Mondragon Unibertsitatea
Escuela Politécnica Superior

Preprocessing

What? When? How?
Where? and why?

Outline

- Introduction
- Data checking
  - Expert knowledge
  - Initial cleaning
  - Missing values
  - Outliers
- Numeric data standardization & normalization
- Numeric data discretization
  - Unsupervised
  - Supervised
- Feature selection
  - Filters
  - Wrappers
- Feature extraction
  - Principal components analysis (PCA)
- Handling unbalanced data
  - Cost sensitive approaches
  - Sampling methods

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  - Right in terms of data representation and structure, volume, … (problem dependent)

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- Is my data useful? (Reliable, representative, noise-free, …)
- Once my goal and my options in term of ML algorithms (computation or memory limitations, etc.) are clear, how will I evaluate the goodness of my results and infer valid conclusions?

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- Know (if you can) that you will eventually reach there.

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- In real-world problems, data preprocessing takes around **80%** of your **working time**.
- It is crucial for the subsequent steps. The **bigger** your **data**, the **more important** their preprocessing process.

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  - Set **bounds** to the modeling choices.

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- Just have a look and see what comes out, if the volume of your data allows it.

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    - More **advanced techniques** requiring some data analysis, such as k-nearest neighbours or expectation & maximization algorithm.

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- When detected, the record is ignored or imputed (risky).

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- Moreover, we cannot obviate the curse of dimensionality effect, i.e. in high-dimensional spaces all data is sparse. In simple words, all distances become huge.

- Therefore, if the algorithm we plan to apply after preprocessing implies distances and/or we are in a high-dimensional problem, we should transform all the features to a similar scale.

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- In general, do **not** standardize or normalize your data unless you have a good reason for doing so.
- Other **transformations** from Statistics (logit, square root, power, Box-Cox, angular, etc.) are not considered because they are part of the posterior processing phase.

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- In general, the computational cost of algorithms with discrete attributes is lower than their continuous versions.

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  - **Equal-frequency**. Divide the range into *k* ranges with the same frequency. Better than equal-width in terms of clumping, but could produce odd artifacts with frequent or special values.

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- As a positive **side effect**, the methods in which k is not fixed in advance can be used as part of the **feature selection** step (still to come) to **detect irrelevant features**, when $k = 1$.

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  - A measurement of the **importance** of the features. This allows us to rank the features. Then we could get a subset by fixing a threshold for a cut-point of the importance.

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  - Embedded methods: included inside the algorithm (outside preprocessing).
- Examples of filters: **Correlation-based feature selection** (different definitions of correlation), **InfoGain** (mutual information), **ReliefF** (distance to the nearest sample from the same class and from a different class), **simmetrical uncertainty** (entropy of the sample and the class).

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- We will have a deeper look to the most famous unsupervised (and linear) method: **principal component analysis** (PCA).

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- **Principal Components Analysis**

Principal component analysis

- Based on the decomposition given by:

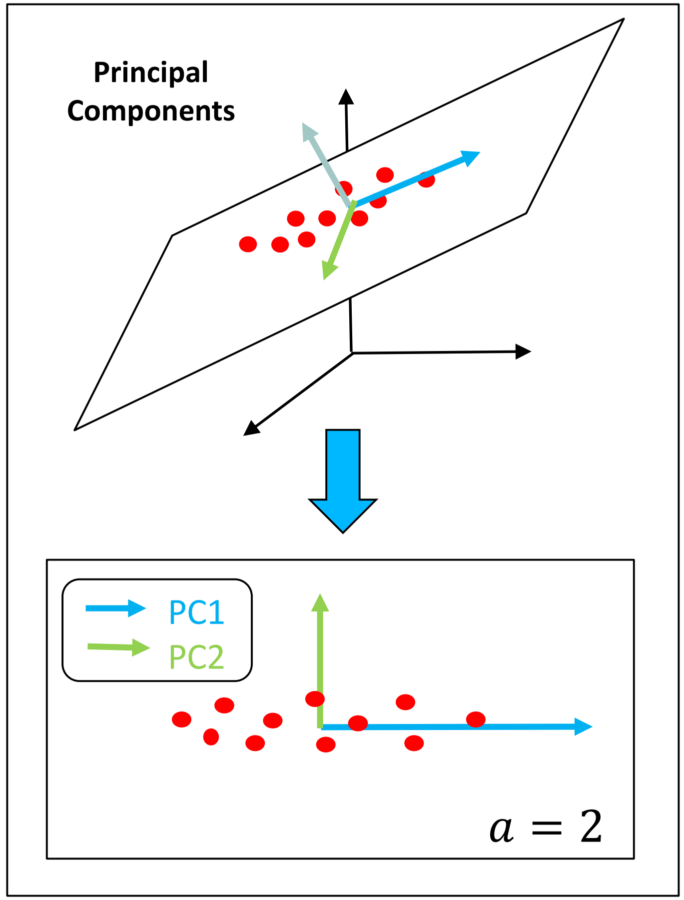
$$X = T_a P_a^T + E_a \qquad a \equiv \#PCs$$

- The PCs (LVs) are selected by maximizing scores variance

- $P \equiv$ Loadings => Coefficients of the linear combination that defines the PCs

- $T \equiv$ Scores => Coordinates of the data in the new axes

- $E \equiv$ Residuals (null if $a = N$)



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- Example: If the proportion of minority class samples is p, a usual approach is to consider an error in the prediction of the majority class $(1-p)/p$ times more relevant than an error in the prediction of the minority class.

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  - Undersampling removes samples that could contain relevant discriminant information.
  - Oversampling incorporates artificial/redundant information that could drive models (depending on their characteristics) towards non-realistic conclusions.

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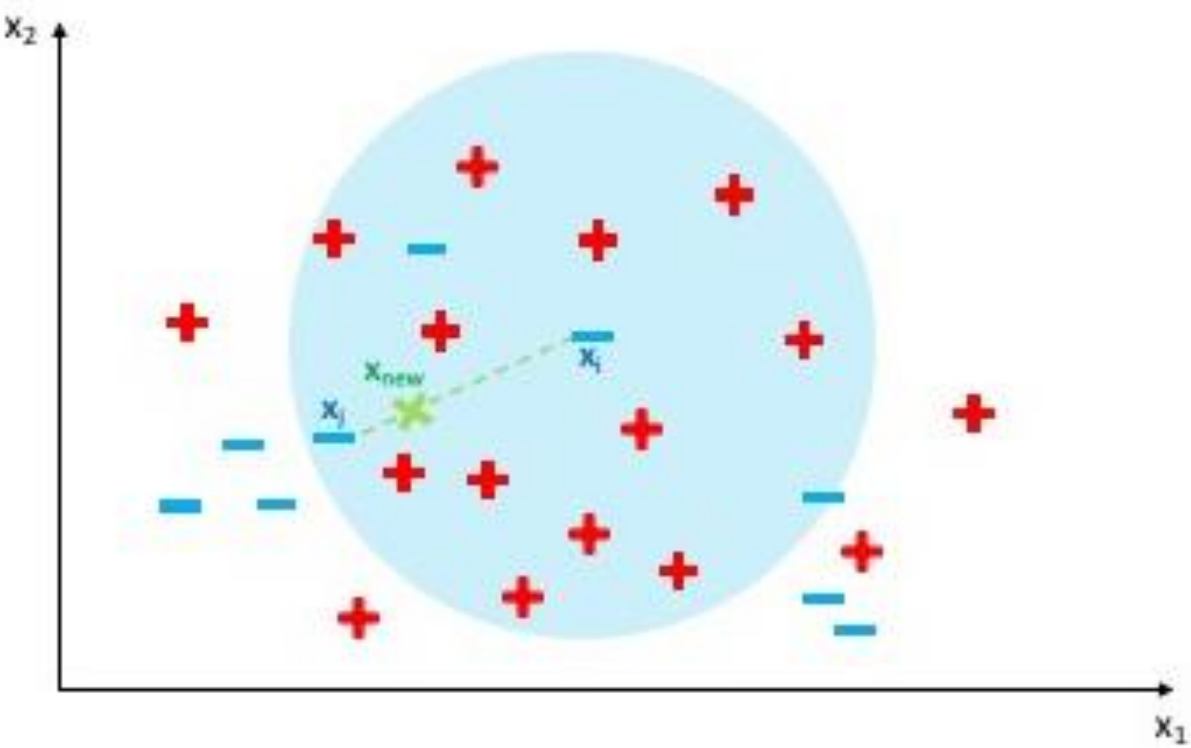

