mlp-week03

January 29, 2021

1 Machine Learning in Python - Workshop 3

1.1 1. Setup

1.1.1 1.1 Packages

In the cell below we will load the core libraries we will be using for this workshop and setting some sensible defaults for our plot size and resolution.

[1]:
```
# Display plots inline
%matplotlib inline

# Data libraries
import pandas as pd
import numpy as np

# Plotting libraries
import matplotlib.pyplot as plt
import seaborn as sns

# Plotting defaults
plt.rcParams['figure.figsize'] = (8,5)
plt.rcParams['figure.dpi'] = 80

# sklearn modules
from sklearn.linear_model import LinearRegression
```

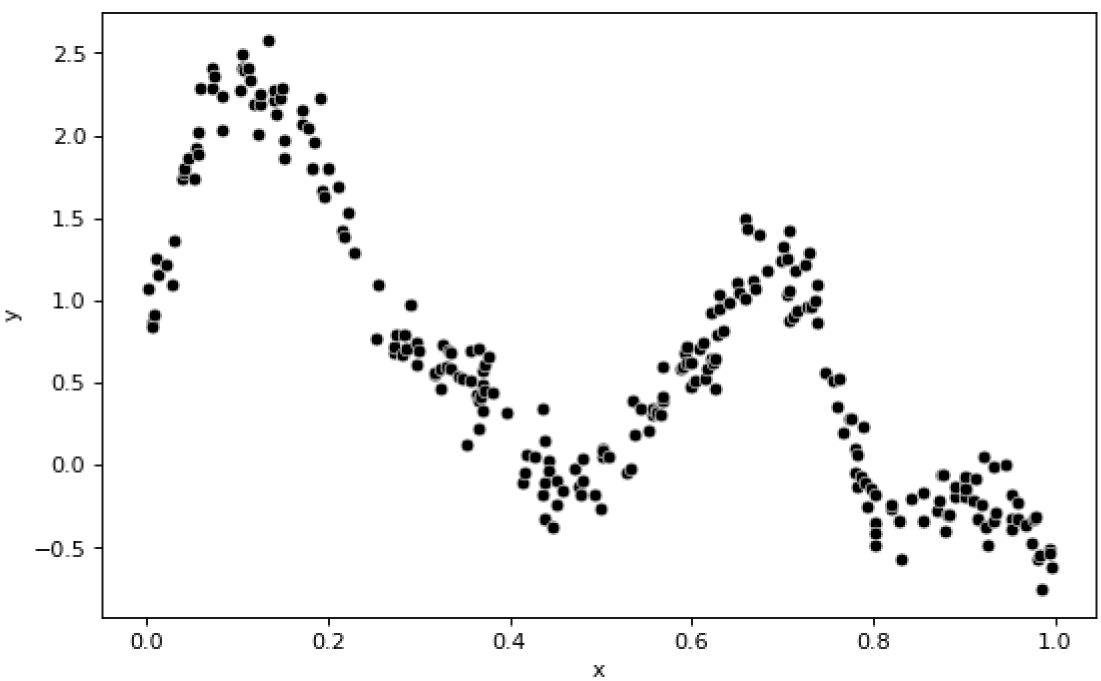
1.1.2 1.2 Data

The data set we will be using today is synthetic data that was generated via a random draw from a Gaussian Process model. The resulting data represent an unknown smooth function $y = f(x) + \epsilon$. We will be implementing a variety of approaches for deriving a parameterized model of this function using least squares regression.

We can read the data in from `gp.csv` and generate a scatter plot to get a sense of the shape of the function.

[2]:
```python
d = pd.read_csv("gp.csv")
n = d.shape[0] # number of rows

sns.scatterplot(x='x', y='y', data=d, color="black")
d
```

[2]:
```
            x         y
0    0.002189  1.070772
1    0.006209  0.863336
2    0.006764  0.846165
3    0.009349  0.916748
4    0.012407  1.258828
..        ...       ...
245  0.982005 -0.540678
246  0.983324 -0.751002
247  0.992081 -0.510908
248  0.993567 -0.537508
249  0.994654 -0.621642

[250 rows x 2 columns]
```

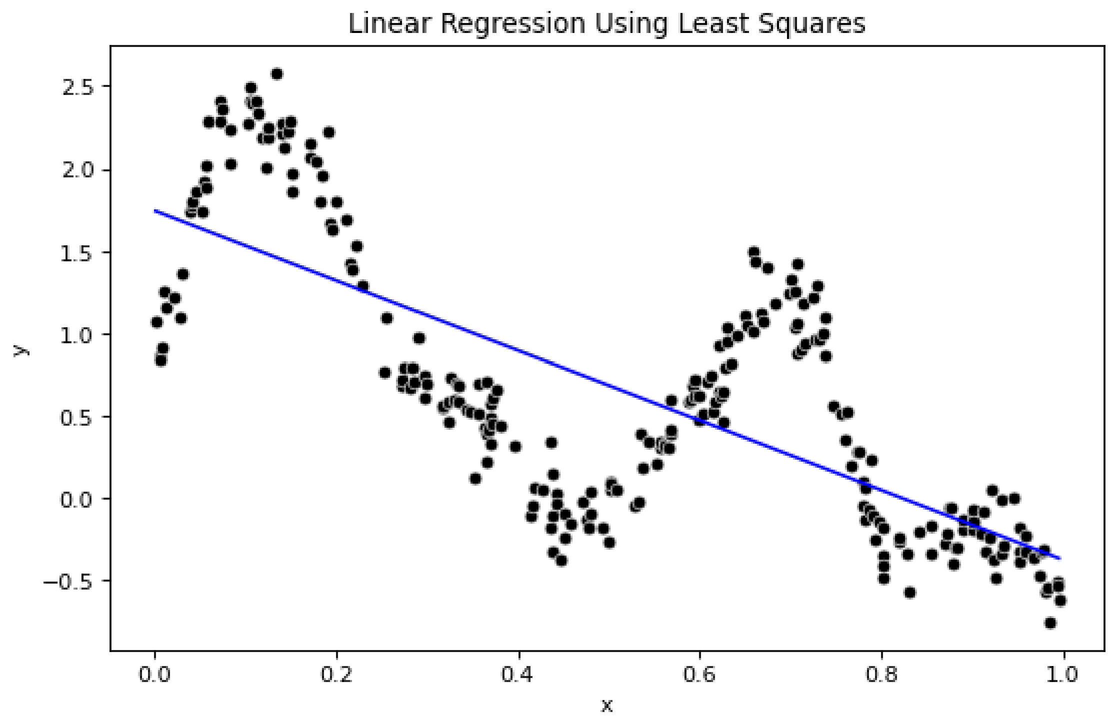


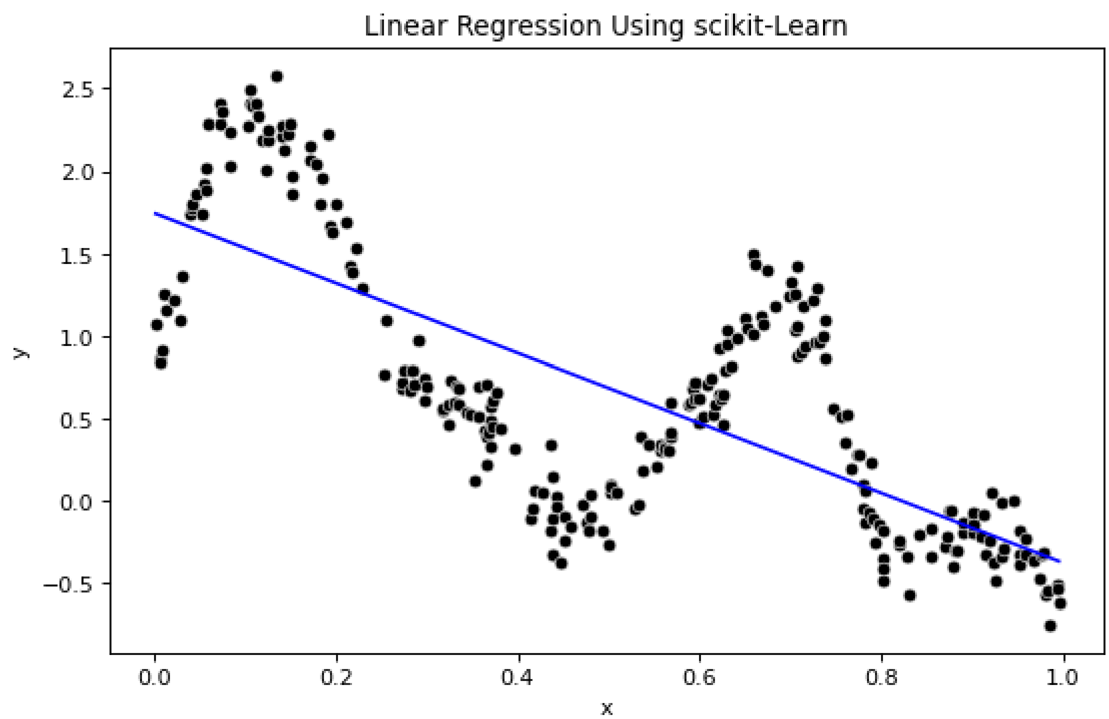
1.1.3 Exercise 1

Fit a linear regression model to these data, and create a plot of the regression line overlayed on the original data. Your models predictions should be stored in a new column in `d` called `pred_lm`.

