# Overfitting and Cross validation Part 1

#### **COMPLEXITY AND OVERFITTING**

# MODEL COMPLEXITY

- A model becomes more complex if new terms are included (polynomial terms, interactions, nonlinear terms, etc.)
- Adding complexity helps the model to identify new patterns useful for prediction
- We should increase the model complexity but not beyond the point where the model starts overfitting

#### **COMPLEXITY AND OVERFITTING**

# UNDERFITTING

The model has not yet identified all important patterns from the training data set

# OVERFITTING

The model has started to learn patterns that are specific to the training data but not to new data sets



# Example 1 Polynomial Regression

#### **EXAMPLE 1**

The Auto.csv file contains information about 392 cars

- mpg (miles per gallon)
- cylinders (between 4 and 8 cylinders)
- displacement (engine displacement in cubic inches)
- horsepower (engine horsepower)
- weight (pounds)
- acceleration (number of seconds to accelerate from 0 to 69 mph)
- year (Model year)
- origin (1. American, 2. European, 3. Japanese)
- name (vehicle name)

#### **EXAMPLE 1**

The Auto.csv file contains the following information about 392 cars

- mpg (miles per gallon)
- cylinders (between 4 and 8 cylinders)
- displacement (engine displacement in cubic inches)
- horsepower (engine horsepower)
- weight (pounds)
- acceleration (number of seconds to accelerate from 0 to 69 mph)
- year (Model year)
- origin (1. American, 2. European, 3. Japanese)
- name (vehicle name)

Use cross validation to find the best polynomial model to predict the car's mileage (mpg) using predictor horsepower

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import PolynomialFeatures

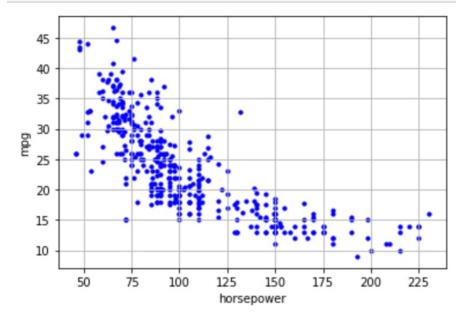
auto = pd.read_csv('Auto.csv')
auto[:5]
```

	mpg	cylinders	displacement	horsepower	weight	acceleration	year	origin	name
0	18.0	8	307.0	130	3504	12.0	70	1	chevrolet chevelle malibu
1	15.0	8	350.0	165	3693	11.5	70	1	buick skylark 320
2	18.0	8	318.0	150	3436	11.0	70	1	plymouth satellite
3	16.0	8	304.0	150	3433	12.0	70	1	amc rebel sst
4	17.0	8	302.0	140	3449	10.5	70	1	ford torino

What polynomial degree best predicts the data?

```
hp = auto.horsepower
mpg = auto.mpg
```

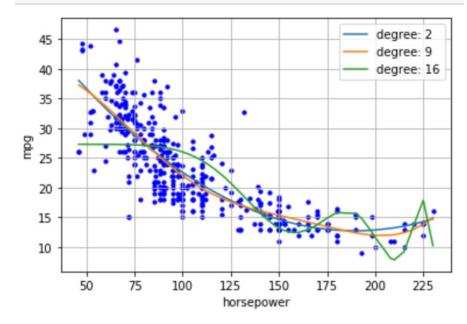
```
plt.scatter(hp,mpg,c='b',s=10)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



What polynomial degree best predicts the data?

```
hp = auto.horsepower
mpg = auto.mpg
```

```
plt.scatter(hp,mpg,c='b',s=10)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



# **POLYNOMIAL REGRESSION – LINEAR MODEL**

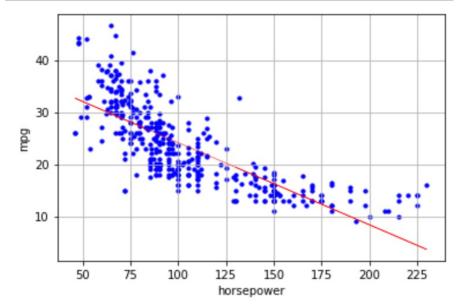
```
hp = auto.horsepower
mpg = auto.mpg
# predictors must be an array
# (not vector or series)
hp.shape
(392,)
hp1 = hp.values.reshape(-1,1)
hp1.shape
(392, 1)
hp1[:5]
array([[130],
       [165],
      [150],
       [150],
       [140]])
```

# **POLYNOMIAL REGRESSION – LINEAR MODEL**

