# Preprocessing

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**CPDSAI** 

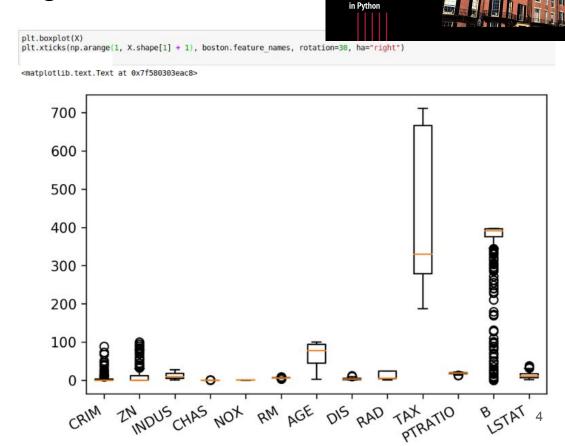
### Preprocessing

- Process raw feature vector into suitable form
- There are several common preprocessing methods
  - Standardization and scaling
  - Encoding categorical features
  - Discretization
  - Imputation
  - Pipeline
    - GridSearchCV
    - Column Transformer

## Standardization and scaling

## Standardization and scaling

- Each feature comes in different scale e.g.
  - Tax ranges (300-700)
  - Age ranges (20-100)
- Difficulties to visualize the data
- Degrade the predictive performance of many machine learning algorithms
- Unscaled data can also slow down or even prevent the convergence of many gradient-based estimators.



Boston

Dataset

**Housing Price** 

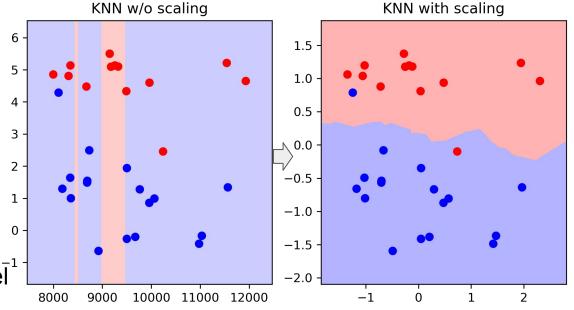
Machine Learning Project

#### Aim of standardization and scaling

We want the values of all features to be in the same scale

#### Benefits:

 There are some models that need the features in the same scale; for example, the KNN model



 In determining the importance of features in a linear model by comparing the coefficient of the features, we need the features to be in the same scale

#### Sklearn instructions

#### Same as modelling process

- Define the operation: specify the model
- Fit the data: standard scaler find mean and variance of X
- Transform the data: calculate the Z score of each feature

# StandardScaler in sklearn

```
>>> from sklearn import preprocessing
>>> import numpy as np
>>> X train = np.array([[ 1., -1., 2.],
                       [2., 0., 0.],
...
                        [0., 1., -1.]])
. . .
>>> scaler = preprocessing.StandardScaler().fit(X train)
>>> scaler
StandardScaler()
>>> scaler.mean
array([1. ..., 0. ..., 0.33...])
>>> scaler.scale
array([0.81..., 0.81..., 1.24...])
>>> X scaled = scaler.transform(X train)
>>> X scaled
array([[ 0. ..., -1.22..., 1.33...],
      [ 1.22..., 0. ..., -0.26...],
      [-1.22..., 1.22..., -1.06...]])
```

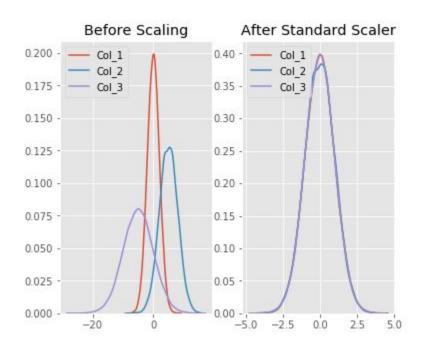
#### Standard scaler

calculating z-score: subtract mean, divided by standard deviation

$$z_f^{(i)} = rac{x_f^{(i)} - \mu_f}{\sigma_f^2}$$
 , where  ${ ext{x}^{(i)}}_{ ext{f}}$  is

the fth feature of the ith instance

- Usually good, but doesn't guarantee particular min and max values
- Can be influenced by outliers



https://michael-fuchs-python.netlify.app/2019/08/3 1/feature-scaling-with-scikit-learn/

### California Housing dataset

**Number of Instances:** 

20640

**Number of Attributes:** 

8 numeric, predictive attributes and the target

**Attribute Information:** 

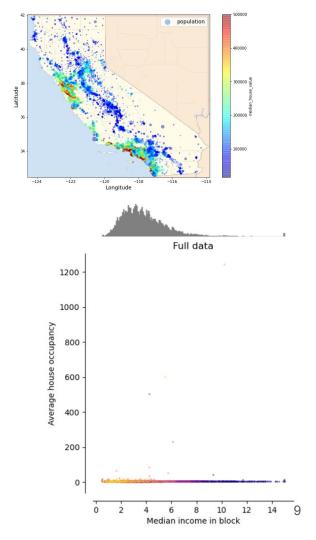
- MedInc median income in block group
- HouseAge median house age in block group
- AveRooms average number of rooms per household
- · AveBedrms average number of bedrooms per household
- · Population block group population
- AveOccup average number of household members
- Latitude block group latitude
- · Longitude block group longitude

#### Target: median house value

- A large majority of the median income are compacted to a specific range, [0, 10]
- The average house occupancy is mostly in the range [0,6] with outliers more than 1,200

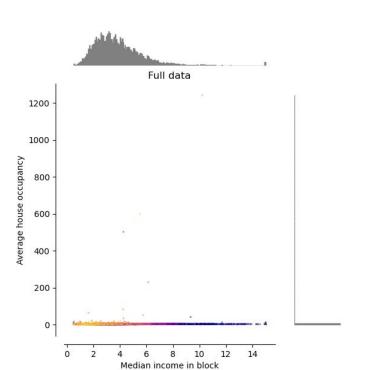
https://www.dcc.fc.up.pt/~ltorgo/Regression/cal\_housing.html

https://github.com/amansingh9097/California-hou sing-price-prediction?tab=readme-ov-file

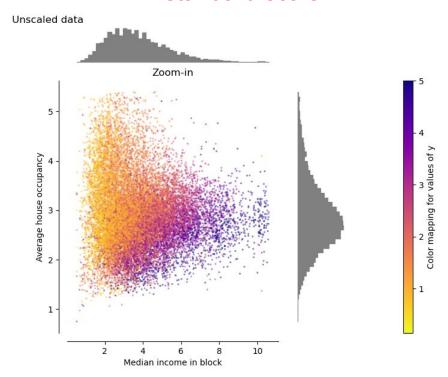


#### StandardScaler





- Is it good?
- What's wrong with the standard scaler?



## Other kinds of scaling

- Minmax scaling: keep the transform values between 0 and 1
  - Fit: find min and max values of each *f* feature

$$\hat{x}^{(i)} = rac{x^{(i)} - \min_f}{\max_f - \min_f}$$

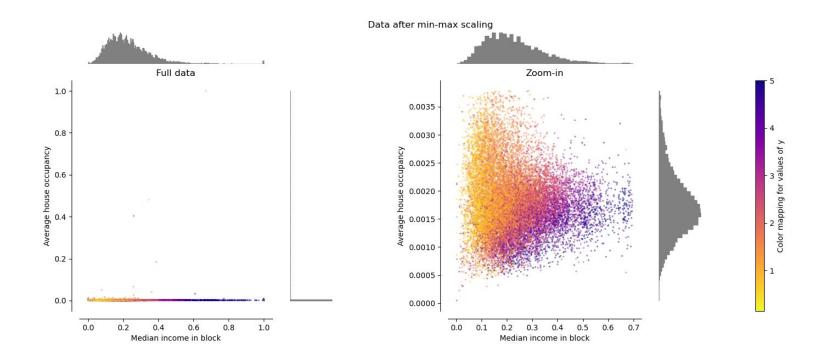
- Transform: calculate the normalized value
- Robust scaling: using median and quartile instead of mean and variance to reduce effect of outliers  $z_f^{(i)}=rac{x_f^{(i)}-m_f}{IOR}$ 
  - Fit: find median and quartile of each *f* feature
  - Transform: calculate the scaled value as in the z score
    - IQR: the range between the 1st quartile (25th quantile) and the 3rd quartile (75th quantile);  $m_f$ : the median

#### MinMaxScaler

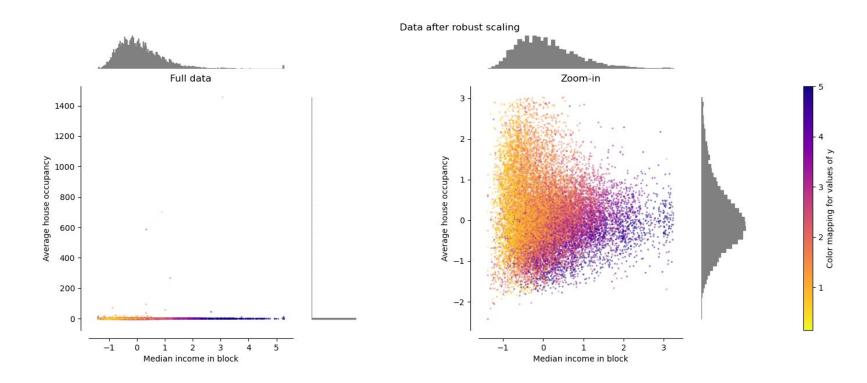
• The same instance of the transformer can then be applied to some new test data unseen during the fit call

```
>>> X_test = np.array([[-3., -1., 4.]])
>>> X_test_minmax = min_max_scaler.transform(X_test)
>>> X_test_minmax
array([[-1.5 , 0. , 1.66666667]])
```

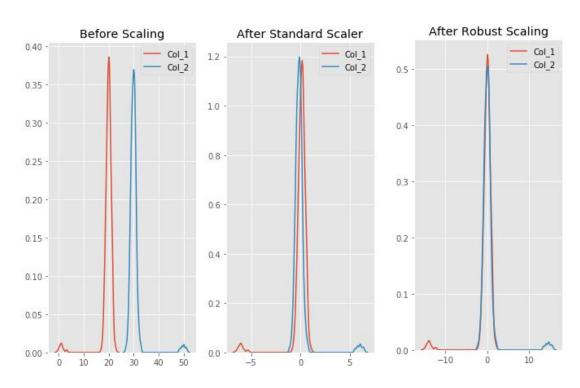
#### MinMaxScaler



### RobustScaler



# StandardScaler vs RobustScaler



#### Data leakage during pre-processing

What's wrong with this?

```
# Load your dataset
X, y = datasets.load_iris(return_X_y=True)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
# Initialize the scaler
scaler = StandardScaler()
X train scaled = scaler.fit transform(X train)
X test scaled = scaler.fit transform(X test)
# Initialize the KNN classifier with a specified number of neighbors
knn = KNeighborsClassifier(n neighbors=7)
#Prediction
y_pred = knn.fit(X_train_scaled, y_train).predict(X_test_scaled)
print(y pred)
#Evaluate the model using accuracy
accuracy = accuracy score(y test, y pred)
print(f'Accuracy: {accuracy:.2f}')
```

## **Encoding**

## Categorical encoding

- Mapping categorical values into numerical values
- Ordinal encoding: mapped to integer value directly
- One-hot encoding: mapped each value into each new column

### Ordinal encoding

- Same as modelling process
  - Define the operation: specify the model
  - Fit the data: find all possible values in feature f
  - Transform the data: mapping integers to the values
- Let the model determine possible values from the training set
- Predefine the possible values (we must predefine all features)
- Features such as: ["male", "female"], ["from Europe", "from US", "from Asia"]
   ["uses Firefox", "uses Chrome", "uses Safari", "uses Internet Explorer"]
- Such features can be efficiently coded as integers, for instance ["male", "from US", "uses Internet Explorer"] could be expressed as [0, 1, 3]
- A feature vector ["female", "from Asia", "uses Chrome"] can be represented as [1, 2, 1]

## sklearn.preprocessing.OrdinalEncoder()

```
>>> enc = preprocessing.OrdinalEncoder()
>>> X = [['male', 'from US', 'uses Safari'], ['female', 'from Europe', 'uses Firefox']]
>>> enc.fit(X)
OrdinalEncoder()
>>> enc.transform([['female', 'from US', 'uses Safari']])
array([[0., 1., 1.]])
```

#### Warning:

- 'using Safari' and 'using Firefox' have no order relationship. Suppose that we assign the value 0 and 1 to 'using Safari' and 'using Firefox' respectively, the model could interpret as they are close to each other.
- Encode 'using Chrome' as 2, some models would interpret that 'using Chrome' is closer to 'using Safari than 'using Firefox, because 2 is closer to 1 than 0.

#### One-hot Encoder

	boro	salary	
0	Manhatten	103	
1	Queens	89 1 142	
2	Manhatten		
3	Brooklyn 54		
4	Brooklyn	63	
5	Bronx	219	



	salary	boro_Bronx	boro_Brooklyn	boro_Manhatten	boro_Queens
0	103	0.0	0.0	1.0	0.0
1	89	0.0	0.0	0.0	1.0
2	142	0.0	0.0	1.0	0.0
3	54	0.0	1.0	0.0	0.0
4	63	0.0	1.0	0.0	0.0
5	219	1.0	0.0	0.0	0.0

- Transform each categorical feature with n\_categories possible values into n\_categories binary features, with one of them 1, and all others 0.
- Pros: No false proximity issue as in ordinal encoding
- Cons: Could cause a lot more features, if the feature contains many categorical values

## sklearn.preprocessing.OneHotEncoder()

## Handle unknown value in OneHotEncoder()

#### What will happen?

```
enc = preprocessing.OneHotEncoder()
X = [['male', 'from US', 'uses Safari'], ['female', 'from Europe', 'uses Firefox']]
enc.fit(X)
enc.transform([['female', 'from Asia', 'uses Chrome']]).toarray()
```

#### How to solve this?

#### Handle unknown value in OneHotEncoder()

#### What will happen?

```
>>> enc = preprocessing.OneHotEncoder(handle_unknown='infrequent_if_exist')
>>> X = [['male', 'from US', 'uses Safari'], ['female', 'from Europe', 'uses Firefox']]
>>> enc.fit(X)
OneHotEncoder(handle_unknown='infrequent_if_exist')
>>> enc.transform([['female', 'from Asia', 'uses Chrome']]).toarray()
array([[1., 0., 0., 0., 0., 0.]])
```

With handle\_unknown='infrequent\_if\_exist' specified and unknown categories are encountered during transform, no error will be raised but the resulting one-hot encoded columns for this feature will be all zeros or considered as an infrequent category if enabled

# Missing values as an additional category (only in sklearn Version 1.0)

```
X = [['male', 'Safari'],['female',None],[np.nan, 'Firefox']]
enc = preprocessing.OneHotEncoder(handle unknown='error').fit(X)
enc.categories
[array(['female', 'male', nan], dtype=object),
 array(['Firefox', 'Safari', None], dtype=object)]
enc.transform(X).toarray()
array([[0., 1., 0., 0., 1., 0.],
       [1., 0., 0., 0., 0., 1.],
       [0., 0., 1., 1., 0., 0.]
```

#### One-hot encoding: sparse representation

Normally, most entries from one-hot encoding would be zeros

Sklearn uses sparse representation to encode only entries with value 1 to save resources.

If we want to see the actual data we need to convert it to ordinary array, using toarray()

```
one hot mapped value:
   (0, 1)
                 1.0
  (0, 2)
                 1.0
  (0, 4)
                 1.0
                 1.0
                 1.0
                 1.0
```

```
print(enc.transform([['male', 'from America', 'uses Safari']]).toarray())
[[0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 1.]]
```

## Discretization

#### Discretization

- Quantization or binning
- partitioning continuous features into discrete values
- In sklearn, use **k-bin discretizer**: dividing each feature into k bins and assigning the values of the feature into corresponding bins.
- sklearn.preprocessing.KBinsDiscretizer(n\_bins=5, \*,
  encode='onehot', strategy='quantile', dtype=None)

### sklearn.preprocessing.KBinsDiscretizer

```
sklearn.preprocessing.KBinsDiscretizer(n_bins=5, *, encode='onehot', strategy='quantile', dtype=None)
```

#### encode: {'onehot', 'onehot-dense', 'ordinal'}, default='onehot'

Method used to encode the transformed result.

#### onehot

Encode the transformed result with one-hot encoding and return a sparse matrix. Ignored features are always stacked to the right.

#### onehot-dense

Encode the transformed result with one-hot encoding and return a dense array. Ignored features are always stacked to the right.

#### ordinal

Return the bin identifier encoded as an integer value.

#### sklearn.preprocessing.KBinsDiscretizer

```
sklearn.preprocessing.KBinsDiscretizer(n_bins=5, *,
encode='onehot', strategy='quantile', dtype=None)
```

strategy: {'uniform', 'quantile', 'kmeans'}, default='quantile'

Strategy used to define the widths of the bins.

#### uniform

All bins in each feature have identical widths.

#### quantile

All bins in each feature have the same number of points.

#### kmeans

Values in each bin have the same nearest center of a 1D k-means cluster.

## sklearn.preprocessing.Binarizer()

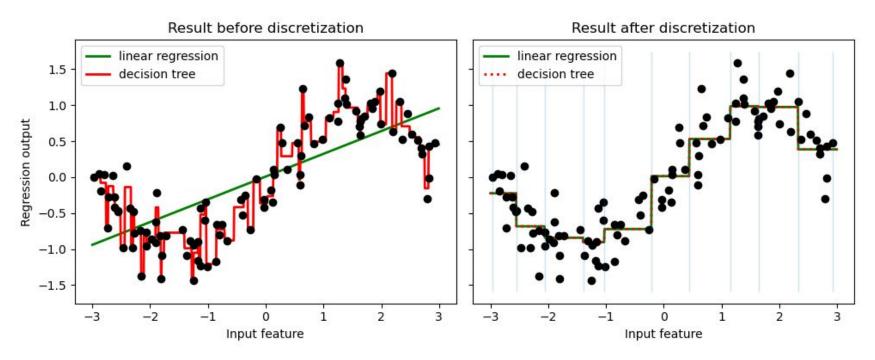
- Feature Binarization
- Setting the threshold and divide the value into two groups
- This method is equivalent to KBinsDiscretizer when k=2.

class sklearn.preprocessing.Binarizer(\*, threshold=0.0, copy=True)

 Feature values below or equal to this are replaced by 0, above it by 1. Threshold may not be less than 0 for operations on sparse matrices.

## sklearn.preprocessing.Binarizer()

## Benefits of discretization: Using KBinsDiscretizer to discretize continuous features



After discretization, linear regression and decision tree make exactly the same prediction.

## **Transformation summary**

Feature type	Transformation
Continuous: numerical values	<ul> <li>Standard Scaling, Min-Max</li> <li>Scaling</li> <li>Discretization</li> </ul>
<b>Nominal:</b> categorical, unordered features ( <i>True</i> or <i>False</i> )	• One-hot encoding (0, 1)
Ordinal: categorical, ordered features (movie ratings)	• Ordinal encoding (0, 1, 2, 3)

## Data imputation

### Univariate feature imputation

- Univariate feature imputation by using the statistics, such as mean or median, of the missing feature alone.
- sklearn.impute.SimpleImputer(\*, missing\_values=nan, strategy='mean',
  fill value=None, verbose=0, copy=True, add indicator=False)

Strategy can be mean, mode, median or constant

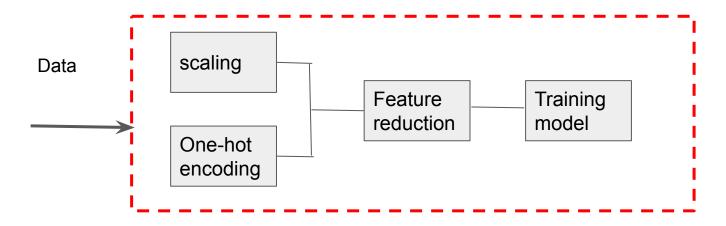
#### Multivariate feature imputation

- Imputes missing values by considering the values of other feature together with the missing feature.
- Operation:
  - y: feature with missing values treated as target vector
  - X: the other feature columns treated as feature vector
- A regressor is fit on (X, y) for known y. Then, the regressor is used to predict the missing values of y.

# Data pipelining

# Pipeline

- Pipelining is the operation that allows us to chain multiple operations into a single instruction
- Very beneficial for streaming data



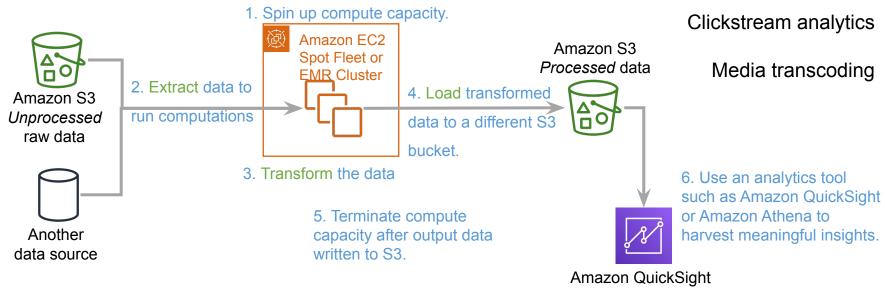
# Amazon S3 use case 3: Data store for computation and analytics



#### Data store for computation and large-scale analytics

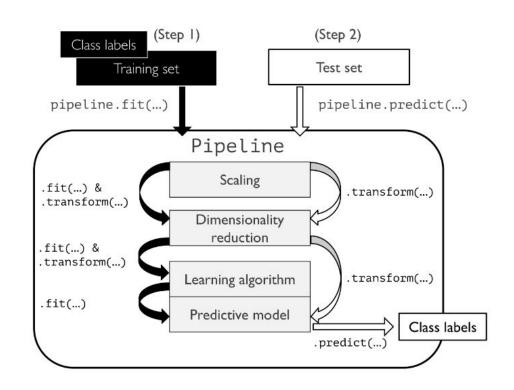
Example data integration and preparation pattern

Financial transaction analysis



#### sklearn.pipeline.make\_pipeline

- Construct a Pipeline from the given estimators.
- Sequentially apply a list of transforms and a final estimator.
- Intermediate steps of the pipeline must be 'transforms', that is, they must implement fit and transform methods.
- The final estimator only needs to implement fit.



#### sklearn.pipeline.make\_pipeline

```
from sklearn.linear_model import Ridge
X, y = boston.data, boston.target
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
ridge = Ridge().fit(X_train_scaled, y_train)

X_test_scaled = scaler.transform(X_test)
ridge.score(X_test_scaled, y_test)
```

0.634

```
from sklearn.pipeline import make_pipeline
pipe = make_pipeline(StandardScaler(), Ridge())
pipe.fit(X_train, y_train)
pipe.score(X_test, y_test)
```

0.634

## sklearn.pipeline.Pipeline

```
pipe = make_pipeline(T1(), T2(), Classifier())
                               Classifier
pipe.fit(X, y)
                              T2.transfrom(X1) X2 Classifier.fit(X2, y)
pipe.predict(X')
X \xrightarrow{\text{T1.transform}(X')} X \xrightarrow{\text{1}} 1 \xrightarrow{\text{T2.transform}(X'1)} X \xrightarrow{\text{2}} 2 \xrightarrow{\text{classifier.predict}(X'2)} V
```

#### sklearn.pipeline.Pipeline

- Must assign the name of each process whereas make\_pipeline assign the name automatically.
- The steps in this command is a list of (key, value) pairs, where the key is a string containing the name you want to give for this step and value is an estimator object

## sklearn.pipeline.Pipeline

- An estimator's parameter can be set using '\_\_' syntax (double underscore)
- pipe.set\_params(knn3\_\_n\_neighbors=
  5).fit(X\_train,
  y\_train).score(X\_test, y\_test)
- can access each step by indexing the list of the pipeline
- What is the output of pipe[0]?

```
pipe.steps[1]
('knn3', KNeighborsClassifier())
pipe[1]
KNeighborsClassifier
KNeighborsClassifier()
pipe['knn3']
KNeighborsClassifier
```

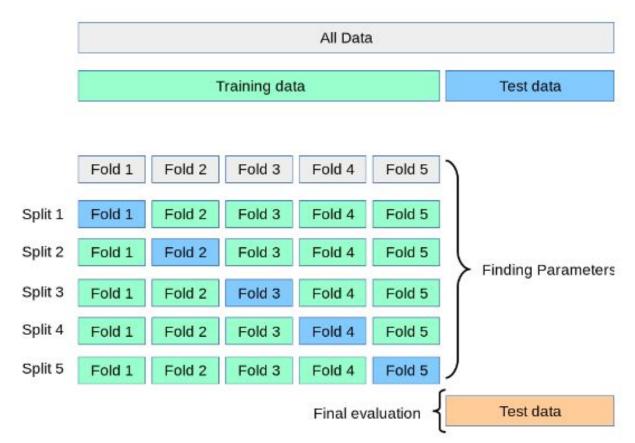
KNeighborsClassifier()

## Data leakage

- Scaling the whole dataset could cause information leakage
- We must split the dataset into training and test datasets, then, we fit training set and use the fitted model to scale the test set
- In case performing cross validation, we cannot split training set and validation set

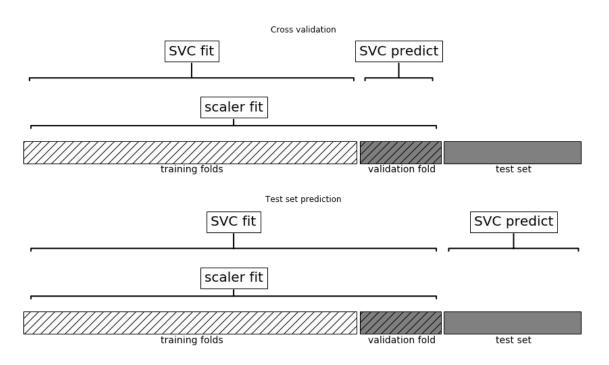
We have to use data pipeline

#### N-fold Cross-validation revisit

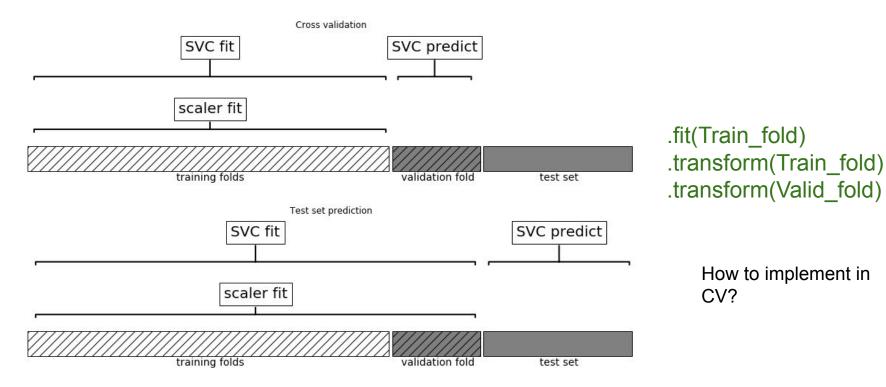


## Information leakage

When we perform scaling, it must be ensured that the validation dataset is excluded from scaling process. Otherwise the information leakage could occur.



# No information leakage



#### Example of Information leakage

Where does the leakage occur?

```
#information leakage
b cancer=load breast cancer()
X, y = b cancer.data, b cancer.target
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
est = LogisticRegression(max iter=400)
#Scaling
from sklearn.preprocessing import StandardScaler
from sklearn.model selection import cross val score
scale = StandardScaler()
X train scaled=scale.fit transform(X train)
scores = cross val score(est, X train scaled, y train, cv=5)
print(f'{scores.mean():.4f}')
```

# Use pipeline to prevent information leakage

 Earlier, the whole training set (train fold + validate fold) is used for scaling -> Leakage

```
#No information leakage
#Scaling
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import make_pipeline
pipe = make_pipeline(StandardScaler(),est)
scores = cross_val_score(pipe, X_train, y_train, cv=5)
```

#### Use pipeline to prevent information leakage

For KNN

**Best Practice** 

```
from sklearn.neighbors import KNeighborsRegressor
knn_pipe = make_pipeline(StandardScaler(), KNeighborsRegressor())
scores = cross_val_score(knn_pipe, X_train, y_train, cv=10)
np.mean(scores), np.std(scores)
```

(0.745, 0.106)

#### Grid-Search with Cross-Validation

```
from sklearn.model selection import cross val score
X train, X test, y train, y test = train test split(X, y)
cross val scores = []
for i in neighbors:
    knn = KNeighborsClassifier(n neighbors=i)
    scores = cross val score(knn, X train, y train, cv=10)
    cross val scores.append(np.mean(scores))
print("best cross-validation score: {:.3f}".format(np.max(cross val scores)))
best n neighbors = neighbors[np.argmax(cross val scores)]
print("best n neighbors: {}".format(best n neighbors))
knn = KNeighborsClassifier(n neighbors=best n neighbors)
knn.fit(X train, y train)
print("test-set score: {:.3f}".format(knn.score(X test, y test)))
best cross-validation score: 0.969
best n neighbors: 9
test-set score: 0.944
```

#### **GridSearchCV**

Grid search is the process of performing hyper parameter tuning in order to determine the optimal values for a given model.

- Called Meta-estimator
- Can specify the estimator, parameters
- Retrain the model with the best parameter settings.

```
from sklearn.model_selection import GridSearchCV

X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y)

param_grid = {'n_neighbors': np.arange(1, 30, 2)}
grid = GridSearchCV(KNeighborsClassifier(), param_grid=param_grid, cv=10, return_train_score=True)
grid.fit(X_train, y_train)
print("best mean cross-validation score: {:.3f}".format(grid.best_score_))
print("best parameters: {}".format(grid.best_params_))

print("test-set score: {:.3f}".format(grid.score(X_test, y_test)))
```

```
best mean cross-validation score: 0.972
best parameters: {'n_neighbors': 3}
test-set score: 0.958
```

#### Naming steps

```
from sklearn.neighbors import KNeighborsRegressor
from sklearn.pipeline import make pipeline
knn pipe = make pipeline(StandardScaler(), KNeighborsRegressor())
print(knn pipe.steps)
[('standardscaler', StandardScaler()), ('kneighborsregressor', KNeighborsRegressor())]
from sklearn.pipeline import Pipeline
pipe = Pipeline((("scaler", StandardScaler()), ("regressor", KNeighborsRegressor())))
```

## Pipeline and GridSearchCV

```
from sklearn.model_selection import GridSearchCV
knn pipe = make pipeline(StandardScaler(), KNeighborsRegressor())
param grid = {'kneighborsregressor n neighbors':range(1, 10, 2)}
grid = GridSearchCV(knn pipe, param grid, cv = 10)
grid.fit(X train, y train)
print(grid.best params )
print(grid.score(X test, y test))
{'kneighborsregressor n neighbors': 7}
```

- 0.8409275659949514
- Use Pipeline inside GridSearchCV
- Use keys as stepname parametername since multiple steps could have parameters with same name

#### Column transformer

- Different columns need different preprocessing treatments e.g. some columns need one-hot processing, while some need standardization.
- Cannot apply OneHotEncoder() or StandardScaler() directly because all columns would receive these treatments together.
- In column transformer, we can specify different columns for different treatments
- If we want more than two or more stages process, we might have to use pipeline together with columns transformer

#### Column transformer

```
numeric features = ['age', 'fare']
numeric transformer = Pipeline(steps=[
    ('imputer', SimpleImputer(strategy='median')),
    ('scaler', StandardScaler())])
categorical features = ['embarked', 'sex', 'pclass']
categorical_transformer = OneHotEncoder(handle_unknown='ignore')
preprocessor = ColumnTransformer(
    transformers=[
        ('num', numeric transformer, numeric features),
        ('cat', categorical transformer, categorical features)])
# Append classifier to preprocessing pipeline.
# Now we have a full prediction pipeline.
clf = Pipeline(steps=[('preprocessor', preprocessor),
                      ('classifier', LogisticRegression())])
```

- Apply Median Imputer and Standard Scaler for numeric features (age, fare)
- Apply One-hot Encoder for categorical features (embarked, sex, pclass)
- Pipeline can simplify this implementation

# Summary

- Pipeline: to specify all ML steps with one command e.g. scaling -> define model -> cross validation
- GridSearchCV is used to find hyper-parameters using brute-force approaches. Set parameters by dictionary: {'parametername':search range}
- With make\_pipeline or Pipeline, we can reference every step used in GridSearchCV in Pipeline
- GridSearchCV inside pipeline: set keys as stepname\_parametername

#### References

- Andreas C. Müller and Sarah Guido. Introduction to Machine
- Learning with Python: A Guide for Data Scientists. O'Reilly Media; 1st edition.
- Andreas C. Müller, COMS W4995 Applied Machine Learning, Columbia University, Spring 2019.
- https://scikit-learn.org/stable/auto\_examples/preprocessing/index.html
- https://scikit-learn.org/1.5/modules/generated/sklearn.pipeline.Pipeline.html