E34

September 6, 2024

1 Exercise Week 34

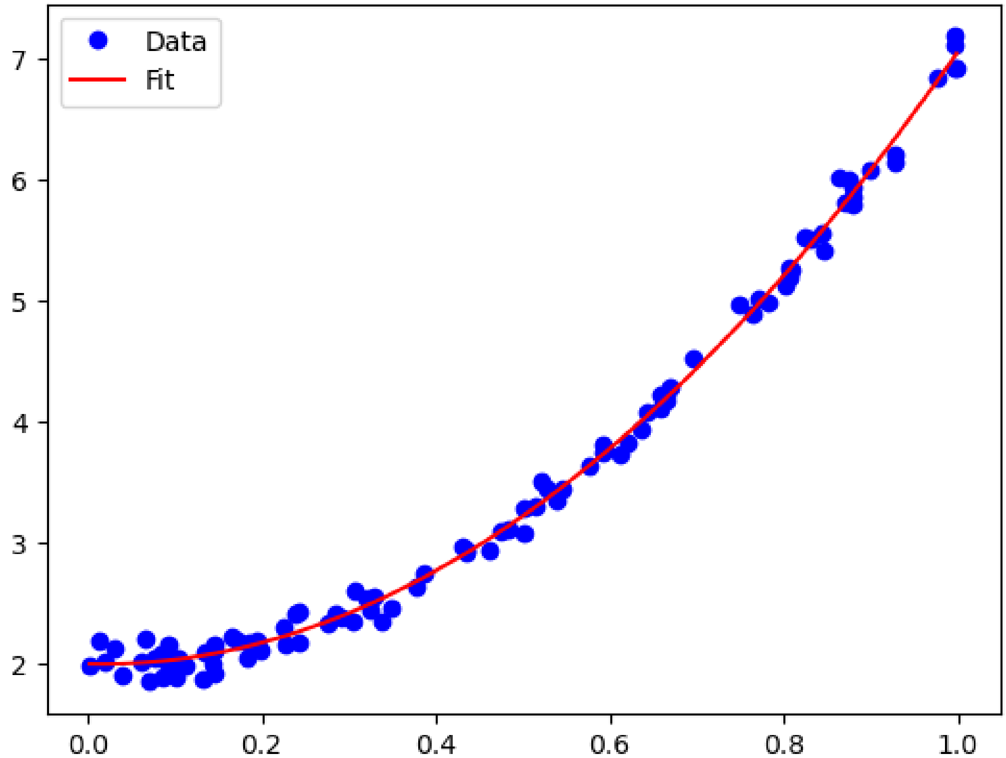
1.1 Exercise 2: Making your own data and exploring scikit-learn

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import PolynomialFeatures
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.model_selection import train_test_split
```

[2]:
```
n = 100
x = np.random.rand(n,1)
idx = np.argsort(x, axis=0).flatten()
x = x[idx] # Always sort sooner rather than later
y = 2.0+5*x*x+0.1*np.random.randn(n,1)
```

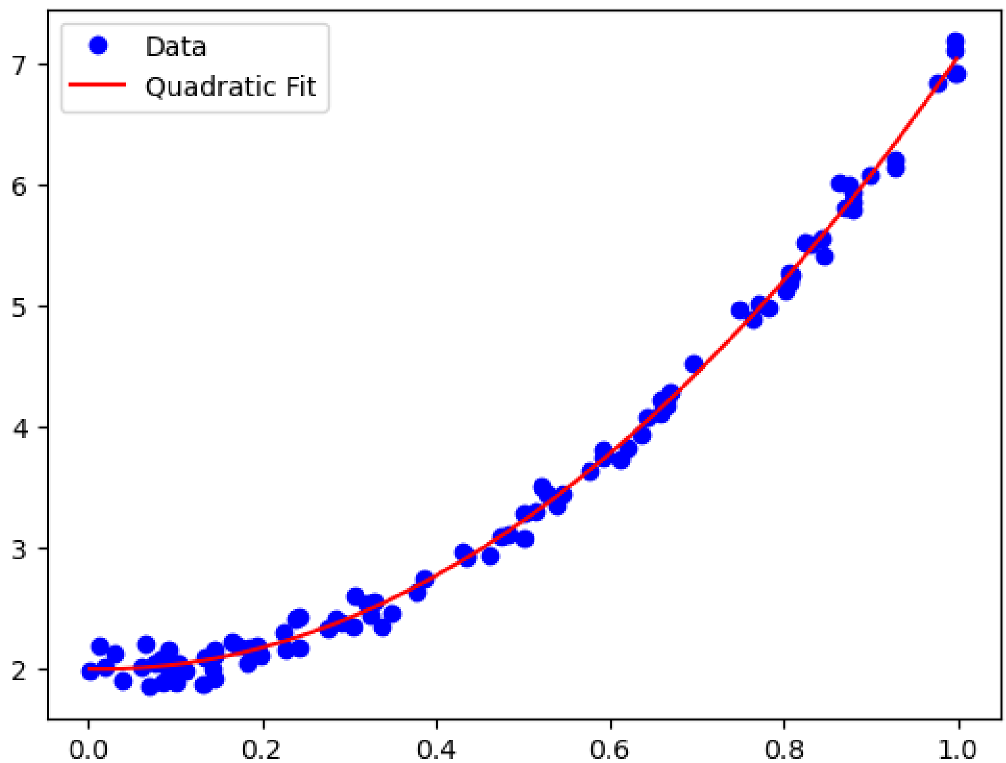
1.1.1 1. My Code

[3]:
```
# Design matrix
X = np.ones((n,3))
X[:,1] = x.flatten()
X[:,2] = x.flatten()**2

# Coefficients and model
  = np.linalg.inv(X.T @ X) @ X.T @ y
y_pred = X @

plt.plot(x,y, "bo", label="Data")
plt.plot(x, y_pred, "r", label="Fit")
plt.legend()
plt.show()
```



1.1.2 2. Scikit-learn

[4]:
```
poly2 = PolynomialFeatures(degree=2).fit(x, y)
X = poly2.fit_transform(x)

# Penta line fit (?)
plf5 = LinearRegression().fit(X, y)
y_pred = plf5.predict(X)

plt.plot(x, y, 'bo', label='Data')
plt.plot(x, y_pred, "r", label="Quadratic Fit")
plt.legend()
plt.show()
```



1.1.3 3. *MSE* & R^2

Mean Squared Errror (χ^2): A function which measures the average square error between our prediction and the data. With more datapins n, we can have more confidence in our model. This should be minimized.

$$\chi(\vec{y}, \tilde{y}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \tilde{y}_i)^2$$

R^2: A function which measures how well our model can predict new values. The max score is 1, and the worst score is $-\infty$. A score of 0 means the same y-value for all predictions.

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

[5]:

```
MSE = mean_squared_error(y, y_pred)
R2 = r2_score(y, y_pred)
print(f'{MSE = :.2e}, {R2 = :.2%}')
```

```
MSE = 9.50e-03, R2 = 99.61%
```

1.2 Exercise 3: Split data in test and training data

1.2.1 a) Manual 5-deg polynomial design matrix and split

[6]:
```
np.random.seed()
n = 100
# Make data set.
x = np.linspace(-3, 3, n).reshape(-1, 1)
y = np.exp(-x**2) + 1.5 * np.exp(-(x-2)**2) + np.random.normal(0, 0.1, x.shape)

# Manual design matrix
X = np.ones((n, 5))
X[:,1] = x.flatten()
X[:,2] = x.flatten()**2
X[:,3] = x.flatten()**3
X[:,4] = x.flatten()**4

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)
  = np.linalg.inv(X.T @ X) @ X.T @ y
```

1.2.2 b) Predictions and MSE calculation

[7]:
```
y_tilde = X_train @
y_pred = X_test @

MSE_train = mean_squared_error(y_train, y_tilde)
MSE_test = mean_squared_error(y_test, y_pred)