```
hp = auto.horsepower
mpg = auto.mpg
# predictors must be an array
# (not vector or series)
hp.shape
(392,)
hp1 = hp.values.reshape(-1,1)
hp1.shape
(392, 1)
hp1[:5]
array([[130],
       [165],
       [150],
       [150],
       [140]])
```

```
model1 = LinearRegression().fit(hp1,mpg)
yhat = model1.predict(hp1)
```

```
plt.scatter(hp,mpg,c='b',s=10)
plt.plot(hp,yhat,c='r',lw=0.5)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



# **POLYNOMIAL REGRESSION – LINEAR MODEL**

```
hp = auto.horsepower
mpg = auto.mpg
# predictors must be an array
# (not vector or series)
hp.shape
(392,)
hp1 = hp.values.reshape(-1,1)
hp1.shape
(392, 1)
hp1[:5]
array([[130],
       [165],
       [150],
       [150],
       [140]])
```

```
model1 = LinearRegression().fit(hp1,mpg)
yhat = model1.predict(hp1)

plt.scatter(hp,mpg,c='b',s=10)
plt.plot(hp,yhat,c='r',lw=0.5)
plt.xlabel('horsepower')
```

plt.ylabel('mpg')

plt.grid()

```
linear model is underfitting the train dataset
```

```
hp1[:5]
array([[130],
       [165],
       [150],
       [150],
       [140]])
poly2 = PolynomialFeatures(degree=2)
hp2 = poly2.fit transform(hp1)
# hp2 is array (no need to reshape)
```

hp1[:5]

# **POLYNOMIAL REGRESSION – QUADRATIC MODEL**

```
array([[130],
       [165],
       [150],
       [150],
       [140]])
poly2 = PolynomialFeatures(degree=2)
hp2 = poly2.fit transform(hp1)
hp2[:5]
array([[1.0000e+00, 1.3000e+02, 1.6900e+04]
       [1.0000e+00, 1.6500e+02, 2.7225e+04]
       [1.0000e+00, 1.5000e+02, 2.2500e+04]
       [1.0000e+00, 1.5000e+02, 2.2500e+04]
       [1.0000e+00, 1.4000e+02, 1.9600e+04]
# hp2 is array (no need to reshape)
```

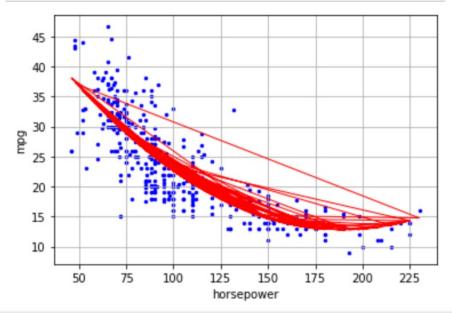
fit\_transform() adds a column of ones and a column of squared values to hp1

```
hp1[:5]
array([[130],
       [165],
       [150],
       [150],
       [140]])
poly2 = PolynomialFeatures(degree=2)
hp2 = poly2.fit transform(hp1)
hp2[:5]
array([[1.0000e+00, 1.3000e+02, 1.6900e+04]
       [1.0000e+00, 1.6500e+02, 2.7225e+04]
       [1.0000e+00, 1.5000e+02, 2.2500e+04]
       [1.0000e+00, 1.5000e+02, 2.2500e+04]
       [1.0000e+00, 1.4000e+02, 1.9600e+04]
# hp2 is array (no need to reshape)
```

```
0 1.0 130.0 16900.0
1 1.0 165.0 27225.0
2 1.0 150.0 22500.0
3 1.0 150.0 22500.0
4 1.0 140.0 19600.0
```

model2 = LinearRegression().fit(hp2,mpg)
yhat2 = model2.predict(hp2)

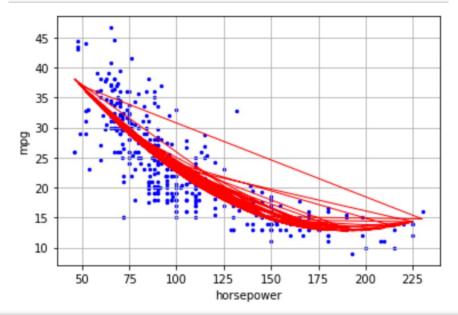
```
plt.scatter(hp,mpg,c='b',s=6)
plt.plot(hp,yhat2,c='r',lw=1)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



hp (and hp2) is not sorted.
Connecting unsorted points
yields this plot
(see previous slide)

