

Data Preprocessing

COMP3314
Machine Learning

Introduction

- Preprocessing a dataset is a crucial step
 - o Garbage in, garbage out
 - Quality of data and amount of useful information it contains are key factors
- Data-gathering methods are often loosely controlled, resulting in out-of-range values (e.g., Income: −100), impossible data combinations (e.g., Sex: Male, Pregnant: Yes), missing values, etc.
- Preprocessing is often the most important phase of a machine learning project

Outline

- In this chapter you will learn how to ...
 - Remove and impute missing values from the dataset
 - Get categorical data into shape
 - Select relevant features
- Specifically, we will looking at the following topics
 - Dealing with missing data
 - Nominal and ordinal features
 - Partitioning a dataset into training and testing sets
 - Bringing features onto the same scale
 - Selecting meaningful features
 - Sequential feature selection algorithms
 - Random forests

Dealing with Missing Data

- Missing data is common in real-world applications
 - Samples might be missing one or more values
- ML models are unable to handle this
- Two ways to handle this
 - Remove entries
 - Imputing missing values from other samples and features

Identifying Missing Values

• Consider the following simple example generated from <u>CSV</u>

```
import pandas as pd
from io import StringIO
import sys
csv_data = \
'''A,B,C,D
1.0,2.0,3.0,4.0
5.0,6.0,,8.0
10.0,11.0,12.0,'''
df = pd.read_csv(StringIO(csv_data))
df
```

	A	В	C	D
0	1.0	2.0	3.0	4.0
1	5.0	6.0	NaN	8.0
2	10.0	11.0	12.0	NaN

- For larger data, it can be tedious to look for missing values
 - Use the isnull method to return a DataFrame with Boolean values that indicate whether a cell
 - contains a numeric value (False), or if
 - data is missing (True)
- Use sum() to count the number of missing values per column

df.isnull().sum()

B 0
C 1
D 1
dtype: int64

COMP 3314

- A B C D

 1.0 2.0 3.0 4.0

 5.0 6.0 NaN 8.0

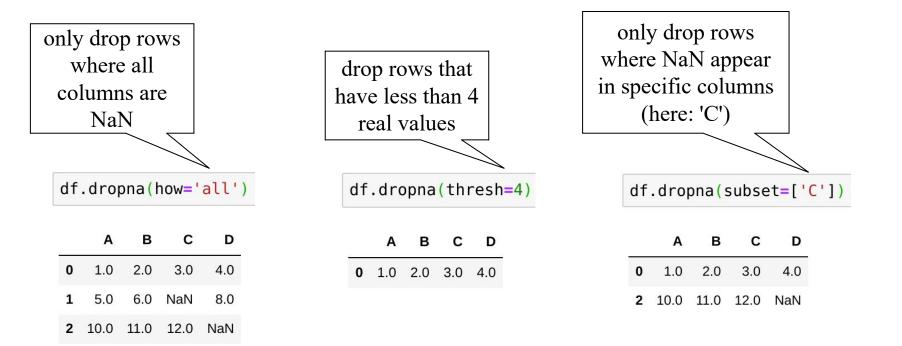
 0.0 11.0 12.0 NaN
- One option is to simply remove the corresponding features (columns) or samples (rows)
- Rows with missing values can be dropped via the dropna method with argument axis=0

• Columns with missing values can be dropped via the dropna method with argument axis=1

2.0

Dropna

• The dropna method supports several additional parameters that can come in handy



Remove Missing Data

- Convenient approach
- Disadvantage
 - May remove too many samples
 - Risk losing valuable information
 - Our classifier may need them to discriminate between classes
 - Could make a reliable analysis impossible
- Alternative approach: Interpolation

Interpolation

- Estimate missing values from the other training samples in our dataset
- Example: Mean imputation
 - Replace missing value with the mean value of the entire feature column

```
from sklearn.impute import SimpleImputer
import numpy as np
                                                                     [5. 6. nan 8.]
imr = SimpleImputer(missing values=np.nan, strategy='mean')
                                                                     [10. 11. 12. nan]]
print(df.values)
imr = imr.fit(df.values)
imputed data = imr.transform(df.values)
print(imputed data)
                                                                    mean and median are for
                                                                      numerical data only,
                            Try to change to:
                                                                 most frequent and constant can
                                  median
                                                                  be used for numerical data or
                                 most frequent
                                                                             strings
                                  constant, fill value=42
```

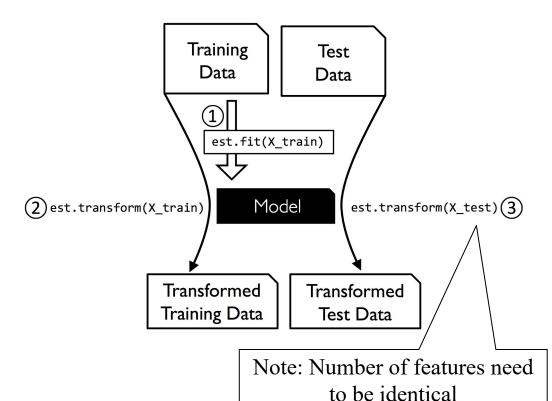
- SimpleImputer is a Transformer class
 - Used for data transformation
 - Two essential methods
 - fit
 - transform
- Estimator class

COMP 3314

- Very similar to transformer class
 - Two essential methods
 - fit
 - predict
 - Transform (optional)

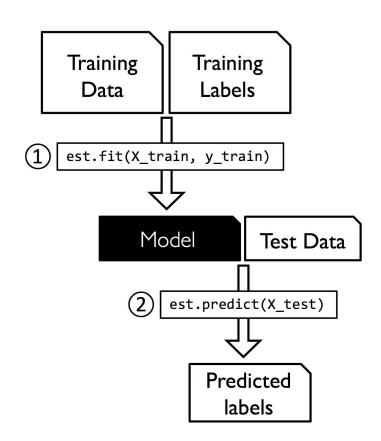
Transformer - Fit and Transform

- fit method
 - Used to learn the parameters from the training data
- transform method
- Uses those parameters to transform the data



Estimator - Fit and Predict

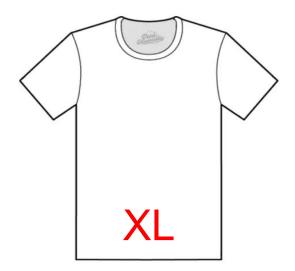
- Use fit method to learn parameters
 - Additionally provide class labels
- Use predict method to make predictions about unlabeled data

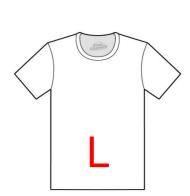


Handling Categorical Data

- We have been exclusively working with numerical data
- How to handle categorical data? —
- Example of categorical data

A categorical feature can take on one of a limited, and usually fixed, number of possible values



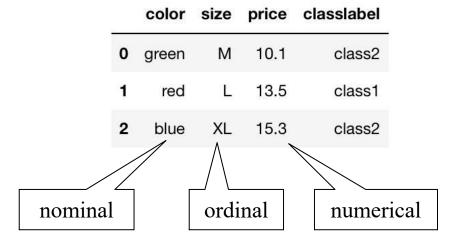




Categorical Data

- It is common that real-world datasets contain categorical features
 - O How to deal with this type of data?
- Nominal features vs ordinal features
 - Ordinal features can be sorted / ordered
 - E.g., t-shirt size, because we can define an order XL>L>M
 - Nominal features don't imply any order
 - E.g., t-shirt color

Example Dataset



Mapping Ordinal Features

M 10.1 class2 0 green L 13.5 red class1 blue XL 15.3 class2

To ensure correct interpretation of ordinal features, convert string values to integers

```
size mapping = {'XL': 3, 'L': 2, 'M': 1}
df2['size'] = df2['size'].map(size mapping)
df2
```

	color	size	price	classlabel
0	green	1	10.1	class2
1	red	2	13.5	class1
2	blue	3	15.3	class2

Reverse-mapping to go back

<pre>inv_size_mapping df2['size'] = df</pre>				
df2	[5126]	•map(±nv_	_bize_map	,ping)

	color	size	price	classlabel
0	green	М	10.1	class2
1	red	L	13.5	class1
2	blue	XL	15.3	class2

Encoding Class Labels

- Most models require integer encoding for class labels
 - Note: class labels are not ordinal, and it doesn't matter which integer number we assign to a particular string label

```
import numpy as np
class_mapping = {label: idx for idx, label in enumerate(np.unique(df2['classlabel']))}
df2['classlabel'] = df2['classlabel'].map(class_mapping)
df2
```

	color	size	price	classlabel
0	green	1	10.1	1
1	red	2	13.5	0
2	blue	3	15.3	1

```
inv_class_mapping = {v: k for k, v in class_mapping.items()}
df2['classlabel'] = df2['classlabel'].map(inv_class_mapping)
df2
```

	color	size	price	classlabel
0	green	1	10.1	class2
1	red	2	13.5	class1
2	blue	3	15.3	class2

LabelEncoder

• Alternatively, there is a convenient LabelEncoder class directly implemented in scikit-learn to achieve this

```
from sklearn.preprocessing import LabelEncoder
class_le = LabelEncoder()
y = class_le.fit_transform(df2['classlabel'].values)
y
array([1, 0, 1])

Class_le.inverse_transform(y)
array(['class2', 'class1', 'class2'], dtype=object)
Shortcut of calling fit
and transform
separately
```

One-Hot Encoding

• We could use a similar approach to transform the nominal color column of our dataset, as follows

- Problem:
 - Model may assume that green > blue, and red > green
 - This could result in suboptimal model
- Workaround: Use one-hot encoding
 - Create a dummy feature for each unique value of nominal features
 - \blacksquare E.g., a blue sample is encoded as blue = 1, green = 0, red = 0

One-Hot Encoding

 Use the OneHotEncoder available in scikit-learn's preprocessing module

```
-1 means unknown
                                                            dimension and we want
1 from sklearn.preprocessing import OneHotEncoder
2 X = df2[['color', 'size', 'price']].values
                                                             numpy to figure it out
3 print(X)
4 color_ohe = OneHotEncoder()
5 print(color_ohe.fit_transform(X[:, 0].reshape(-1, 1)).toarray())
['green' 1 10.1]
                                                        Apply to only a
['red' 2 13.5]
['blue' 3 15.3]]
                                                         single column
[[0. 1. 0.]
[0. 0. 1.]
[1. 0. 0.]]
```

One-Hot Encoding via ColumnTransformer

- To selectively transform columns in a multi-feature array, use ColumnTransformer
 - Accepts a list of (name, transformer, column(s)) tuple

```
Only modify the first
 1 from sklearn.compose import ColumnTransformer
                                                                 column
 2 X = df2[['color', 'size', 'price']].values
 3 c transf = ColumnTransformer([
                                ('onehot', OneHotEncoder(), [0]),
                                ('nothing', 'passthrough', [1, 2])
 7 c transf.fit transform(X).astype(float)
array([[ 0. , 1. , 0. , 1. , 10.1],
       [0., 0., 1., 2., 13.5],
       [ 1. , 0. , 0. , 3. , 15.3]])
```

One-Hot Encoding - Via Pandas

- An even more convenient way to create those dummy features via one-hot encoding is to use the get_dummies method implemented in pandas
 - get_dummies will only convert string columns

```
        price
        size
        color_blue
        color_green
        color_red

        0
        10.1
        1
        0
        1
        0

        1
        13.5
        2
        0
        0
        1

        2
        15.3
        3
        1
        0
        0
```

One-Hot Encoding - Dropping First Feature

- Note that we do not lose any information by removing one dummy column
 - E.g., if we remove the column color_blue, the feature information is still preserved since if we observe color_green=0 and color_red=0, it implies that the observation must be blue

```
pd.get_dummies(df2[['price', 'color', 'size']], drop_first=True)

price size color_green color_red

0 10.1 1 1 0

1 13.5 2 0 1

2 15.3 3 0 0

ohct.fit_transform(X)[:, 1:]

array([[1.0, 0.0, 1, 10.1], [0.0, 1.0, 2, 13.5], [0.0, 0.0, 3, 15.3]], dtype=object)
```

UCI Wine Dataset

• The <u>UCI wine dataset</u> consists of 178 wine samples with 13 features describing their different chemical properties

[1 2 3]

	Class label	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanaoid phenois	Proanthocyanins	Color intensity	Hue	OD280/OD315 of diluted wines	Proline
0	1	14.23	1.71	2.43	15.6	127	2.80	3.06	0.28	2.29	5.64	1.04	3.92	1065
1	1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.26	1.28	4.38	1.05	3.40	1050
2	1	13.16	2.36	2.67	18.6	101	2.80	3.24	0.30	2.81	5.68	1.03	3.17	1185
3	1	14.37	1.95	2.50	16.8	113	3.85	3.49	0.24	2.18	7.80	0.86	3.45	1480
4	1	13.24	2.59	2.87	21.0	118	2.80	2.69	0.39	1.82	4.32	1.04	2.93	735

UCI Wine Dataset: Training-Testing

• Let's first divide the dataset into separate training and testing sets

```
from sklearn.model_selection import train_test_split
X, y = df_wine.iloc[:, 1:].values, df_wine.iloc[:, 0].values
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=0, stratify=y)
print(X_train.shape)
print(X_test.shape)
print(y_train.shape)
print(y_test.shape)

(124, 13)
(54, 13)
(124,)
(54,)
```

UCI Wine Dataset: Training-Testing

- It is important to balance the trade-off between inaccurate estimation of generalization error and withholding too much information from the learning algorithm
- In practice, the most commonly used splits are 60:40, 70:30, or 80:20, depending on the size of the initial dataset
 - For large datasets, 90:10 or 99:1 splits are also common and appropriate
- Instead of discarding the allocated test data after model training and evaluation, we can retrain a classifier on the entire dataset as it could improve the predictive performance of the model
 - While this approach is generally recommended, it could lead to worse generalization performance

Feature Scaling

- The majority of ML algorithms require feature scaling
 - Decision trees and random forests are two of few ML algorithms that don't require feature scaling
- Importance
 - Consider the squared error function in Adaline for two dimensional features where one feature is measured on a scale from 1 to 10 and the second feature is measured on a scale from 1 to 100,000
 - The second feature would contribute to the error with a much higher significance
- Two common approaches to bring different features onto the same scale
 - Normalization
 - E.g., rescaling features to a range of [0, 1]
 - Standardization
 - E.g., center features at mean 0 with standard deviation 1

Feature Scaling - Normalization

- Most often, normalization refers to the rescaling of features to a range of [0, 1]
- To normalize our data, we can simply apply a min-max scaling to each feature column
 - \circ A new value $x^{(i)}_{norm}$ of a sample $x^{(i)}$ is calculated as follows

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

• Here x_{min} is the smallest value in a feature column and x_{max} the largest

```
from sklearn.preprocessing import MinMaxScaler
mms = MinMaxScaler()
X_train_norm = mms.fit_transform(X_train)
X_test_norm = mms.transform(X_test)
```

```
print(X_train[:,0].max(axis=0))
print(X_train[:,0].min(axis=0))
print(X_train_norm[:,0].max(axis=0))
print(X_train_norm[:,0].min(axis=0))
print(X_test_norm[:,0].max(axis=0))
print(X_test_norm[:,0].min(axis=0))

14.83
11.41
1.0
0.0
0.871345029239766
-0.111111111111111116
```

Feature Scaling - Standardization

- Standardization is more practical for various reasons including retaining useful information about outliers
- A new value $x^{(i)}_{std}$ of a sample $x^{(i)}$ is calculated as follows

$$x_{std}^{(i)} = \frac{x^{(i)} - \mu_x}{\sigma_x}$$

- Here μ_x is the sample mean of feature column and σ_x the corresponding standard deviation
- Similar to the MinMaxScaler class, scikit-learn also implements a class for standardization

```
from sklearn.preprocessing import StandardScaler
stdsc = StandardScaler()
X_train_std = stdsc.fit_transform(X_train)
X_test_std = stdsc.fit_transform(X_test)
```

```
print(X_train[:,0].mean(axis=0))
print(X_train[:,0].std(axis=0))
print(X_train_std[:,0].mean(axis=0))
print(X_train_std[:,0].std(axis=0))

13.033548387096777
0.8233685663454646
6.87935371750596e-15
0.999999999999998
-1.133095674900999e-15
1.0
```

Normalization vs. Standardization

• The following example illustrates the difference between standardization and normalization

```
ex = np.array([0, 1, 2, 3, 4, 5])

print('standardized: ', (ex-ex.mean()) / ex.std())
print('normalized: ', (ex-ex.min()) / ex.max() - ex.min())

standardized: [-1.46385011 -0.87831007 -0.29277002 0.29277002 0.87831007 1.46385011]
normalized: [0. 0.2 0.4 0.6 0.8 1.]
```

Robust Scaler

- More advanced methods for feature scaling are available in sklearn
- The <u>RobustScaler</u> is especially helpful and recommended if working with small datasets that contain many outliers

Feature Selection

- Selects a subset of relevant features
 - Simplify model for easier interpretation
 - Shorten training time
 - Avoid curse of dimensionality
 - Reduce overfitting
- Feature selection \neq feature extraction (covered in next chapter)
 - \circ Selecting subset of the features \neq creating new features
- We are going to look at two techniques for feature selection
 - L1 Regularization
 - Sequential Backward Selection (SBS)

• L2 regularization (penalty) used in chapter 3

$$L2: \|\mathbf{w}\|_{2}^{2} = \sum_{j=1}^{m} w_{j}^{2}$$

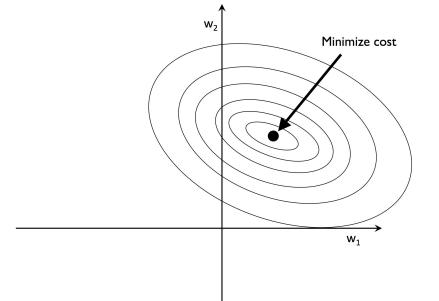
• Another approach: L1 regularization (penalty)

$$L1: \left\| \boldsymbol{w} \right\|_1 = \sum_{j=1}^m \left| w_j \right|$$

- This will usually yield sparse feature weights
 - Most feature weights will be zero
- Sparsity can be useful in practice if we have a high dimensional dataset with many features that are irrelevant
- L1 regularization can be taken as a technique for feature selection

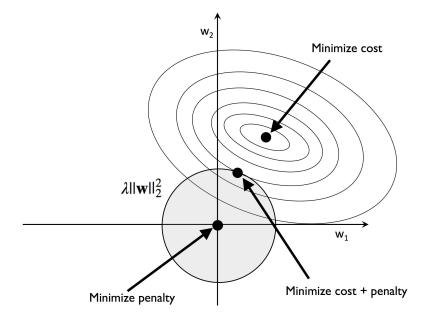
Geometric Interpretation

- To better understand how L1 regularization encourages sparsity, let's take a look at a geometric interpretation of regularization
- Consider the sum of squared errors cost function used for Adaline
- Plot of the contours of a convex cost function for two coefficients w₁ and w₂



Geometric Interpretation: L2 Regularization

- Regularization adds a penalty to the cost function to encourage smaller weights
 - O By increasing the regularization strength λ we shrink the weights towards zero and decrease the dependency of our model on the training data

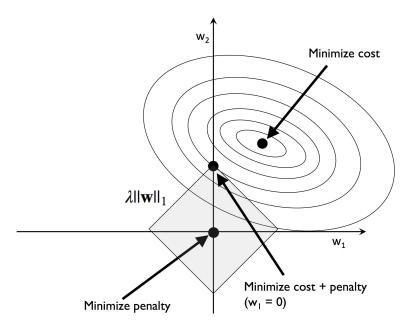


Geometric Interpretation: L1 Regularization

• Since the L1 penalty is the sum of the absolute weight coefficients we can represent it as a diamond-shape

• It is more likely that the optimum is located on the axes, which encourages

sparsity



Mathematical details can be found in Section 3.4 of

The Elements of Statistical Learning

1.56356565 -0.81863112 -0.49263067

Sparse Solution

• We can simply set the penalty parameter to '11' for models in scikit-learn that support L1 regularization

```
from sklearn.linear_model import LogisticRegression
lr = LogisticRegression(penalty = 'l1', C=1.0, solver='liblinear', multi_class='ovr')
lr.fit(X_train_std, y_train)
print('Training accuracy:',lr.score(X_train_std, y_train))
print('Test accuracy:', lr.score(X_test_std, y_test))
Training accuracy: 1.0
```

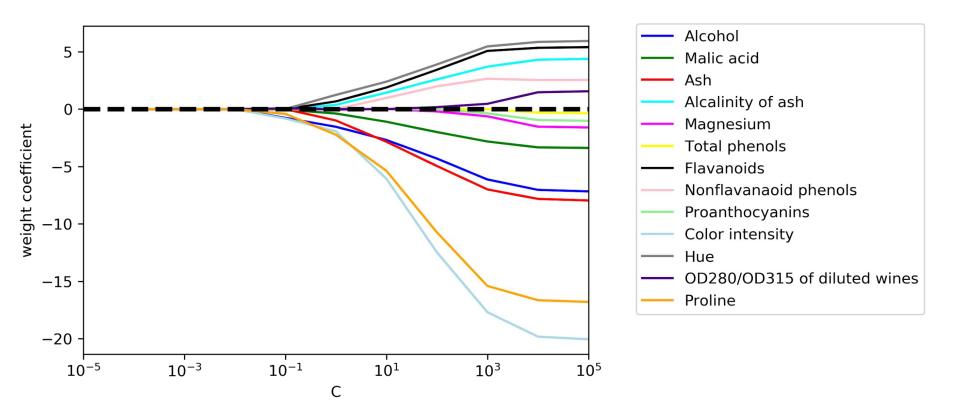
Test accuracy: 1.0

• In scikit-learn, w_0 corresponds to intercept_ and w_j (for j > 0) corresponds to the

-2.4378634 0.

0.

Sparse Solution - Regularization Strength



Sequential Backward Selection (SBS)

- Reduces an initial d-dimensional space to a k-dimensional subspace (k < d) by automatically selecting features that are most relevant
- Idea:
 - Sequentially remove features until desired feature number is reached
 - Define a criterion function J to be maximized
 - E.g., performance of the classifier after removal
 - Use a validation subset of the training set for performance evaluation
 - Eliminate the feature that causes the least performance loss

SBS

Steps:

COMP 3314

- 1. Initialize the algorithm with k = dd is the dimensionality of the full feature space $\mathbf{X_d}$
- 2. Determine the feature $\mathbf{x}^{-} = \operatorname{argmax} J(\mathbf{X}_{\mathbf{k}} \mathbf{x})$ that maximizes the criterion function J
- function J

 3. Remove the feature **x** from the feature set

$$\mathbf{X}_{\mathbf{k-1}} = \mathbf{X}_{\mathbf{k}} - \mathbf{x}^{-1}$$
$$k = k - 1$$

- 4. Terminate if *k* equals the number of desired features; otherwise, go to step 2
 - In the following we will implement SBS in Python from scratch

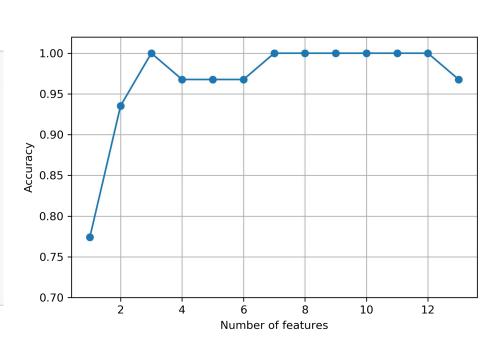
42

COMP 3314

from sklearn.base import clone

```
def init (self, estimator, k features, scoring=accuracy score, test size=0.25, random state=1):
    self.scoring = scoring
   self.estimator = clone(estimator)
   self.k features = k features
   self.test size = test size
   self.random_state = random_state
def fit(self, X, y):
   X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=self.test_size, random state=self.random state)
    dim = X train.shape[1]
    self.indices = tuple(range(dim))
    self.subsets = [self.indices ]
   score = self. calc score(X train, y train, X test, y test, self.indices )
    self.scores = [score]
   while dim > self.k features:
        scores = []; subsets = []
        for p in combinations(self.indices , r=dim - 1):
            score = self._calc_score(X_train, y_train, X_test, y_test, p)
            scores.append(score)
            subsets.append(p)
        best = np.argmax(scores)
        self.indices = subsets[best]
        self.subsets .append(self.indices )
        dim -= 1
        self.scores .append(scores[best])
    self.k_score_ = self.scores_[-1]
    return self
def transform(self, X):
    return X[:, self.indices ]
def calc score(self, X train, y train, X test, y test, indices):
   self.estimator.fit(X_train[:, indices], y_train)
   y_pred = self.estimator.predict(X_test[:, indices])
    score = self.scoring(y test, y pred)
    return score
```

```
import matplotlib.pyplot as plt
from sklearn.neighbors import KNeighborsClassifier
knn = KNeighborsClassifier(n_neighbors=5)
sbs = SBS(knn, k_features=1)
sbs.fit(X_train_std, y_train)
k_feat = [len(k) for k in sbs.subsets_]
plt.plot(k_feat, sbs.scores_, marker='o')
plt.ylim([0.7, 1.02])
plt.ylabel('Accuracy')
plt.xlabel('Number of features')
plt.grid()
plt.tight_layout()
plt.show()
```



SBS - Analyzing the Result

• The smallest feature subset (k = 3) that yielded such a good performance on the validation dataset has the following features

```
k3 = list(sbs.subsets_[10])
print(df_wine.columns[1:][k3])

Index(['Alcohol', 'Malic acid', 'OD280/OD315 of diluted wines'], dtype='object')
```

• The accuracy of the KNN classifier on the original test set is as follows

```
knn.fit(X_train_std, y_train)
print('Training accuracy:', knn.score(X_train_std, y_train))
print('Test accuracy:', knn.score(X_test_std, y_test))
Training accuracy: 0.967741935483871
Test accuracy: 0.9814814814814815
```

• The three-feature subset has the following accuracy

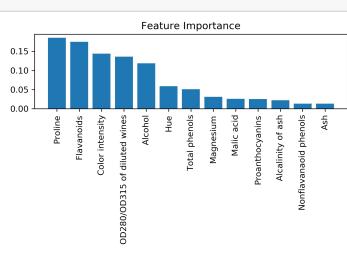
Feature Selection Algorithms in scikit-learn

- There are many more feature selection algorithms available via scikit-learn
- A comprehensive discussion of the different feature selection methods is beyond the scope of this lecture
 - A good summary with illustrative examples can be found <u>here</u>

Assessing Feature Importance

- We can determine relevant features using random forest
 - Measure the feature importance as the averaged information gain
- The random forest implementation in scikit-learn already collects the feature importance values for us
 - Access them via the feature_importances_ attribute after fitting a RandomForestClassifier
- In the following we will train a forest of 500 trees on the Wine dataset and rank the 13 features by their respective importance measures

```
from sklearn.ensemble import RandomForestClassifier
feat_labels = df_wine.columns[1:]
forest = RandomForestClassifier(n_estimators=500, random_state=1)
forest.fit(X_train, y_train)
importances = forest.feature_importances_
indices = np.argsort(importances)[::-1]
for f in range(X_train.shape[1]):
    print("%2d) %-*s %f" % (f + 1, 30, feat_labels[indices[f]], importances[indices[f]]))
plt.title('Feature Importance')
plt.bar(range(X_train.shape[1]), importances[indices], align='center')
plt.xticks(range(X_train.shape[1]), feat_labels[indices], rotation=90)
plt.xlim([-1, X_train.shape[1]])
plt.tight_layout()
plt.show()
```

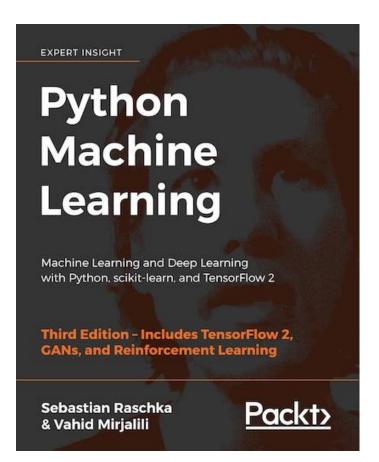


Conclusion

- Handle missing data correctly
- Encode categorical variables correctly
- Map ordinal and nominal feature values to integer representations
- L1 regularization can help us to avoid overfitting by reducing the complexity of a model
- Used a sequential feature selection algorithm to select meaningful features from a dataset

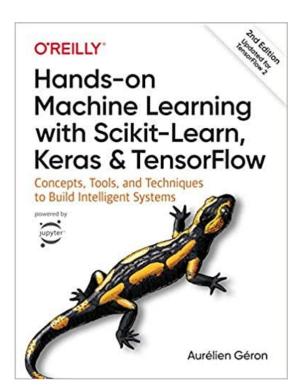
References

- Most materials in this chapter are based on
 - o <u>Book</u>
 - o <u>Code</u>



References

- Some materials in this chapter are based on
 - o <u>Book</u>
 - o Code



References

- The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition
 - Trevor Hastie, Robert Tibshirani, Jerome Friedman
- https://web.stanford.edu/~hastie/ElemStatLearn/
- Pandas User Guide: Working with missing data