



Politecnico
di Torino



Data Science Lab

Scikit-learn
Regression

Andrea Pasini
Flavio Giobergia
Elena Baralis

DataBase and Data Mining Group



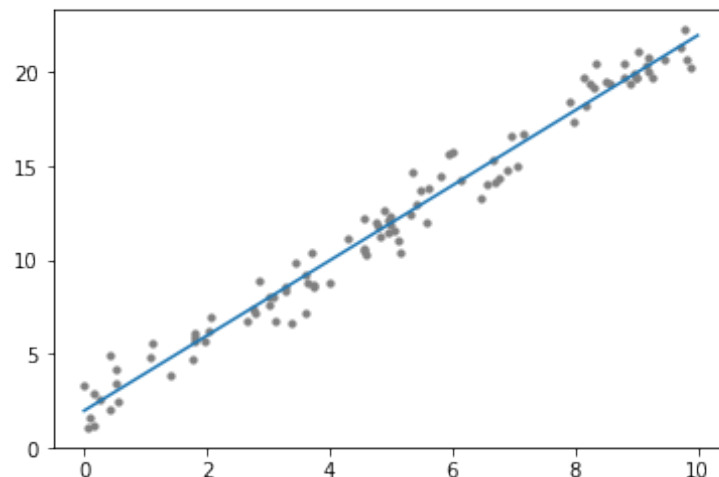
Linear regression

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

$$f(\mathbf{x}) = w_0 + \mathbf{w}^T \mathbf{x} = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_n x_n$$

- Simple linear regression (1 input feature)

$$f(x) = w_1 x_1 + w_0$$



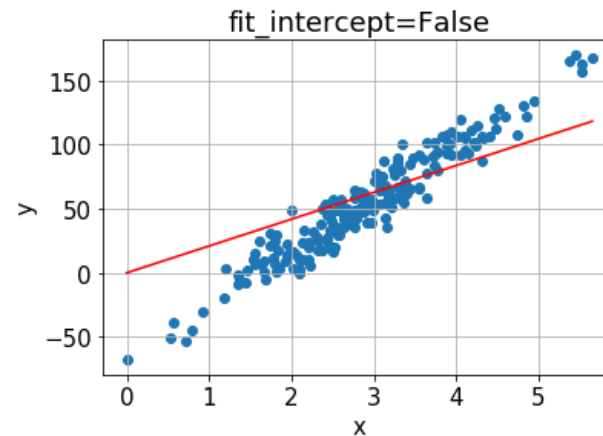
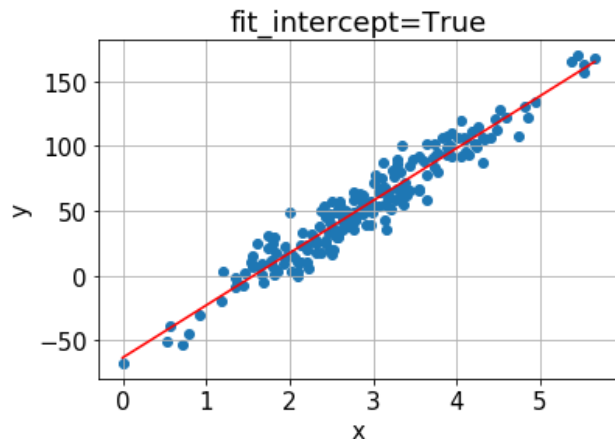


- Regression with Scikit-learn

```
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





- 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**)
 - $y_{\text{test_pred}}$ (\hat{y}): the prediction made by your model



- MAE (Mean Absolute Error)

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

- MSE (Mean Squared Error)

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

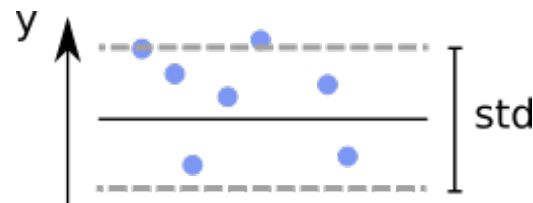
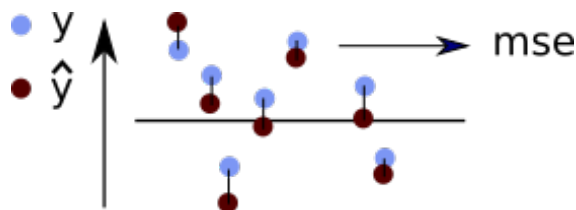
- Both positive numbers
 - MSE tends to penalize less errors close to 0



- 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)
```