[3]:
```
# Method 1 - Using Least Squares

X = np.c_[
    np.ones(n),
    d.x
]

y = np.array(d.y)

beta = np.linalg.solve(X.T @ X, X.T @ y)

yhat = X @ beta

d['pred_lm'] = yhat

plt.title('Linear Regression Using Least Squares')
sns.scatterplot(x='x', y='y', data=d, color="black")
sns.lineplot(x="x", y="pred_lm", color="blue", data=d)


# Method 2 - Using scikit-Learn

linear_model = LinearRegression(fit_intercept = False).fit(X, d.y)
beta2 = linear_model.coef_

d['pred_lm2'] = linear_model.predict(X)

plt.figure()
plt.title('Linear Regression Using scikit-Learn')
sns.scatterplot(x='x', y='y', data=d, color="black")
sns.lineplot(x="x", y="pred_lm2", color="blue", data=d)

# We see that with both forms we get the same linear model plotted.
```

[3]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fac4e4d6ad0>
```


Linear Regression Using Least Squares
y
x
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0


Linear Regression Using scikit-Learn
y
x
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

1.1.4 Exercise 2

Calculate the mean squared error of your linear model's predictions. The function `mean_squared_error` from `sklearn.metrics` will be useful for this. See the functions documentation here.

[4]:
```
from sklearn.metrics import mean_squared_error

mse = mean_squared_error(d.y, d.pred_lm)
print(mse)
```

```
0.30684493321337125
```

1.2 2. Polynomial Regression

Polynomial regression is a straight forward approach to capturing simple non-linear relationships between a feature and our response variable. At its core, polynomial regression amounts to the inclusion of additional columns in the model matrix that are powers of the feature of interest.

1.2.1 2.1 By hand

For a single feature and low order polynomials this is can be done by hand. For example, if we want to fit a quadratic model to these data we can do the following,

[5]:
```
y = d.y
X = np.c_[
    np.ones(n),
    d.x,
    d.x**2
]

l = LinearRegression(fit_intercept = False).fit(X,y)

print(l.coef_)
```

```
[ 1.96397561 -3.42899677  1.30199921]
```

Which gives us the following model for the data,

$$\hat{y} = 1.96 - 3.43x + 1.30x^2$$

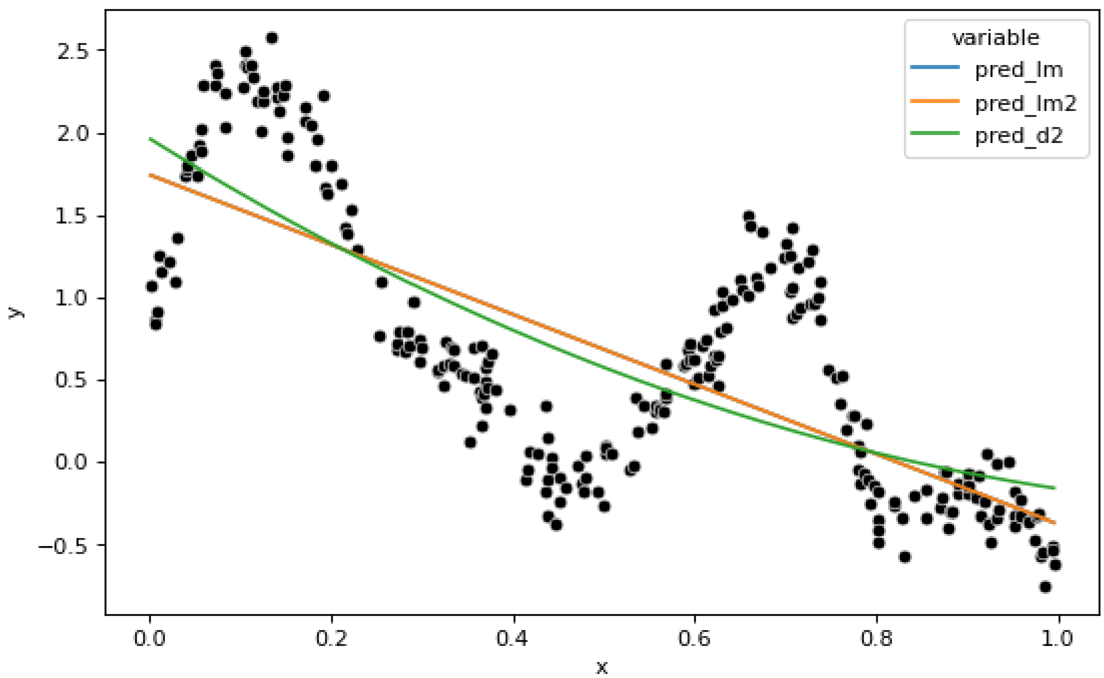
The predictons of this model are then,

[6]:
```
d["pred_d2"] = l.predict(X)

sns.scatterplot(x='x', y='y', data=d, color="black")
```

```
sns.lineplot(x='x', y='value', hue="variable", data=pd.
 ↪melt(d,id_vars=["x","y"]))

d
```

[6]:

```
            x         y   pred_lm  pred_lm2   pred_d2
0    0.002189  1.070772  1.741303  1.741303  1.956474
1    0.006209  0.863336  1.732770  1.732770  1.942737
2    0.006764  0.846165  1.731590  1.731590  1.940841
3    0.009349  0.916748  1.726103  1.726103  1.932033
4    0.012407  1.258828  1.719609  1.719609  1.921633
..        …         …         …         …         …
245  0.982005 -0.540678 -0.339009 -0.339009 -0.147754
246  0.983324 -0.751002 -0.341809 -0.341809 -0.148902
247  0.992081 -0.510908 -0.360403 -0.360403 -0.156408
248  0.993567 -0.537508 -0.363558 -0.363558 -0.157661
249  0.994654 -0.621642 -0.365865 -0.365865 -0.158574

[250 rows x 5 columns]
```



Note that the predicted values from this model form a curve rather than a straight line - specifically we have found the quadratic curve that best fits our data. We have used the pandas function `melt` to restructure our data frame, this is not strictly needed here but will be necessary for later examples. See the pandas documentation on `melt` for futher details.

1.2.2 Exercise 3

Calculate the mean square error of this quadratic polynomial model. How does it compare to the linear model we previously fit?

[7]:
```
mse2 = mean_squared_error(d.y, d.pred_d2)
print(mse2)
```

```
0.2969616424742076
```

Using a model of degree two, we fit the data slightly better - resulting in a lower mse. Ideally, we should use a higher degree polynomial to reduce mse even further.

A cubic model can be similarly fit by adding a column containing x^3 to the previous model matrix (`X`). Note that by convention when fitting a polynomial model of degree n we include all powers from 0 to n, so for a cubic model our model matrix should include x^0, x^1, x^2, and x^3.

[8]:
```
X = np.c_[X, d.x**3]
l = LinearRegression(fit_intercept = False).fit(X,y)

print(l.coef_)
```

```
[ 2.36985684 -8.49429068 13.95066369 -8.39215284]
```

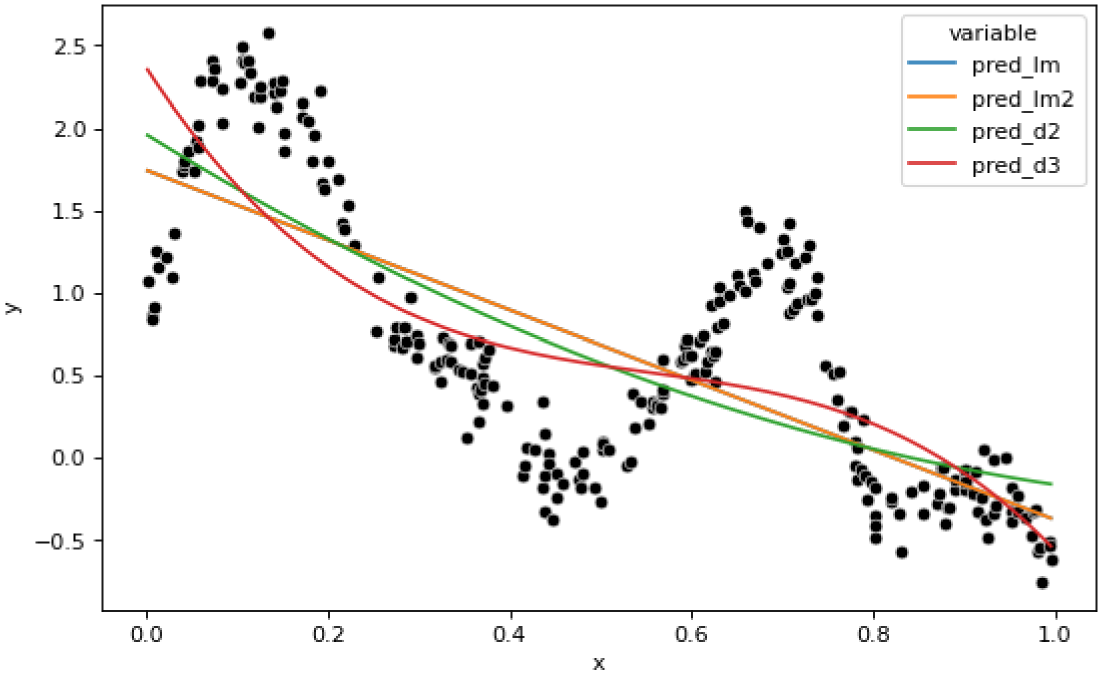
This gives us a cubic model with the form,

$$\hat{y} = 2.37 - 8.49x + 13.9x^2 - 8.39x^3$$

and predictions of this model are then,

[9]:
```
d["pred_d3"] = l.predict(X)

sns.scatterplot(x='x', y='y', data=d, color="black")
sns.lineplot(x='x', y='value', hue="variable", data=pd.
 ↪melt(d,id_vars=["x","y"]))
```

[9]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fac4e386dd0>
```



1.2.3 Exercise 4

Calculate the mean square error of the cubic polynomial model. How does this model compare to your previous models?

[10]:
```
mse = mean_squared_error(d.y, d.pred_d3)
print(mse)
```

```
0.27124908717801827
```

The mse has reduced further

1.2.4 2.2 sklearn and polynomial features

sklearn has a built in function called `PolynomialFeatures` which can be used to simplify the process of including polynomial features in a model. This function is included in the *preprocessing* module of sklearn, as with other python functions we can import it as follows.

[11]:
```
from sklearn.preprocessing import PolynomialFeatures
```

Construction and use of this and other transformers is similar to what we have already seen with `LinearRegression`, we construct a `PolynomialFeatures` object in which we set basic options (e.g. the degree of the polynomial) and then apply the transformation to our data via `fit_transform` method. This will generate a new model matrix which includes the polynomial features up to the degree we have specified.

