# Machine Learning in Physics: Models

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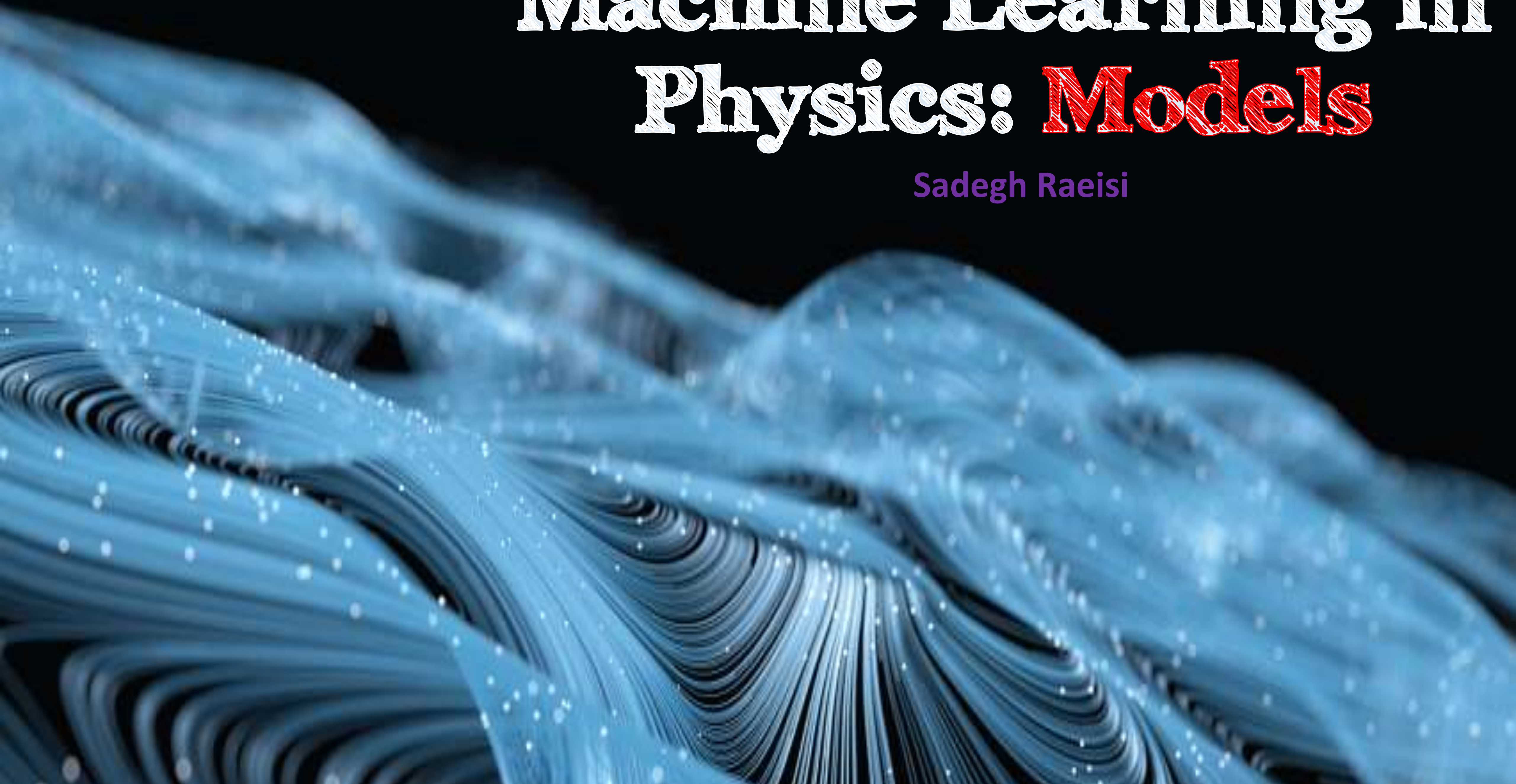
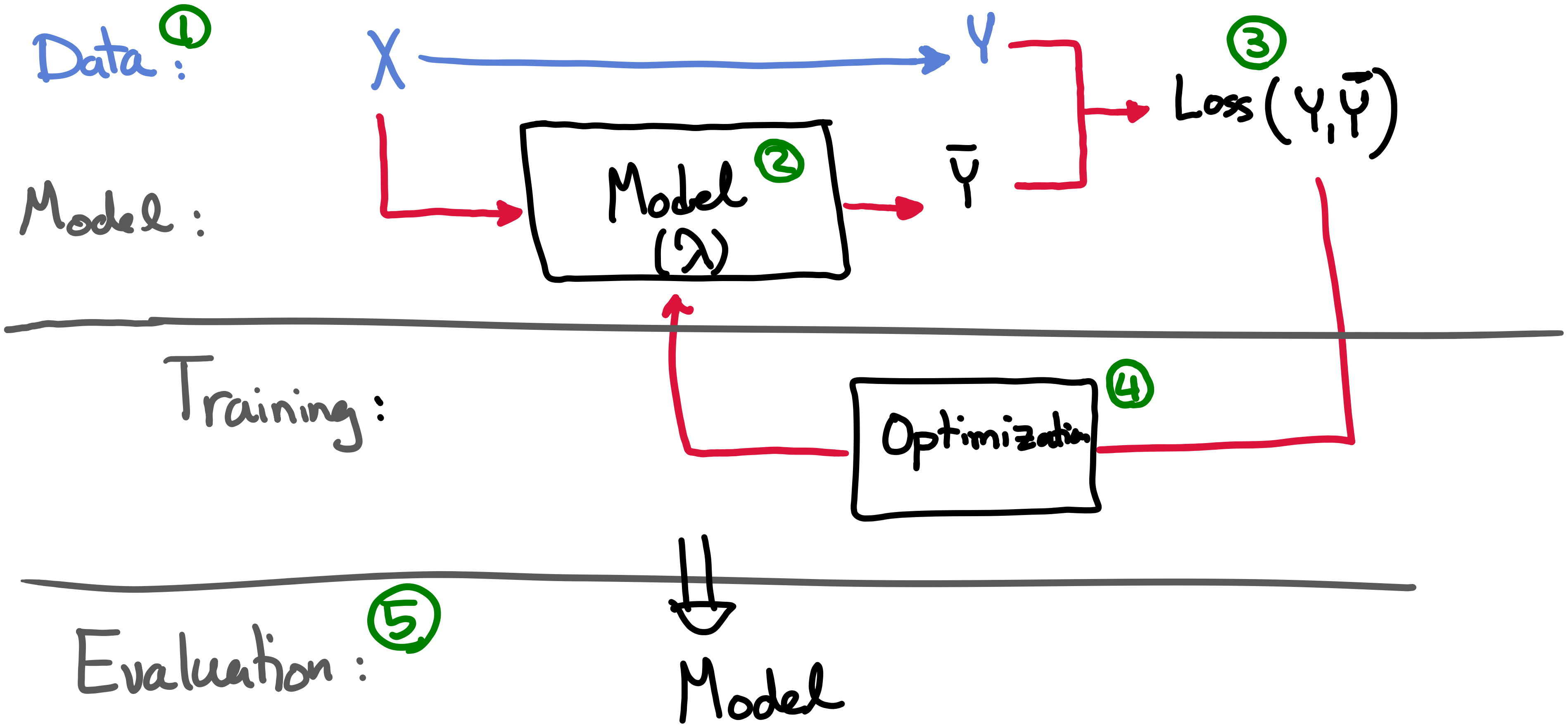