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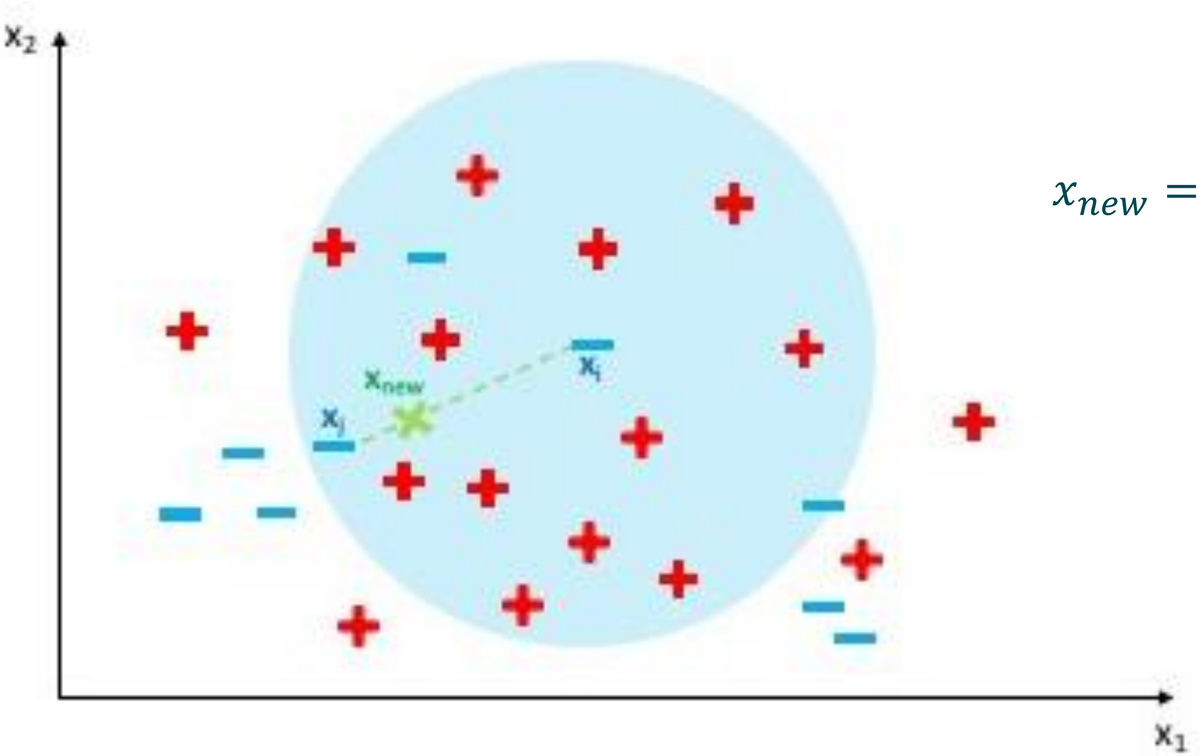

$$x_{new} = \lambda x_i + (1 - \lambda) x_j$$

Imbalanced data

- Oversampling methods

❖ Selection methods:

❑ Random oversampling. With or without replacement, pure or guided,…

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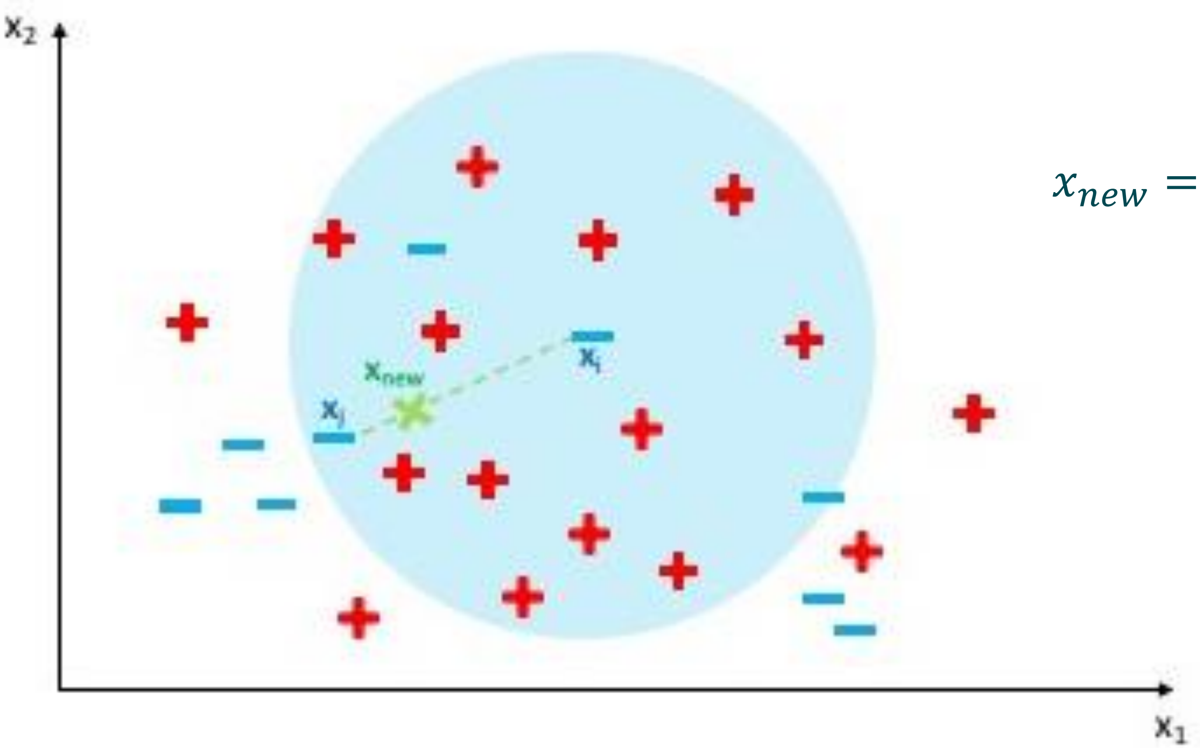