To demonstrate the core features we will start with a toy example and then replicate the models we constructed in Section 2.1. Below we construct our sample data vector and then pass it into the transformer,

[12]:
```
x = np.array([1,2,3,4]) # Initial data
```

[13]:
```
PolynomialFeatures(degree = 2).fit_transform(x)
```

```
 ␣
↪---------------------------------------------------------------------------

 ValueError                                Traceback (most recent call␣
↪last)

 <ipython-input-13-d08876eb1631> in <module>
----> 1 PolynomialFeatures(degree = 2).fit_transform(x)


 /opt/conda/lib/python3.7/site-packages/sklearn/base.py in␣
↪fit_transform(self, X, y, **fit_params)
    688         if y is None:
    689             # fit method of arity 1 (unsupervised transformation)
--> 690             return self.fit(X, **fit_params).transform(X)
    691         else:
    692             # fit method of arity 2 (supervised transformation)


 /opt/conda/lib/python3.7/site-packages/sklearn/preprocessing/_data.py in␣
↪fit(self, X, y)
   1511         """
   1512         n_samples, n_features = self._validate_data(
-> 1513             X, accept_sparse=True).shape
   1514         combinations = self._combinations(n_features, self.degree,
   1515                                           self.interaction_only,


 /opt/conda/lib/python3.7/site-packages/sklearn/base.py in␣
↪_validate_data(self, X, y, reset, validate_separately, **check_params)
    418                     f"requires y to be passed, but the target y is␣
↪None."
    419                 )
```

```
--> 420             X = check_array(X, **check_params)
    421             out = X
    422         else:


    /opt/conda/lib/python3.7/site-packages/sklearn/utils/validation.py in␣
↪inner_f(*args, **kwargs)
     70                           FutureWarning)
     71         kwargs.update({k: arg for k, arg in zip(sig.parameters,␣
↪args)})
---> 72         return f(**kwargs)
     73     return inner_f
     74


    /opt/conda/lib/python3.7/site-packages/sklearn/utils/validation.py in␣
↪check_array(array, accept_sparse, accept_large_sparse, dtype, order, copy,␣
↪force_all_finite, ensure_2d, allow_nd, ensure_min_samples,␣
↪ensure_min_features, estimator)
    621                     "Reshape your data either using array.
↪reshape(-1, 1) if "
    622                     "your data has a single feature or array.
↪reshape(1, -1) "
--> 623                     "if it contains a single sample.".format(array))
    624
    625         # in the future np.flexible dtypes will be handled like␣
↪object dtypes


    ValueError: Expected 2D array, got 1D array instead:
array=[1 2 3 4].
Reshape your data either using array.reshape(-1, 1) if your data has a␣
↪single feature or array.reshape(1, -1) if it contains a single sample.
```

When we run the above code we get an error because currently `x` is a 1D vector when the `fit_transform` function is expected a 2D array (the same will also happen with `LinearRegression`'s `fit` method). To solve this we need to make sure that the value we pass has the correct dimensions, `x.reshape(-1, 1)` is suggested by the error and corrects the issue.

[14]:
```
PolynomialFeatures(degree = 2).fit_transform(x.reshape(-1,1))
```

[14]:
```
array([[ 1.,  1.,  1.],
       [ 1.,  2.,  4.],
       [ 1.,  3.,  9.],
       [ 1.,  4., 16.]])
```

Alternatively, we can alsu use the `np.c_` function to construct the matrix.

[15]:
```python
PolynomialFeatures(degree = 2).fit_transform(np.c_[x]) # Order 2 polynomial␣
↪model matrix for x
```

[15]:
```
array([[ 1.,  1.,  1.],
       [ 1.,  2.,  4.],
       [ 1.,  3.,  9.],
       [ 1.,  4., 16.]])
```

[16]:
```python
PolynomialFeatures(degree = 3).fit_transform(np.c_[x]) # Order 3 polynomial␣
↪model matrix for x
```

[16]:
```
array([[ 1.,  1.,  1.,  1.],
       [ 1.,  2.,  4.,  8.],
       [ 1.,  3.,  9., 27.],
       [ 1.,  4., 16., 64.]])
```

Note that when we use this transform we get all of the polynomial transformations of x from **0** to `degree`. In this case, the 0 degree column is equivalent to the intercept column. If for some reason we did not want to include this we can construct `PolynomialFeatures` with `include_bias=False`.

[17]:
```python
PolynomialFeatures(degree = 3, include_bias=False).fit_transform(np.c_[x])
```

[17]:
```
array([[ 1.,  1.,  1.],
       [ 2.,  4.,  8.],
       [ 3.,  9., 27.],
       [ 4., 16., 64.]])
```

We can now apply this to our original data by storing the result as `X` then passing this new model matrix to the linear regression fit method.

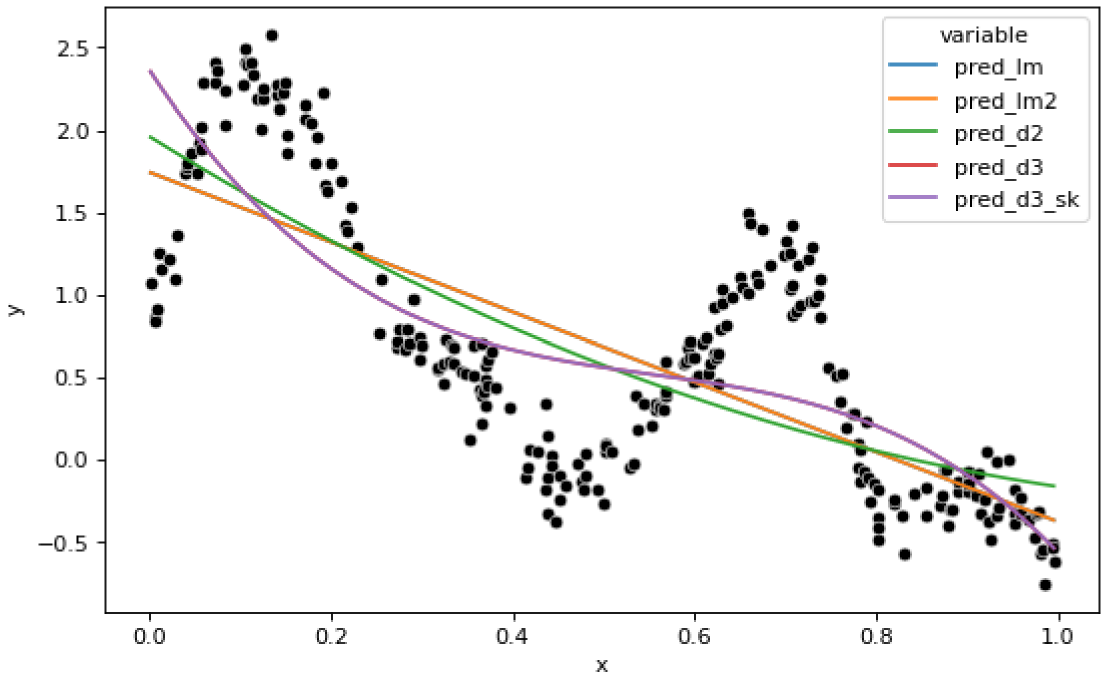
[18]:
```python
X = PolynomialFeatures(degree = 3).fit_transform(np.c_[d.x])

l = LinearRegression(fit_intercept = False).fit(X,d.y)
print(l.coef_)
```

```
[ 2.36985684 -8.49429068 13.95066369 -8.39215284]
```

These values match those we obtained from the earlier cubic model, and we can also see this when plotting the model predictons.

[19]:
```python
d["pred_d3_sk"] = l.predict(X)

sns.scatterplot(x='x', y='y', data=d, color="black")
sns.lineplot(x='x', y='value', hue="variable", data=pd.
↪melt(d,id_vars=["x","y"]))
```

[19]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fac4e1562d0>
```



We can not even see the `pred_d3` line as it is being overplotted by the `pred_d3_sk` line.

1.2.5 2.3 Pipelines

You may have noticed that `PolynomialFeatures` takes a model matrix as input and returns a new model matrix as output which is then used as the input for `LinearRegression`. This is not an accident, and by structuring the library in this way sklearn is designed to enable the connection of these steps together, into what sklearn calls a *pipeline*.

We can modularize and simply our code somewhat by creating a pipeline that takes our original data, performs a polynomial feature transform and then feeds the results into a linear regression. We can accomplish this via the `make_pipeline` function from the `pipeline` module.

[20]:
```
from sklearn.pipeline import make_pipeline

poly_model = make_pipeline(
    PolynomialFeatures(degree=4),
    LinearRegression()
)

print(poly_model)
```

```
Pipeline(steps=[('polynomialfeatures', PolynomialFeatures(degree=4)),
                ('linearregression', LinearRegression())])
```

The resulting object represents a new "model" which can then be fit to data.

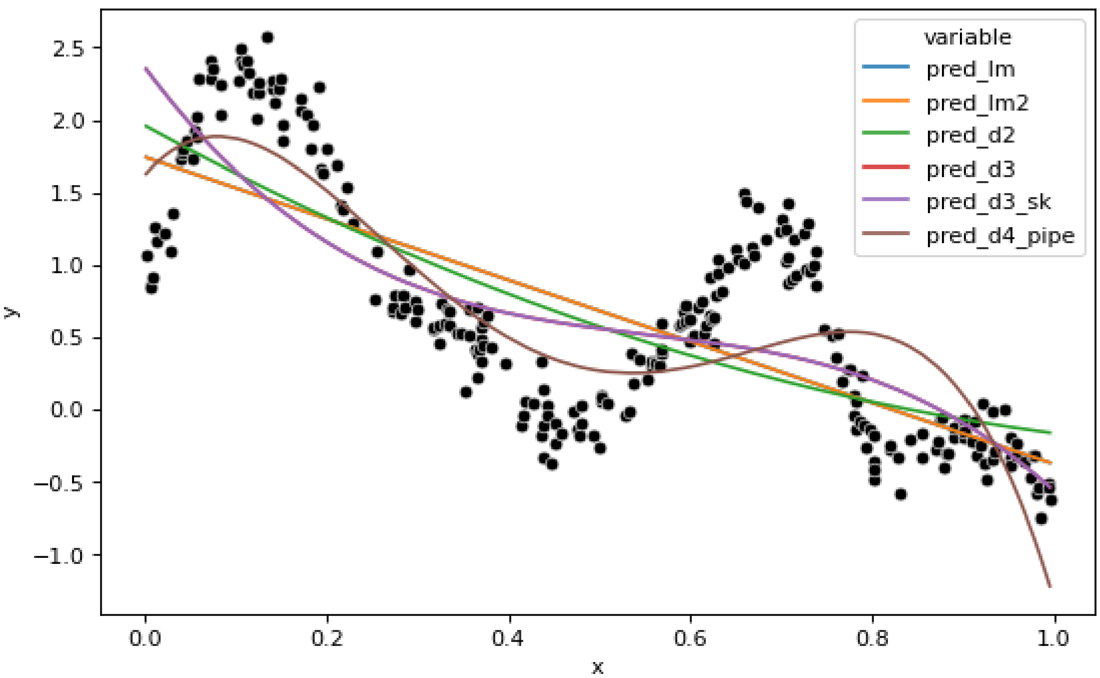
[21]:
```
p = poly_model.fit(np.c_[d.x], d.y)
print(p)
```

```
Pipeline(steps=[('polynomialfeatures', PolynomialFeatures(degree=4)),
                ('linearregression', LinearRegression())])
```

and used to create predictions just like our previous `LinearRegression` model.

[22]:
```
d['pred_d4_pipe'] = p.predict(np.c_[d.x])

sns.scatterplot(x='x', y='y', data=d, color="black")
sns.lineplot(x='x', y='value', hue="variable", data=pd.
 ↪melt(d,id_vars=["x","y"]))
```

[22]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fac4e097a50>
```



The returned object is a `Pipeline` object so it will not provide direct access to step properties, such as the coefficients for the regression model.