# Supervised: Ingredients



# Outline

- A Simple model
- Linear vs non-linear
- Inherently non-linear models

# Notation

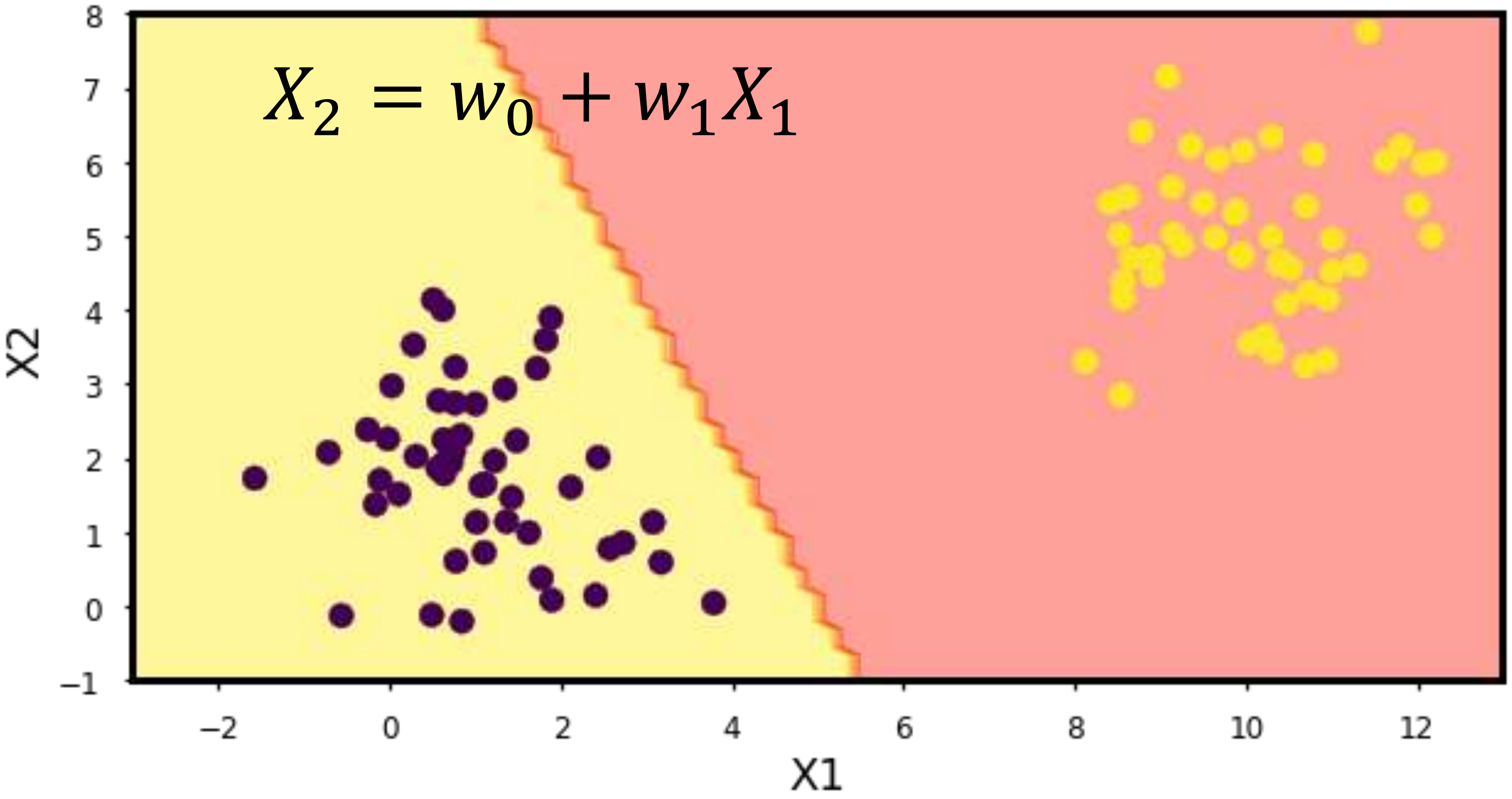
Features of the sample

Label of the sample

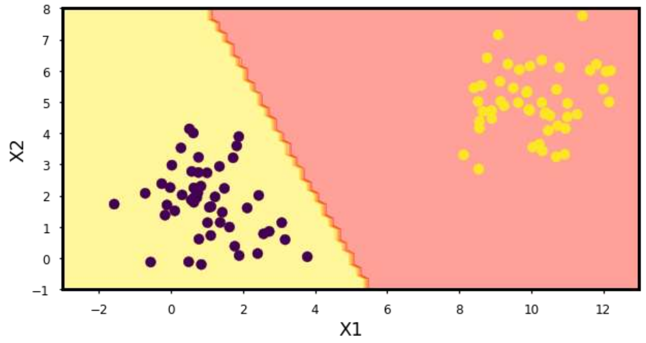
$$f_w(\vec{X}^i) = \bar{Y}$$

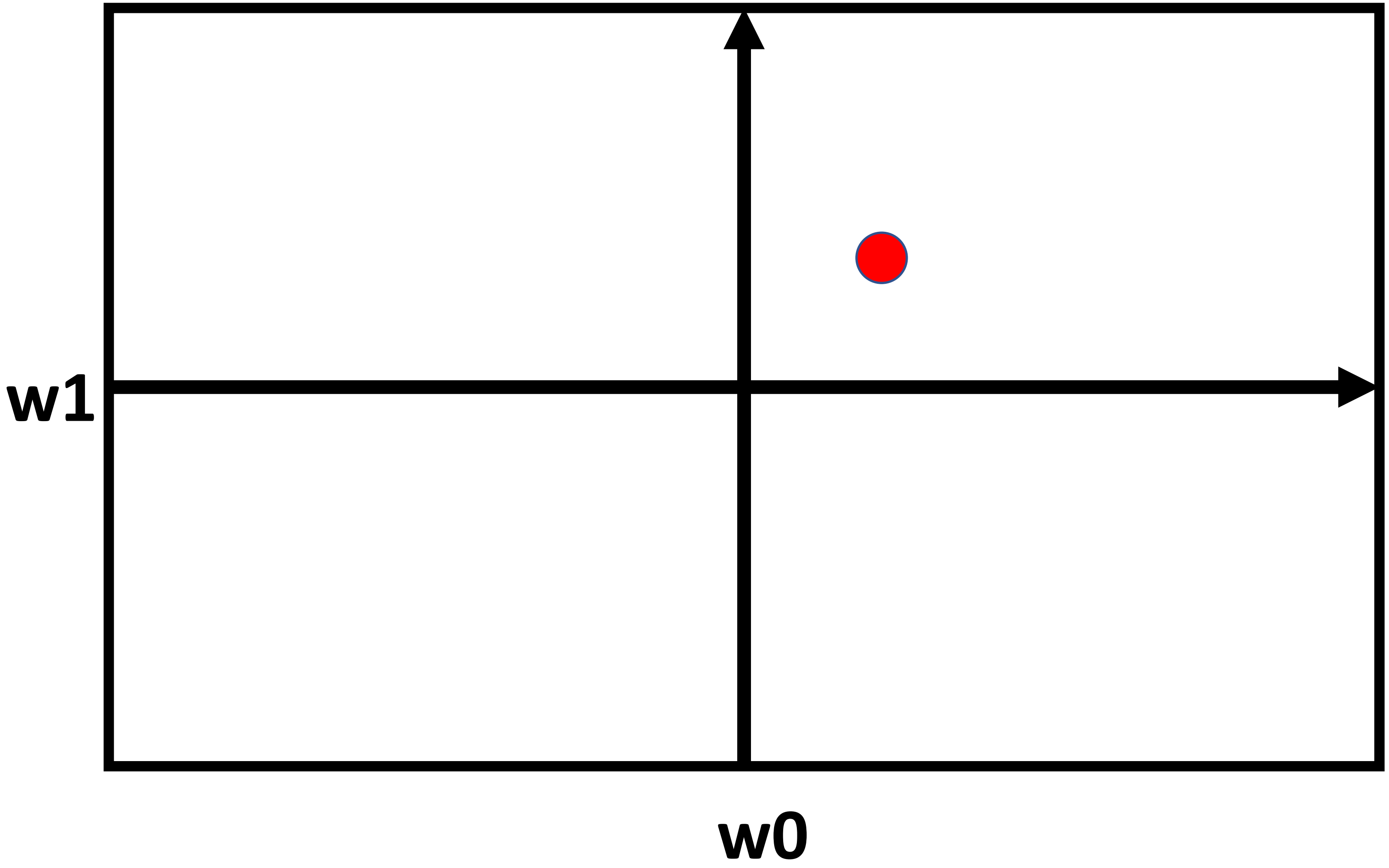
Parameters of the model

# Feature space and decision boundary



# Model space



# A Simple Model

# Simplest model possible

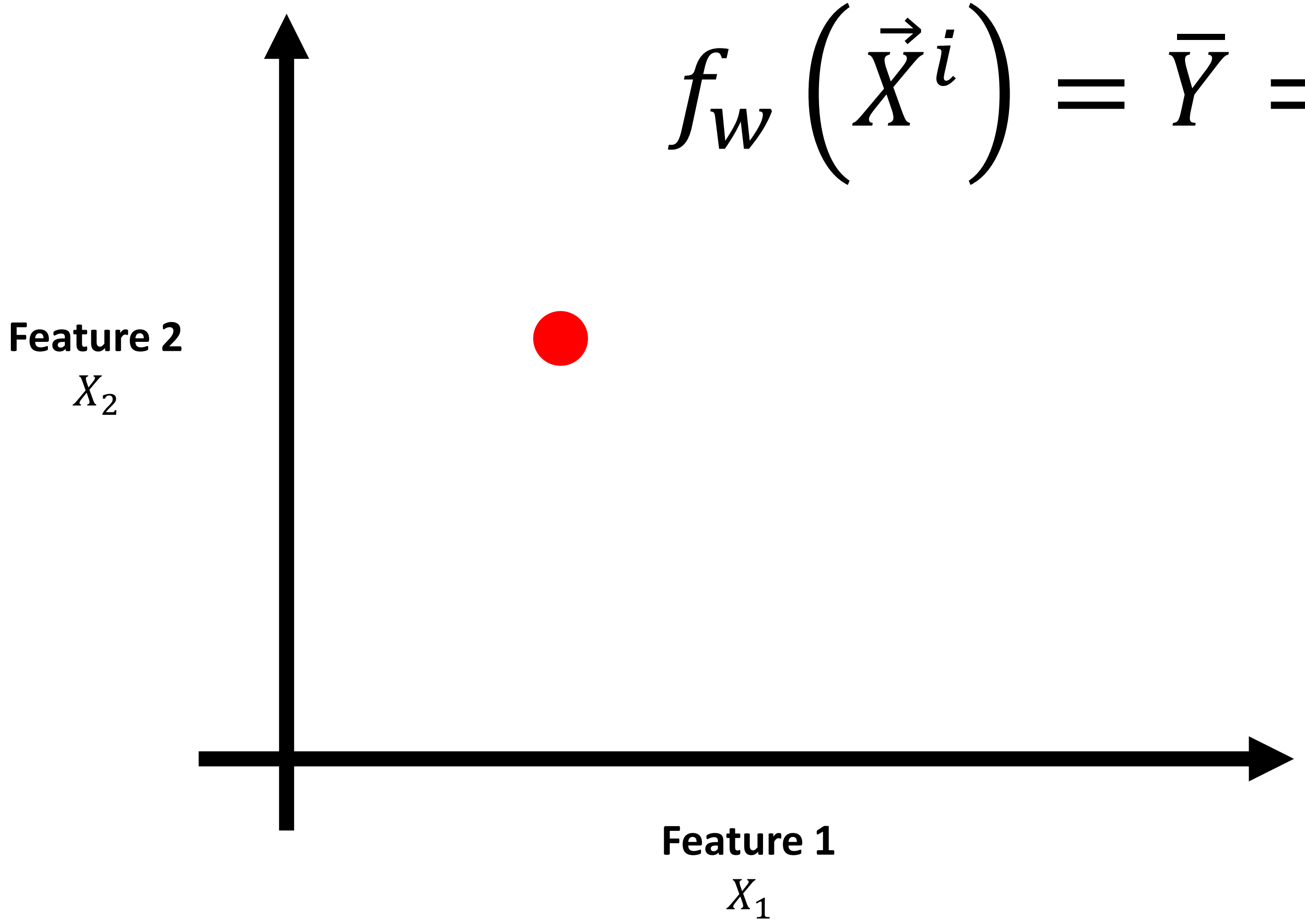
$$f_w\left(\vec{X}^i\right) = \text{const.}$$

# Simplest model possible: linear model

$$f_w\left(\vec{X}^i\right) = \sum_j w_j X_j^{(i)}$$

# One sample

$$f_w\left(\vec{X}^i\right) = \bar{Y} = w_2X_2 + w_1X_1 + w_0$$



# Vectorization

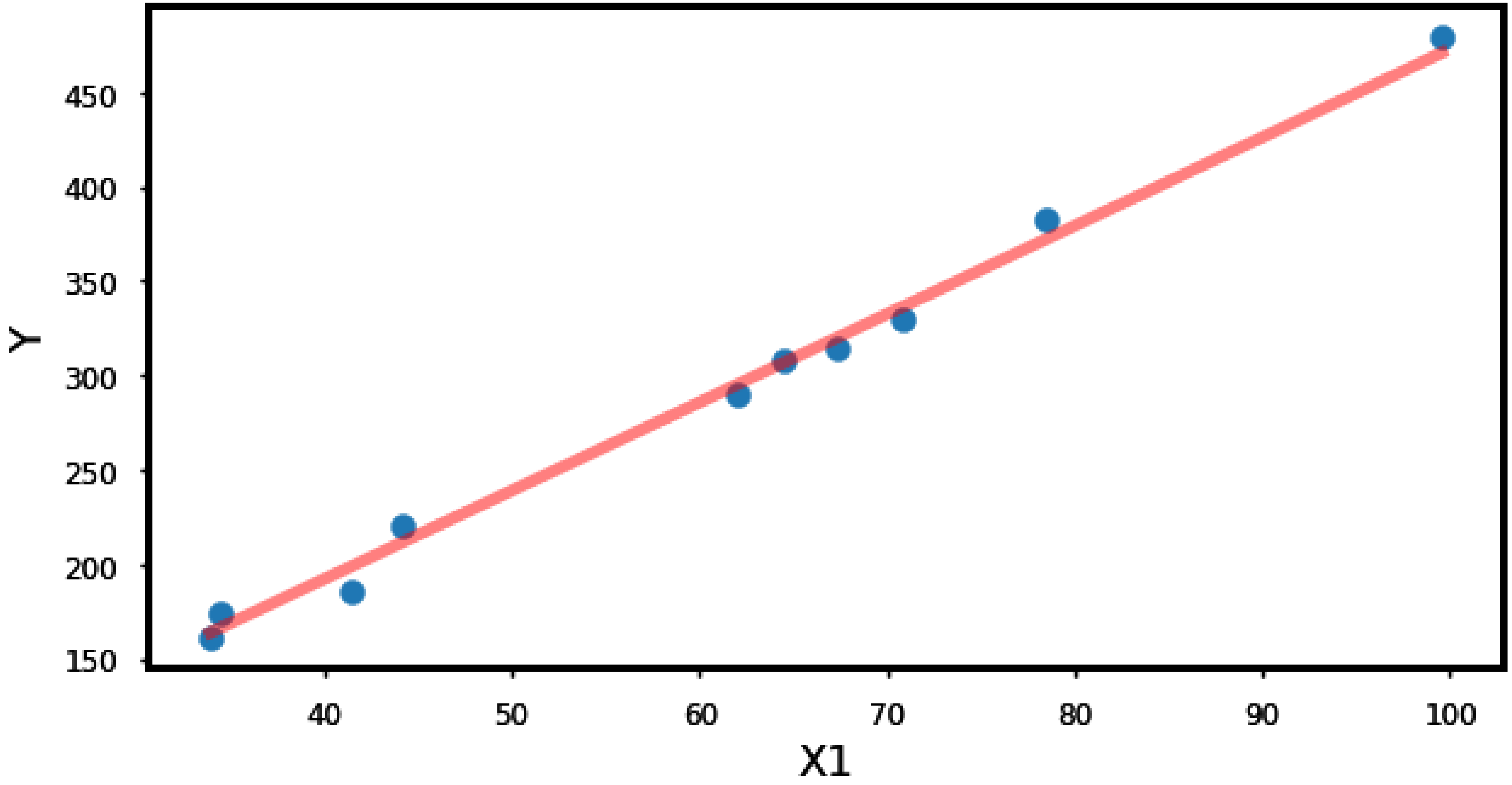
$$f_w\left(\vec{X}^i\right) = \sum_j w_j \, X_j^{(i)}$$