print(f'{MSE_train = :.2e}')
print(f'{MSE_test = :.2e}')
```

```
MSE_train = 2.47e-02
MSE_test = 3.86e-02
```

1.2.3 c) Scikit-learn 15-deg polynomial design matrix and split

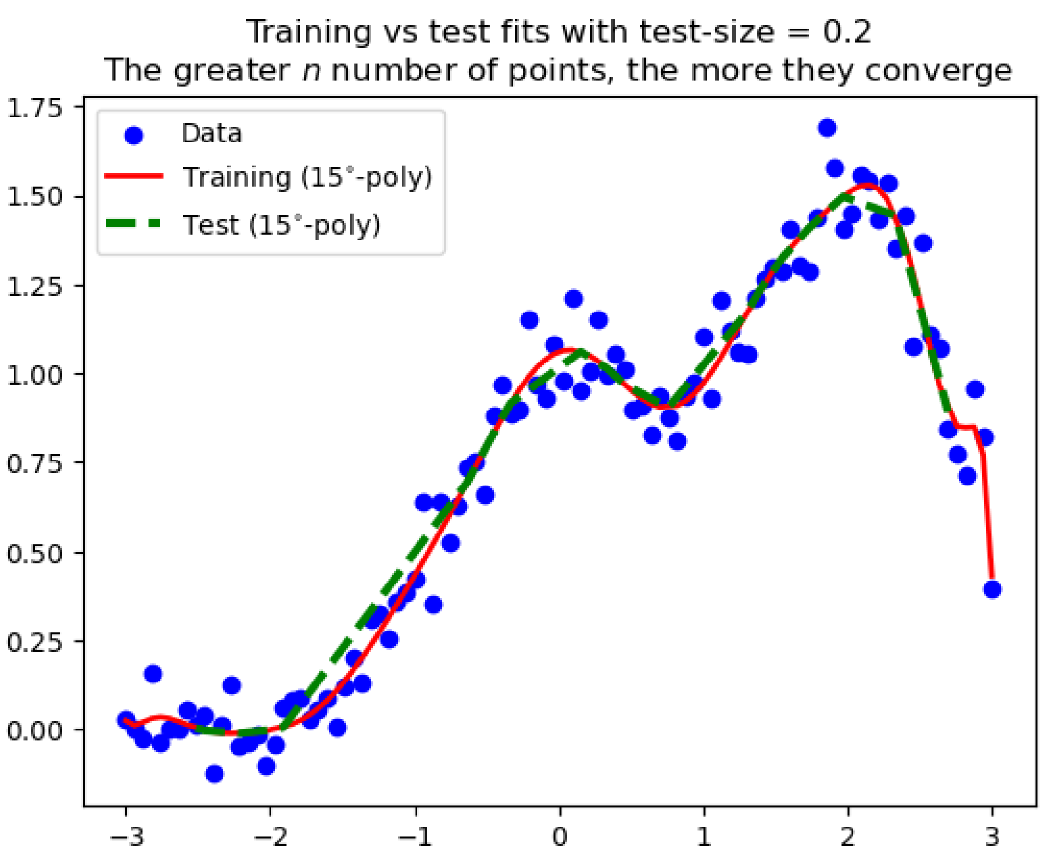
[8]:
```
poly15 = PolynomialFeatures(degree=15).fit(x, y)
X = poly15.fit_transform(x)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)


# Sorting columns as values are picked at random
idx_train = np.argsort(X_train[:,1])
idx_test = np.argsort(X_test[:,1])
X_test = X_test[idx_test]
X_train = X_train[idx_train]

  = np.linalg.inv(X.T @ X) @ X.T @ y
```

```
y_tilde = X_train @
y_pred = X_test @

MSE_train = mean_squared_error(y_train, y_tilde)
MSE_test = mean_squared_error(y_test, y_pred)

print(F'{MSE_train = :.2e}')
print(F'{MSE_test = :.2e}')
```

```
MSE_train = 4.82e-01
MSE_test = 5.70e-01
```

[9]:

```
plt.scatter(x, y, c="b", label="Data")

plt.plot(X_train[:,1], y_tilde, c="r", label="Training ($15^{\circ}$-poly)",␣
 ↪linewidth=2)
plt.plot(X_test[:,1], y_pred, c="green", label="Test ($15^{\circ}$-poly)",␣
 ↪linewidth=3, linestyle='--')
plt.legend()
plt.title(f'Training vs test fits with test-size = 0.2\nThe greater $n$ number␣
 ↪of points, the more they converge')
plt.show()
```



1.2.4 Conclusion

- The greater the number n of data points, the more accurate our model will be. With a high n, the test and training data was more similar.
- The MSE was consistently lower for the 5th degree polynomial by an order of magnitude, as $\mathrm{MRE}_5 \approx 10^{-2}$ and $\mathrm{MRE}_{15} \approx 10^{-1}$. This might shows that the 15th degree polynomial is overfitting the data.