Data Science and Machine Learning for Engineering Applications

Scikit-Learn
Regression

Politecnico di Torino

DataBase and Data Mining Group

Salvatore Greco
Andrea Pasini
Flavio Giobergia
Elena Baralis
Tania Cerquitelli

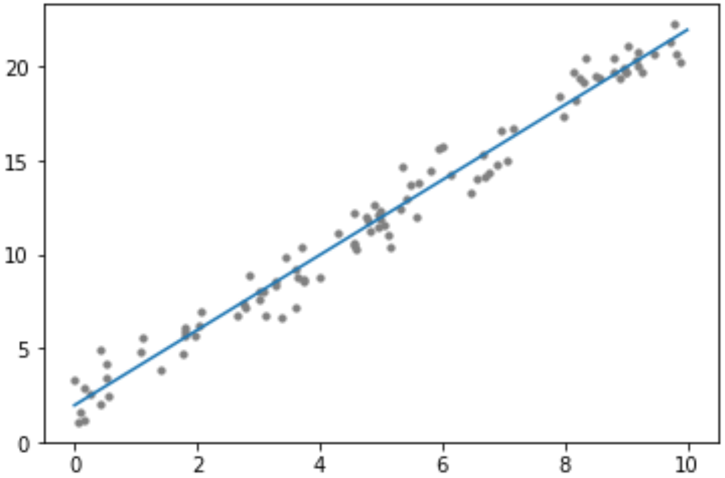
Linear regression

- Linear model to predict a single real value based on some input features

$$f(\mathbf{x}) = w_0 + \mathbf{w}^T\mathbf{x} = w_0 + w_1x_1 + w_2x_2 + \ldots + w_nx_n$$

- Simple linear regression (1 input feature)

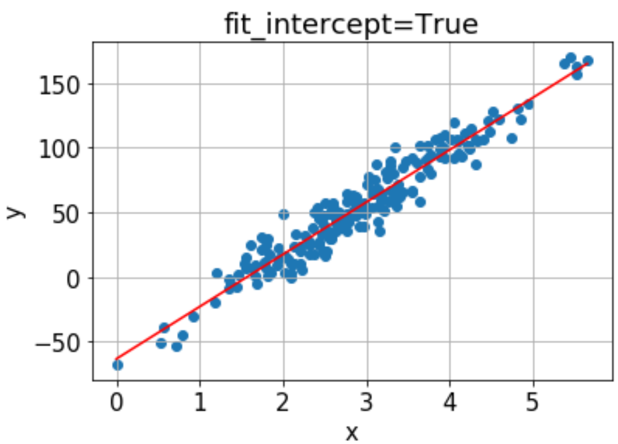
$$f(\mathbf{x}) = w_1x_1 + w_0$$

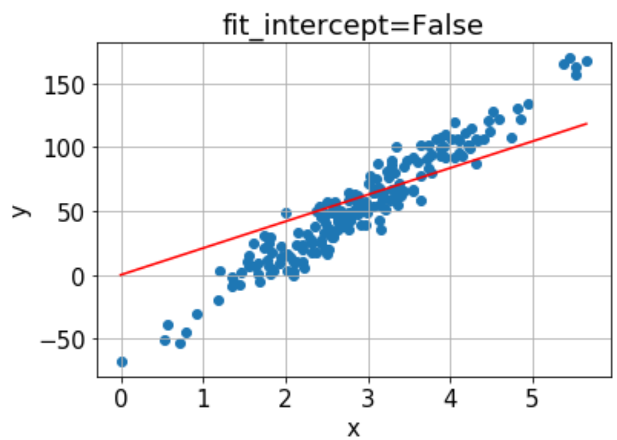


- Regression with Scikit-learn

```python
from sklearn.linear_model import LinearRegression
reg = LinearRegression(fit_intercept = True)
reg.fit(X_train, y_train)
y_test_pred = reg.predict(X_test)
```

  - The hyperparameter **fit_intercept** specifies whether the intercept will be computed during training
    - Default is True





Evaluating regression

- Evaluation metrics for regression:
  - MAE (Mean Absolute Error)
  - MSE (Mean Squared Error)
  - R^2

- Evaluated by comparing the two vectors
  - y_test (y): the expected result (**ground truth**)
  - y_test_pred ($\hat{y}$): the prediction made by your model

Evaluating regression

- MAE (Mean Absolute Error)

$$MAE = \frac{1}{n}\sum_{i} |y_i - \hat{y}_i|$$

- MSE (Mean Squared Error)

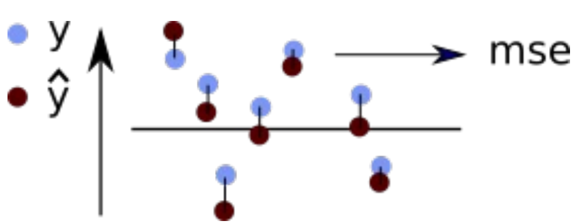
$$MSE = \frac{1}{n}\sum_{i} (y_i - \hat{y}_i)^2$$

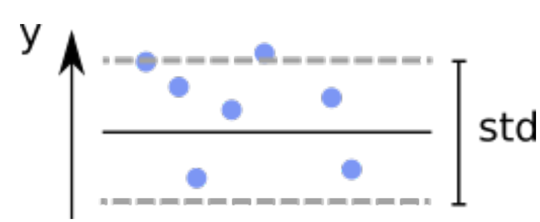
- Both positive numbers
  - MSE tends to penalize less errors close to 0

- R^2 (R squared)
  - It represents the proportion of variance explained by the predictions

$$R^2 = 1 - \frac{MSE}{std^2}$$

  - R^2 is close to 1 when you have good predictions
  - R^2 **negative** or **close to 0** means wrong predictions





- Evaluating regression with Scikit-learn

```
from sklearn.metrics import r2_score
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error

# Compute R2, MAE and MSE:
r2 = r2_score(y_test, y_test_pred)
mae = mean_absolute_error(y_test, y_test_pred)
mse = mean_squared_error(y_test, y_test_pred)
```

Evaluating regression

- Evaluation with cross_val_score()

```
from sklearn.model_selection import cross_val_score


reg = LinearRegression()
r2 = cross_val_score(reg, X, y, cv=5, scoring='r2')
```

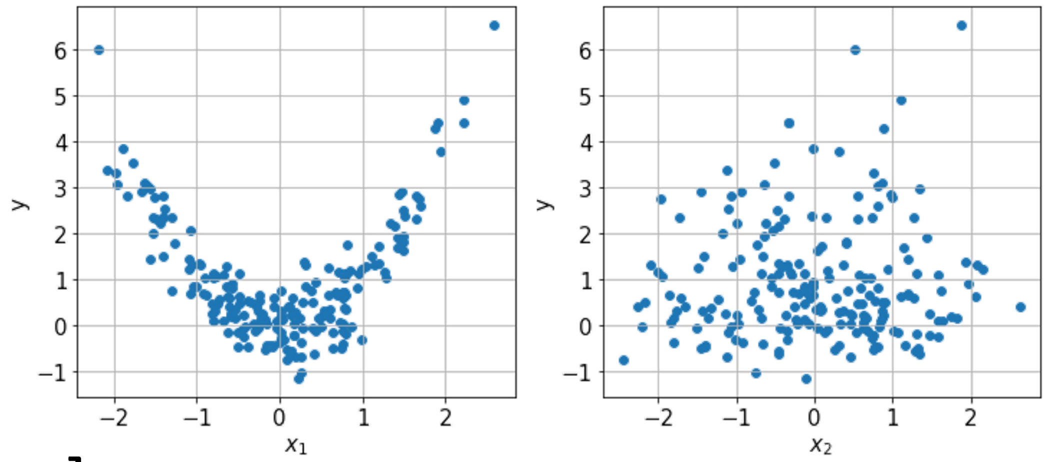
- Parameters:
  - cv = number of partitions for cross-validation
  - scoring = scoring function for the evaluation
    - E.g. ‘r2’, ‘**neg**_mean_squared_error’
- Similarly, we can use cross_val_predict()

Notebook Examples

- 4b-Scikitlearn-Linear-Regression.ipynb
  - 1. Simple linear regression
  - 2. Linear regression with multiple input features

- Polynomial regression
  - Useful when the data does not follow a linear trend
- **It consists of:**
  - Computing new **features** that are power functions of the input features
  - Applying **linear** regression on the new features

- Example



input vector = [x_1, x_2]

degree(2) features = [1, x_1 , x_2 , x_1^2 , x_2^2 , x_1x_2]

$$f(x) = w_0 + w_1x_1 + w_2x_2 + w_3x_1^2 + w_4x_2^2 + w_5x_1x_2$$

Polynomial regression

- Extracting polynomial features

```
from sklearn.preprocessing import PolynomialFeatures
poly = PolynomialFeatures(5)
X_poly = poly.fit_transform(X)
```

- Input
  - degree
    - Integer: the maximal degree of the computed features
    - Tuple: min and max degrees of the computed features
  - interaction_only: if True, only include interactions
  - include_bias: if True, add a bias column (column of ones)
- Output (of fit_transform())
  - A 2D **NumPy array** with the new feature matrix

Polynomial regression

- Building a **pipeline** with polynomial features and linear regression

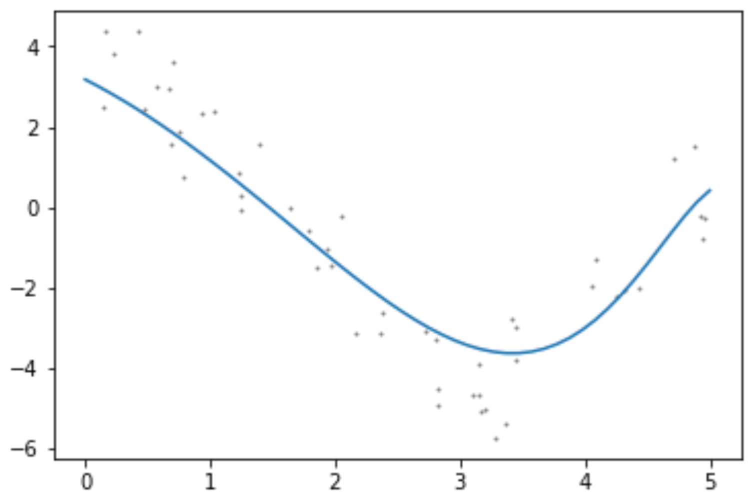
```
from sklearn.pipeline import make_pipeline
reg = make_pipeline(PolynomialFeatures(5), LinearRegression())
reg.fit(X_train, y_train)
y_test_pred = ret.predict(X_test)
```

- Pipelines are objects that allow concatenating multiple Scikit-learn models

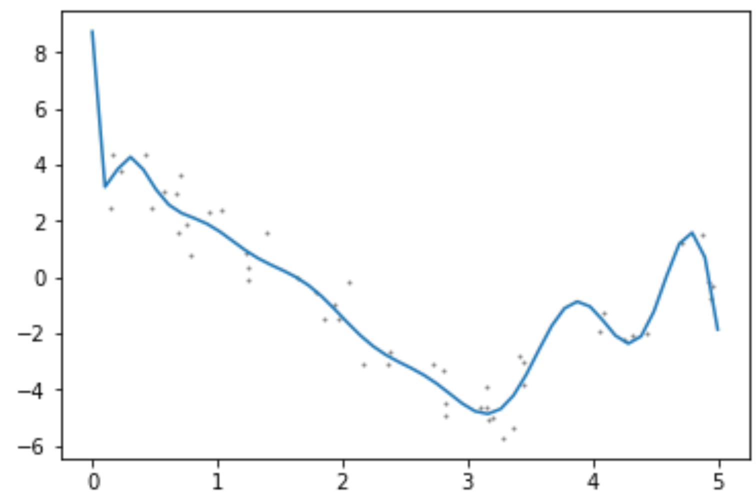
Polynomial regression

- Higher polynomial degree means higher **capacity** of your model, but …
  - Pay attention to not **overfit** your data
  - Overfitting occurs in these cases when you have few samples and a model that has high capacity

Correct regression



Overfitting



Polynomial regression

- To avoid this form of overfitting
  - Use more training data (if possible)
  - Use lower model complexity (capacity)
  - Use regularization techniques
    - E.g. Ridge, Lasso

- **Ridge** and **Lasso** are two techniques for training a linear regression (or a linear regression with polynomial features)
- They try to assign values **closer to zero** to the coefficients assigned to features that are not useful for the regression
- This effect can **decrease the complexity** of the model when necessary

- When training normal linear regression you **minimize the MSE** to compute the coefficients
- When training **Ridge** you minimize

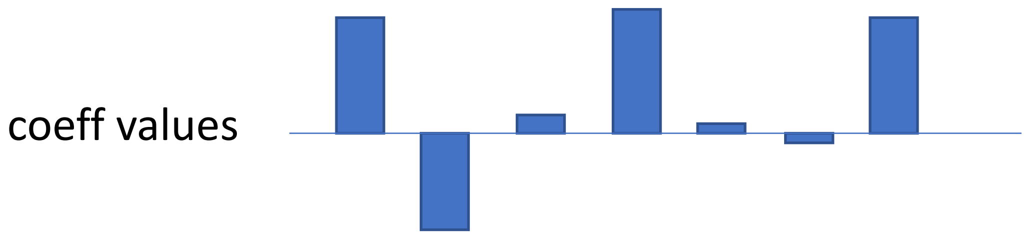
$$MSE + \alpha(\sum_i w_i^2)$$

- When training **Lasso** you minimize

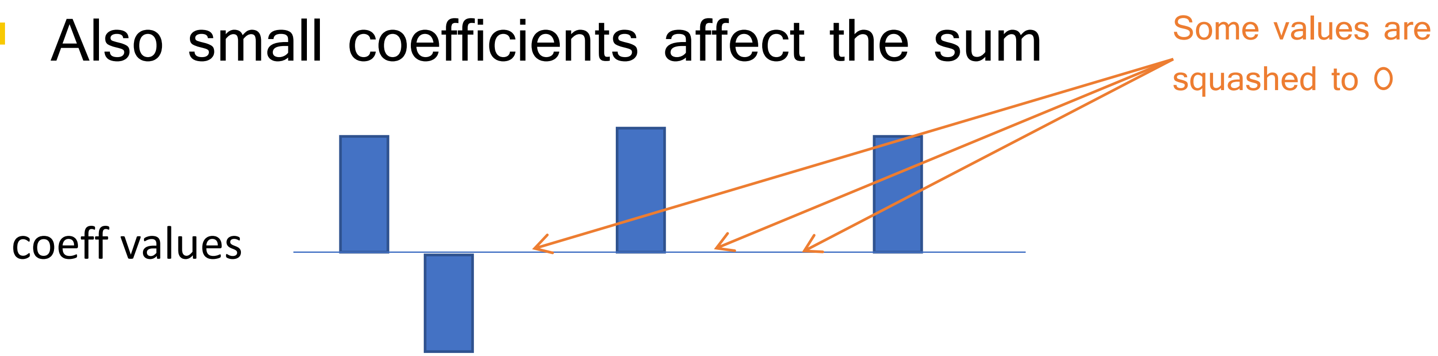
$$MSE + \alpha(\sum_i |w_i|)$$

Polynomial regression

- **Ridge** tends to lower uniformly all the coefficients
  - Coefficients already close to 0 have little effect on the sum of **squares** (if $x \approx 0$, $x^2 < x$)



- **Lasso** tends to assign the value 0 to **some** coefficients (feature selection)
  - Also small coefficients affect the sum



- **Ridge:**

```python
from sklearn.linear_model import Ridge
reg = Ridge(alpha=0.5)
```

- **Lasso:**

```python
from sklearn.linear_model import Lasso
reg = Lasso(alpha=0.5)
```

Notebook Examples

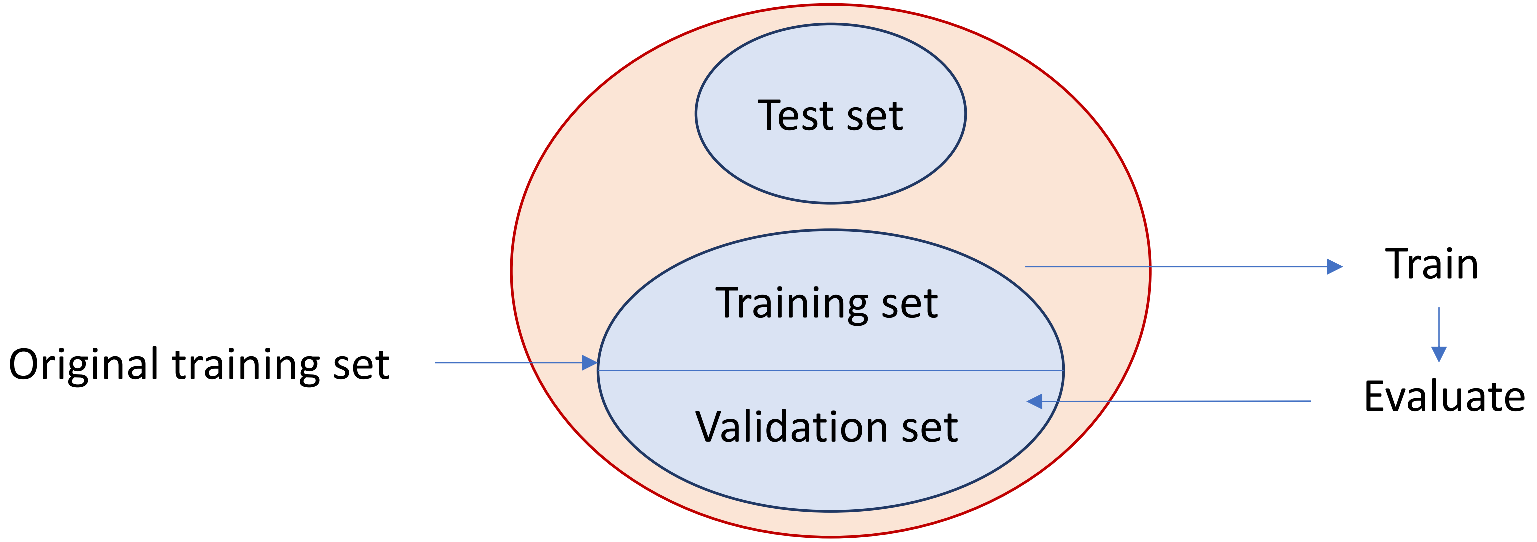
- **4c-Scikitlearn-Polynomial-Regression.ipynb**
  - **1. Polynomial regression**
  - **2. Overfitting and regularization**

Hyperparameters selection

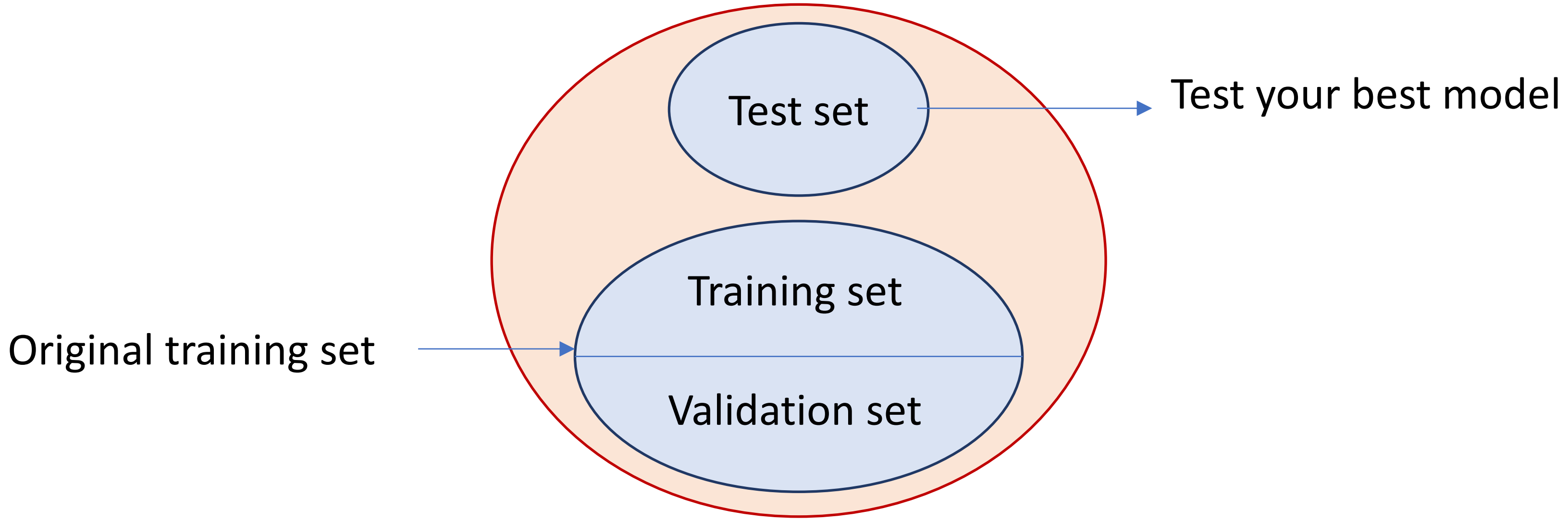
- Hyperparameters vs parameters
  - Hyperparameters are selected by the user
  - Parameters are computed by the algorithm during training
- **Important**: hyperparameters cannot be set by finding the values that give the best results on the test set
  - This methodology **will overfit the test set**
  - We would be using **information from the test data** to select some **training** hyperparameters

Hyperparameters selection

- There are two valid methodologies
- 1. Use hold-out to divide training data in 2 parts
  - Fit different model configurations on the **training** set
  - Pick the best one by evaluating the performance on the **validation** set

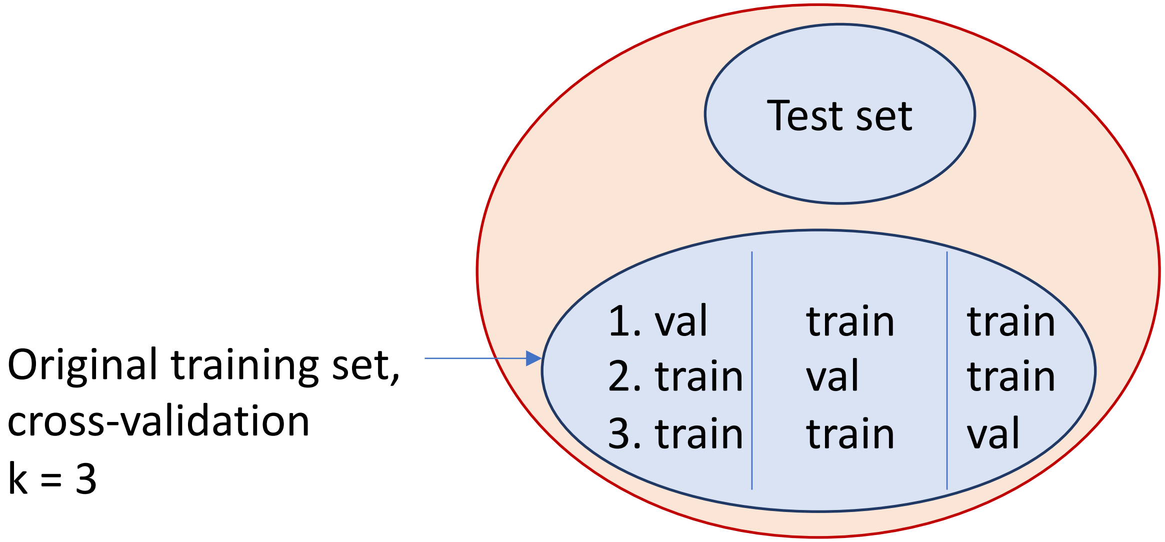


- Finally test the selected model on the actual **test set** to have a measure of how well the selected hyperparameters work with new data

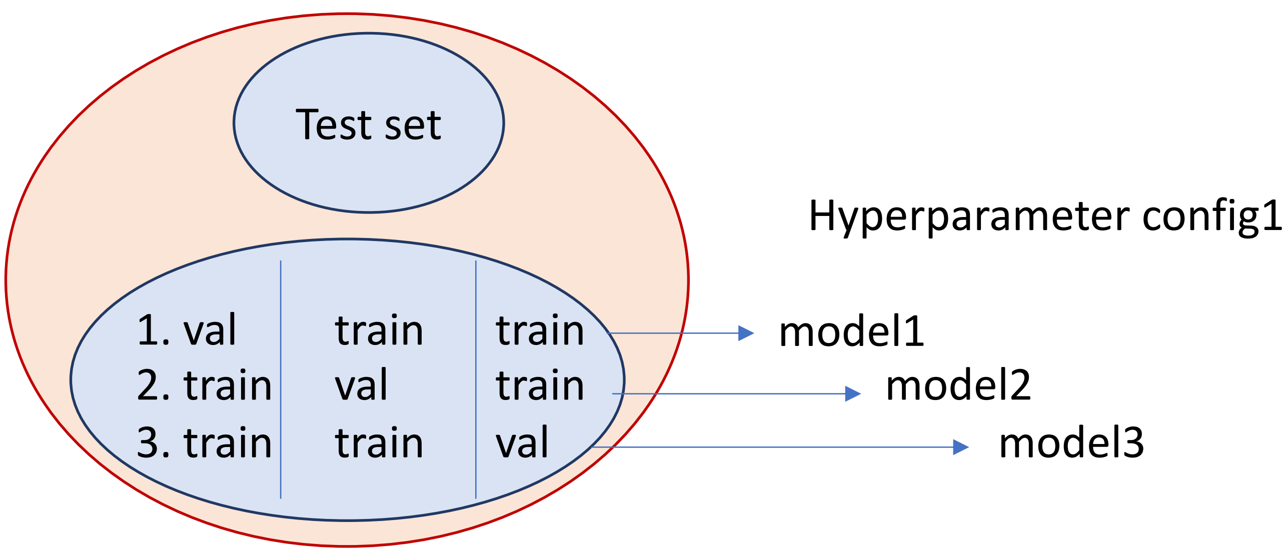


Hyperparameters selection

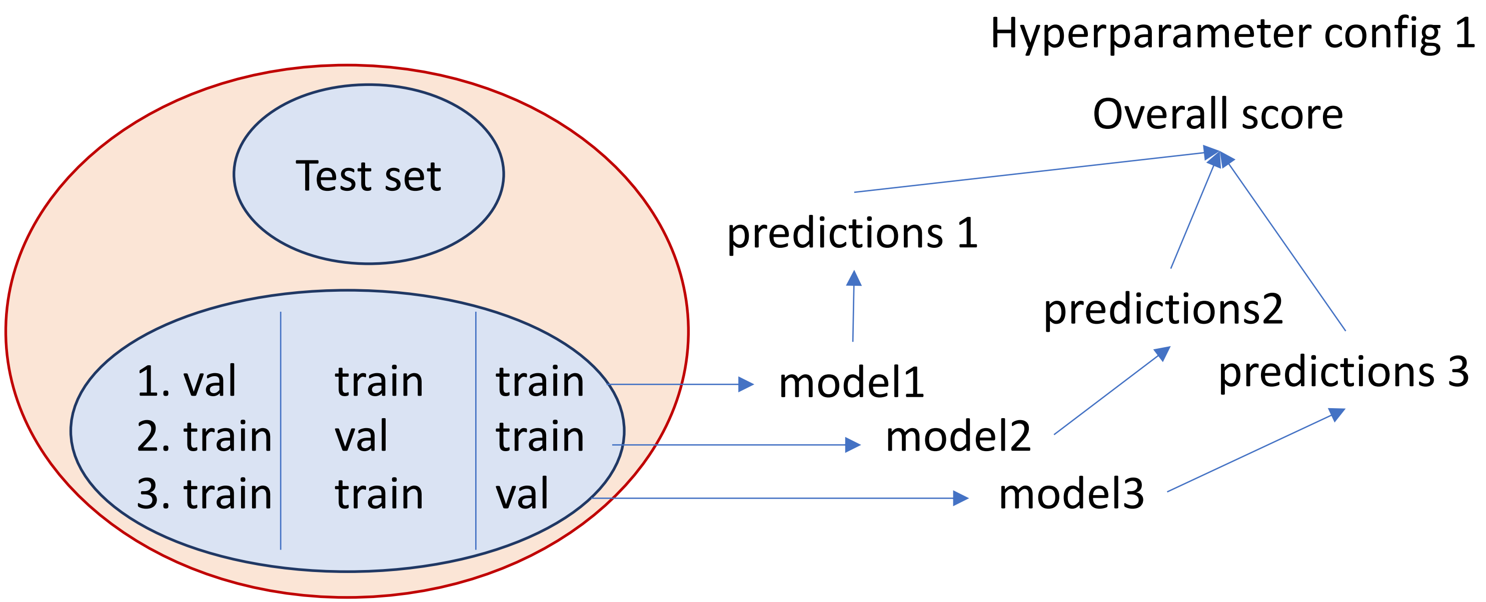
- 2. Use cross-validation (k-fold) on training data
  - At each **iteration** 1 partition of the training data is used as **validation** set, the others are used to **train** the models



- 2. Use cross-validation (k-fold) on training data
  - For a given **configuration** we train k **models** on the training partitions and evaluate them on the **validation** partition



- 2. Use cross-validation (k-fold) on training data
  - For each model configuration compute the **overall** scores on the validation partitions
  - Select the configuration with the **highest** overall score



Hyperparameters selection

- This second methodology can be easily performed in Scikit-learn
  - First define a **dictionary** with the **parameter values** that you want to tune
  - E.g. for Ridge regression:

```
param_grid = {'alpha' : [0.1, 0.2],
              'fit_intercept' : [True, False]}
```

  - With this grid Scikit-learn will try all the **combinations**:
    - {alpha=0.1,fit_intercept=True}
    - {alpha=0.1,fit_intercept=False}
    - {alpha=0.2,fit_intercept=True}
    - {alpha=0.2,fit_intercept=False}

- Then define a model and call GridSearchCV

```
from sklearn.model_selection import GridSearchCV
reg = Ridge()
gridsearch = GridSearchCV(reg, param_grid, scoring='r2', cv=5)
gridsearch.fit(X_train, y_train)
```

- This code will pick the best configuration of the param grid, for Ridge model,
  - According to the $\mathbf{R^2}$ score
  - Using a cross validation with **k=5** partitions

Hyperparameters selection

- The best parameter configuration can be found in the *best_params_* attribute of the gridsearch object
- An instance of the model with the best configuration is available in best_estimator_
  - **Important**: it is trained on the **whole dataset**!

```
...
gridsearch.fit(X_train, y_train)
print(gridsearch.best_params_['alpha'])
print(gridsearch.best_params_['fit_intercept')

best_configured_model = gridsearch.best_estimator_
```

Notebook Examples

- **4c-Scikitlearn-Polynomial-Regression.ipynb**
  - **3. Grid-search to select model hyperparameters**