Introduction to Statistical Learning with Applications

CM3: Cross-validation, model selection, and bias-variance

Pedro L. C. Rodrigues

IN OUR PREVIOUS EPISODES…

Our current worflow

1. We want to estimate the values of Y based on predictors $X_1, \ldots, X_p$
2. We are given a set of N examples of y_i with corresponding $x_{i1}, \ldots, x_{ip}$
3. We estimate parameters $\hat{\beta}$ that minimize $\frac{1}{N}\sum_{i=1}^{N}(y_i - \beta^T x_i)^2$
4. We do statistical inference on the values of the $\hat{\beta}_j$

$$x_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix}$$

IN OUR PREVIOUS EPISODES...

We do **statistical inference** on the values of $\hat{\beta}_j$

1 We are given a dataset $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$

2 We assume that each data point is

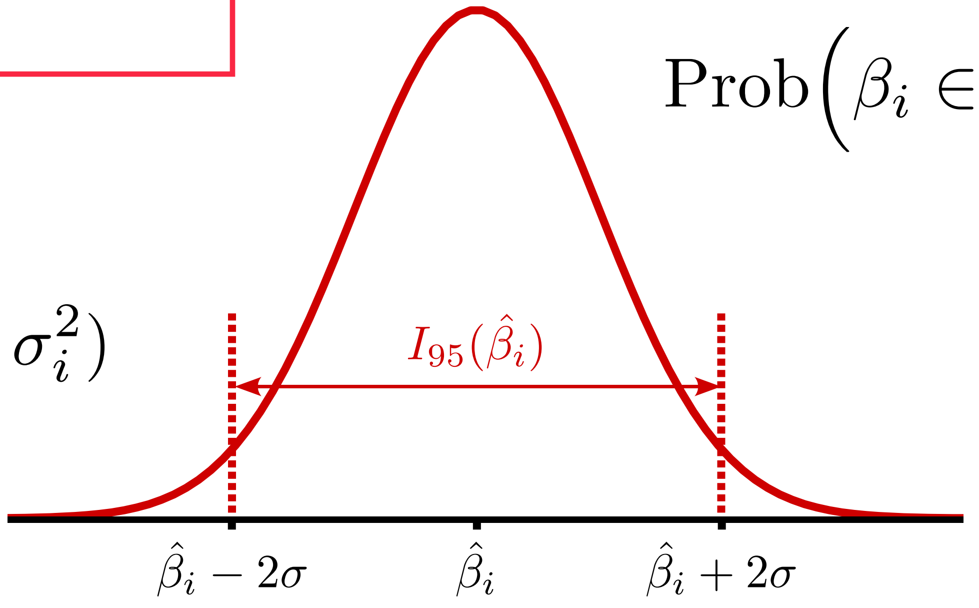
$$y_i = \beta_0 + \sum_{k=1}^{p} \beta_k x_{ik} + \varepsilon_i$$

3 We assume the noise is **Gaussian** IID

$$\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

$$\text{Prob}\Big(\beta_i \in I_{95}(\hat{\beta}_i)\Big) = 0.95$$

$$\hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_p \end{bmatrix} \longrightarrow \hat{\beta}_i \sim \mathcal{N}(\beta_i, \sigma_i^2)$$



IN OUR PREVIOUS EPISODES...

We do **statistical inference** on the values of $\hat{\beta}_j$

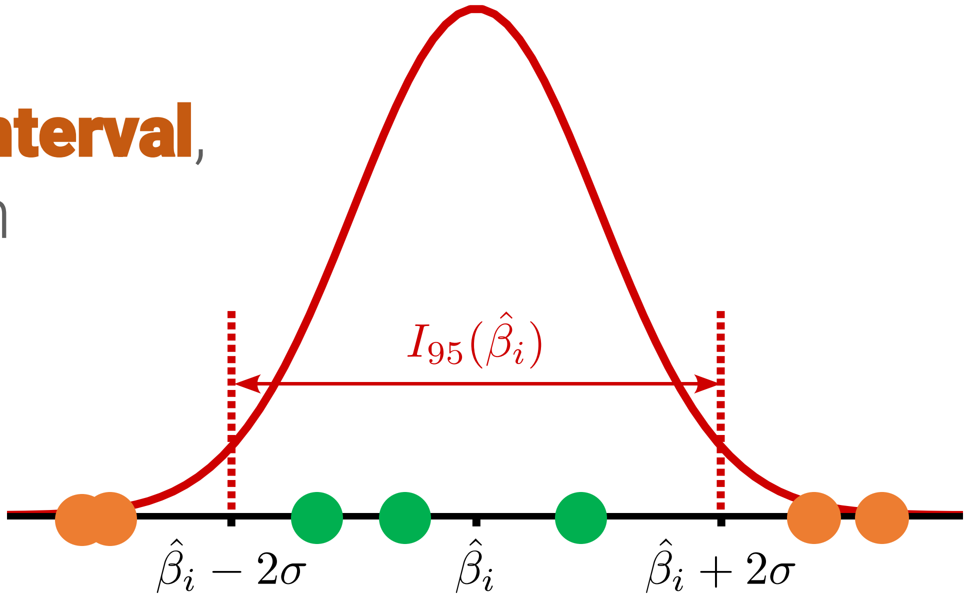
Note that even if we had data generated with $\beta_i = 0$ our estimate is a RV

$$\boxed{\hat{\beta}_i \sim \mathcal{N}(0, \sigma^2) \longrightarrow \text{Very likely that } \hat{\beta}_i \neq 0}$$

Therefore, we would like to check whether the number that we get for this estimate is one that could **indeed come from such distribution**

If it is a **number too far off from the confidence interval**, then it might in fact mean that the distribution with zero-mean is not a good one to describe the data

This is the intuition behind the statistical tests!



IN OUR PREVIOUS EPISODES...

However, in practice we're often more interested in the **predictions**!

Is there a natural way of describing the statistics of the predicted values?

Remember that if we assume a linear model for the data, then

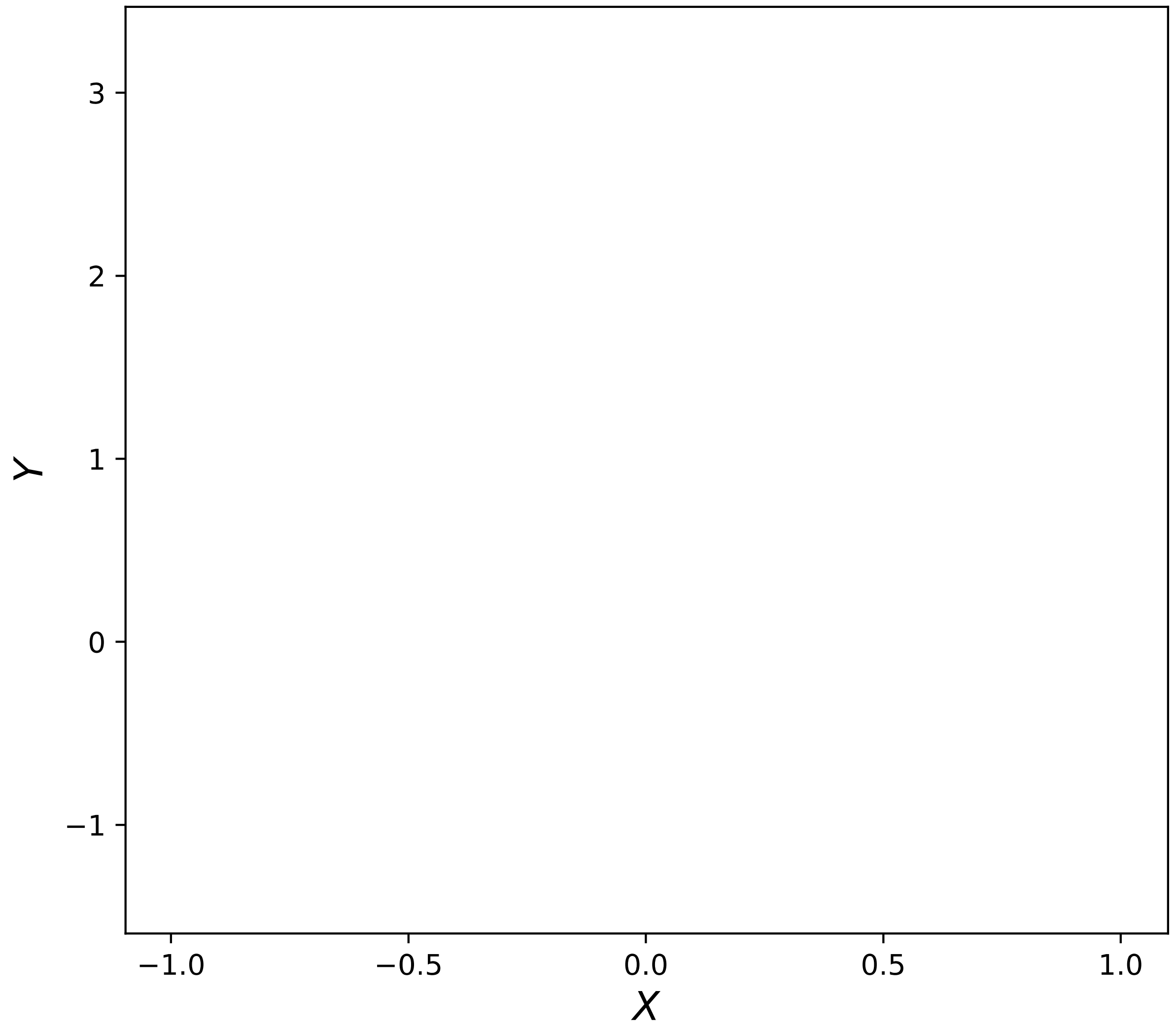
$$\mathbb{E}[Y \mid X = x] = m(x) = \beta_0 + \sum_{k=1}^{p} \beta_k x_k = x^\top \beta$$

Using our limited dataset, we can build

$$\hat{m}(x) = x^\top \hat{\beta} \sim \mathcal{N}(x^\top \beta, \Sigma_m) \text{ with } \Sigma_m = x^\top \Sigma_\beta x$$

IN OUR PREVIOUS EPISODES…

But what if we can’t assume a linear model? Nor Gaussian?



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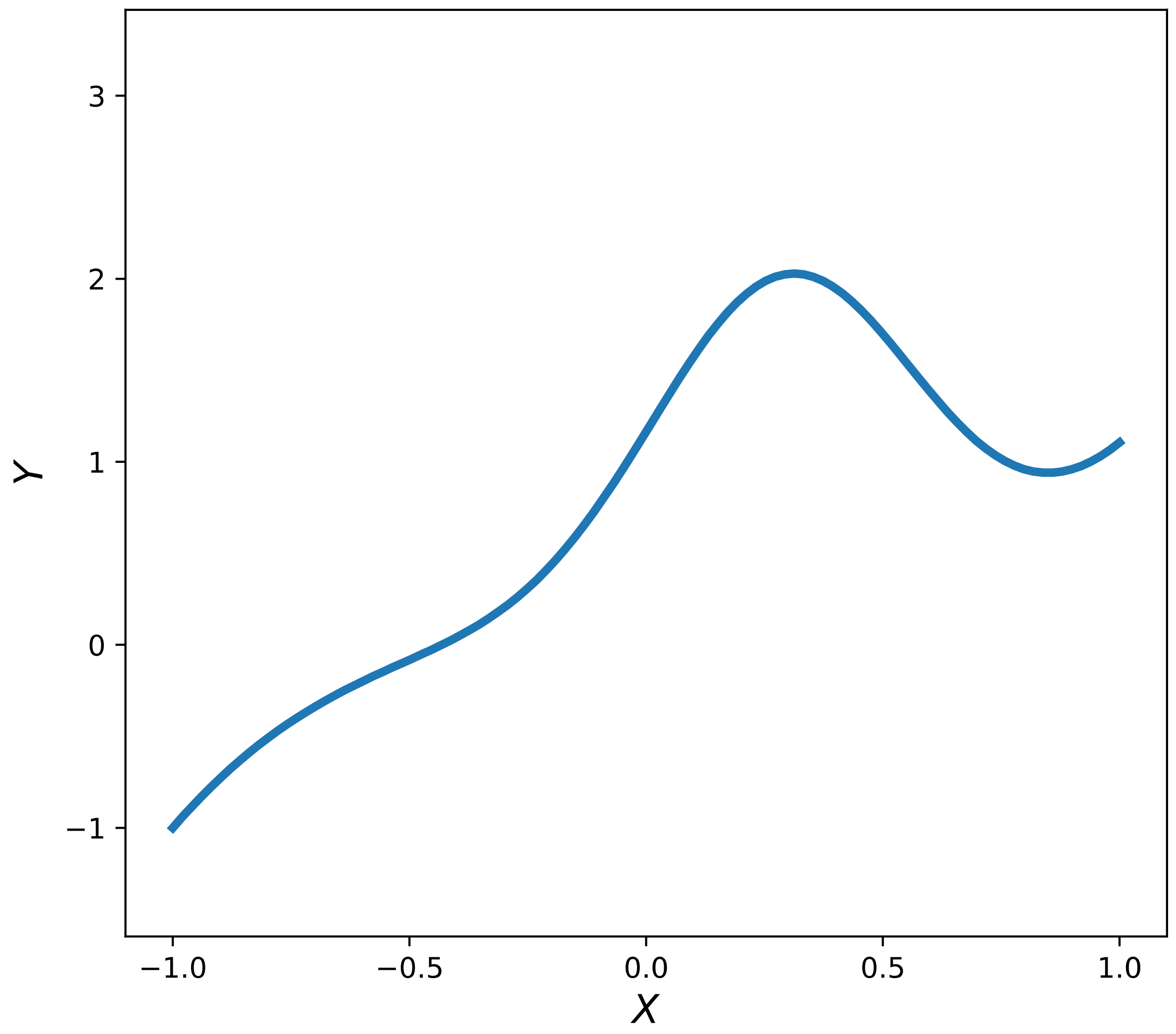

