Polynomial Regression

Introduction

Polynomial regression means transforming your features into quadratic (squared) or higher-order polynomial terms so that you can model a non-linear relationship using linear regression.

Objectives

You will be able to:

- Determine if polynomial regression would be useful for a specific model or set of data
- Create polynomial terms out of independent variables in linear regression
- Interpret coefficients of linear regression models that contain polynomial terms

Polynomial Functions

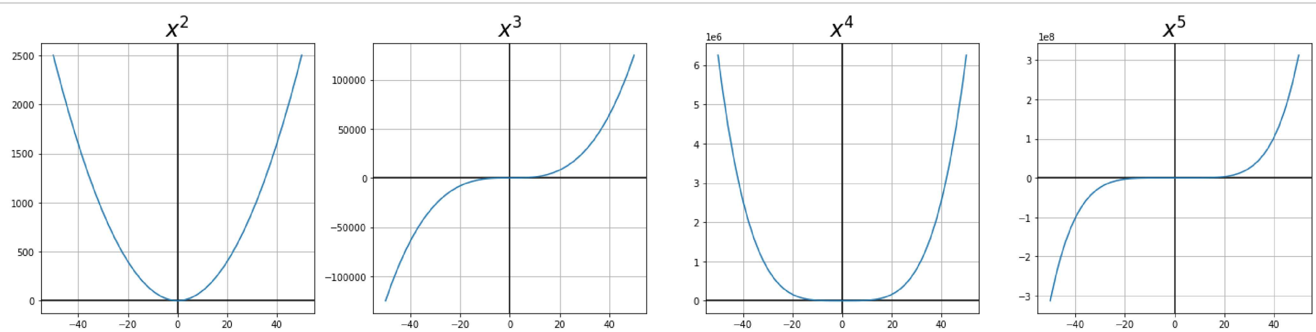
In data science we typically define ***polynomial*** to mean a feature raised to a power of 2 or higher. (This is a looser definition than you might have learned in math class.) The power that the feature is raised to is called the ***degree*** of the polynomial.

Below we plot some examples of polynomials with different degrees:

In [1]:
```
import matplotlib.pyplot as plt
import matplotlib as mpl
import numpy as np
%matplotlib inline
mpl.rcParams["axes.grid"] = True

x = np.linspace(-50, 50, 50)
fig, axes = plt.subplots(ncols=4, figsize=(20,5))
for i, ax in enumerate(axes):
    ax.axhline(0, color="black")
    ax.axvline(0, color="black")
    degree = i + 2
    ax.plot(x, x**degree)
    ax.set_title(f"$x^{degree}$", {"fontsize": 24})

fig.tight_layout()
```



Similar to an interaction term, a polynomial term can also be added to a linear function in the form $y = mx + b$. Below we demonstrate some examples using a polynomial of degree 2, also called a ***quadratic*** function, which is represented in the form $y = ax^2 + bx + c$.

This is one of the most common polynomials you'll see in data science and the associated curved shape is called a ***parabola***. Parabolas can have various shapes and positions depending on the coefficients used.