$$= \vec{w}.\vec{X}^i$$

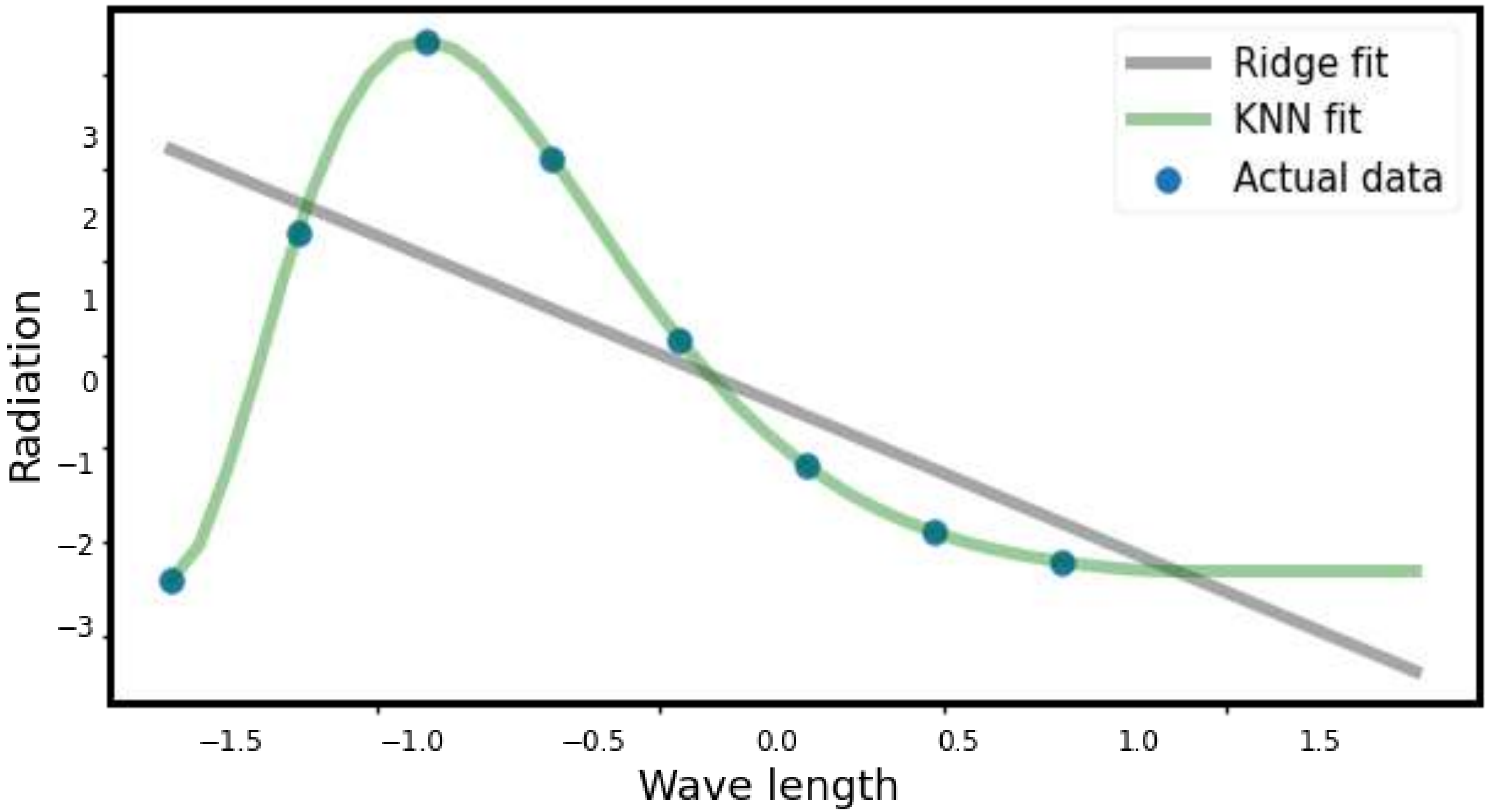
$$\vec{w} = (w_0, w_1, \cdots w_{nf})$$

$$\vec{X} = (1, X_1, \cdots X_{nf})$$

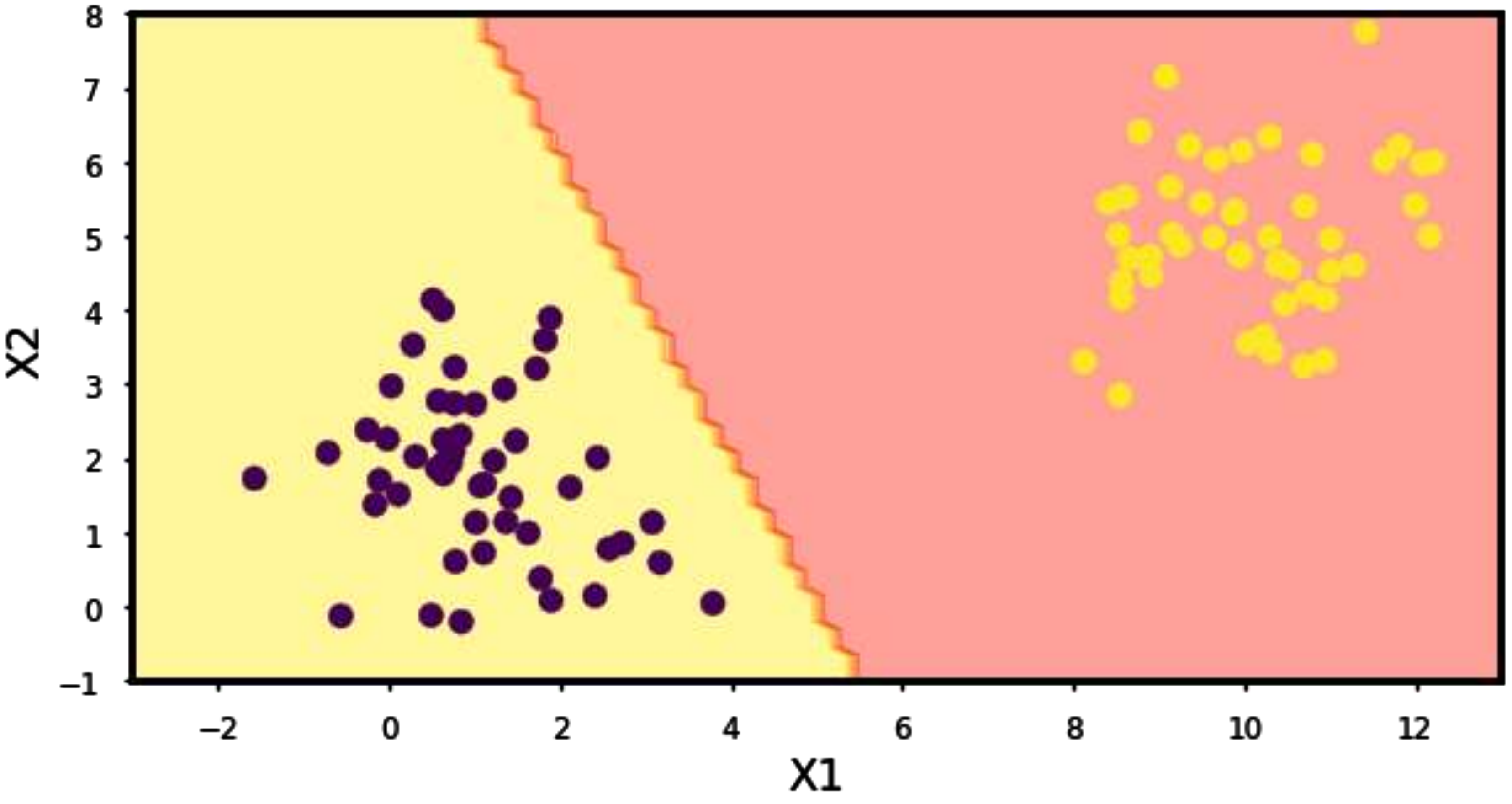
# Regression



# Regression

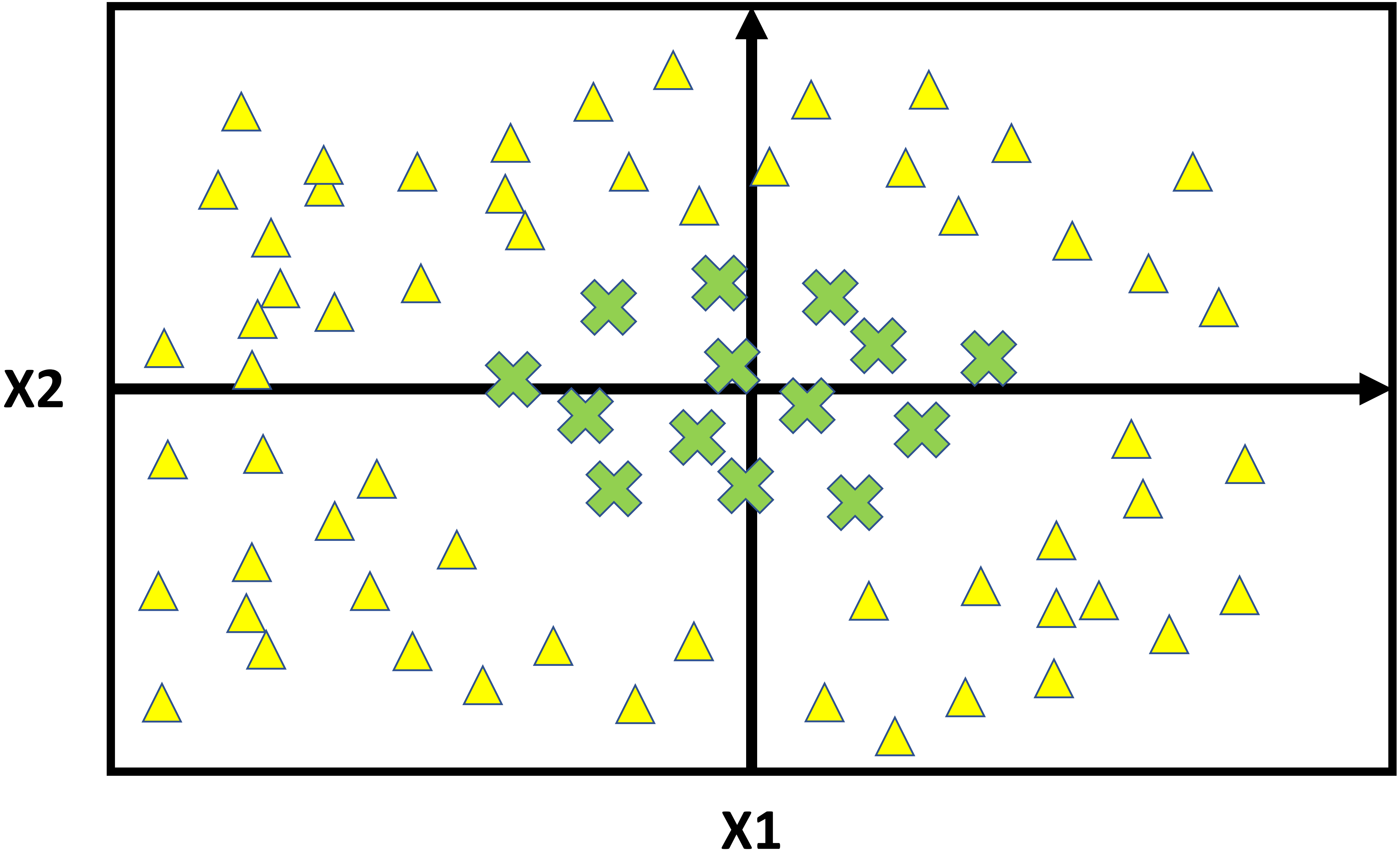

Ridge fit
KNN fit
Actual data
Radiation
Wave length
3
2
1
0
−1
−2
−3
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

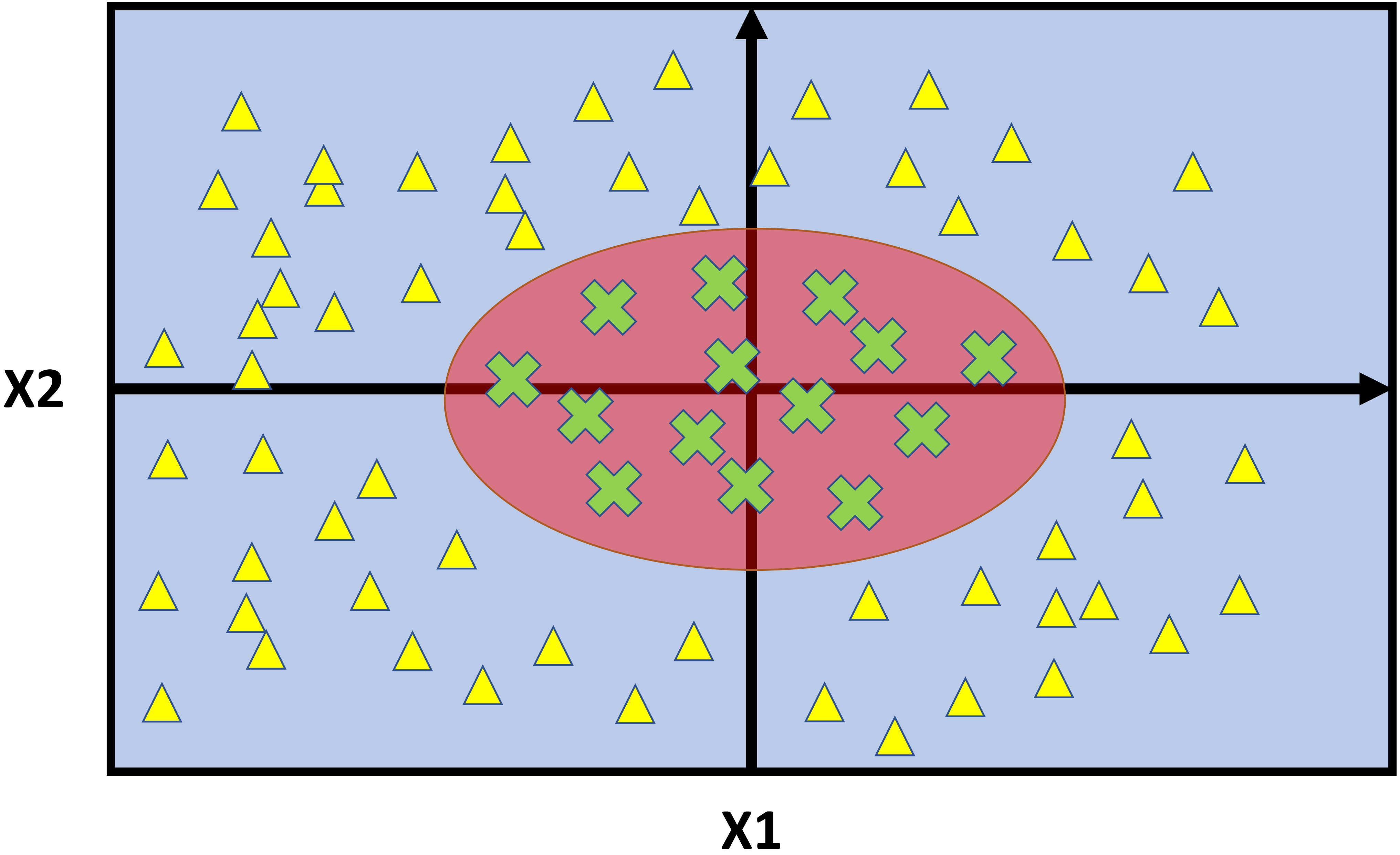
# Classification



# What is a good fit?

# Linear
# vs.
# Non-linear


X2
X1



X2
X1

# Polynomial models

# How can we make a quadratic model?

Example:

$$\vec{X} = (X_1, X_2)$$

$$f_w\left(\vec{X}^i\right) = w_0 + w_1 X_1 + w_2 X_2$$

$$\boldsymbol{+ w_3 X_1^2 + w_4 X_1 X_2 + w_5 X_2^2}$$

# How?

## 1. Feature Transformation

$$\vec{X} \Rightarrow \Phi(X)$$

Example: Quadratic model

$$\vec{X} = (1, X_1, X_2) \quad \Rightarrow \Phi(X) = (1, X_1, X_2, X_1^2, X_2^2, X_1 X_2)$$

