in \mathbb{R}^p, w_0 \in \mathbb{R}} \max_{\alpha \in \mathbb{R}_+^n} L(w, w_0, \alpha) = L(\hat{w}, \hat{w}_0, \hat{\alpha}) = \max_{\alpha \in \mathbb{R}_+^n} \min_{w \in \mathbb{R}^p, w_0 \in \mathbb{R}} L(w, w_0, \alpha)$$

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$$y_j^2 = 1$$

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In practice averaging:  $\hat{w}_0 \equiv \frac{1}{|S|} \sum_{j \in S} y_j - \sum_{i \in S} \hat{\alpha}_i y_i x_i^T x_j$

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## Dual Problem:

Maximize  $-\frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i x_j + \sum_{i=1}^n \alpha_i$

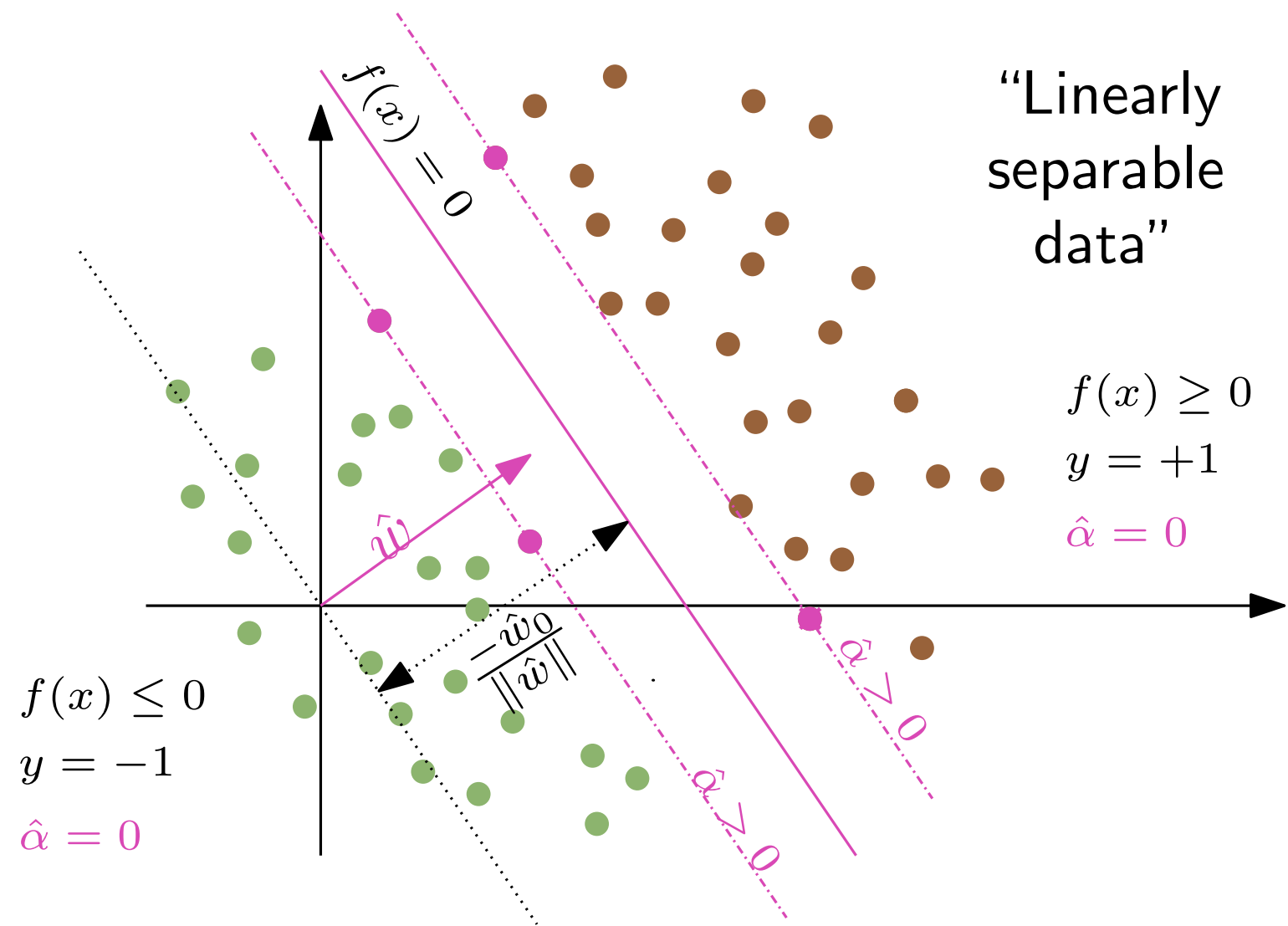
Subject to  $\alpha \in \mathbb{R}_+^n$ ,  $\sum_{i=1}^n \alpha_i y_i = 0$ .

## Final prediction:

$$f(\mathbf{x}) = \hat{w}^T \mathbf{x} + \hat{w}_0$$

$$\text{with: } \hat{w} = \sum_{i \in S} \hat{\alpha}_i y_i x_i \quad S = \{i : \alpha_i > 0\}$$

$$\hat{w}_0 = \frac{1}{|S|} \sum_{j \in S} y_j - \sum_{i \in S} \hat{\alpha}_i y_i x_i^T x_j$$

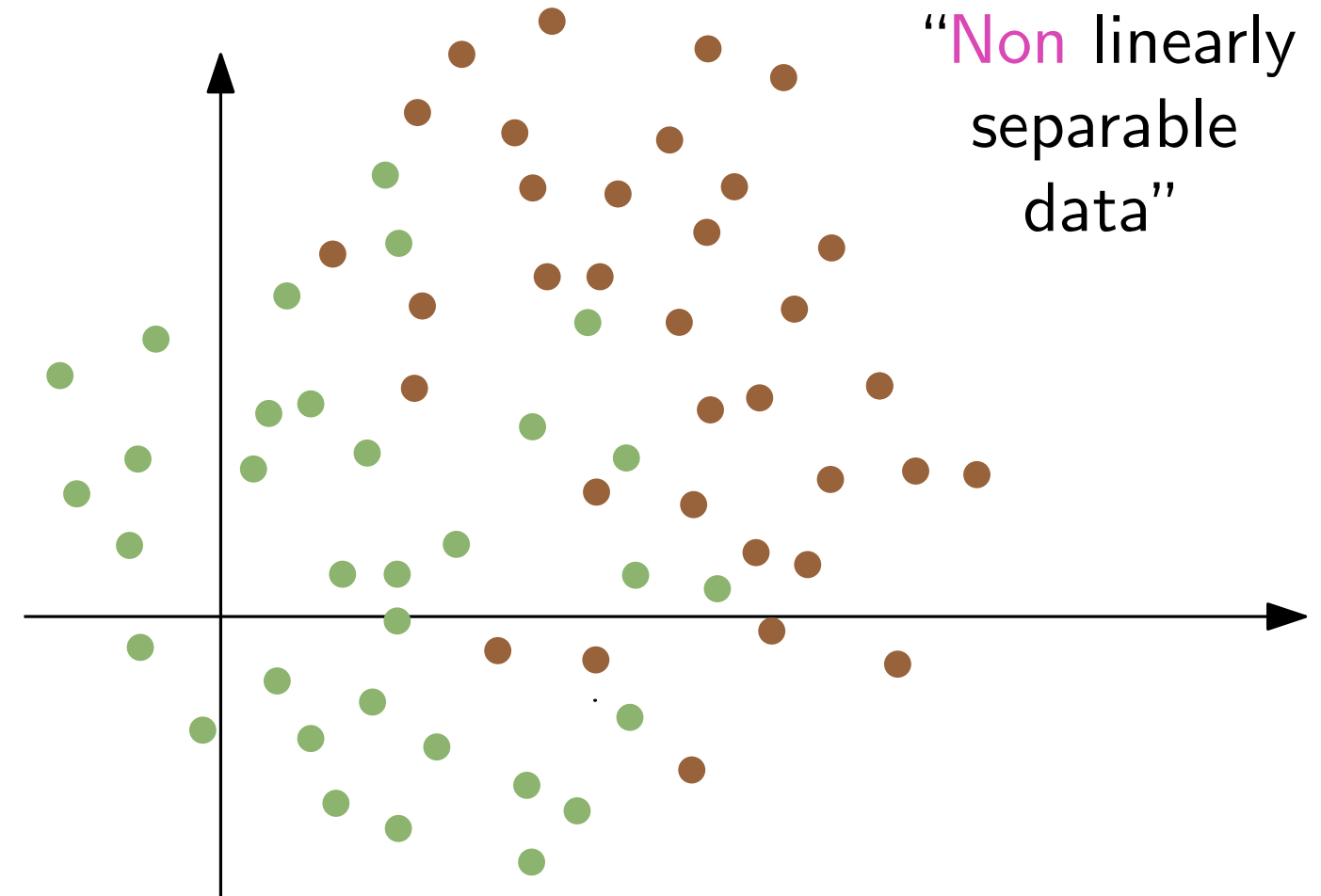




# Soft Margin SVM

## Primal Problem:

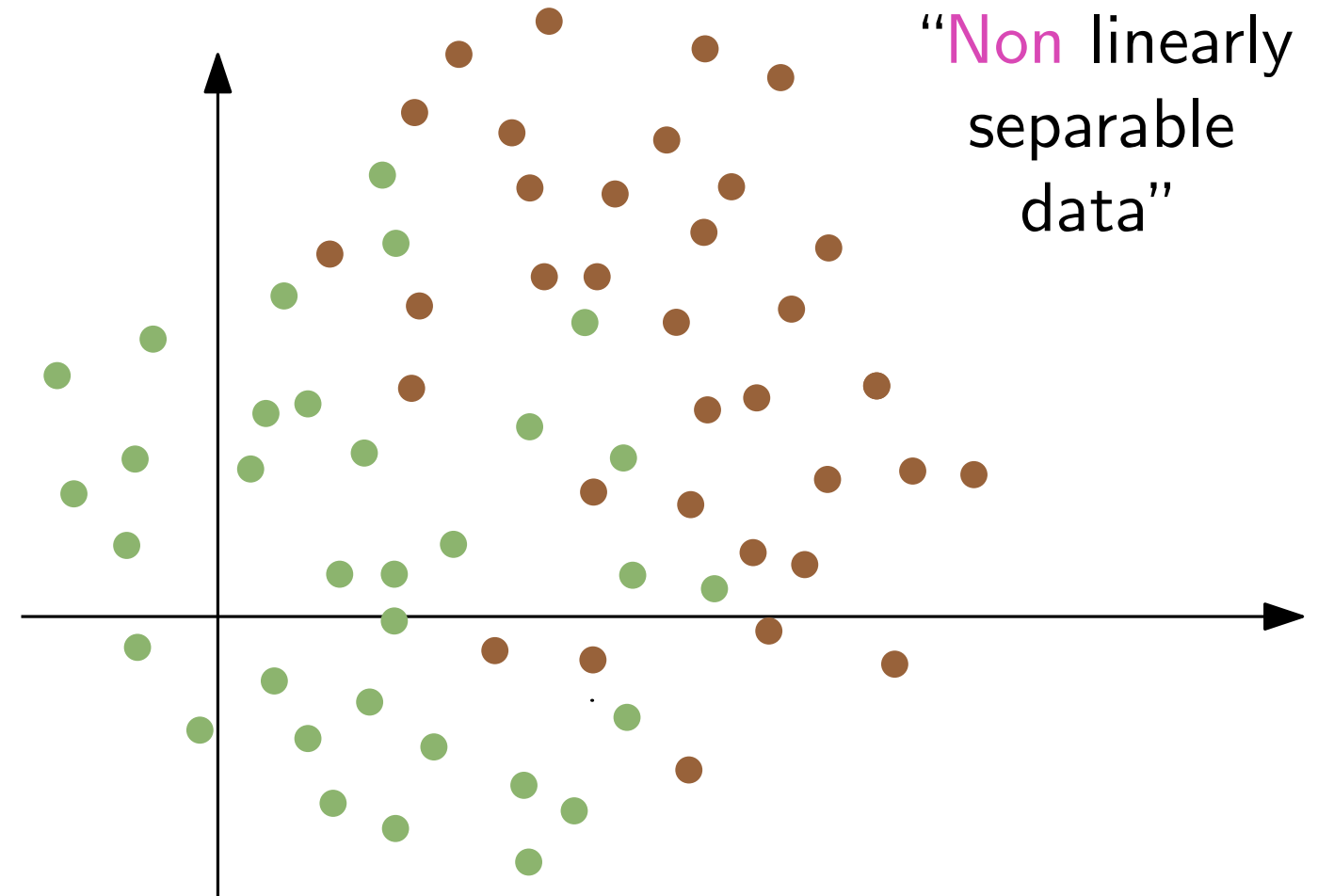
Minimize  $\frac{1}{2} \|w\|^2$  subject to  $\forall i \in [n] : y_i(w^T x_i + w_0) \geq 1$



# Soft Margin SVM

## Primal Problem:

Minimize  $\frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i$  subject to  $\forall i \in [n] : y_i(w^T x_i + w_0) \geq 1 - \xi_i, \quad \xi_i > 0$



# Soft Margin SVM

## Primal Problem:

Minimize  $\frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i$  subject to  $\forall i \in [n] : y_i(w^T x_i + w_0) \geq 1 - \xi_i, \quad \xi_i > 0$

## Dual Problem:

Maximize  $-\frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i x_j + \sum_{i=1}^n \alpha_i$

Subject to  $\alpha \in [0, C]^n, \sum_{i=1}^n \alpha_i y_i = 0$ .

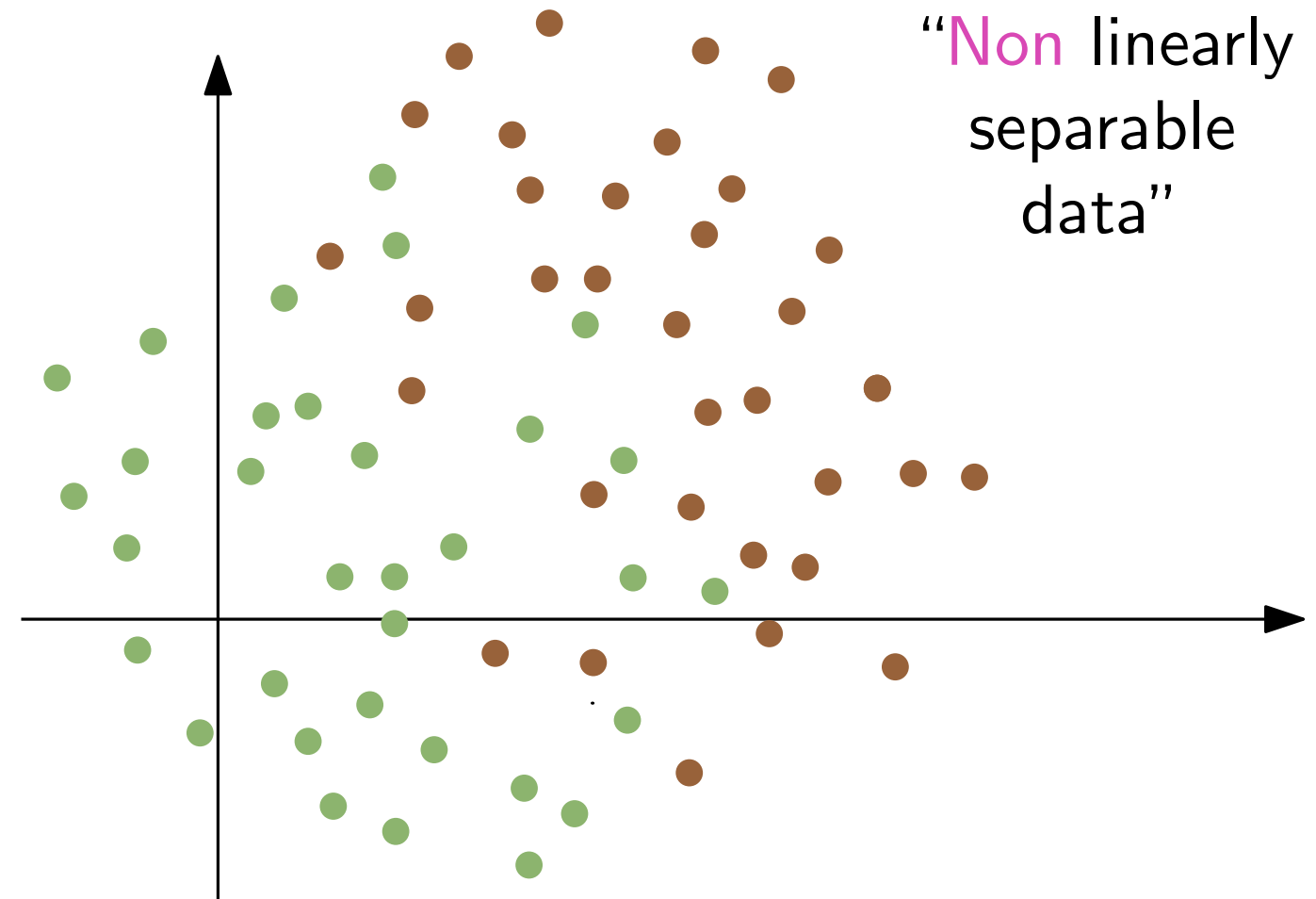
## Final prediction:

$$f(x) = \hat{w}^T x + \hat{w}_0$$

(Same kind  
of inferences  
as before)

with:  $\hat{w} = \sum_{i \in S} \hat{\alpha}_i y_i x_i$

$$\hat{w}_0 = \frac{1}{|S|} \sum_{j \in S} y_j - \sum_{i \in S} \hat{\alpha}_i y_i x_i^T x_j$$



# Soft Margin SVM

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Maximize  $-\frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i x_j + \sum_{i=1}^n \alpha_i$

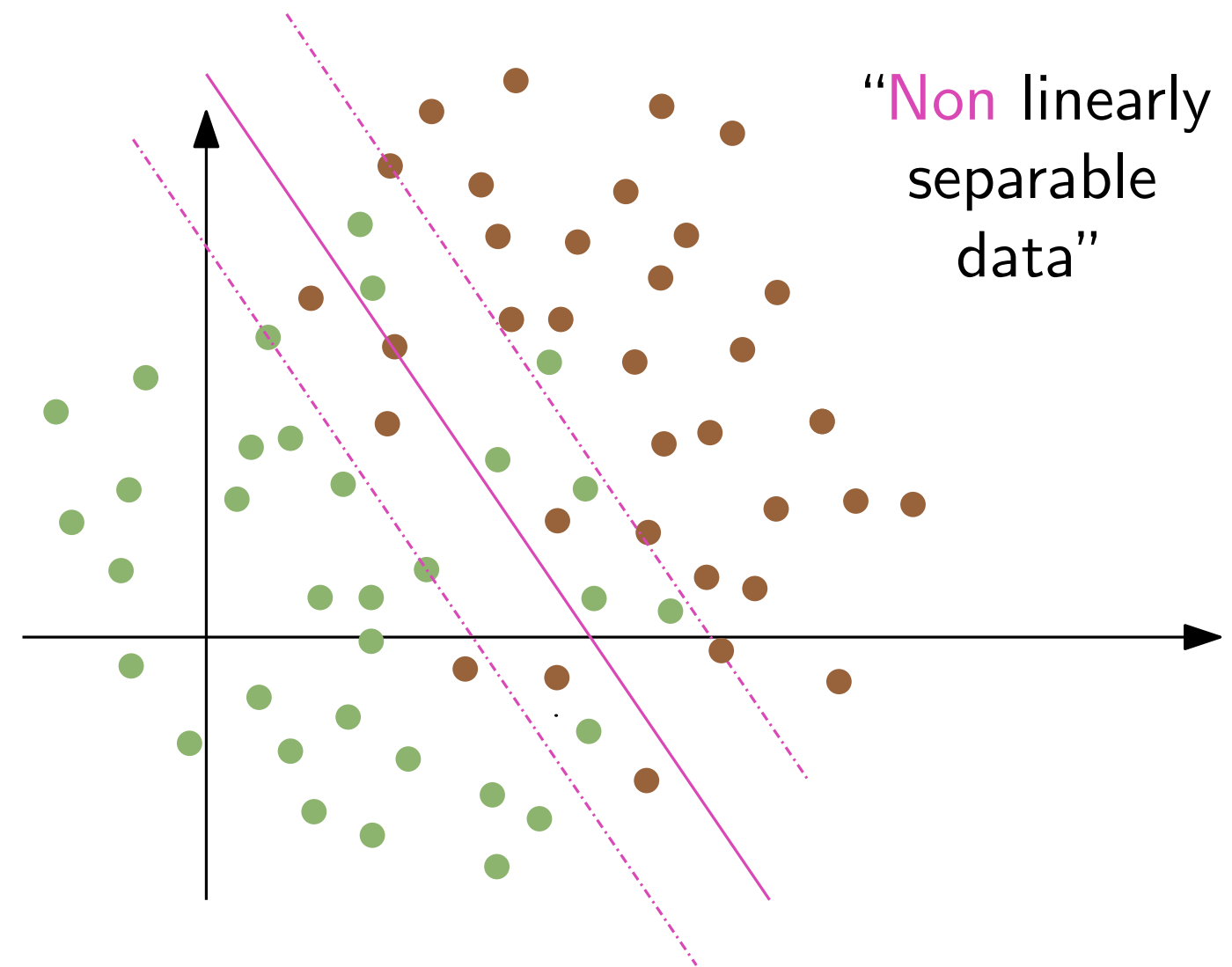
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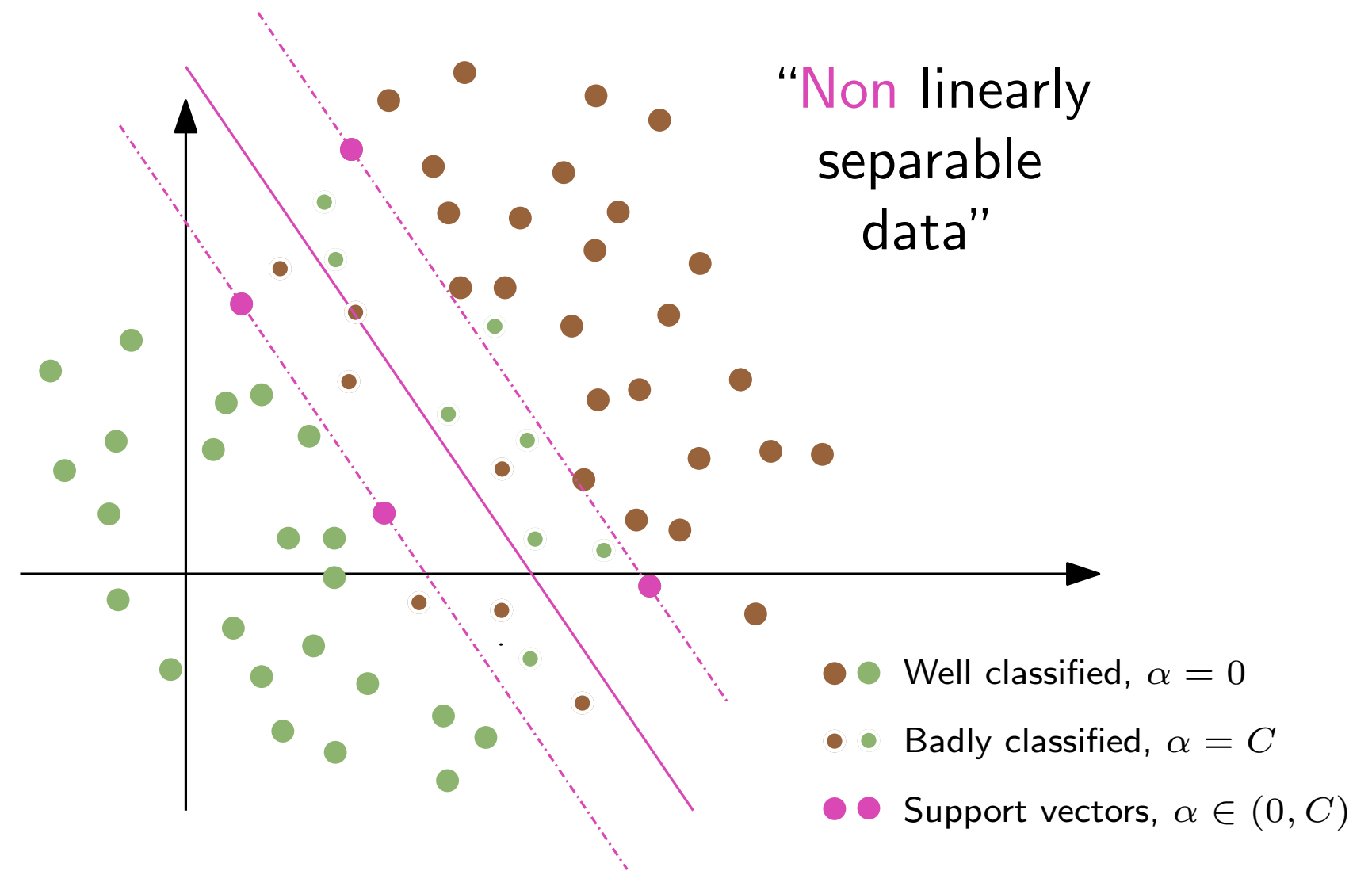
Subject to  $\alpha \in [0, C]^n, \sum_{i=1}^n \alpha_i y_i = 0$ .

## Final prediction:

$$f(x) = \hat{w}^T x + \hat{w}_0$$

$$\text{with: } \hat{w} = \sum_{i \in S} \hat{\alpha}_i y_i x_i$$

$$\hat{w}_0 = \frac{1}{|S|} \sum_{j \in S} y_j - \sum_{i \in S} \hat{\alpha}_i y_i x_i^T x_j$$



# Kernel trick with SVM

Minimize:  $\sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j - \sum_{i=1}^n \alpha_i$

Subject to: •  $\forall i \in [n] : 0 \leq \alpha_i \leq C$

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

Then:

$$\bullet f(t) = \sum_{i \in S} \hat{\alpha}_i y_i \mathbf{x}_i^T \mathbf{x}_i + \hat{w}_0$$

$$\bullet \hat{w}_0 = \frac{1}{|S|} \sum_{i \in S} \left( y_i - \sum_{j \in S} \hat{\alpha}_j y_j \mathbf{x}_j^T \mathbf{x}_i \right)$$

# Kernel trick with SVM

Minimize:  $\sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j K(x_i, x_j) - \sum_{i=1}^n \alpha_i$

Subject to: •  $\forall i \in [n] : 0 \leq \alpha_i \leq C$

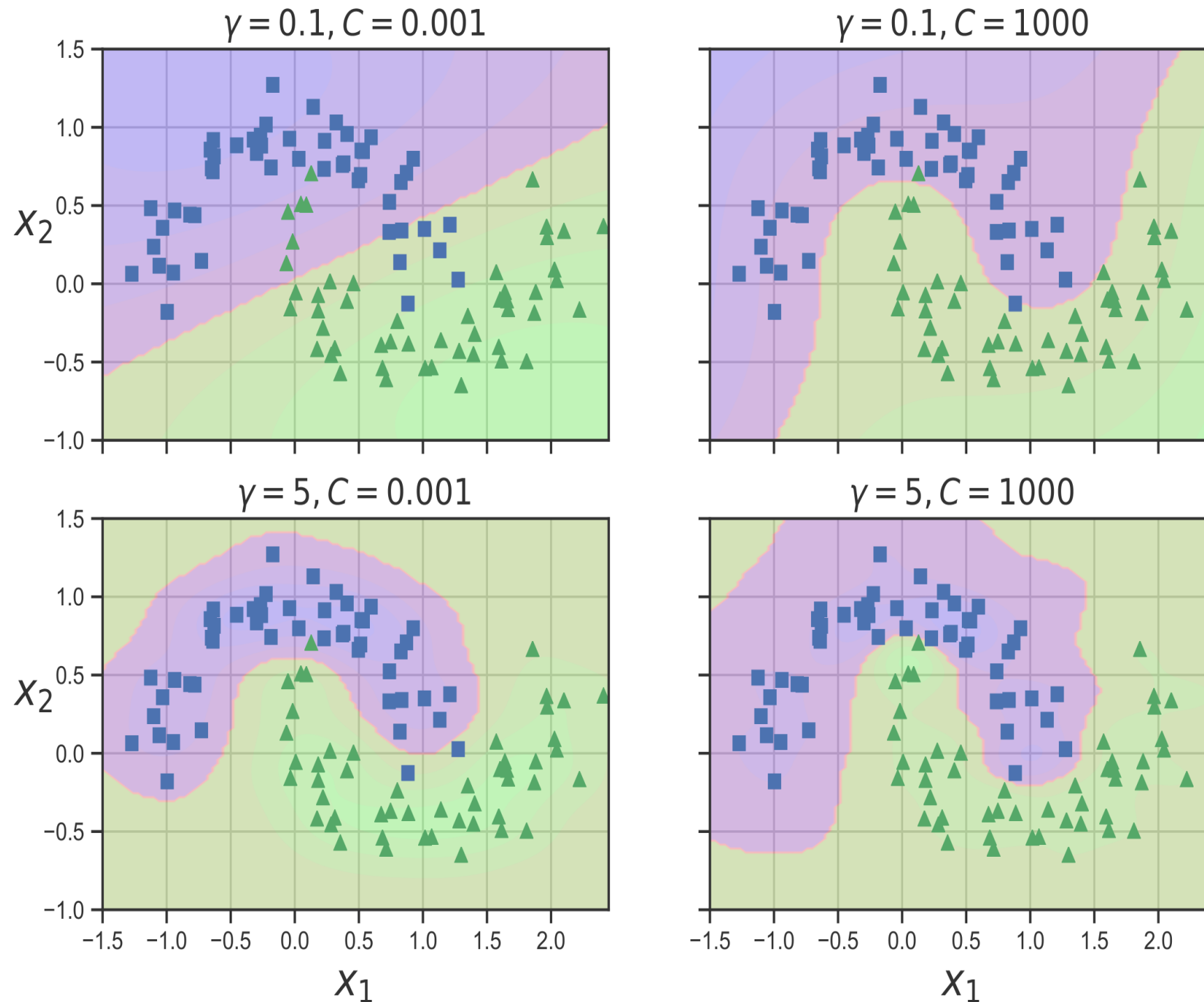
$$\bullet \sum_{i=1}^n \alpha_i y_i = 0$$

Then:

$$\bullet f(t) = \sum_{i \in S} \hat{\alpha}_i y_i K(x, x_i) + \hat{w}_0$$

$$\bullet \hat{w}_0 = \frac{1}{|S|} \sum_{i \in S} \left( y_i - \sum_{j \in S} \hat{\alpha}_j y_j K(x_j, x_i) \right)$$

# Kernel trick with SVM



Minimize:  $\sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j K(x_i, x_j) - \sum_{i=1}^n \alpha_i$

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Then:

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Exmple with  $K(x, z) = \exp(-\gamma \|x - z\|^2)$