Randomly selected from the neighborhood of xi

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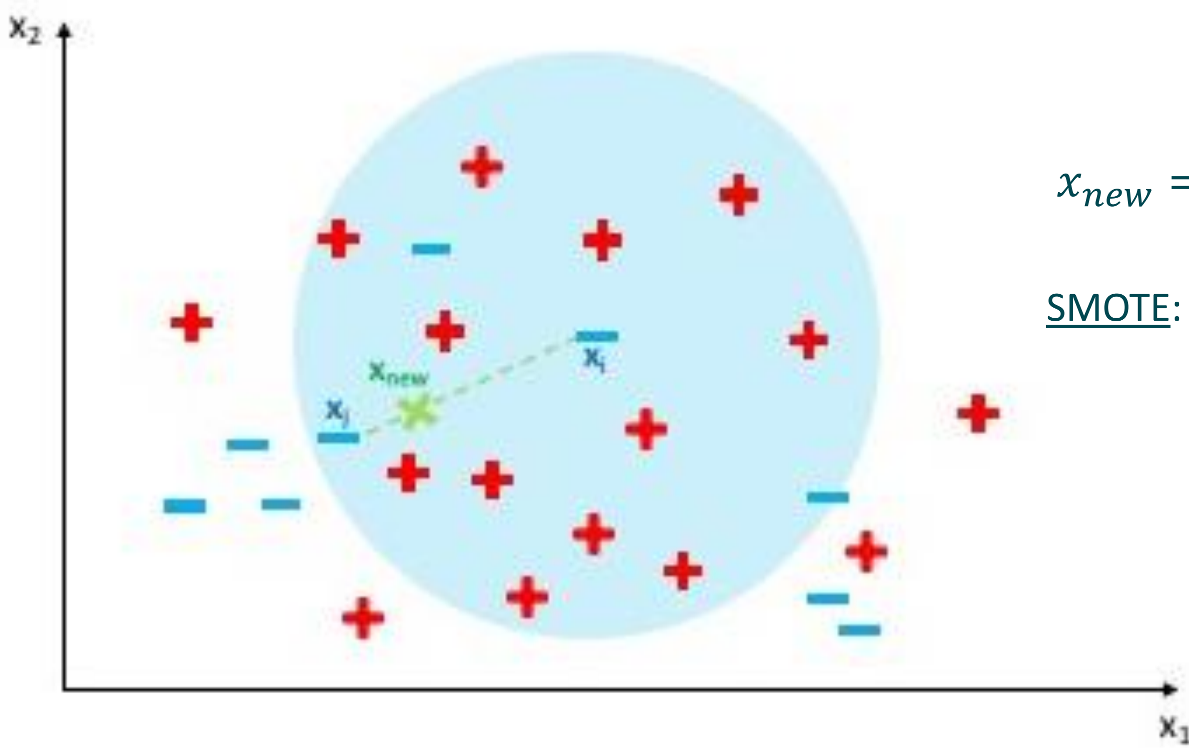

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<u>SMOTE</u>: Neighborhood by KNN, where K is pre-fixed

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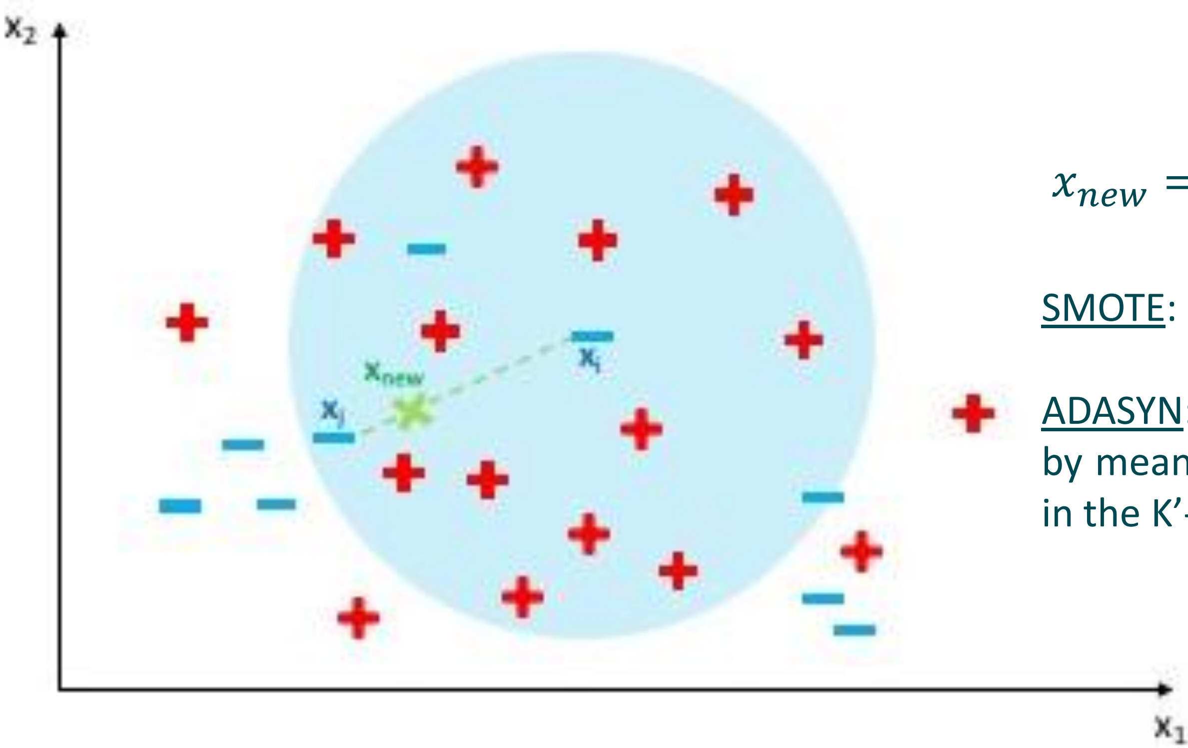

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SMOTE: Neighborhood by KNN, where K is pre-fixed

ADASYN: Neighborhood by K-NN, where K is estimated by means of the density of the minority class samples in the K'-NN (K' is pre-fixed and "big")

Imbalanced data

- *Oversampling methods*

Imbalanced data

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Imbalanced data

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<u>Problem</u>: Both suffer in presence of extreme values (outliers or not)
<u>Solution</u>: Design variants where they are not that relevant

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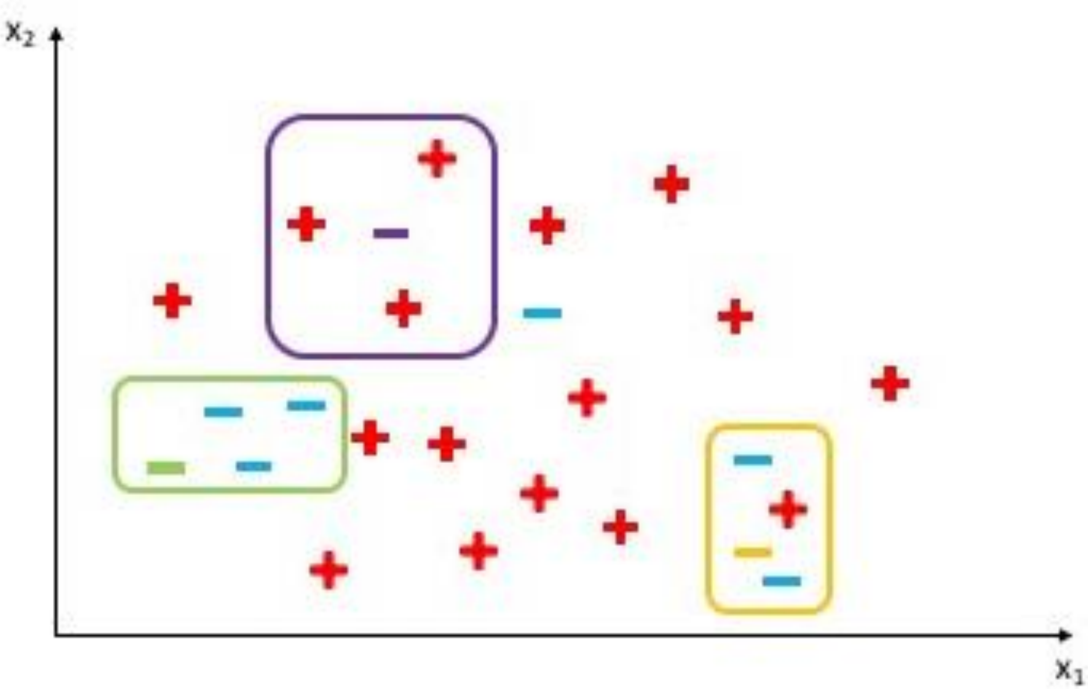

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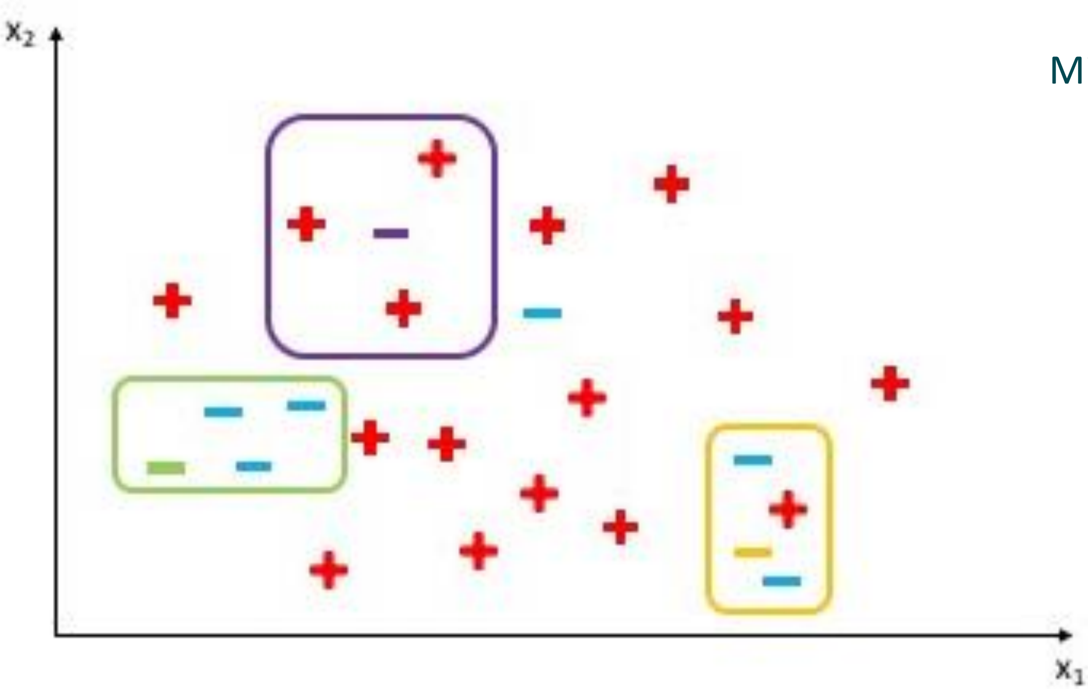

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Imbalanced data

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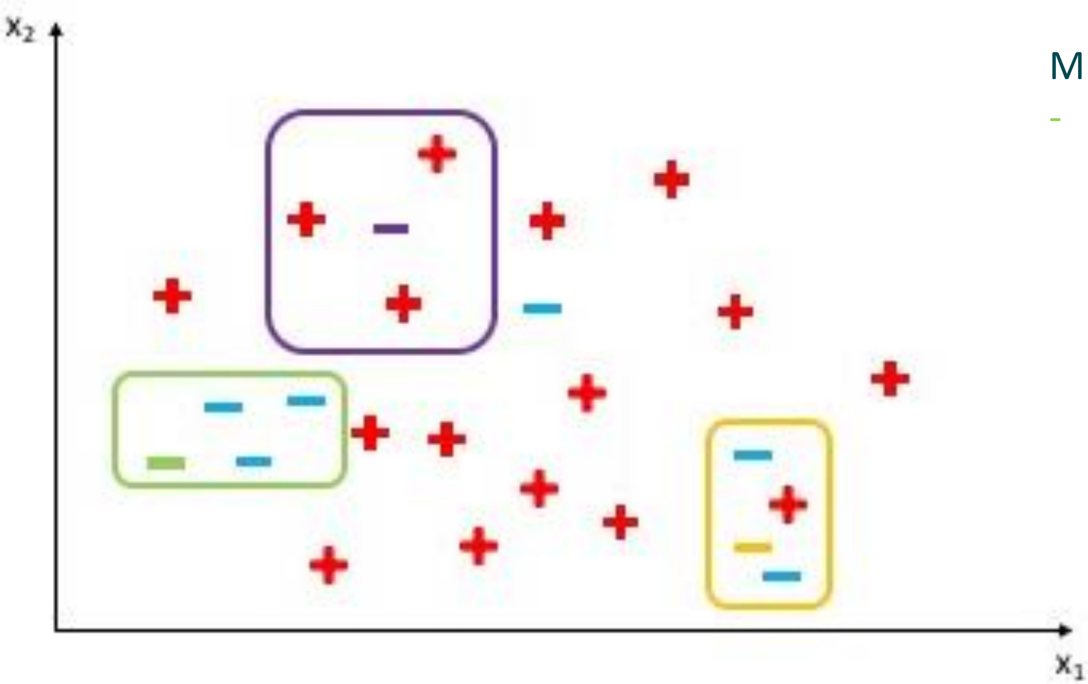

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Imbalanced data

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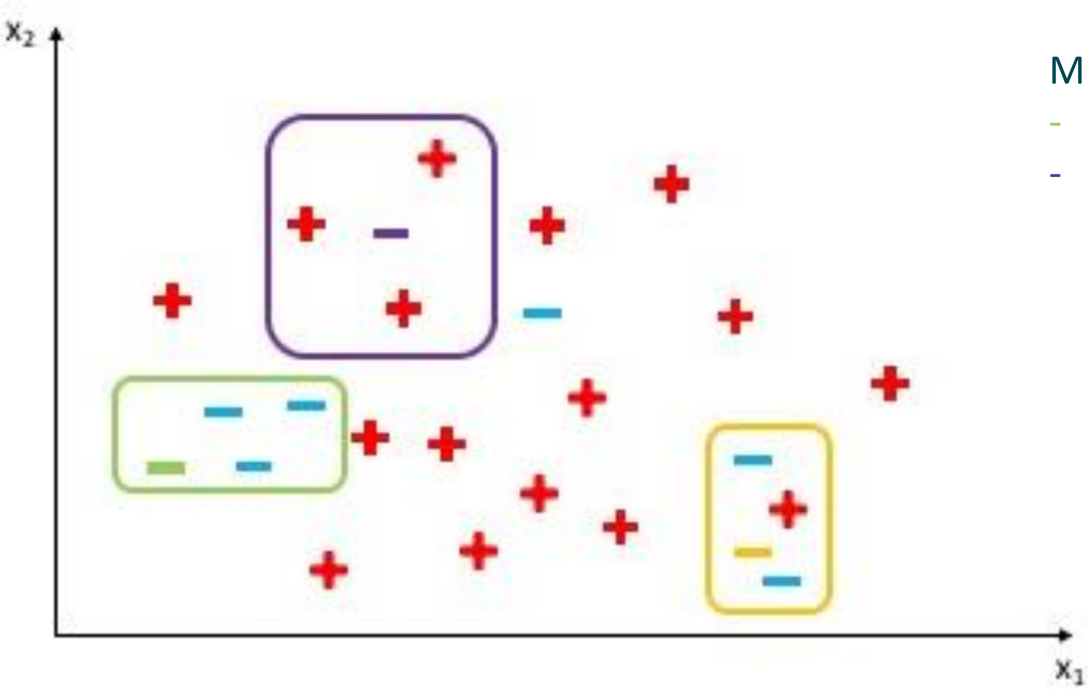

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Imbalanced data

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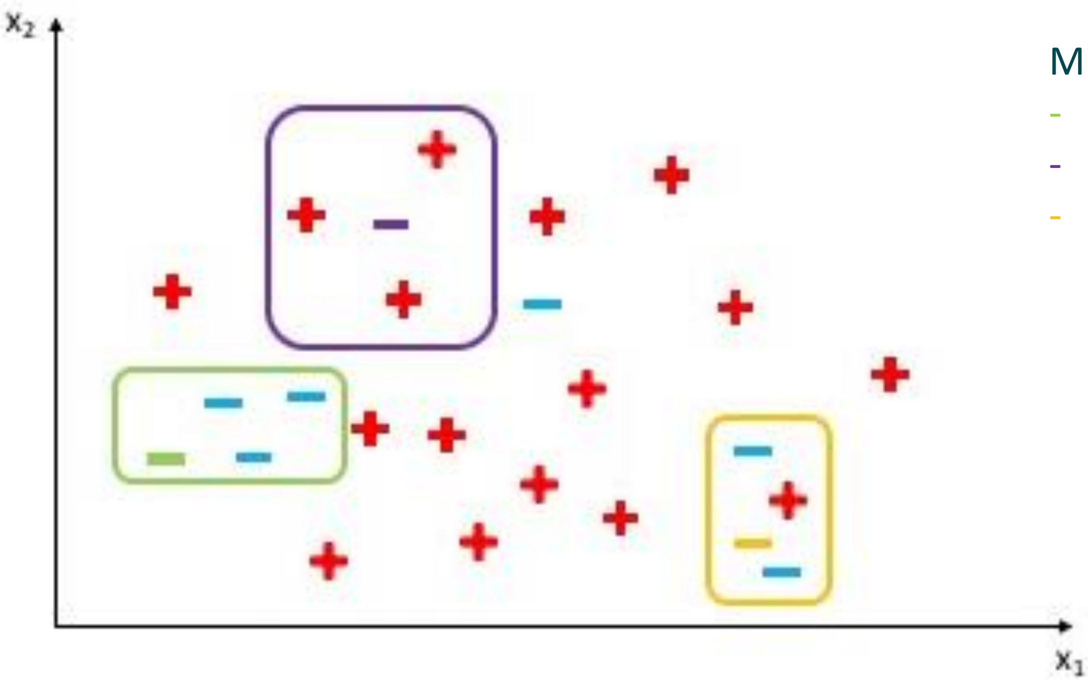

Minority class samples are classified as:

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Imbalanced data

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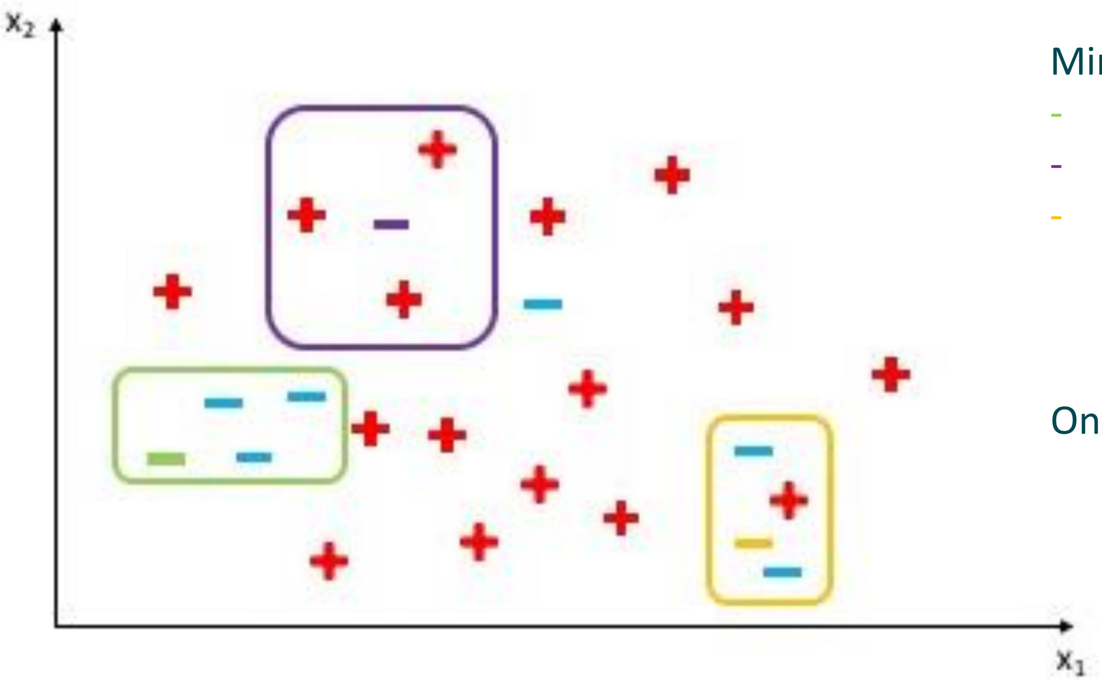

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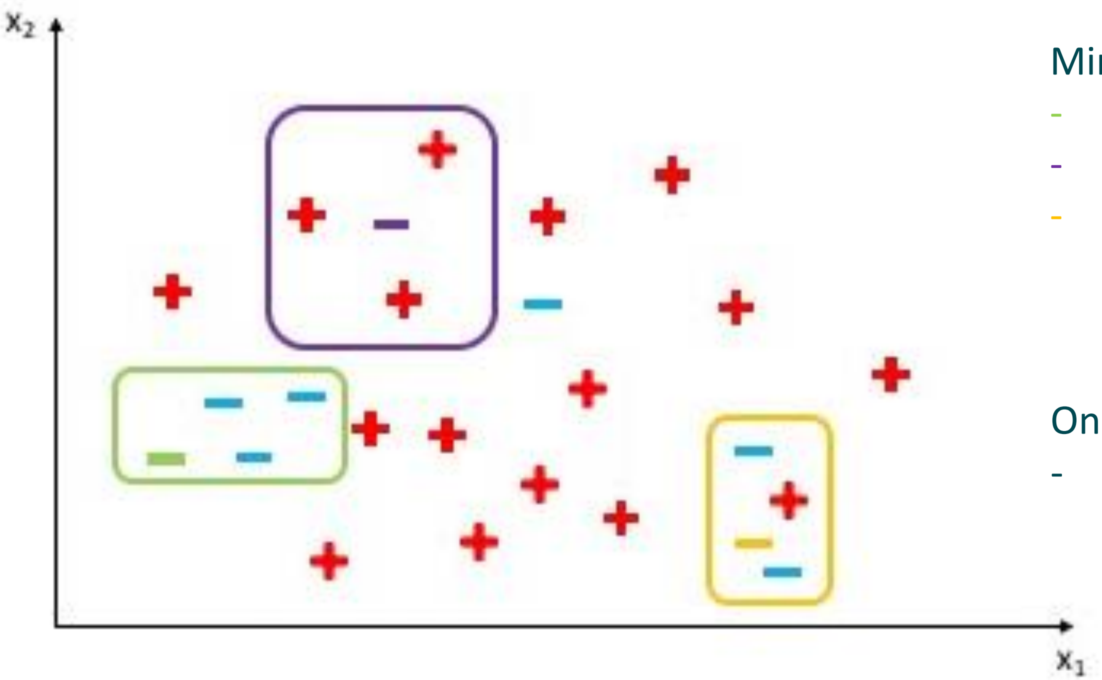

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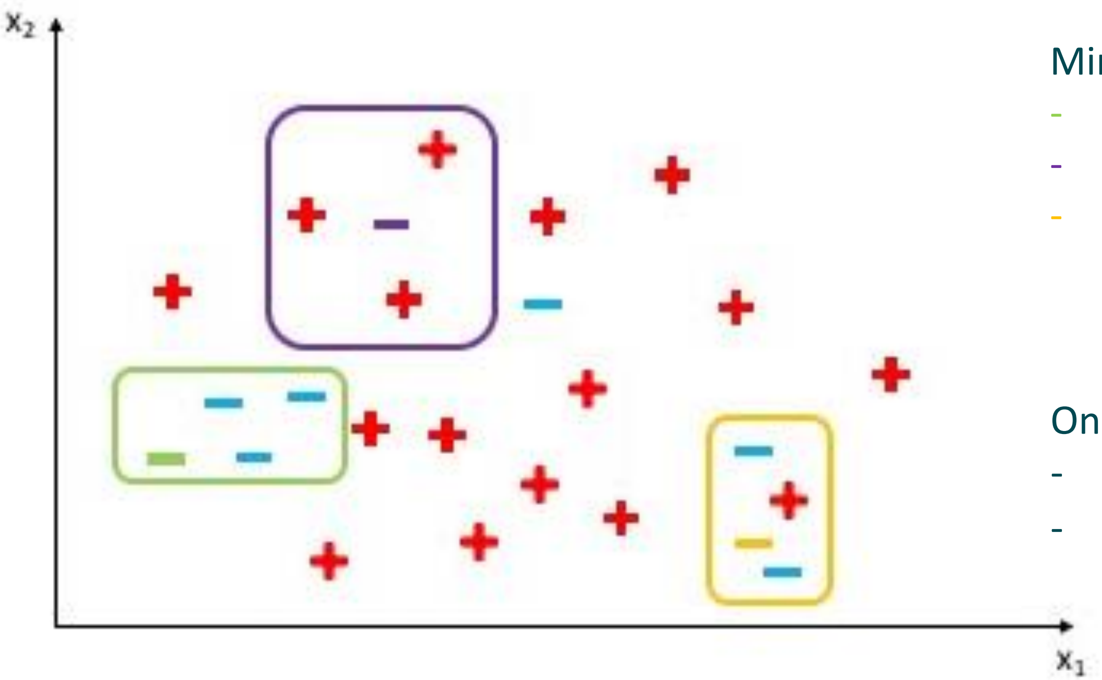

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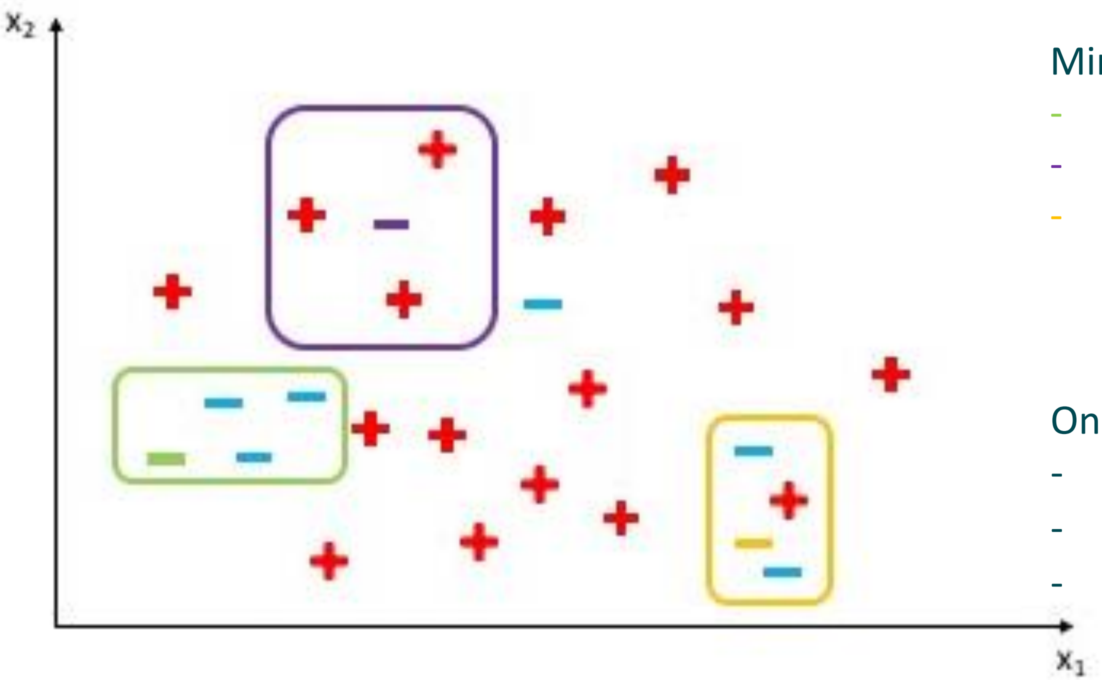

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Imbalanced data

- Undersampling methods

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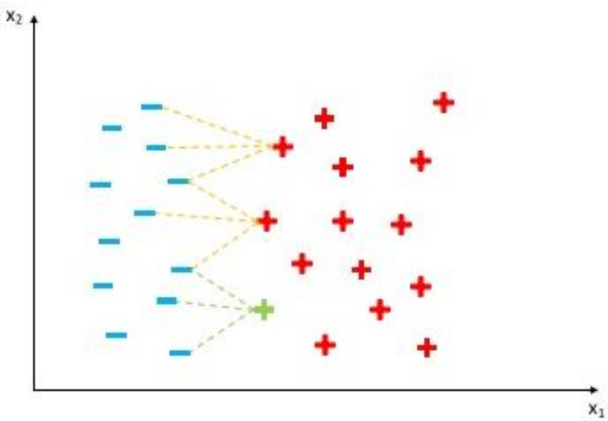
    - *Random undersampling*. Pure or guided,…
    - *NearMiss*. Majority class samples are selected using certain heuristic rules. Three main variants:
      - NearMiss-1
      - NearMiss-2
      - NearMiss-3

Imbalanced data

NearMiss-1

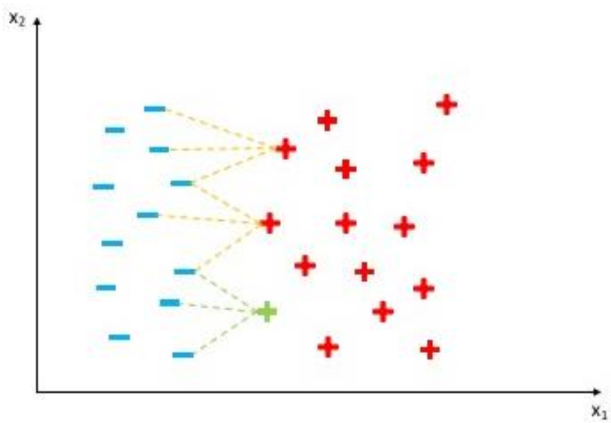


The heuristic rule is the minimum average distance to the N closest minority class samples.

Here N = 3 and the selected sample is depicted in green.

Imbalanced data

NearMiss-1



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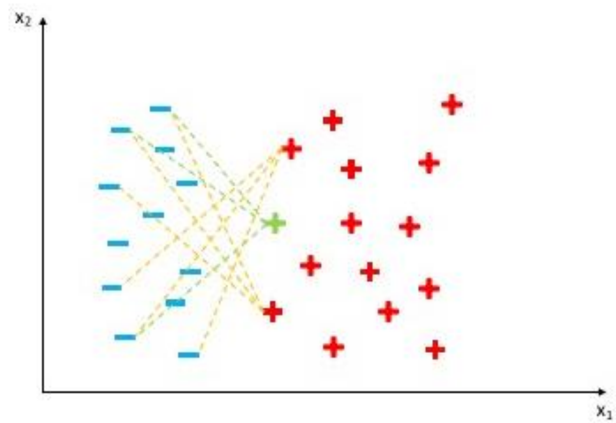
NearMiss-2



The heuristic rule is the minimum average distance to the N farthest minority class samples.

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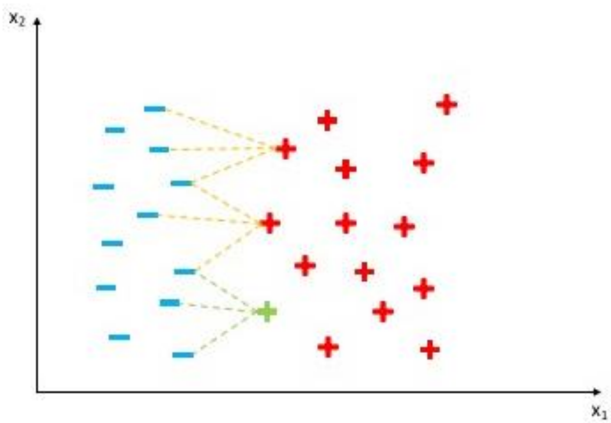
Imbalanced data

NearMiss-1



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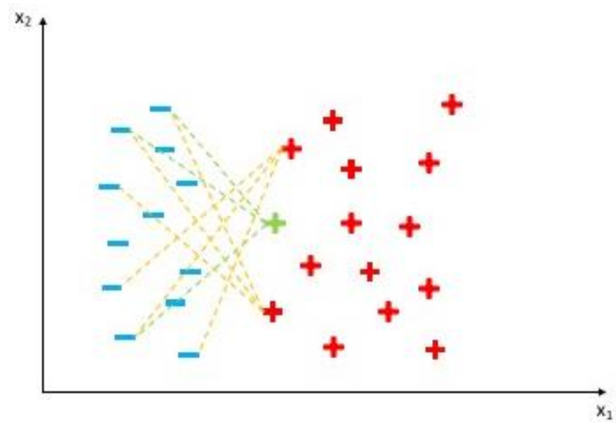

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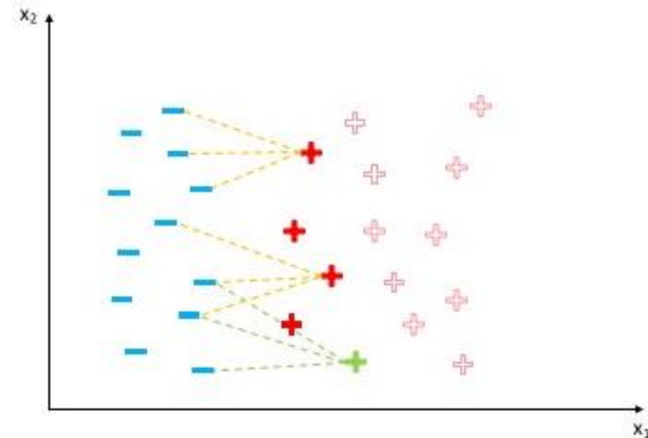
NearMiss-3



The heuristic rule has two steps: First, keep the M nearest majority class neighbors for each minority class sample (dark red).
Second, select the majority class sample with maximum average distance to its N minority class nearest neighbors.

Here M = 5, N = 3 and the selected sample is depicted in green.

Imbalanced data

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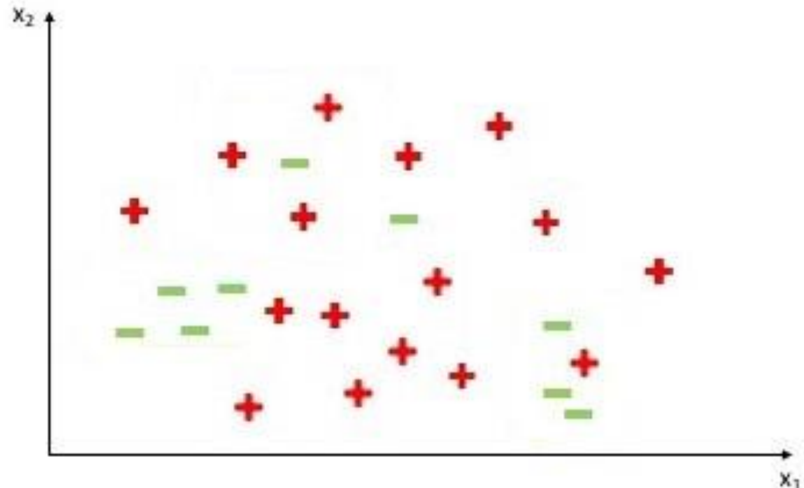

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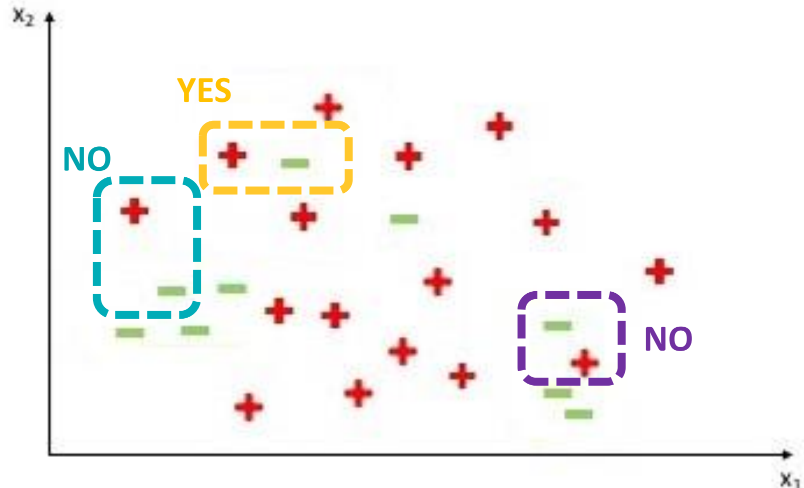

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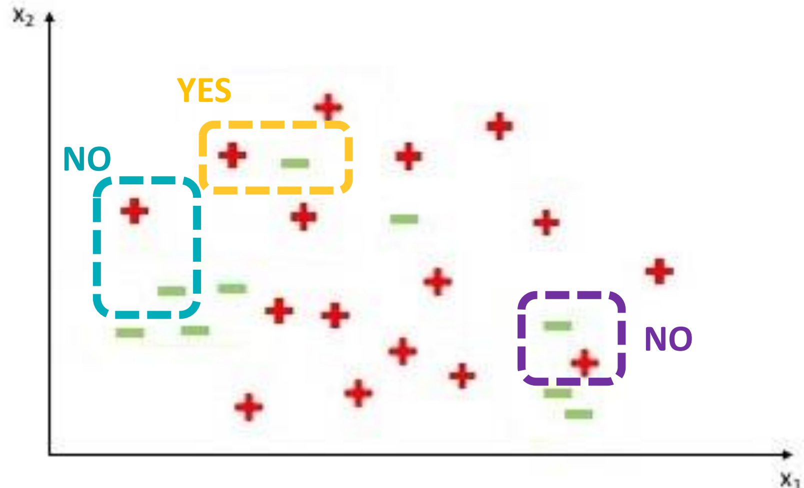
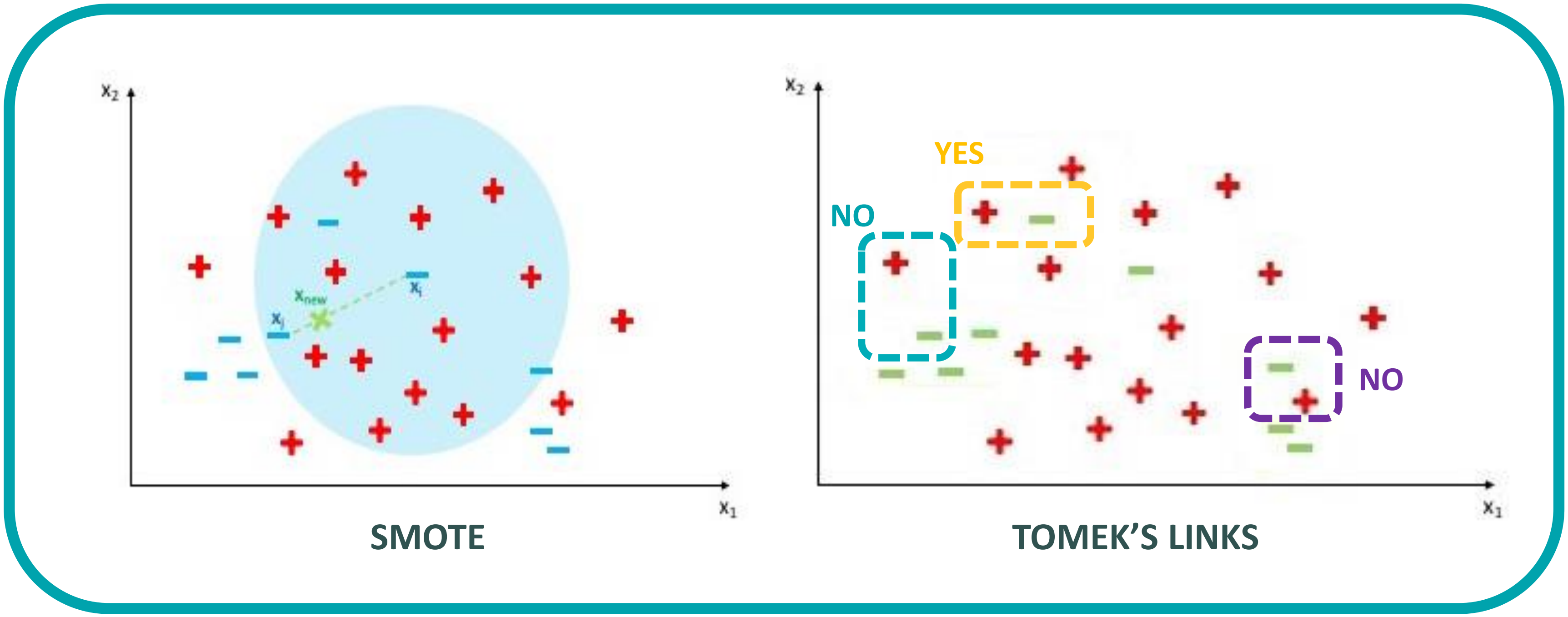


Two possible alternatives:
- Delete both samples
- Delete only the majority class sample ($\boldsymbol{y}$).

Imbalanced data

- Mixed
  - *Random oversampling + random undersampling*
  - SMOTE + Tomek's links (ejemple)
  - SMOTE + ENN



Python functions

Tarea	Entorno	Función	Uso
Read CSV	Pandas	pd.read_csv()	Load data in comma separated values format
Cleaning	Pandas	df.drop()	Columns deletion (df is the dataframe name)
Missing values	Pandas	df.isnull()	Localization
Missing values	Numpy	np.isnan()	Localization
Missing values	Pandas	df.drop()	Rows deletion
Missing values	Scikit-learn	SimpleImputer()	Missing values imputation
Outliers	Scikit-learn	EllipticEnvelope()	Mahalanobis hull
Outliers	Seaborn	sns.boxplot()	Boxplot (ocular inspection)
Discretization	Scikit-learn	KBinsDiscretizer()	Discretization (several opcions using the function parameters)
Selection	Scikit-learn	SelectKBest(), SelectPercentile(), GenericUnivariateSelect()	Several estrategies. The last one is totally configurable.
Extraction	Scikit-learn	PCA.fit(), PCA.transform()	Principal components analysis: calculation and application
Extraction	Scikit-learn	KernelPCA.fit(), KernelPCA.transform(), KernelPCA.fit_transform()	Kernel principal components analysis (no lineal): calculation, application y both
Imbalanced Data	Imbalanced-learn	SMOTE(), ADASYN(), BorderlineSMOTE(), NearMiss(), TomekLinks()	Imbalance correction

Mondragon Unibertsitatea
Escuela Politécnica Superior

Eskerrik asko

Muchas gracias

Thank you

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