```
model2 = LinearRegression().fit(hp2,mpg)
yhat2 = model2.predict(hp2)
```

```
plt.scatter(hp,mpg,c='b',s=6)
plt.plot(hp,yhat2,c='r',lw=1)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



sort by *horsepower,* then transform, fit, and plot again

```
d2 = auto.sort_values('horsepower')
d2[:5]
```

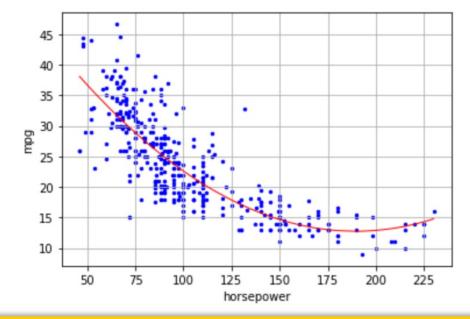
rs	mpg	cylinders	displacement	horsepower	weight	acceleration	year	origin
19	26.0	4	97.0	46	1835	20.5	70	2
101	26.0	4	97.0	46	1950	21.0	73	2
324	43.4	4	90.0	48	2335	23.7	80	2
323	44.3	4	90.0	48	2085	21.7	80	2
242	43.1	4	90.0	48	1985	21.5	78	2

```
mpg = d2.mpg
hp = d2.horsepower
hp1 = hp.values.reshape(-1,1)
```

```
poly2 = PolynomialFeatures(degree=2)
hp2 = poly2.fit_transform(hp1)
```

```
model2 = LinearRegression().fit(hp2,mpg)
yhat2 = model2.predict(hp2)
```

```
plt.scatter(hp,mpg,c='b',s=6)
plt.plot(hp,yhat2,c='r',lw=1)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



# **POLYNOMIAL REGRESSION – MODEL DEGREE 5**

# Model (degree 5)

```
poly5 = PolynomialFeatures(degree=5)
hp5 = poly5.fit transform(hp1)
hp5.shape
(392, 6)
df5 = pd.DataFrame(hp5)
df5[:5]
       hp
0 1.0
       46.0 2116.0
                  97336.0 4477456.0 205962976.0
1 1.0
       46.0 2116.0
                  97336.0 4477456.0 205962976.0
2 1.0
       48.0 2304.0 110592.0 5308416.0 254803968.0
3 1.0
       48.0 2304.0 110592.0 5308416.0 254803968.0
4 1.0 48.0 2304.0 110592.0 5308416.0 254803968.0
```

# **POLYNOMIAL REGRESSION – MODEL DEGREE 5**

# Model (degree 5)

```
poly5 = PolynomialFeatures(degree=5)
hp5 = poly5.fit_transform(hp1)
hp5.shape

(392, 6)
```

```
df5 = pd.DataFrame(hp5)
df5[:5]
```

```
        0
        1
        2
        3
        4
        5

        0
        1.0
        46.0
        2116.0
        97336.0
        4477456.0
        205962976.0

        1
        1.0
        46.0
        2116.0
        97336.0
        4477456.0
        205962976.0

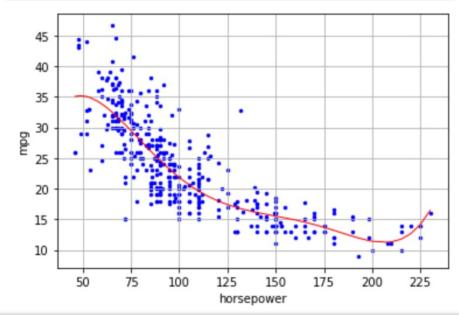
        2
        1.0
        48.0
        2304.0
        110592.0
        5308416.0
        254803968.0

        3
        1.0
        48.0
        2304.0
        110592.0
        5308416.0
        254803968.0

        4
        1.0
        48.0
        2304.0
        110592.0
        5308416.0
        254803968.0
```