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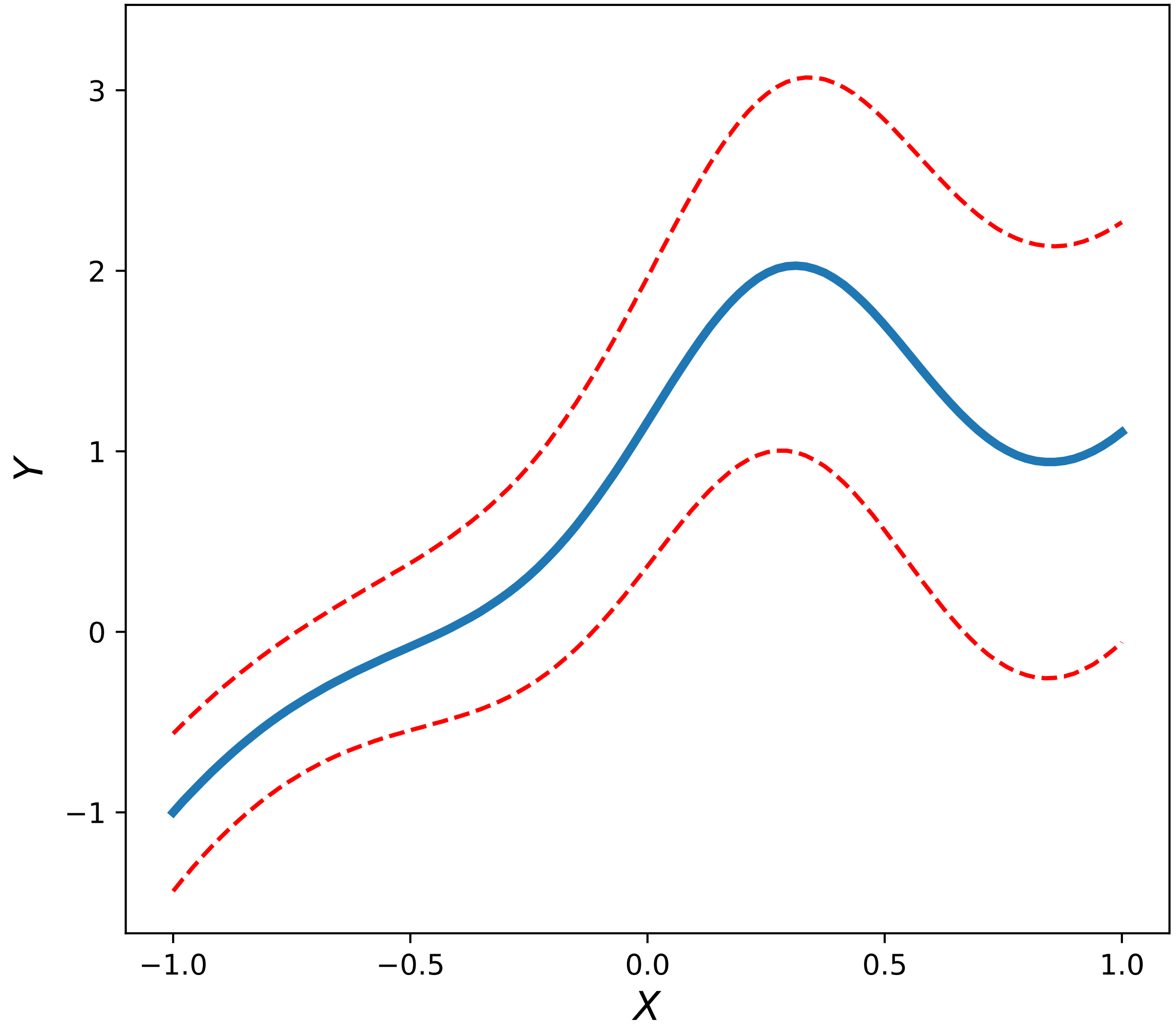

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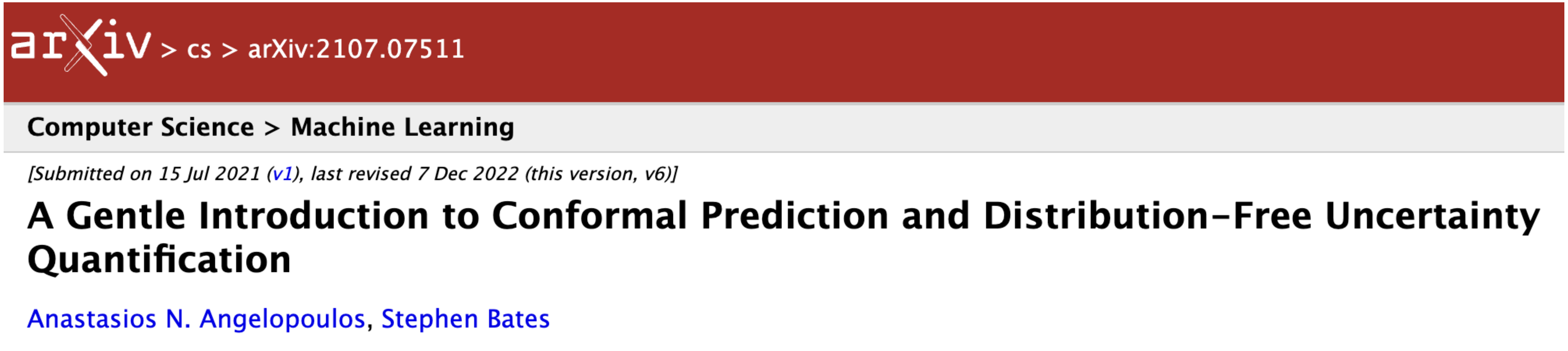

arXiv > cs > arXiv:2107.07511

Computer Science > Machine Learning

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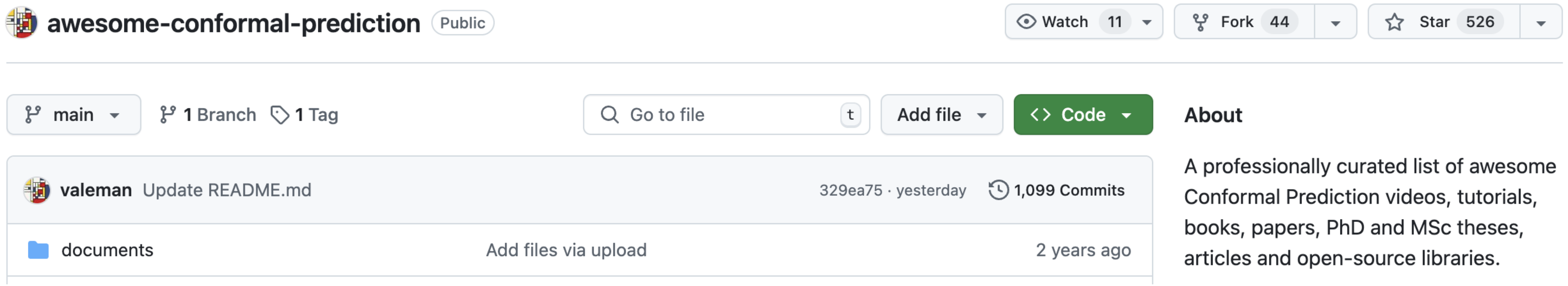
A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification

Anastasios N. Angelopoulos, Stephen Bates



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IN OUR PREVIOUS EPISODES...

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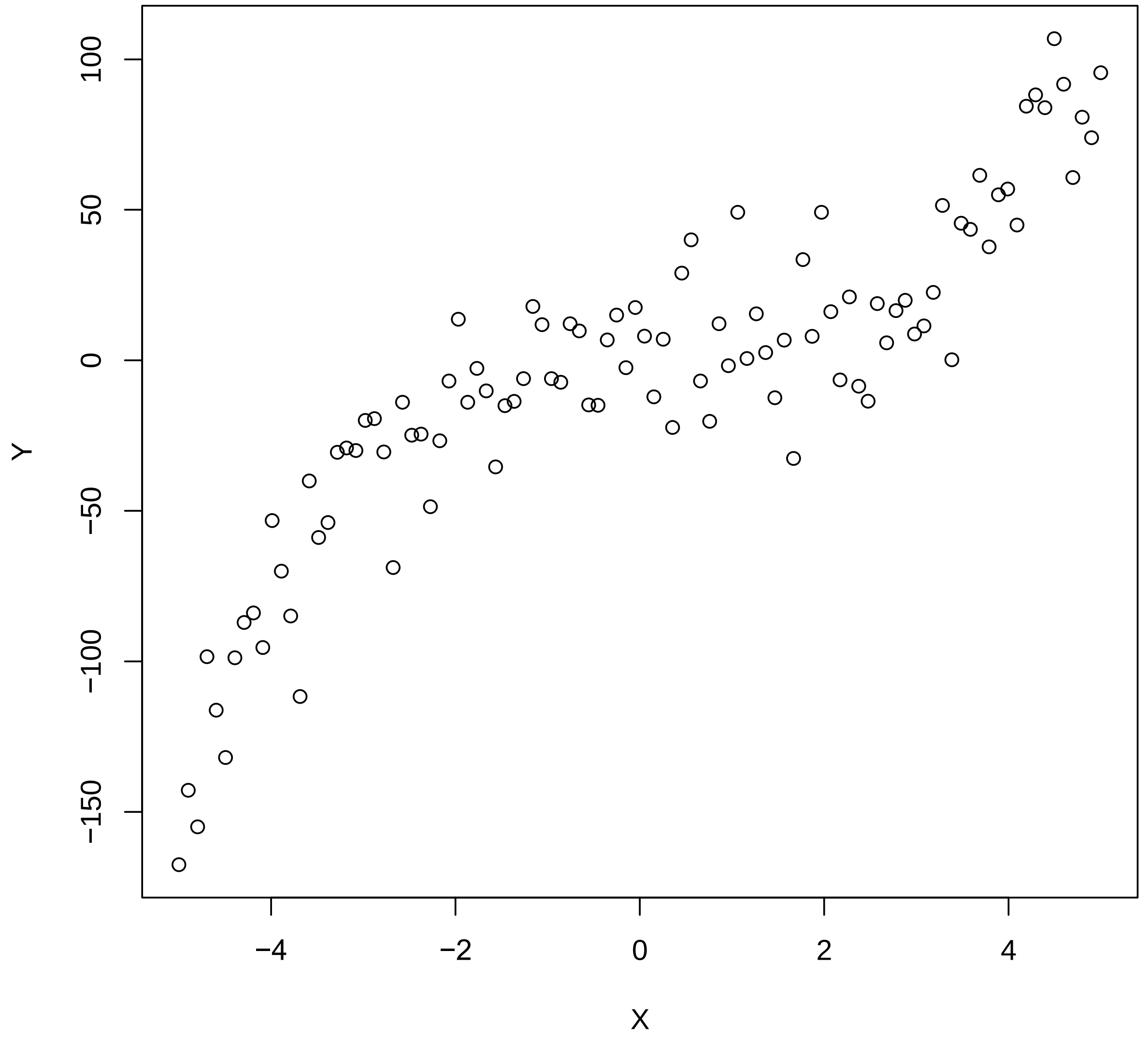
4. We do statistical inference on the values of the $\hat{\beta}_j$
5. How can we **assess the quality** of a model?

$$x_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix}$$

- What makes a model **good**?
- Estimating the quality of a model
- Comparing and selecting models

What makes a model good?



