

The dashed line and solid line are exactly on top of each other, meaning the linear regression model and the decision tree make exactly the same predictions. For each bin, they predict a constant value. As features are constant within each bin, any model must predict the same value for all points within a bin. Comparing what the models learned before binning the features and after, we see that the linear model became much more flexible, because it now has a different value for each bin, while the decision tree model got much less flexible. Binning features generally has no beneficial effect for tree-based models, as these models can learn to split up the data anywhere. In a sense, that means decision trees can learn whatever binning is most useful for predicting on this data. Additionally, decision trees look at multiple features at once, while binning is usually done on a per-feature basis. However, the linear model benefited greatly in expressiveness from the transformation of the data.

If there are good reasons to use a linear model for a particular dataset—say, because it is very large and high-dimensional, but some features have nonlinear relations with the output—binning can be a great way to increase modeling power.

## Interactions and Polynomials

Another way to enrich a feature representation, particularly for linear models, is adding *interaction features* and *polynomial features* of the original data. This kind of feature engineering is often used in statistical modeling, but it's also common in many practical machine learning applications.

As a first example, look again at [Figure 4-2](#). The linear model learned a constant value for each bin in the wave dataset. We know, however, that linear models can learn not only offsets, but also slopes. One way to add a slope to the linear model on the binned data is to add the original feature (the x-axis in the plot) back in. This leads to an 11-dimensional dataset, as seen in [Figure 4-3](#):

**In[17]:**

```
X_combined = np.hstack([X, X_binned])
print(X_combined.shape)
```

**Out[17]:**

```
(100, 11)
```

**In[18]:**

```
reg = LinearRegression().fit(X_combined, y)

line_combined = np.hstack([line, line_binned])
plt.plot(line, reg.predict(line_combined), label='linear regression combined')

for bin in bins:
    plt.plot([bin, bin], [-3, 3], ':', c='k')
```

```
plt.legend(loc="best")
plt.ylabel("Regression output")
plt.xlabel("Input feature")
plt.plot(X[:, 0], y, 'o', c='k')
```

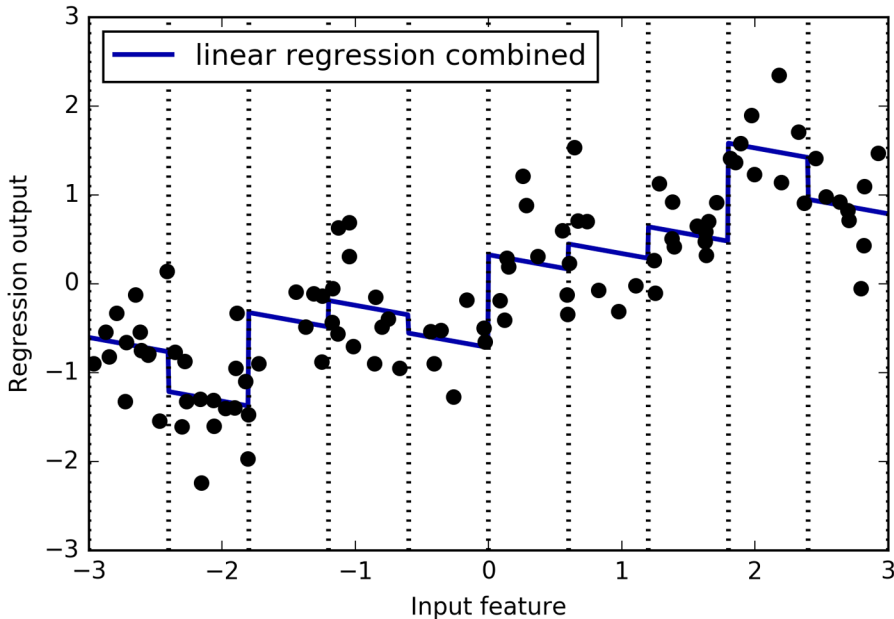


Figure 4-3. Linear regression using binned features and a single global slope

In this example, the model learned an offset for each bin, together with a slope. The learned slope is downward, and shared across all the bins—there is a single x-axis feature, which has a single slope. Because the slope is shared across all bins, it doesn't seem to be very helpful. We would rather have a separate slope for each bin! We can achieve this by adding an interaction or product feature that indicates which bin a data point is in *and* where it lies on the x-axis. This feature is a product of the bin indicator and the original feature. Let's create this dataset:

**In[19]:**

```
X_product = np.hstack([X_binned, X * X_binned])
print(X_product.shape)
```

**Out[19]:**

```
(100, 20)
```

The dataset now has 20 features: the indicators for which bin a data point is in, and a product of the original feature and the bin indicator. You can think of the product

feature as a separate copy of the x-axis feature for each bin. It is the original feature within the bin, and zero everywhere else. Figure 4-4 shows the result of the linear model on this new representation:

**In[20]:**

```
reg = LinearRegression().fit(X_product, y)

line_product = np.hstack([line_binned, line * line_binned])
plt.plot(line, reg.predict(line_product), label='linear regression product')

for bin in bins:
    plt.plot([bin, bin], [-3, 3], ':', c='k')

plt.plot(X[:, 0], y, 'o', c='k')
plt.ylabel("Regression output")
plt.xlabel("Input feature")
plt.legend(loc="best")
```

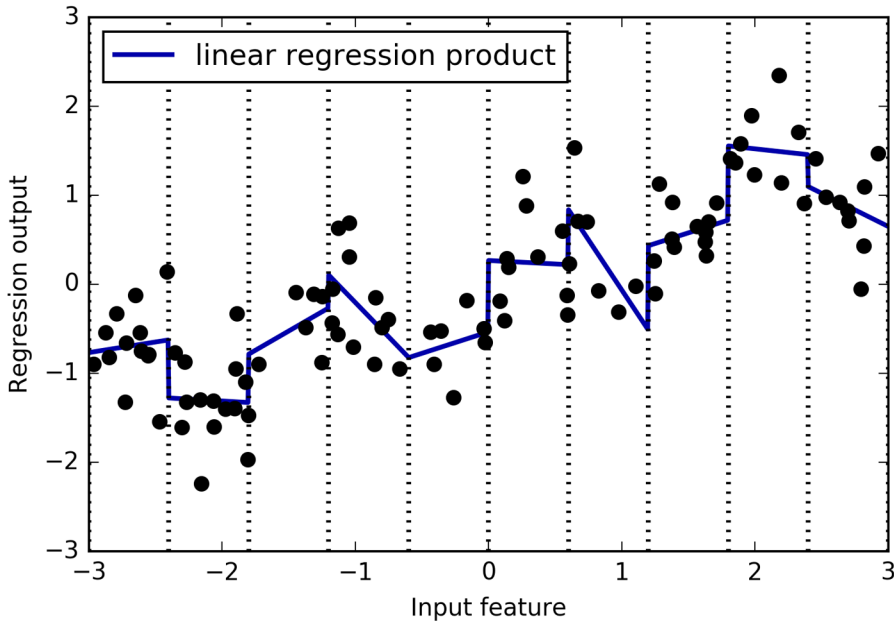


Figure 4-4. Linear regression with a separate slope per bin

As you can see, now each bin has its own offset and slope in this model.

Using binning is one way to expand a continuous feature. Another one is to use *polynomials* of the original features. For a given feature  $x$ , we might want to consider  $x^2$ ,  $x^3$ ,  $x^4$ , and so on. This is implemented in `PolynomialFeatures` in the preprocessing module:

**In[21]:**

```
from sklearn.preprocessing import PolynomialFeatures

# include polynomials up to x ** 10:
# the default "include_bias=True" adds a feature that's constantly 1
poly = PolynomialFeatures(degree=10, include_bias=False)
poly.fit(X)
X_poly = poly.transform(X)
```

Using a degree of 10 yields 10 features:

**In[22]:**

```
print("X_poly.shape: {}".format(X_poly.shape))
```

**Out[22]:**

```
X_poly.shape: (100, 10)
```

Let's compare the entries of  $X_{\text{poly}}$  to those of  $X$ :

**In[23]:**

```
print("Entries of X:\n{}".format(X[:5]))
print("Entries of X_poly:\n{}".format(X_poly[:5]))
```

**Out[23]:**

```
Entries of X:
[[-0.753]
 [ 2.704]
 [ 1.392]
 [ 0.592]
 [-2.064]]
Entries of X_poly:
[[ -0.753    0.567   -0.427    0.321   -0.242    0.182
  -0.137    0.103   -0.078    0.058]
 [  2.704    7.313   19.777   53.482  144.632  391.125
 1057.714 2860.360 7735.232 20918.278]
 [  1.392    1.938    2.697    3.754    5.226    7.274
 10.125   14.094   19.618   27.307]
 [  0.592    0.350    0.207    0.123    0.073    0.043
  0.025    0.015    0.009    0.005]
 [ -2.064    4.260   -8.791   18.144  -37.448   77.289
 -159.516  329.222 -679.478 1402.367]]
```

You can obtain the semantics of the features by calling the `get_feature_names` method, which provides the exponent for each feature:

In[24]:

```
print("Polynomial feature names:\n{}".format(poly.get_feature_names()))
```

Out[24]:

```
Polynomial feature names:  
['x0', 'x0^2', 'x0^3', 'x0^4', 'x0^5', 'x0^6', 'x0^7', 'x0^8', 'x0^9', 'x0^10']
```

You can see that the first column of `X_poly` corresponds exactly to `X`, while the other columns are the powers of the first entry. It's interesting to see how large some of the values can get. The second column has entries above 20,000, orders of magnitude different from the rest.

Using polynomial features together with a linear regression model yields the classical model of *polynomial regression* (see Figure 4-5):

In[26]:

```
reg = LinearRegression().fit(X_poly, y)  
  
line_poly = poly.transform(line)  
plt.plot(line, reg.predict(line_poly), label='polynomial linear regression')  
plt.plot(X[:, 0], y, 'o', c='k')  
plt.ylabel("Regression output")  
plt.xlabel("Input feature")  
plt.legend(loc="best")
```

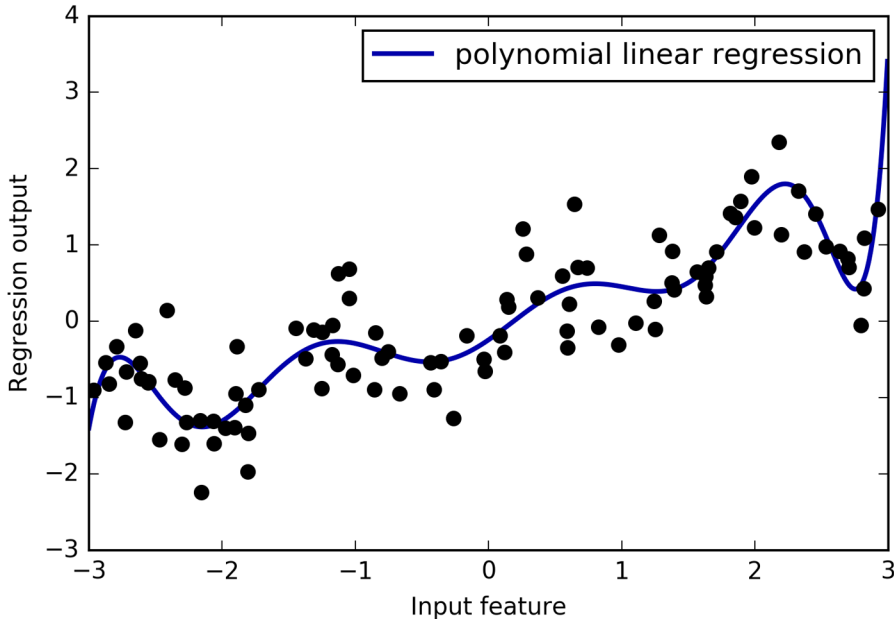


Figure 4-5. Linear regression with tenth-degree polynomial features

As you can see, polynomial features yield a very smooth fit on this one-dimensional data. However, polynomials of high degree tend to behave in extreme ways on the boundaries or in regions with little data.