[23]:
```
print(p.coef_)
```

```
␣
↪---------------------------------------------------------------------------
```

```
AttributeError                            Traceback (most recent call␣
↪last)

<ipython-input-23-806ff5269aa8> in <module>
----> 1 print(p.coef_)


AttributeError: 'Pipeline' object has no attribute 'coef_'
```

If we want access to the attributes or methods of a particular step we need to first access that step using either its name or position.

[24]:
```
print(p.named_steps['linearregression'].coef_)
```

```
[  0.           7.39051417 -57.67175293 102.72227443 -55.38181361]
```

[25]:
```
print(p.steps[1][1].intercept_) # second subset is necessary here because
                                # each step is a tuple of a name and the
                                # model / transform object
```

```
1.6136636604768269
```

Also note that both the `'linearregression'` and `'polynomialfeatures'` step introduce a column of ones into the model matrix. This potentially introduces a rank deficiency in our model matrix, however sklearn handles this by fixing the coefficient of the duplicate intercept column to 0. The result however is that the intercept is now stored in `intercept_` and not `coef_`. If we wished to avoid this we would need to construct our pipeline using `LinearRegression(fit_intercept=False)`.

[26]:
```
p = make_pipeline(
    PolynomialFeatures(degree=4),
    LinearRegression(fit_intercept = False)
).fit(
    np.c_[d.x],
    d.y
)

print(p.named_steps['linearregression'].coef_)
print(p.named_steps['linearregression'].intercept_)
```

```
[  1.61366366   7.39051417 -57.67175293 102.72227443 -55.38181361]
0.0
```

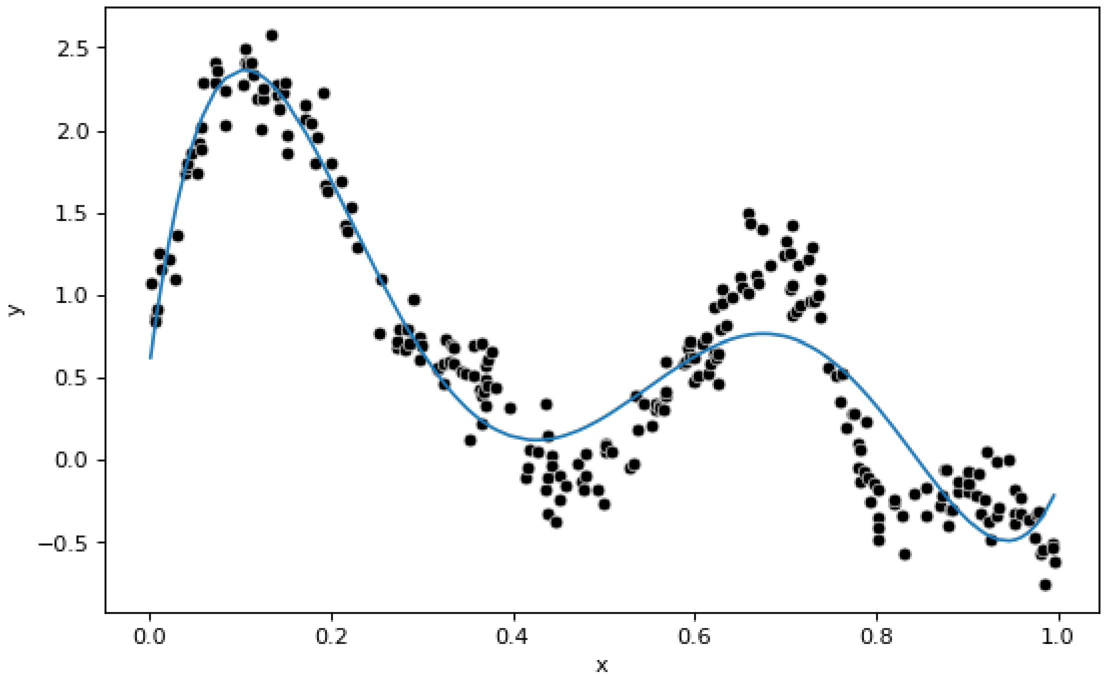
1.2.6 2.4 Putting it all together

So far each time we've wanted to fit a polynomial regression model we've had to set up the various data objects and then create the sklearn model and transformation objects and then get a final result of the coefficients or a plot - because of this the preceeding cells contain a lot of duplicated code which is something we should be trying to avoid.

Our modeling task here is like many other programming tasks, when we find ourselves reusing the same code over and over it is time to consider writing a function. Below I have implemented a function called `poly_reg` that allows the user to provide a data frame and specific the names of the `x` column an d `y` column as well as the degree of the polynomial we would like to fit. The function returns the original data frame with the model predictions added as well as the model coefficients in a tuple.

[27]:
```
def poly_reg(data, x = 'x', y = 'y', degree=1, plot_data = True, plot_fit =␣
 ↪True):
    X = np.c_[data[x]]
    Y = data[y]

    p = make_pipeline(
        PolynomialFeatures(degree=degree),
        LinearRegression(fit_intercept=False)
    )

    m = p.fit(X,Y)

    pred_col = 'pred_d'+str(degree)
    data[pred_col] = m.predict(X)

    if plot_data:
        sns.scatterplot(x=data[x], y=data[y], color="black")

    if plot_fit:
        sns.lineplot(x=data[x], y=data[pred_col])

    return (data, m.steps[1][1])
```

[28]:
```
_, _ = poly_reg(d, degree=5)
```

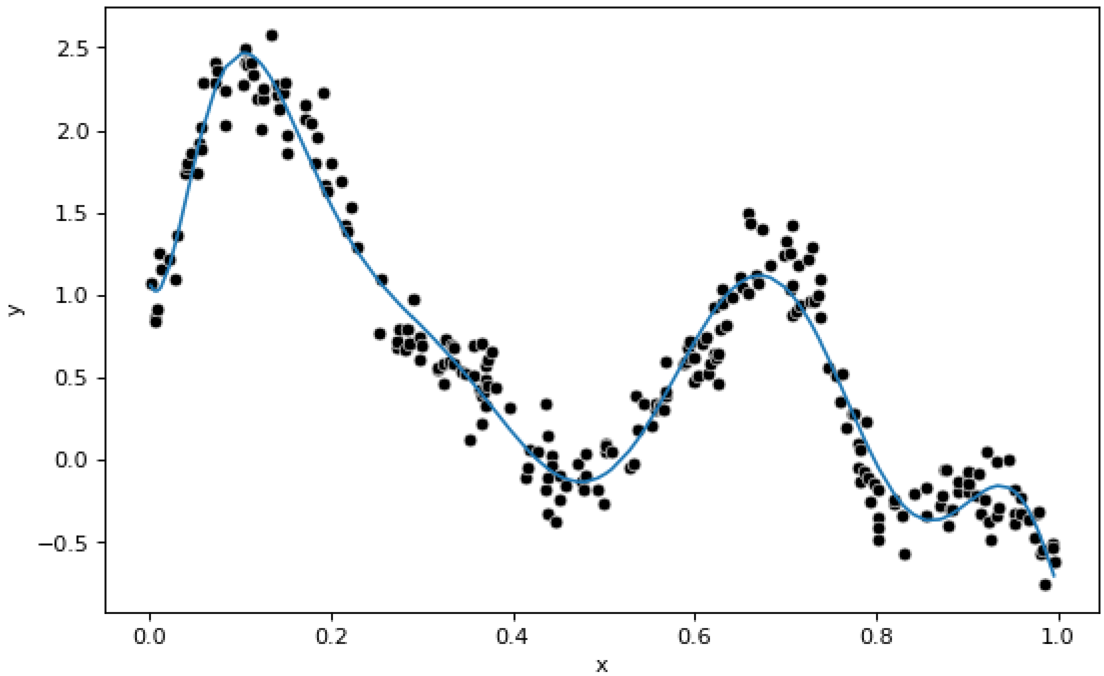


Since we are not using either the data frame or model coefficients we unpack them into `_`.

1.2.7 Exercise 5

Use the `poly_reg` function to fit a variety of different polynomial models to the data. What values of `degree` provides the best fit (judged qualitatively not quantitatively).

[29]:
```
degrees = [
    #5,6,7,8,
    #9,
    10,
    #11,
    #12,
    #13,
    #14,
    #20
]

for i in degrees:
    poly_reg(d, degree=i)

# It looks like values above 10 provide a good fit
```



1.2.8 Exercise 6

In the cell below we have provided a copy of the `poly_reg` function, modify this function such that it returns a 3rd value that is the mean square error of the predictions for the model. Check that the value returned by the function matches the MSE you calculated in **Exercises 2-4**.

[30]:
```
def poly_reg_mse(data, x = 'x', y = 'y', degree=1, plot_data = True, plot_fit =␣
 ↪True):
    X = np.c_[data[x]]
    Y = data[y]

    p = make_pipeline(
        PolynomialFeatures(degree=degree),
        LinearRegression(fit_intercept=False)
    )

    m = p.fit(X,Y)

    pred_col = 'pred_d'+str(degree)
    data[pred_col] = m.predict(X)

    #print(data.y)
```

```
    #print()

    mse = mean_squared_error(data.y, m.predict(X))

    if plot_data:
        sns.scatterplot(data[x],data[y], color="black")

    if plot_fit:
        sns.lineplot(data[x],data[pred_col])

    return (data, m.steps[1][1], mse)
```

Below are three calls to this function which report these MSE values.