Suppose our data is generated as

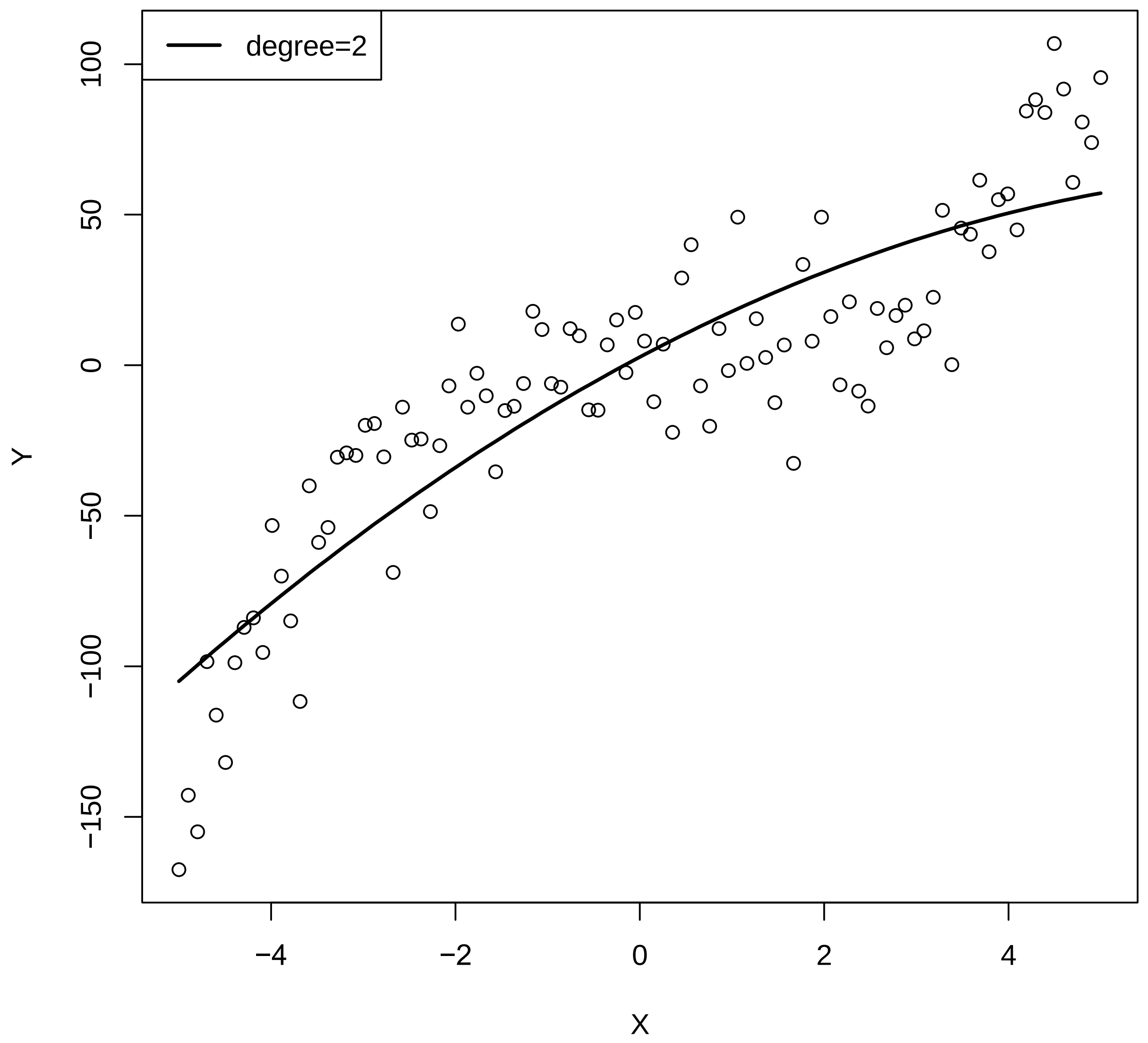
$$Y = \beta_0 + \sum_{i=1}^{d} \beta_i X^i + \varepsilon$$

we can run multiple linear regression with

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^d \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_1 & x_N^2 & \dots & x_N^d \end{bmatrix}$$

What's the best choice for *d* ?

What makes a model good?



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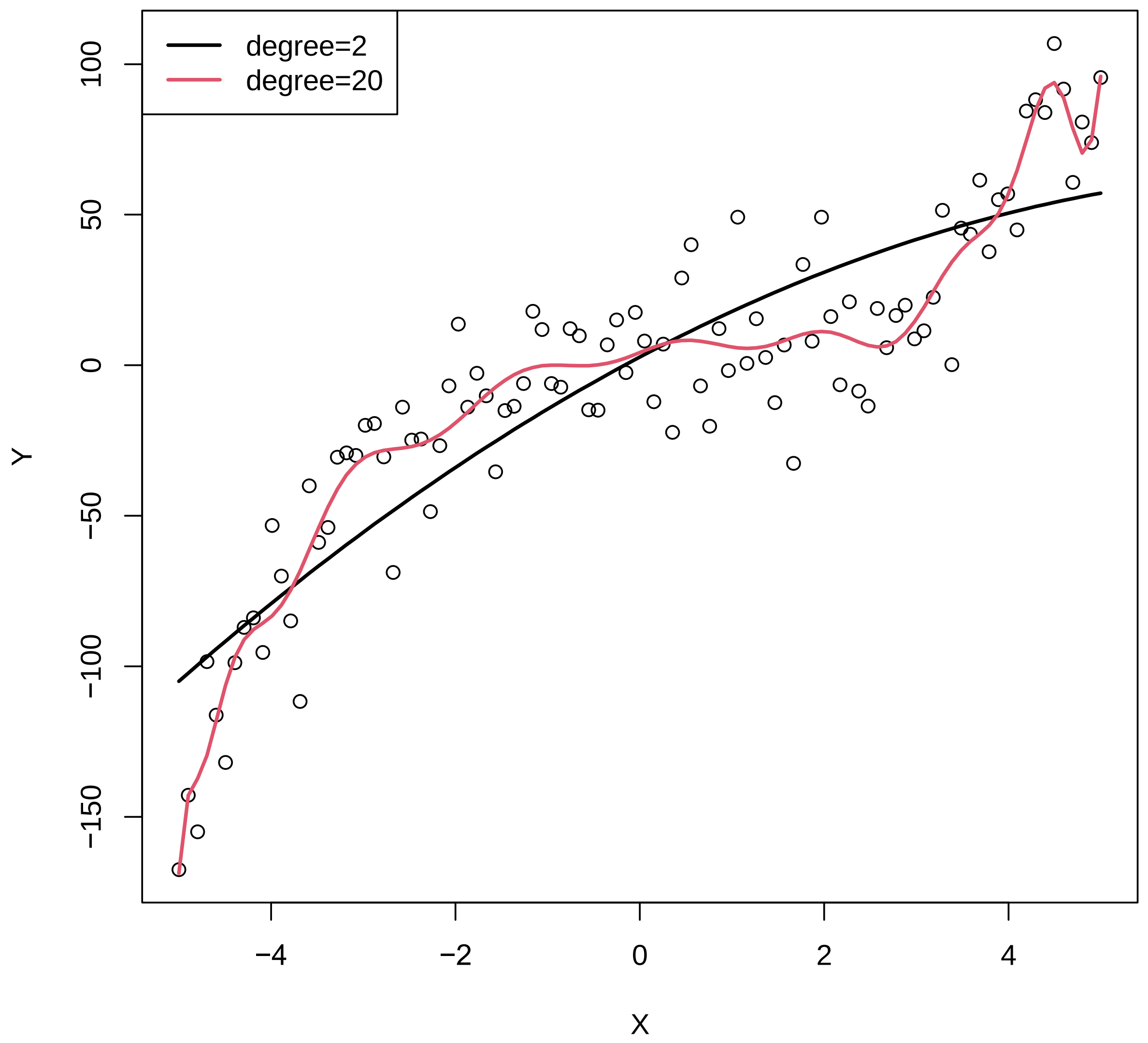

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What's the best choice for *d* ?

What makes a model good? – The generalization error

Remember that our goal in regression is to minimize the generalization error:

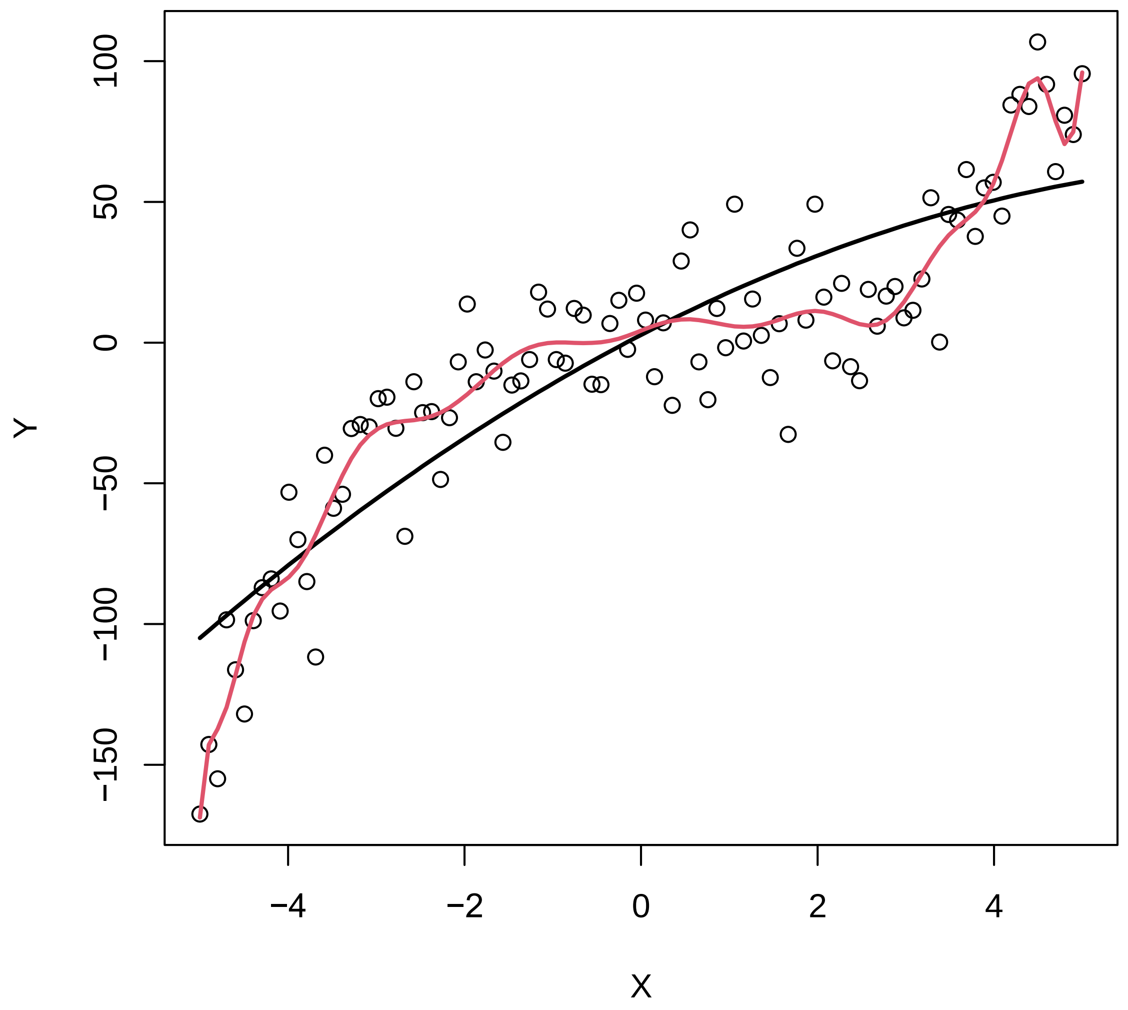
$$\boxed{\mathcal{L}(r) = \mathbb{E}_{Y,X}\left[\left(Y - r(X)\right)^2\right]}$$

