Data preprocessing

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Types of features

- nominal
  - {MALE, FEMALE}
  - {RED, GREEN, BLUE}
- ordinal
  - {SATISFACTORY, GOOD, VERY_GOOD}
  - {'M', 'L', 'XL'}
- interval-scaled
  - temperature in Celsius degrees
- ratio-scaled
  - temperature in Kelvins
  - mass in kilograms

Data imputation

- removal of columns or rows with missing values
- imputation of missing values with mean, median or mode
- imputation of missing values with the most fequent values, zero value or random value
- imputation of missing values with k-NN method

Feature encoding

Ordinal encoding

- imposes order between nominal values

{RED, GREEN, BLUE}

RED	→	0
GREEN	→	1
BLUE	→	2

Feature encoding

One-hot encoding

- impractical for large number of categories
- relation between ordinal values are lost

{RED, GREEN, BLUE}

$$\begin{array}{lclcl}
\text{RED} & \rightarrow & [1, 0, 0] & & [1, 0] \\
\text{GREEN} & \rightarrow & [0, 1, 0] & \rightarrow & [0, 1] \\
\text{BLUE} & \rightarrow & [0, 0, 1] & & [0, 0]
\end{array}$$

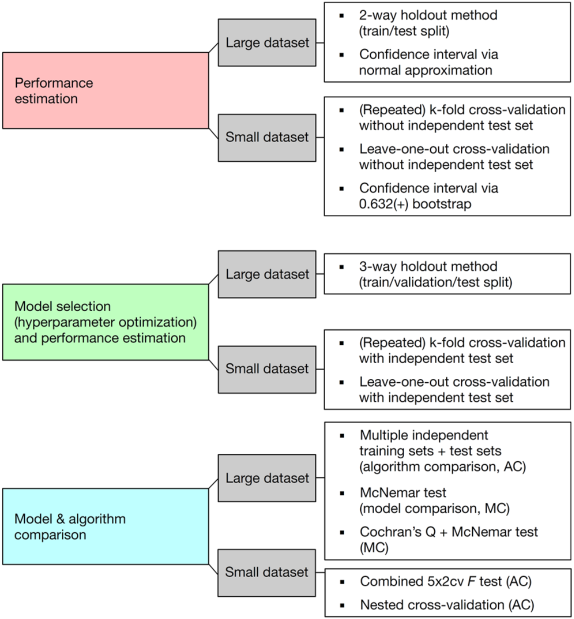
Dummy variable encoding

$$\begin{array}{lcl}
\text{RED} & \rightarrow & [1, 0] \\
\text{GREEN} & \rightarrow & [0, 1] \\
\text{BLUE} & \rightarrow & [0, 0]
\end{array}$$

Feature scaling

- normalization (max-min scaling)
  $x \leftarrow \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$
- standarization
  $x \leftarrow \frac{x - \mu}{\sigma}$
- soft-max scaling
  $y \leftarrow \frac{x - \mu}{r\sigma}$
  $x \leftarrow \frac{1}{1 + \exp(-y)}$

Evaluation



Performance estimation

Large dataset

- 2-way holdout method (train/test split)
- Confidence interval via normal approximation

Small dataset

- (Repeated) k-fold cross-validation without independent test set
- Leave-one-out cross-validation without independent test set
- Confidence interval via 0.632(+) bootstrap

Model selection (hyperparameter optimization) and performance estimation

Large dataset

- 3-way holdout method (train/validation/test split)

Small dataset

- (Repeated) k-fold cross-validation with independent test set
- Leave-one-out cross-validation with independent test set

Model & algorithm comparison

Large dataset

- Multiple independent training sets + test sets (algorithm comparison, AC)
- McNemar test (model comparison, MC)
- Cochran's Q + McNemar test (MC)

Small dataset

- Combined 5x2cv *F* test (AC)
- Nested cross-validation (AC)

References I

[1] https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.04-Feature-Engineering.ipynb

[2] https://github.com/rasbt/machine-learning-book/tree/main/ch04

[3] Sebastian Raschka,
Model Evaluation, Model Selection and Algorithm Selection in Machine Learning, 2018.