[31]:
```
_, _, mse_d1 = poly_reg_mse(d, degree=1, plot_data=False, plot_fit=False)
_, _, mse_d2 = poly_reg_mse(d, degree=2, plot_data=False, plot_fit=False)
_, _, mse_d3 = poly_reg_mse(d, degree=3, plot_data=False, plot_fit=False)


print("deg=1:", mse_d1)
print("deg=2:", mse_d2)
print("deg=3:", mse_d3)
```

```
deg=1: 0.3068449332133712
deg=2: 0.2969616424742076
deg=3: 0.27124908717801816
```

1.2.9 Exercise 7

Construct a data frame called `poly_res` with the columns `degree` and `mse`. `degree` should contain the integer values 1 to 20 and `mse` should contain the mean squared errors, calculated using the function `poly_reg_mse`, for each of the different `degree` values.

[32]:
```
high_degree= 21
degreelist = np.linspace(1,high_degree,num=high_degree, dtype = int)
mses = []

for i in degreelist:
    _, _, mse = poly_reg_mse(d, degree=i, plot_data=False, plot_fit=False)
    mses.append(mse)

dictionary1 = {'degree' : degreelist, 'mse' : mses}

poly_res= pd.DataFrame(data=dictionary1)
```

```
poly_res
```

[32]:

	degree	mse
0	1	0.306845
1	2	0.296962
2	3	0.271249
3	4	0.203277
4	5	0.077071
5	6	0.076422
6	7	0.067818
7	8	0.047326
8	9	0.043203
9	10	0.031921
10	11	0.027017
11	12	0.026995
12	13	0.026437
13	14	0.026291
14	15	0.023590
15	16	0.023289
16	17	0.019938
17	18	0.019937
18	19	0.019881
19	20	0.019872
20	21	0.019873

[33]:

```
#np.linspace?
#np.append?
pd.DataFrame?

#np.linspace(1,20,num=20, dtype = int)
```

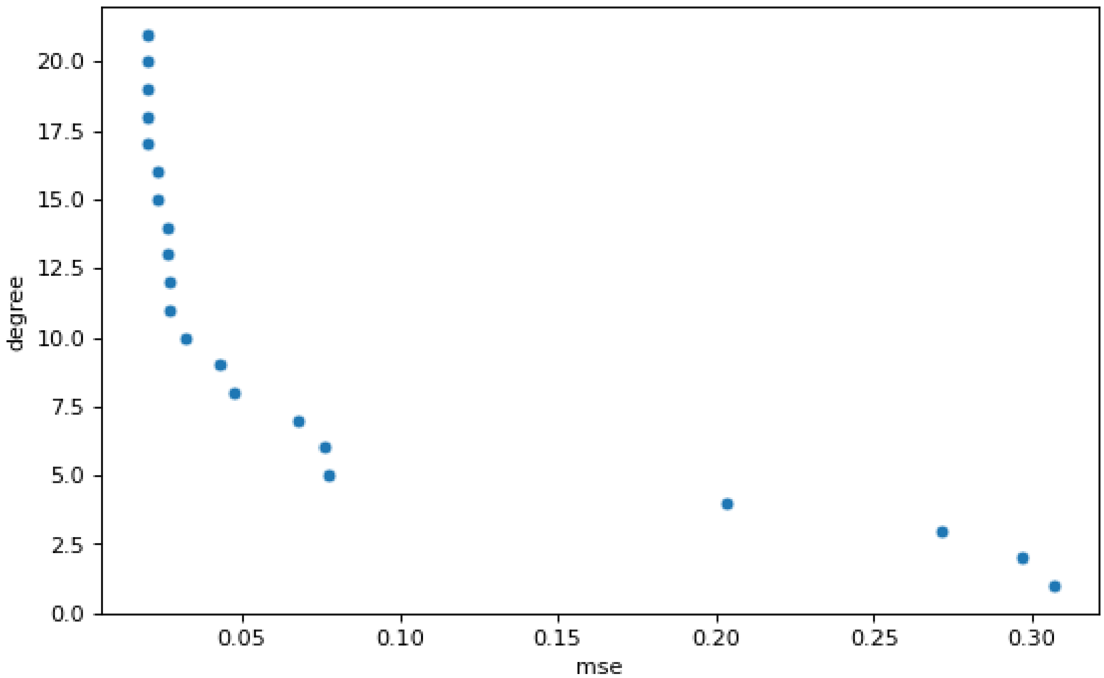
1.2.10 Exercise 8

Create a plot of `degree` vs. `mse` using the `poly_res` data frame you created above. Based on this comment on what model appears to best fit the data.

[34]:

```
sns.scatterplot(x = poly_res.mse,y = poly_res.degree)
#plt.yticks(np.linspace(0,20,num=20,dtype = int))

# If we consider the model with the lowest mse to be the best fit then the
↪model of degree 20 fits the data best
```

[34]: <matplotlib.axes._subplots.AxesSubplot at 0x7fac4df37b50>



1.2.11 Exercise 9

Based on your findings in the preceding exercises, can we find the "optimal model" using this kind of approach? Explain why or why not.

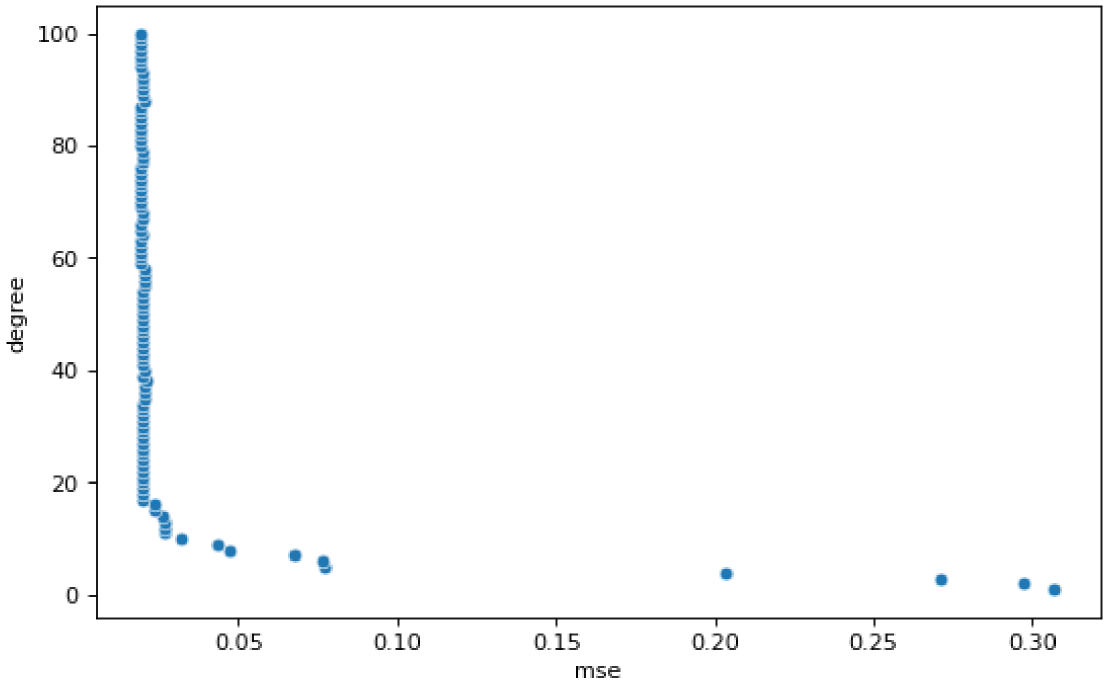
I beleive that we cannot find an optimal model in this way. The simple mean squared error is a one dimensional metric attempting to describe a two dimensional problem and so we will always encounter a problem.

We can see that if we calcualte the mse up to degree 100,

[35]:
```
high_degree= 100
degreelist = np.linspace(1,high_degree,num=high_degree, dtype = int)
mses = []

for i in degreelist:
    _, _, mse = poly_reg_mse(d, degree=i, plot_data=False, plot_fit=False)
    mses.append(mse)

dictionary1 = {'degree' : degreelist, 'mse' : mses}

poly_res= pd.DataFrame(data=dictionary1)
```

```
sns.scatterplot(x = poly_res.mse,y = poly_res.degree)
print(poly_res.min())
```

```
degree    1.000000
mse       0.019166
dtype: float64
```



It appears that the mse falls to a minimum value of 0.019166 over the first 100 iterations. However, not indicating an optimal model.

1.3 3. Regression Trees (via feature engineering)

Later in this course we will be covering proper regression tree models, including the algorithms for fitting them. For today we will be exploring a simplified version of these models as a way of further exploring feature engineering via sklearn's feature transformers and pipelines.

Here we will consider a simple basis function of the form,

$$f_j(x; a_j, b_j) = \begin{cases} 1 & \text{if } a_j \leq x < b_j \\ 0 & \text{otherwise} \end{cases}$$

This reflects one possible basis function that we might choose to better fit our data. In order to use these functions to transform our data, we will need to choose the values of a and b as well as the number of basis functions to use M. Given those choices our goal is to then to fit the model,

$$y_i = \beta_1 f(x_i; a_1, b_1) + \beta_2 f(x_i; a_2, b_2) + \ldots + \beta_M f(x_i; a_M, b_M)$$

1.3.1 Exercise 10

Explain why we are not able to directly use the least squares approach to find optimal values of a, b, and M to fit our data.

The least squares estimate in this case is just $\hat{w}_m = \bar{y}_m$ (from lectures) and so gives us no information about a,b or M.

1.3.2 3.1 With pandas

For our example today, we will keep things simple and divide our `x` values up into 11 equal sized pieces: $[0, 0.1)$, $[0.1, 0.2)$, $\ldots$, $[0.9, 1)$. This can be achieved using pandas' `cut` function as follows,

[36]:
```
d = pd.read_csv("gp.csv") # Get a clean copy of the data

d["x_bin"] = pd.cut(d.x, np.linspace(0,1,11))
print(d)
```

```
            x         y       x_bin
0    0.002189  1.070772  (0.0, 0.1]
1    0.006209  0.863336  (0.0, 0.1]
2    0.006764  0.846165  (0.0, 0.1]
3    0.009349  0.916748  (0.0, 0.1]
4    0.012407  1.258828  (0.0, 0.1]
..        …         …          …
245  0.982005 -0.540678  (0.9, 1.0]
246  0.983324 -0.751002  (0.9, 1.0]
247  0.992081 -0.510908  (0.9, 1.0]
248  0.993567 -0.537508  (0.9, 1.0]
249  0.994654 -0.621642  (0.9, 1.0]

[250 rows x 3 columns]
```

`np.linspace` is used here to specify the cut points and returns the array `[0,0.1,...,0.9,1]`. The results new column `x_bin` now contains a categorical variable for the interval containing the `x` value for that row.

We can then use pandas' `get_dummies` to transform this categorical variable using one hot encoding. After brief examination you should be able to see that this is equivalent applying the 11 basis functions (columns) to each of the `x` values (rows) using the ranges we've described.

[37]:
```
pd.get_dummies(d.x_bin)
```

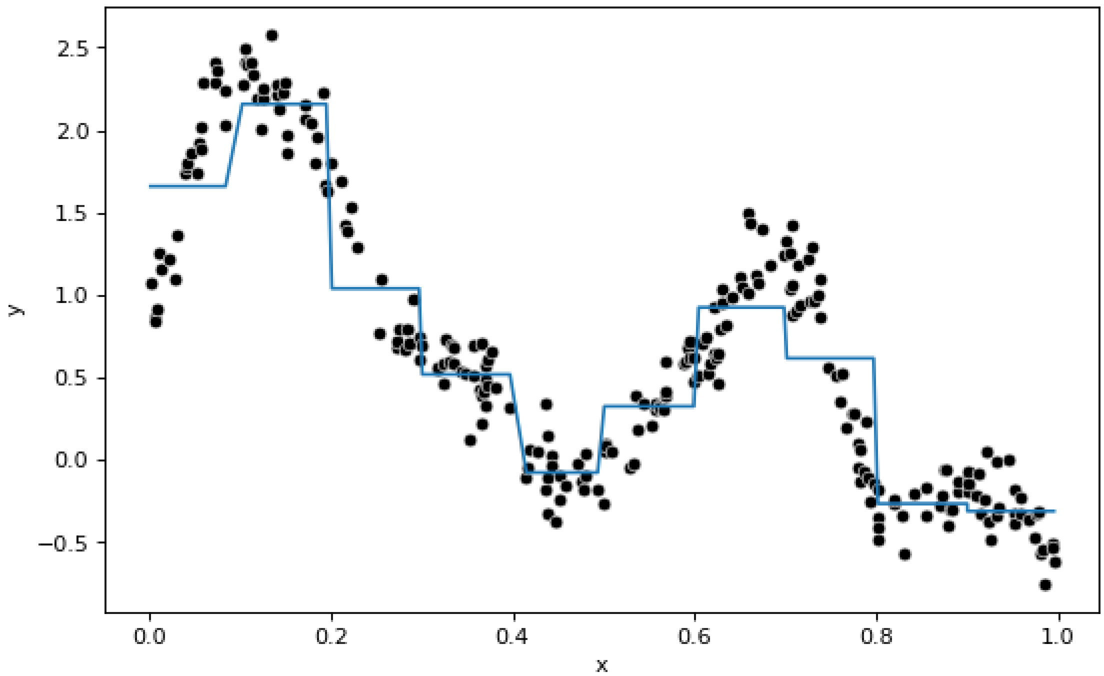
[37]:
```
     (0.0, 0.1]  (0.1, 0.2]  (0.2, 0.3]  (0.3, 0.4]  (0.4, 0.5]  (0.5, 0.6]  \
0             1           0           0           0           0           0
1             1           0           0           0           0           0
2             1           0           0           0           0           0
3             1           0           0           0           0           0
4             1           0           0           0           0           0
..          ...         ...         ...         ...         ...         ...
245           0           0           0           0           0           0
246           0           0           0           0           0           0
247           0           0           0           0           0           0
248           0           0           0           0           0           0
249           0           0           0           0           0           0

     (0.6, 0.7]  (0.7, 0.8]  (0.8, 0.9]  (0.9, 1.0]
0             0           0           0           0
1             0           0           0           0
2             0           0           0           0
3             0           0           0           0
4             0           0           0           0
..          ...         ...         ...         ...
245           0           0           0           1
246           0           0           0           1
247           0           0           0           1
248           0           0           0           1
249           0           0           0           1

[250 rows x 10 columns]
```

We can then fit a linear regression model using only these dummy variable and obtain the following model fit,

[38]:
```
X = pd.get_dummies(d.x_bin)
y = d.y

l = LinearRegression(fit_intercept=False).fit(X,y)
d["pred_M11"] = l.predict(X)
```

[39]:
```
sns.scatterplot(x='x', y='y', data=d, color="black")
sns.lineplot(x='x', y='pred_M11', data=d)
```

[39]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fac4de44d50>
```



1.3.3 Exercise 11

Calculate the mean squared error of this model. How does it compare to the polynomial models we fit previously?

[41]:
```
mse = mean_squared_error(d.y, d.pred_M11)
print(mse)

# This MSE is equivalent to between a degree 3 and 4 polynomial
```

```
0.0985882258438611
```

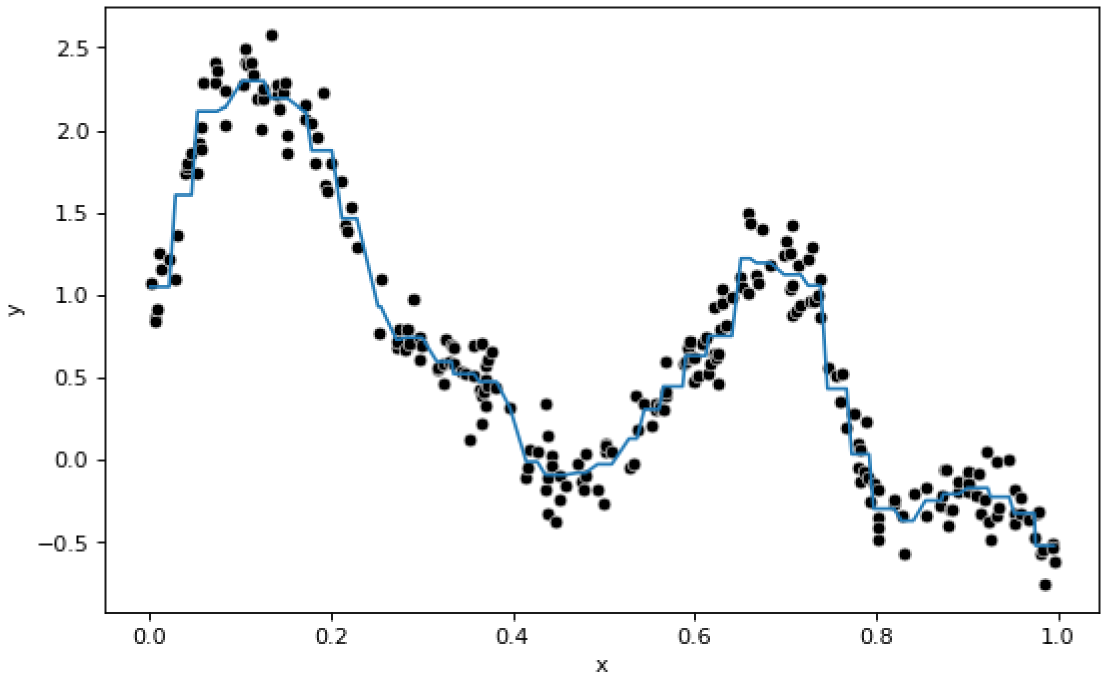
1.3.4 Exercise 12

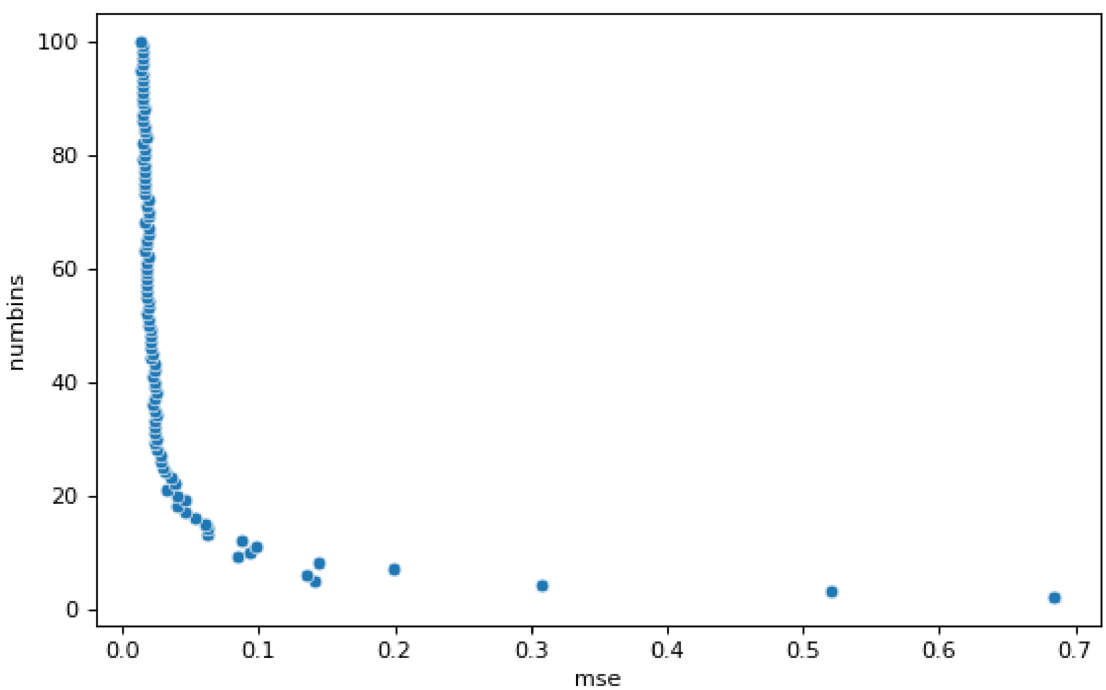
Repeat this fitting procedure, but vary the number of bins being used (by changing the 3rd parameter in `np.linspace`). How does the MSE compare to the previous models?

[75]:
```
def RegressionTree(data, num_bins=1, plot_data = True,return_mse = True):
    data["x_bin"] = pd.cut(data.x, np.linspace(0,1,num_bins))
```

```
    X = pd.get_dummies(data.x_bin)
    y = data.y

    l = LinearRegression(fit_intercept=False).fit(X,y)
    data["pred_M11"] = l.predict(X)

    if plot_data:
        sns.scatterplot(x='x', y='y', data=data, color="black")
        sns.lineplot(x='x', y='pred_M11', data=data)

    mse1 = mean_squared_error(data.y, data.pred_M11)
    if return_mse:
        return mse1
    return

data = pd.read_csv("gp.csv") # Get a clean copy of the data
mse2 = RegressionTree(data,num_bins=40)
print(mse2)
#data[:20]

high_degree= 100
degreelist = np.linspace(2,high_degree,num=high_degree-1, dtype = int)
mses = []

for i in degreelist:
    mse = RegressionTree(data,num_bins=i, plot_data = False)
    #print(mse)
    mses.append(mse)

dictionary2 = {'numbins' : degreelist, 'mse' : mses}

reg_tree_res= pd.DataFrame(data=dictionary2)
#print(reg_tree_res)

plt.figure()
sns.scatterplot(x = reg_tree_res.mse,y = reg_tree_res.numbins)
print(reg_tree_res.min())
```

```
0.023510607859067777
numbins    2.000000
mse        0.013284
dtype: float64
```





Here, we have plotted the first 100 regression trees and we see that the mse decreases as the number of bins increases. It is also true that the lowest mse for a regression tree is 0.01324 which is considerably lower than the best polynomial mse of 0.019166. It appears that this method gives us the lowest mse of all our previous attempts.

1.3.5 3.2 With sklearn

A similar process can be achieved with sklearn's `KBinsDiscretizer` from the *preprocessing* submodule.

[76]:
```
from sklearn.preprocessing import KBinsDiscretizer
```

The key arguments for this transformer are `n_bins` which determines the number of bins, `encode` which determines how the transformed values are encoded, and `strategy` which is used to determine bin widths. To (almost) replicate our results from pandas we will use `strategy="uniform"` and `encode="onehot-dense"`.

[77]:
```
kb_disc = KBinsDiscretizer(n_bins=10, strategy="uniform", encode="onehot-dense")
kb_disc
```

[77]:
```
KBinsDiscretizer(encode='onehot-dense', n_bins=10, strategy='uniform')
```

We can examine where the transformer has selected the bin edges to be located by calling the fit method on our features and then printing the `bin_edges_` attribute.

[78]:
```
X = np.c_[d.x]
kb_disc.fit(X).bin_edges_
```

[78]:
```
array([array([0.00218943, 0.10143587, 0.20068231, 0.29992875, 0.39917519,
       0.49842163, 0.59766807, 0.69691451, 0.79616095, 0.89540739,
       0.99465383])], dtype=object)
```

These cut points differ slightly from those we obtained from pandas, this is happening because we are using the data to derive the cut points and since the `x` values are randomly generated the data does not begin exactly at 0 and end at 1.

If we want to match pandas exactly, we can provide new data which is used to fit the transformer and then apply that to our data using the `transform` later.

[79]:
```
x_range = np.array([0,1])
kb_disc.fit(x_range.reshape(-1,1)).bin_edges_
```

[79]:
```
array([array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1. ])],
      dtype=object)
```

To obtain the transformed feature, we need to call `transform` with the feature to transform.

[80]:
```
kb_disc.fit(x_range.reshape(-1,1)).transform(X)
```

```
[80]: array([[1., 0., 0., …, 0., 0., 0.],
             [1., 0., 0., …, 0., 0., 0.],
             [1., 0., 0., …, 0., 0., 0.],
             …,
             [0., 0., 0., …, 0., 0., 1.],
             [0., 0., 0., …, 0., 0., 1.],
             [0., 0., 0., …, 0., 0., 1.]])
```

If instead we used `fit_transform` we will get the bin edges from the first example above, this will be the default behavior of the transformer if we use it in a pipeline.

```
[81]: kb_disc.fit_transform(X)
```

```
[81]: array([[1., 0., 0., …, 0., 0., 0.],
             [1., 0., 0., …, 0., 0., 0.],
             [1., 0., 0., …, 0., 0., 0.],
             …,
             [0., 0., 0., …, 0., 0., 1.],
             [0., 0., 0., …, 0., 0., 1.],
             [0., 0., 0., …, 0., 0., 1.]])
```

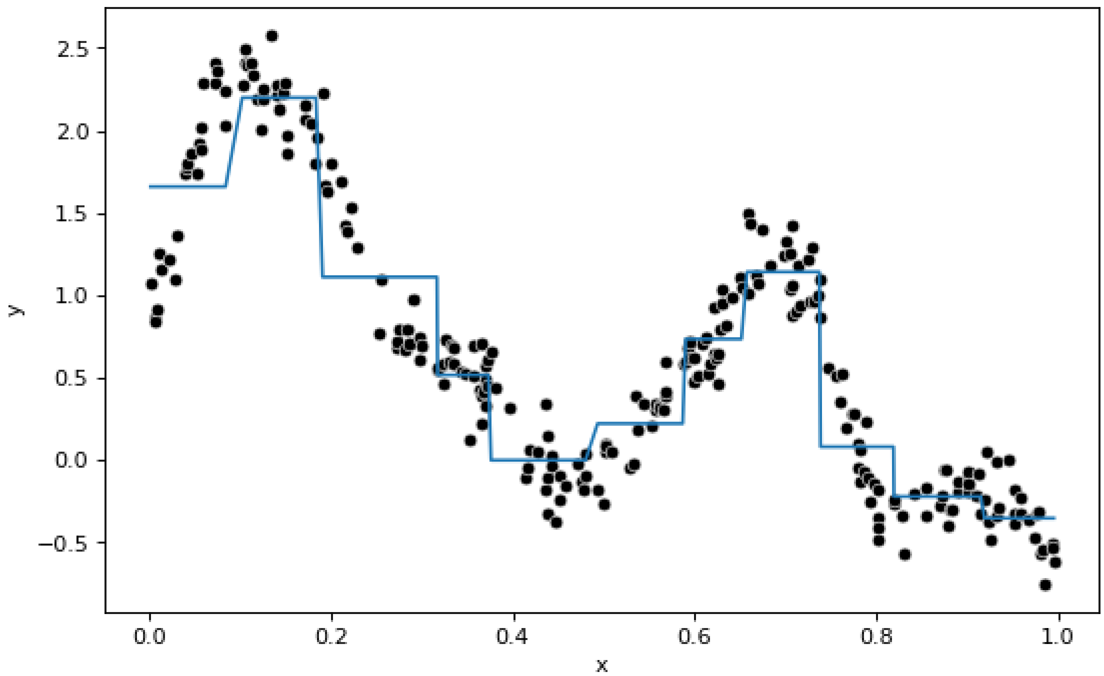
The two data frames above look similar, but are very slightly different due to the different bin edges used.

Just like our polynomial regression model, we can combine this transformed with the model using a pipeline. This combined with some plotting and diagnostic code is below.

```
[82]: def reg_tree(data, x = 'x', y = 'y',
                   n_bins=10, strategy = "uniform",
                   x_range = np.array([0,1]),
                   plot_data = True, plot_fit = True):

          X = np.c_[data[x]]
          Y = data[y]

          p = make_pipeline(
              KBinsDiscretizer(n_bins=n_bins, strategy=strategy,␣
      ↪encode="onehot-dense"),
              LinearRegression(fit_intercept=False) # Since we are using onehot above␣
      ↪we
          )                                          # need to remove the intercept␣
      ↪here

          m = p.fit(X,Y)

          pred_col = 'pred_rt_M'+str(n_bins)
          data[pred_col] = m.predict(X)
```

```
    if plot_data:
        sns.scatterplot(x=data[x], y=data[y], color="black")

    if plot_fit:
        sns.lineplot(x=data[x], y=data[pred_col])

    return (data, m)
```

[83]:
```
_, _  = reg_tree(d, n_bins=11, strategy="quantile")
```

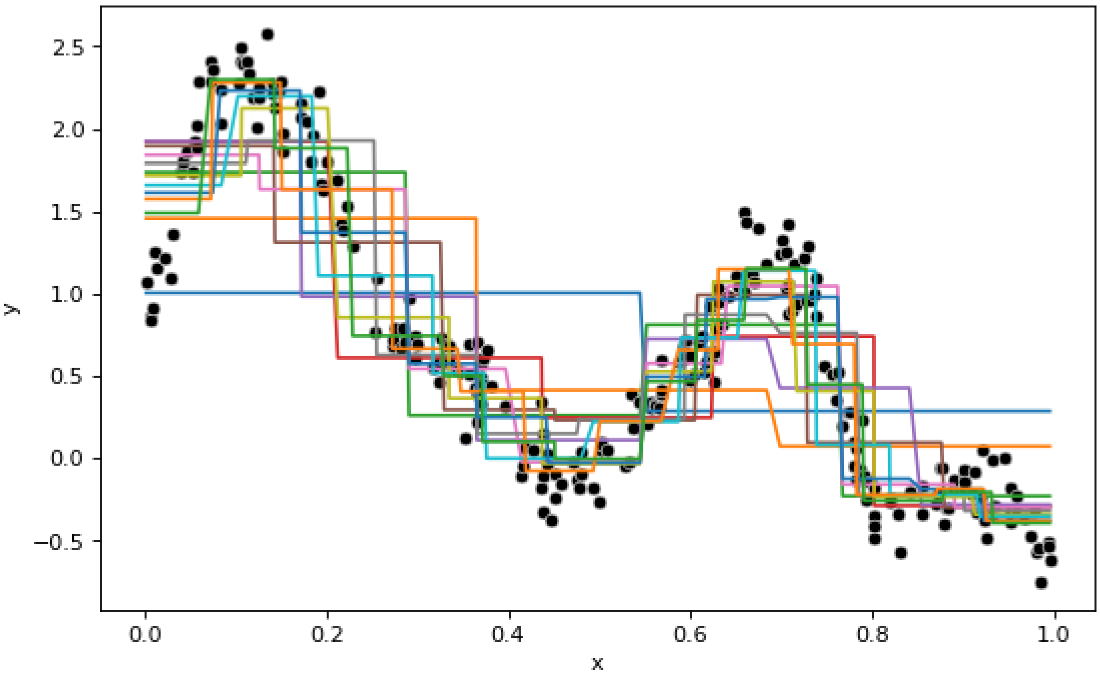


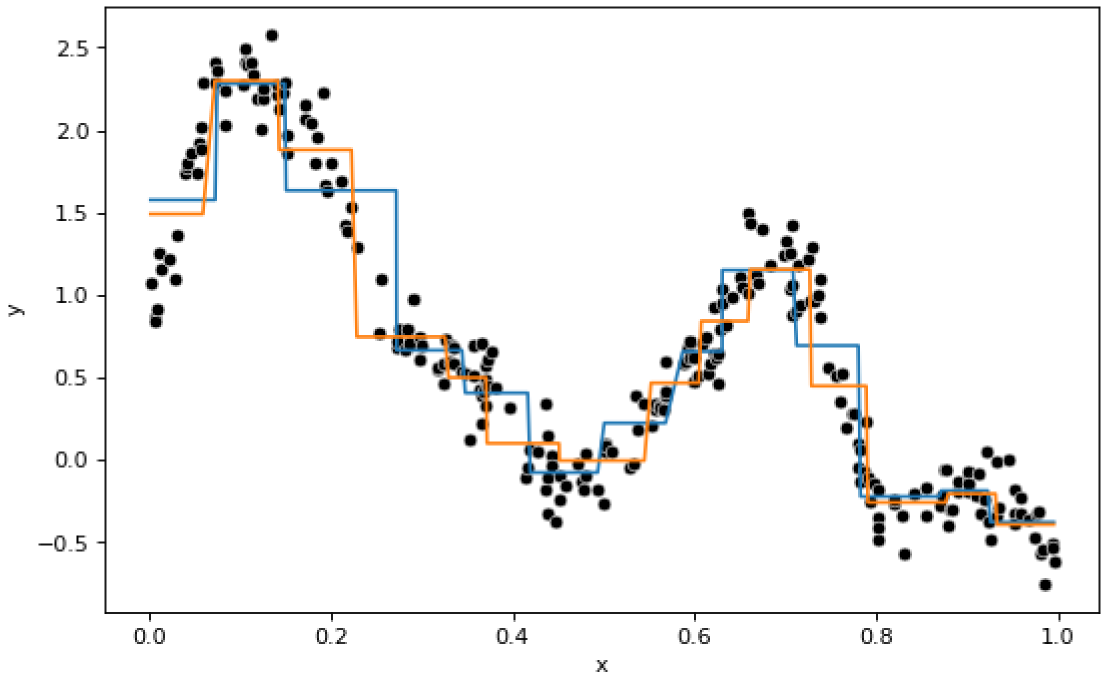
1.3.6 Exercise 13

Use the `reg_tree` function to fit a variety of different discretized models to the data. What value of `n_bins` provides the best fit (judged qualitatively not quantitatively).

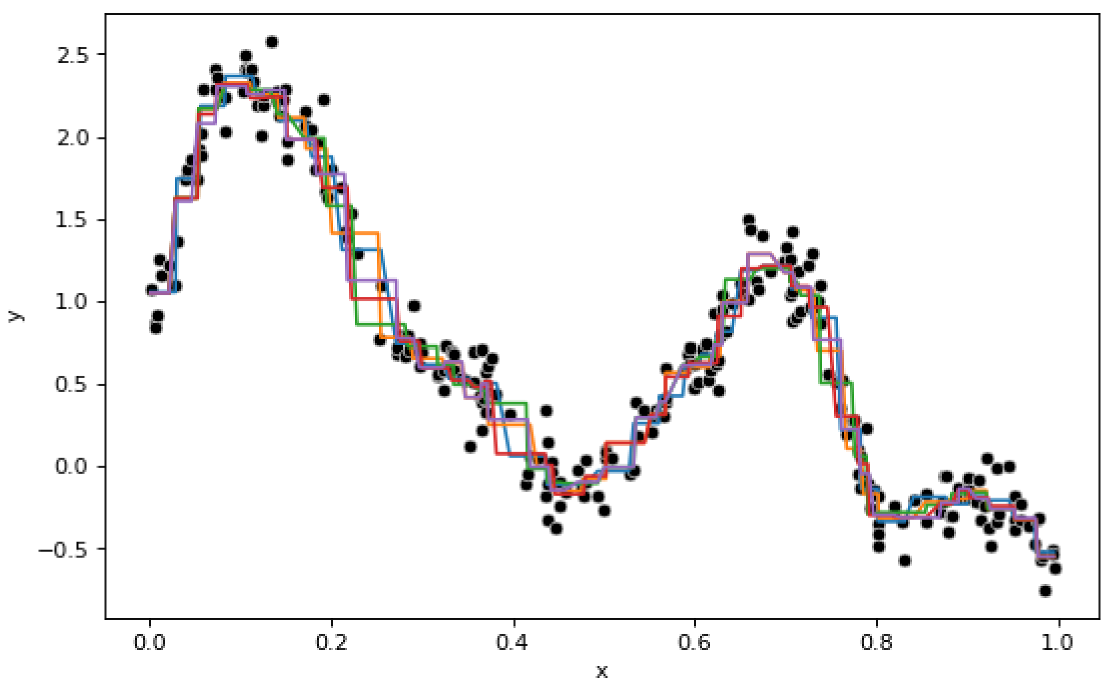
[93]:
```
for i in range(2,15):
    _, _  = reg_tree(d, n_bins=i, strategy="quantile")
plt.figure()
for i in range(13,15):
    _, _  = reg_tree(d, n_bins=i, strategy="quantile")
plt.figure()
for i in range(35,40):
```

```python
    _, _  = reg_tree(d, n_bins=i, strategy="quantile")
plt.figure()
for i in range(80,85):
    _, _  = reg_tree(d, n_bins=i, strategy="quantile")

# It appears that higher values of n_bins provide the best fit.
```

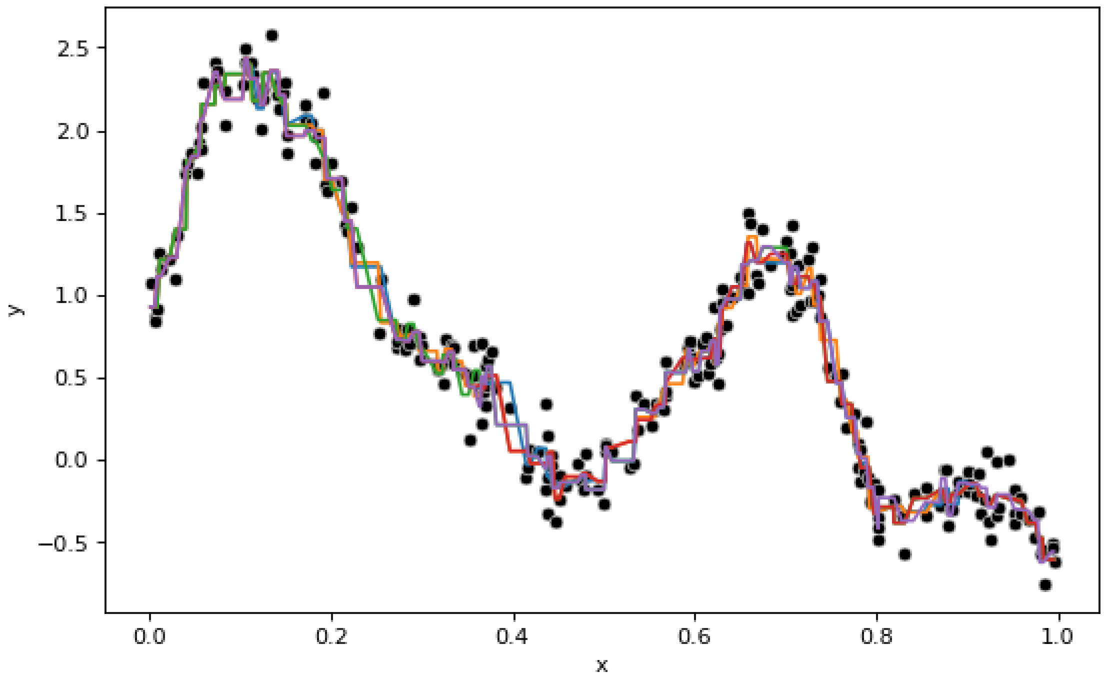




2.5
2.0
1.5
1.0
0.5
0.0
−0.5
y
0.0
0.2
0.4
0.6
0.8
1.0
x



2.5
2.0
1.5
1.0
0.5
0.0
−0.5
y
0.0
0.2
0.4
0.6
0.8
1.0
x



1.3.7 Exercise 14

Based on what you've seen in Exercise 13, how do you think the quality of fit changes as `n_bins` increases?

An n_bins increases, the quality of fit also increases. However, there is a point at which we begin to overfit the data. This point is difficult to judge solely qualitatively.

1.4 3. Competing the worksheet

At this point you have hopefully been able to complete all the preceeding exercises. Now is a good time to check the reproducibility of this document by restarting the notebook's kernel and rerunning all cells in order.

Once that is done and you are happy with everything, you can then run the following cell to generate your PDF and turn it in on gradescope under the `mlp-week03` assignment.

[95]:
```
!jupyter nbconvert --to pdf mlp-week03.ipynb
```

```
[NbConvertApp] Converting notebook mlp-week03.ipynb to pdf
[NbConvertApp] Support files will be in mlp-week03_files/
```

```
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Making directory ./mlp-week03_files
[NbConvertApp] Writing 104558 bytes to ./notebook.tex
[NbConvertApp] Building PDF
[NbConvertApp] Running xelatex 3 times: ['xelatex', './notebook.tex', '-quiet']
[NbConvertApp] Running bibtex 1 time: ['bibtex', './notebook']
[NbConvertApp] WARNING | bibtex had problems, most likely because there were no
citations
[NbConvertApp] PDF successfully created
[NbConvertApp] Writing 591841 bytes to mlp-week03.pdf
```

[ ]: