Day 06 - Polynomial Regression Models

Sept. 24, 2020

From Pre-Class Assignment

Challenging bits

- How to fit data with more than one feature
- How to determine a good fit when multiple features are used
- How to make sure `OLS` is doing the fit that I want

You will get more practice with this today.

Things that are still important:

- What is a regression model?
- How does a regression model work?
- What are the concerns about fitting with a line (or other function)?
- How do we determine if the fit is good?

Let's start by making some data

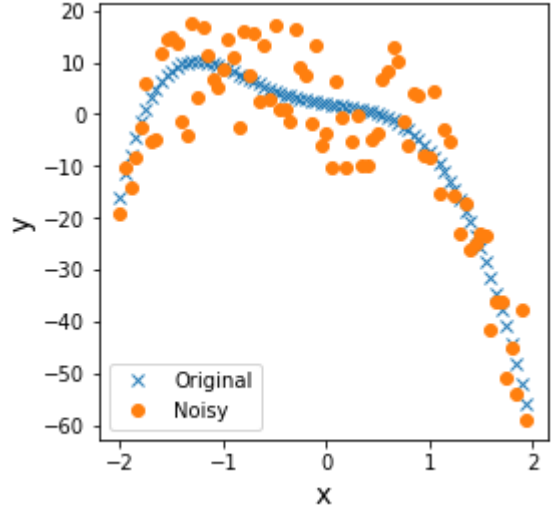
We will use quintic data: $y = 5x^5 + 3x^4 - 6x^3 + 2x^2 - 3x + 2$ from x = -2 to +2

In [13]:
```
import statsmodels.api as sm
import numpy as np
import matplotlib.pyplot as plt

x_ary = np.arange(-2, 2, 0.05)
y_ary = +x_ary**5 - 3*x_ary**4 - 6*x_ary**3 + 2*x_ary**2 - 3*x_ary + 2
y_noisy = y_ary + np.random.uniform(-15, 15.0, len(y_ary))

fig = plt.figure(figsize=(4,4))
plt.plot(x_ary, y_ary, 'x')
plt.plot(x_ary, y_noisy, 'o')
plt.xlabel('x', fontsize = 14)
plt.ylabel('y', fontsize = 14)
plt.legend(['Original', 'Noisy'])
```

Out[13]:
```
<matplotlib.legend.Legend at 0x7fe3c17cd950>
```



Let's make a model using up to x^{10}

Our model will try to fit:

$$y = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + c_5 x^5 + c_6 x^6 + c_7 x^7 + c_8 x^8 + c_9 x^9 + c_{10} x^{10} + \epsilon$$

to the noisy data. `statsmodels` will estimate the c_i each time we make the model. We will be able to set different c_i's to zero to reduce the complexity of the model.

In [2]:
```
import pandas as pd

column_names = ['x0','x1','x2','x3','x4','x5','x6','x7','x8','x9','x10']

const_values = np.ones(len(x_ary))

data = np.array([const_values, x_ary, x_ary**2, x_ary**3, x_ary**4,
                 x_ary**5,x_ary**6, x_ary**7, x_ary**8, x_ary**9,
                 x_ary**10])

df = pd.DataFrame(data.T, columns = column_names)
df.head()
```

Out[2]:

	x0	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10
0	1.0	-2.00	4.0000	-8.000000	16.000000	-32.000000	64.000000	-128.000000	256.000000	-512.000000	1024.000000
1	1.0	-1.95	3.8025	-7.414875	14.459006	-28.195062	54.980371	-107.211724	209.062862	-407.672580	794.961532
2	1.0	-1.90	3.6100	-6.859000	13.032100	-24.760990	47.045881	-89.387174	169.835630	-322.687698	613.106626
3	1.0	-1.85	3.4225	-6.331625	11.713506	-21.669987	40.089475	-74.165529	137.206229	-253.831523	469.588318
4	1.0	-1.80	3.2400	-5.832000	10.497600	-18.895680	34.012224	-61.222003	110.199606	-198.359290	357.046723

Ok let's run an OLS model using only the constant term

$$y_0 = c_0 + \epsilon$$

In [3]:
```
model = sm.OLS(y_noisy, df['x0']) # make the model
results = model.fit()
results.summary()
```

Out[3]:

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.000
Model:	OLS	**Adj. R-squared:**	0.000
Method:	Least Squares	**F-statistic:**	nan
Date:	Thu, 24 Sep 2020	**Prob (F-statistic):**	nan
Time:	09:46:18	**Log-Likelihood:**	-344.68
No. Observations:	80	**AIC:**	691.4
Df Residuals:	79	**BIC:**	693.7
Df Model:	0		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
x0	-5.1967	2.024	-2.568	0.012	-9.225	-1.169

Omnibus:	11.732	**Durbin-Watson:**	0.520
Prob(Omnibus):	0.003	**Jarque-Bera (JB):**	12.091
Skew:	-0.893	**Prob(JB):**	0.00237
Kurtosis:	3.664	**Cond. No.**	1.00

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

That was bad ($R^2 = 0$). Let's add the linear term.

$$y_1 = c_1 x + c_0 + \epsilon$$

That is better ($R^2 = 0.457$). Let's add the quadratic term

$$y_2 = c_2 x^2 + c_1 x + c_0 + \epsilon$$

In [5]:
```
model = sm.OLS(y_noisy, df[['x0','x1', 'x2']]) # make the model
results = model.fit()
results.summary()
```

Out[5]:

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.724
Model:	OLS	**Adj. R-squared:**	0.716
Method:	Least Squares	**F-statistic:**	100.8
Date:	Thu, 24 Sep 2020	**Prob (F-statistic):**	3.13e-22
Time:	09:46:18	**Log-Likelihood:**	-293.24
No. Observations:	80	**AIC:**	592.5
Df Residuals:	77	**BIC:**	599.6
Df Model:	2		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
x0	5.2172	1.616	3.228	0.002	1.999	8.435
x1	-10.7548	0.934	-11.511	0.000	-12.615	-8.894
x2	-8.0096	0.904	-8.862	0.000	-9.809	-6.210

Omnibus:	8.591	**Durbin-Watson:**	1.859
Prob(Omnibus):	0.014	**Jarque-Bera (JB):**	3.271
Skew:	0.144	**Prob(JB):**	0.195
Kurtosis:	2.052	**Cond. No.**	3.21

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Ok let's run this for each choice with increasing powers of x

$$y_0 = c_0 + \epsilon$$
$$y_1 = c_1 x + c_0 + \epsilon$$
$$\cdots$$
$$y_{10} = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + c_5 x^5 + c_6 x^6 + c_7 x^7 + c_8 x^8 + c_9 x^9 + c_{10} x^{10} + \epsilon$$

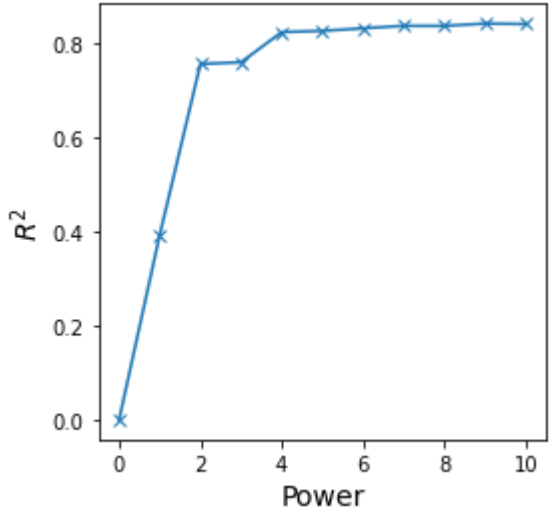
In [14]:

```
rsqr_arry = []
columns = []

for column in column_names:

    columns.append(column)
    model = sm.OLS(y_noisy, df[columns]) # make the model
    results = model.fit()                # run the OLS fit
    rsqr_arry.append(results.rsquared_adj)

fig = plt.figure(figsize=(4,4))
plt.plot(np.arange(0,11,1), rsqr_arry, 'x-')
plt.xlabel('Power', fontsize = 14)
plt.ylabel(r'$R^2$', fontsize = 14);
```



The quality of the fit "saturates" at x^5

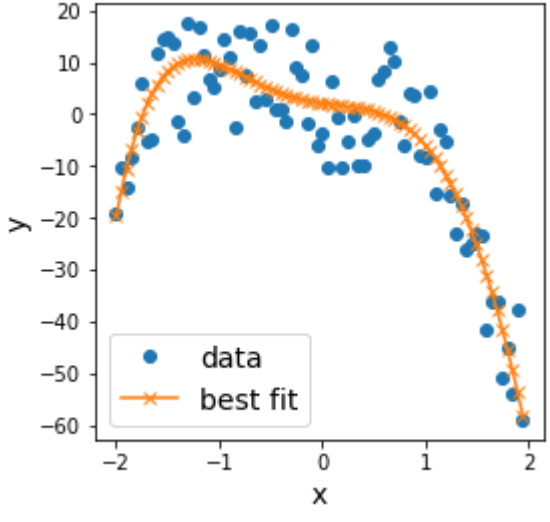
As we might have expected, $y_5 = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + c_5 x^5 + \epsilon$ produces the "best" model

In [16]:
```
best_fit = ['x0', 'x1', 'x2', 'x3', 'x4', 'x5']

model = sm.OLS(y_noisy, df[best_fit]) # make the model
results_b = model.fit()

fig = plt.figure(figsize=(4,4))
plt.plot(x_ary, y_noisy, 'o')
plt.plot(x_ary, results_b.predict(), '-x')
plt.xlabel('x', fontsize = 14)
plt.ylabel('y', fontsize = 14)
plt.legend(['data', 'best fit'], fontsize = 14)
```

Out[16]:
```
<matplotlib.legend.Legend at 0x7fe39009a690>
```



Let's look at the fits of other models

Linear fit: $y_1 c_1 x + c_0 + \epsilon$

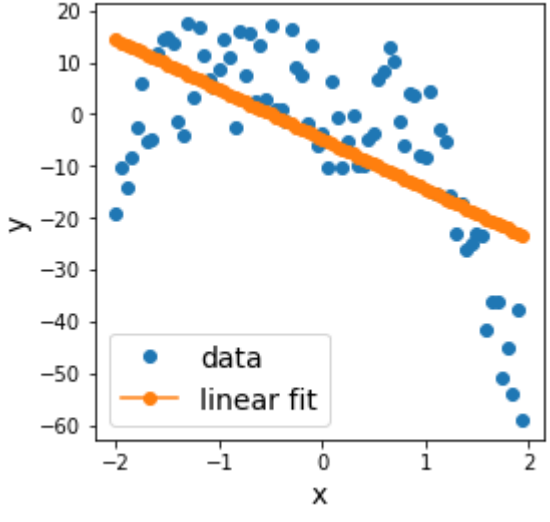
This is underfitting!

In [17]:
```
linear_fit = ['x0','x1']

model = sm.OLS(y_noisy, df[linear_fit]) # make the model
results_l = model.fit()

fig = plt.figure(figsize=(4,4))
plt.plot(x_ary, y_noisy, 'o')
plt.plot(x_ary, results_l.predict(), '-o')
plt.xlabel('x', fontsize = 14)
plt.ylabel('y', fontsize = 14)
plt.legend(['data', 'linear fit'], fontsize = 14)
```

Out[17]:
```
<matplotlib.legend.Legend at 0x7fe3c12b4cd0>
```



Let's look at the fits of other models

Full fit:
$y = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + c_5 x^5 + c_6 x^6 + c_7 x^7 + c_8 x^8 + c_9 x^9 + c_{10} x^{10}$$
$+ \epsilon$

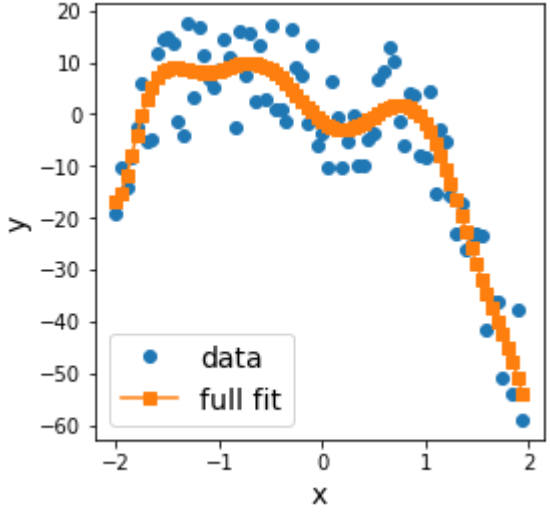
This is overfitting!