# How?

## 2. Kernel

Often we are interested in a scalar product $\langle \nu^{(1)}, \nu^{(2)} \rangle$

$$\begin{tikzcd}
\boldsymbol{\nu}^{(1)}, \boldsymbol{\nu}^{(2)} \arrow[r, Rightarrow] \arrow[dr, Rightarrow] & \boldsymbol{\Phi}(\boldsymbol{\nu}^{(1)}), \boldsymbol{\Phi}(\boldsymbol{\nu}^{(2)}) \arrow[r, Rightarrow] & \langle \boldsymbol{\Phi}(\boldsymbol{\nu}^{(1)}), \boldsymbol{\Phi}(\boldsymbol{\nu}^{(2)}) \rangle \\
& \boldsymbol{K}(\boldsymbol{\nu}^{(1)}, \boldsymbol{\nu}^{(2)}) = \langle \boldsymbol{\Phi}(\boldsymbol{\nu}^{(1)}), \boldsymbol{\Phi}(\boldsymbol{\nu}^{(2)}) \rangle &
\end{tikzcd}$$

# Example:

$$\Phi\left(\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}\right) = \begin{bmatrix} X_1^2 \\ X_2^2 \\ \sqrt{2}X_1X_2 \end{bmatrix}$$

$$\left\langle \mathbf{\Phi}\left(\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}\right), \mathbf{\Phi}\left(\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}\right) \right\rangle$$

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$$= \boldsymbol{X_1^2 Z_1^2 + X_2^2 Z_2^2 + 2X_1X_2Z_1Z_2}$$

# Example:

$$\mathrm{K}(X, Z) = \langle X, Z \rangle^2$$

$$\langle X, Z \rangle^2 = \left\langle \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} \right\rangle^{\mathbf{2}}$$

# Example:

$$\mathrm{K}(X, Z) = \langle X, Z \rangle^2$$

$$\langle X, Z \rangle^2 = \left\langle \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} \right\rangle^{\mathbf{2}} = (\boldsymbol{X_1 Z_1} + \boldsymbol{X_2 Z_2})^{\mathbf{2}}$$

# Example:

$$\mathrm{K}(X,Z) = \langle X,Z\rangle^2$$

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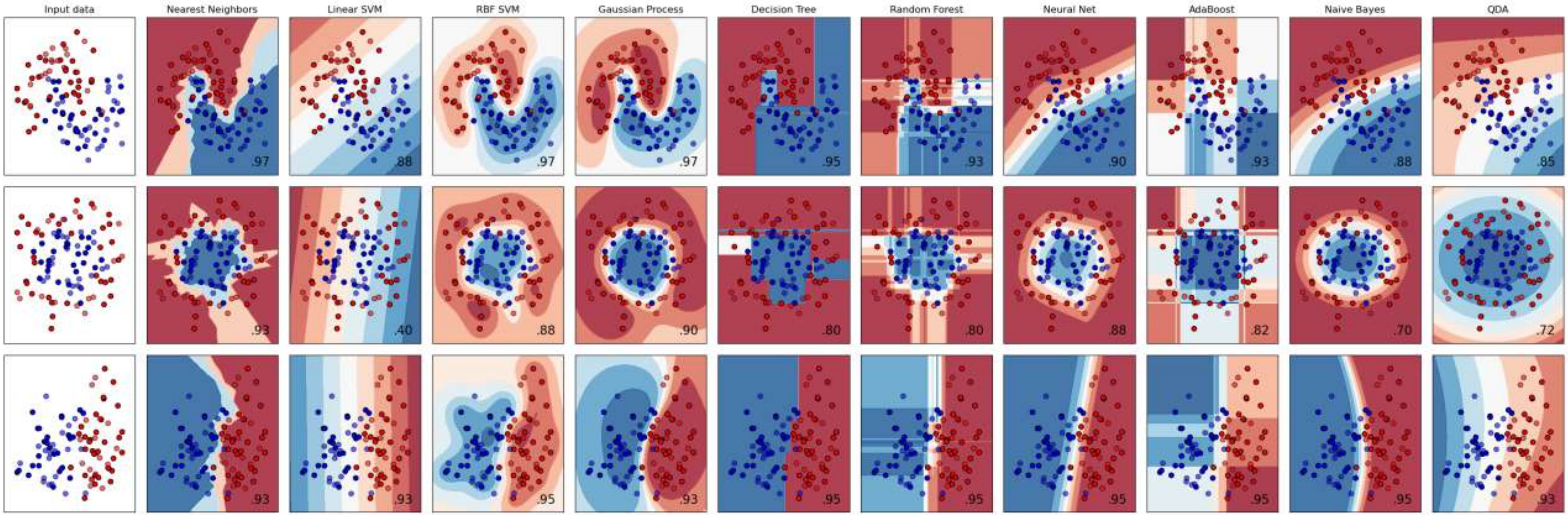
$$= \boldsymbol{X_1^2 Z_1^2} + \boldsymbol{X_2^2 Z_2^2} + \mathbf{2}\boldsymbol{X_1 X_2 Z_1 Z_2} = \left\langle \boldsymbol{\Phi}\left(\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}\right), \boldsymbol{\Phi}\left(\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}\right) \right\rangle$$