```
model5 = LinearRegression().fit(hp5,mpg)
yhat5 = model5.predict(hp5)
```

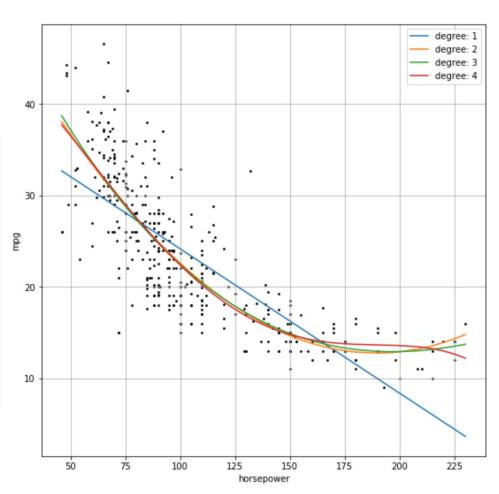
```
plt.scatter(hp,mpg,c='b',s=6)
plt.plot(hp,yhat5,c='r',lw=1)
plt.xlabel('horsepower')
plt.ylabel('mpg')
plt.grid()
```



# POLYNOMIAL REGRESSION - MODELS DEGREE 1 TO 4 (LOOP)

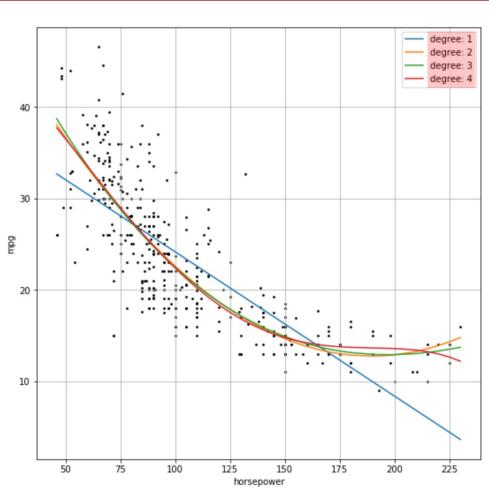
# Model (degree 5)

# Models (all up to degree 4)



# Models (all up to degree 4)

labels for the legend items



# Holdout cross-validation to select the best polynomial model

# **CROSS VALIDATION**

#### DataFrame with variables

```
list1 = ['horsepower','mpg']
df = auto[list1]
df[:5]
```

# horsepower mpg 0 130 18.0 1 165 15.0 2 150 18.0 3 150 16.0 4 140 17.0

# Select response and predictor(s)

```
mpg = df.mpg
hp1 = df.drop(['mpg'],axis = 1)
hp1[:5]
```

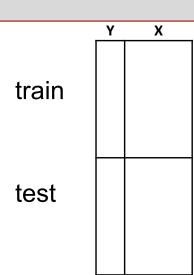
	horsepower			
0	130			
1	165			
2	150			
3	150			
4	140			

mpg	pg[:5]					
0	18.0					
1	15.0					
2	18.0					
3	16.0					
4	17.0					

# **HOLDOUT CROSS VALIDATION**

# Split the data into

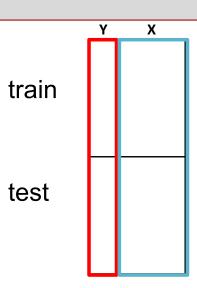
- Train set 50%
- Test set 50%



# **HOLDOUT CROSS VALIDATION**

# Split the data into

- Train set 50%
- Test set 50%



```
from sklearn.model_selection import train_test_split
```

```
hp_train,hp_test,mpg_train,mpg_test = train_test_split(hp1,mpg,
test_size=0.5,
random_state=1)
```

# Model (degree 2)

add a column of ones and a column of squared values to hp train, hp test

```
form = PolynomialFeatures(degree=2)
hp_train_2 = form.fit_transform(hp_train)
hp_test_2 = form.fit_transform(hp_test)
```

# Model (degree 2)

- train set used to fit() the model
- test set used to predict yhat values

```
form = PolynomialFeatures(degree=2)
hp_train_2 = form.fit_transform(hp_train)
hp_test_2 = form.fit_transform(hp_test)
```

```
m2 = LinearRegression().fit(hp_train_2,mpg_train)
yhat2 = m2.predict(hp_test_2)
```

# Model (degree 2)

```
form = PolynomialFeatures(degree=2)
hp_train_2 = form.fit_transform(hp_train)
hp_test_2 = form.fit_transform(hp_test)

m2 = LinearRegression().fit(hp_train_2,mpg_train)
```

```
# mspe
res2 = (yhat2 - mpg_test)**2
mspe2 = np.mean(res2)
mspe2
```

18.848292603275382

yhat2 = m2.predict(hp test 2)

# Model (degree 5)

```
form = PolynomialFeatures(degree=5)
hp_train_5 = form.fit_transform(hp_train)
hp_test_5 = form.fit_transform(hp_test)

m5 = LinearRegression().fit(hp_train_5,mpg_train)
```

```
res5 = (yhat5 - mpg_test)**2
mspe5 = np.mean(res5)
mspe5
```

18.324168662607967

yhat5 = m5.predict(hp test 5)

# Model (all degrees)

# into a loop

```
form = PolynomialFeatures(degree=5)
hp_train_5 = form.fit_transform(hp_train)
hp_test_5 = form.fit_transform(hp_test)

m5 = LinearRegression().fit(hp_train_5,mpg_train)
yhat5 = m5.predict(hp_test_5)

res5 = (yhat5 - mpg_test)**2
mspe5 = np.mean(res5)
mspe5
```

18.324168662607967

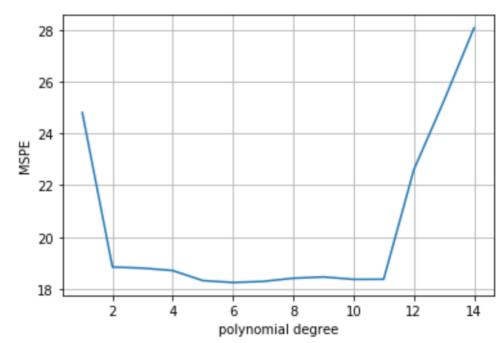
# Models (all degrees)

```
mspe = []
for i in range(1,15):
    form = PolynomialFeatures(degree=i)
    hp_train_i = form.fit_transform(hp_train)
    hp_test_i = form.fit_transform(hp_test)
    model = LinearRegression().fit(hp_train_i,mpg_train)
    yhat_i = model.predict(hp_test_i)
    sqres = (yhat_i - mpg_test)**2
    mspe_i = np.mean(sqres)
    mspe.append(mspe_i)
```

# Models (all degrees)

```
mspe.insert(0,np.nan)
         mspe
          [nan,
degree 1 \rightarrow 24.80212062059357,
degree 2 \rightarrow 18.848292603275382,
          18.805111358625545,
           18.711722273821835,
           18.324168662607967,
           18.25139104995864,
           18.29312744057875,
           18.415019005606478,
           18.46497960020678,
           18.371543424469433,
           18.376202865567404,
           22.59569142528774,
          25.260683389280025,
degree 14
          28.071751024475821
```

```
plt.plot(mspe)
plt.xlabel('polynomial degree')
plt.ylabel('MSPE')
plt.grid()
```

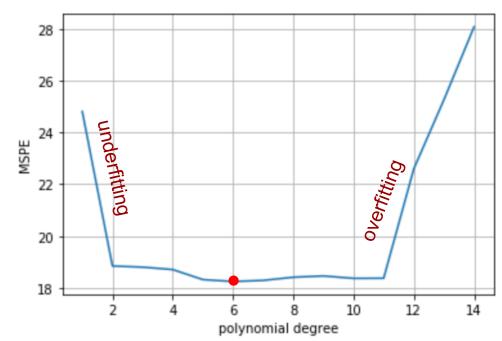


#### **POLYNOMIAL REGRESSION - VALIDATION APPROACH**

```
mspe.insert(0,np.nan)
         mspe
         [nan,
          24.80212062059357,
          18.848292603275382,
          18.805111358625545,
          18.711722273821835,
          18.324168662607967,
degree 6 \rightarrow 18.25139104995864,
          18.29312744057875,
          18.415019005606478,
          18.46497960020678,
          18.371543424469433,
          18.376202865567404,
          22.59569142528774,
          25.260683389280025,
          28.071751024475821
```

polynomial degree 6 is best model

```
plt.plot(mspe)
plt.xlabel('polynomial degree')
plt.ylabel('MSPE')
plt.grid()
```



### **POLYNOMIAL REGRESSION**

# to select the best polynomial model

for KFold CV and LOOCV

no need to split into train and test sets

from sklearn.model\_selection import cross\_val\_score

mspel = cross\_val\_score(LinearRegression(), hpl, mpg, cv = LeaveOneOut(), scoring = measure)

for KFold CV and LOOCV from sklearn.model\_selection import cross\_val\_score from sklearn.model\_selection import LeaveOneOut

no need to split into train and test sets

from sklearn.model selection import cross val score

24.231513517929226

-cvmspe1

## degree 2 model

linear model

19.24821312448941

# All degrees

#### mspe values