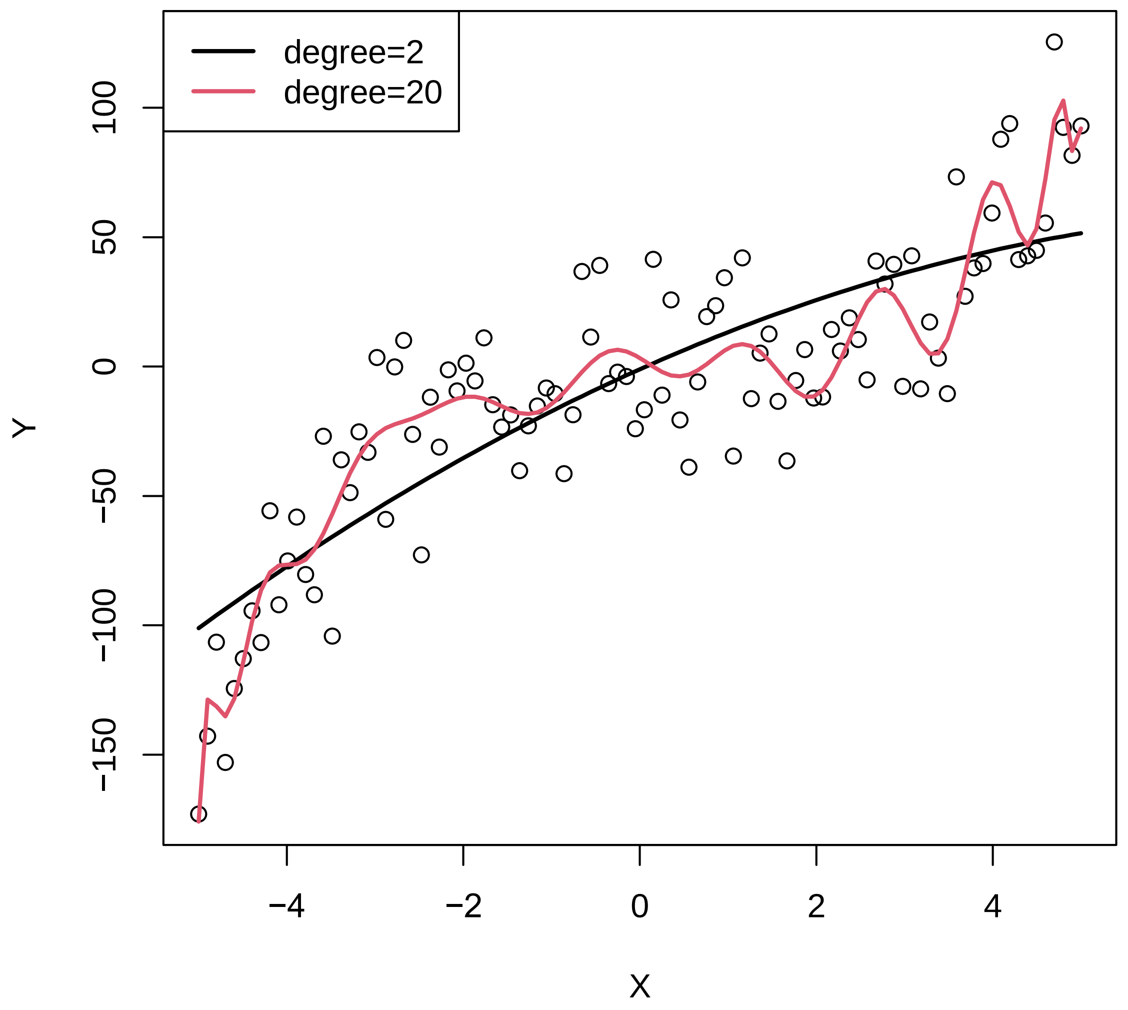
Intuitively, we can expect this error to be decomposed into a few informative parts:

- The **irreducible error**: can we ever predict Y from X with zero prediction error? Probably not, since we always assume having some observation error ε in the data model.
- The **estimation bias**: when estimating the conditional expectation, we always have to choose a family of approximators, which may not be sufficiently flexible.
- The **estimation variance**: for families of approximators that are too flexible, it might happen that for every small change in the observed data points, the estimates change a lot.

What makes a model good?

Estimation variance. The same model fit on two slightly different datasets.





What makes a model good?

What makes a model good? – The bias-variance tradeoff

Remember that the data model is assumed to be $Y = r(X) + \varepsilon$ with $\mathrm{Var}(\varepsilon) = \sigma^2$

We use a training dataset $\mathcal{D} = \left\{(y_i, x_i)\right\}_{i=1}^{i=N}$ to estimate $\hat{r}_{\mathcal{D}}$

For new observation x we write the bias-variance decomposition conditioned on x as

$$\begin{aligned}
\mathcal{L}\left(\hat{r}_{\mathcal{D}}(x)\right) &= \mathbb{E}_{Y,X}\left[\left(Y - \hat{r}_{\mathcal{D}}(X)\right)^2 \,\middle|\, X = x\right] \\
&= \mathbb{E}_{Y,X}\left[\left(Y - r(X) + r(X) - \hat{r}_{\mathcal{D}}(X)\right)^2 \,\middle|\, X = x\right] \\
&= \mathbb{E}_{Y,X}\left[\left(Y - r(X)\right)^2 \,\middle|\, X = x\right] + \mathbb{E}_{Y,X}\left[\left(r(X) - \hat{r}_{\mathcal{D}}(X)\right)^2 \,\middle|\, X = x\right] \\
&= \underbrace{\mathbb{E}_{Y,X}\left[\left(Y - r(X)\right)^2 \,\middle|\, X = x\right]}_{\text{Irreducible error } \sigma^2} + \underbrace{\left(\mathbb{E}_{Y,X}\left[r(X) - \hat{r}_{\mathcal{D}}(X) \,\middle|\, X = x\right]\right)^2}_{\text{Squared estimation bias}} + \underbrace{\mathrm{Var}\left(\hat{r}_{\mathcal{D}}(X) \,\middle|\, X = x\right)}_{\text{Estimation variance}}
\end{aligned}$$

- What makes a model **good**?
- ☞ Estimating the quality of a model
- Comparing and selecting models

Estimating the quality of a model

How can we estimate the generalization error of an approximator model in practice?

$$\mathcal{L}(\hat{r}_{\mathcal{D}}) = \mathbb{E}_{Y,X}\left[\Big(Y - \hat{r}_{\mathcal{D}}(X)\Big)^2\right]$$

We don't know the $p(Y, X)$

Estimating the quality of a model

How can we estimate the generalization error of an approximator in practice?

$$\mathcal{L}(\hat{r}_{\mathcal{D}}) = \mathbb{E}_{Y,X}\left[\Big(Y - \hat{r}_{\mathcal{D}}(X)\Big)^2\right] \approx \underline{\frac{1}{M}\sum_{i=1}^{M}\Big(y_i - \hat{r}_{\mathcal{D}}(x_i)\Big)^2} = L(\hat{r}_{\mathcal{D}}, \mathcal{X}) \quad \text{with} \quad \mathcal{X} = \Big\{(y_i, x_i)\Big\}_{i=1}^{i=M}$$

We don't know the $p(Y,X)$

So we approximate it with M data points

Note that for $\mathcal{D} = \Big\{(y_i, x_i)\Big\}_{i=1}^{i=N}$ we have $\hat{r}_{\mathcal{D}} = \underset{r \in \mathcal{F}}{\operatorname{argmin}}\ L(r, \mathcal{D})$

We want to minimize one quantity but can only estimate a proxy of it

One-slide reminder of the law of large numbers (LLN)

Whenever we want to approximate an expectation, we can use the LLN

$$\mathbb{E}_X\left[f(X)\right] = \int f(x)p(x)\mathrm{d}x \approx \frac{1}{N}\sum_{n=1}^{N} f(x_i)$$

with N **independent** and identically distributed samples $x_i \sim p(x)$

This result will be useful many times in our class and is ubiquitous in machine learning

Approximate weighted integral $\longleftrightarrow$ **Average of random IID samples**

This is also used in computer graphics, statistical physics, econometry, etc.

Estimating the quality of a model

How can we estimate the generalization error of an approximator in practice?

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Question: Can we say that $\mathcal{L}(\hat{r}_{\mathcal{D}}) \approx L(\hat{r}_{\mathcal{D}}, \mathcal{D})$?

ABSOLUTELY NOT!

In fact $\mathcal{L}(\hat{r}_{\mathcal{D}}) \geq L(\hat{r}_{\mathcal{D}}, \mathcal{D})$ i.e. the true generalization error is larger than the estimated one

The optimism of the training error

Different ways of seeing the problem:

- Intuitively, since $\hat{r}_{\mathcal{D}} = \underset{r \in \mathcal{F}}{\operatorname{argmin}}\ L(r, \mathcal{D})$ then $L(\hat{r}_{\mathcal{D}}, \mathcal{D})$ will always look small…

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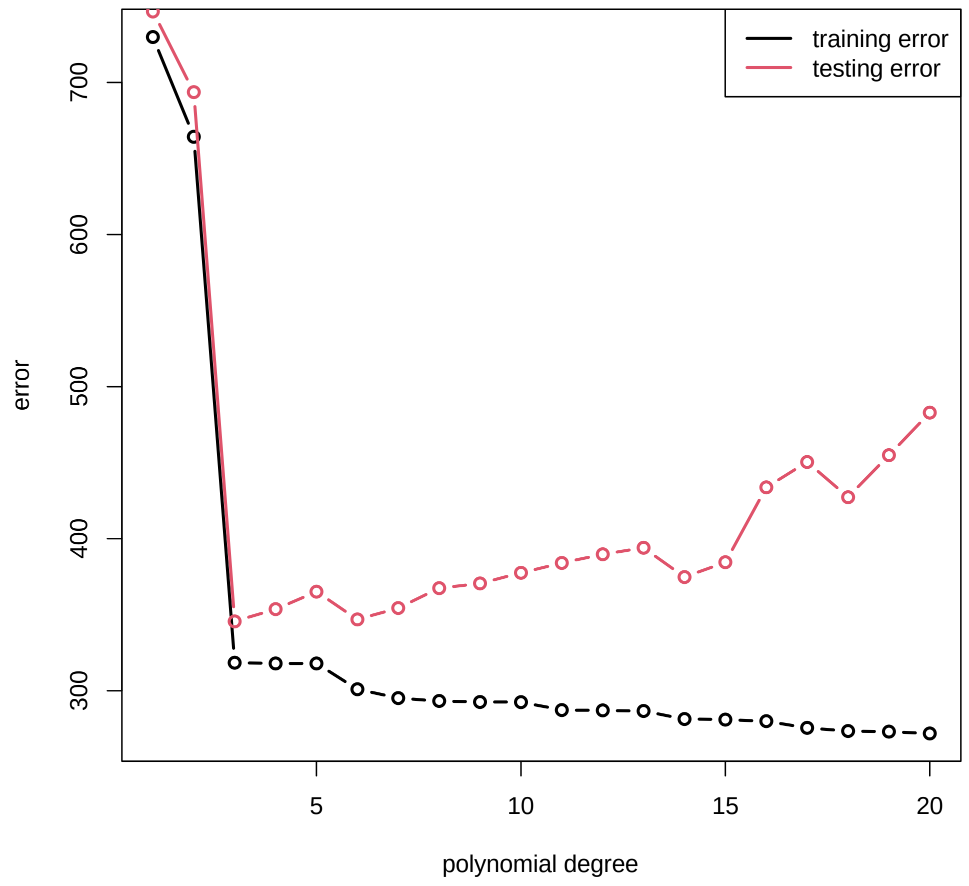
- Consider our example with polynomials
  - Increasing the degree improves training error
  - But the testing error grows!