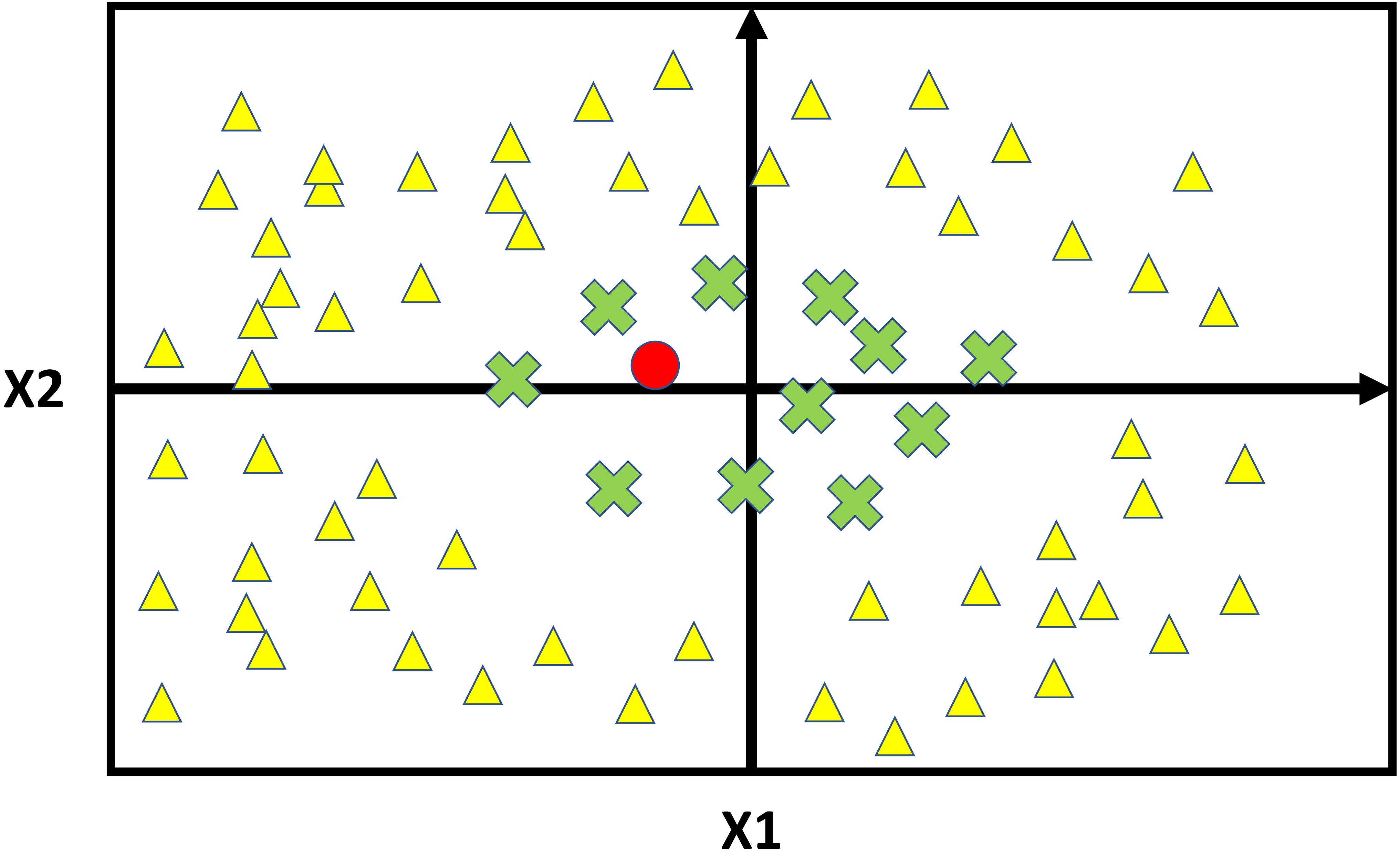
# Inherently non-linear models

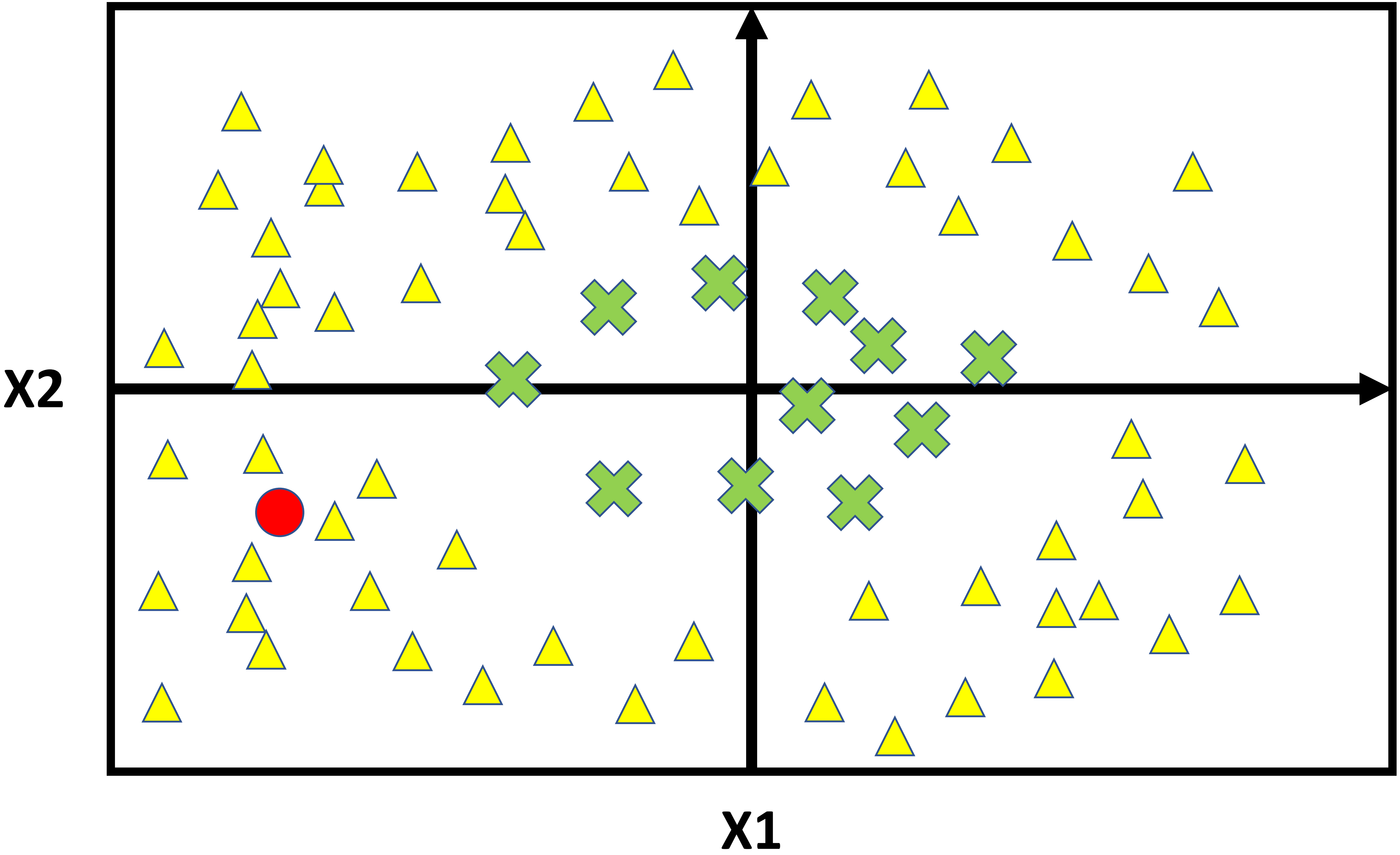
# There are many different techniques …

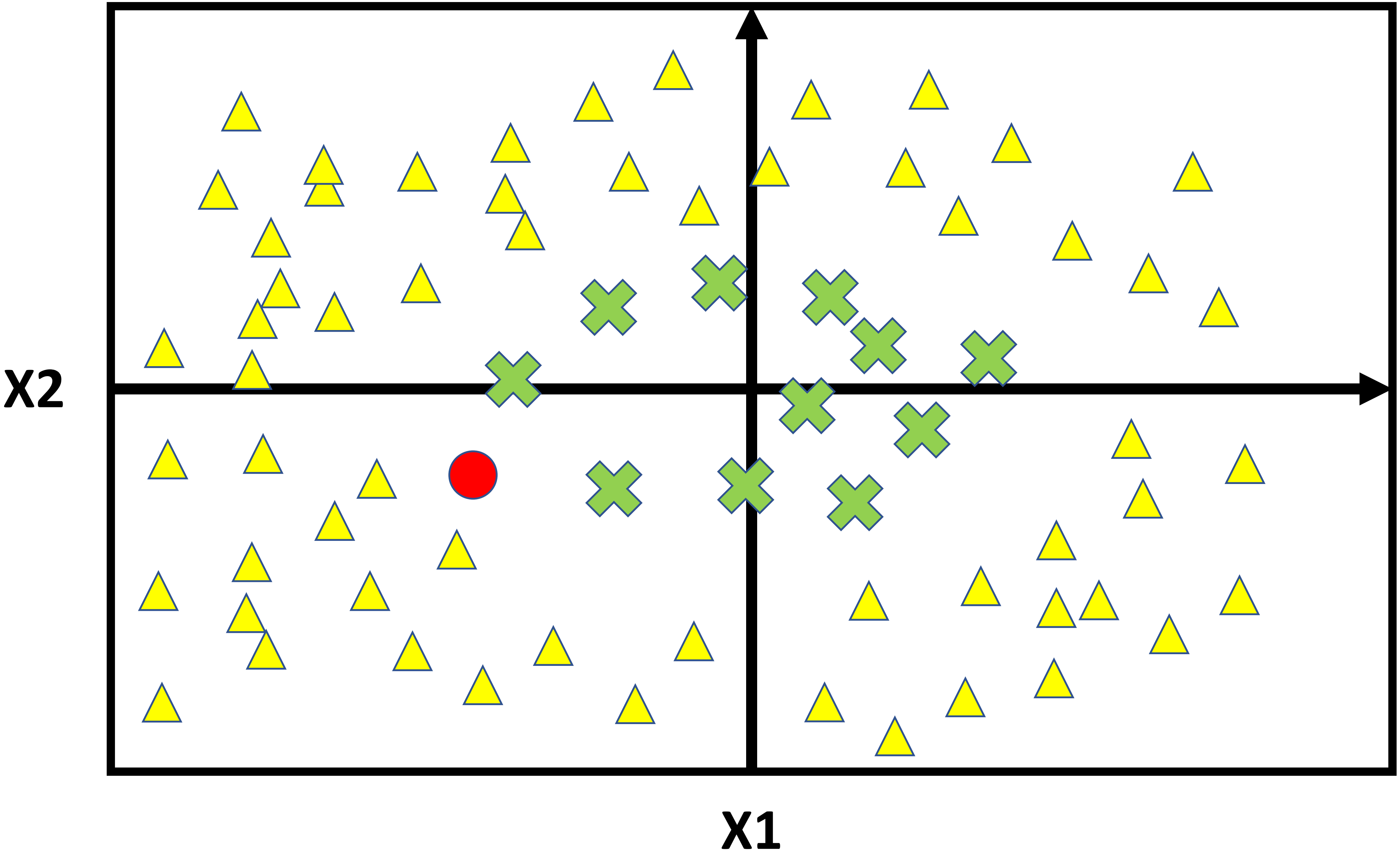



[Classifier comparison — scikit-learn 1.0 documentation]()

# K Nearest neighbours KNN


X2
X1


X2
X1


X2
X1

# Variables of the KNN model

- How many neighbours?
- Policy?
  - Majority
  - Weighted distance
- Metric

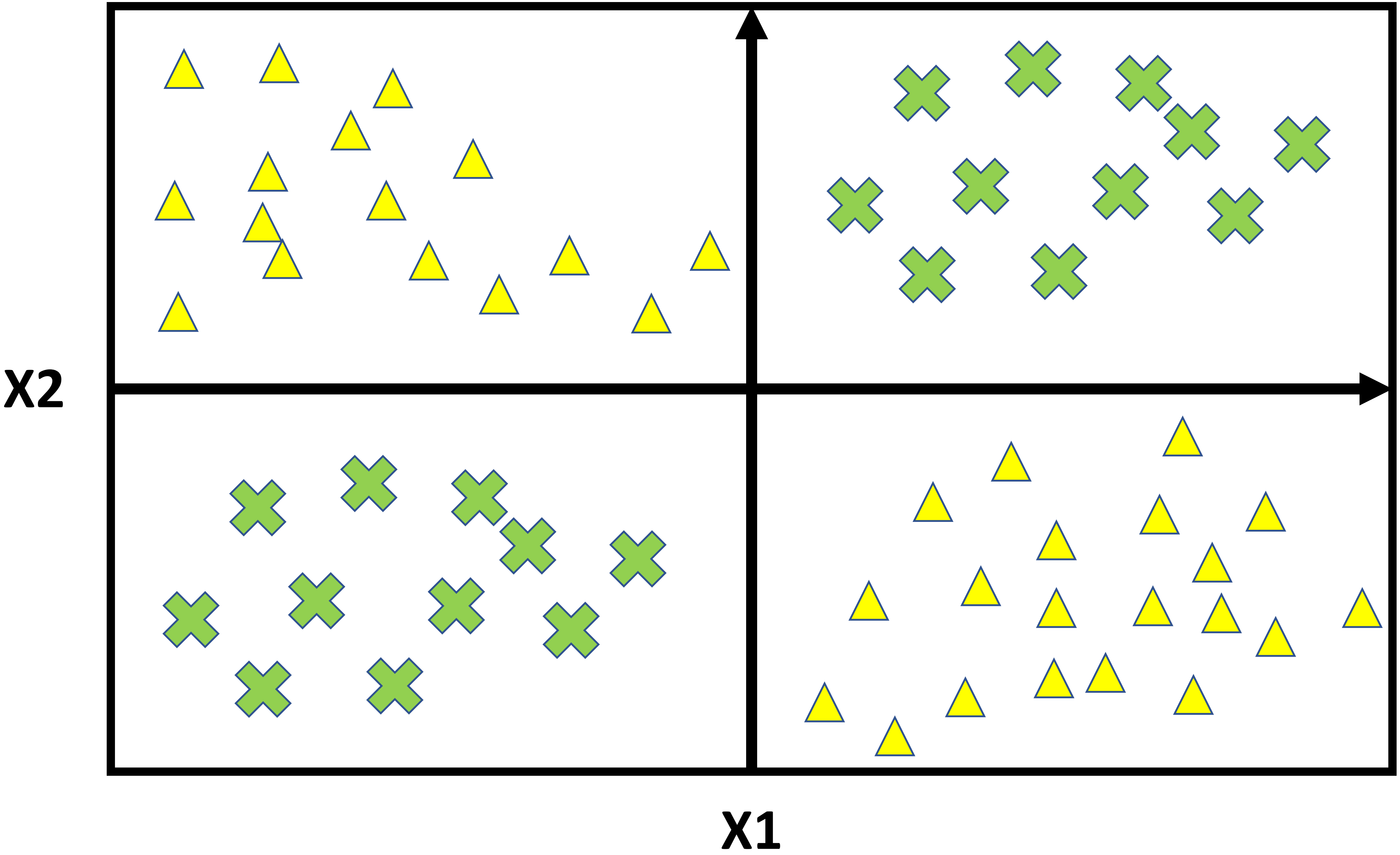
# Learning vs memorizing

- Training is roughly equivalent to storing all the data points
- Prediction:
    - Cross-checking the input with the stored data points.

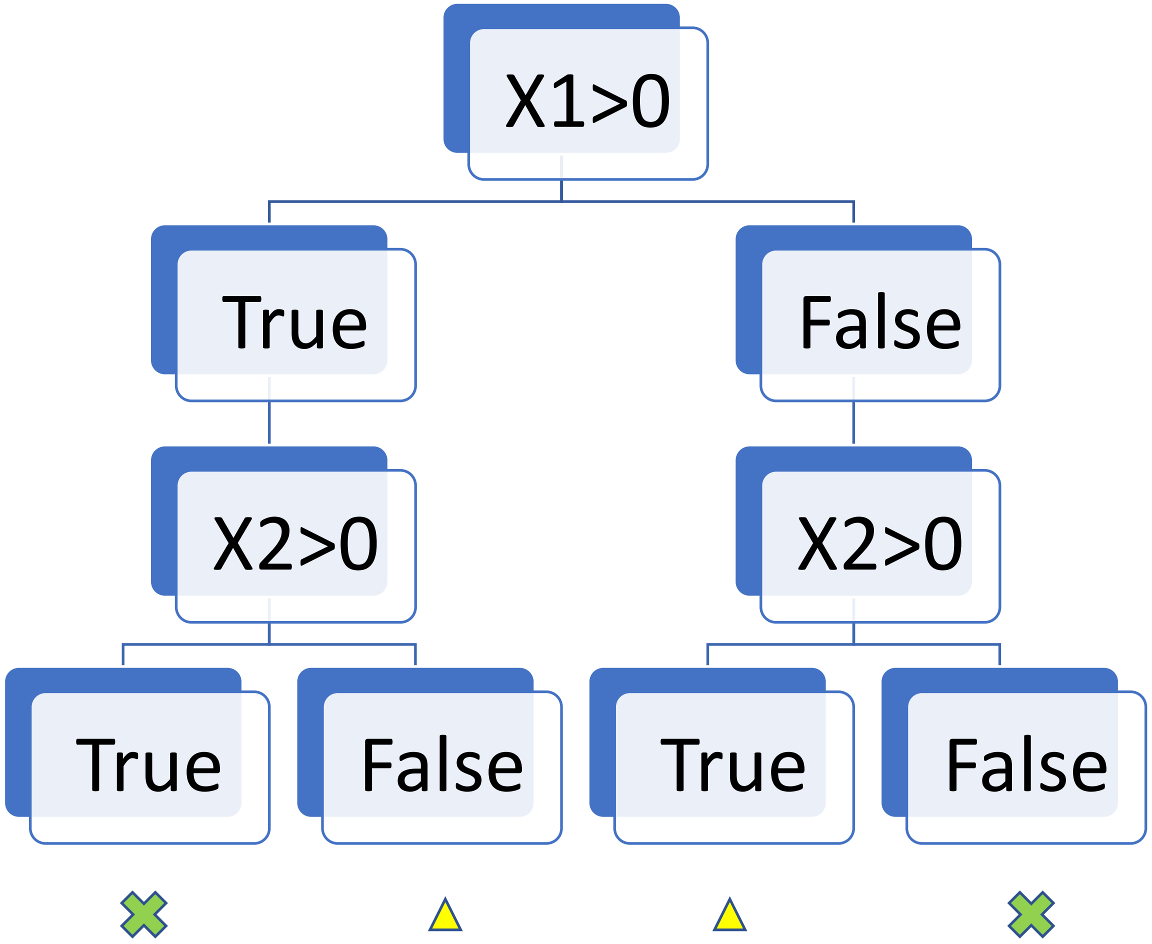
# What happens if

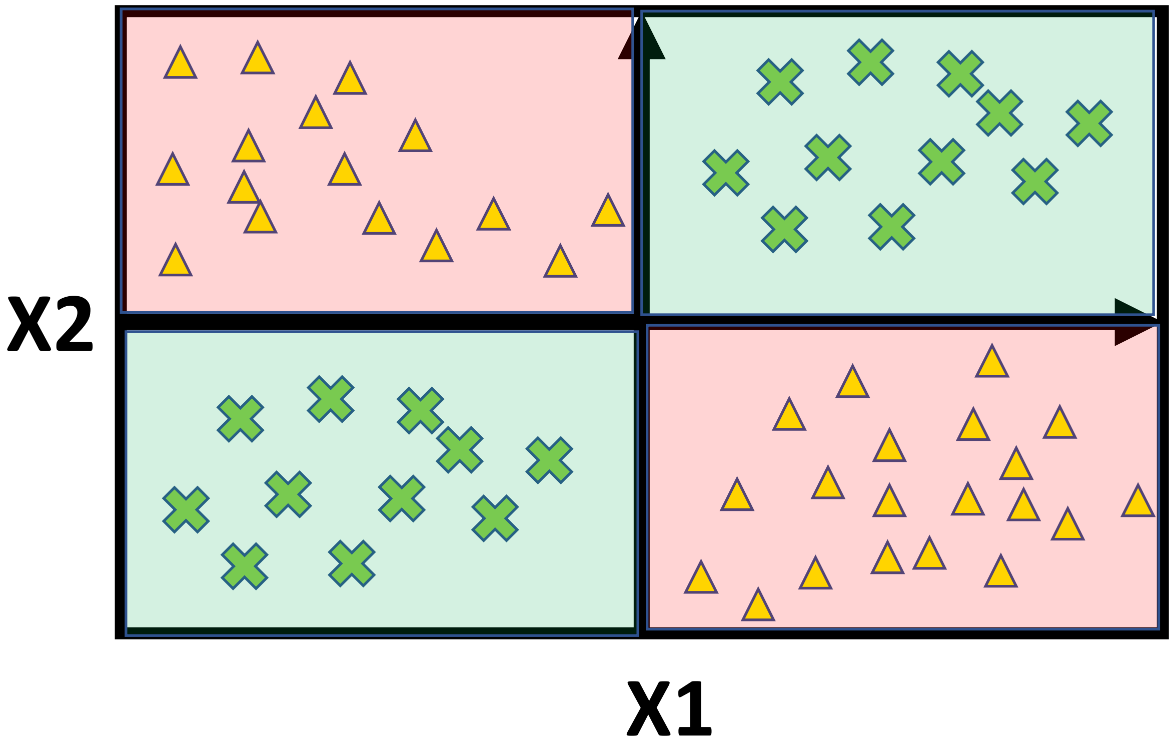
- $k \to n_s$?
- $k \to 1$?

