

Aprendizado de Máquina e Reconhecimento de Padrões 2021.2



Scikit-Learn Design Principles

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Preliminary Concepts

Model Hyperparameters

Properties that are **external** to the model and whose value **cannot be estimated from data**.

Examples:

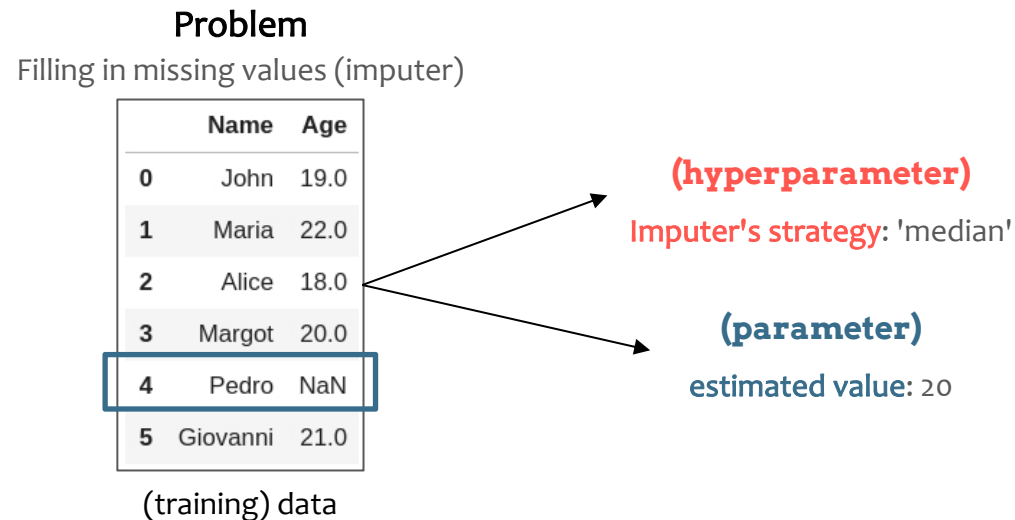
- **Imputer's strategy**: 'median'
- **Number of neighbors for KNN**: 3

Model Parameters

Properties that are **internal** to the model and whose value **can be estimated from data**.

Examples:

- **Estimated value for missing values**: 20 (median)
- **Estimated coefficients of a linear regression**.



Main Interfaces (API) of Scikit-Learn

Estimators

- Main and core interface of Scikit-learn;
- Any object that can **estimate** some **parameters** based on a dataset;
- Estimation (learning/training) is performed by the **fit()** method;
- **Hyperparameters** needed to guide the estimation must be set as a class attribute in the constructor.

```
# unsupervised learning
estimator.fit(X_train)

# supervised learning
estimator.fit(X_train, y_train)
```

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Transformers

- **Estimators** which can also **transform** data with **transform()** or **fit_transform()**;
- Preprocessing, feature selection, feature extraction and dimensionality reduction algorithms are all provided as **transformers** within the library;

```
new_data = transformer.transform(data)
new_data = transformer.fit_transform(data)
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Predictors

- Estimators that can also **predict** a value.
- From a trained model, predictors return **predicted labels (numeric or categorical)** for a given **input features** by using the **predict()** method.
- Some predictors may also provide **probabilities** and prediction **scores** by using, respectively, **predict_proba()** and **score()**.

```
prediction = predictor.predict(data)
probability = predictor.predict_proba(data)
score = model.score(data)
```

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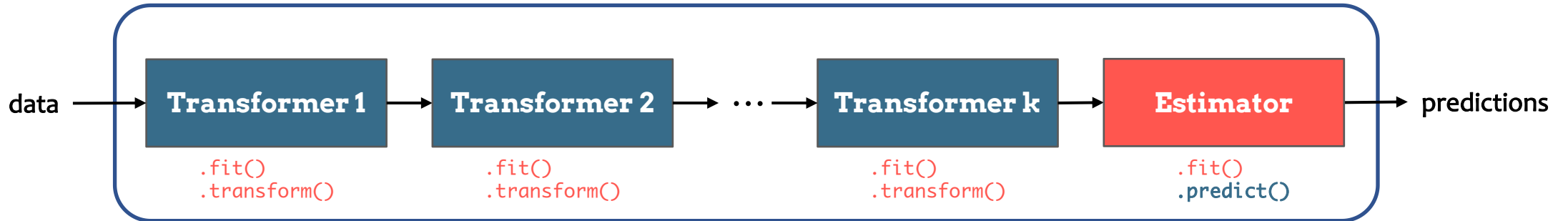
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Predictors are commonly referred to as **estimators**.

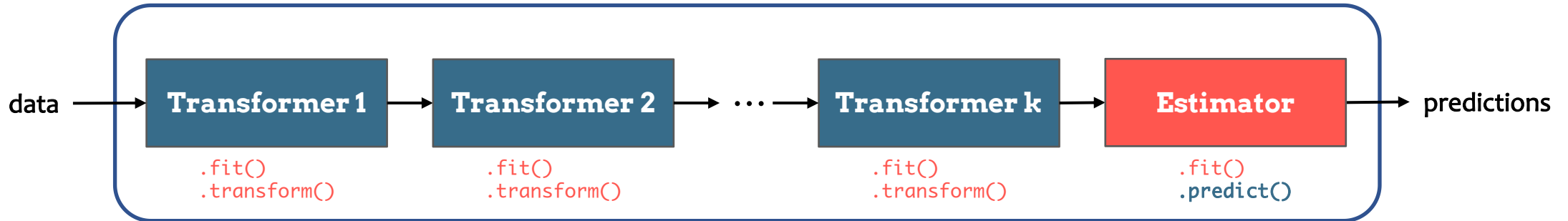
Scikit-Learn Pipelines

- A **scikit-learn Pipeline** is an object that sequentially applies a **list of transforms** and a **final estimator (predictor)**;



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- The **Pipeline** is build using a list of (key, value) pairs, where:
 - the **key** a string containing the **name** you want to give this step, and the **value** is an **estimator object**;

```
from sklearn.impute import SimpleImputer
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LinearRegression

from sklearn.pipeline import Pipeline

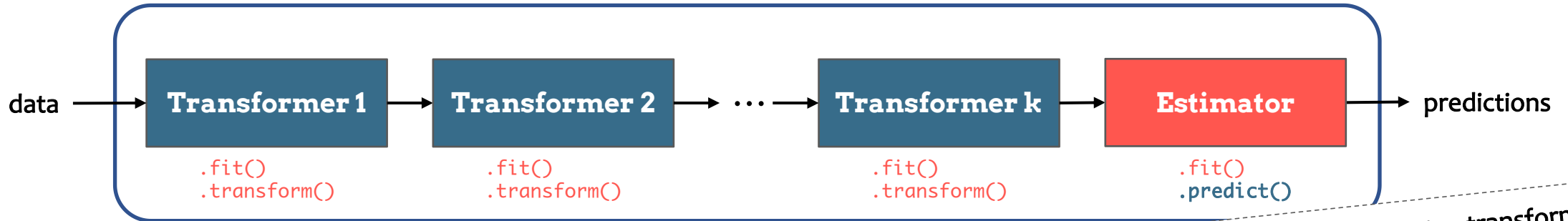
pipeline = Pipeline([
    ('imputer', SimpleImputer(strategy="median")),
    ('scaler', StandardScaler()),
    ('linear_regression', LinearRegression())
])

pipeline.fit(X_train, y_train)

y_test_pred = pipeline.predict(X_test)
```


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If the last estimator is a **transformer**, its `fit_transform()` method will be executed so that the **output** will be the **final transformed data**.

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