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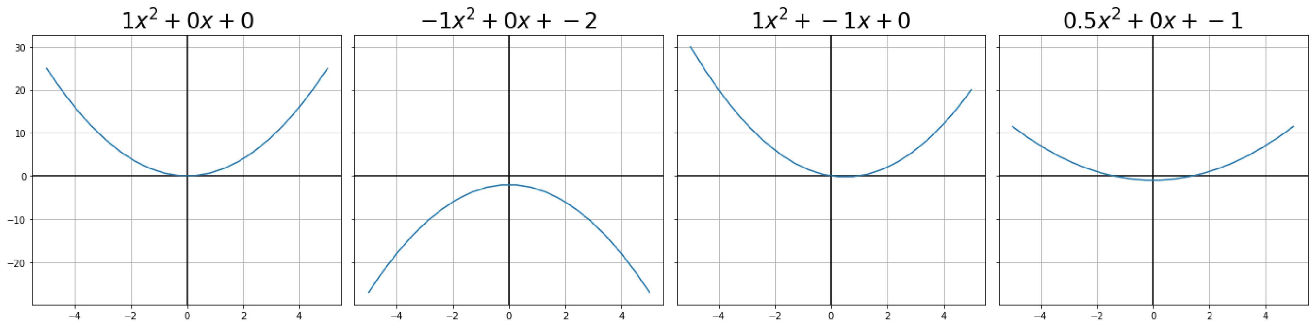
In [2]:
```
fig, axes = plt.subplots(ncols=4, figsize=(20,5), sharey=True)

coefficients = (
    (1, 0, 0),
    (-1, 0, -2),
    (1, -1, 0),
    (0.5, 0, -1)
)
x = np.linspace(-5, 5, 20)
for i, (a, b, c) in enumerate(coefficients):
    ax = axes[i]
    ax.axhline(0, color="black")
    ax.axvline(0, color="black")
    ax.plot(x, a * x**2 + b * x + c)
    ax.set_title(f"${a}x^2 + {b}x + {c}$", {"fontsize": 24})

fig.tight_layout()
```



Attempting Linear Regression on a Non-Linear Relationship

The dataset `'yields.csv'` , with just 21 cases, contains measurements of the yields from an experiment done at six different levels of temperature in degrees Fahrenheit.

In [3]:
```
import pandas as pd

yld = pd.read_csv('yield.csv', sep='\s+', index_col=0)
yld.head()
```

Out[3]:

i	Temp	Yield
1	50	3.3
2	50	2.8
3	50	2.9
4	50	3.2
5	60	2.7

Let's plot temperature vs. yield.

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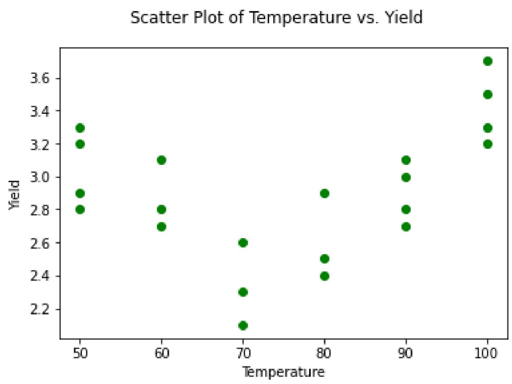
In [4]:
```
mpl.rcParams["axes.grid"] = False

y = yld['Yield']
X = yld.drop(columns='Yield', axis=1)

fig, ax = plt.subplots()
ax.scatter(X, y, color='green')
ax.set_xlabel('Temperature')
ax.set_ylabel('Yield')
fig.suptitle("Scatter Plot of Temperature vs. Yield");
```



It's clear that this relationship is not linear. Let's try and fit a linear regression anyways and see how the model performs:

In [5]:
```
import statsmodels.api as sm
linear_results = sm.OLS(y, sm.add_constant(X)).fit()
```

In [6]:
```
linear_results.params
```

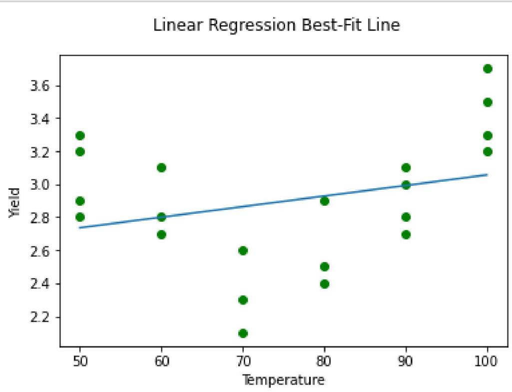
Out[6]:
```
const    2.415106
Temp     0.006404
dtype: float64
```

In [7]:
```
linear_results.rsquared
```

Out[7]:
```
0.08605718085106395
```

We are explaining about 9% of the variance in yield. Let's look at that model on a graph:

In [8]:
```
fig, ax = plt.subplots()
ax.scatter(X, y, color='green')
ax.plot(X, linear_results.predict(sm.add_constant(X)))
ax.set_xlabel('Temperature')
ax.set_ylabel('Yield')
fig.suptitle("Linear Regression Best-Fit Line");
```



This is clearly not a good fit for the data. The data points seem to form a parabola shape, so let's try creating a polynomial term to see if it improves!