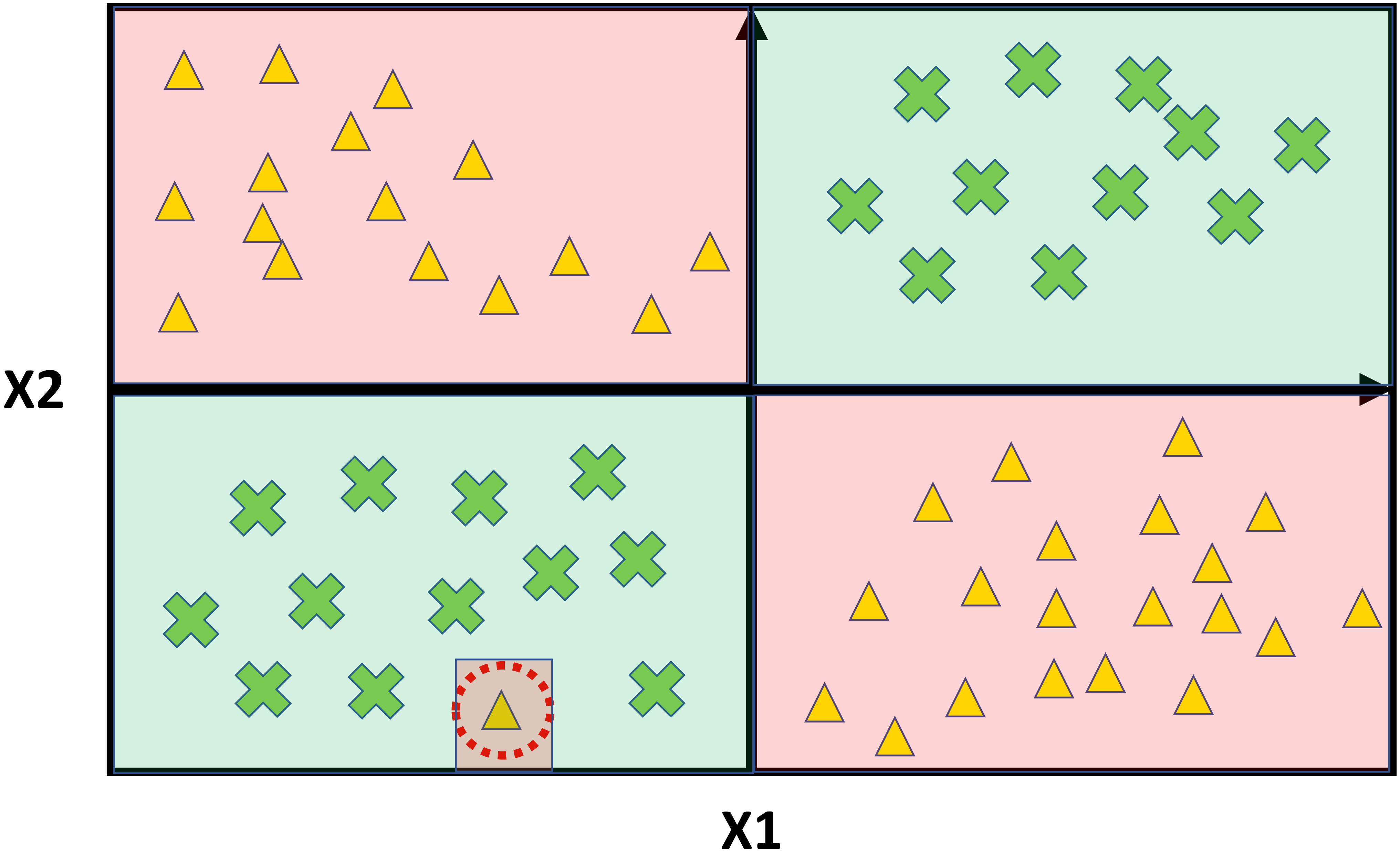
# Decision Trees


X2
X1

# Decision tree




X2
X1

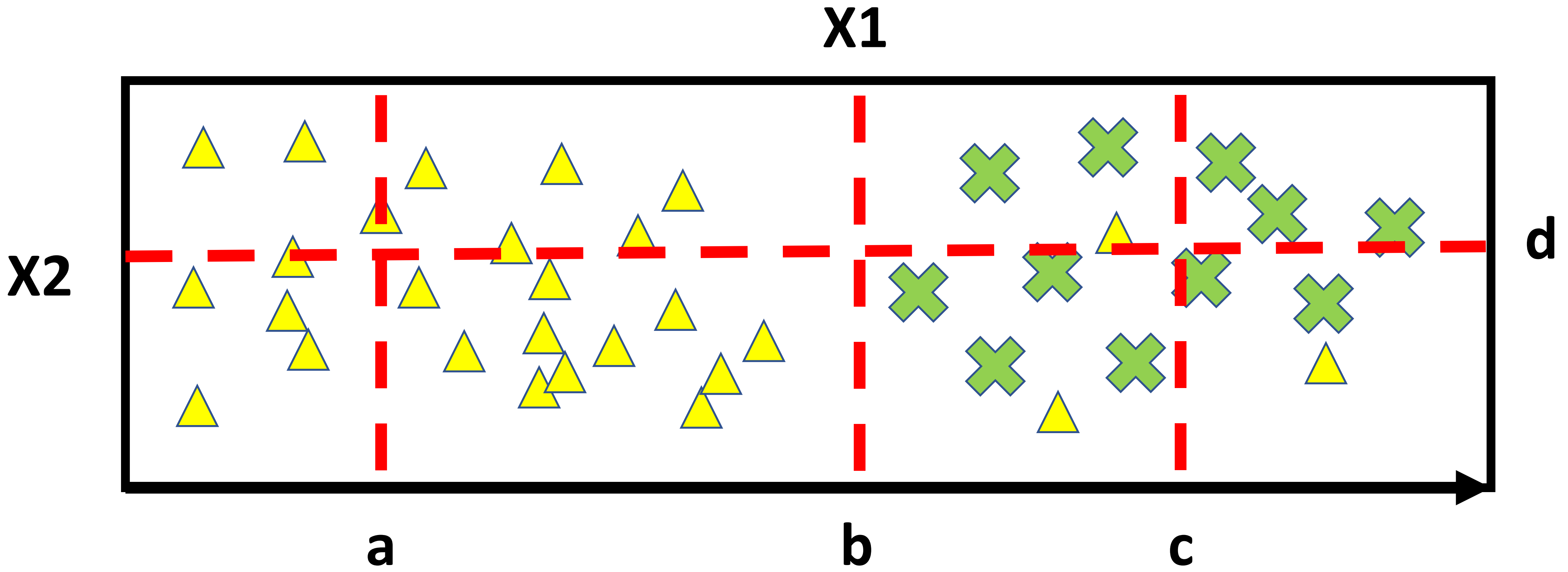
# What is the main variable?

Depth of the tree

# What happens if $depth \to \infty$?

# What are we optimizing?
# What is the objective?

- What is the most informative questions to ask?
  - Information gain
  - Variance reduction




X2 > d

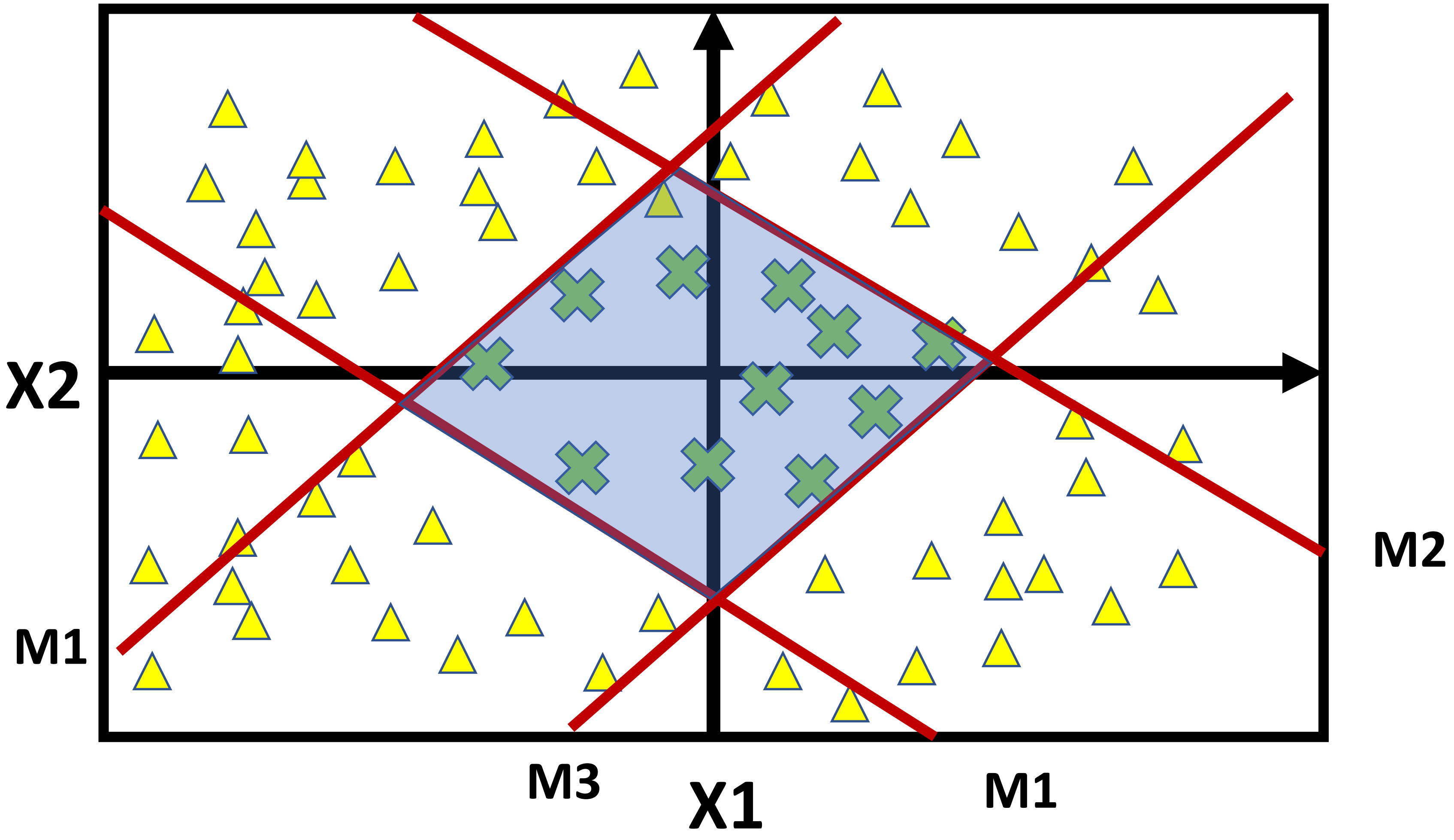
X1 > a

X1 > b

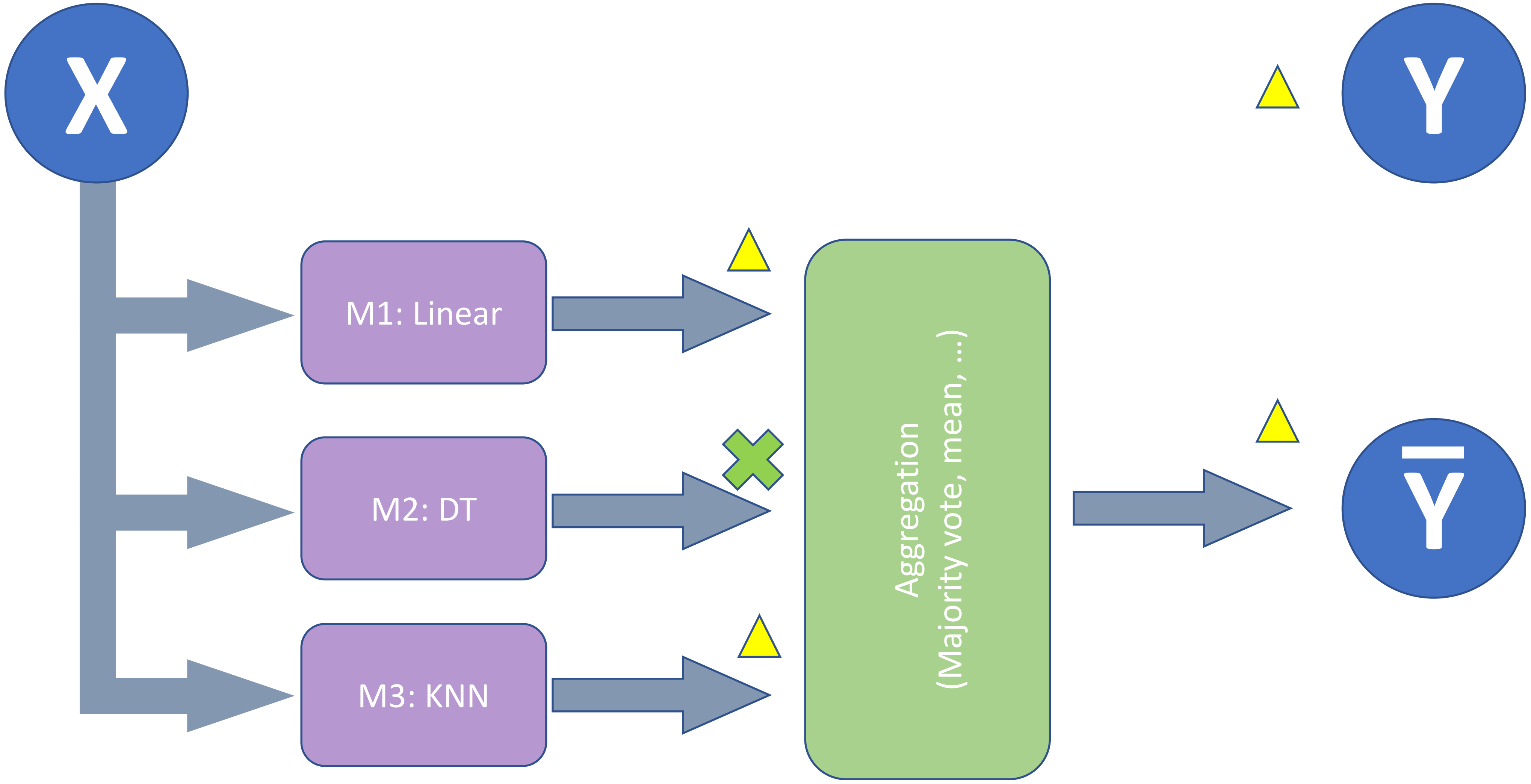
X1 > c

# Ensemble Techniques

# Intuition

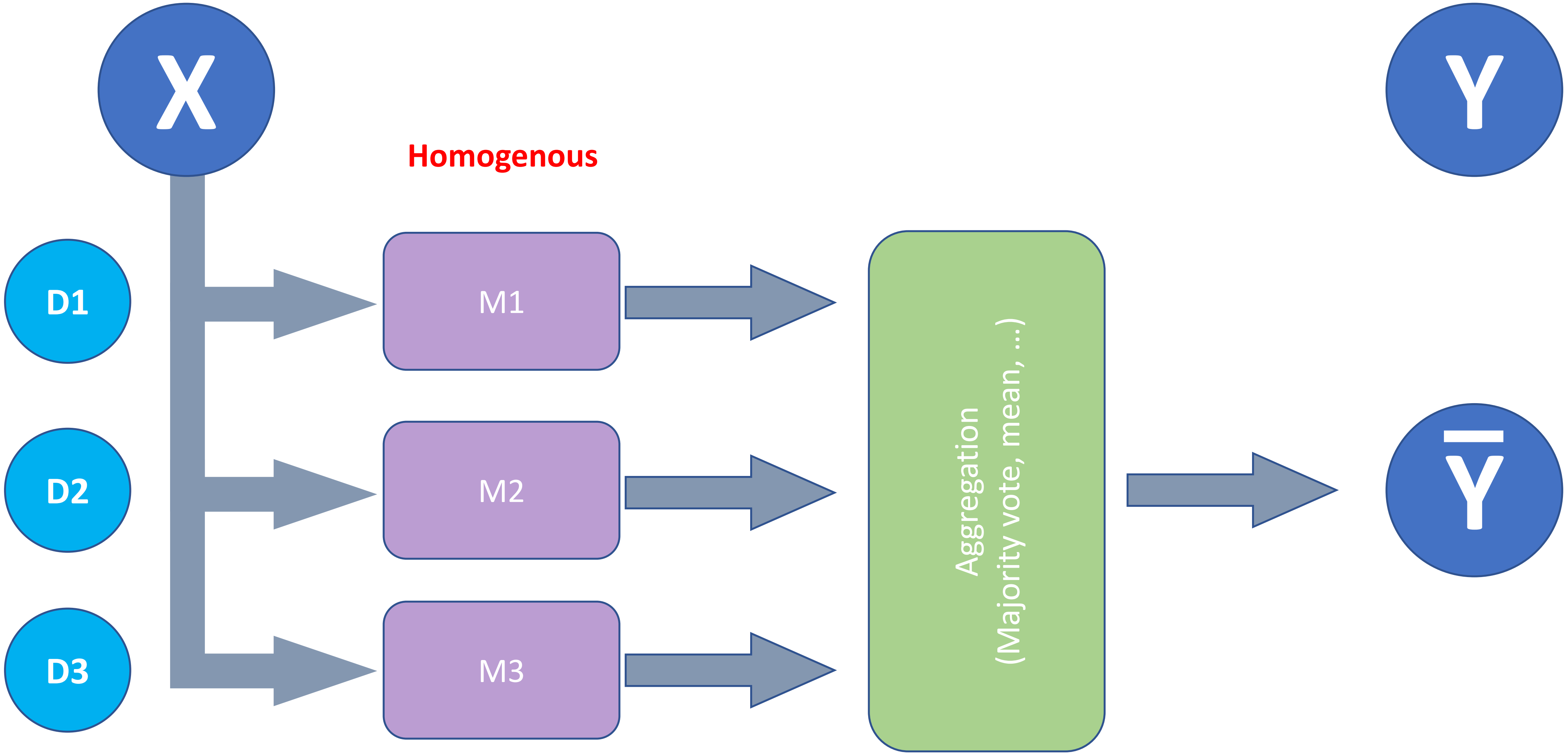


# Simplest way to aggregate models



# Bagging (Bootstrap aggregating)

$D_i$ is a subset of X.



# Example of Bagging: Random Forest

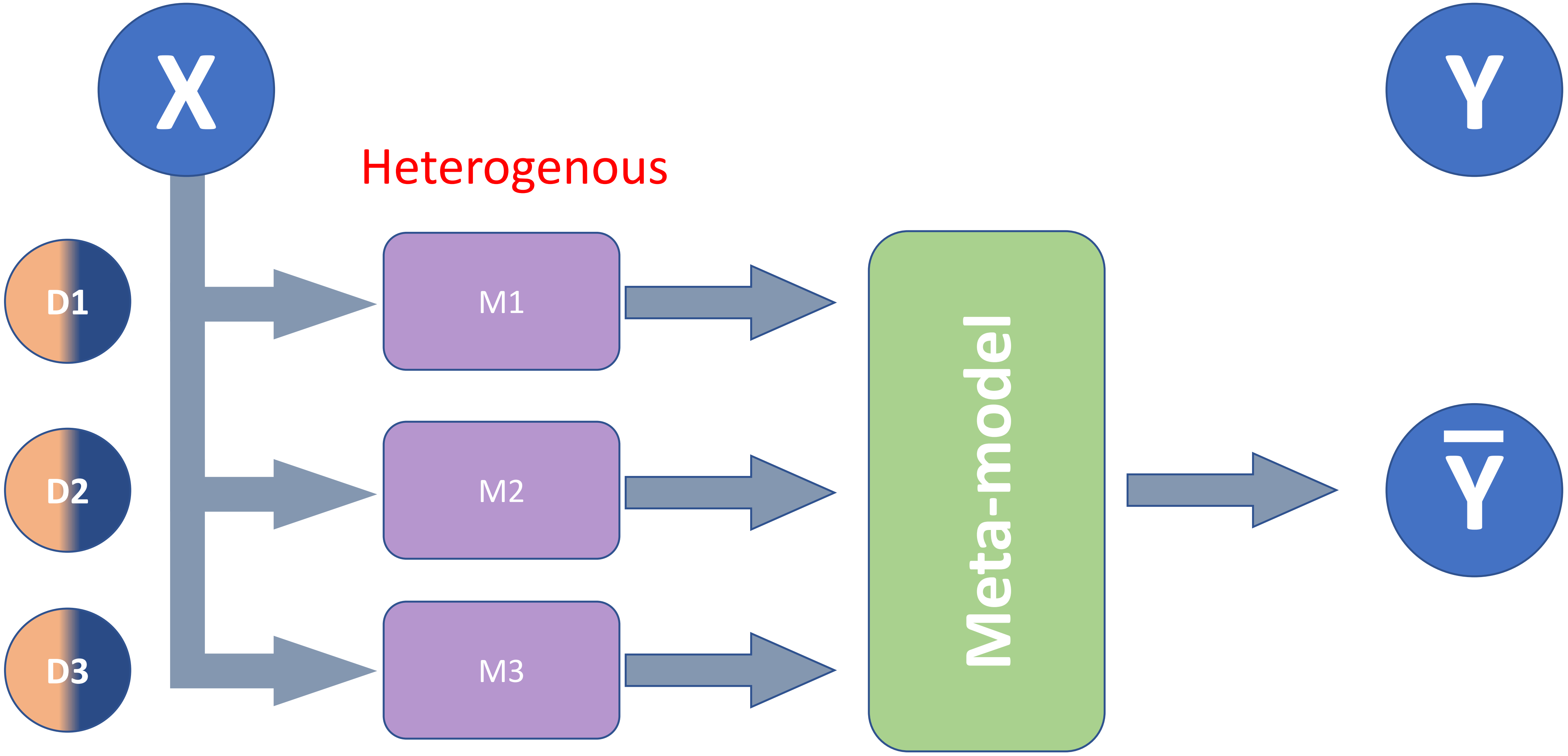
# Boosting

- Sequential improvement

  Put more emphasis on the mislabelled samples and try to force the models to do better.

- Examples:
  - Adaboost
  - Gradient boosting

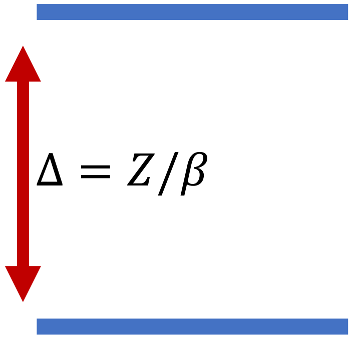
# Stacking



# Activation Function: Logistic Regression

$$f_w\left(\vec{X}^i\right) = \left(\sum_j w_j \, X_j^{(i)}\right)$$

$$\text{Sigmoid}(Z) = \frac{1}{1 + e^{-Z}}$$



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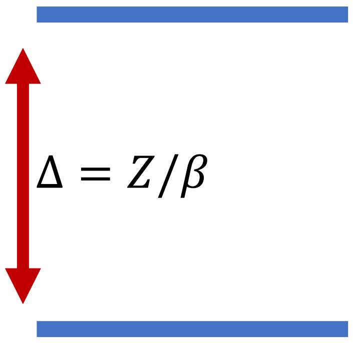
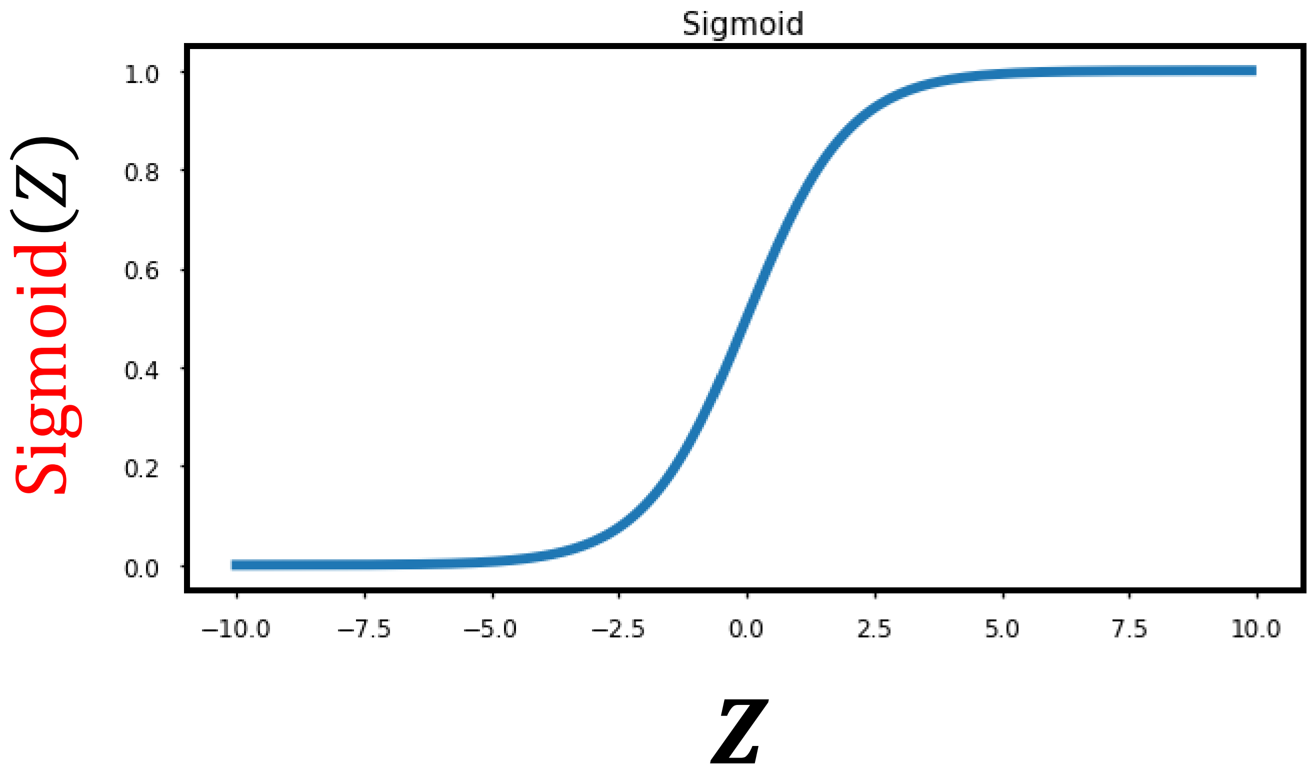


# Is this a linear or non-linear model?

How can we use
activation functions
to make
non-linear Models?