In [18]:
```
full_fit = ['x0','x1','x2','x3','x4','x5','x6','x7','x8','x9','x10']

model = sm.OLS(y_noisy, df[full_fit]) # make the model
results_f = model.fit()

fig = plt.figure(figsize=(4,4))
plt.plot(x_ary, y_noisy, 'o')
plt.plot(x_ary, results_f.predict(), '-s')
plt.xlabel('x', fontsize = 14)
plt.ylabel('y', fontsize = 14)
plt.legend(['data', 'full fit'], fontsize = 14)
```

Out[18]:
```
<matplotlib.legend.Legend at 0x7fe3d1265e50>
```

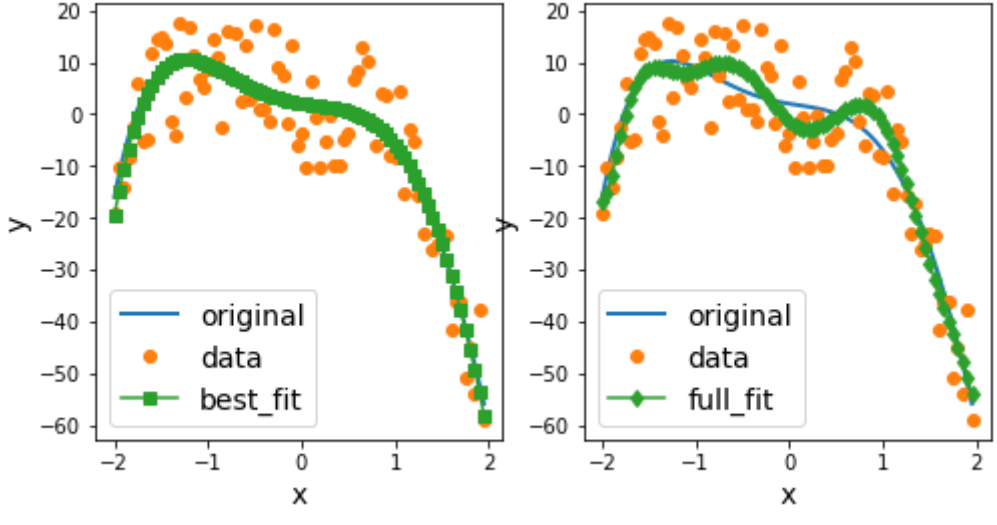


Let’s compare the best fit to the full fit

In [19]:
```
fig,(ax1, ax2) = plt.subplots(1, 2, figsize = (8,4))

ax1.plot(x_ary, y_ary, '-', lw = 2)
ax1.plot(x_ary, y_noisy, 'o')
ax1.plot(x_ary, results_b.predict(), '-s')
ax2.plot(x_ary, y_ary, '-', lw = 2)
ax2.plot(x_ary, y_noisy, 'o')
ax2.plot(x_ary, results_f.predict(), '-d')
ax1.set_xlabel('x', fontsize = 14)
ax2.set_xlabel('x', fontsize = 14)
ax1.set_ylabel('y', fontsize = 14)
ax2.set_ylabel('y', fontsize = 14)
ax1.legend(['original', 'data', 'best_fit'], fontsize = 14)
ax2.legend(['original', 'data', 'full_fit'], fontsize = 14)
```

Out[19]:
```
<matplotlib.legend.Legend at 0x7fe3b8546f90>
```



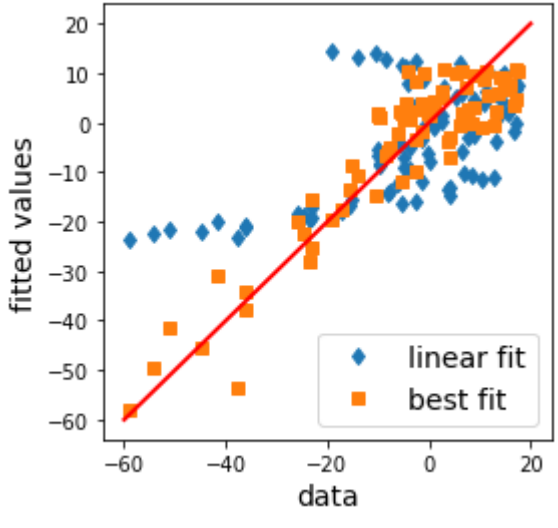
Let's compare the data to the fitted values

We would expect a perfect model to produce a line.

In [21]:
```
fig = plt.figure(figsize = (4,4))
plt.plot(y_noisy, results_l.predict(), 'd')
plt.plot(y_noisy, results_b.predict(), 's')

plt.plot([-60,20], [-60,20], '-r', lw=2)
plt.xlabel('data', fontsize = 14)
plt.ylabel('fitted values', fontsize = 14)
plt.legend(['linear fit', 'best fit'], fontsize = 14)
```

Out[21]:
```
<matplotlib.legend.Legend at 0x7fe3a0813dd0>
```



Questions, Comments, Concerns?