$L(\hat{r}_{\mathcal{D}}, \mathcal{D})$ is the **training** error

$L(\hat{r}_{\mathcal{D}}, \mathcal{X})$ with $\mathcal{X} \neq \mathcal{D}$ is the **testing** error

Error on unseen data



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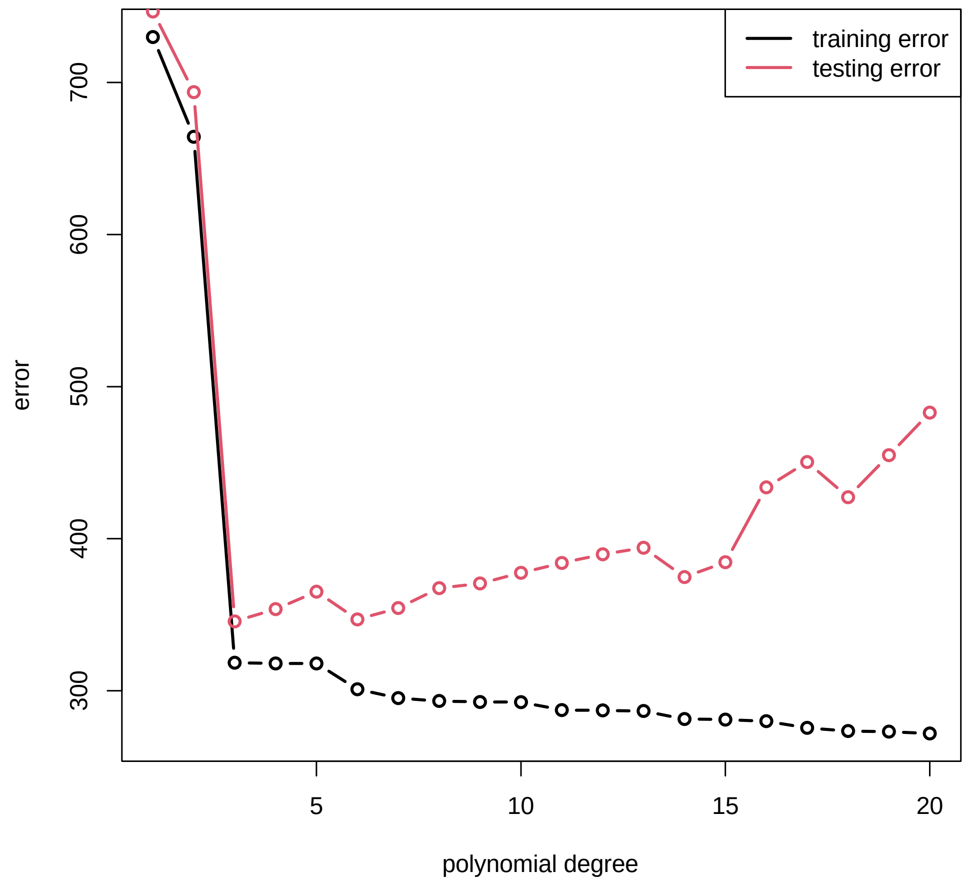
- Consider our example with polynomials
  - Increasing the degree improves training error
  - But the testing error grows!
- Mathematical illustration on linear regression

$$\mathcal{D} = \left\{(x_i, y_i)\right\}_{i=1}^{i=N} \quad \mathcal{D}' = \left\{(x_i, y_i')\right\}_{i=1}^{i=N} \quad Y = \beta_0 + \sum_{k=1}^{p} \beta_k X_k + \varepsilon$$

(same predictors but different observations because of noise)

$$\mathbb{E}\Big[L(\hat{r}_{\mathcal{D}}, \mathcal{D}')\Big] = \mathbb{E}\Big[L(\hat{r}_{\mathcal{D}}, \mathcal{D})\Big] + \frac{2}{N}\sigma^2(p+1)$$



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2 We train regressor on $\mathcal{D}$ that minimizes

$$\hat{r}_{\mathcal{D}} = \underset{r \in \mathcal{H}}{\operatorname{argmin}} \; \frac{1}{N} \sum_{i=1}^{N} \Big(y_i - r(x_i) \Big)^2$$

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$$\mathcal{L}(\hat{r}_{\mathcal{D}}) = \mathbb{E}_{(X,Y)}\Big[\Big(Y - \hat{r}_{\mathcal{D}}(X)\Big)^2\Big]$$

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4 But we can only obtain an approximation

$$L(\hat{r}_{\mathcal{D}}, \mathcal{X}) = \frac{1}{M} \sum_{i=1}^{M} \Big(y_i - \hat{r}_{\mathcal{D}}(x_i)\Big)^2$$

such that
$$\mathcal{X} = \{x_i, y_i\}_{i=1}^{M}$$
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such that $\mathcal{X} = \{x_i, y_i\}_{i=1}^{M}$, $(x_i, y_i) \sim p(x, y)$

! Beware the optimism of training error!

$$\underline{L(\hat{r}_{\mathcal{D}}, \mathcal{D})} \leq L(\hat{r}_{\mathcal{D}}, \mathcal{X})$$

This was the criterion used during the training

The optimism of the training error

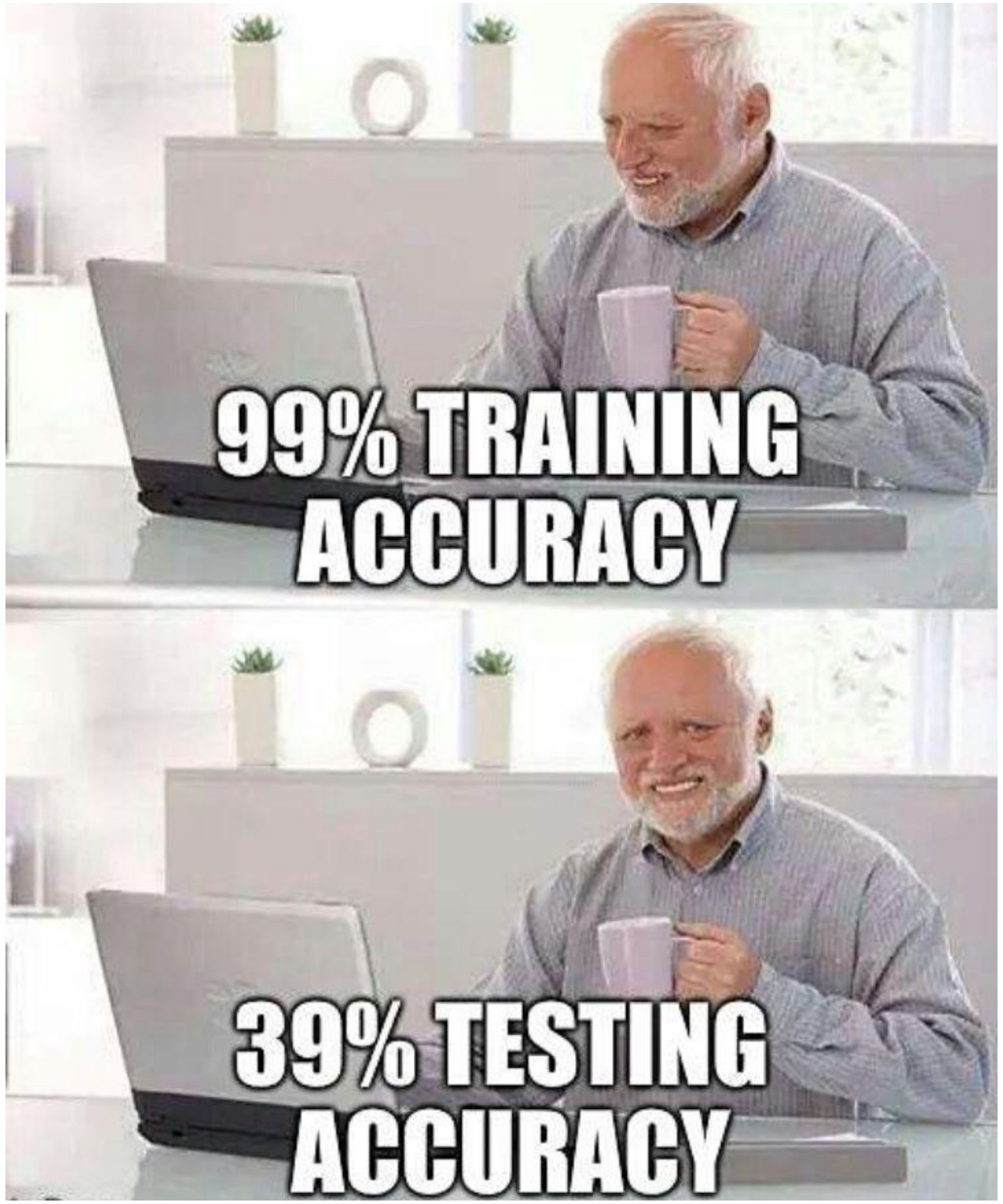
Conclusion:

- We can only know if a model is good or not if we **correctly evaluate** its performance

- The objective function that we minimize when training a model (**training error**) is never the same as the one we are actually interested in minimizing (**test error**)

$$\hat{r}_{\mathcal{D}} = \underset{r \in \mathcal{F}}{\operatorname{argmin}} \frac{1}{M} \sum_{i=1}^{M} \Big(y_i - r(x_i)\Big)^2$$

$$\mathcal{L}(\hat{r}_{\mathcal{D}}) = \mathbb{E}_{(X,Y)}\left[\Big(Y - \hat{r}_{\mathcal{D}}(X)\Big)^2\right]$$



Cross-validation

We are given a dataset with N datapoints $\mathcal{D} = \left\{(y_i, x_i)\right\}_{i=1}^{i=N}$

How can we estimate the **generalization error** of a model we train on this dataset?

Remember: We should evaluate the model on samples that were not used for training

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- **Strategy 1 : Single hold-out test point**

We fit a model on the first N-1 training samples, calling it $\hat{r}^{(-N)}$

Treat the last sample (X_N, Y_N) as a test sample and estimate generalization error as

$$\mathcal{L}(\hat{r}) \approx \left(y_N - \hat{r}^{(-N)}(x_N)\right)^2$$

The estimator is easy to calculate but we can expect a rather large variance.

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- **Strategy 2 : Leave one out cross-validation (LOOCV)**

We fit N models on N-1 training samples, holding out x_i at each time to get $\hat{r}^{(-i)}$

The test error is approximate as

$$\mathcal{L}(\hat{r}) \approx \frac{1}{N} \sum_{i=1}^{N} \left(y_i - \hat{r}^{(-i)}(x_i)\right)^2$$

The variance decreases, but the computational burden is much higher

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How can we estimate the **generalization error** of a model we train on this dataset?

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- **Strategy 3 : K-Fold cross-validation**

Split the training dataset randomly into K folds so to have $\mathcal{D}_1 \cup \cdots \cup \mathcal{D}_K = \mathcal{D}$

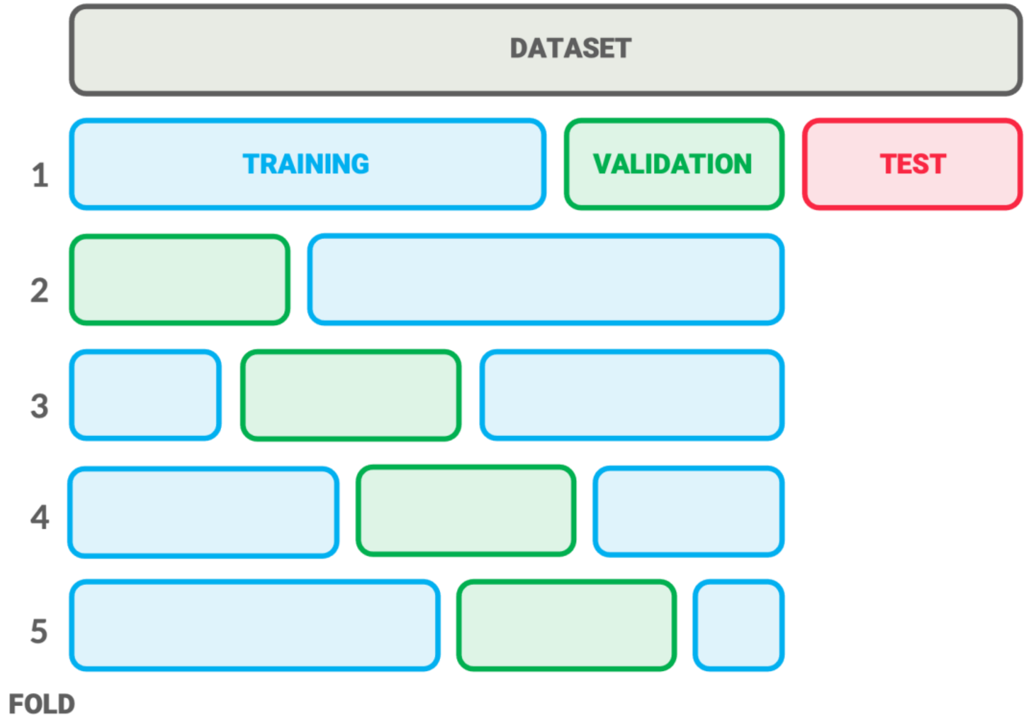
For k=1,...,K fit a model $\hat{r}^{(-k)}$ on a training set except that excludes $\mathcal{D}_k$

$$\mathcal{L}(\hat{r}) \approx \frac{1}{K} \underbrace{\sum_{k=1}^{K}}_{\text{Take average over folds}} \left(\underbrace{\frac{1}{N_k} \sum_{i \in \mathcal{D}_k} \Big(y_i - \hat{r}^{(-k)}(x_i) \Big)^2}_{\text{Estimate test error for each fold}} \right)$$

Cross-validation

Strategy 3 : K-Fold cross-validation

Note that the errors calculated in each fold are not IID random variables, since the models share some of their data points.
↳ **Question:** What does this imply?