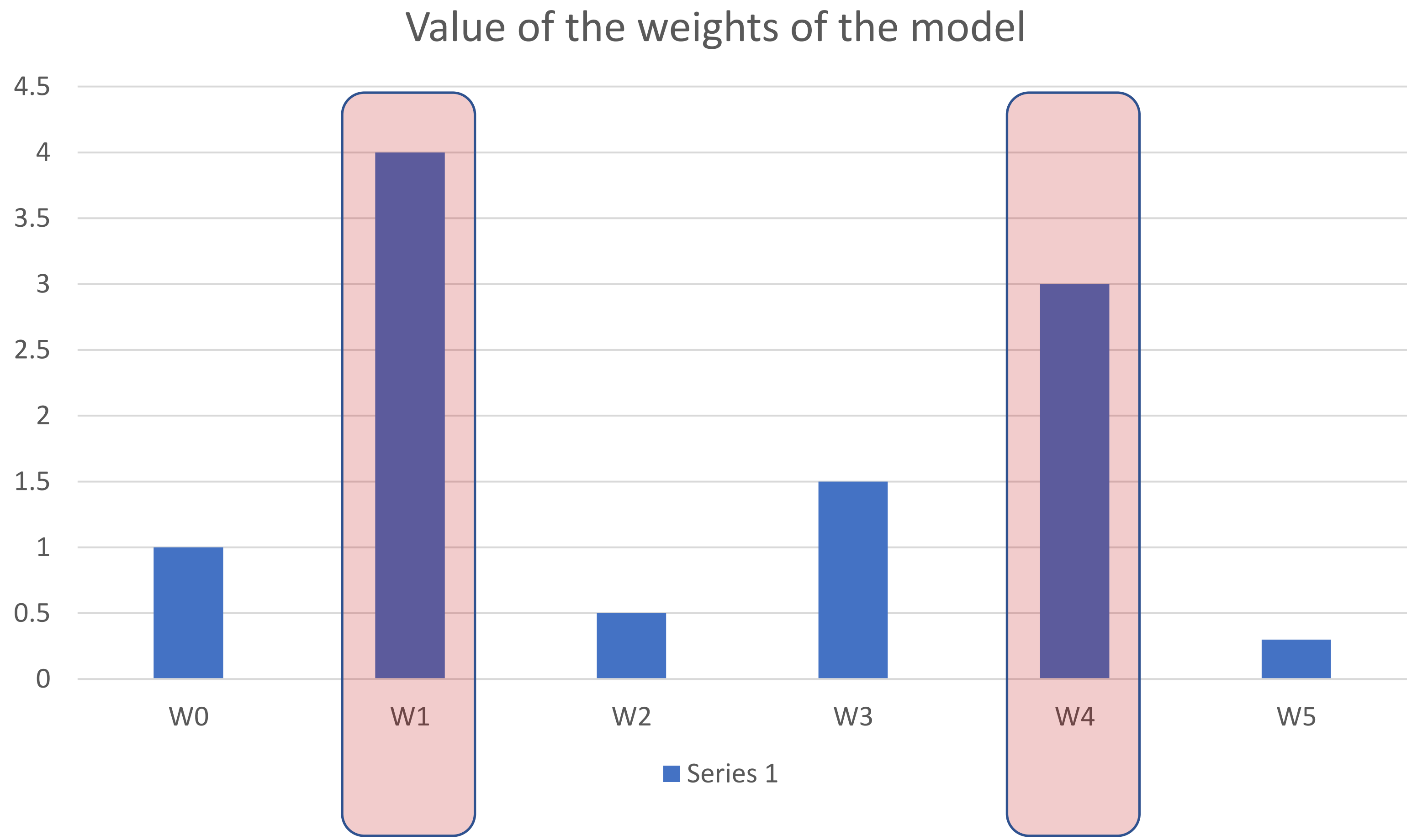
# Importance of Features

# How can we define the importance of features?

Which one is more important?
Some ordering in the significance of different features

# Linear models

$$f_w\left(\vec{X}^i\right) = \sum_j w_j X_j^{(i)}$$



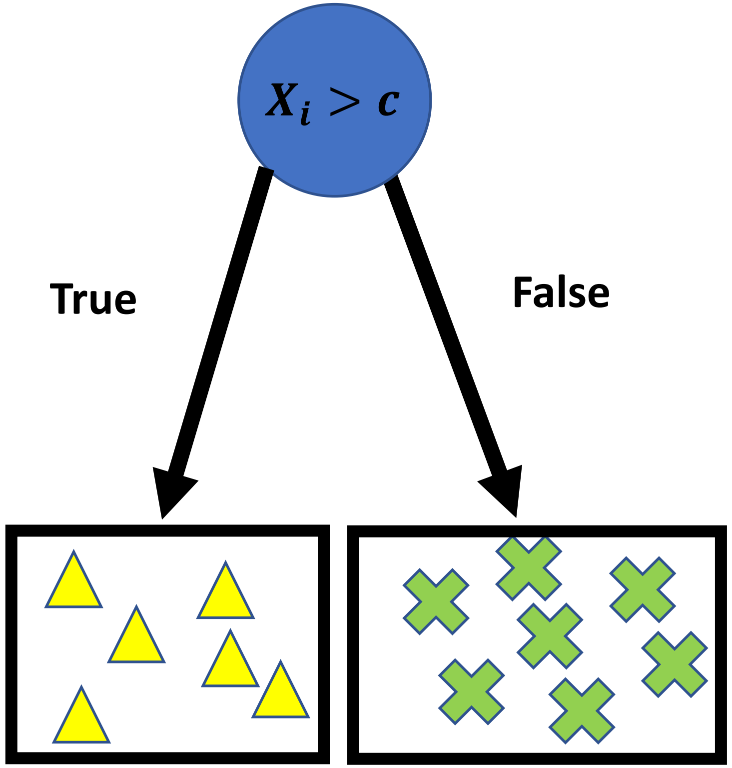
# Decision trees

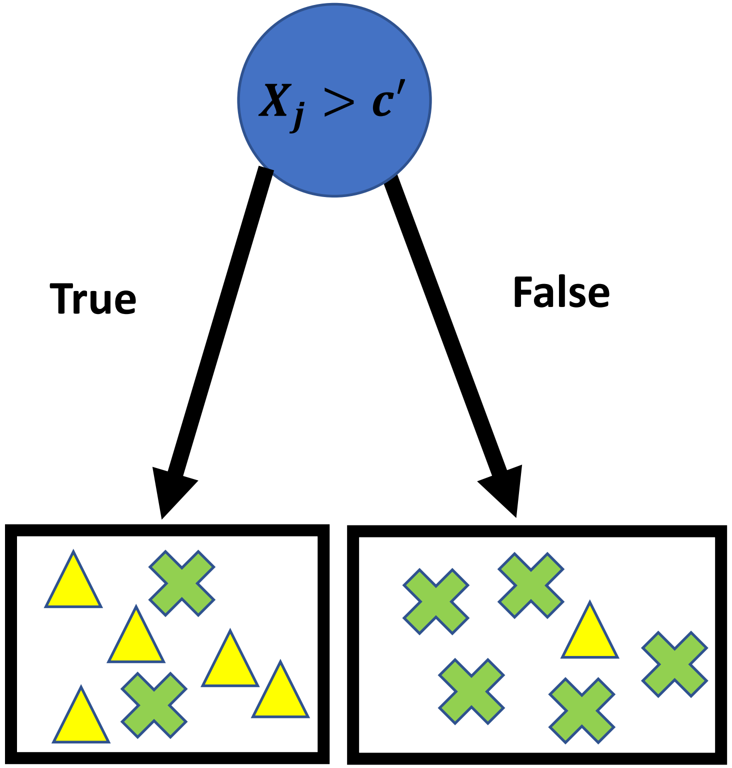
How can we define feature importance?

Information gain/Change in variance

# Information gain/Change in variance

Which is better?



# KNN

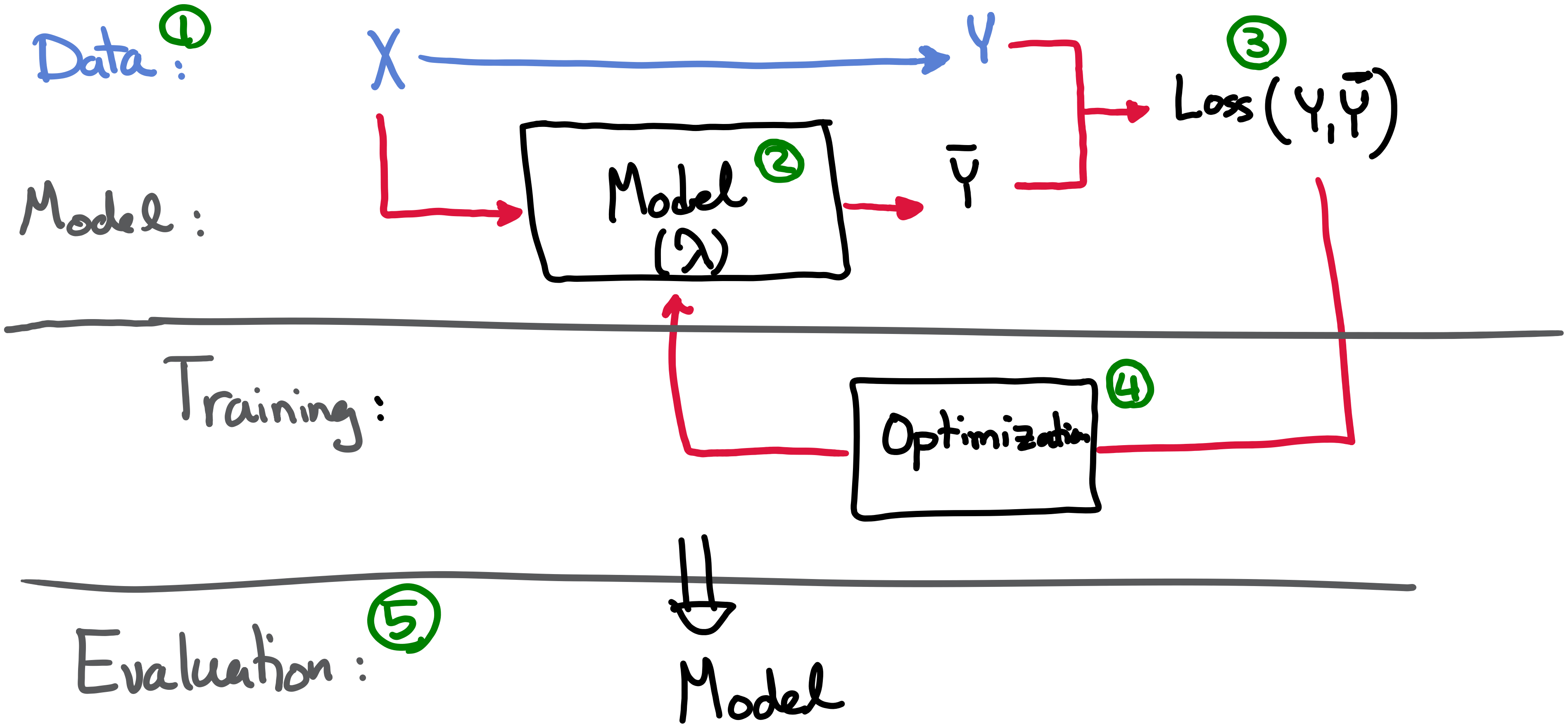
How would you define feature importance for KNN?

# Which Model?

# Comparison

| | Linear | DT | KNN | Random Forest |
|---|---|---|---|---|
| Performance | | | | |
| Idea | | | | |
| Training time | | | | |
| Prediction time | | | | |
| Explainability/ Interpretability | | | | |
| | | | | |

# So far …


Data: ①
X
Y
Model: 
Model ② (λ)
Ȳ
③ Loss(Y, Ȳ)
Training:
Optimization ④
Evaluation: ⑤
Model