LECTURE 16

`sklearn` and Feature Engineering

Transforming data to improve model performance.

Data Science, Spring 2024@ Knowledge Stream

Sana Jabbar

Goals for this Lecture

Lecture 16

Last few lectures: underlying theory of modeling

This lecture: putting things into practice!

- using `sklearn`, a useful Python library for building and fitting models
- Techniques for selecting features to improve model performance

Implementing Models in Code

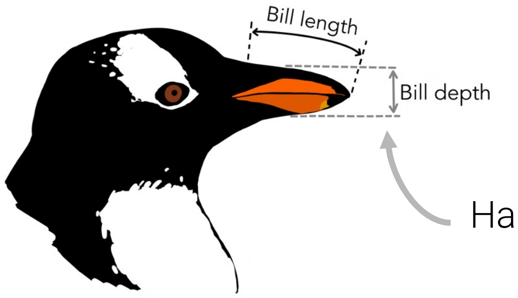
Lecture 16

Demo: `penguins`

We have the dataset **`penguins`**.

	species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	sex
0	Adelie	Torgersen	39.1	18.7	181.0	3750.0	Male
1	Adelie	Torgersen	39.5	17.4	186.0	3800.0	Female
2	Adelie	Torgersen	40.3	18.0	195.0	3250.0	Female
4	Adelie	Torgersen	36.7	19.3	193.0	3450.0	Female
5	Adelie	Torgersen	39.3	20.6	190.0	3650.0	Male

We want to predict a penguin's bill depth given its flipper length and body mass.



Hard to measure without bites.

Performing Ordinary Least Squares in Python

We previously derived the OLS estimate for the optimal model parameters:

$$\hat{\theta} = \left(\mathbb{X}^\top \mathbb{X}\right)^{-1} \mathbb{X}^\top \mathbb{Y}$$

In Python:

Transpose	Inverse	Matrix Multiplication
`matrix.T`	`np.linalg.inv(matrix)`	`matrix_1 @ matrix_2`

```
theta_hat = np.linalg.inv(X.T @ X) @ X.T @ Y
```

sklearn

Lecture 16

- Implementing Models in Code
- **sklearn**
- Feature Engineering
- One-Hot Encoding
- Polynomial Features
- Complexity and Overfitting

`sklearn`: a Standard Library for Model Creation

So far, we have been doing the "heavy lifting" of model creation ourselves – via calculus, ordinary least squares, or gradient descent

In Data science, we will use Scikit-Learn, commonly called **`sklearn`**

```
import sklearn
my_model = linear_model.LinearRegression()
my_model.fit(X, y)
my_model.predict(X)
```

`sklearn`: a Standard Library for Model Creation

`sklearn` uses an object-oriented programming. Different types of models are defined as their own classes. To use a model, we initialize an instance of the model class. .

The `sklearn` Workflow

At a high level, there are three steps to creating an **`sklearn`** model:

1

Initialize a new model instance
Make a "copy" of the model template

2

Fit the model to the training data
Save the optimal model parameters

3

Use fitted model to make predictions
Fitted model outputs predictions for y

The `sklearn` Workflow

At a high level, there are three steps to creating an **`sklearn`** model:

1	Initialize a new model instance *Make a "copy" of the model template*	`my_model = lm.LinearRegression()`
2	Fit the model to the training data *Save the optimal model parameters*	`my_model.fit(X, y)`
3	Use fitted model to make predictions *Fitted model makes predictions for y*	`my_model.predict(X)`

To extract the fitted parameters: `my_model.coef_` and `my_model.intercept_`

Feature Engineering

Lecture 16

Feature Engineering

Feature engineering is the process of transforming raw features into more informative features for use in modeling

Allows us to:

- Capture domain knowledge
- Express non-linear relationships using linear models
- Use non-numeric features in models

Feature Functions

A **feature function** describes the transformations we apply to raw features in the dataset to create transformed features. Often, the dimension of the *featurized* dataset increases.

Example: a feature function that adds a squared feature to the design matrix

	hp	mpg
0	130.00	18.00
1	165.00	15.00
2	150.00	18.00
...	...	...
395	84.00	32.00
396	79.00	28.00
397	82.00	31.00

392 rows × 2 columns

Φ

	hp	hp^2	mpg
0	130.00	16900.00	18.00
1	165.00	27225.00	15.00
2	150.00	22500.00	18.00
...	...	...	...
395	84.00	7056.00	32.00
396	79.00	6241.00	28.00
397	82.00	6724.00	31.00

392 rows × 3 columns

Dataset of raw features:

$$\mathbb{X} \in \mathbb{R}^{n \times p}$$

After applying the feature function Φ:

$$\Phi(\mathbb{X}) \in \mathbb{R}^{n \times p'}$$

Feature Functions

A **feature function** describes the transformations we apply to raw features in the dataset to create transformed features. Often, the dimension of the *featurized* dataset increases.

Linear models trained on transformed data are sometimes written using the symbol Φ instead of X:

$$\hat{y} = \theta_0 + \theta_1 x + \theta_2 x^2$$
$$\hat{\mathbb{Y}} = \mathbb{X}\theta$$

$$\hat{y} = \theta_0 + \theta_1 \phi_1 + \theta_2 \phi_2$$
$$\hat{\mathbb{Y}} = \Phi\theta$$

Shorthand for "the design matrix after feature engineering"

One-Hot Encoding

Lecture 16

- Implementing Models in Code
- `sklearn`
- Feature Engineering
- **One-Hot Encoding**
- Polynomial Features
- Complexity and Overfitting

Regression Using Non-Numeric Features

In `tips` dataset we used when first exploring regression

	total_bill	size	day
0	16.99	2	Sun
1	10.34	3	Sun
2	21.01	3	Sun
3	23.68	2	Sun
4	24.59	4	Sun

Before, we were limited to only using numeric features in a model – `total_bill` and `size`

By performing feature engineering, we can incorporate *non-numeric* features like the day of the week

One-hot Encoding

One-hot encoding is a feature engineering technique to transform non-numeric data into numeric features for modeling

- Each category of a categorical variable gets its own feature
  - Value = 1 if a row belongs to the category
  - Value = 0 otherwise

Original data
Sunday
Sunday
Thursday
Thursday
Saturday

Sunday	Thursday	Saturday
1	0	0
1	0	0
0	**1**	0
0	**1**	0
0	0	**1**

One-hot encoding

Regression Using the One-Hot Encoding

The one-hot encoded features can then be used in the design matrix to train a model

	total_bill	size	day_Fri	day_Sat	day_Sun	day_Thur
0	16.99	2	0.0	0.0	1.0	0.0
1	10.34	3	0.0	0.0	1.0	0.0
2	21.01	3	0.0	0.0	1.0	0.0
3	23.68	2	0.0	0.0	1.0	0.0
4	24.59	4	0.0	0.0	1.0	0.0

Raw features | One-hot encoded features

$$\hat{y} = \theta_1(\text{total\_bill}) + \theta_2(\text{size}) + \theta_3(\text{day\_Fri}) + \theta_4(\text{day\_Sat}) + \theta_5(\text{day\_Sun}) + \theta_6(\text{day\_Thur})$$

In shorthand: $\hat{y} = \theta_1\phi_1 + \theta_2\phi_2 + \theta_3\phi_3 + \theta_4\phi_4 + \theta_5\phi_5 + \theta_6\phi_6$

Regression Using the One-Hot Encoding

Using `sklearn` to fit the new model:

$$\hat{y} = \theta_1(\text{total\_bill}) + \theta_2(\text{size}) + \theta_3(\text{day\_Fri}) + \theta_4(\text{day\_Sat}) + \theta_5(\text{day\_Sun}) + \theta_6(\text{day\_Thur})$$

	Model Coefficient
Feature	
total_bill	0.092994
size	0.187132
day_Fri	0.745787
day_Sat	0.621129
day_Sun	0.732289
day_Thur	0.668294

Interpretation: how much the fact that it is Friday impacts the predicted tip

Regression Using the One-Hot Encoding

Party of 3, $50 total bill, eating on a Friday:

$$\hat{y} = \theta_1(\text{total\_bill}) + \theta_2(\text{size}) + \theta_3(\text{day\_Fri}) + \theta_4(\text{day\_Sat}) + \theta_5(\text{day\_Sun}) + \theta_6(\text{day\_Thur})$$

$$\hat{y} = 0.092994(50) + 0.187132(3) + 0.745787(1) + 0.621129(0) + 0.732289(0) + 0.668294(0)$$

	Model Coefficient
Feature	
total_bill	0.092994
size	0.187132
day_Fri	0.745787
day_Sat	0.621129
day_Sun	0.732289
day_Thur	0.668294

$$\hat{y} = 5.9568643$$

One-hot Encode Wisely!

Any set of one-hot encoded columns will always sum to a column of all ones.

Original data
Sunday
Sunday
Thursday
Thursday
Saturday

→

Sunday	Thursday	Saturday	Bias
1	0	0	1
1	0	0	1
0	1	0	1
0	1	0	1
0	0	1	1

The bias column is a linear combination of the OHE columns

If we also include a bias column in the design matrix, there will be linear dependence in the model. $\mathbb{X}^\top\mathbb{X}$ is not invertible, and our OLS estimate $\hat{\theta} = (\mathbb{X}^\top\mathbb{X})^{-1}\mathbb{X}^\top\mathbb{Y}$ fails.

How to resolve? Omit one of the one-hot encoded columns *or* do not include an intercept term

One-hot Encode Wisely!

How to resolve? Omit one of the one-hot encoded columns *or* do not include an intercept term

Adjusted design matrices:

Sunday	Thursday	~~Saturday~~	Bias
1	0	~~0~~	1
1	0	~~0~~	1
0	1	~~0~~	1
0	1	~~0~~	1
0	0	~~1~~	1

or

Sunday	Thursday	Saturday	~~Bias~~
1	0	0	~~1~~
1	0	0	~~1~~
0	1	0	~~1~~
0	1	0	~~1~~
0	0	1	~~1~~

We still retain the same information – in both approaches, the omitted column is simply a linear combination of the remaining columns

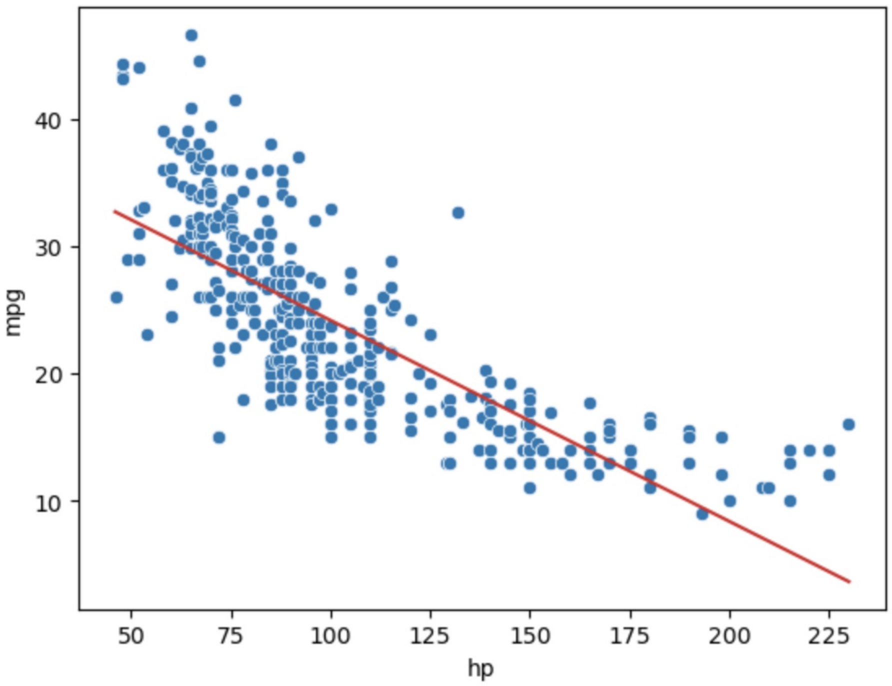
Polynomial Features

Lecture 16

- `sklearn`
- Feature Engineering
- One-Hot Encoding
- **Polynomial Features**
- Complexity and Overfitting

Accounting for Curvature

We've seen a few cases now where models with linear features have performed poorly on datasets with a clear non-linear curve.



$$\hat{y} = \theta_0 + \theta_1(\text{hp})$$

MSE: 23.94

When our model uses only a single linear feature (**hp**), it cannot capture non-linearity in the relationship

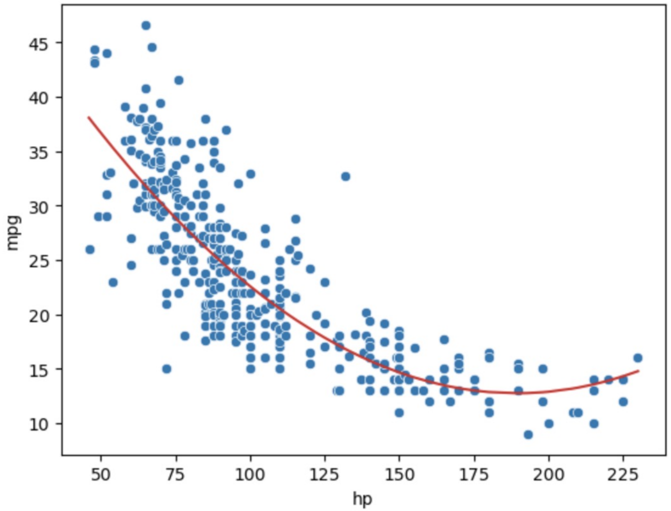
Solution: incorporate a non-linear feature!

Polynomial Features

We create a new feature: the square of the **hp**

$$\hat{y} = \theta_0 + \theta_1(\text{hp}) + \theta_2\left(\text{hp}^2\right)$$

This is still a **linear model**. Even though there are non-linear *features*, the model is linear with respect to θ



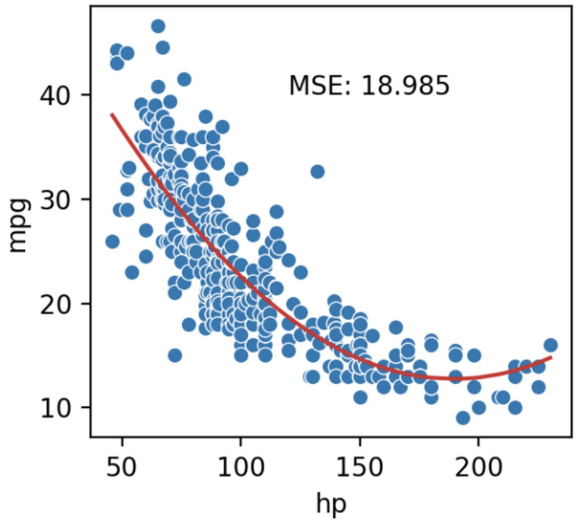
Degree of model: 2
MSE: 18.98

Looking a lot better: our predictions capture the curvature of the data.

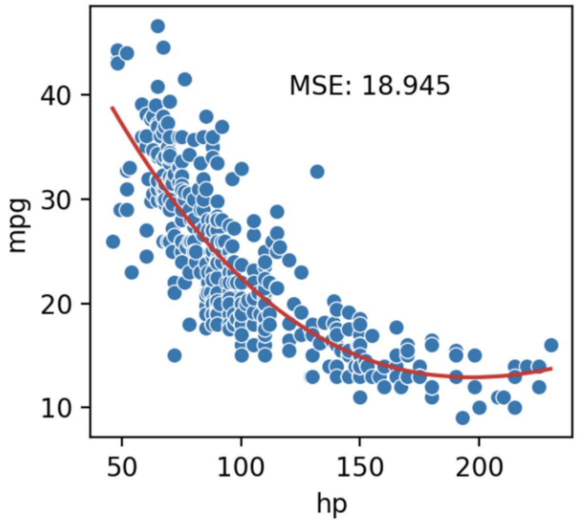
Polynomial Features

What if we add more polynomial features?

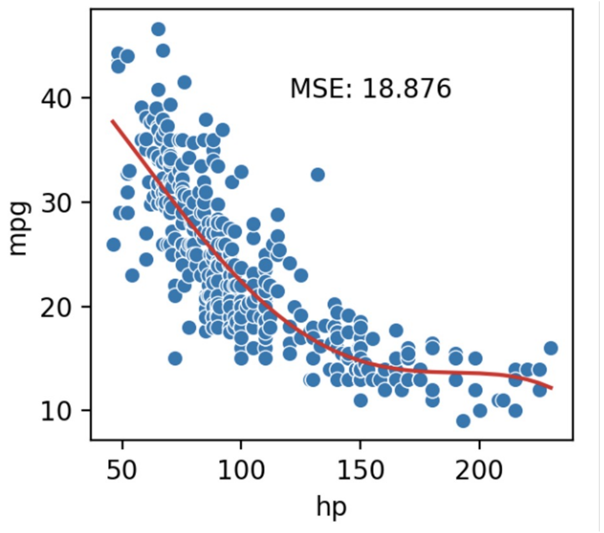
$$\hat{y} = \theta_0 + \theta_1(\text{hp}) + \theta_2\left(\text{hp}^2\right)$$



$$\hat{y} = \theta_0 + \theta_1(\text{hp}) + \theta_2\left(\text{hp}^2\right) + \theta_3\left(\text{hp}^3\right)$$



$$\hat{y} = \theta_0 + \theta_1(\text{hp}) + \theta_2\left(\text{hp}^2\right) + \theta_3\left(\text{hp}^3\right) + \theta_4\left(\text{hp}^4\right)$$



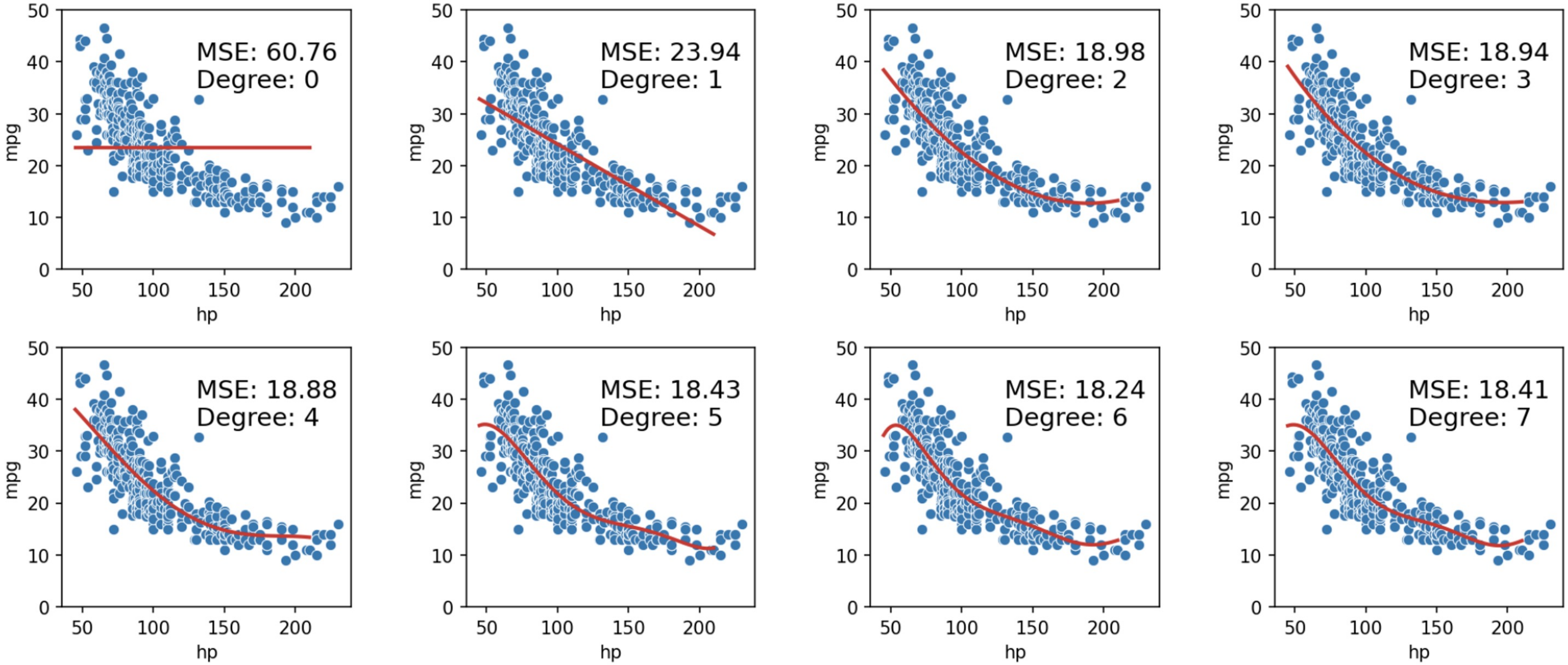
MSE continues to decrease with each additional polynomial term

Complexity and Overfitting

Lecture 16

- `sklearn`
- Feature Engineering
- One-Hot Encoding
- Polynomial Features
- **Complexity and Overfitting**

How Far Can We Take This?

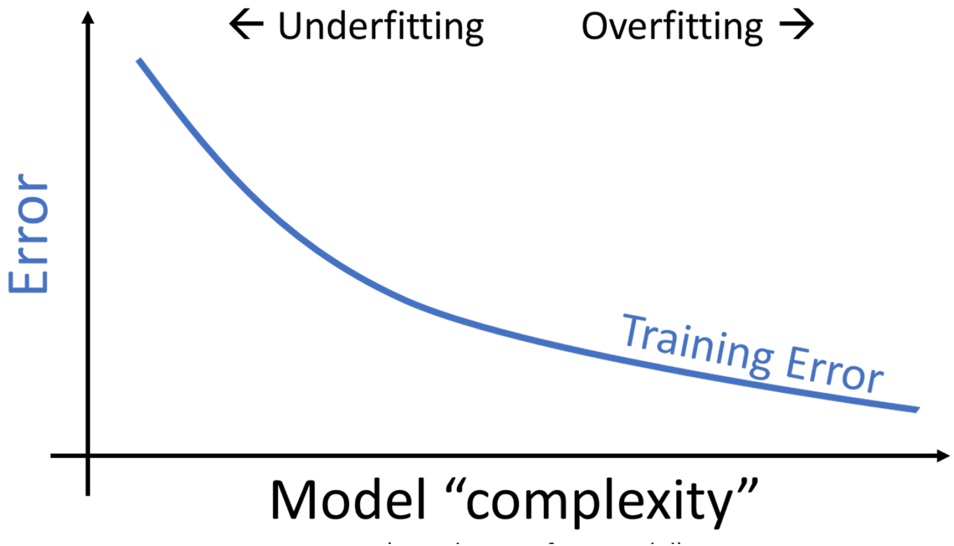


Model Complexity

As we continue to add more and more polynomial features, the MSE continues to decrease

Equivalently: as the **model complexity** increases, its *training error* decreases

General trend for an arbitrary dataset

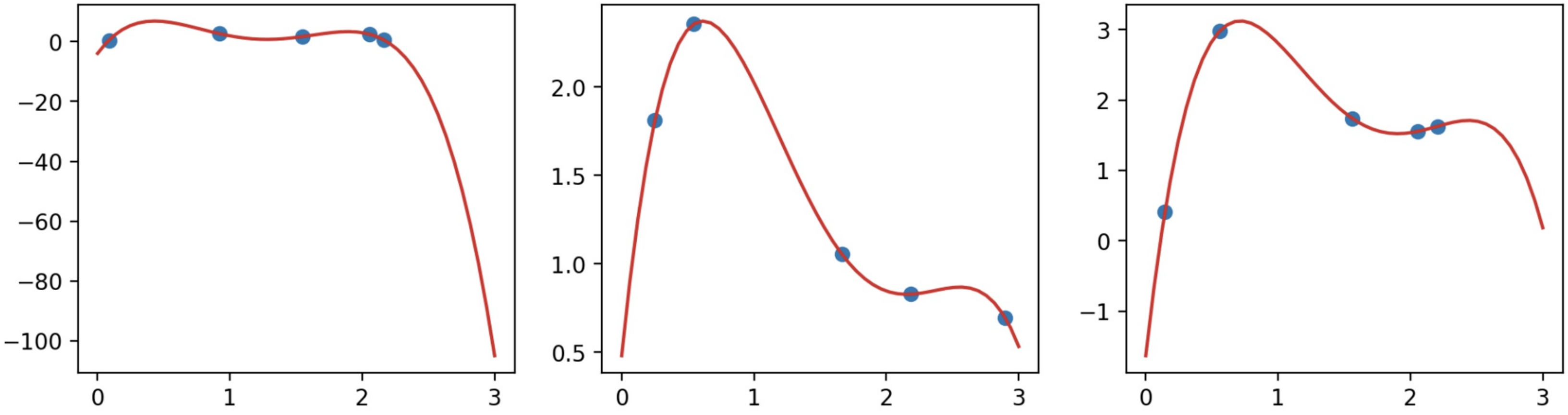


Seems like a good deal?

An Extreme Example: Perfect Polynomial Fits

Math fact: given N non-overlapping data points, we can always find a polynomial of degree N-1 that goes through all those points.

For example, there always exists a degree-4 polynomial curve that can perfectly model a dataset of 5 datapoints

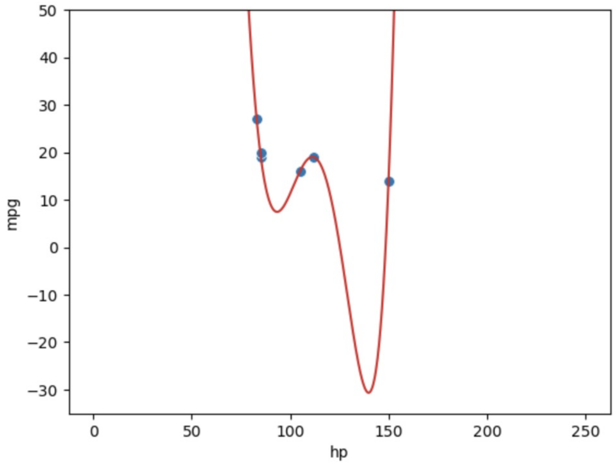


Model Performance on Unseen Data

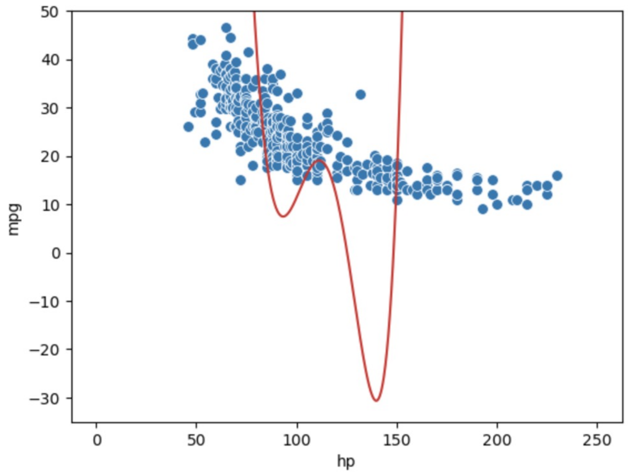
New (more realistic) example:

- We are given a training dataset of just 6 datapoints
- We want to train a model to then make predictions on a *different* set of points

We may be tempted to make a highly complex model (eg degree 5)



Complex model makes perfect predictions on the training data...



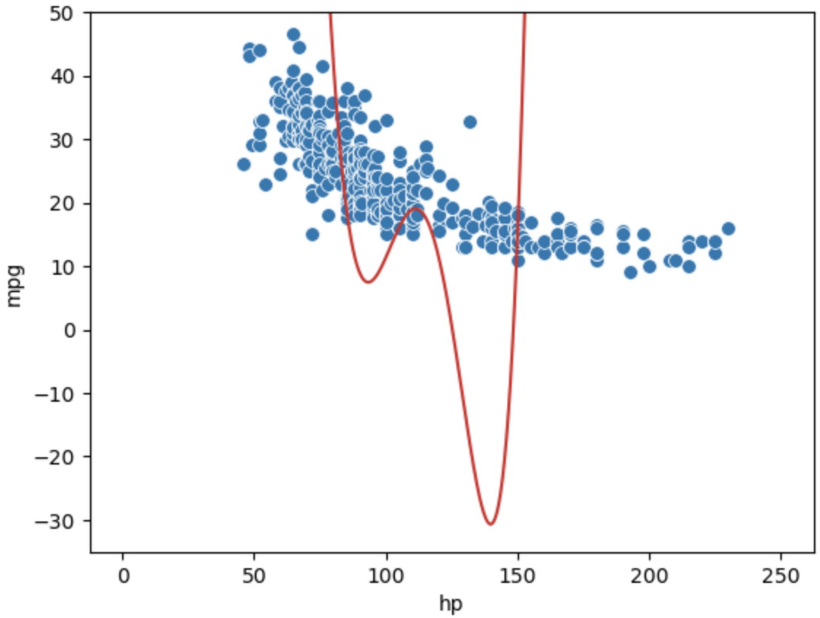
...but performs *horribly* on the rest of the population!

Model Performance on Unseen Data

What went wrong?

- The complex model **overfit** to the training data – it essentially “memorized” these 6 training points
- The overfitted model does not **generalize** well to data it did not encounter during training

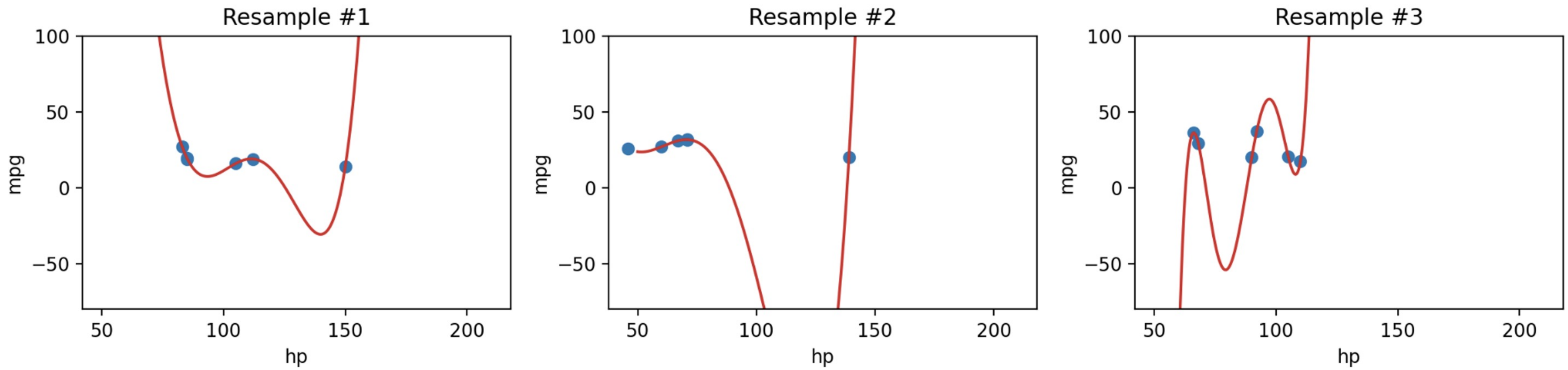
This is a problem: we want models that are generalizable to “unseen” data



Model Variance

Complex models are sensitive to the specific dataset used to train them – they have high **variance**, because they will *vary* depending on what datapoints are used for training them

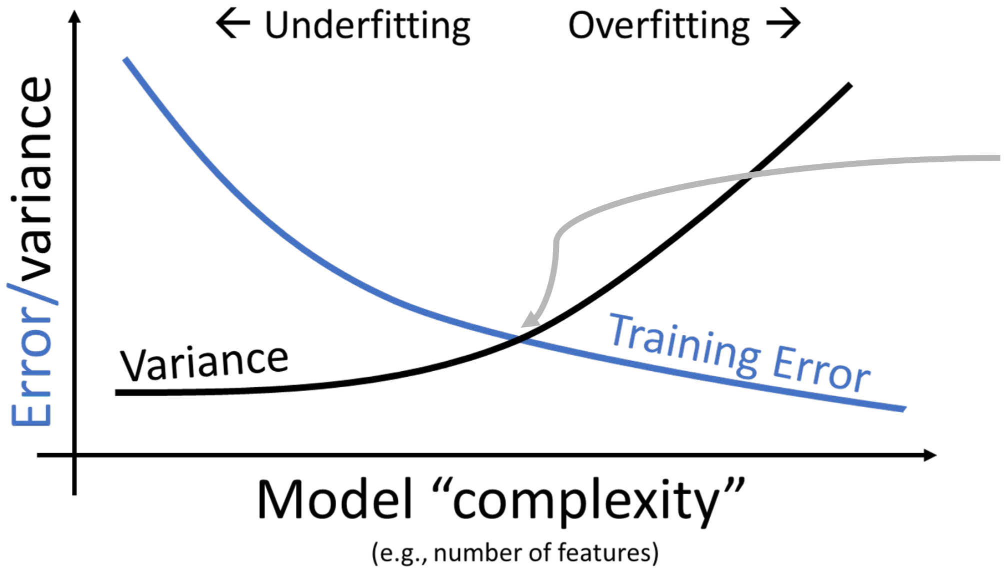
Our degree-5 model varies erratically when we fit it to different samples of 6 points from `vehicles`



Error, Variance, and Complexity

We face a dilemma:

- We know that we can **decrease training error** by increasing model complexity
- However, models that are *too* complex start to overfit and do not generalize well – their **high variance** means they can't be reapplied to new datasets



Our goal: find this "sweet spot"

Stay tuned for future lectures covering this!