A Quadratic Relationship

Adding a Squared Term

Creating a 2nd-degree polynomial (squared term) is pretty straightforward, using `pandas` broadcasting. Let's call ours `Temp_sq` :

In [9]:
```
X_quad = X.copy()
X_quad['Temp_sq'] = X_quad['Temp']**2
X_quad
```

Out[9]:

i	Temp	Temp_sq
1	50	2500
2	50	2500
3	50	2500
4	50	2500
5	60	3600
6	60	3600
7	60	3600
8	70	4900
9	70	4900
10	70	4900
11	80	6400
12	80	6400
13	80	6400
14	90	8100
15	90	8100
16	90	8100
17	90	8100
18	100	10000
19	100	10000
20	100	10000
21	100	10000

Building a Quadratic Model

Now let's fit a linear regression on `Temp` and `Temp_sq` :

In [10]:
```
squared_results = sm.OLS(y, sm.add_constant(X_quad)).fit()
```

Viewing Quadratic Model Results

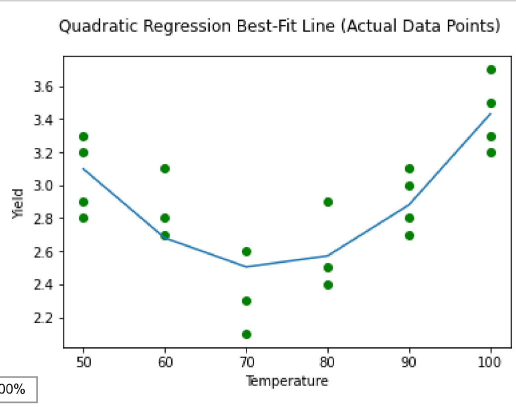
In [11]:
```
squared_results.rsquared
```

Out[11]: 0.6948165884110555

That's a much better metric! But what did we actually just do?

Let's plot our new model's predictions:

In [12]:
```
fig, ax = plt.subplots()
ax.scatter(X_quad["Temp"], y, color='green')
ax.plot(X_quad["Temp"], squared_results.predict(sm.add_constant(X_quad)))
ax.set_xlabel('Temperature')
ax.set_ylabel('Yield')
fig.suptitle("Quadratic Regression Best-Fit Line (Actual Data Points)");
```



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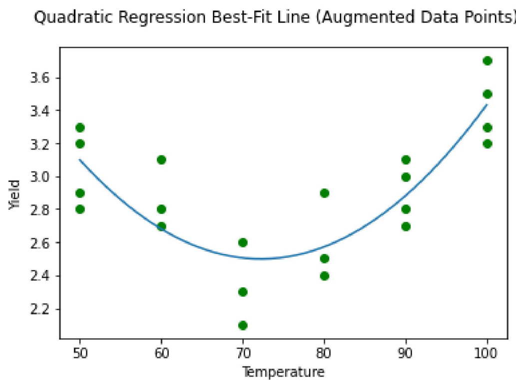
Note that you get a seemingly "piecewise linear" function here, because the yields were only measured at 50, 60, 70, 80, 90 and 100. In reality, this model generates a smooth curve, as denoted below.

In [13]:
```
X_smooth = pd.DataFrame(np.linspace(50, 100, 50), columns=['Temp'])
X_smooth['Temp_sq'] = X_smooth['Temp'] ** 2

fig, ax = plt.subplots()
ax.scatter(X["Temp"], y, color='green')
ax.plot(X_smooth["Temp"], squared_results.predict(sm.add_constant(X_smooth)))
ax.set_xlabel('Temperature')
ax.set_ylabel('Yield')
fig.suptitle("Quadratic Regression Best-Fit Line (Augmented Data Points)");
```



Interpreting Quadratic Model Results

Because we added a squared term to our model, we went from fitting this regression model:

$$\hat{y} = \hat{\beta_0} + \hat{\beta_1}x$$

To fitting this regression model:

$$\hat{y} = \hat{\beta_0} + \hat{\beta_1}x + \hat{\beta_2}x^2$$

Based on our improved R-Squared score as well as qualitatively inspecting the graphs of the best-fit lines, it looks like we have a better model. But how would we interpret these results?

In [14]:
```
squared_results.params
```

Out[14]:
```
const      8.817531
Temp      -0.174928
Temp_sq    0.001211
dtype: float64
```

In [15]:
```
squared_results.pvalues
```

Out[15]:
```
const      2.122009e-07
Temp       1.868031e-05
Temp_sq    1.145398e-05
dtype: float64
```

Since all of the p-values are below a standard alpha of 0.05, let's plug in those values. The function created by our fitted model is $y = 0.0012x^2 - 0.17x + 8.8$.

Intercept

The interpretation of the intercept is essentially the same as any other intercept. When all features have a value of 0, we expect the target to be about 8.8. As is often the case, this is not particularly interpretable, because we don't have any data points where `Temp` is equal to 0. We might consider centering the `Temp` values if interpretation of the intercept matters.

x and x^2 Coefficients

We have essentially added an interaction term of `Temp` with itself. This means that a "one-at-a-time" interpretation is not possible, because there can't be a 1-unit increase of `Temp` while `Temp_sq` is held constant at 0.

Instead they must be interpreted together. So, for each increase of 1 degree of `Temp`, we see a change of -0.17 + (0.0012 x `Temp`) in `Yield`.

We can also incorporate more of a quadratic-specific explanation. Because the `Temp_sq` coefficient is positive (and based on looking at the graph), we know that this parabola has a minimum value at its vertex. To calculate the minimum point, the formula is $(-b / 2a, c - b^2 / 4a)$ (you can find the longer derivation for this formula [here (https://youtu.be/r2oywW2A-6M)](https://youtu.be/r2oywW2A-6M)).

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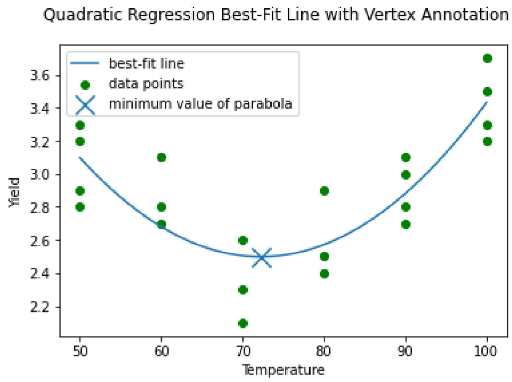
In [16]:
```
a = squared_results.params["Temp_sq"]
b = squared_results.params["Temp"]
c = squared_results.params["const"]

x_vertex, y_vertex = (-b / (2 * a), c - (b ** 2) / (4 * a))
x_vertex, y_vertex
```

Out[16]:
```
(72.24853453215083, 2.4983975303475425)
```

Below we plot this point on the graph as well:

In [17]:
```
fig, ax = plt.subplots()
ax.scatter(X["Temp"], y, color='green', label="data points")
ax.plot(X_smooth["Temp"], squared_results.predict(sm.add_constant(X_smooth)), label="best-fit line")
ax.scatter(x_vertex, y_vertex, s=200, marker="x", label="minimum value of parabola")
ax.legend()
ax.set_xlabel('Temperature')
ax.set_ylabel('Yield')
fig.suptitle("Quadratic Regression Best-Fit Line with Vertex Annotation");
```



Using this point, we can say that for `Temp` values below about 72, the `Yield` decreases as the `Temp` increases until it reaches a minimum expected `Yield` of about 2.5. Then for `Temp` values above about 72, the `Yield` increases as the `Temp` increases.

