

Bias-Variance Trade-Off &

Polynomial Regression

Session-3



SUMMARY of PREVIOUS CLASS



- **Residuals**
 - Sum and mean of the Residuals are always Zero
 - Residuals are normally distributed for Suitable Linear Regression.
- **Regression Error Metrics**
 - MAE, MSE, RMSE...
- **Scikit-learn Library and ML**
 - 5 Steps: Import, Split Data, Model Building and Fit, Prediction, Evaluation

SUMMARY of PREVIOUS CLASS



Model Building

1- Import Library

```
[18] import numpy as np
     import pandas as pd
     from sklearn.model_selection import train_test_split
     from sklearn.linear_model import LinearRegression
     from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
[18] ✓ 0.1s
```

2- Data Preparation / Train-Test Split

```
[19] df = pd.read_csv("Advertising.csv")
     X = df.drop(columns = "sales") #df[["TV", "radio", "newspaper"]]
     y = df["sales"]
     X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3, random_state = 42)
[19] ✓ 0.1s
```

3- Model Building and Fitting

```
model = LinearRegression()
model.fit(X_train, y_train)
```

4- Prediction

```
[21] y_pred = model.predict(X_test)
[21] ✓ 0.5s
```

Python

5- Evaluation

```
[22] mae = mean_absolute_error(y_test, y_pred)
     mse = mean_squared_error(y_test, y_pred)
     rmse = np.sqrt(mean_squared_error(y_test, y_pred))
     R2_score = r2_score(y_test, y_pred)
     print("Model Performance Evaluation:")
     print("-----")
     print(f"R2_score \t\t: {R2_score}")
     print(f"MAE \t\t\t: {mae}")
     print(f"MSE \t\t\t: {mse}")
     print(f"RMSE \t\t\t: {rmse}")
[22] ✓ 1.1s
```

Python

```
... Model Performance Evaluation:
-----
R2_score      : 0.8609466508230368
MAE          : 1.5116692224549086
MSE          : 3.796797236715219
RMSE         : 1.9485372043446385
```



Introduction to Bias-Variance Trade-Off

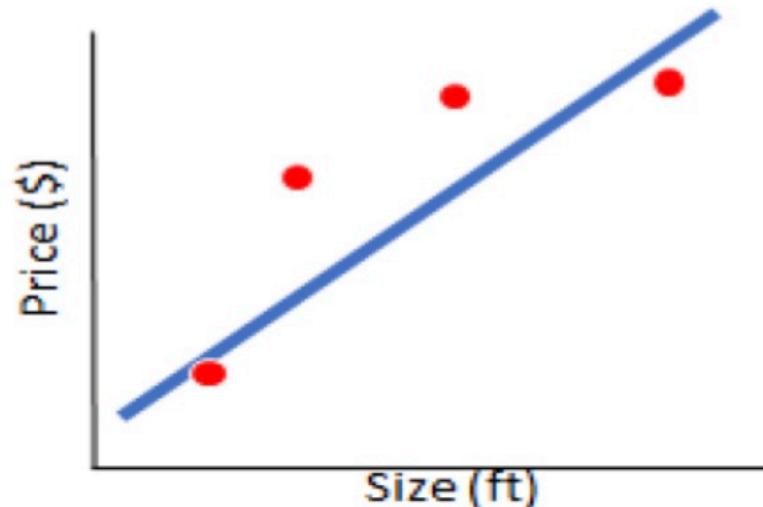
Underfitting and Overfitting Problems

Training Error vs. Validation Error (Test Error)

Polynomial Regression



Introduction to Bias-Variance Trade-Off



Models with **too few** parameters may not fit the data well (**high bias**),

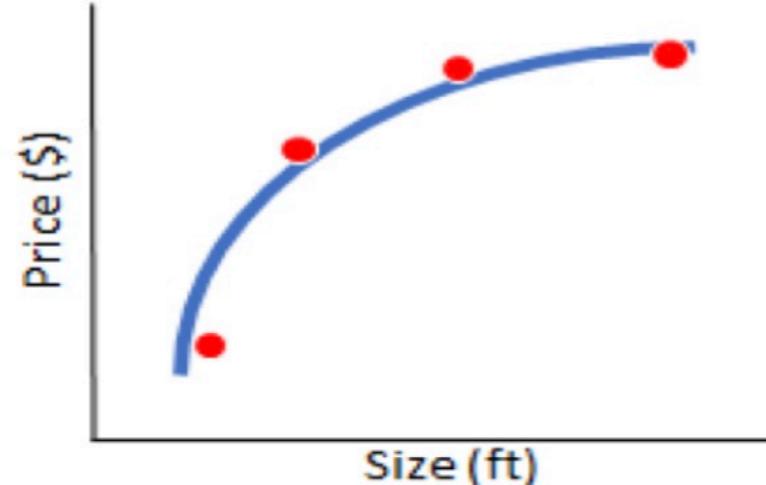
but the scores in the test set are the same as in the train set. (**low variance**)



Simple

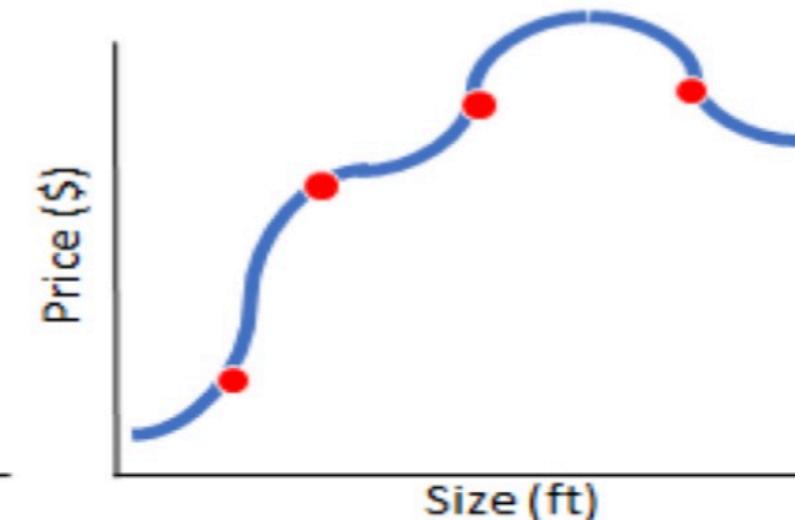


UNDERFIT



Just Right

Ideally, we would like to choose a model that both accurately **captures the regularities** in the training data, but also **generalizes well** to unseen data. (**low bias & low variance**)



Models with **too many** parameters may fit the **training data** well (**low bias**),

but the scores on the test set are much lower than on the train set (**high variance**)



Complex



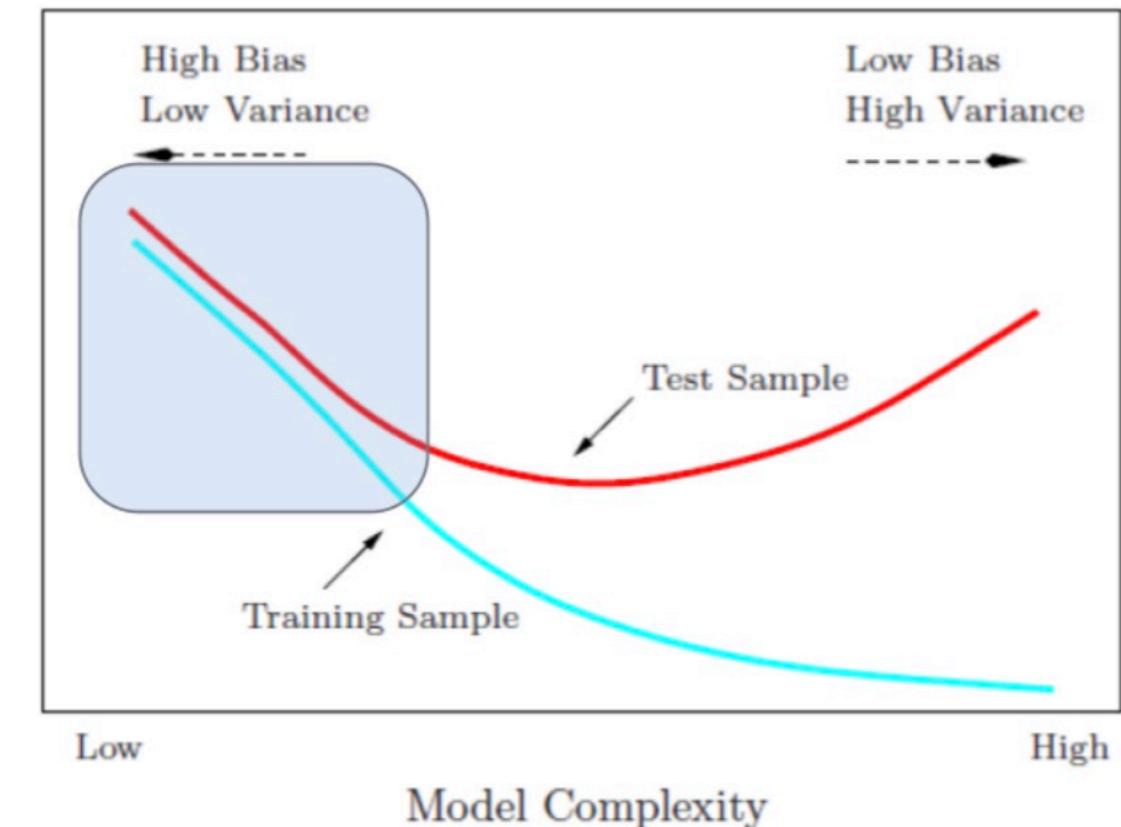
OVERFIT

Underfitting and Overfitting Problems

HOW TO RECOGNIZE ?

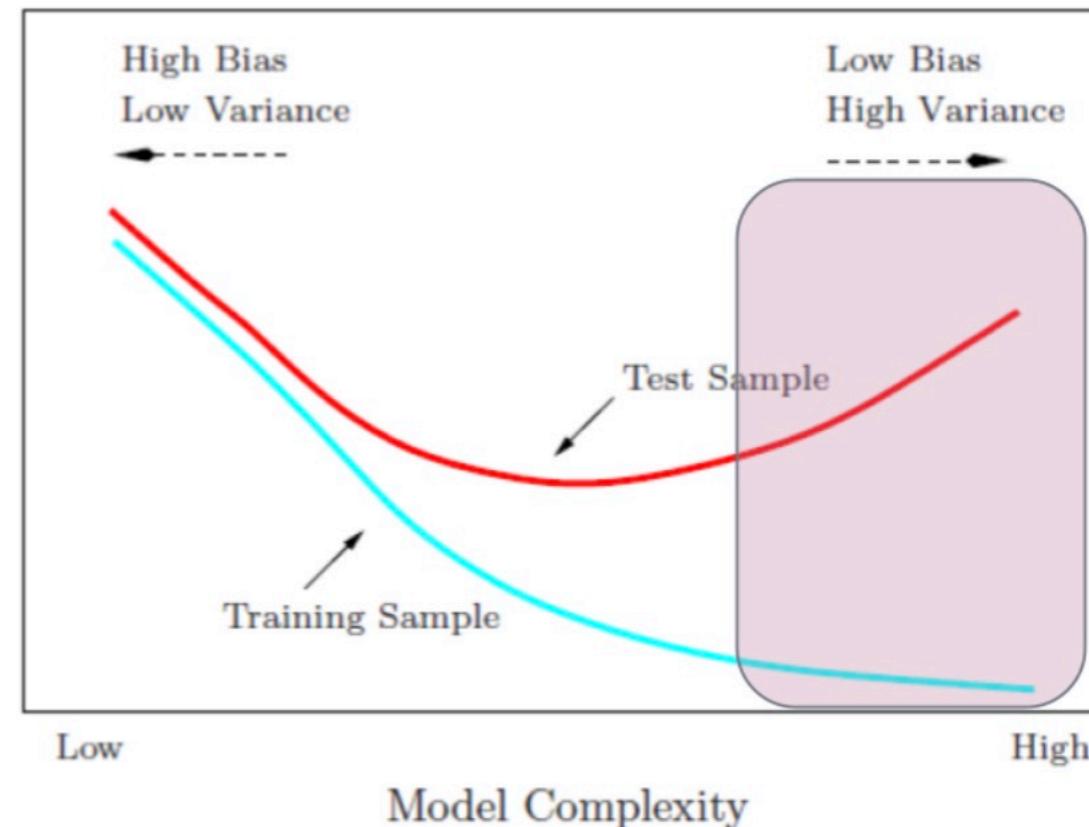
UNDERFITTING

High training error and **high** test error

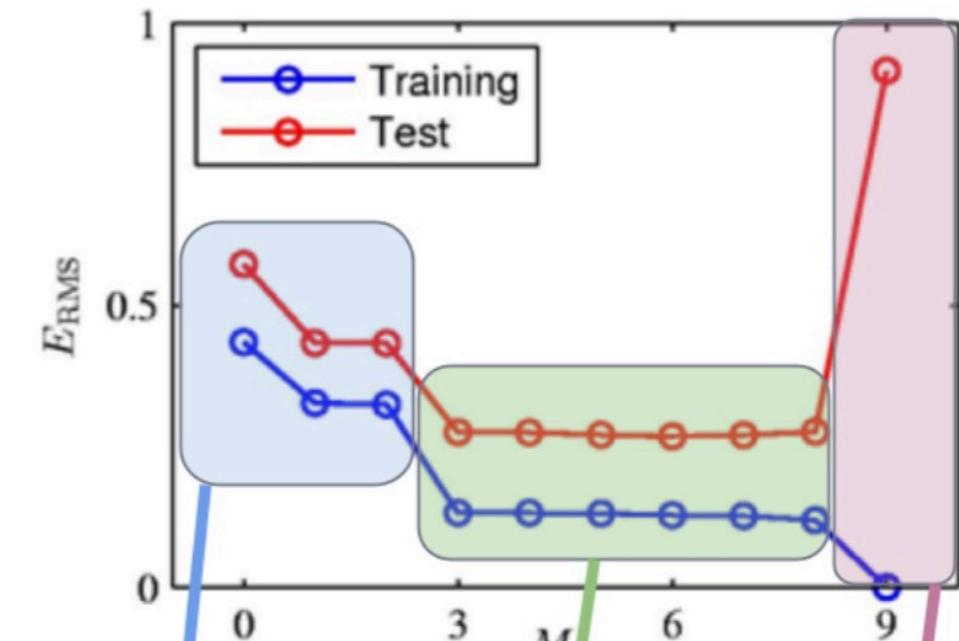
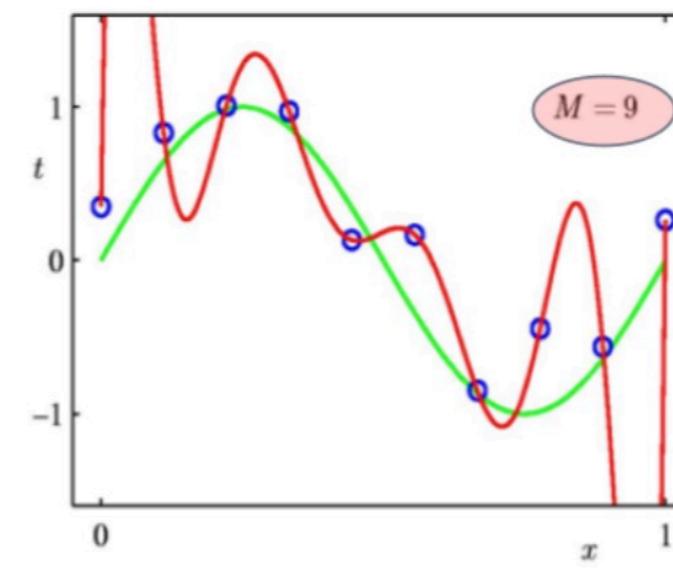
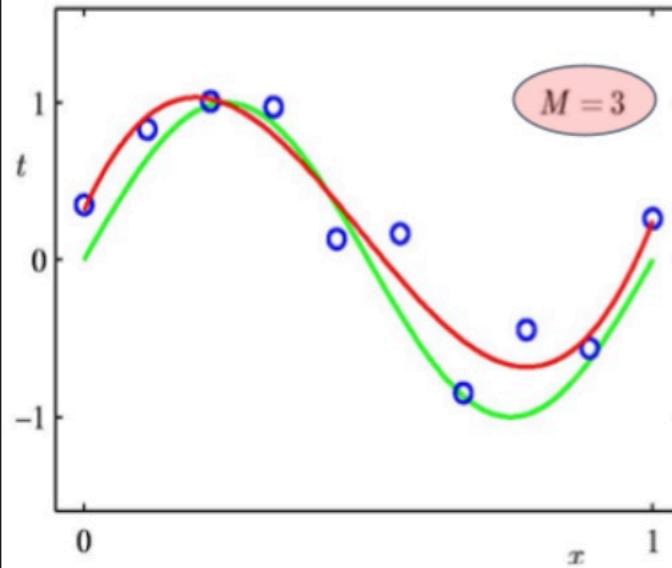
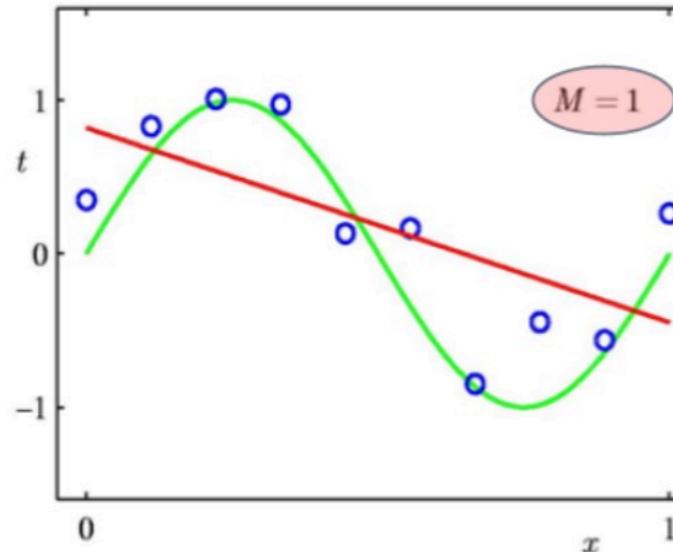
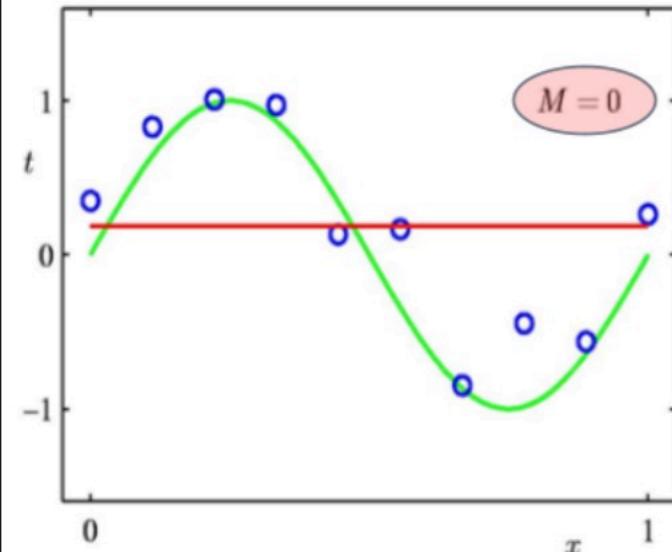


OVERFITTING

Low training error and **high** test error



Underfitting and Overfitting Problems

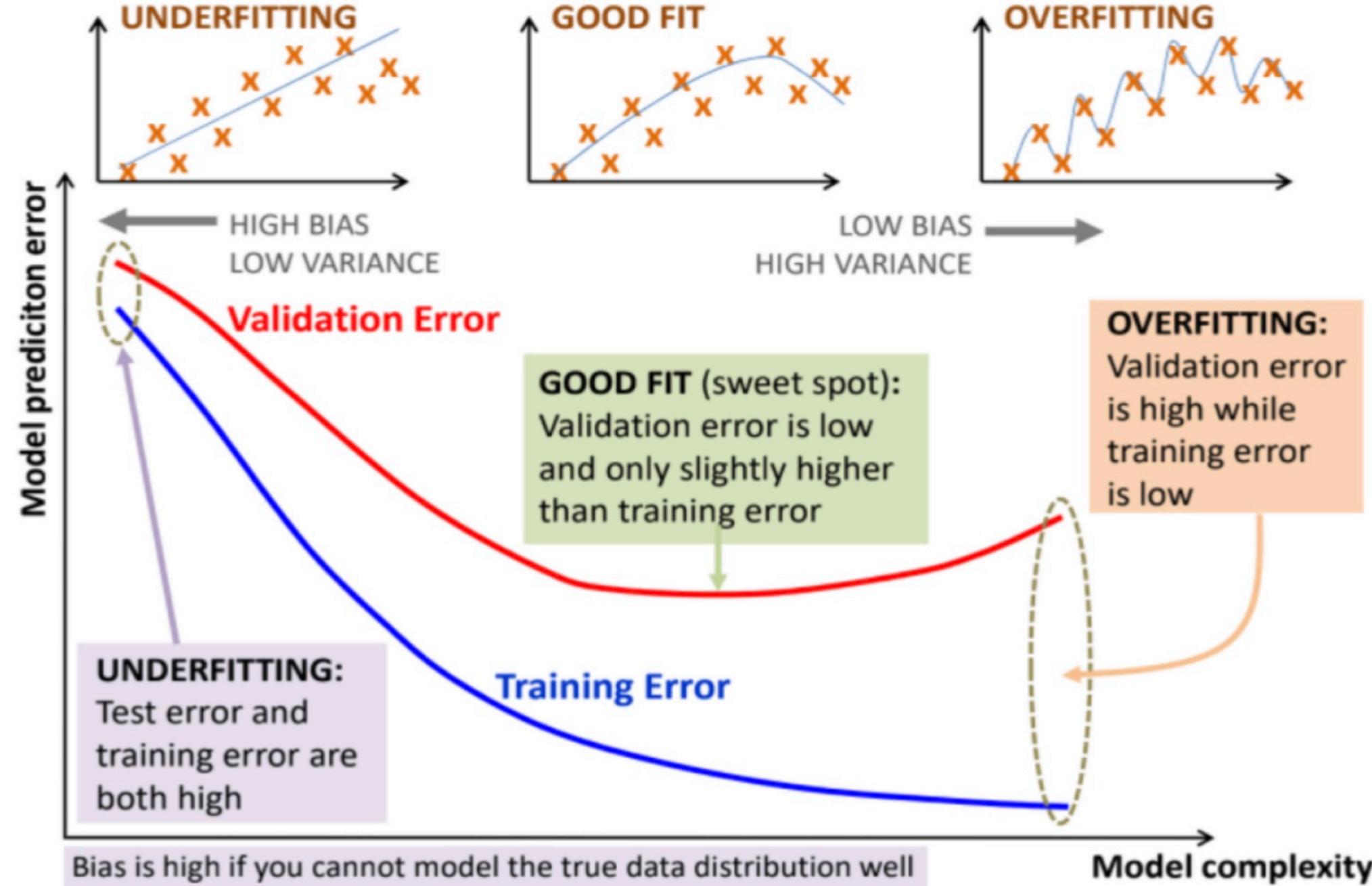


Underfit



Overfit

Training Error vs. Validation Error (Test Error)



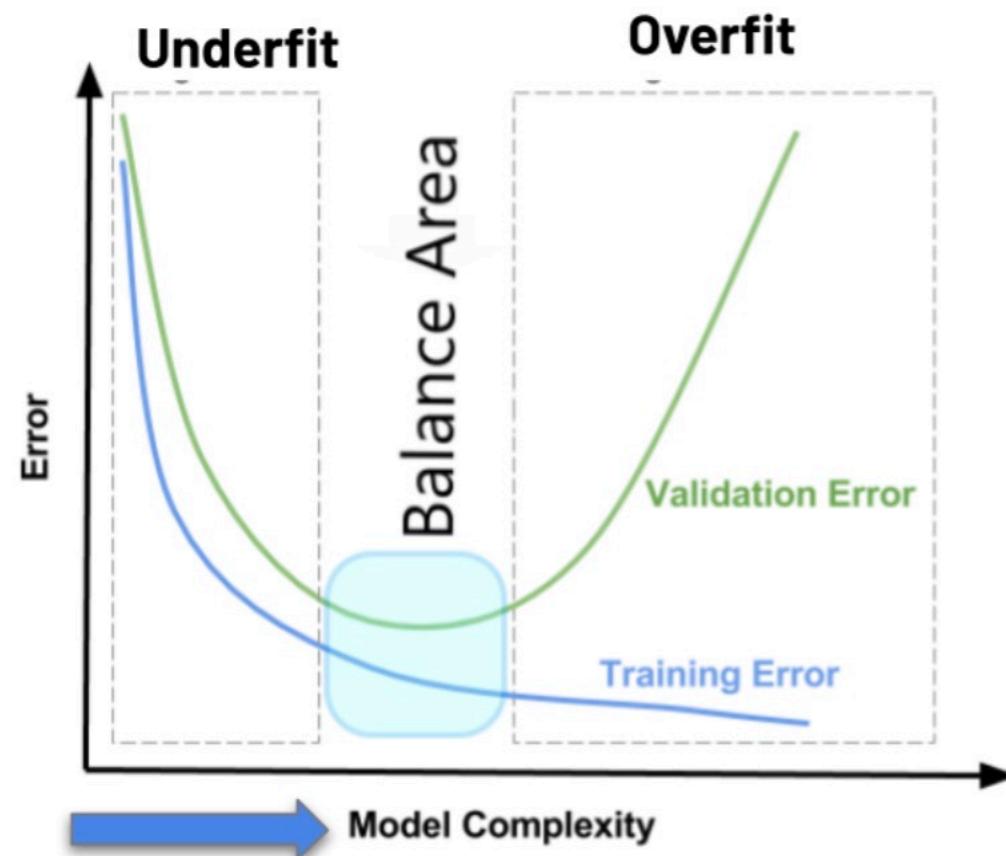
Underfitting and Overfitting Problems



HOW TO DEAL WITH

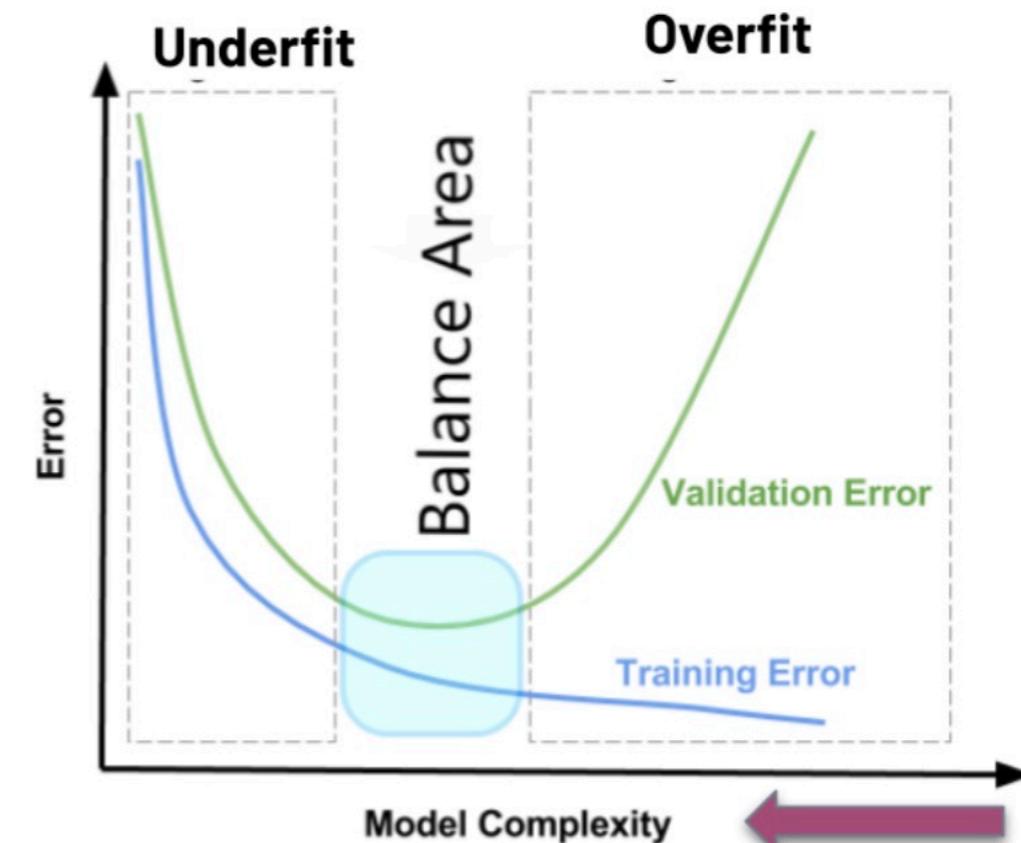
UNDERFITTING ?

- Find a **more complex** model



OVERTFITTING ?

- Decrease the number of parameters
- More training data / **Cross Validation**
- **Regularization (Lasso&Ridge)**



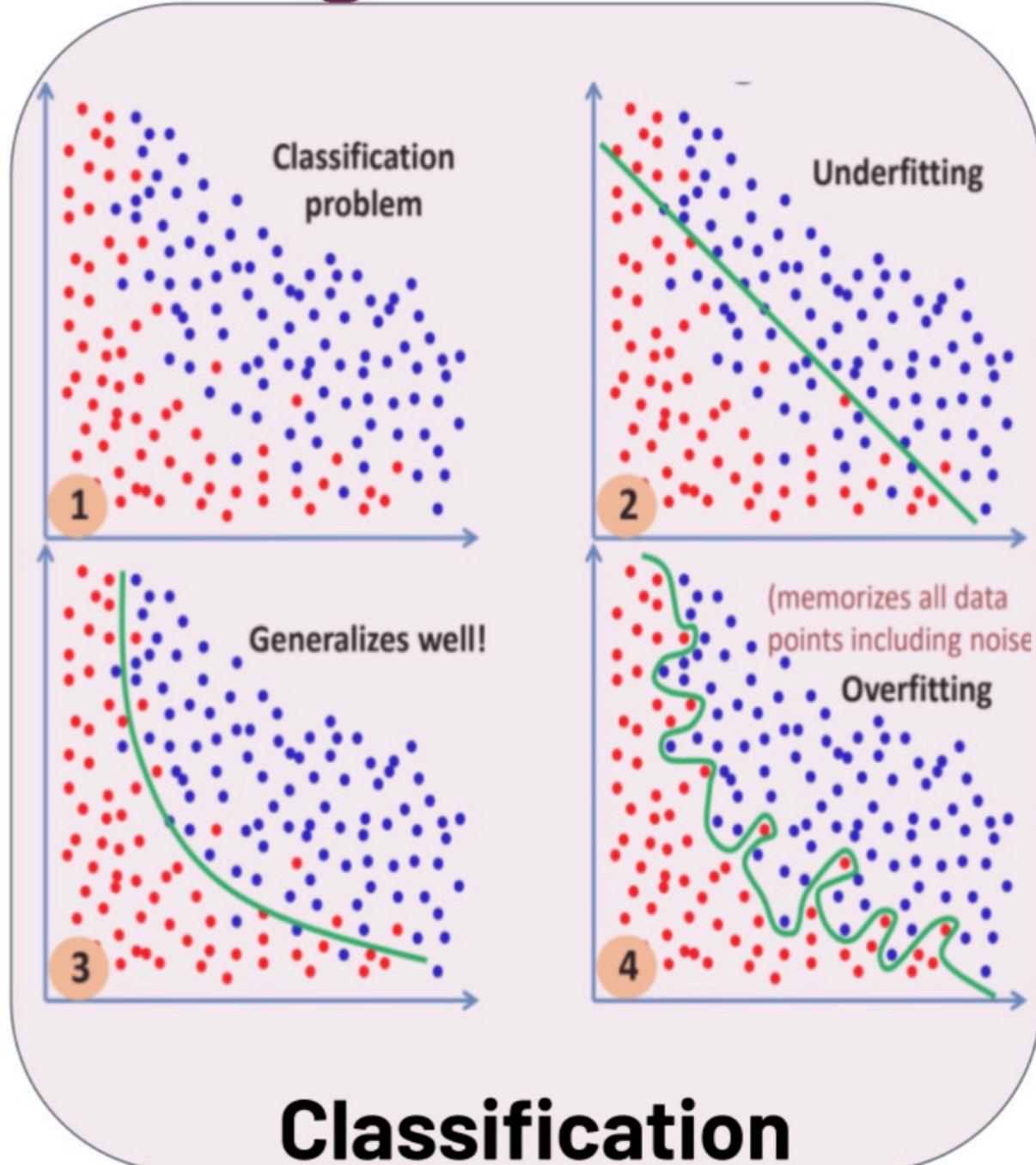
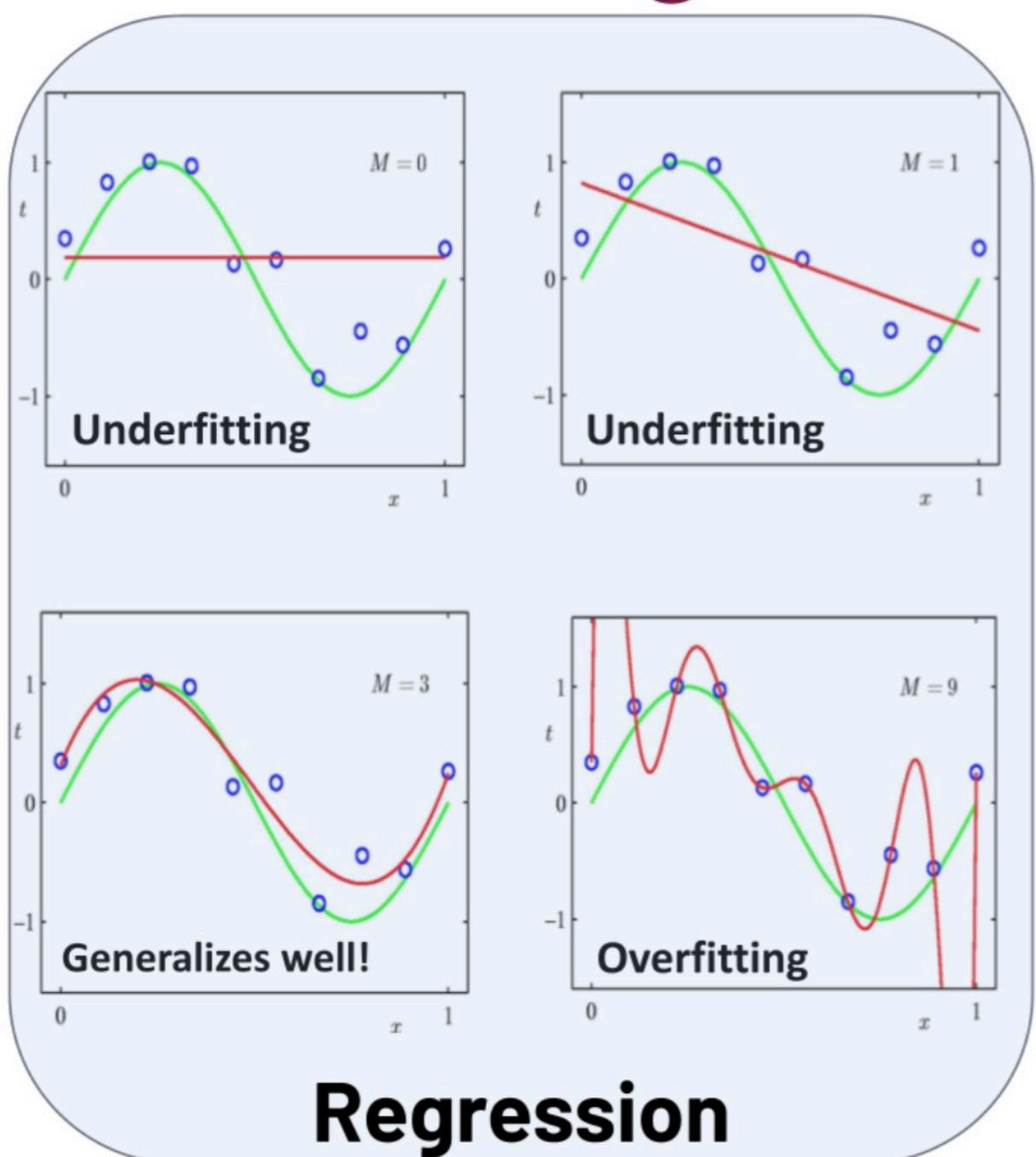
Underfitting and Overfitting Problems

Summary

	MODEL				
	Bias	Variance	Complexity	Flexibility	Generalizability
Underfitting: An overly simple model	High	Low	Low	Low	High
Overfitting: Modeling the noise as well	Low	High	High	High	Low

Ref: <https://cambridgecoding.wordpress.com/2016/03/24/misleading-modelling-overfitting-cross-validation-and-the-bias-variance-trade-off/>

Underfitting and Overfitting Problems





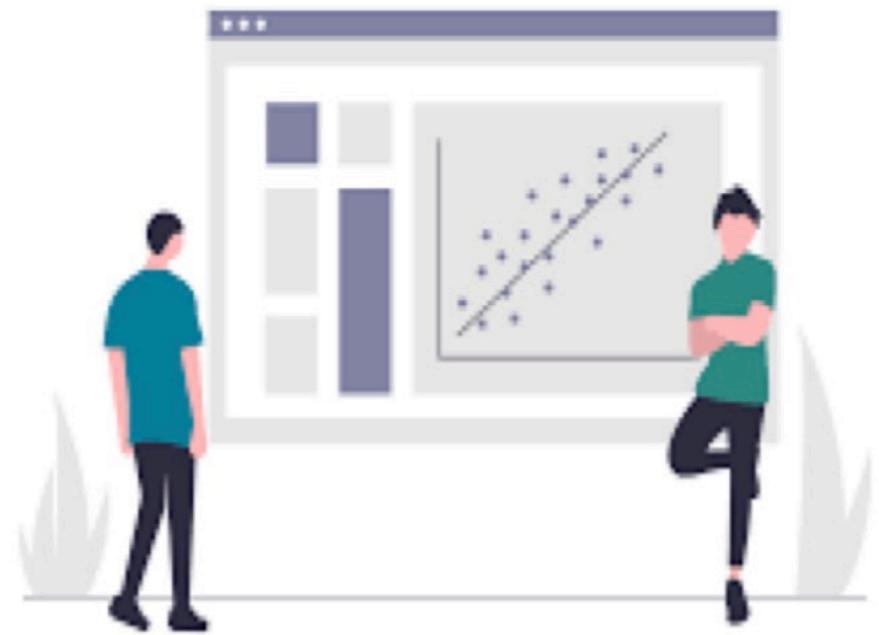
Regression (cont.)

Session-3

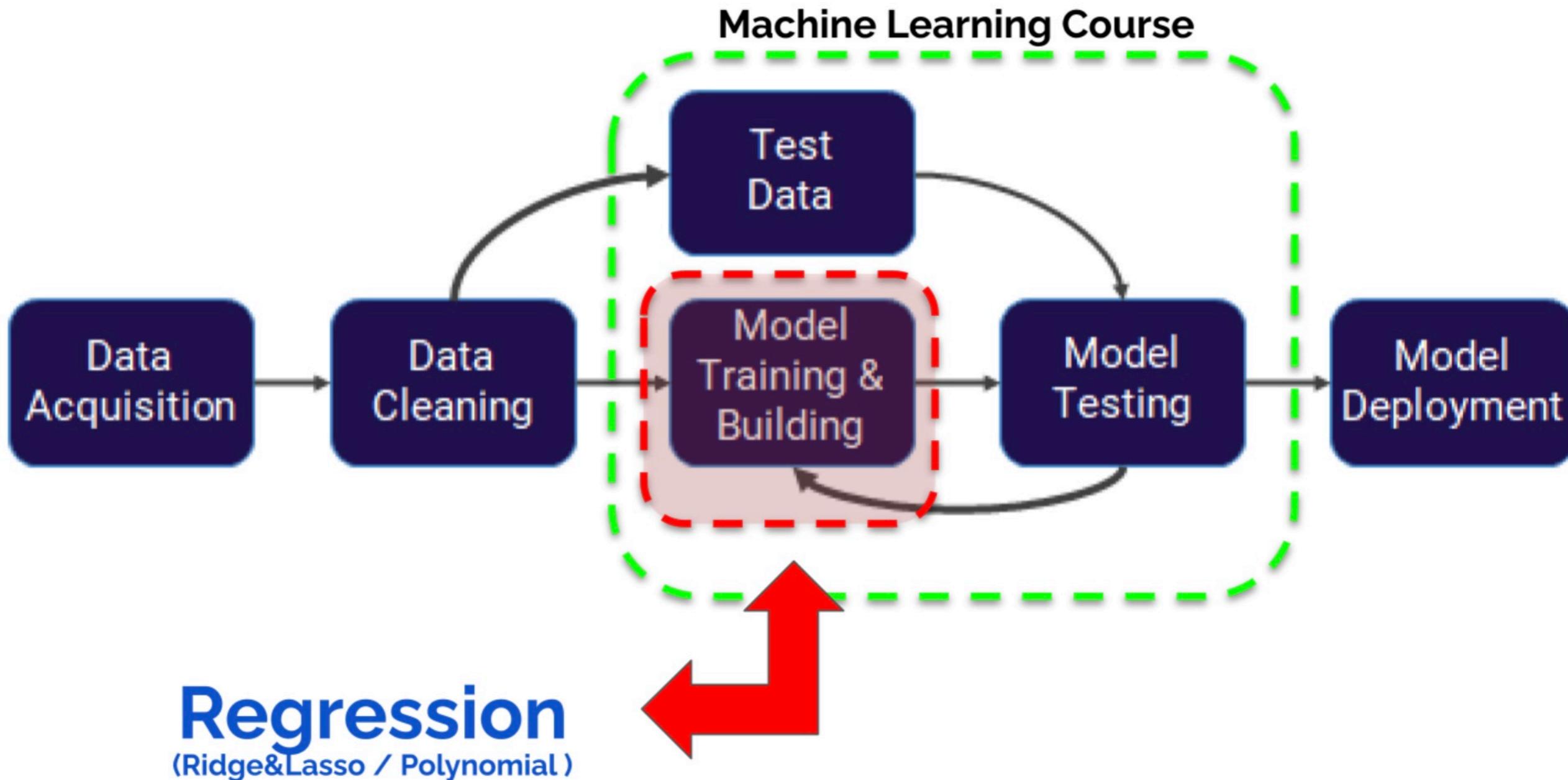




Polynomial Regression



Where are we?



Polynomial Regression



Types of Regression Models

Simple Linear Regression

A linear regression model that estimates the relationship between **one independent** variable and **one dependent** variable using a straight line.

$$Y = \theta_0 + \theta_1 x$$

Multi Linear Regression

A linear regression model that estimates the relationship between **several independent** variables (features) and **one dependent** variable.

Polynomial Regression

A special case of multiple linear regression. It also works with non linear relationship. The relationship between the independent variable x and dependent variable y is modeled as an **nth degree polynomial** in x.

$$Y = \theta_0 + \theta_1 x + \theta_2 x^2$$

Advantages:

- Give info about the relevance of the features
- Works good irrespective of data size

Disadvantages:

Assumptions of linear regression

Advantages:

Works good on nonlinear probs.

Disadvantages:

Need to choose right polynomial degree for good bias/variance trade off.

Polynomial Regression

Linear regression: $Y = \beta_0 + \beta_1 X$

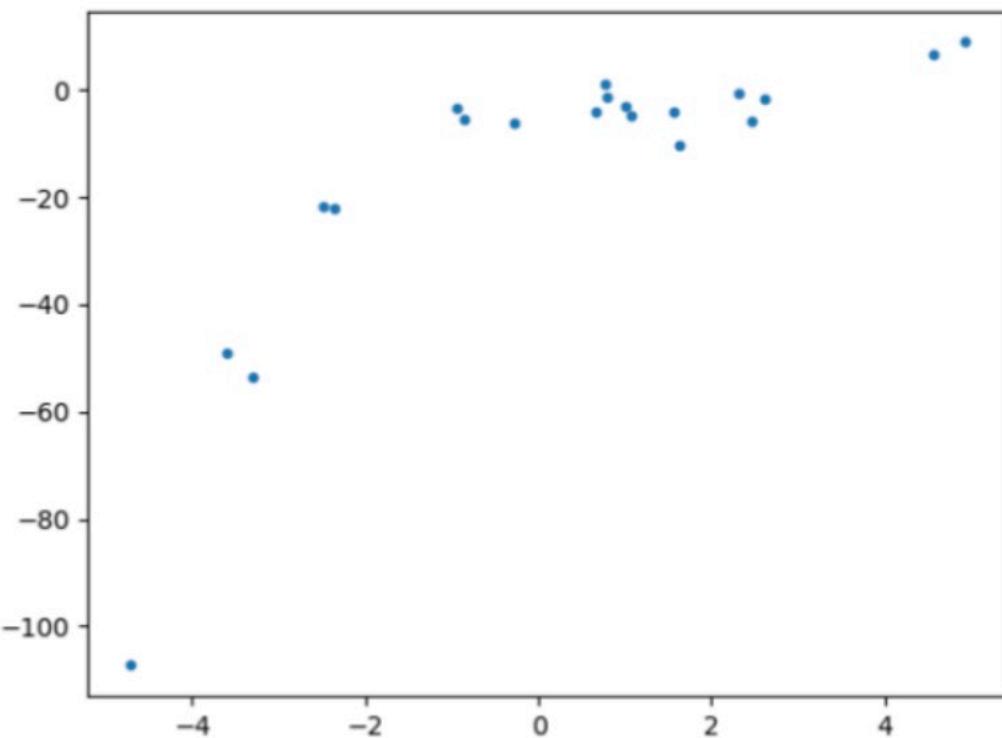
Linear regression: $Y = \beta_0 + \beta_1 X^2$

Nonlinear regression: $Y = \beta_1 X^{\beta_2}$

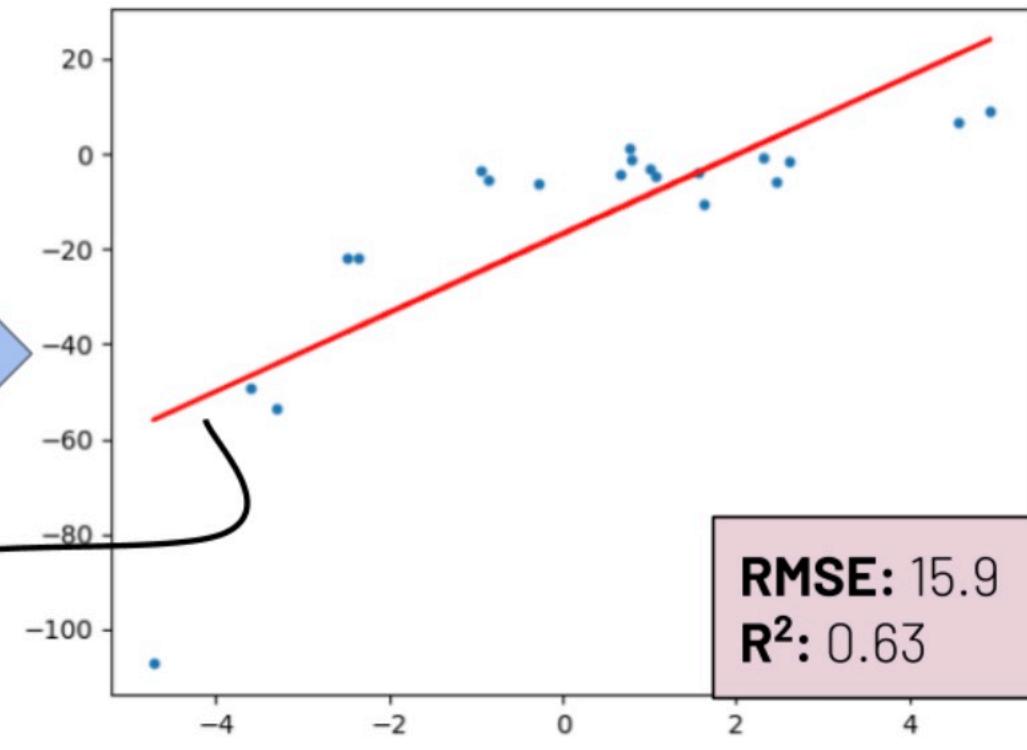
Nonlinear regression: - $Y = \beta_0 + (\beta_2 - \beta_1)e^{-\beta_3 X^{\beta_4}}$

Nonlinear regression: $Y = \beta_1 \cos(X_1 + \beta_2) + \beta_3 \cos(2X_2 + \beta_4)$

Polynomial Regression



fitted Simple
Lin.Reg.



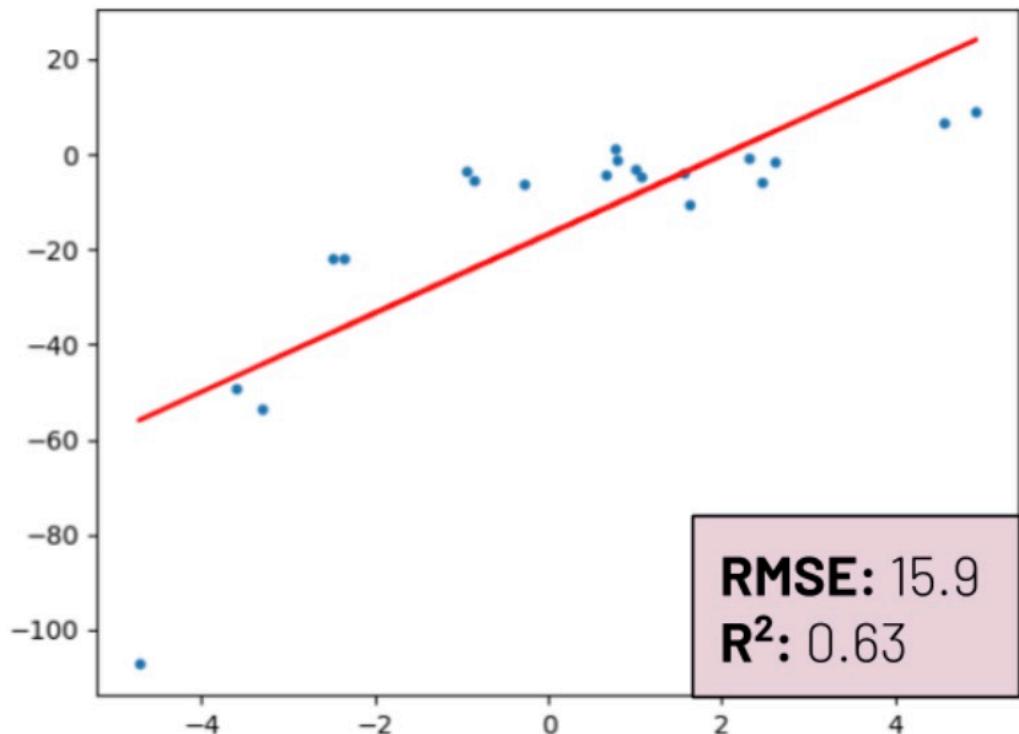
The regression line is **unable to capture the patterns** in the data. This is an example of **under-fitting**.

To overcome under-fitting, we need to **increase the complexity** of the model.

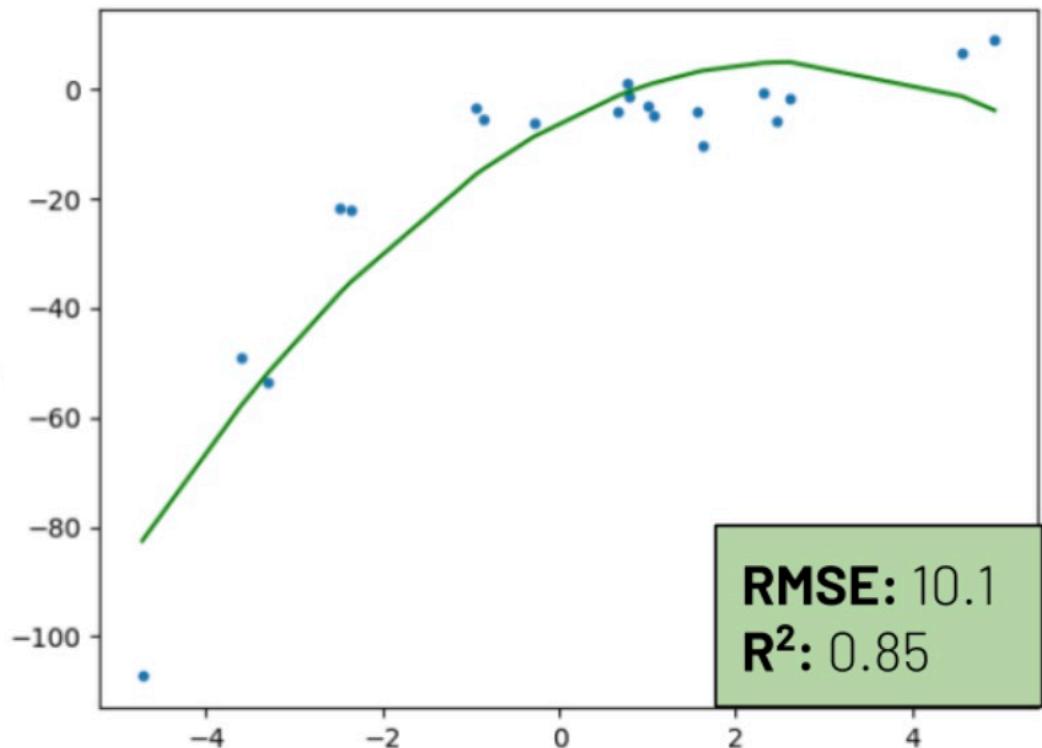
Polynomial Regression



To generate a higher order equation we can **add powers of the original features as new features.**



added powers of
features



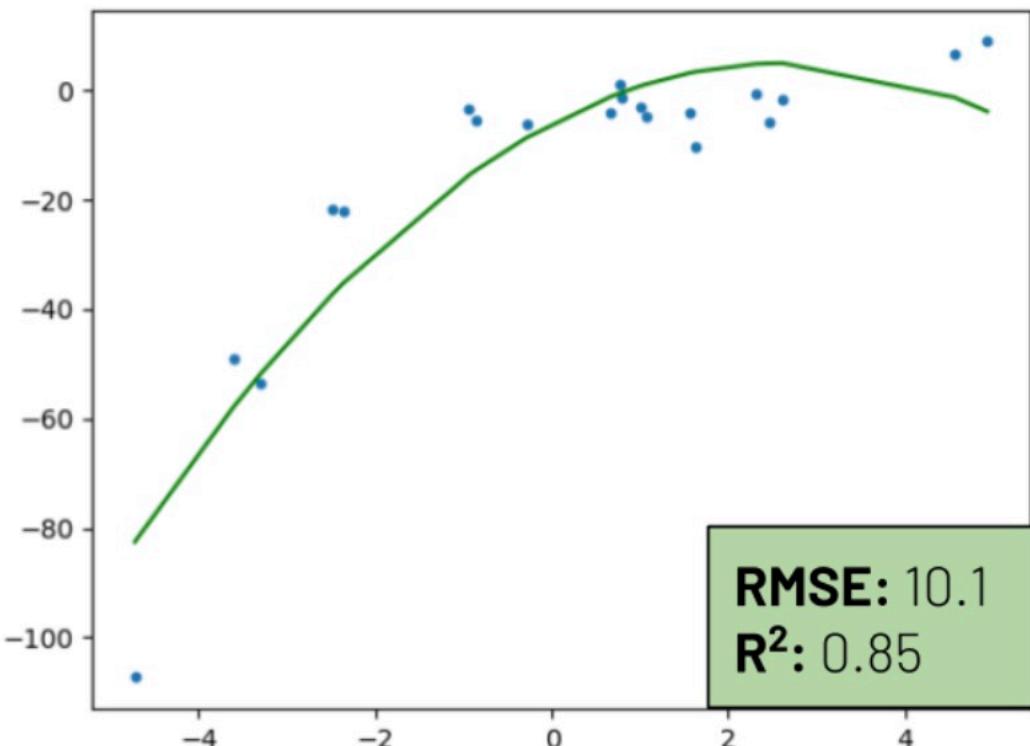
$$Y = \theta_0 + \theta_1 x$$

$$Y = \theta_0 + \theta_1 x + \theta_2 x^2$$

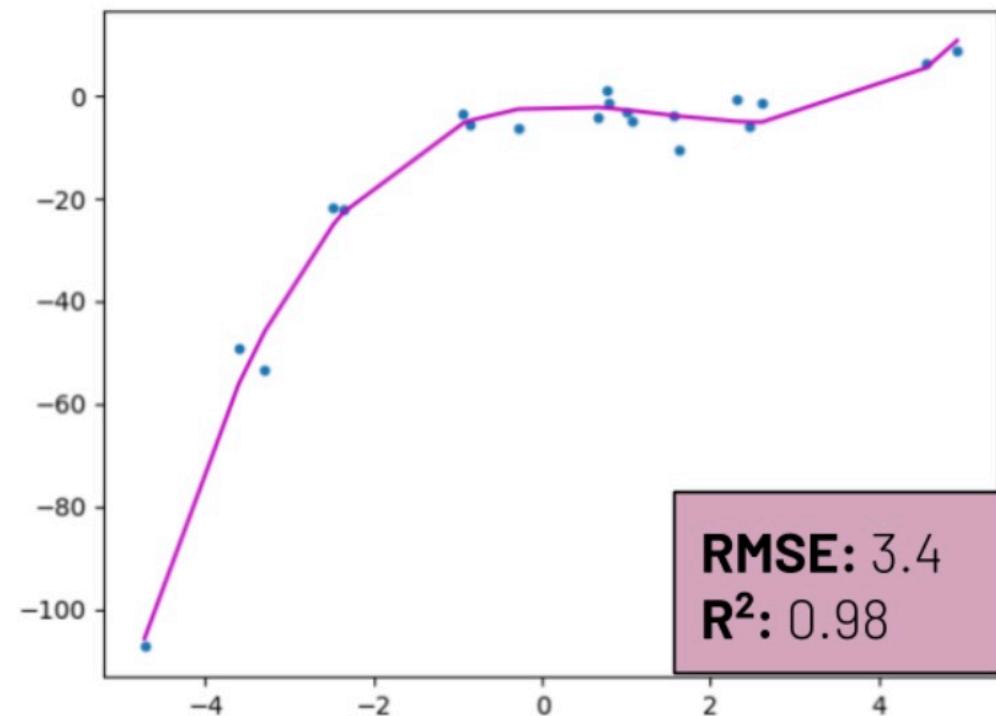
Polynomial Regression



If we try to **fit a cubic curve (degree=3)** to the dataset, we can see that it is **more successfully generalized** than the quadratic (degree=2) and the linear plots (degree=1).

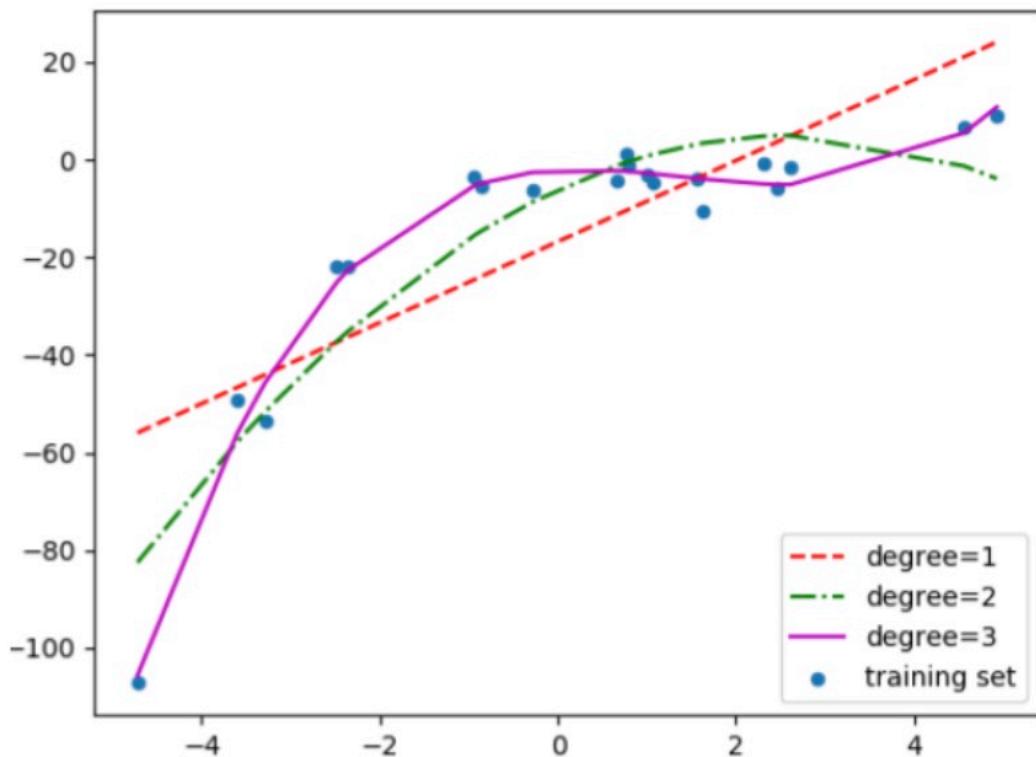


fit a cubic curve
(degree=3)

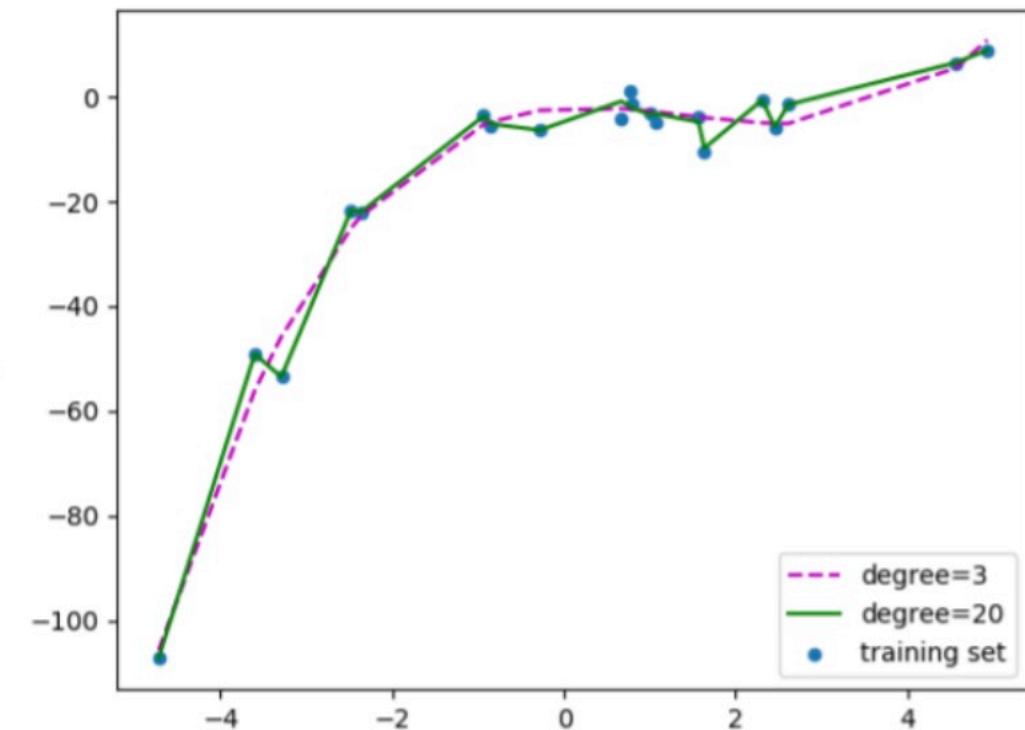


Polynomial Regression

If we further **increase the degree to 20**, we can see that the curve memorize the data points. This is an example of **overfitting**.



degree 1,2,3 to 20



How do we choose an optimal degree?

Bias Variance Trade-off