```
[nan,

24.231513517929226,

19.24821312448941,

19.33498406411397,

19.424430309411886,

19.033211842978396,

18.973012737758705,

19.125639655104838,

19.22423029373206,

19.133856501117357,

18.945837436861932,

19.1250385409314,

24.14841810216805,

27.76341869209905]
```

# 

#### best mspe values

```
[nan,
24.231513517929226,
19.24821312448941,
19.33498406411397,
19.424430309411886,
19.033211842978396,
                        degree 6
18.973012737758705,
19.125639655104838,
19.22423029373206,
19.133856501117357,
                        degree 10
18.945837436861932,
19.1250385409314,
24.14841810216805,
27.763418692099051
```

```
plt.plot(cvmspe)
                                                   plt.xlabel('polynomial degree')
                                                   plt.ylabel('MSPE')
model = LinearRegression()
                                                   plt.grid()
cvmspe = [-cvmspe1]
                                                           underfitting
for i in range(2,14):
    form = PolynomialFeatures(degree = i)
                                                      28
    hp_i = form.fit_transform(hp1)
    mspe = cross_val score(model,hp i,mpg,
                              cv = LeaveOneOut(),
                              scoring = measure)
                                                      24
    cvmspe.append(-mspe.mean())
                                                      22
cvmspe.insert(0,np.nan)
                                                      20
                                                                                            12
                                                                       polynomial degree
```

best models are degree 10 and 6

#### **POLYNOMIAL REGRESSION**

# K-Fold cross-validation to select the best polynomial model

#### **POLYNOMIAL REGRESSION – KFold Cross Validation**

```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold

measure = 'neg_mean_squared_error'
```

#### linear model

Cesar Acosta Ph.D.

#### **POLYNOMIAL REGRESSION – KFold Cross Validation**

```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold

measure = 'neg_mean_squared_error'
```

#### linear model

Cesar Acosta Ph.D.

#### **POLYNOMIAL REGRESSION - KFold Cross-validation**

## All polynomial models up to degree 13

#### **POLYNOMIAL REGRESSION - KFold Cross-validation**

# All polynomial models up to degree 13

```
[nan,

31.447014088557513,

24.34715884367356,

24.34607807898161,

24.35538965780616,

23.57323974697034,

23.407797059555385, degree 6

23.646448063420337,

23.892270279390385,

23.918015840113277,

23.862407621094167,

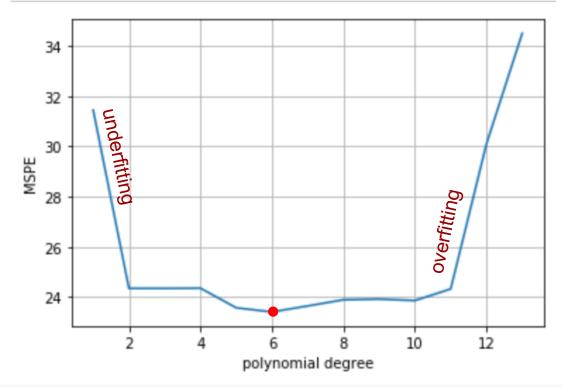
24.323550189304466,

30.101687309472418,

34.50104373957487]
```

## **POLYNOMIAL REGRESSION - KFold Cross-validation**

```
plt.plot(cvmspe)
plt.xlabel('polynomial degree')
plt.ylabel('MSPE')
plt.grid()
```



best model is degree 6

## **Sklearn - Cross Validation Summary**

```
from sklearn.model selection import train test split
                 hp train, hp test, mpg train, mpg test = train test split(hp1, mpg,
                                                                         test size=0.5,
HOLDOUT
                                                                         random state=1)
Cross Validation
                 m2 = LinearRegression().fit(hp train 2,mpg train)
                 yhat2 = m2.predict(hp test 2)
                 # mspe
                 res2 = (yhat2 - mpg test)**2
                 mspe2 = np.mean(res2)
                 measure = 'neg mean squared error'
                 from sklearn.model selection import cross val score
k-Fold
                 from sklearn.model selection import KFold
                 mspel = cross val score(LinearRegression(),hp1,mpg,
Cross Validation
                                           cv = KFold(n splits = 5),
                                           scoring = measure)
                 mspel.mean()
```