Higher-Order Relationships

The use of polynomials is not restricted to quadratic relationships. You can explore cubic or higher order relationships as well!

Adding Polynomial Terms

You could write custom `pandas` code to achieve this, but there is also a tool we can import from the `preprocessing` module of scikit-learn called `PolynomialFeatures`.

Let's test it out with a degree of 6.

In [18]:
```
from sklearn.preprocessing import PolynomialFeatures

poly = PolynomialFeatures(6)
X_poly = poly.fit_transform(X)
```

Take a look at what these transformed features really look like. As you can see, `PolynomialFeatures` transformed the X value of a single 50 into 50^0 through 50^6! The first value of 1 (50^0) represents the intercept in the linear regression, which you can read more about in the [PolynomialFeatures documentation (https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.PolynomialFeatures.html)](https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.PolynomialFeatures.html).

In [19]:
```
feature_names = poly.get_feature_names(input_features=X.columns)

print(f'The transformed feature names are: {feature_names}')
print('------------------')
print(f'The first row of transformed data is: {X_poly[0]}')
```

```
The transformed feature names are: ['1', 'Temp', 'Temp^2', 'Temp^3', 'Temp^4', 'Temp^5', 'Temp^6']
------------------
The first row of transformed data is: [1.0000e+00 5.0000e+01 2.5000e+03 1.2500e+05 6.2500e+06 3.1250e+08
 1.5625e+10]
```

We can also make the result back into a dataframe for easier viewing:

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In [20]:
```
X_poly = pd.DataFrame(X_poly, columns=feature_names, index=X.index)
X_poly
```

Out[20]:

i	1	Temp	Temp^2	Temp^3	Temp^4	Temp^5	Temp^6
1	1.0	50.0	2500.0	125000.0	6250000.0	3.125000e+08	1.562500e+10
2	1.0	50.0	2500.0	125000.0	6250000.0	3.125000e+08	1.562500e+10
3	1.0	50.0	2500.0	125000.0	6250000.0	3.125000e+08	1.562500e+10
4	1.0	50.0	2500.0	125000.0	6250000.0	3.125000e+08	1.562500e+10
5	1.0	60.0	3600.0	216000.0	12960000.0	7.776000e+08	4.665600e+10
6	1.0	60.0	3600.0	216000.0	12960000.0	7.776000e+08	4.665600e+10
7	1.0	60.0	3600.0	216000.0	12960000.0	7.776000e+08	4.665600e+10
8	1.0	70.0	4900.0	343000.0	24010000.0	1.680700e+09	1.176490e+11
9	1.0	70.0	4900.0	343000.0	24010000.0	1.680700e+09	1.176490e+11
10	1.0	70.0	4900.0	343000.0	24010000.0	1.680700e+09	1.176490e+11
11	1.0	80.0	6400.0	512000.0	40960000.0	3.276800e+09	2.621440e+11
12	1.0	80.0	6400.0	512000.0	40960000.0	3.276800e+09	2.621440e+11
13	1.0	80.0	6400.0	512000.0	40960000.0	3.276800e+09	2.621440e+11
14	1.0	90.0	8100.0	729000.0	65610000.0	5.904900e+09	5.314410e+11
15	1.0	90.0	8100.0	729000.0	65610000.0	5.904900e+09	5.314410e+11
16	1.0	90.0	8100.0	729000.0	65610000.0	5.904900e+09	5.314410e+11
17	1.0	90.0	8100.0	729000.0	65610000.0	5.904900e+09	5.314410e+11
18	1.0	100.0	10000.0	1000000.0	100000000.0	1.000000e+10	1.000000e+12
19	1.0	100.0	10000.0	1000000.0	100000000.0	1.000000e+10	1.000000e+12
20	1.0	100.0	10000.0	1000000.0	100000000.0	1.000000e+10	1.000000e+12
21	1.0	100.0	10000.0	1000000.0	100000000.0	1.000000e+10	1.000000e+12

Building a Polynomial Model

Now you can fit a linear regression model with your transformed data. Note that you do **not** need to use `sm.add_constant` because `PolynomialFeatures` has already added a constant.

In [21]:
```
poly_results = sm.OLS(y, X_poly).fit()
```

Viewing Polynomial Model Results

Let's start by comparing R-Squared values again.

In [22]:
```
print(f"""
Comparing R-Squared Results:
Linear Regression:             {linear_results.rsquared}
Quadratic Regression:          {squared_results.rsquared}
6th Degree Polynomial Regression: {poly_results.rsquared}
""")
```

```
Comparing R-Squared Results:
Linear Regression:             0.08605718085106395
Quadratic Regression:          0.6948165884110555
6th Degree Polynomial Regression: 0.7591134874665022
```

It looks like we have a marginal improvement in R-Squared for the 6th degree polynomial regression compared to the quadratic (2nd degree polynomial) regression. What does this look like in terms of the graph?

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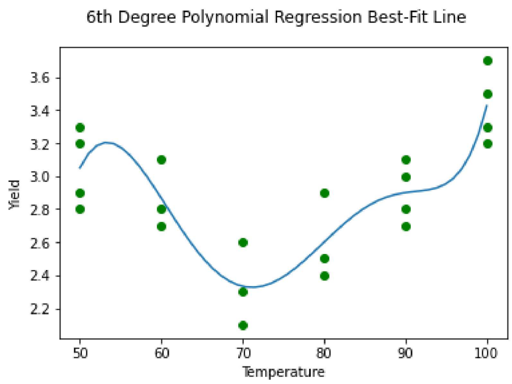
In [23]:
```
X_smooth = poly.transform(X_smooth.drop(columns=["Temp_sq"]))

fig, ax = plt.subplots()
ax.scatter(X["Temp"], y, color='green')
ax.plot(X_smooth[:, 1], poly_results.predict(X_smooth))
ax.set_xlabel('Temperature')
ax.set_ylabel('Yield')
fig.suptitle("6th Degree Polynomial Regression Best-Fit Line");
```



That's a much more complex curve!

Given how few data points we actually have, it's difficult to tell whether this is really a better fit than the quadratic model just by looking at the graph.

Interpreting Polynomial Model Results

Let's check out the coefficients and p-values:

In [24]:
```
poly_results.params
```

Out[24]:
```
1        -6.516328e-01
Temp     -7.686863e+00
Temp^2    5.488636e-01
Temp^3   -1.516236e-02
Temp^4    2.048805e-04
Temp^5   -1.359511e-06
Temp^6    3.553543e-09
dtype: float64
```

In [25]:
```
poly_results.pvalues
```

Out[25]:
```
1         0.137393
Temp      0.137404
Temp^2    0.133079
Temp^3    0.134236
Temp^4    0.137672
Temp^5    0.142381
Temp^6    0.147712
dtype: float64
```

We are now up to 7 coefficients and **none** of them are statistically significant at an alpha of 0.05 -- not even the intercept. If the goal is to generate inferential insights, this model is not especially useful.

Additional Resources

- Check out this resource (https://www.khanacademy.org/math/algebra/x2f8bb11595b61c86:quadratic-functions-equations) for a refresher on parabolas and the relationship between quadratic graphs and formulas
- Wondering why we always seem to use every lower degree term instead of skipping to a higher degree? This resource (https://maxhfarrell.com/bus41100/handout_41100_PolynomialRegression.pdf) demonstrates how that would be similar to skipping the intercept term and involve making undue assumptions

Summary

Great! You now know how to include polynomials in your linear models. Let's go ahead and practice this knowledge!

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