Lecture 05

Data Preprocessing and Machine Learning with Scikit-Learn

(Computational Foundations Part 3/3)

STAT 451: Intro to Machine Learning, Fall 2021
Sebastian Raschka

Where we currently are in this course ...

Part I: Introduction

- Lecture 1: What is Machine Learning? An Overview.
- Lecture 2: Intro to Supervised Learning: KNN

Part II: Computational Foundations

- Lecture 3: Using Python, Anaconda, IPython, Jupyter Notebooks
- Lecture 4: Scientific Computing with NumPy, SciPy, and Matplotlib

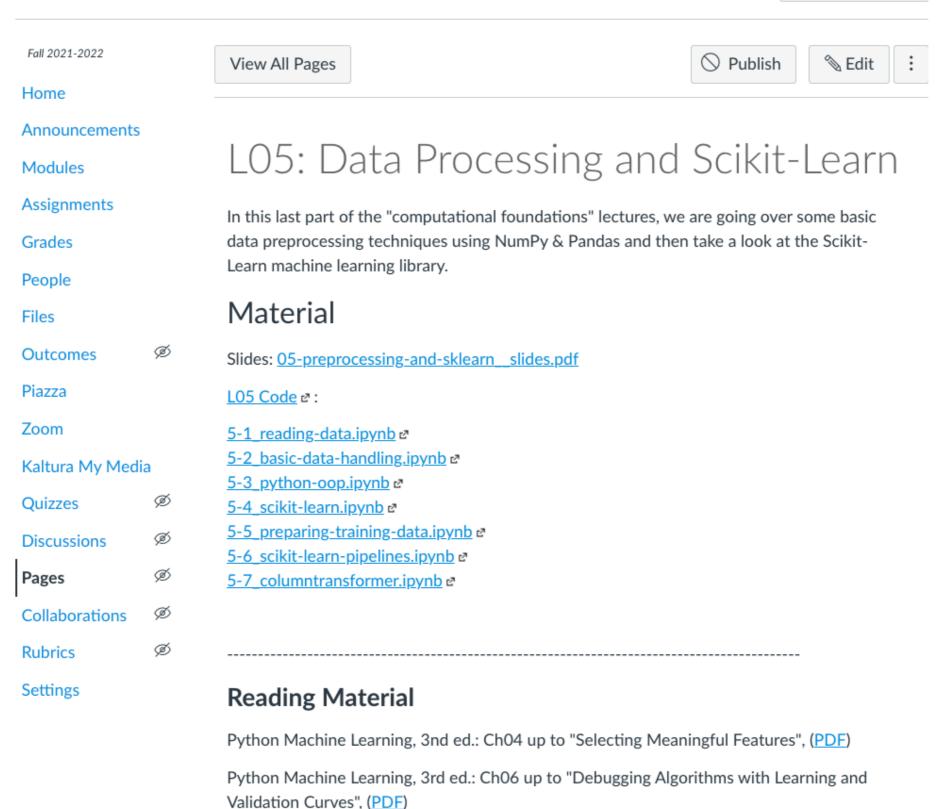


Lecture 5: Data Preprocessing and Machine Learning with Scikit-Learn

Part III: Tree-Based Methods

- Lecture 6: Decision Trees
- Lacture 7: Encamble Methods

6∂ Student View

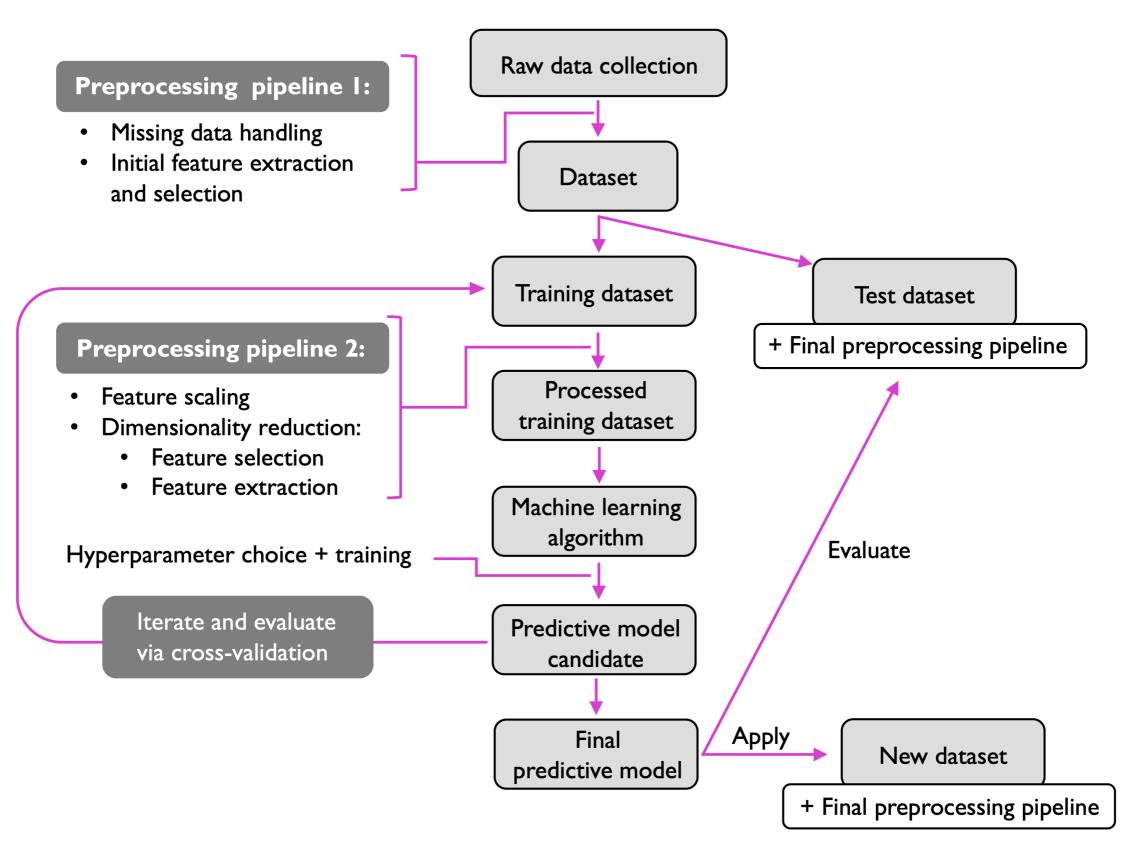


Previous

Lecture 5 (Data Preprocessing and ML with Scikit-Learn) Topics

- 1. Reading a Dataset from a Tabular Text File
- 2. Basic Data Handling
- 3. Object Oriented Programming (OOP) & Python Classes
- 4. Machine Learning with Scikit-learn
- 5. Preparing Training Data & Transformer API
- 6. Scikit-learn Pipelines
- 7. Heterogeneous Datasets

Machine Learning Workflow



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Reading a Dataset from a Tabular Text File

The Iris Dataset



Iris-Setosa



Iris-Versicolor



Iris-Virginica

Sometimes Useful: Executing "Bash" Terminal Commands Via "!"

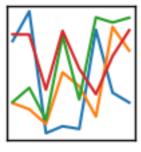
```
!head iris.csv
```

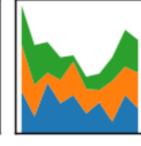
```
Id,SepalLength[cm],SepalWidth[cm],PetalLength[cm],PetalWidth[cm],Species
1,5.1,3.5,1.4,0.2,Iris-setosa
2,4.9,3.0,1.4,0.2,Iris-setosa
3,4.7,3.2,1.3,0.2,Iris-setosa
4,4.6,3.1,1.5,0.2,Iris-setosa
5,5.0,3.6,1.4,0.2,Iris-setosa
6,5.4,3.9,1.7,0.4,Iris-setosa
7,4.6,3.4,1.4,0.3,Iris-setosa
8,5.0,3.4,1.5,0.2,Iris-setosa
9,4.4,2.9,1.4,0.2,Iris-setosa
```

A DataFrame Library for Data Wrangling









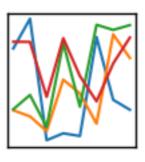
https://pandas.pydata.org

pandas is short for "PANel DAta S"

Pandas Paper: McKinney, Wes. "Data structures for statistical computing in python." Proceedings of the 9th Python in Science Conference. Vol. 445. 2010.









https://pandas.pydata.org

```
import pandas as pd

df = pd.read_csv('iris.csv')
df.head()
```

	Id	SepalLength[cm]	SepalWidth[cm]	PetalLength[cm]	PetalWidth[cm]	Species
0	1	5.1	3.5	1.4	0.2	Iris-setosa
1	2	4.9	3.0	1.4	0.2	Iris-setosa
2	3	4.7	3.2	1.3	0.2	Iris-setosa
3	4	4.6	3.1	1.5	0.2	Iris-setosa
4	5	5.0	3.6	1.4	0.2	Iris-setosa

df.shape

(150, 6)

```
import pandas as pd
pd.read_csv?
Signature:
pd.read csv(
    filepath_or_buffer: Union[str, pathlib.Path, IO[~AnyStr]],
    sep=',',
    delimiter=None,
    header='infer',
    names=None,
    index_col=None,
    usecols=None,
    squeeze=False,
    prefix=None,
    mangle_dupe_cols=True,
    dtype=None,
    engine=None,
    converters=None,
    true_values=None,
    false_values=None,
    skipinitialspace=False,
    skiprows=None,
    skipfooter=0,
    nrows=None,
    na_values=None,
    keep_default_na=True,
    na_filter=True,
    verbose=False,
    skip_blank_lines=True,
    parse_dates=False,
    infer_datetime_format=False,
    keep_date_col=False,
    date_parser=None,
    dayfirst=False,
    cache_dates=True,
    iterator=False,
    chunksize=None,
    compression='infer',
    thousands=None,
```

decimal: str = '.',
lineterminator=None,

quotechar='"',

Many additional options exist ...

E.g., processing a large file iteratively ...

```
in_csv = 'my_large.csv'
chunksize = 100000 # number of lines to process at each iteration
# columns that should be read from the CSV file
columns = ['molecule_id', 'charge', 'drugsnow', 'hba', 'hbd']
# Get number of lines in the CSV file
nlines = subprocess.check_output(['wc', '-l', in_csv])
nlines = int(nlines.split()[0])
# Iteratively read CSV and dump lines into the SQLite table
for i in range(0, nlines, chunksize): # change 0 -> 1 if your csv file contains a column header
   df = pd.read csv(in csv,
            header=None, # no header, define column header manually later
            nrows=chunksize, # number of rows to read at each iteration
            skiprows=i) # skip rows that were already read
   # do something with the data in df
```

Source: https://github.com/rasbt/python-reference/blob/master/useful-scripts/large-csv to sqlite.py

For scaling Pandas, also check out

Modin: https://github.com/modin-project/modin

Visit the complete documentation on readthedocs: https://modin.readthedocs.io

Scale your pandas workflow by changing a single line of code.

```
import modin.pandas as pd
import numpy as np

frame_data = np.random.randint(0, 100, size=(2**10, 2**8))
df = pd.DataFrame(frame_data)
```

and Dask: https://github.com/dask/dask/

```
from dask.distributed import Client, progress
client = Client(n_workers=2, threads_per_worker=2, memory_limit='1GB')
client

import dask
import dask.dataframe as dd
df = dask.datasets.timeseries()
```

```
df2 = df[df.y > 0]
df3 = df2.groupby('name').x.std()
df3

Dask Series Structure:
npartitions=1
    float64
...
Name: x, dtype: float64
Dask Name: sqrt, 157 tasks
```

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Lecture 5 (Data Preprocessing and ML with Scikit-Learn) Topics

1. Reading a Dataset from a Tabular Text File

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- 7. Heterogeneous Datasets

Python Function

```
def some_func(x):
    return 'Hello World ' + str(x)
some_func(123)
```

'Hello World 123'

Regular Function vs Lambda Function

```
def some_func(x):
    return 'Hello World ' + str(x)
some_func(123)
```

'Hello World 123'

```
f = lambda x: 'Hello World ' + str(x)
f(123)
```

'Hello World 123'

```
import pandas as pd

df = pd.read_csv('iris.csv')
df.head()
```

	Id	SepalLength[cm]	SepalWidth[cm]	PetalLength[cm]	PetalWidth[cm]	Species
0	1	5.1	3.5	1.4	0.2	Iris-setosa
1	2	4.9	3.0	1.4	0.2	Iris-setosa
2	3	4.7	3.2	1.3	0.2	Iris-setosa
3	4	4.6	3.1	1.5	0.2	Iris-setosa
4	5	5.0	3.6	1.4	0.2	Iris-setosa

Column-based Data Processing via Lambda Functions and ".apply"

```
df['Species'] = df['Species'].apply(lambda x: 0 if x=='Iris-setosa' else x)
df.head()
```

	ld	SepalLength[cm]	SepalWidth[cm]	PetalLength[cm]	PetalWidth[cm]	Species
0	1	5.1	3.5	1.4	0.2	0
1	2	4.9	3.0	1.4	0.2	0
2	3	4.7	3.2	1.3	0.2	0
3	4	4.6	3.1	1.5	0.2	0
4	5	5.0	3.6	1.4	0.2	0

Column-based Data Processing via Dictionaries and ".map"

S	Specie	ecie	es
			0
			0
			0
			0
		1	0

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Quick Inspections via "head" and "tail"

df.tail()

	Id	SepalLength[cm]	SepalWidth[cm]	PetalLength[cm]	PetalWidth[cm]	Species
145	146	6.7	3.0	5.2	2.3	2
146	147	6.3	2.5	5.0	1.9	2
147	148	6.5	3.0	5.2	2.0	2
148	149	6.2	3.4	5.4	2.3	2
149	150	5.9	3.0	5.1	1.8	2

Accessing the Underlying NumPy Array(s) via the ".values" Attribute

"Creating*" the Label Vector "y" and Design Matrix "X"

```
y = df['Species'].values
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
 X = df.iloc[:, 1:5].values
X[:5]
array([[5.1, 3.5, 1.4, 0.2],
```

```
array([[5.1, 3.5, 1.4, 0.2], [4.9, 3. , 1.4, 0.2], [4.7, 3.2, 1.3, 0.2], [4.6, 3.1, 1.5, 0.2], [5. , 3.6, 1.4, 0.2]])
```

* why did I put "Creating" in quotation marks?

A Library with Additional Data Science & Machine Learning-related Functions



http://rasbt.github.io/mlxtend/

Raschka, Sebastian. "MLxtend: Providing machine learning and data science utilities and extensions to Python's scientific computing stack." *The Journal of Open Source Software* 3.24 (2018).

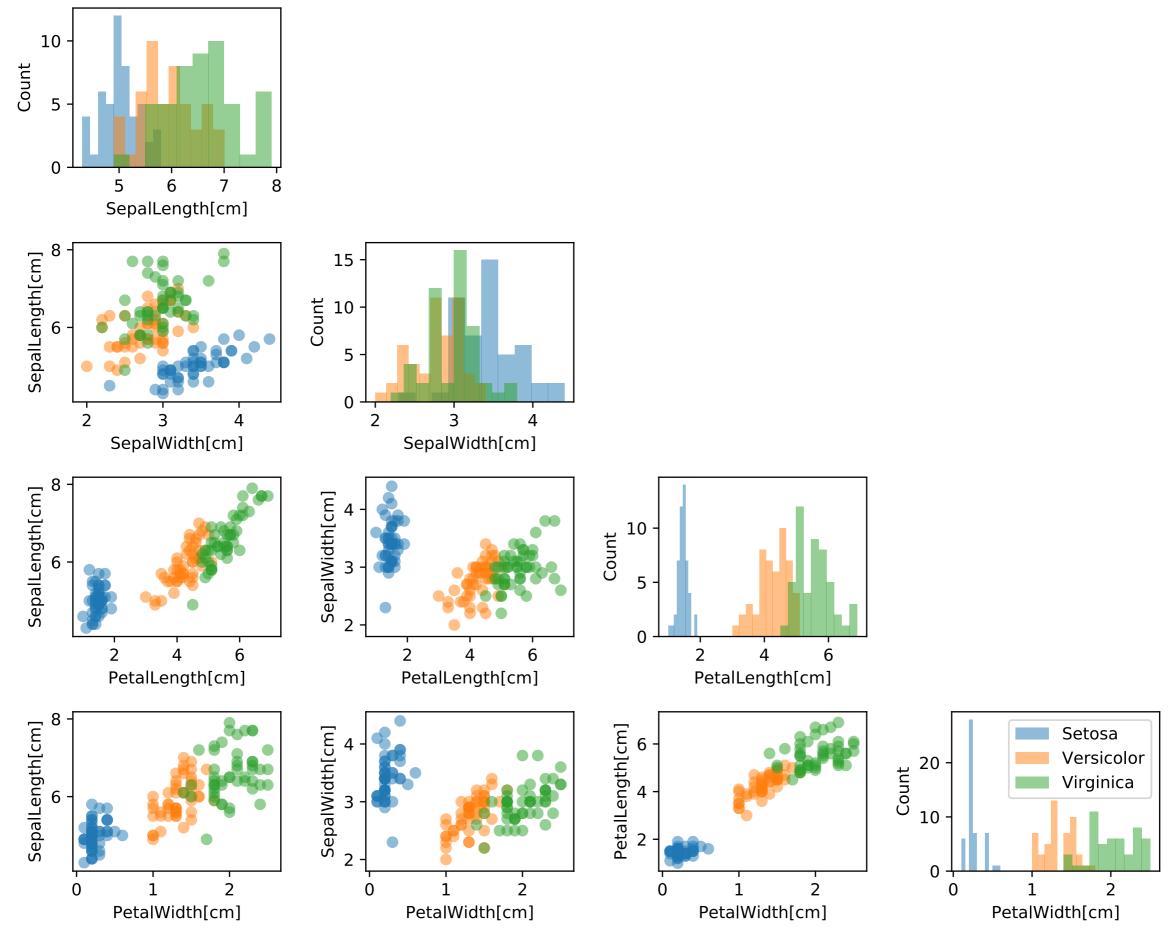
Exploratory Data Analysis (EDA)

```
%matplotlib inline
import matplotlib.pyplot as plt
from mlxtend.data import iris_data
from mlxtend.plotting import scatterplotmatrix

names = df.columns[1:5]

fig, axes = scatterplotmatrix(X[y==0], figsize=(10, 8), alpha=0.5)
fig, axes = scatterplotmatrix(X[y==1], fig_axes=(fig, axes), alpha=0.5)
fig, axes = scatterplotmatrix(X[y==2], fig_axes=(fig, axes), alpha=0.5, names=names)

plt.tight_layout()
plt.legend(labels=['Setosa', 'Versicolor', 'Virginica'])
plt.show()
```



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Splitting a Dataset into Train, Validation, and Test Subsets

```
import numpy as np
indices = np.arange(X.shape[0])
rng = np.random.RandomState(123)
permuted_indices = rng.permutation(indices)
permuted_indices
```

Splitting a Dataset into Train, Validation, and Test Subsets

```
import numpy as np
indices = np.arange(X.shape[0])
rng = np.random.RandomState(123)
permuted_indices = rng.permutation(indices)
permuted_indices
array([ 72, 112, 132, 88, 37, 138, 87, 42, 8, 90, 141, 33, 59,
      116, 135, 104, 36, 13, 63, 45, 28, 133, 24, 127, 46, 20,
       31, 121, 117, 4, 130, 119, 29, 0, 62, 93, 131, 5, 16,
       82, 60, 35, 143, 145, 142, 114, 136, 53, 19, 38, 110, 23,
       9, 86, 91, 89, 79, 101, 65, 115, 41, 124, 95, 21, 11,
      103, 74, 122, 118, 44, 51, 81, 149, 12, 129, 56, 50, 25,
      128, 146, 43, 1, 71, 54, 100, 14, 6, 80, 26, 70, 139,
       30, 108, 15, 18, 77, 22, 10, 58, 107, 75, 64, 69, 3,
       40, 76, 134, 34, 27, 94, 85, 97, 102, 52, 92, 99, 105,
       7, 48, 61, 120, 137, 125, 147, 39, 84, 2, 67, 55, 49,
      68, 140, 78, 144, 111, 32, 73, 47, 148, 113, 96, 57, 123,
      106, 83, 17, 98, 66, 126, 109])
```

Splitting a Dataset into Train, Validation, and Test Subsets

```
import numpy as np
indices = np.arange(X.shape[0])
rng = np.random.RandomState(123)
permuted_indices = rng.permutation(indices)
permuted_indices
        00, 170, 70, 177, 111, 32, 73, 77, 170, 113,
       106, 83, 17, 98, 66, 126, 109])
train_size, valid_size = int(0.65*X.shape[0]), int(0.15*X.shape[0])
test_size = X.shape[0] - (train_size + valid_size)
print(train_size, valid_size, test_size)
97 22 31
train_ind = permuted_indices[:train_size]
valid_ind = permuted_indices[train_size:(train_size + valid_size)]
test_ind = permuted_indices[(train_size + valid_size):]
X_train, y_train = X[train_ind], y[train_ind]
X_valid, y_valid = X[valid_ind], y[valid_ind]
X_test, y_test = X[test_ind], y[test_ind]
```

(Later, we will see how to do this more conveniently)

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(97, 4)

Lecture 5 (Data Preprocessing and ML with Scikit-Learn) Topics

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To get a better understanding of the scikit-learn API, we need to understand the main concepts behind Object Oriented Programming (OOP) & classes in Python

```
class VehicleClass():
   def __init__(self, horsepower):
        "This is the 'init' method"
        # this is a class attribute:
        self.horsepower = horsepower
   def horsepower_to_torque(self, rpm):
        "This is a regular method"
        torque = self.horsepower * rpm / 5252
        return torque
   def tune_motor(self):
        self.horsepower *= 2
   def _private_method(self):
        print('this is private')
   def ___very_private_method(self):
        print('this is very private')
```

```
class VehicleClass():
    def __init__(self, horsepower):
        "This is the 'init' method"
        # this is a class attribute:
        self.horsepower = horsepower
    def horsepower_to_torque(self, rpm):
        "This is a regular method"
        torque = self.horsepower * rpm / 5252
        return torque
    def tune_motor(self):
        self.horsepower *= 2
    def _private_method(self):
        print('this is private')
    def __very_private_method(self):
        print('this is very private')
```

```
# instantiate an object:
car1 = VehicleClass(horsepower=123)
print(car1.horsepower)
```

123

```
class VehicleClass():
    def __init__(self, horsepower):
        "This is the 'init' method"
        # this is a class attribute:
        self.horsepower = horsepower
    def horsepower_to_torque(self, rpm):
        "This is a regular method"
        torque = self.horsepower * rpm / 5252
        return torque
    def tune_motor(self):
        self.horsepower *= 2
    def _private_method(self):
        print('this is private')
    def __very_private_method(self):
        print('this is very private')
```

```
# instantiate an object:
car1 = VehicleClass(horsepower=123)
print(car1.horsepower)

123

car1.horsepower_to_torque(rpm=5000)

117.0982482863671

car1.tune_motor()
car1.horsepower_to_torque(rpm=5000)

234.1964965727342
```

```
class VehicleClass():
    def __init__(self, horsepower):
        "This is the 'init' method"
        # this is a class attribute:
        self.horsepower = horsepower
    def horsepower_to_torque(self, rpm):
        "This is a regular method"
        torque = self.horsepower * rpm / 5252
        return torque
    def tune_motor(self):
        self.horsepower *= 2
    def _private_method(self):
        print('this is private')
    def __very_private_method(self):
        print('this is very private')
```

```
class VehicleClass():
                                             Python Classes
   def __init__(self, horsepower):
       "This is the 'init' method"
       # this is a class attribute:
       self.horsepower = horsepower
   def horsepower_to_torque(self, rpm):
       "This is a regular method"
       torque = self.horsepower * rpm / 5252
       return torque
   def tune_motor(self):
       self.horsepower ∗= 2
   def private method(self):
       print('this is private')
   def __very_private_method(self):
       print('this is very private')
```

```
car1._private_method()
  this is private
  car1.__very_private_method()
                                            Traceback (most recent call last)
  AttributeError
  <ipython-input-23-818c47ec0aa2> in <module>()
  ---> 1 car1.__very_private_method()
 AttributeError: 'VehicleClass' object has no attribute '__very_private_method'
  car1._VehicleClass__very_private_method()
this is very private
```

```
class CarClass(VehicleClass):

    def __init__(self, horsepower):
        super().__init__(horsepower)
        self.num_wheels = 4

new_car = CarClass(horsepower=123)
print('Number of wheels:', new_car.num_wheels)
print('Horsepower:', new_car.horsepower)
new_car.tune_motor()
print('Horsepower:', new_car.horsepower)
```

Number of wheels: 4

Horsepower: 123 Horsepower: 246

K-Nearest Neighbors Implementation

```
class KNNClassifier(object):
    def __init__(self, k, dist_fn=None):
        self.k = k
        if dist_fn is None:
            self.dist_fn = self._euclidean_dist
   def _euclidean_dist(self, a, b):
        dist = 0.
        for ele_i, ele_j in zip(a, b):
            dist += ((ele_i - ele_j)**2)
        dist = dist**0.5
        return dist
   def _find_nearest(self, x):
        dist_idx_pairs = []
        for j in range(self.dataset_.shape[0]):
            d = self.dist_fn(x, self.dataset_[j])
            dist_idx_pairs.append((d, j))
        sorted_dist_idx_pairs = sorted(dist_idx_pairs)
        return sorted_dist_idx_pairs
   def fit(self, X, y):
        self.dataset_ = X.copy()
        self.labels_ = y.copy()
        self.possible_labels_ = np.unique(y)
   def predict(self, X):
        predictions = np.zeros(X.shape[0], dtype=int)
        for i in range(X.shape[0]):
            k_nearest = self._find_nearest(X[i])[:self.k]
            indices = [entry[1] for entry in k_nearest]
            k_labels = self.labels_[indices]
            counts = np.bincount(k_labels,
                                 minlength=self.possible_labels_.shape[0])
            pred_label = np.argmax(counts)
            predictions[i] = pred_label
        return predictions
```

K-Nearest Neighbors Implementation

```
class KNNClassifier(object):
   def __init__(self, k, dist_fn=None):
       self.k = k
       if dist_fn is None:
           self.dist_fn = self._euclidean_dist
   def _euclidean_dist(self, a, b):
       dist = 0.
       for ele_i, ele_j in zip(a, b):
           dist += ((ele_i - ele_j)**2)
       dist = dist**0.5
       return dist
   def _find_nearest(self, x):
       dist_idx_pairs = []
       for j in range(self.dataset_.shape[0]):
           d = self.dist_fn(x, self.dataset_[j])
           dist_idx_pairs.append((d, j))
       sorted
                knn_model = KNNClassifier(k=3)
       return
                knn_model.fit(X_train, y_train)
   def fit(se
       self.d
       self.l
                print(knn_model.predict(X_valid))
       self.p
   def predic
                             1 1 0 0 1 2 0 0 1 1 1 2 1 1 1 2 0 0
       predic
       for i
           k nearest = self. find nearest(X[i])[:self.k]
           indices = [entry[1] for entry in k_nearest]
           k_labels = self.labels_[indices]
           counts = np.bincount(k_labels,
                               minlength=self.possible_labels_.shape[0])
           pred_label = np.argmax(counts)
           predictions[i] = pred_label
       return predictions
```

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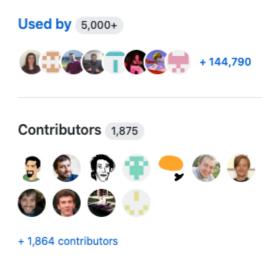
The "Main" Machine Learning Library for Python



http://scikit-learn.org

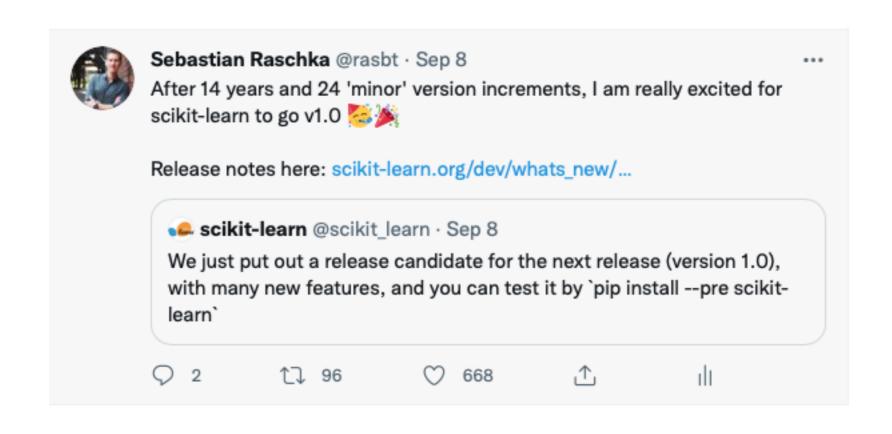
Scikit-learn was initially developed by David Cournapeau as a Google summer of code project in 2007. Later Matthieu Brucher joined the project and started to use it as a part of his thesis work.

Original author(s): David Cournapeau
Written in: Python, Cython, C and C++
Initial release: June 2007; 13 years ago



Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V. and Vanderplas, J., 2011. Scikit-learn: Machine learning in Python. *the Journal of Machine Learning Research*, 12, pp.2825-2830.

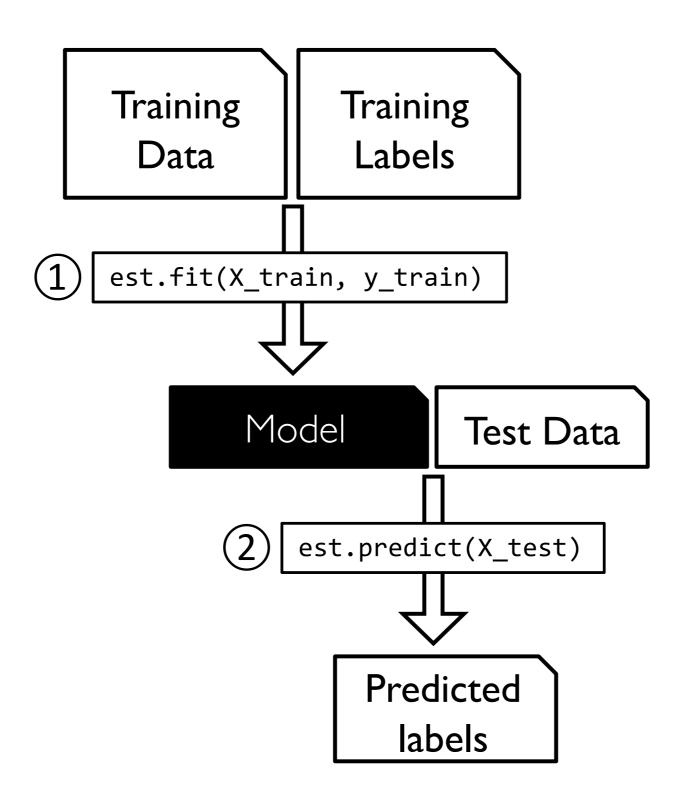
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The Scikit-learn Estimator API (an OOP Paradigm)

```
class SupervisedEstimator(...):
    def __init__(self, hyperparam_1, ...):
        self.hyperparm_1
    def fit(self, X, y):
        self.fit_attribute_
        return self
    def predict(self, X):
        return y_pred
    def score(self, X, y):
        return score
    def _private_method(self):
    . . .
```

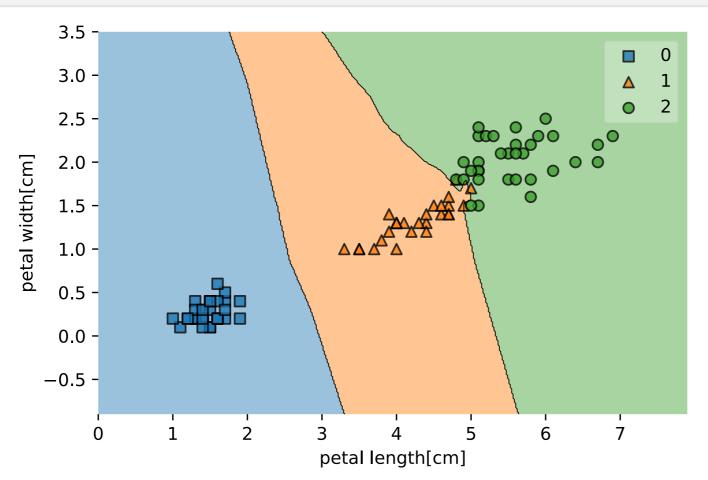
The Scikit-learn Estimator API



A 3-Nearest Neighbor Classifier & 2 Iris Features

```
from sklearn.neighbors import KNeighborsClassifier
from mlxtend.plotting import plot_decision_regions

knn_model = KNeighborsClassifier(n_neighbors=3)
knn_model.fit(X_train[:, 2:], y_train)
plot_decision_regions(X_train[:, 2:], y_train, knn_model)
plt.xlabel('petal length[cm]')
plt.ylabel('petal width[cm]')
plt.savefig('images/decisionreg.pdf')
plt.show()
```



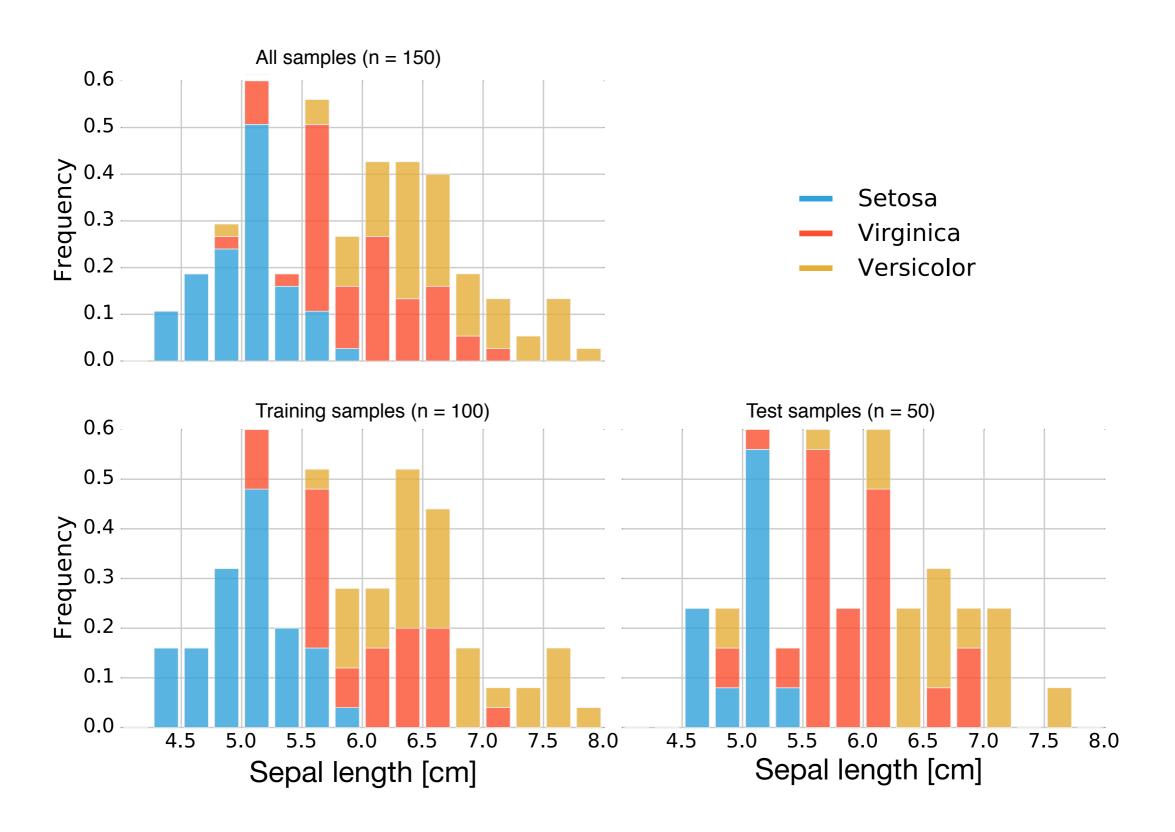
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Lecture 5 (Data Preprocessing and ML with Scikit-Learn) Topics

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- 6. Scikit-learn Pipelines
- 7. Heterogeneous Datasets

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Issues with Random Subsampling ...



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Stratified Splits

```
from sklearn.model_selection import train_test_split
X_temp, X_test, y_temp, y_test = \
        train_test_split(X, y, test_size=0.2,
                         shuffle=True, random_state=123, stratify=y)
np.bincount(y_temp)
array([40, 40, 40])
X_train, X_valid, y_train, y_valid = \
        train_test_split(X_temp, y_temp, test_size=0.2,
                         shuffle=True, random_state=123, stratify=y_temp)
X_train.shape
(96, 4)
```

Normalization: Min-Max Scaling

$$x_{norm}^{[i]} = \frac{x^{[i]} - x_{min}}{x_{max} - x_{min}}$$

Normalization: Min-Max Scaling

$$x_{norm}^{[i]} = \frac{x^{[i]} - x_{min}}{x_{max} - x_{min}}$$

```
x = np.arange(6).astype(float)
x

array([0., 1., 2., 3., 4., 5.])

x_norm = (x - x.min()) / (x.max() - x.min())
x_norm

array([0., 0.2, 0.4, 0.6, 0.8, 1.])
```

Normalization: Standardization

$$x_{std}^{[i]} = \frac{x^{[i]} - \mu_x}{\sigma_x}$$

Normalization: Standardization

$$x_{std}^{[i]} = \frac{x^{[i]} - \mu_x}{\sigma_x}$$

Normalization: Standardization

```
df = pd.DataFrame([1, 2, 1, 2, 3, 4])
df[0].std()
```

1.1690451944500122

```
df[0].values.std()
```

1.0671873729054748

Sample vs Population Standard Deviation

$$s_{x} = \sqrt{\frac{1}{n-1} \sum_{n=1}^{i=1} (x^{[i]} - \bar{x})^{2}}$$

$$\sigma_{x} = \sqrt{\frac{1}{n} \sum_{i=1}^{i=1} (x^{[i]} - \mu_{x})^{2}}$$

Sample vs Population Standard Deviation

```
df = pd.DataFrame([1, 2, 1, 2, 3, 4])
df[0].std()
```

1.1690451944500122

1.0671873729054748

1.1690451944500122

$$S_{x} = \sqrt{\frac{1}{n-1} \sum_{n=1}^{i=1} (x^{[i]} - \bar{x})^{2}}$$

$$\sigma_{x} = \sqrt{\frac{1}{n} \sum_{i=1}^{i=1} (x^{[i]} - \mu_{x})^{2}}$$

```
mu, sigma = X_train.mean(axis=0), X_train.std(axis=0)

X_train_std = (X_train - mu) / sigma
X_valid_std = (X_valid - mu) / sigma
X_test_std = (X_test - mu) / sigma
```

Given 3 training examples:

- example1: 10 cm -> class 2

- example2: 20 cm -> class 2

- example3: 30 cm -> class 1

Estimate:

mean: 20 cm

standard deviation: 8.2 cm

Given 3 training examples:

```
- example1: 10 cm -> class 2
```

- example2: 20 cm -> class 2
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Estimate:

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Standardize:

- example1: -1.21 -> class 2

- example2: 0.00 -> class 2

- example3: 1.21 -> class 1

Given 3 training examples:

- example1: 10 cm -> class 2

- example2: 20 cm -> class 2

- example3: 30 cm -> class 1

Estimate:

mean: 20 cm standard deviation: 8.2 cm

Standardize (z scores):

- example1: -1.21 -> class 2

- example2: 0.00 -> class 2

- example3: 1.21 -> class 1

Assume you have the classification rule:

$$h(z) = \begin{cases} \text{class 2} & \text{if } z \leq 0.6\\ \text{class 1} & \text{otherwise} \end{cases}$$

Given 3 training examples:

- example1: 10 cm -> class 2

- example2: 20 cm -> class 2

- example3: 30 cm -> class 1

Estimate:

mean: 20 cm standard deviation: 8.2 cm

Standardize (z scores):

- example1: -1.21 -> class 2

- example2: 0.00 -> class 2

- example3: 1.21 -> class 1

$$h(z) = \begin{cases} \text{class 2} & \text{if } z \leq 0.6\\ \text{class 1} & \text{otherwise} \end{cases}$$

Given 3 NEW examples:

- example4: 5 cm -> class?

- example5: 6 cm -> class?

- example6: 7 cm -> class?

Estimate "new" mean and std.:

- example5: -1.21 -> class 2

- example6: 0.00 -> class 2

- example7: 1.21 -> class 1

Given 3 training examples:

- example1: 10 cm -> class 2

- example2: 20 cm -> class 2

- example3: 30 cm -> class 1

Estimate:

mean: 20 cm standard deviation: 8.2 cm

Standardize (z scores):

- example1: -1.21 -> class 2

- example2: 0.00 -> class 2

- example3: 1.21 -> class 1

$$h(z) = \begin{cases} \text{class 2} & \text{if } z \leq 0.6\\ \text{class 1} & \text{otherwise} \end{cases}$$

- example4: 5 cm -> class?

- example5: 6 cm -> class?

- example6: 7 cm -> class?

Estimate "new" mean and std.:

- example5: -1.21 -> class 2

- example6: 0.00 -> class 2

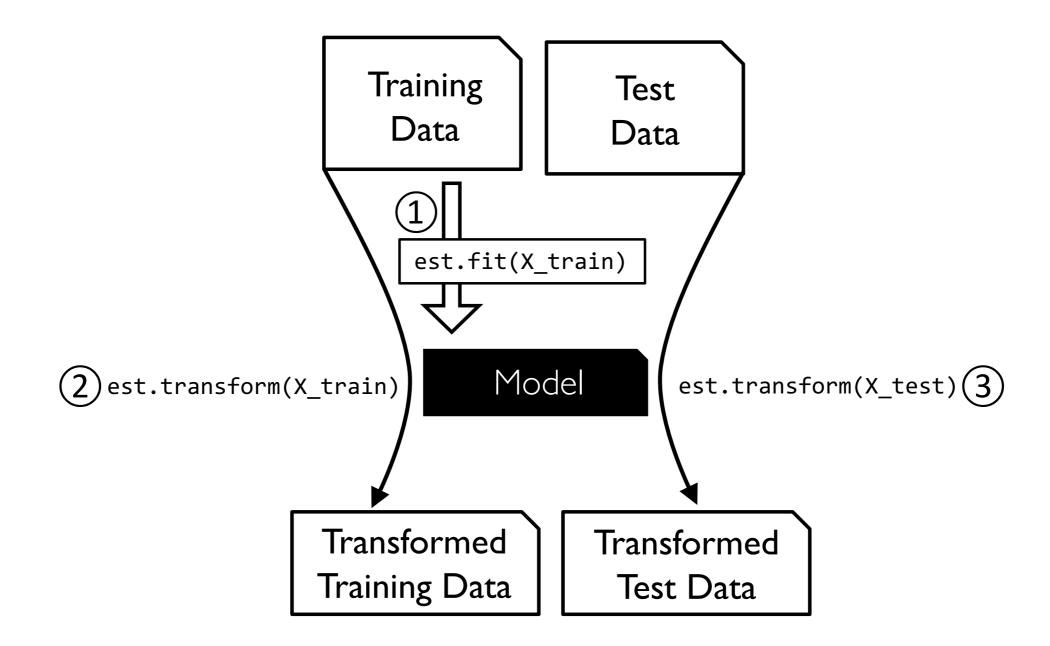
- example7: 1.21 -> class 1

- example5: -18.37

- example6: -17.15

- example7: -15.92

The Scikit-Learn Transformer API



The Scikit-Learn Transformer API

```
from sklearn.preprocessing import MinMaxScaler
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
scaler.fit(X_train)
X_train_std = scaler.transform(X_train)
X_valid_std = scaler.transform(X_valid)
X_test_std = scaler.transform(X_test)
```

Working with Categorical Data

```
df = pd.read_csv('categoricaldata.csv')
df
```

ŀ	classlabe	price	size	color	
1	class	10.1	М	green	0
2	class2	13.5	L	red	1
1	class	15.3	XXL	blue	2

Categorical Data -> Ordinal Data

	color	size	price	classlabel
0	green	2	10.1	class1
1	red	3	13.5	class2
2	blue	5	15.3	class1

Categorical Data -> Nominal Data color size price classlabel (Class Labels)

	COIOI	3126	price	Classianci
0	green	2	10.1	class1
1	red	3	13.5	class2
2	blue	5	15.3	class1

```
from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
df['classlabel'] = le.fit_transform(df['classlabel'])
df
```

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	color	size	price	classlabel
0	green	2	10.1	0
1	red	3	13.5	1
2	blue	5	15.3	0

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One-hot Encoding for Categorical (Nominal) Features

	color	size	price	classlabel
0	green	2	10.1	0
1	red	3	13.5	1
2	blue	5	15.3	0

pd.get_dummies(df)

	size	price	classlabel	color_blue	color_green	color_red
0	2	10.1	0	0	1	0
1	3	13.5	1	0	0	1
2	5	15.3	0	1	0	0

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One-hot Encoding for Categorical (Nominal) Features

pd.get_dummies(df)

	size	price	classlabel	color_blue	color_green	color_red
0	2	10.1	0	0	1	0
1	3	13.5	1	0	0	1
2	5	15.3	0	1	0	0

pd.get_dummies(df, drop_first=True)

	size	price	classlabel	color_green	color_red
0	2	10.1	0	1	0
1	3	13.5	1	0	1
2	5	15.3	0	0	0

Lecture 5: Scikit-learn

Additional categorical encoding schemes are available via the scikit-learn compatible category_encoders library: https://contrib.scikit-learn.org/category_encoders/

Dealing with Missing Data

```
df = pd.read_csv('missingdata.csv')
df
```

	Α	В	С	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

Dealing with Missing Data

```
df = pd.read_csv('missingdata.csv')
df
```

	Α	В	С	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

```
# drop rows with missing values:
df.dropna(axis=0)
```

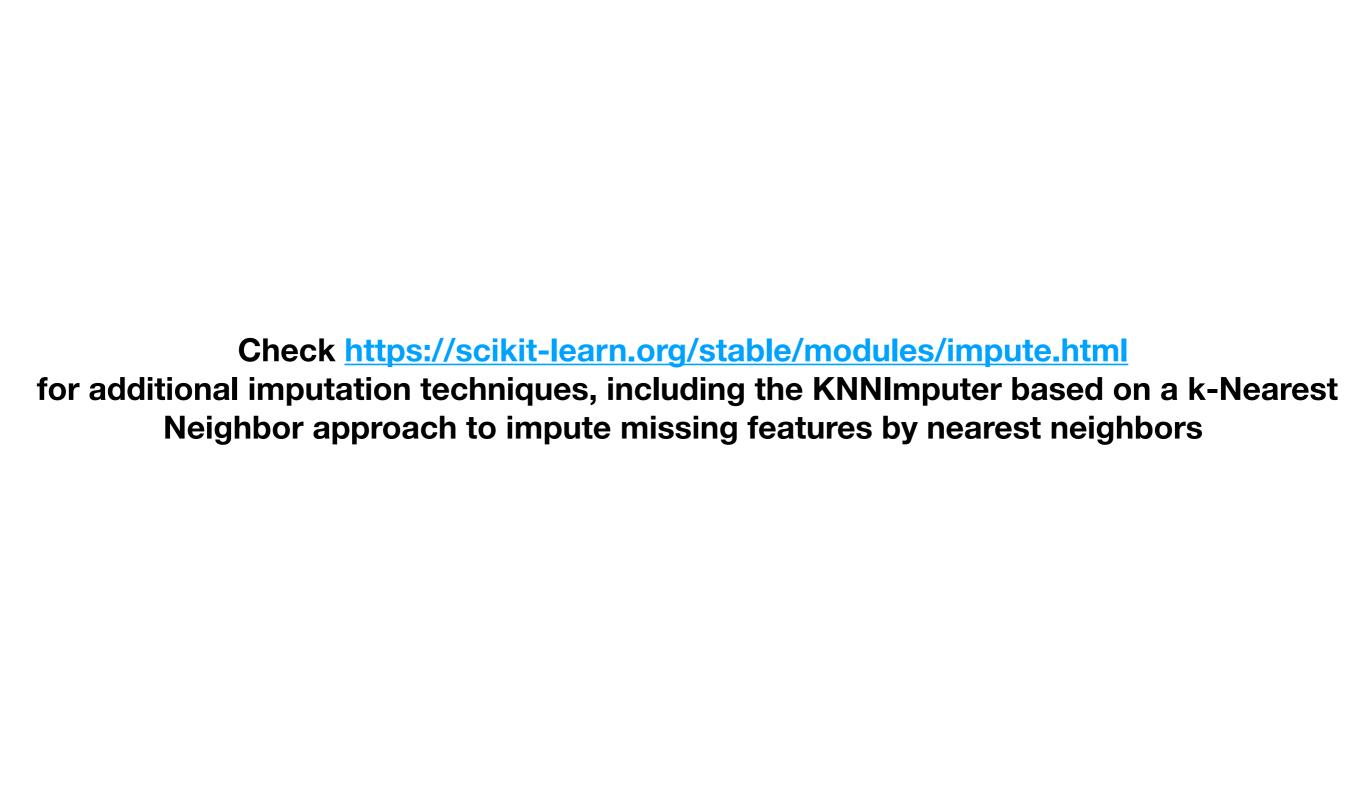
```
A B C DO 1.0 2.0 3.0 4.0
```

```
# drop columns with missing values:
df.dropna(axis=1)
```

	Α	В
0	1.0	2.0
1	5.0	6.0
2	10.0	11.0

Dealing with Missing Data

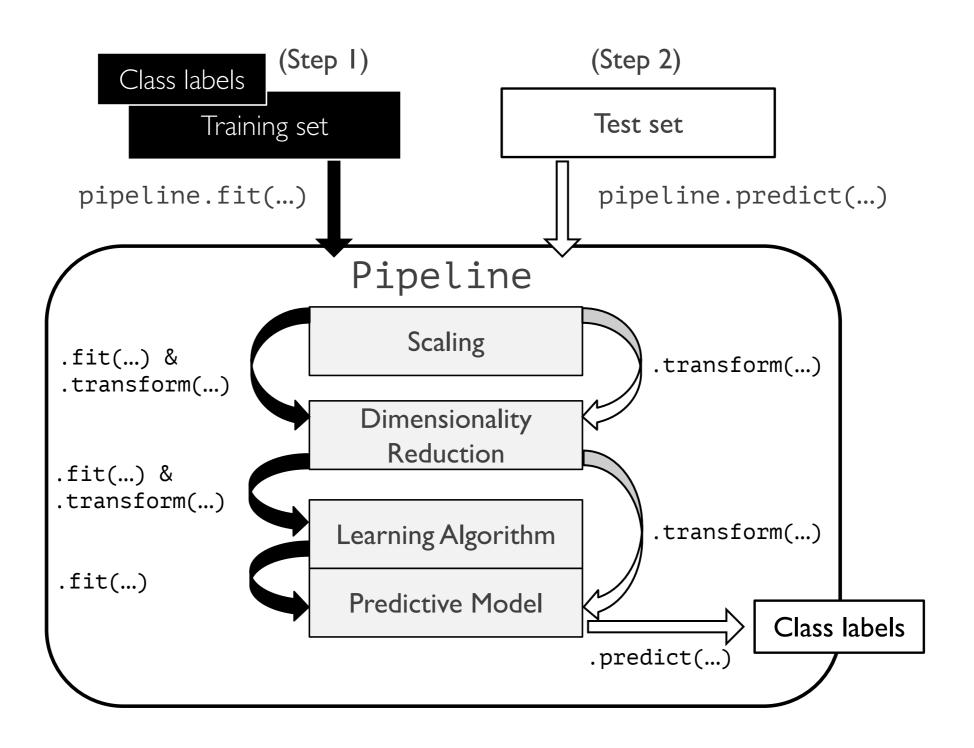
```
X = df.values
X = imputer.fit_transform(df.values)
X
array([[ 1. ,  2. ,  3. ,  4. ],
       [ 5. ,  6. ,  7.5,  8. ],
       [ 10. ,  11. ,  12. ,  6. ]])
```



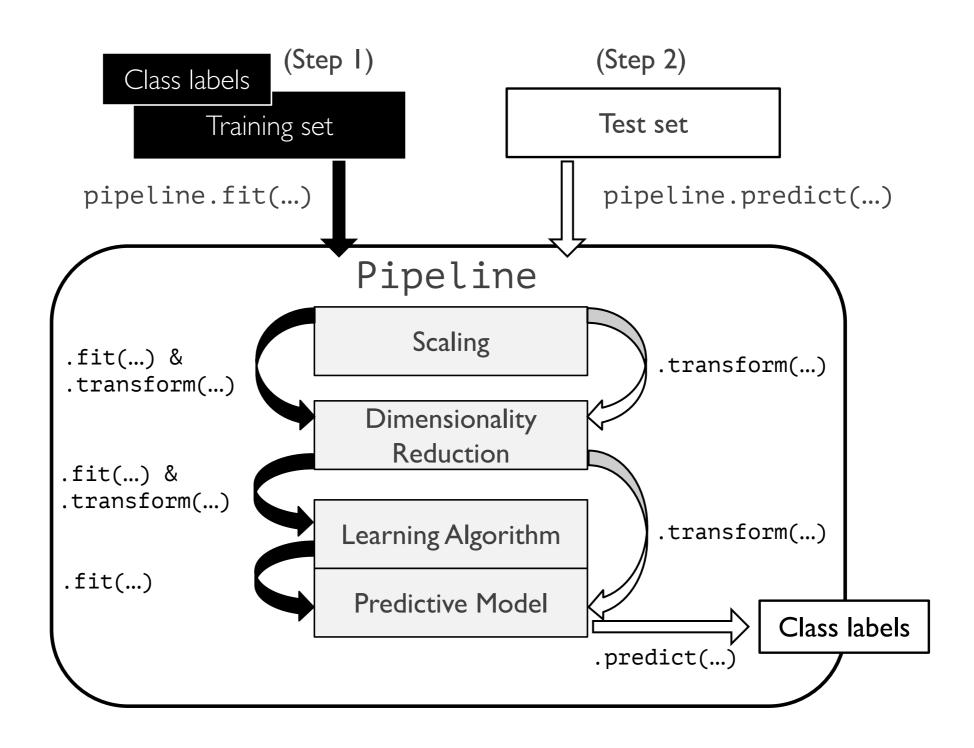
Lecture 5 (Data Preprocessing and ML with Scikit-Learn) Topics

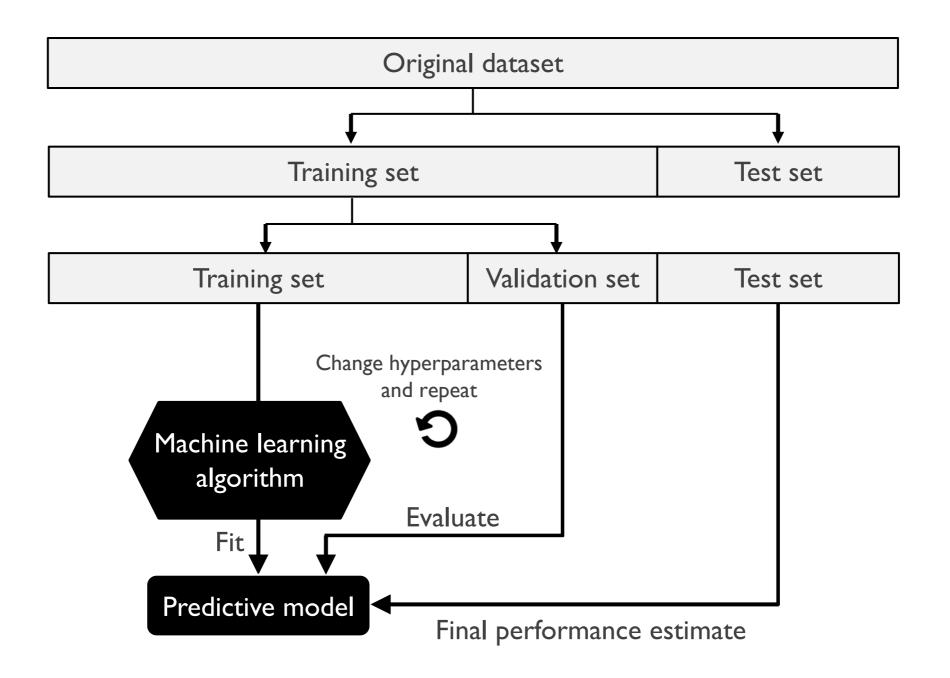
- 1. Reading a Dataset from a Tabular Text File
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```
from sklearn.model_selection import GridSearchCV
from mlxtend.evaluate import PredefinedHoldoutSplit
from sklearn.pipeline import make_pipeline
train_ind, valid_ind = train_test_split(np.arange(X_train.shape[0]),
                                        test_size=0.2, shuffle=True,
                                        random_state=0, stratify=y_train)
pipe = make_pipeline(StandardScaler(),
                     KNeighborsClassifier())
params = {'kneighborsclassifier__n_neighbors': [1, 3, 5],
          'kneighborsclassifier__p': [1, 2]}
split = PredefinedHoldoutSplit(valid_indices=valid_ind)
grid = GridSearchCV(pipe,
                    param_grid=params,
                    cv=split)
grid.fit(X_train, y_train)
GridSearchCV(cv=<mlxtend.evaluate.holdout.PredefinedHoldoutSplit object at 0x128a61d30>,
             estimator=Pipeline(steps=[('standardscaler', StandardScaler()),
                                       ('kneighborsclassifier',
                                        KNeighborsClassifier())]),
             param_grid={'kneighborsclassifier__n_neighbors': [1, 3, 5],
                         'kneighborsclassifier__p': [1, 2]})
```

```
grid.cv results
{'mean_fit_time': array([0.0004158 , 0.00039411, 0.00032306, 0.0003221 , 0.00042081,
        0.00034189]),
 'std_fit_time': array([0., 0., 0., 0., 0., 0.]),
 'mean_score_time': array([0.00058508, 0.00048375, 0.0004611 , 0.0004642 , 0.00054717,
        0.00052381]),
 'std_score_time': array([0., 0., 0., 0., 0., 0.]),
 'param_kneighborsclassifier__n_neighbors': masked_array(data=[1, 1, 3, 3, 5, 5],
             mask=[False, False, False, False, False, False],
        fill_value='?',
             dtype=object),
 'param_kneighborsclassifier__p': masked_array(data=[1, 2, 1, 2, 1, 2],
             mask=[False, False, False, False, False, False],
        fill_value='?',
             dtype=object),
 'params': [{'kneighborsclassifier__n_neighbors': 1,
   'kneighborsclassifier__p': 1},
  {'kneighborsclassifier__n_neighbors': 1, 'kneighborsclassifier__p': 2},
  {'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 1},
  {'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 2},
 {'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 1},
 {'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 2}],
 'split0_test_score': array([0.95, 0.95, 1. , 1. , 0.95, 0.95]),
 'mean_test_score': array([0.95, 0.95, 1. , 1. , 0.95, 0.95]),
 'std_test_score': array([0., 0., 0., 0., 0., 0.]),
 'rank test score': array([3, 3, 1, 1, 3, 3], dtype=int32)}
```

```
grid.cv_results_
{'mean_fit_time': array([0.0004158 , 0.00039411, 0.00032306, 0.0003221 , 0.00042081,
        0.00034189]),
 'std_fit_time': array([0., 0., 0., 0., 0., 0.]),
 'mean_score_time': array([0.00058508, 0.00048375, 0.0004611 , 0.0004642 , 0.00054717,
        0.00052381]),
 'std_score_time': array([0., 0., 0., 0., 0., 0.]),
 'param_kneighborsclassifier__n_neighbors': masked_array(data=[1, 1, 3, 3, 5, 5],
              mask=[False, False, False, False, False, False].
for i,j in zip(grid.cv_results_['params'], grid.cv_results_['mean_test_score']):
   print(i, j)
{'kneighborsclassifier__n_neighbors': 1, 'kneighborsclassifier__p': 1} 0.95
{'kneighborsclassifier__n_neighbors': 1, 'kneighborsclassifier__p': 2} 0.95
{'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 1} 1.0
{'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 2} 1.0
{'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 1} 0.95
{'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 2} 0.95
  {'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 2},
  {'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 1},
  {'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 2}],
 'split0_test_score': array([0.95, 0.95, 1. , 1. , 0.95, 0.95]),
 'mean_test_score': array([0.95, 0.95, 1. , 1. , 0.95, 0.95]),
 'std_test_score': array([0., 0., 0., 0., 0., 0.]),
 'rank test score': array([3, 3, 1, 1, 3, 3], dtype=int32)}
```

```
grid.cv_results_
  {'mean_fit_time': array([0.0004158 , 0.00039411, 0.00032306, 0.0003221 , 0.00042081,
         0.00034189]),
   'std_fit_time': array([0., 0., 0., 0., 0., 0.]),
   'mean_score_time': array([0.00058508, 0.00048375, 0.0004611 , 0.0004642 , 0.00054717,
         0.00052381]),
print(grid.best_score_)
print(grid.best_params_)
1.0
{'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 1}
clf = grid.best estimator
#clf.fit(X_train, y_train)
print('Test accuracy: %.2f%' % (clf.score(X_test, y_test)*100))
Test accuracy: 93.33%
    {'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 1},
    {'kneighborsclassifier__n_neighbors': 3, 'kneighborsclassifier__p': 2},
    {'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 1},
   {'kneighborsclassifier__n_neighbors': 5, 'kneighborsclassifier__p': 2}],
   'split0_test_score': array([0.95, 0.95, 1. , 1. , 0.95, 0.95]),
   'mean_test_score': array([0.95, 0.95, 1. , 1. , 0.95, 0.95]),
   'std_test_score': array([0., 0., 0., 0., 0., 0.]),
   'rank_test_score': array([3, 3, 1, 1, 3, 3], dtype=int32)}
```

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Randomized Search

sklearn.model_selection.RandomizedSearchCV

class sklearn.model_selection. RandomizedSearchCV(estimator, param_distributions, *, n_iter=10, scoring=None, n_jobs=None, iid='deprecated', refit=True, cv=None, verbose=0, pre_dispatch='2*n_jobs', random_state=None, error_score=nan, return_train_score=False)

[source]

n_iter : int, default=10

Number of parameter settings that are sampled. n_iter trades off runtime vs quality of the solution.

Successive Halving

sklearn.model_selection.HalvingGridSearchCV

class sklearn.model_selection.HalvingGridSearchCV(estimator, param_grid, *, factor=3, resource='n_samples',
max_resources='auto', min_resources='exhaust', aggressive_elimination=False, cv=5, scoring=None, refit=True,
error_score=nan, return_train_score=True, random_state=None, n_jobs=None, verbose=0) [source]

Search over specified parameter values with successive halving.

The search strategy starts evaluating all the candidates with a small amount of resources and iteratively selects the best candidates, using more and more resources.

Read more in the User guide.

https://scikit-learn.org/0.24/modules/generated/sklearn.model_selection.HalvingGridSearchCV.html

- like a tournament among candidate parameter combinations
- an iterative selection process where all candidates (the parameter combinations) are evaluated with a small amount of resources at the first iteration
- only some of these candidates are selected for the next iteration, which will be allocated more resources

Lecture 5 (Data Preprocessing and ML with Scikit-Learn) Topics

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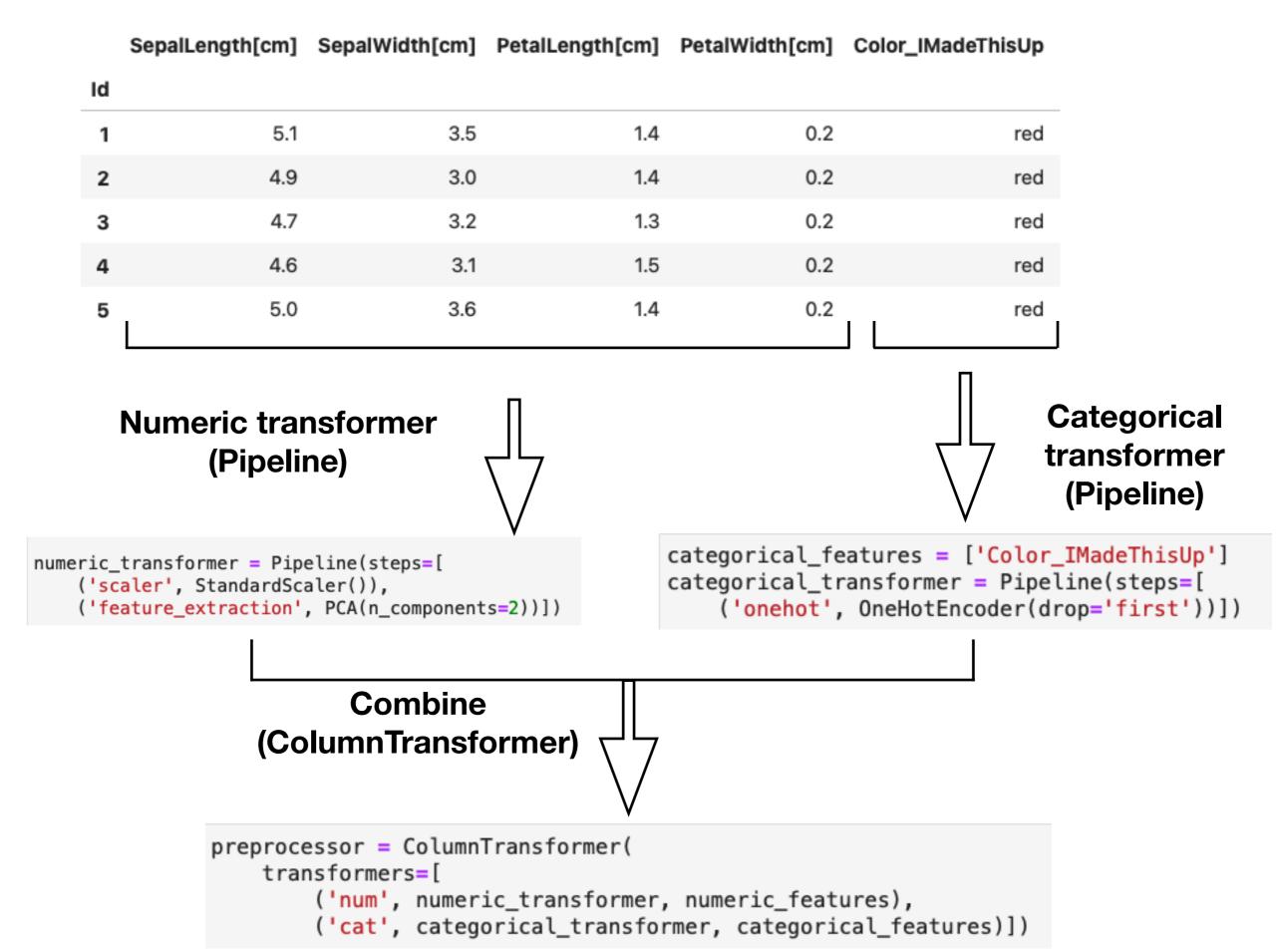
	SepalLength[cm]	SepalWidth[cm]	PetalLength[cm]	PetalWidth[cm]	Color_IMadeThisUp
Id					
1	5.1	3.5	1.4	0.2	red
2	4.9	3.0	1.4	0.2	red
3	4.7	3.2	1.3	0.2	red
4	4.6	3.1	1.5	0.2	red
5	5.0	3.6	1.4	0.2	red
		Г	1		П

Numeric transformer (Pipeline)

```
numeric_transformer = Pipeline(steps=[
    ('scaler', StandardScaler()),
    ('feature_extraction', PCA(n_components=2))])
```

Categorical transformer (Pipeline)

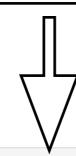
```
categorical_features = ['Color_IMadeThisUp']
categorical_transformer = Pipeline(steps=[
          ('onehot', OneHotEncoder(drop='first'))])
```



```
preprocessor = ColumnTransformer(
    transformers=[
        ('num', numeric_transformer, numeric_features),
        ('cat', categorical_transformer, categorical_features)])
```

As a result, we get a 4 dimensional feature array (design matrix) if we apply this preprocessor. What are these 4 columns?

Combine (ColumnTransformer)



```
preprocessor = ColumnTransformer(
          transformers=[
                ('num', numeric_transformer, numeric_features),
                ('cat', categorical_transformer, categorical_features)])
```

Use like regular scikitlearn Transformer