- 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'



Notebook Examples

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

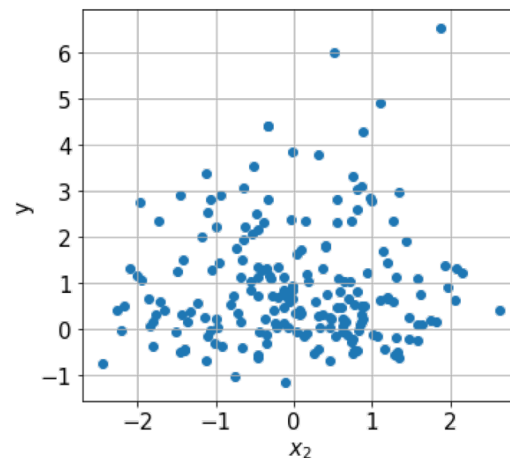
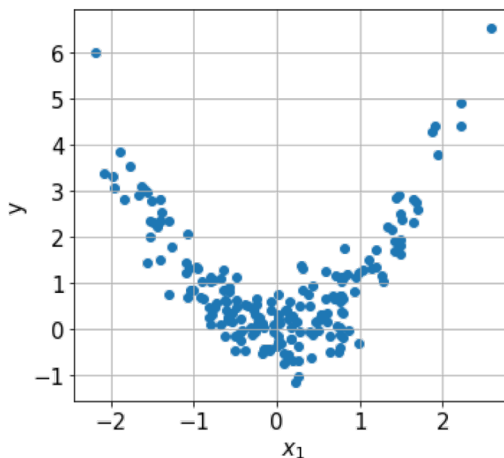




- Polynomial regression
 - Useful when the data does not follow a linear trend
- **It consists of:**
 - Computing new **features** that are power functions of the input features
 - Applying **linear** regression on the new features



- Example



input vector = $[x_1, x_2]$

↓

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

↓

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



- 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



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

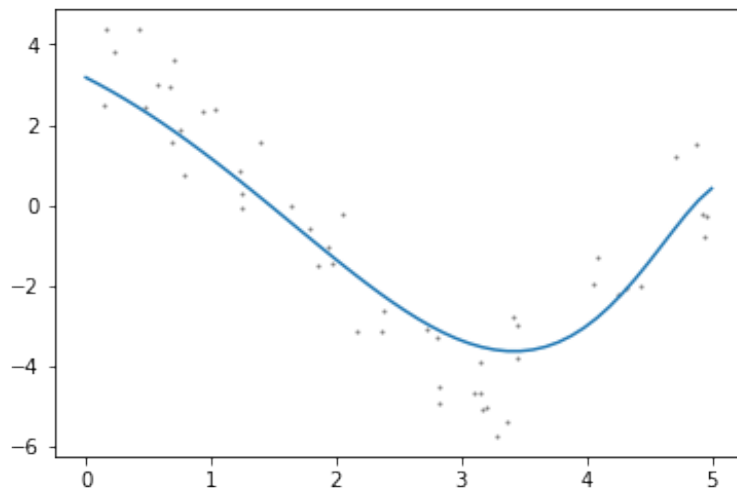
```
from sklearn.pipeline import make_pipeline
reg = make_pipeline(PolynomialFeatures(5), LinearRegression())
reg.fit(X_train, y_train)
y_test_pred = reg.predict(X_test)
```

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

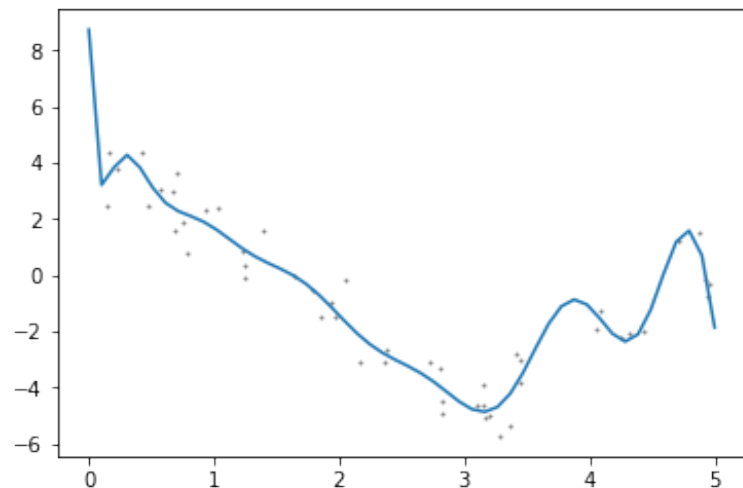


- Higher polynomial degree means higher **capacity** of your model, but ...
 - Pay attention to not **overfit** your data
 - Overfitting occurs in these cases when you have few samples and a model that has high capacity