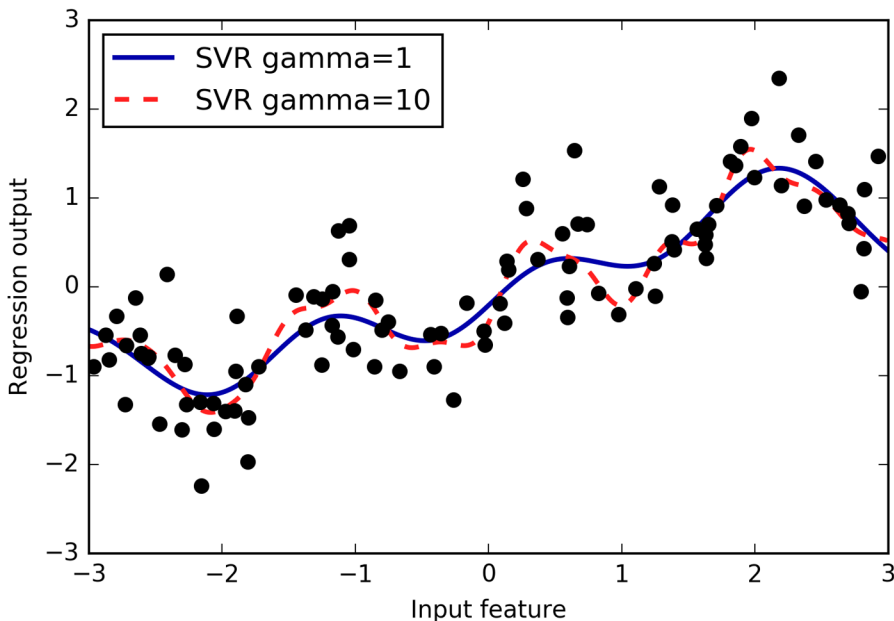
As a comparison, here is a kernel SVM model learned on the original data, without any transformation (see [Figure 4-6](#)):

**In[26]:**

```
from sklearn.svm import SVR

for gamma in [1, 10]:
    svr = SVR(gamma=gamma).fit(X, y)
    plt.plot(line, svr.predict(line), label='SVR gamma={}'.format(gamma))

plt.plot(X[:, 0], y, 'o', c='k')
plt.ylabel("Regression output")
plt.xlabel("Input feature")
plt.legend(loc="best")
```



*Figure 4-6. Comparison of different gamma parameters for an SVM with RBF kernel*

Using a more complex model, a kernel SVM, we are able to learn a similarly complex prediction to the polynomial regression without an explicit transformation of the features.

As a more realistic application of interactions and polynomials, let's look again at the Boston Housing dataset. We already used polynomial features on this dataset in [Chapter 2](#). Now let's have a look at how these features were constructed, and at how much the polynomial features help. First we load the data, and rescale it to be between 0 and 1 using `MinMaxScaler`:

**In[27]:**

```
from sklearn.datasets import load_boston
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

boston = load_boston()
X_train, X_test, y_train, y_test = train_test_split(
    (boston.data, boston.target, random_state=0)

# rescale data
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

Now, we extract polynomial features and interactions up to a degree of 2:

**In[28]:**

```
poly = PolynomialFeatures(degree=2).fit(X_train_scaled)
X_train_poly = poly.transform(X_train_scaled)
X_test_poly = poly.transform(X_test_scaled)
print("X_train.shape: {}".format(X_train.shape))
print("X_train_poly.shape: {}".format(X_train_poly.shape))
```

**Out[28]:**

```
X_train.shape: (379, 13)
X_train_poly.shape: (379, 105)
```

The data originally had 13 features, which were expanded into 105 interaction features. These new features represent all possible interactions between two different original features, as well as the square of each original feature. `degree=2` here means that we look at all features that are the product of up to two original features. The exact correspondence between input and output features can be found using the `get_feature_names` method:

**In[29]:**

```
print("Polynomial feature names:\n{}".format(poly.get_feature_names()))
```

**Out[29]:**

```
Polynomial feature names:
['1', 'x0', 'x1', 'x2', 'x3', 'x4', 'x5', 'x6', 'x7', 'x8', 'x9', 'x10',
 'x11', 'x12', 'x0^2', 'x0 x1', 'x0 x2', 'x0 x3', 'x0 x4', 'x0 x5', 'x0 x6',
 'x0 x7', 'x0 x8', 'x0 x9', 'x0 x10', 'x0 x11', 'x0 x12', 'x1^2', 'x1 x2',
```

```
'x1 x3', 'x1 x4', 'x1 x5', 'x1 x6', 'x1 x7', 'x1 x8', 'x1 x9', 'x1 x10',
'x1 x11', 'x1 x12', 'x2^2', 'x2 x3', 'x2 x4', 'x2 x5', 'x2 x6', 'x2 x7',
'x2 x8', 'x2 x9', 'x2 x10', 'x2 x11', 'x2 x12', 'x3^2', 'x3 x4', 'x3 x5',
'x3 x6', 'x3 x7', 'x3 x8', 'x3 x9', 'x3 x10', 'x3 x11', 'x3 x12', 'x4^2',
'x4 x5', 'x4 x6', 'x4 x7', 'x4 x8', 'x4 x9', 'x4 x10', 'x4 x11', 'x4 x12',
'x5^2', 'x5 x6', 'x5 x7', 'x5 x8', 'x5 x9', 'x5 x10', 'x5 x11', 'x5 x12',
'x6^2', 'x6 x7', 'x6 x8', 'x6 x9', 'x6 x10', 'x6 x11', 'x6 x12', 'x7^2',
'x7 x8', 'x7 x9', 'x7 x10', 'x7 x11', 'x7 x12', 'x8^2', 'x8 x9', 'x8 x10',
'x8 x11', 'x8 x12', 'x9^2', 'x9 x10', 'x9 x11', 'x9 x12', 'x10^2', 'x10 x11',
'x10 x12', 'x11^2', 'x11 x12', 'x12^2']
```

The first new feature is a constant feature, called "1" here. The next 13 features are the original features (called "x0" to "x12"). Then follows the first feature squared ("x0^2") and combinations of the first and the other features.

Let's compare the performance using Ridge on the data with and without interactions:

**In[30]:**

```
from sklearn.linear_model import Ridge
ridge = Ridge().fit(X_train_scaled, y_train)
print("Score without interactions: {:.3f}".format(
    ridge.score(X_test_scaled, y_test)))
ridge = Ridge().fit(X_train_poly, y_train)
print("Score with interactions: {:.3f}".format(
    ridge.score(X_test_poly, y_test)))
```

**Out[30]:**

```
Score without interactions: 0.621
Score with interactions: 0.753
```

Clearly, the interactions and polynomial features gave us a good boost in performance when using Ridge. When using a more complex model like a random forest, the story is a bit different, though:

**In[31]:**

```
from sklearn.ensemble import RandomForestRegressor
rf = RandomForestRegressor(n_estimators=100).fit(X_train_scaled, y_train)
print("Score without interactions: {:.3f}".format(
    rf.score(X_test_scaled, y_test)))
rf = RandomForestRegressor(n_estimators=100).fit(X_train_poly, y_train)
print("Score with interactions: {:.3f}".format(rf.score(X_test_poly, y_test)))
```

**Out[31]:**

```
Score without interactions: 0.799
Score with interactions: 0.763
```



You can see that even without additional features, the random forest beats the performance of Ridge. Adding interactions and polynomials actually decreases performance slightly.

## Univariate Nonlinear Transformations

We just saw that adding squared or cubed features can help linear models for regression. There are other transformations that often prove useful for transforming certain features: in particular, applying mathematical functions like `log`, `exp`, or `sin`. While tree-based models only care about the ordering of the features, linear models and neural networks are very tied to the scale and distribution of each feature, and if there is a nonlinear relation between the feature and the target, that becomes hard to model—particularly in regression. The functions `log` and `exp` can help by adjusting the relative scales in the data so that they can be captured better by a linear model or neural network. We saw an application of that in [Chapter 2](#) with the memory price data. The `sin` and `cos` functions can come in handy when dealing with data that encodes periodic patterns.

Most models work best when each feature (and in regression also the target) is loosely Gaussian distributed—that is, a histogram of each feature should have something resembling the familiar “bell curve” shape. Using transformations like `log` and `exp` is a hacky but simple and efficient way to achieve this. A particularly common case when such a transformation can be helpful is when dealing with integer count data. By count data, we mean features like “how often did user A log in?” Counts are never negative, and often follow particular statistical patterns. We are using a synthetic dataset of counts here that has properties similar to those you can find in the wild. The features are all integer-valued, while the response is continuous:

**In[32]:**

```
rnd = np.random.RandomState(0)
X_org = rnd.normal(size=(1000, 3))
w = rnd.normal(size=3)

X = rnd.poisson(10 * np.exp(X_org))
y = np.dot(X_org, w)
```

Let’s look at the first 10 entries of the first feature. All are integer values and positive, but apart from that it’s hard to make out a particular pattern.

If we count the appearance of each value, the distribution of values becomes clearer: