



# A Light Intro. to Scikit-Learn

Rina BUOY, PhD



ChatGPT 4.0

# Scikit-Learn

- Scikit-Learn is characterized by a clean, uniform, and streamlined API, as well as by very useful and complete online documentation.
- A benefit of this uniformity is that once you understand the basic use and syntax of Scikit-Learn for one type of model, switching to a new model or algorithm is very straightforward.

# ML Data as a Table

one sample

$X =$

Features matrix

1.1	2.2	3.4	5.6	1.0
6.7	0.5	0.4	2.6	1.6
2.4	9.3	7.3	6.4	2.8
1.5	0.0	4.3	8.3	3.4
0.5	3.5	8.1	3.6	4.6
5.1	9.7	3.5	7.9	5.1
3.7	7.8	2.6	3.2	6.3

one feature

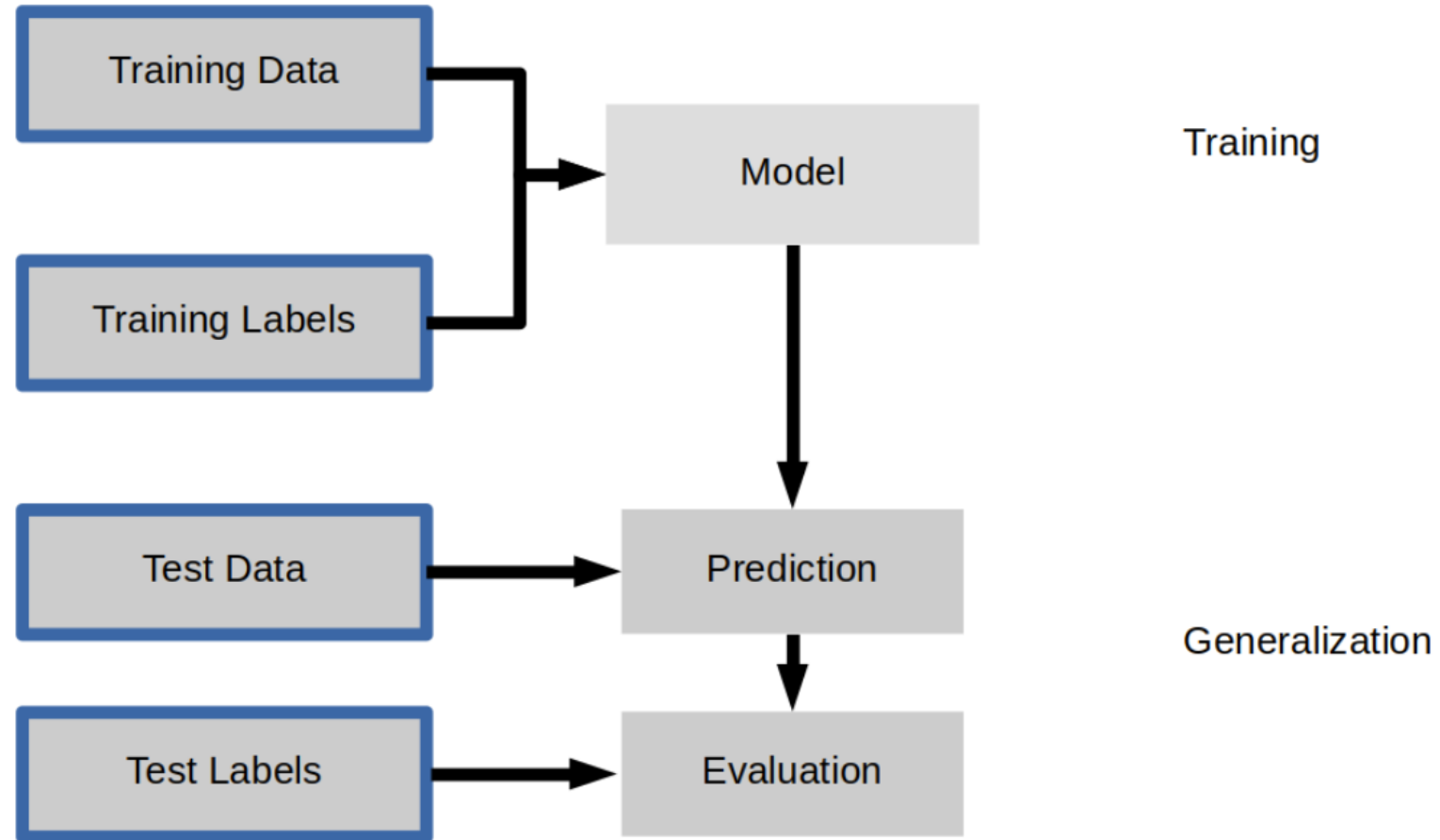
$y =$

Target vector

1.6
2.7
4.4
0.5
0.2
5.6
6.7

outputs / labels

# ML Workflow



# Train-Test Sets

Model Training +  
Setting Selection  
(require  
validation  
dataset)

$X =$

1.1	2.2	3.4	5.6	1.0
6.7	0.5	0.4	2.6	1.6
2.4	9.3	7.3	6.4	2.8
1.5	0.0	4.3	8.3	3.4
0.5	3.5	8.1	3.6	4.6

$y =$

1.6
2.7
4.4
0.5
0.2

Only for  
evaluation

5.1	9.7	3.5	7.9	5.1
3.7	7.8	2.6	3.2	6.3

5.6
6.7

test set

# Scikit-Learn API

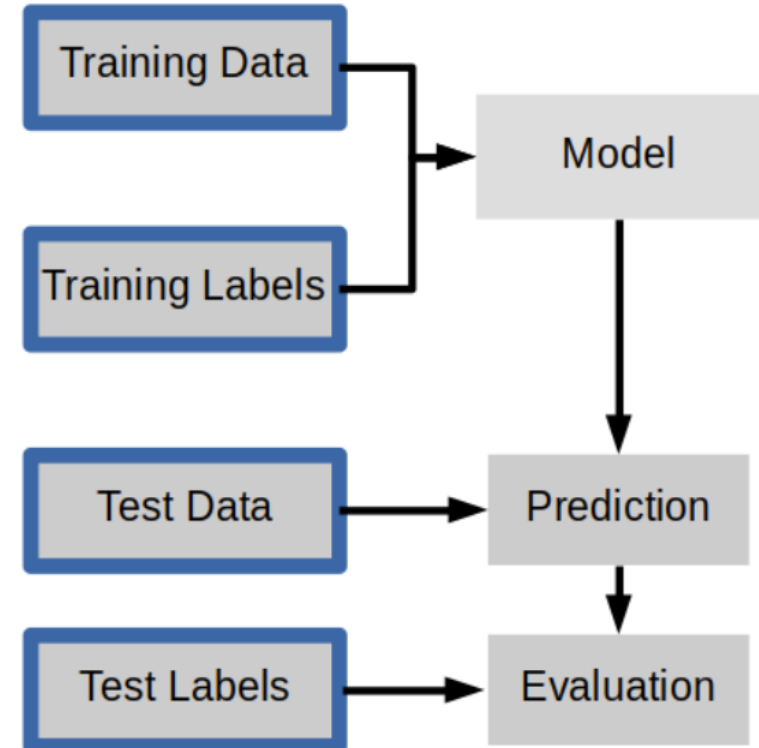
**From sklearn import Model**

```
clf = Model()
```

```
clf.fit(X_train, y_train)
```

```
y_pred = clf.predict(X_test)
```

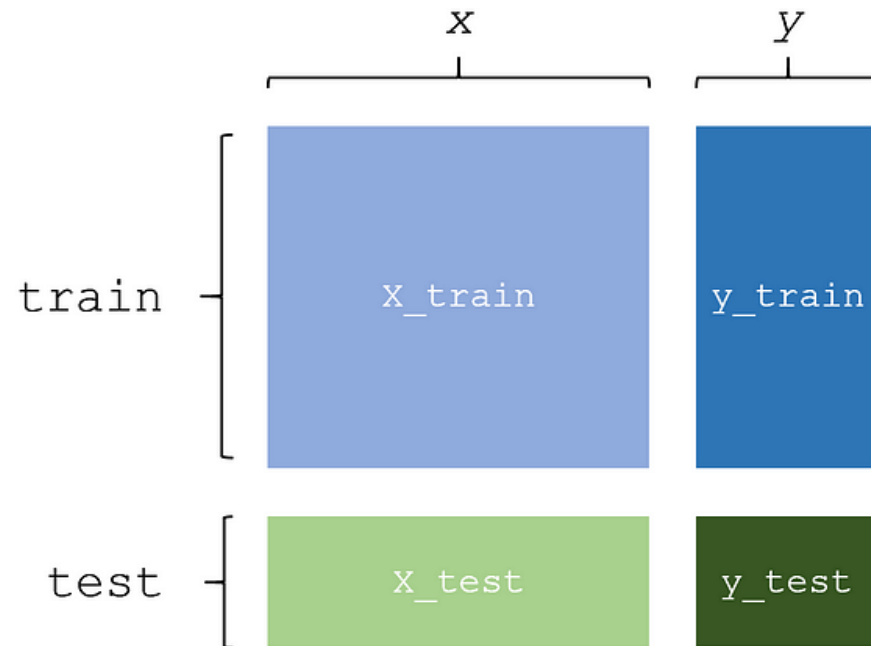
```
clf.score(X_test, y_test)
```



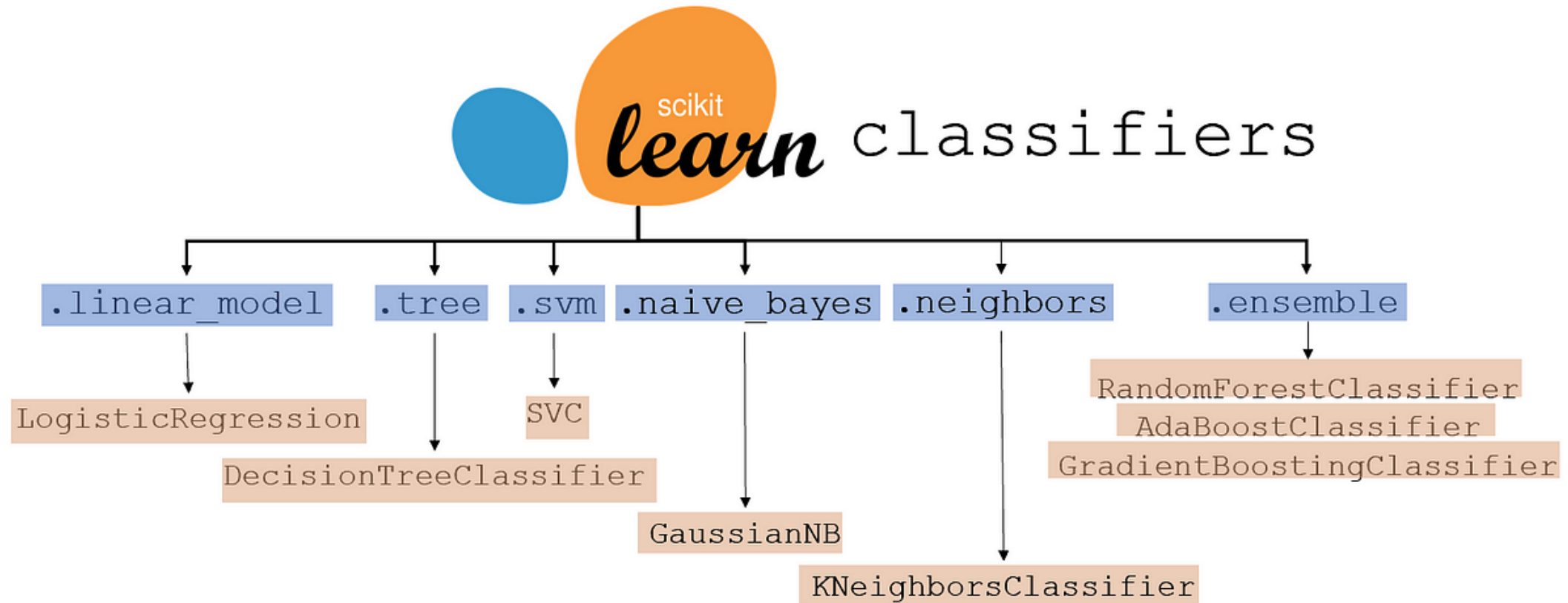


# Train-test-split

```
from sklearn.model_selection import train_test_split  
X_train,X_test,y_train,y_test = train_test_split(X,y,test_size=0.3)
```

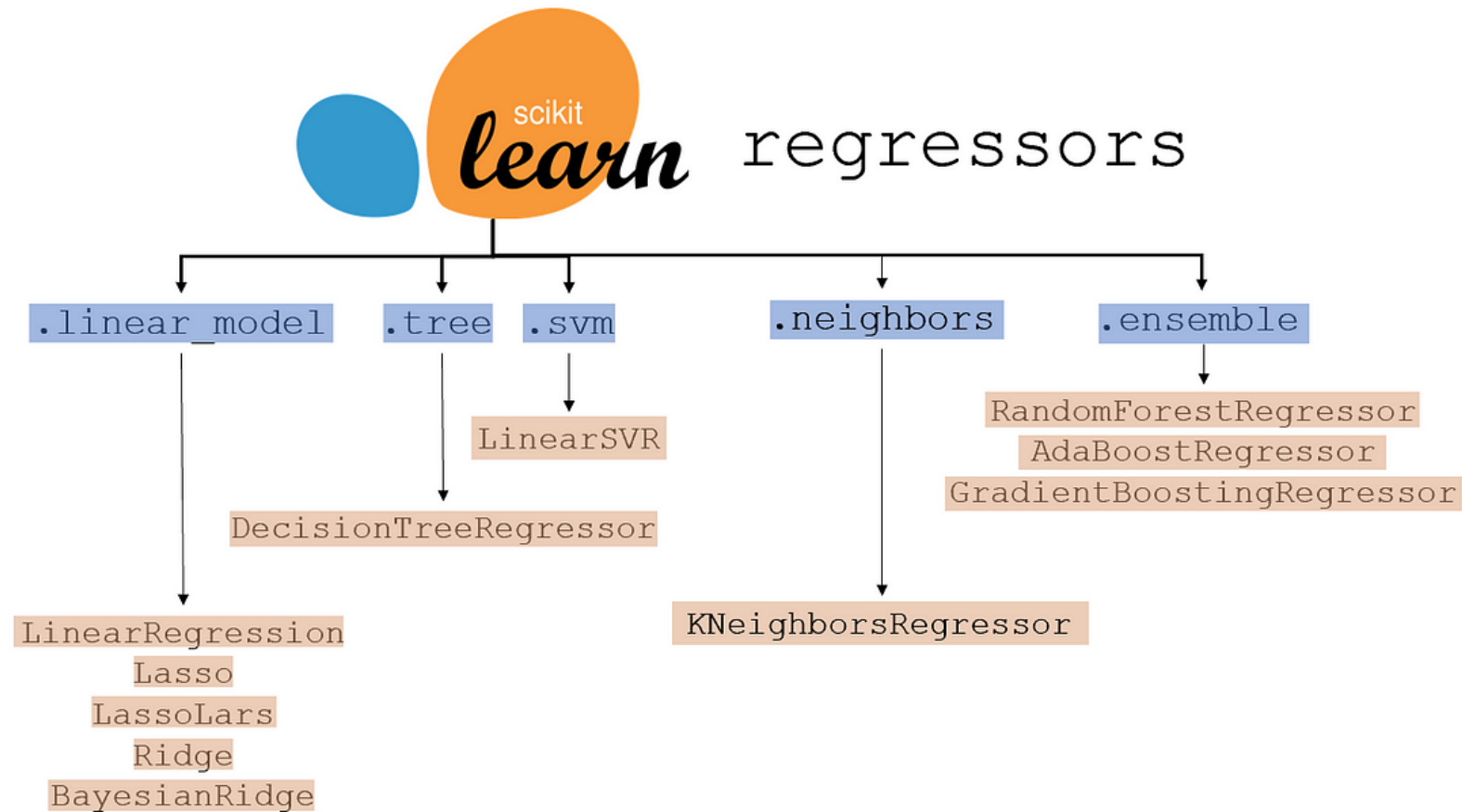


# Scikitlearn Classifiers





# Scikitlearn Regressors

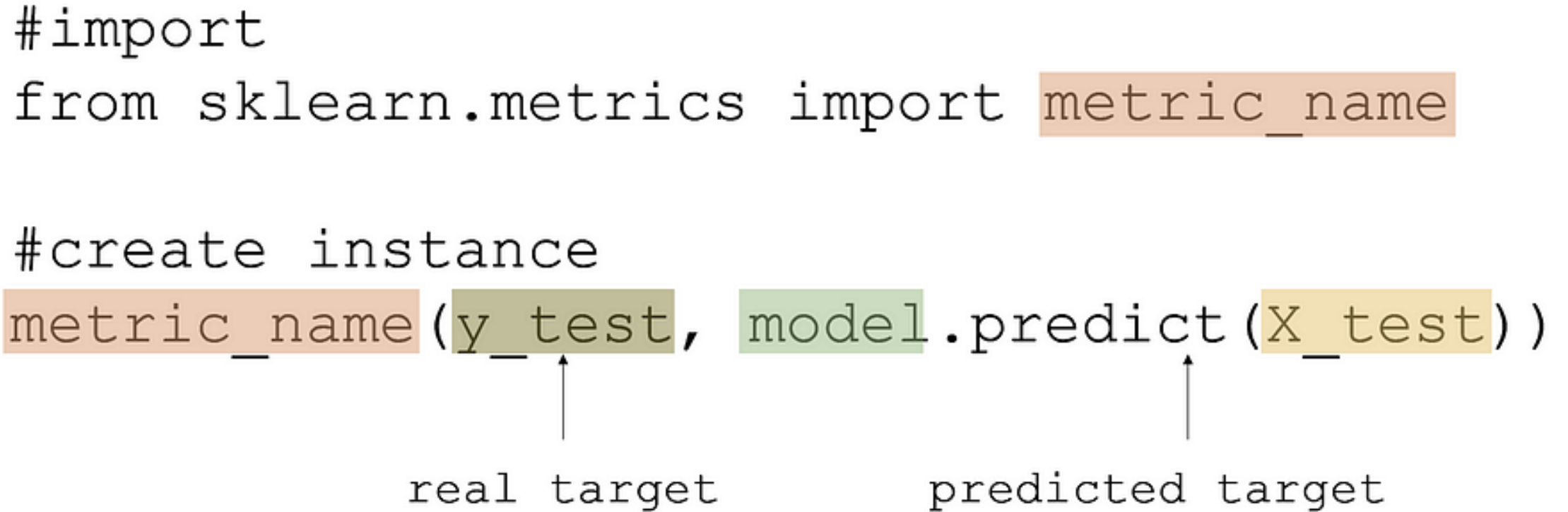


# Evaluating Model Performance

```
#import
from sklearn.metrics import metric_name

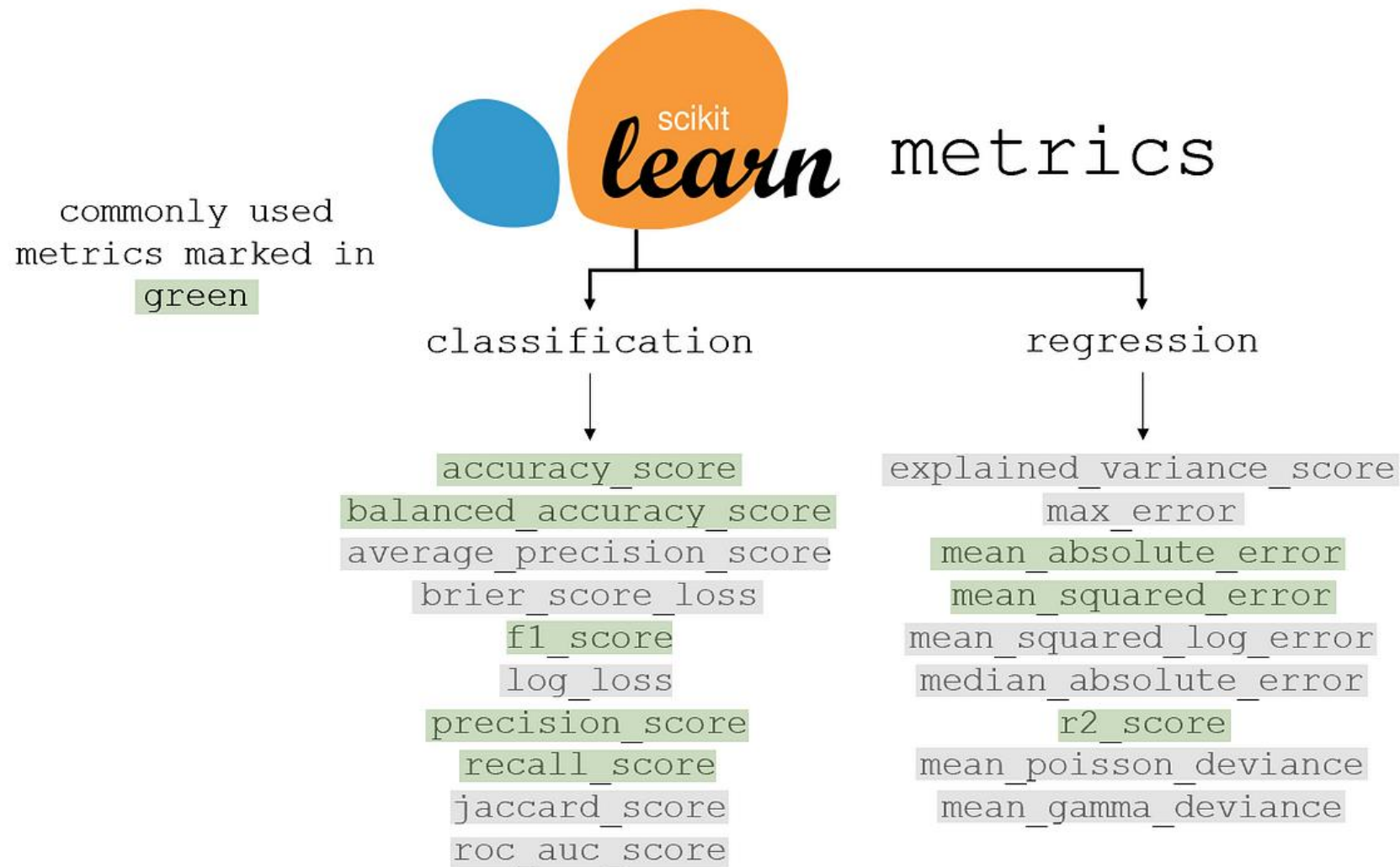
#create instance
metric_name(y_test, model.predict(X_test))
```

real target                      predicted target



The diagram illustrates the process of evaluating a model's performance. It shows a code snippet where a metric function is imported from sklearn.metrics and then called with two arguments: y\_test (the real target) and model.predict(X\_test) (the predicted target). Arrows point from the labels 'real target' and 'predicted target' to the corresponding arguments in the function call.

# Evaluating Model Performance



# Data Transformation

- Standardizing or scaling is the process of ‘reshaping’ the data such that it contains the same information but has a mean of 0 and a variance of 1. By scaling the data, the mathematical nature of algorithms can usually handle data better.

```
from sklearn.preprocessing import StandardScaler  
scaler = StandardScaler()  
scaler.fit(data)  
transformed_data = scaler.transform(data)
```

```
data = scaler.inverse_transform(output_data)
```

# Data Transformation

- Normalizing data puts it on a 0 to 1 scale, something that, similar to standardized data, makes the data mathematically easier to use for the model.

```
from sklearn.preprocessing import Normalizer  
normalize = Normalizer()  
transformed_data = normalize.fit_transform(data)
```

# Data Transformation

- Box-cox transformations involve raising the data to various powers to transform it. Box-cox transformations can normalize data, make it more linear, or decrease the complexity.
- sklearn automatically determines the best series of box-cox transformations to apply to the data to make it better resemble a

```
from sklearn.preprocessing import PowerTransformer
transformer = PowerTransformer(method='box-cox')
transformed_data = transformer.fit_transform(data)
```

# Dealing with Discreet Inputs

- Nominal variables: These variables represent categories without any inherent order or ranking. Examples include colors, types of fruits, or gender.
- Ordinal variables: These variables have a natural ordering or ranking among the categories. For example, ratings such as "low," "medium," and "high" represent ordinal variables.



# One-Hot Encoding

id	color
1	red
2	blue
3	green
4	blue



id	color_red	color_blue	color_green
1	1	0	0
2	0	1	0
3	0	0	1
4	0	1	0

```
from sklearn.preprocessing import OneHotEncoder

# Sample data
data = [['red'], ['green'], ['blue']]

# Initialize the encoder
encoder = OneHotEncoder()

# Fit and transform the data
encoded_data = encoder.fit_transform(data).toarray()

# Print the encoded data
print(encoded_data)
```

# Ordinal Encoding

Original Encoding	Ordinal Encoding
Poor	1
Good	2
Very Good	3
Excellent	4

```
from sklearn.preprocessing import OrdinalEncoder

# Sample data
data = [['low'], ['medium'], ['high']]

# Initialize the encoder
encoder = OrdinalEncoder(categories=[['low', 'medium', 'high']])

# Fit and transform the data
encoded_data = encoder.fit_transform(data)

# Print the encoded data
print(encoded_data)
```

# Hyperparameter Selection

- Scikit-learn's GridSearchCV is an excellent tool for tuning hyperparameters of machine learning models. It exhaustively searches through a specified grid of hyperparameters to find the best ones based on cross-validated performance.

```
from sklearn.model_selection import GridSearchCV
parameters = {'param': [0.1, 0.01, 0.001]}
model = Model()
gs = GridSearchCV(model, parameters, cv=5)
gs.fit(X_train, y_train)
```

```
best_model = gs.best_estimator_
best_model.fit(X_train, y_train)
```

# Example of Complex Search

## Parameters to search

```
# number of trees  
n_estimators=[500, 800, 1500, 2500, 5000]  
# max number of features to consider at every split  
max_features = ['auto', 'sqrt', 'log2']  
# max number of levels in tree  
max_depth = [10, 20, 30, 40, 50]  
max_depth.append(None)  
# Minimum number of samples required to split a node  
min_samples_split = [2, 5, 10, 15, 20]  
# Minimum number of samples required at each leaf node  
min_samples_leaf = [1, 2, 5, 10, 15]
```

```
grid_param = {'n_estimators': n_estimators,  
              'max_features': max_features,  
              'max_depth': max_depth,  
              'min_samples_split': min_samples_split,  
              'min_samples_leaf': min_samples_leaf}
```

# Pipeline

- Scikit-learn's Pipeline is a tool for chaining multiple estimators into one. This is useful when there are a series of steps in your machine learning workflow that need to be executed in a particular sequence, such as data preprocessing, feature engineering, and model training.

```
# Define the steps in the pipeline
steps = [
    ('scaler', StandardScaler()), # Step 1: Data preprocessing (scaling)
    ('pca', PCA()),               # Step 2: Feature reduction (PCA)
    ('svm', SVC())                # Step 3: Model training (Support Vector Machine)
]

# Create the pipeline
pipeline = Pipeline(steps)

# Now you can use the pipeline as a single estimator
pipeline.fit(X_train, y_train)
```

For more

<https://scikit-learn.org/stable/index.html>