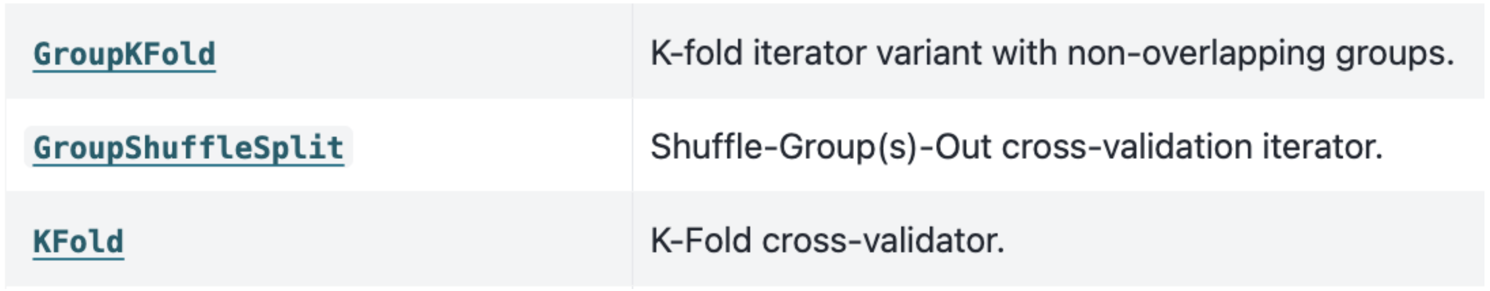
Using scikit learn

```
from sklearn.model_selection import KFold
from sklearn.datasets import fetch_california_housing
from sklearn.linear_model import LinearRegression
kf = KFold(n_splits=5)
dataset = fetch_california_housing()
lm = LinearRegression()
X = dataset.data
y = dataset.target
scores = []
for idx_train, idx_test in kf.split(X):
    X_train, y_train = X[idx_train], y[idx_train]
    X_test, y_test = X[idx_test], y[idx_test]
    lm.fit(X_train, y_train)
    scores.append(lm.score(X_test, y_test))
print(np.mean(scores))
```

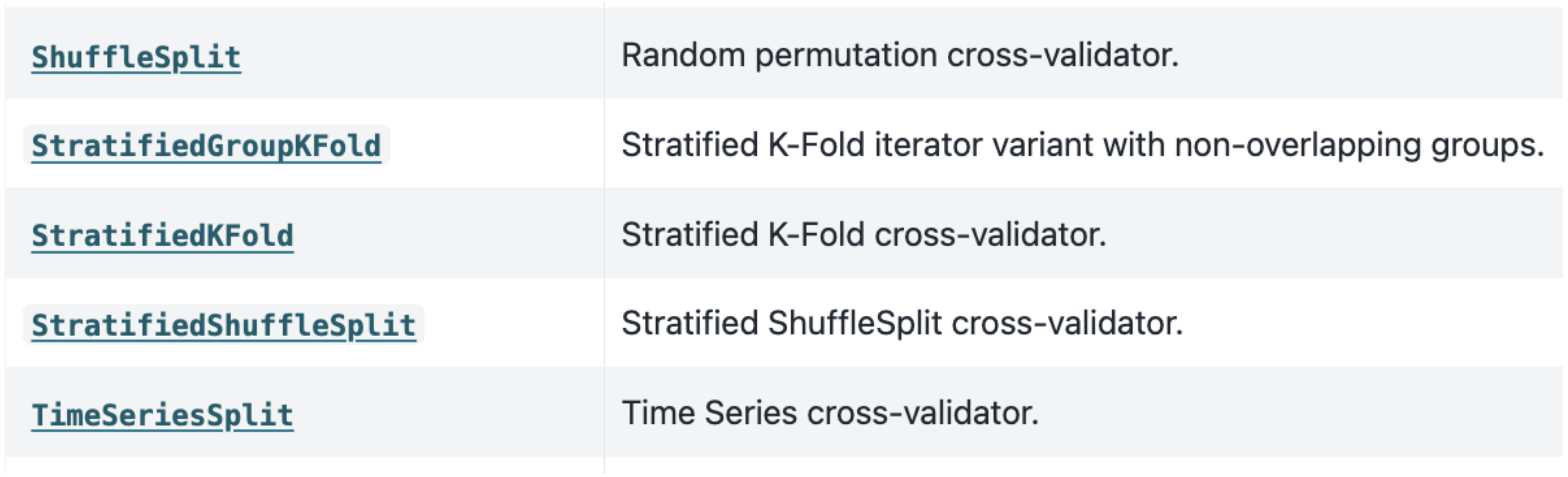
See the documentation for more details

Cross-validation

But there are **several** other strategies!



GroupKFold	K-fold iterator variant with non-overlapping groups.
GroupShuffleSplit	Shuffle-Group(s)-Out cross-validation iterator.
KFold	K-Fold cross-validator.

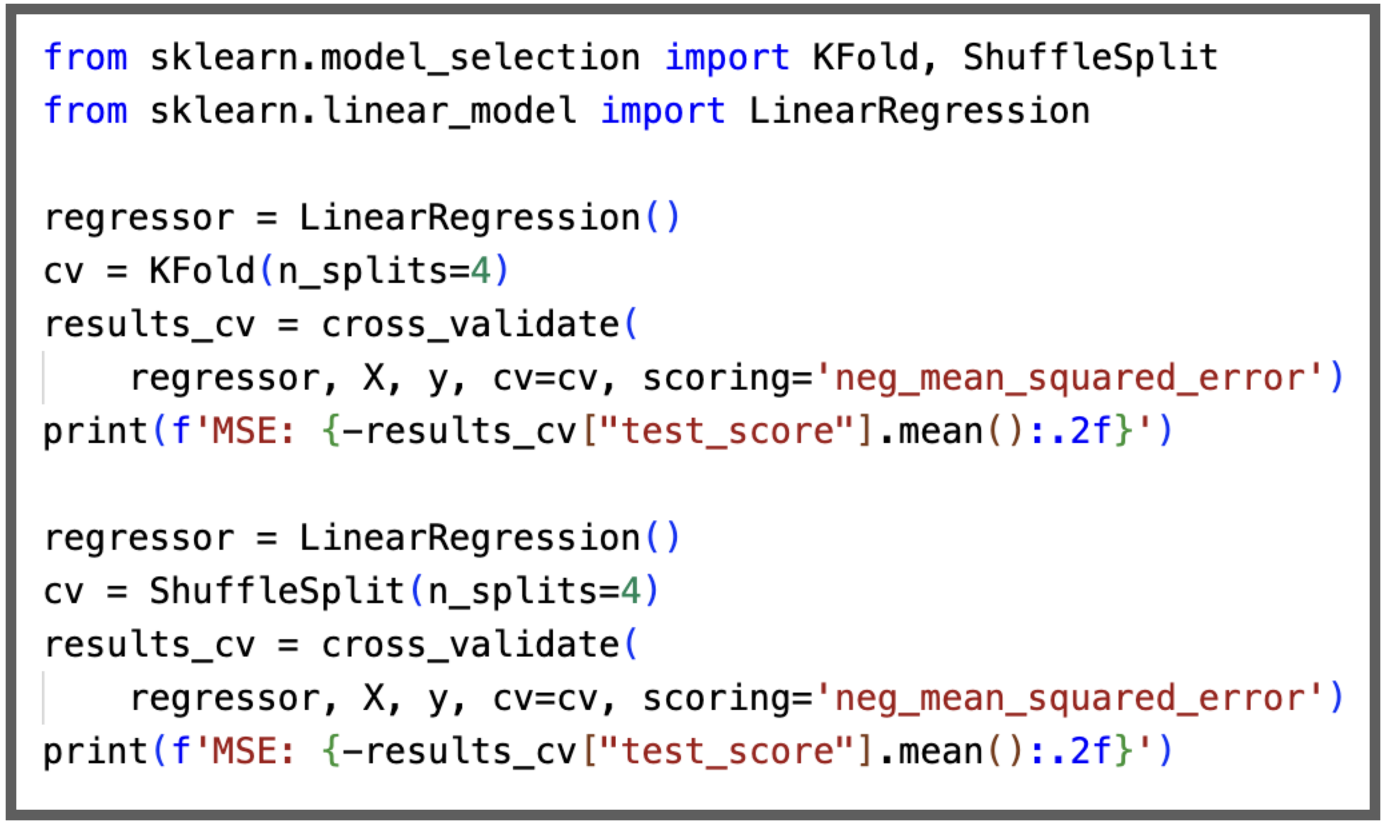


ShuffleSplit	Random permutation cross-validator.
StratifiedGroupKFold	Stratified K-Fold iterator variant with non-overlapping groups.
StratifiedKFold	Stratified K-Fold cross-validator.
StratifiedShuffleSplit	Stratified ShuffleSplit cross-validator.
TimeSeriesSplit	Time Series cross-validator.

