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Machine Learning

Session 4 - T

Data Scaling and Feature Selection

Degree in Applied Data Science

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Data Scaling

- Data scaling refers to the procedure of adjusting the range of features within a dataset to a **comparable scale;**

- Real-world datasets often contain features with **different orders of magnitude, ranges, and measurement units**.

Car	Model	Volume	Weight	CO2
Toyota	Aygo	1.0	790	99
Skoda	Citigo	1.0	929	95
Fiat	500	0.9	865	90
Mini	Cooper	1.5	1140	105
Skoda	Fabia	1.4	1109	90
…	…	…	…	…

Why do we need scaling?

- Some machine learning models are **sensitive to feature scale;**
- Features with larger scales may **dominate the learning process**;
- Models may **converge faster**;
- Model **performance may improve** (specially for models that rely on **distance metrics**);

Data Scaling Methods

- **Standardization** (Z-score normalization): centers the data around mean 0 and standard deviation 1:

$$z = \frac{x_i - \mu}{\sigma}$$

- **Normalization**: scales the data between 0 and 1;

$$x_{\text{norm}} = \frac{x - \min(x)}{\max(x) - \min(x)}$$

- **Min-Max Scaling**: scales data betwenn a maximum and minimum value;

$$X_{scaled} = \frac{X - \min(X)}{\max(X) - \min(X)} (NewMax - NewMin) + NewMin$$

Data Scaling Methods

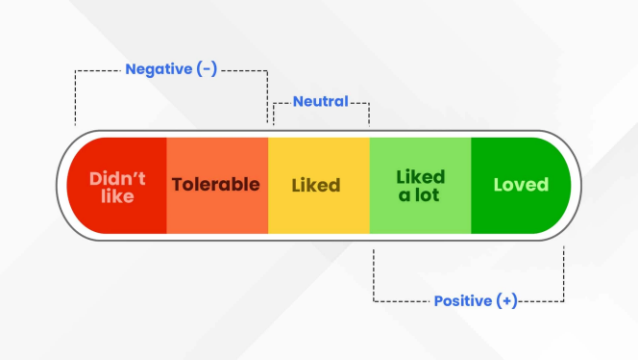
- **Robust Scaling**: Scales data based on the interquartile range, making it robust to outliers;

$$X = \frac{X - Q_1(X)}{Q_3(X) - Q_1(X)}$$

- **Log transformation**: scales data by applying the natural logarithm function;

$$X = log(X)$$

- **Ordinal scaling**: assign integer values to categories with a meaningful order.



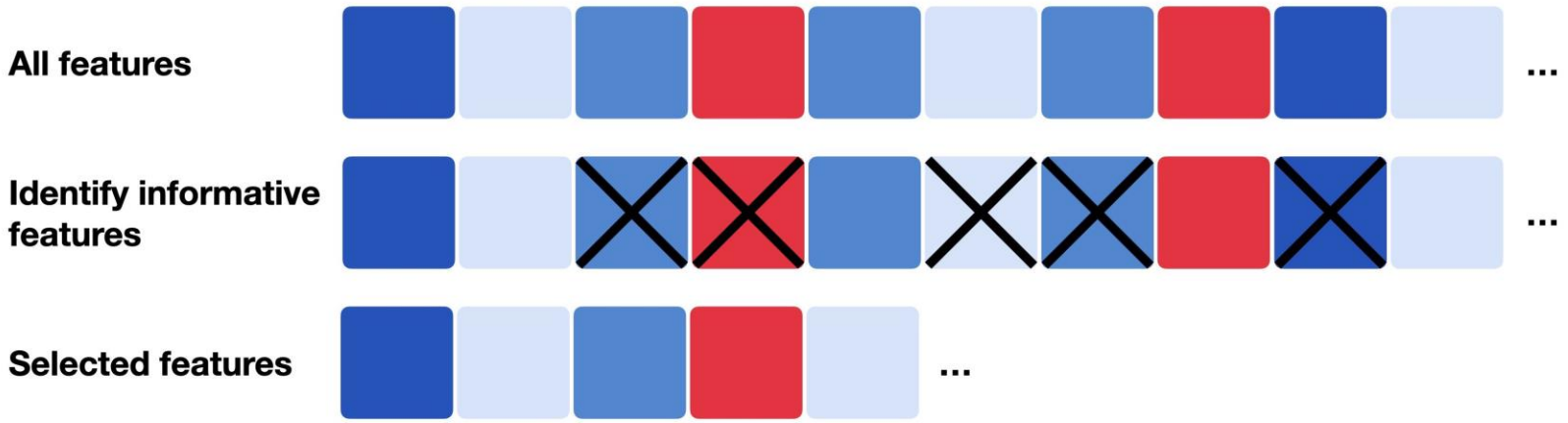
Which Scaling Method to Choose?

- Choose the method that aligns with your **data type**, **distribution**, and **Machine Learning model** to use;

- Methods to use:
  - **Continuous data**:
    - Uniform distribution: Min-Max scaling / normalization;
    - Normally distributed: Z-score standardization;
    - Data with outliers: Robust scaling;
    - Skewed or exponential distribution: Log transformation.
  - **Categorical data**:
    - Ordinal: Ordinal scaling;
    - Nominal: other strattegies like one-hot encoding and frequency encoding.

Feature Selection

- Feature selection is a process of **selecting a subset of the initial features while minimizing the loss of information** related to the final task (classification, regression, etc);



Why Feature Selection?

- In many cases, there are multiple advantages in **reducing the number of input features** used in a model.

- This is especially important when:
  - Dealing with **noisy data**;
  - Handling numerous **low-frequency features**;
  - Data has too **many features compared to samples**;
  - Managing **complex models**;
  - …

https://medium.com/barnbridge/barnbridge-dao-built-for-the-future-3735fbd671c5

Why Feature Selection?

- The reduction of the number of features can:
  - Improve the **model's performance**;
  - Enhance **optimization stability** by removing **multicollinearity**;
  - Increase **computational eficiency**;
  - Reduce **cost of future data collection**;
  - Simplify the model, making it **easier to understand and interpret**;
  - …

- However, it is **not always a necessary step**:
  - Some models have **implicit feature selection**
    - Tree-based models;
  - Models with **regularization**
    - LASSO;
    - RIDGE.

https://www.kaggle.com/code/heyspaceturtle/feature-selection-is-all-u-need

Feature Selection Algorithms

- From the **label perspective** they can be:
  - **Supervised**;
  - **Unsupervised**.

- From the **selection strategy perspective** they can be:
  - **Filter** methods;
  - **Wrapper** methods;
  - **Embbeded** methods.

Feature Selection: Filter Methods

- Filters methods evaluate feature relevance based on **intrinsic data characteristics:**
  - First, features are individually **ranked** based on specific criteria such as **distance, correlation, or entropy;**
  - Second, the **best-ranked features** are selected using a predetermined **threshold**.

Feature Selection: Filter Methods

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- **Unsupervised**:
  - Unsupervised filters compute a metric for each feature **based solely on its values**;
  - Metrics include those measuring variability, such as **variance** (continuous variables) and **entropy** (discrete variables);
  - Selection can occur through **ranking** (e.g., percentile) or by **absolute value**, by keeping all features with a value below/above a specified threshold.

- **Supervised**:
  - Supervised filters use a metric calculated for each input feature, **comparing its values to those of the output**;
  - Metrics include **mutual information** (discrete variables) and **correlations** (continuous variables);
  - Scores may also rely on **univariate statistical tests** applied to the paired sets of values;
  - Different tests may be applied depending on the type of features.

Feature Selection: Filter Methods

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- **Supervised**:
  - For **classification problems** (discrete output):
    - **T-test** may be used for continuous and binary output; for multiclass output, **one-way ANOVA** may be used;
    - **Chi-square** is used for counts/frequencies or binary variables.
  - For **regression problems** (continuous output):
    - **Correlation** is an option for continuous inputs (Pearson or Spearman);
    - **Kendall's rank correlation** for discrete inputs (ordinal).
  - In both cases, **mutual information** can be used as a **non-parametric** alternative.

Feature Selection: Filter Methods

- **Advantages**:
  - Independent of a learning model;
  - Computationally efficient;
  - Suitable for high dimensional data;
- **Disadvantages**:
  - Interactions between features are ignored;
  - May fail to handle redundant features;
  - No interaction with the learning algorithm.

Feature Selection: Filter Methods

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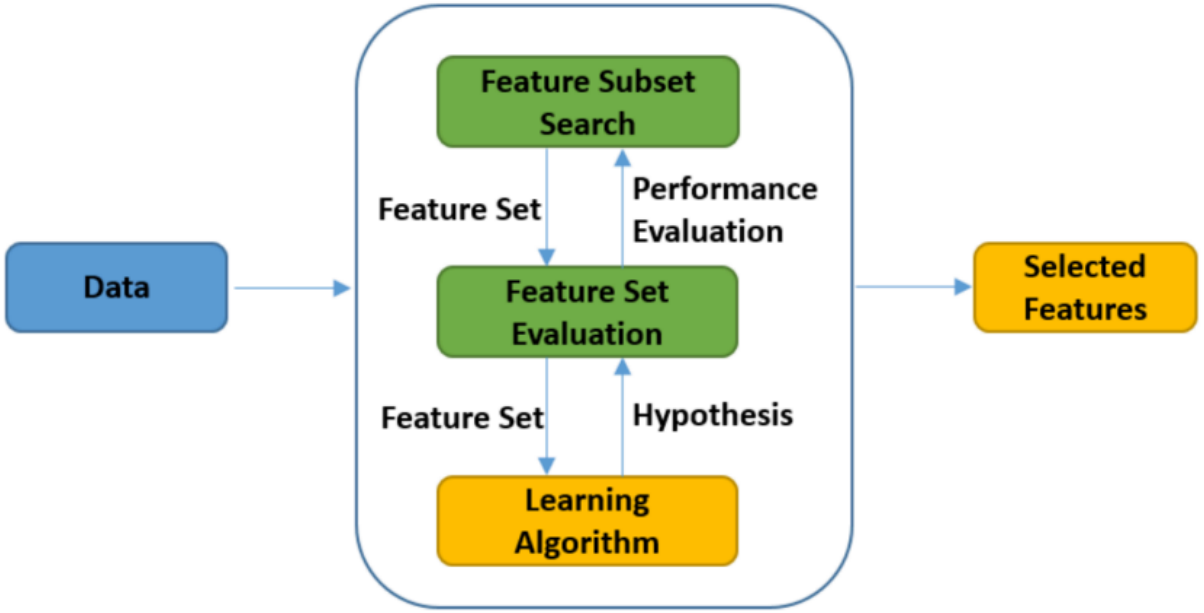
- **Examples**:
  - **VarianceThreshold**: keeps only features whose variance exceeds a specified threshold;
  - **SelectKBest**: selects the top k (user-defined parameter) features based on a scoring function (mutual information, chi2, ANOVA, etc);
  - **SelectPercentile**: selects the top percentage (percentile) of features based on a scoring function (mutual information, chi2, ANOVA, etc).
  - **SelectFpr**, **SelectFdr**, and **SelectFwe**: sseatures are selected based on their significance according to statistical tests. SelectFpr controls the false positive rate, SelectFdr controls the false discovery rate, and SelectFwe controls the family-wise error rate.

Feature Selection: Wrapper Methods

- Wrapper methods directly involve a **learning algorithm** in the feature selection process.
- **Subsets of features** are used to train and test a model iteratively, selecting the subset that optimizes a performance metric.



Feature Selection: Wrapper Methods

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- Subset selection method:
  - **Forward search**:
    - Start with no features;
    - Greedily include the most relevant feature;
    - Stop when the desired number of features is selected.
  - **Backward search**:
    - Start with all the features;
    - Greedily remove the least relevant feature;
    - Stop when the desired number of features is reached.

Feature Selection: Wrapper Methods

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- **Advantages:**
  - Better performance attainability;
  - Take into account interaction between features;
  - Identify feature interactions of higher order.

- **Disadvantages:**
  - Computationally expensive;
  - Prone to overfitting;
  - The learning algorithm is built from scratch for each subset.

Feature Selection: Wrapper Methods

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- **Examples**:
  - **RFE:** recursively selects features by training a model, removing the least important features, and repeating until the desired number of features is reached;
  - **SequentialFeatureSelector**: evaluates different combinations of features by adding or removing features iteratively based on model performance;
  - **SelectFromModel**: selects features based on importance weights provided by a pre-trained model.
  - **Boruta**: all-relevant feature selection method that identifies important features by comparing their importance with that of random shadow features.

Feature Selection: Embedded Methods

- Feature selection is **integrated directly into the model training** process;
- Features are selected or discarded based on their **importance to the model's performance** during training;
- Some examples include **tree-based models** and models with **regularization** (L1/L2).

Feature Selection: Embedded Methods

- **Advantages:**
  - Faster than wrapper methods;
  - Take into account interactions between features;
  - Identify feature dependencies;

- **Disadvantages:**
  - Specific to the learning algorithm;
  - Selection dependent on the learning algorithm.

Feature Selection: Embedded Methods

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- **Examples**:
  - **Lasso Regression**: performs feature selection by penalizing the absolute size of the regression coefficients, effectively shrinking some coefficients to zero and eliminating corresponding features.
  - **Ridge Regression:** performs feature selection by penalizing the square of the regression coefficients, which encourages smaller coefficients and effectively shrinks the impact of less important features.
  - **Random Forests**: ensemble learning method that naturally performs feature selection by assessing the importance of features based on how much they decrease node impurity across multiple decision trees.
  - **Gradient Boosting Machines:** ensemble learning method that builds decision trees sequentially, each focusing on the residuals of the previous trees, effectively performing feature selection by giving more importance to relevant features.

Resources:

- Zheng, A. (2018). Feature Engineering for Machine Learning. Sebastopol, CA: O'Reilly Media.

- Kuhn, M., & Johnson, K. (2019). Feature engineering and selection. Philadelphia, PA: Chapman & Hall/CRC.