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

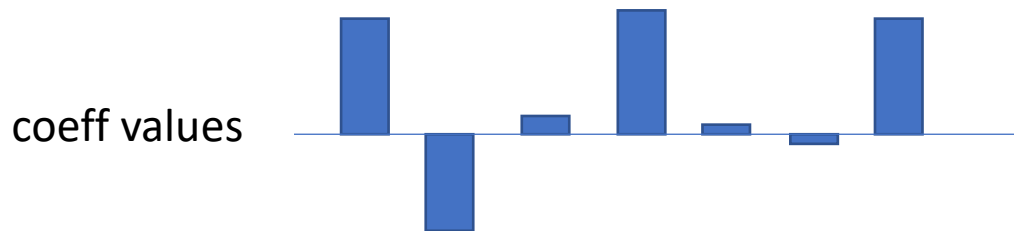
$$MSE + \alpha \left(\sum_i w_i^2 \right)$$

- When training **Lasso** you minimize

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

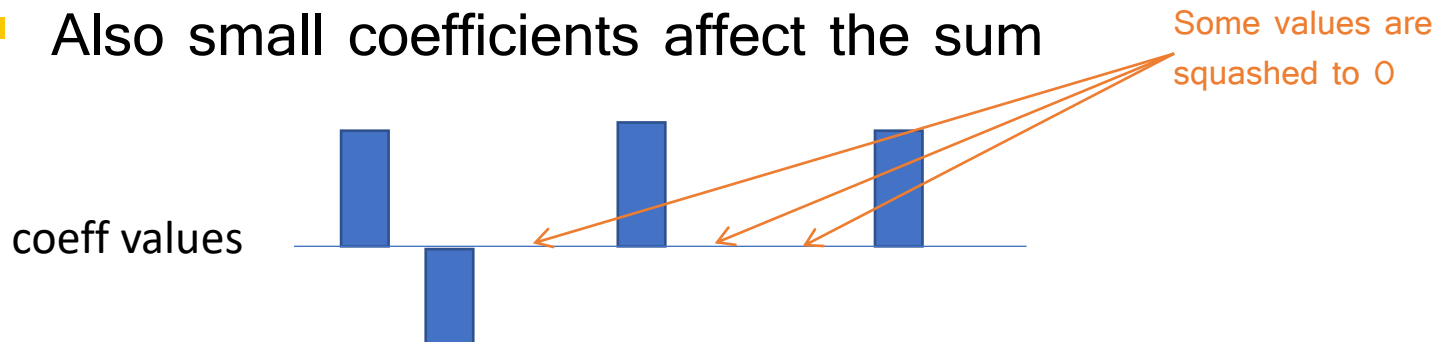


- **Ridge** tends to lower uniformly all the coefficients
 - Coefficients already close to 0 have little effect on the sum of **squares** (if $x \approx 0$, $x^2 < x$)



- **Lasso** tends to assign the value 0 to **some** coefficients (feature selection)

- Also small coefficients affect the sum





- **Ridge:**

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

- **Lasso:**

```
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

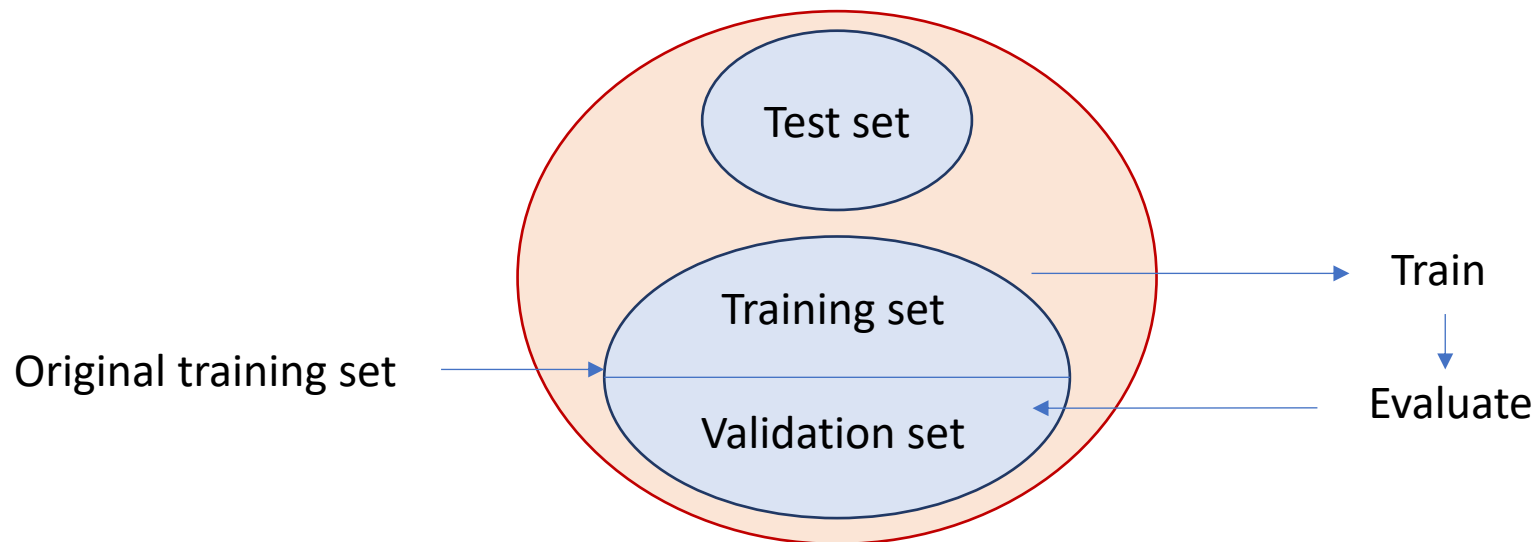




- Hyperparameters vs parameters
 - Hyperparameters are selected by the user
 - Parameters are computed by the algorithm during training
- **Important:** hyperparameters cannot be set by finding the values that give the best results on the test set
 - This methodology **will overfit the test set**
 -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

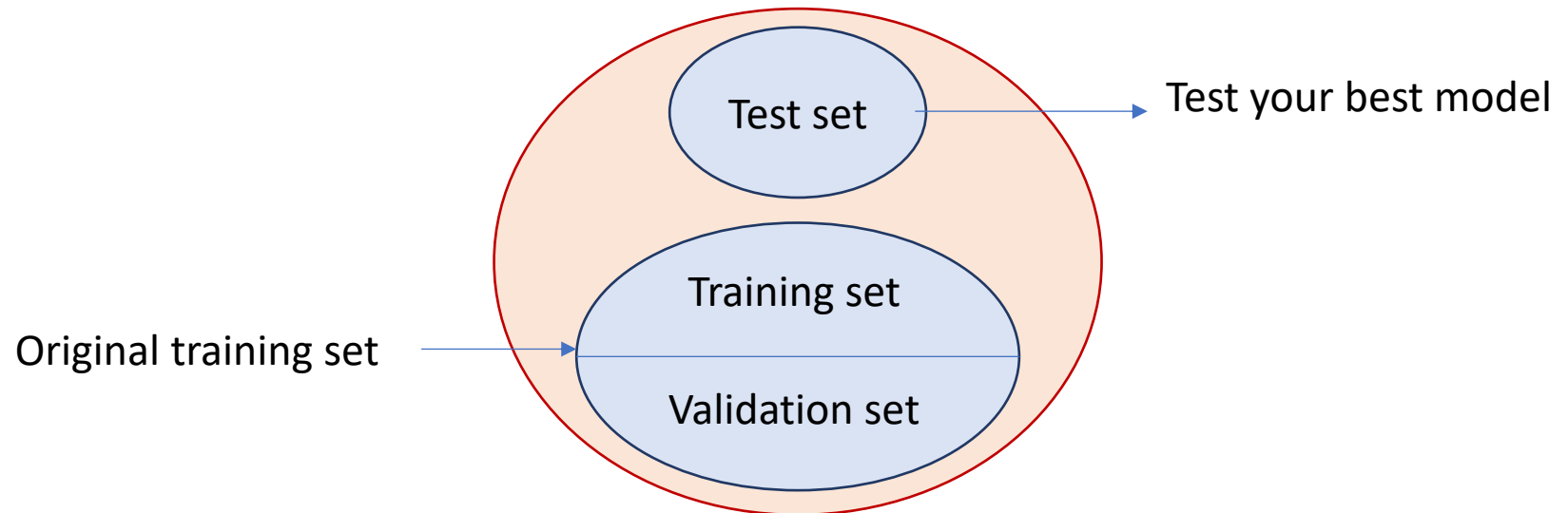


- There are two valid methodologies
- 1. Use hold-out to divide training data in 2 parts
 - Fit different model configurations on the **training** set
 - Pick the best one by evaluating the performance on the **validation** set



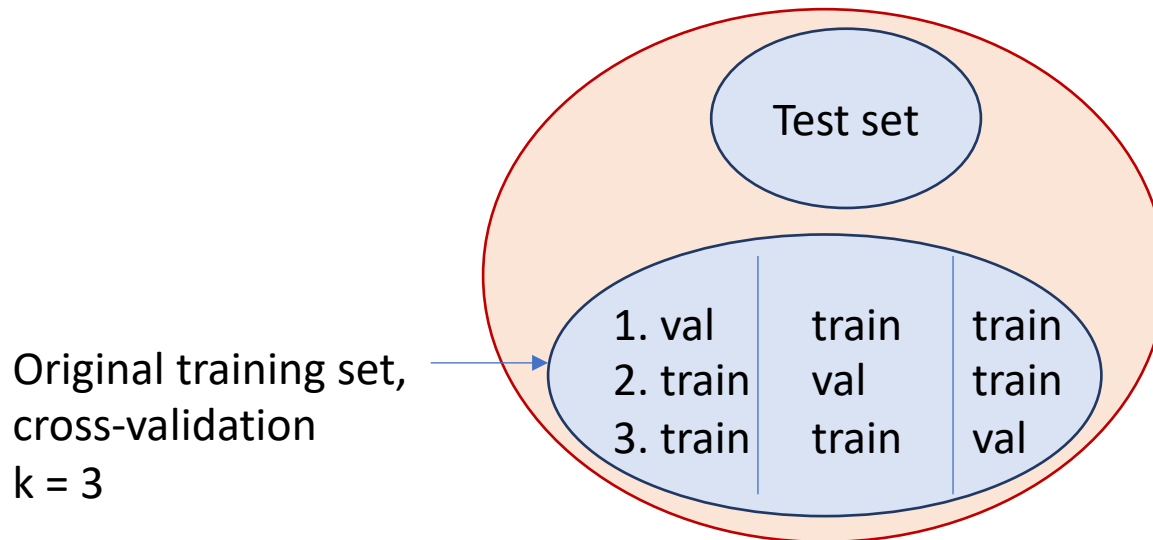


- Finally test the selected model on the actual **test set** to have a measure of how well the selected hyperparameters work with new data



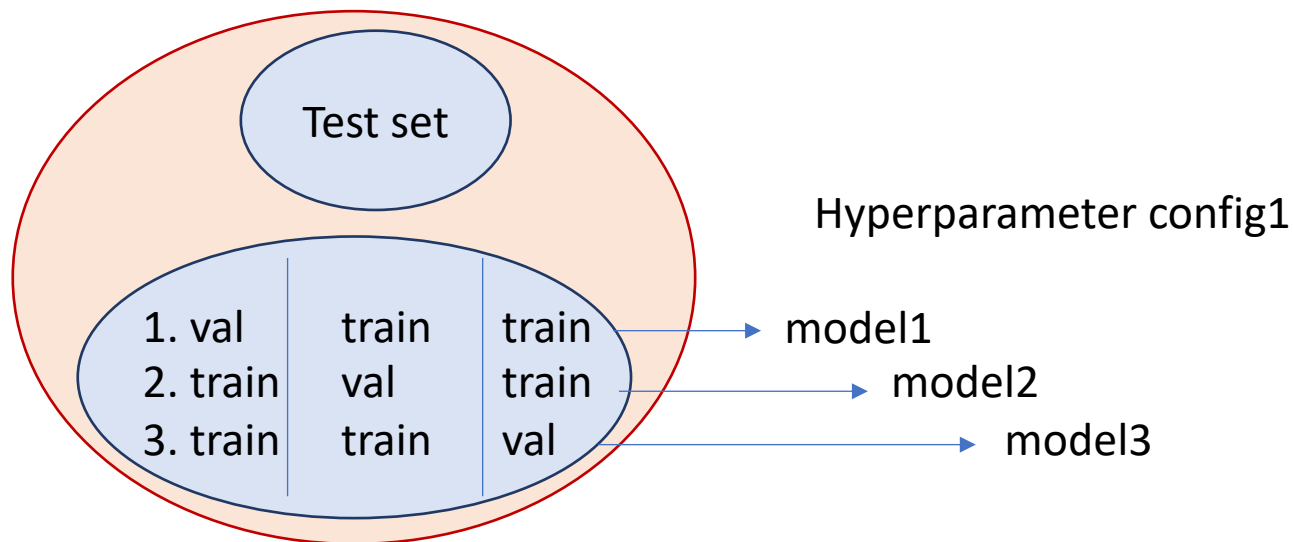


- 2. Use cross-validation (k-fold) on training data
 - At each **iteration** 1 partition of the training data is used as **validation** set, the others are used to **train** the models



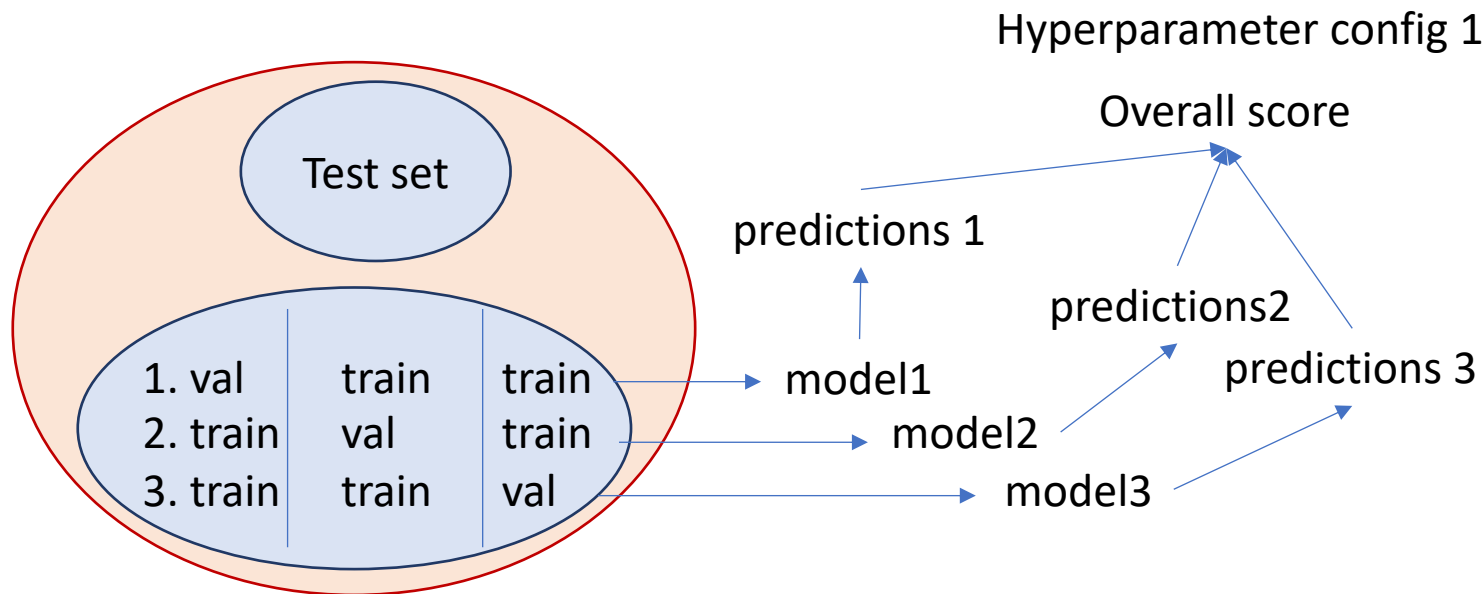


- 2. Use cross-validation (k-fold) on training data
 - For a given **configuration** we train k **models** on the training partitions and evaluate them on the **validation** partition





- 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





- 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 R^2 score
 - Using a cross validation with **k=5** partitions



- 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**