and more…

Cross-validation

(1) Example with the **categorical variables** from last week



```python
from sklearn.model_selection import KFold, ShuffleSplit
from sklearn.linear_model import LinearRegression

regressor = LinearRegression()
cv = KFold(n_splits=4)
results_cv = cross_validate(
    regressor, X, y, cv=cv, scoring='neg_mean_squared_error')
print(f'MSE: {-results_cv["test_score"].mean():.2f}')

regressor = LinearRegression()
cv = ShuffleSplit(n_splits=4)
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```
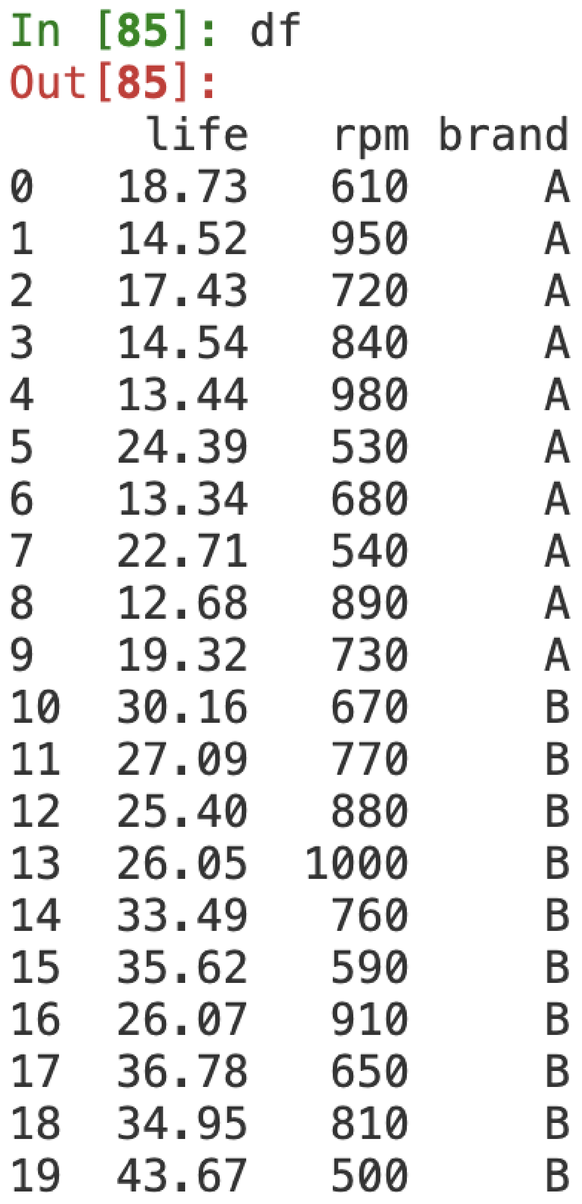

17.50

4.60

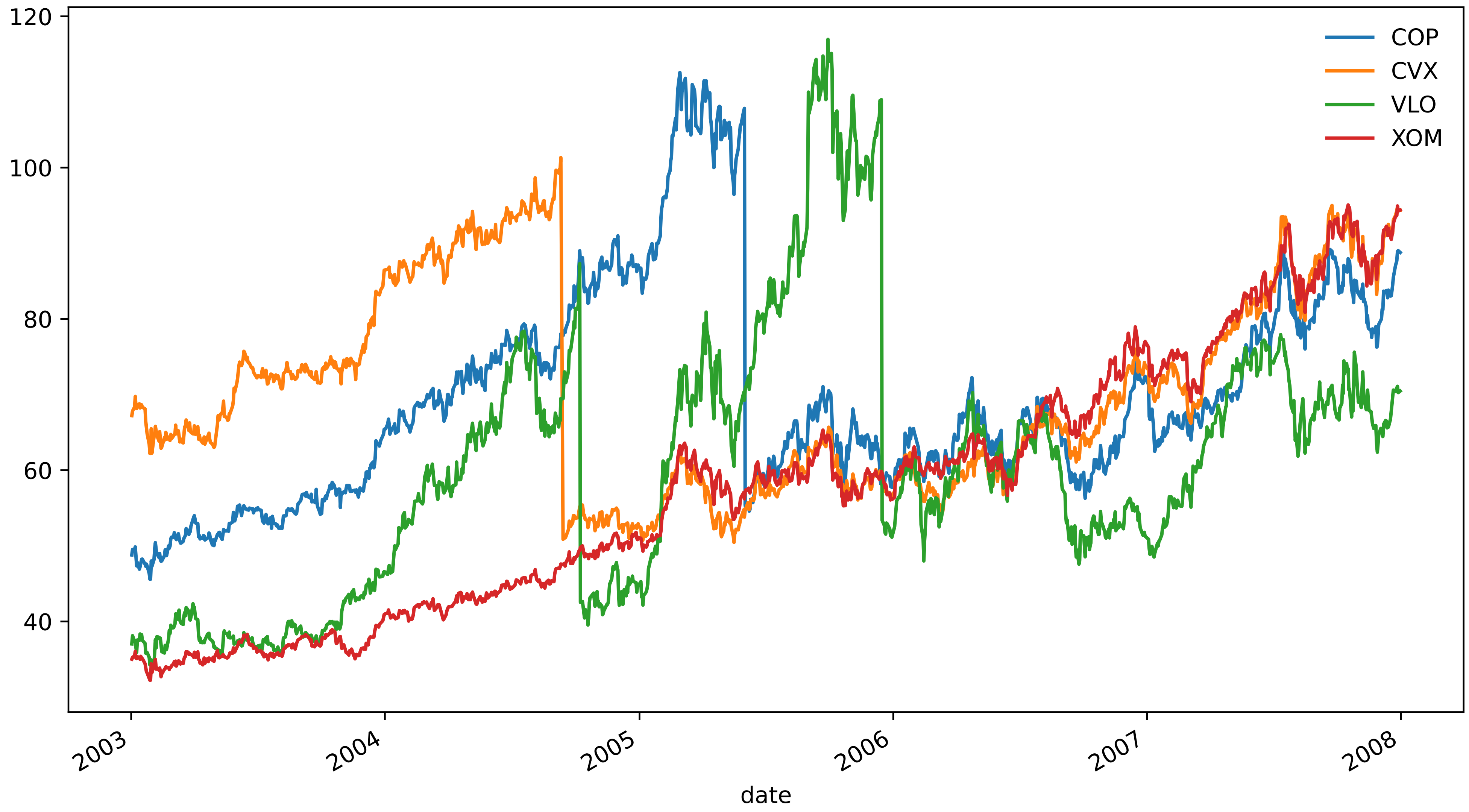


```
In [85]: df
Out[85]:
     life   rpm brand
0   18.73   610     A
1   14.52   950     A
2   17.43   720     A
3   14.54   840     A
4   13.44   980     A
5   24.39   530     A
6   13.34   680     A
7   22.71   540     A
8   12.68   890     A
9   19.32   730     A
10  30.16   670     B
11  27.09   770     B
12  25.40   880     B
13  26.05  1000     B
14  33.49   760     B
15  35.62   590     B
16  26.07   910     B
17  36.78   650     B
18  34.95   810     B
19  43.67   500     B
```

What is going on? 😅

Cross-validation

(2) Example with **financial** time series: predict CVX's quotes based on other quotes



Cross-validation

(2) Example with **financial** time series: predict CVX's quotes based on other quotes

```python
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.model_selection import ShuffleSplit, cross_validate
X = quotes.drop(columns=["CVX"])
y = quotes["CVX"]
regressor = GradientBoostingRegressor()
cv = ShuffleSplit(n_splits=10)
results_cv = cross_validate(regressor, X, y, cv=cv)
print(f'Mean R2: {results_cv["test_score"].mean():.2f}')
```

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

0.95

This looks like an almost perfect prediction! Does it sound right to you?

Cross-validation

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0.95

This looks like an almost perfect prediction! Does it sound right to you?

```python
from sklearn.model_selection import TimeSeriesSplit
cv = TimeSeriesSplit(n_splits=10)
results_cv = cross_validate(regressor, X, y, cv=cv)
print(f'Mean R2: {results_cv["test_score"].mean():.2f}')
```

-3.10

Disappointing, but closer to reality…

Cross-validation

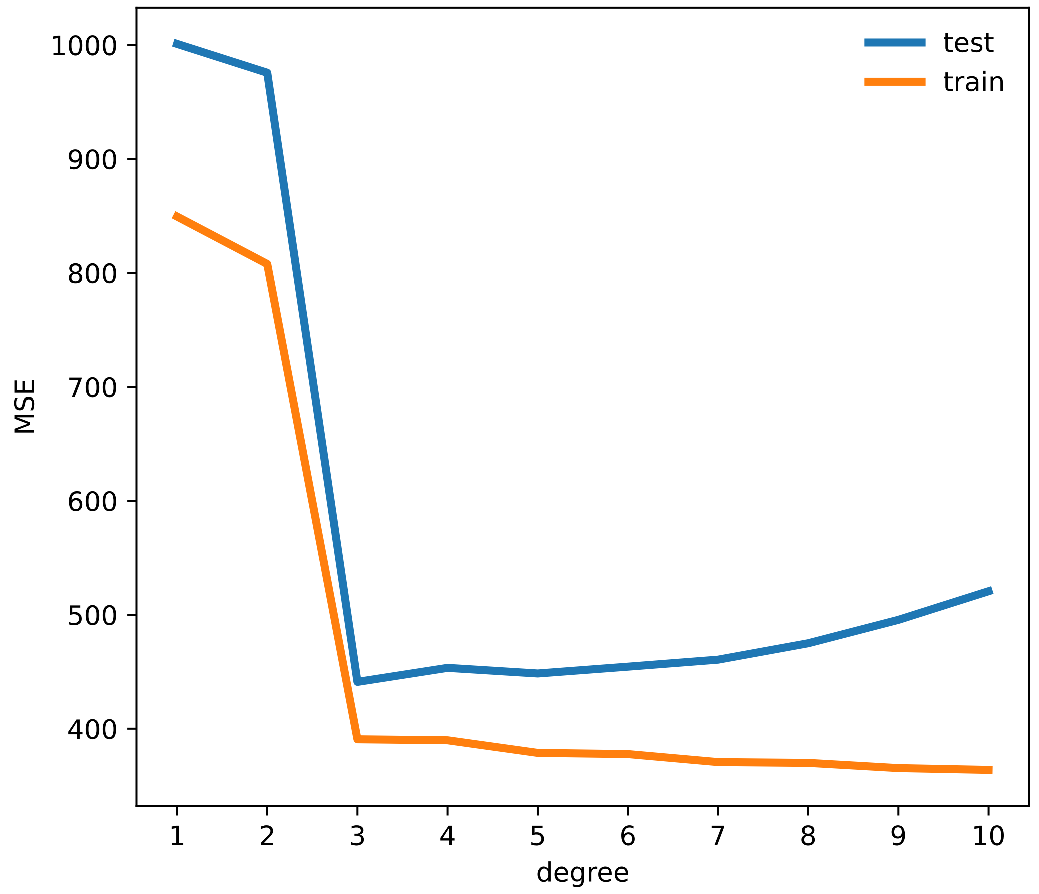
(3) Choosing the best order for the polynomial approximating a dataset

```python
import matplotlib.pyplot as plt
import numpy as np
from sklearn.preprocessing import PolynomialFeatures
from sklearn.pipeline import make_pipeline
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import GridSearchCV, ShuffleSplit

np.random.seed(6)

# generate dataset
N = 100
x = np.linspace(-5, +5, N)
y = x - x**2 + x**3 + 20 * np.random.randn(N)
X = x.reshape(-1, 1)

# instantiate pipeline
poly = PolynomialFeatures(include_bias=False)
lr = LinearRegression()
pipe = make_pipeline(poly, lr)

# instantiate grid search cv
degrees_array = np.arange(1, 10+1)
parameters = {'polynomialfeatures__degree':degrees_array}
cv = ShuffleSplit(n_splits=10)
est = GridSearchCV(estimator=pipe, param_grid=parameters, cv=cv,
                   scoring='neg_mean_squared_error', return_train_score=True)

# get cv results
est.fit(X, y)
cv_test_scores = -est.cv_results_['mean_test_score']
cv_train_scores = -est.cv_results_['mean_train_score']

# plot results
fig, ax = plt.subplots(figsize=(6, 5.4))
ax.plot(degrees_array, cv_test_scores, c='C0', lw=3, label='test')
ax.plot(degrees_array, cv_train_scores, c='C1', lw=3, label='train')
ax.set_xlabel('degree')
ax.set_ylabel('MSE')
ax.set_xticks(degrees_array)
fig.savefig('CM3_cv_figure.pdf', format='pdf')
```

We're using several scikit-learn important concepts : transformers, pipelines, grid search

Cross-validation

(3) Choosing the best order for the polynomial approximating a dataset



We're using several scikit-learn important concepts : transformers, pipelines, grid search

- What makes a model **good**?
- Estimating the quality of a model
- ☞ Comparing and selecting models

Comparing and selecting models

Suppose we are given a dataset with *p* predictors.

We want to estimate a linear model with only a subset of them.

There are mainly **three strategies** for doing this properly:

- **Shrinkage** fits a model with all p predictors but using a modified loss function that drives some parameters to zero automatically. (Razan will talk about this)
- We can use **dimensionality reduction** techniques to project the *p* predictors to a lower-dimensional subspace. (We will see how to do this in CM4 and TP2)
- In **subset selection** we identify a subset of the predictors that seems the most adequate and then fit a model with them.

Comparing and selecting models

When p is large, testing all 2^p possible models can be very time consuming…

So we prefer to proceed greedily with e.g. **forward stepwise selection**

(1) Let $\mathcal{M}_0$ denote a model with no predictors (i.e. just the intercept)

(2) For $k = 0, \ldots, p-1$

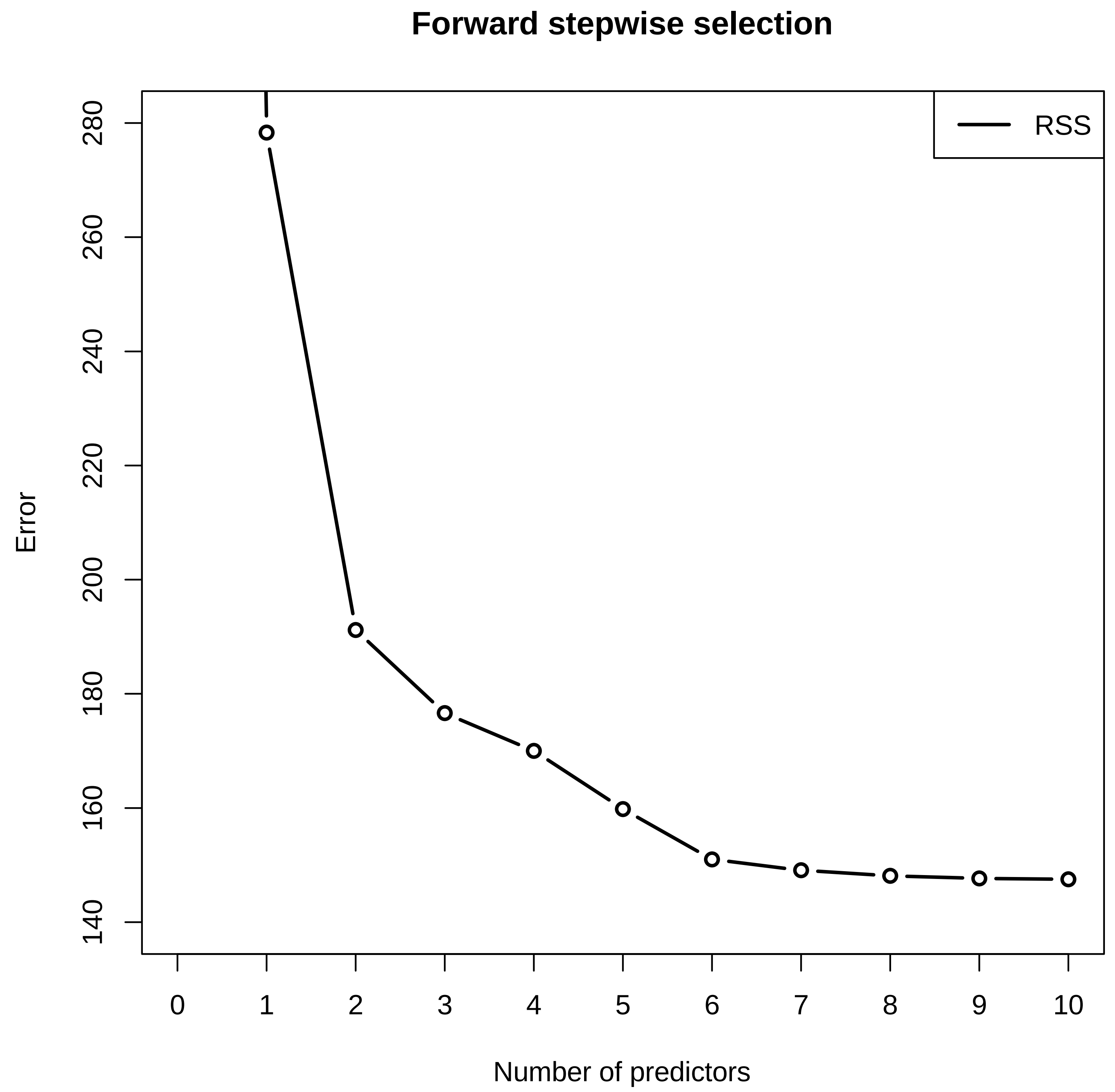
- **(a)** Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$ by one extra predictor
- **(b)** Choose the **best** among these $p-k$ models and call it $\mathcal{M}_{k+1}$

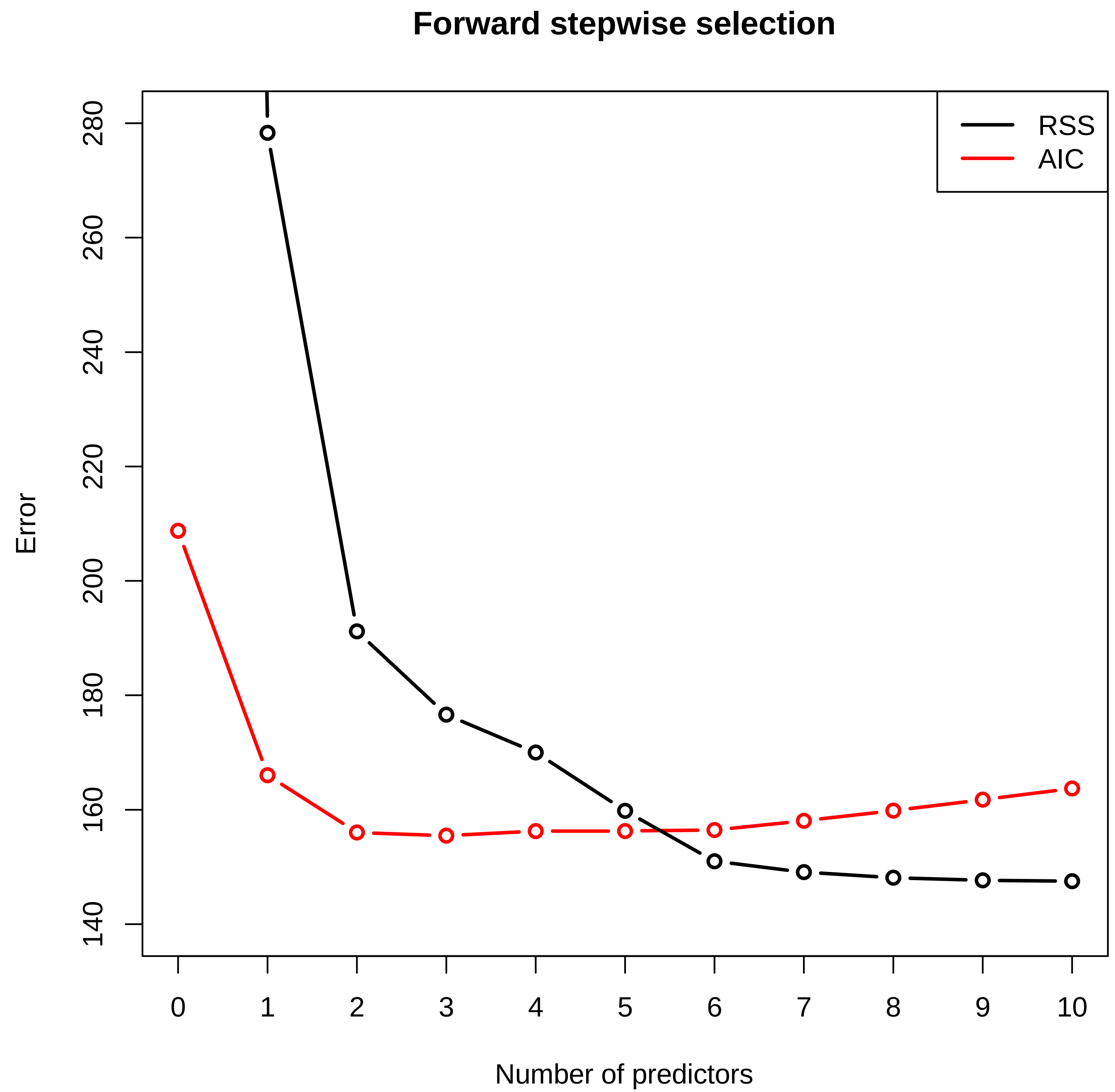
(3) Select single **best** model among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error

Example: Consider the mtcars dataset – we want to predict **mpg**

```
Description:

     The data was extracted from the 1974 _Motor Trend_ US magazine,
     and comprises fuel consumption and 10 aspects of automobile design
     and performance for 32 automobiles (1973-74 models).

Format:

     A data frame with 32 observations on 11 variables.

       [, 1]  mpg   Miles/(US) gallon
       [, 2]  cyl   Number of cylinders
       [, 3]  disp  Displacement (cu.in.)
       [, 4]  hp    Gross horsepower
       [, 5]  drat  Rear axle ratio
       [, 6]  wt    Weight (lb/1000)
       [, 7]  qsec  1/4 mile time
       [, 8]  vs    V/S
       [, 9]  am    Transmission (0 = automatic, 1 = manual)
       [,10]  gear  Number of forward gears
       [,11]  carb  Number of carburetors
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    mpg   R-squared:                       0.869
Model:                            OLS   Adj. R-squared:                  0.807
Method:                 Least Squares   F-statistic:                     13.93
Date:                Fri, 27 Dec 2024   Prob (F-statistic):           3.79e-07
Time:                        15:09:11   Log-Likelihood:                -69.855
No. Observations:                  32   AIC:                             161.7
Df Residuals:                      21   BIC:                             177.8
Df Model:                          10
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
cyl           -0.1114      1.045     -0.107      0.916      -2.285       2.062
disp           0.0133      0.018      0.747      0.463      -0.024       0.050
hp            -0.0215      0.022     -0.987      0.335      -0.067       0.024
drat           0.7871      1.635      0.481      0.635      -2.614       4.188
wt            -3.7153      1.894     -1.961      0.063      -7.655       0.224
qsec           0.8210      0.731      1.123      0.274      -0.699       2.341
vs             0.3178      2.105      0.151      0.881      -4.059       4.694
am             2.5202      2.057      1.225      0.234      -1.757       6.797
gear           0.6554      1.493      0.439      0.665      -2.450       3.761
carb          -0.1994      0.829     -0.241      0.812      -1.923       1.524
intercept     12.3034     18.718      0.657      0.518     -26.623      51.229
==============================================================================
```


Forward stepwise selection
RSS
Error
280
260
240
220
200
180
160
140
0
1
2
3
4
5
6
7
8
9
10
Number of predictors


Forward stepwise selection
RSS
AIC
Error
280
260
240
220
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0
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5
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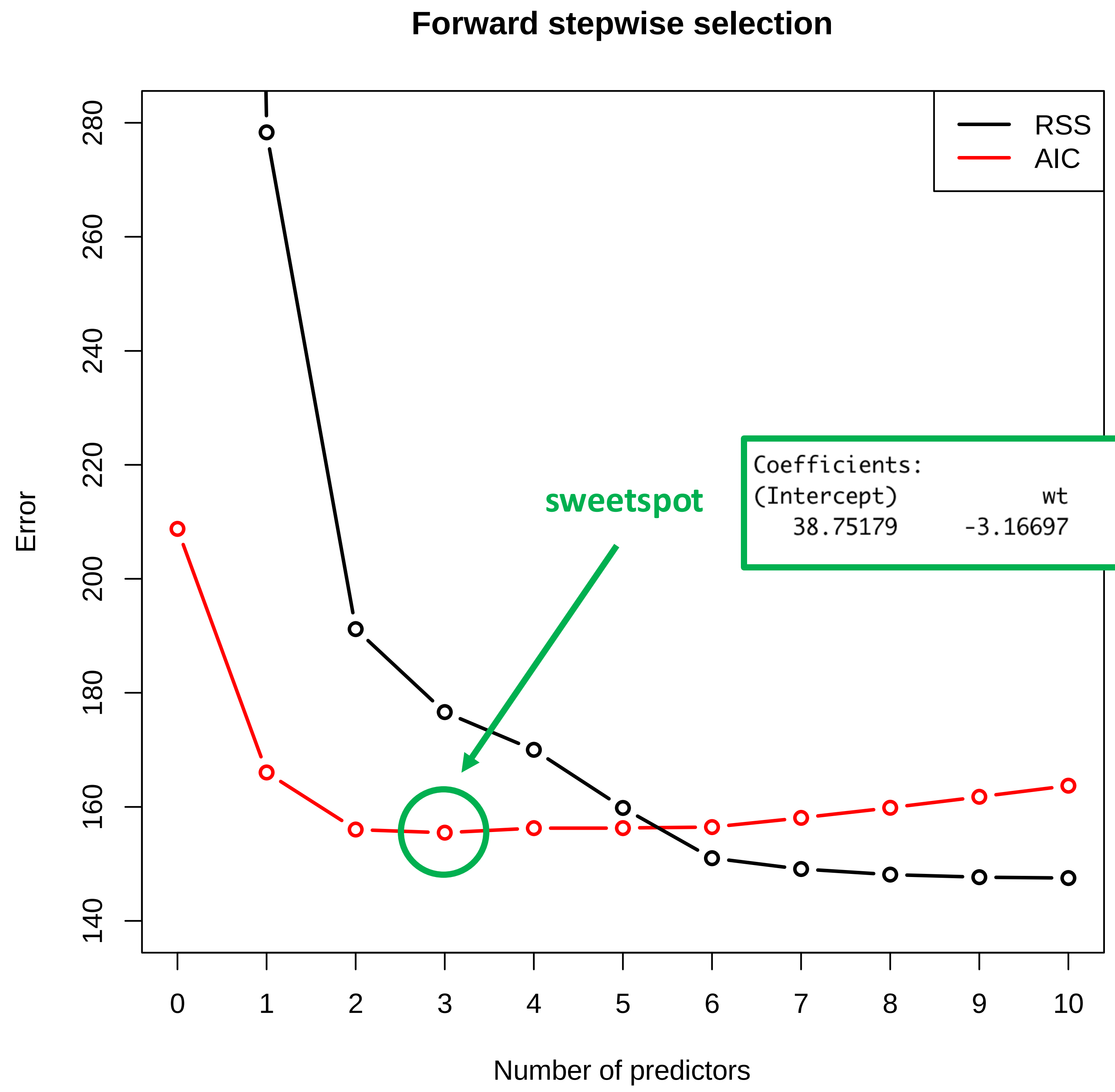
Number of predictors



```
Coefficients:
(Intercept)           wt          cyl           hp
   38.75179     -3.16697     -0.94162     -0.01804
```

Reminder

We have a TD this Friday at 17h00 !