Optimization: Overfitting

Industrial AI Lab.

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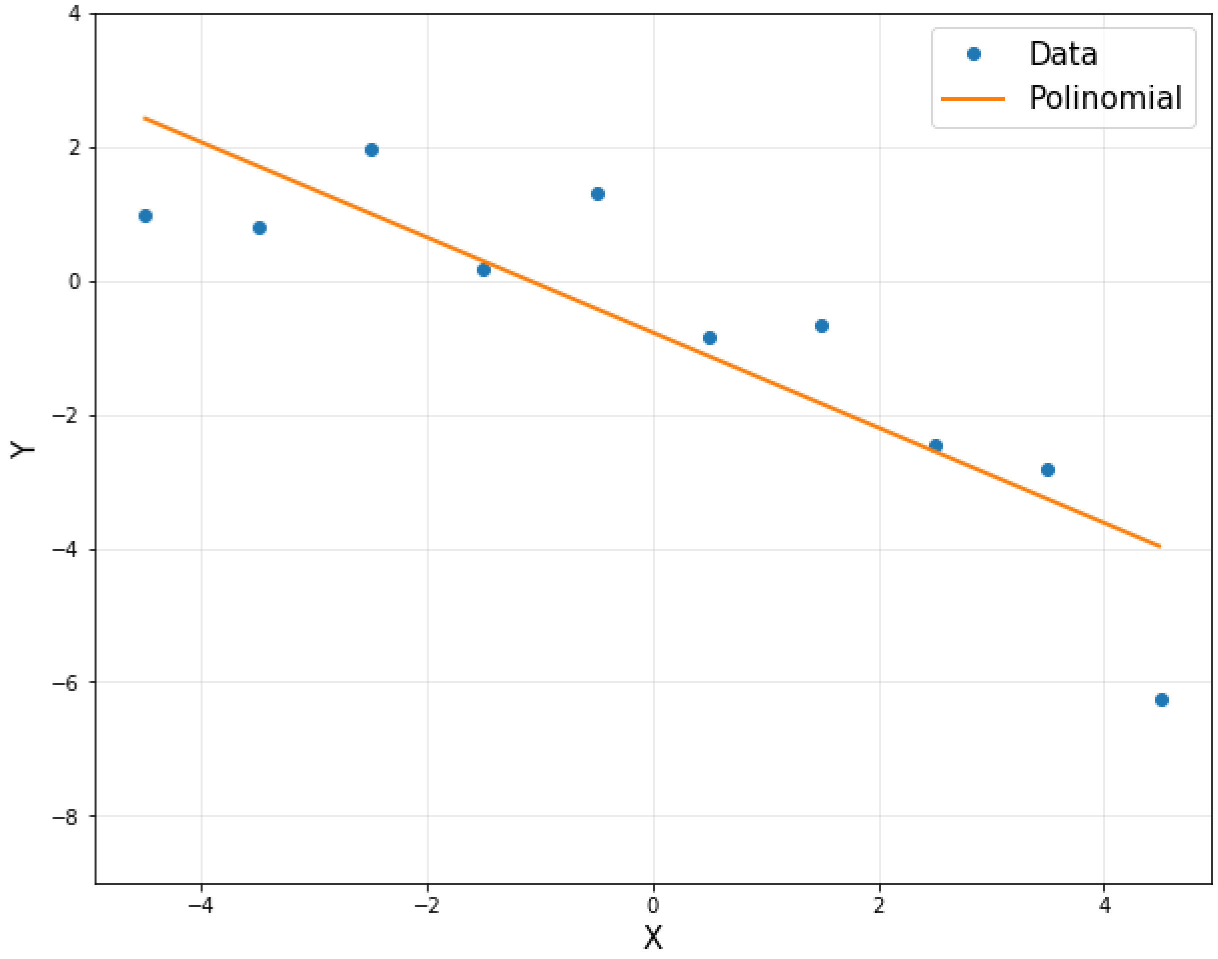
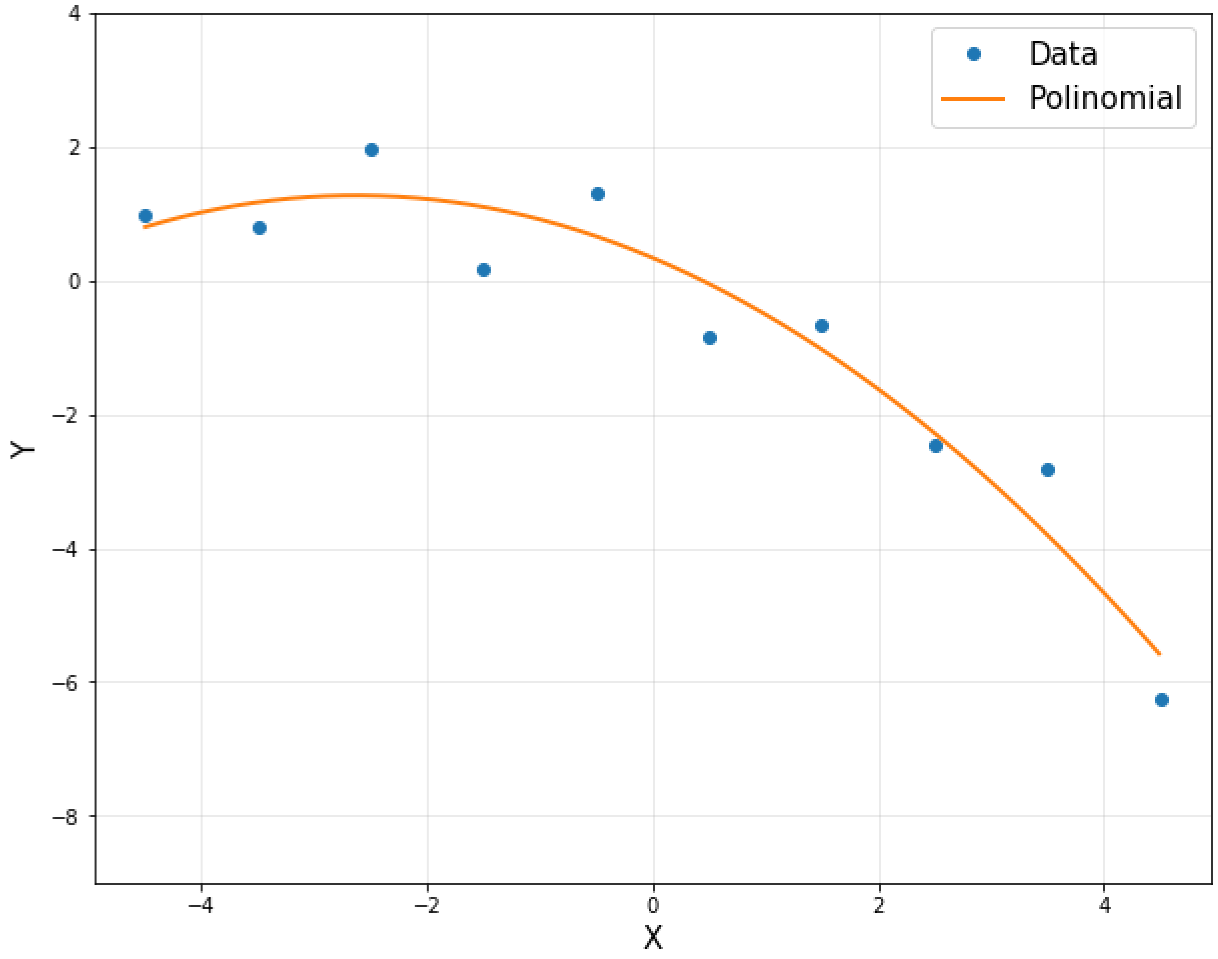
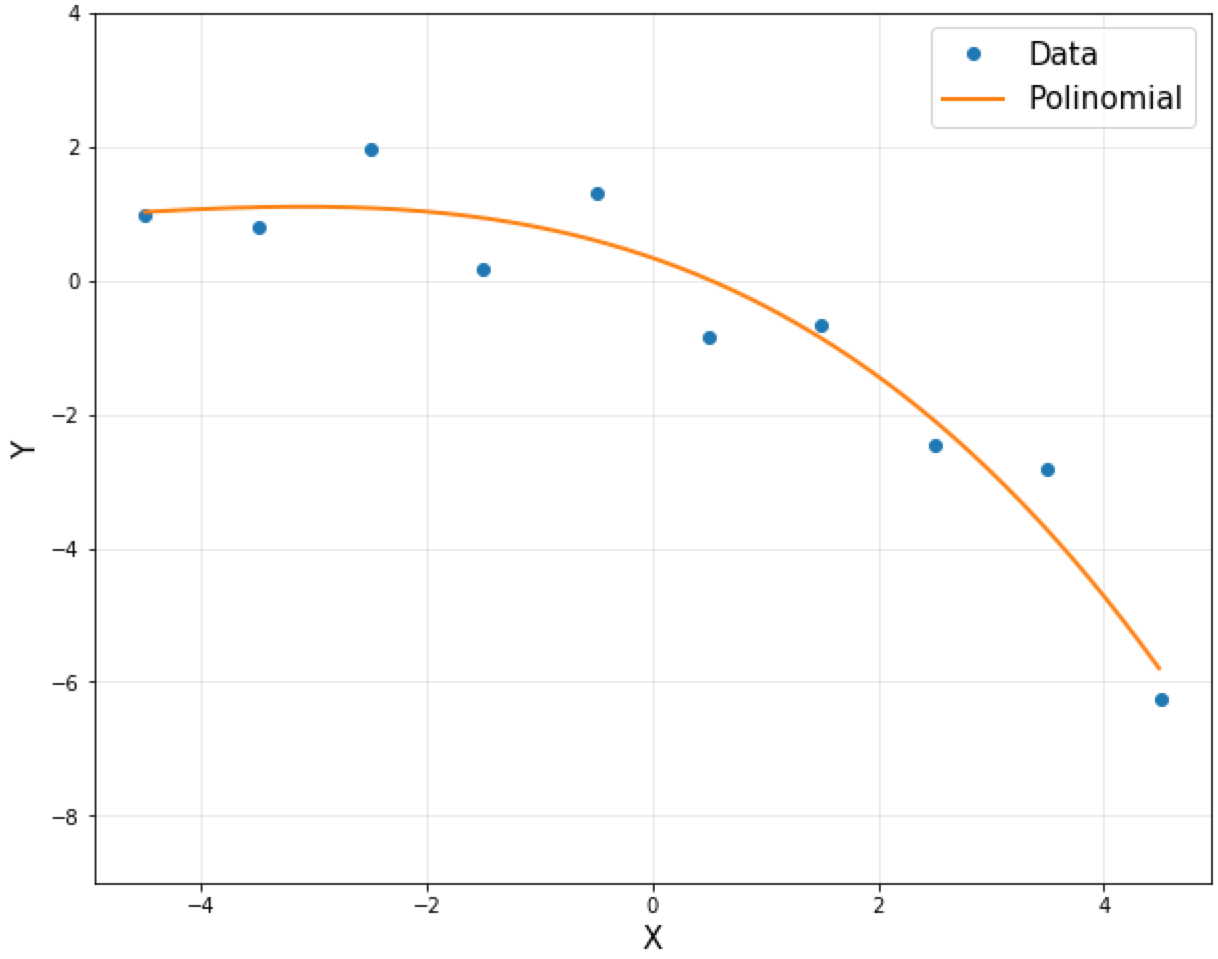
Polynomial Regression (d = 1)



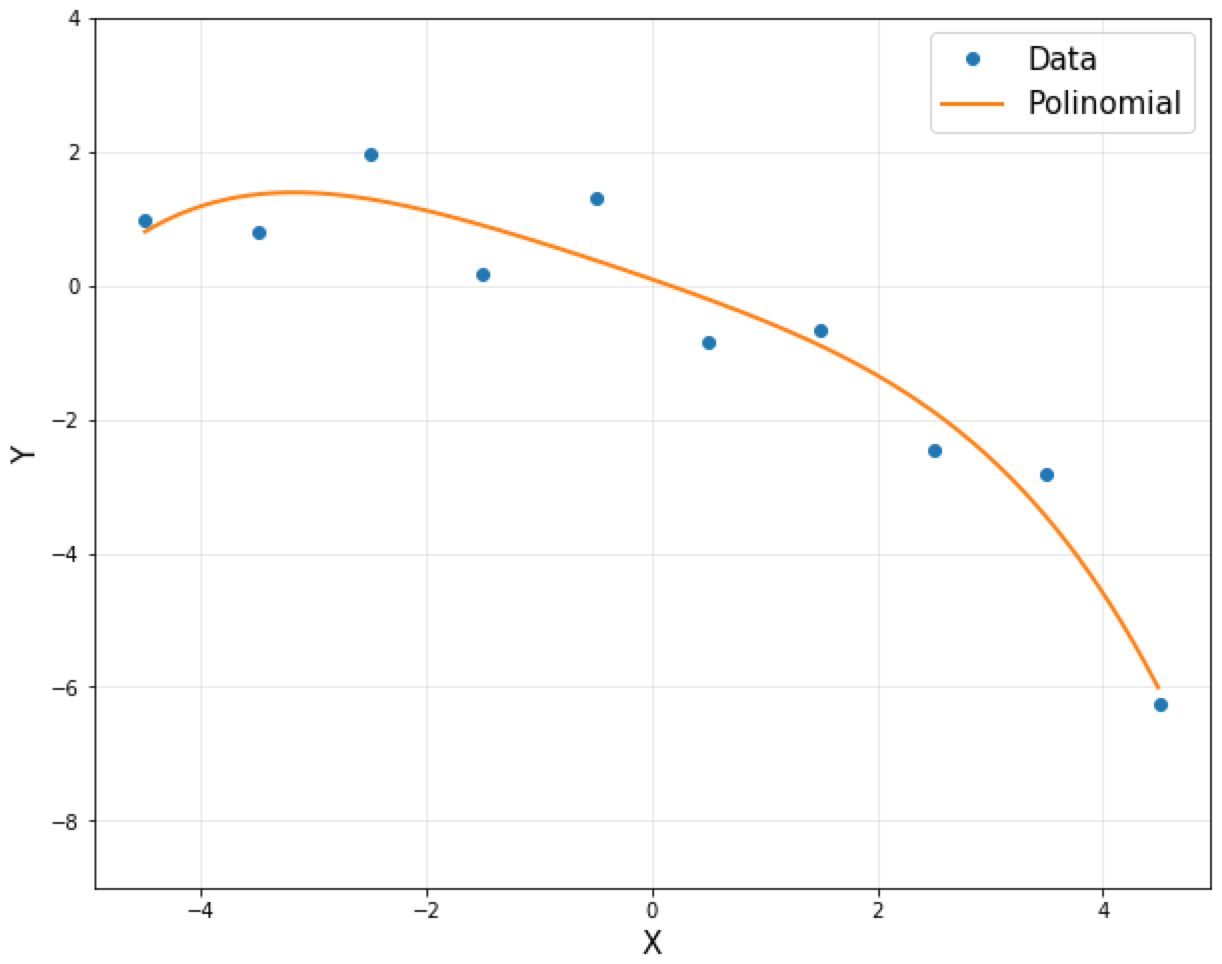
Polynomial Regression (d = 2)



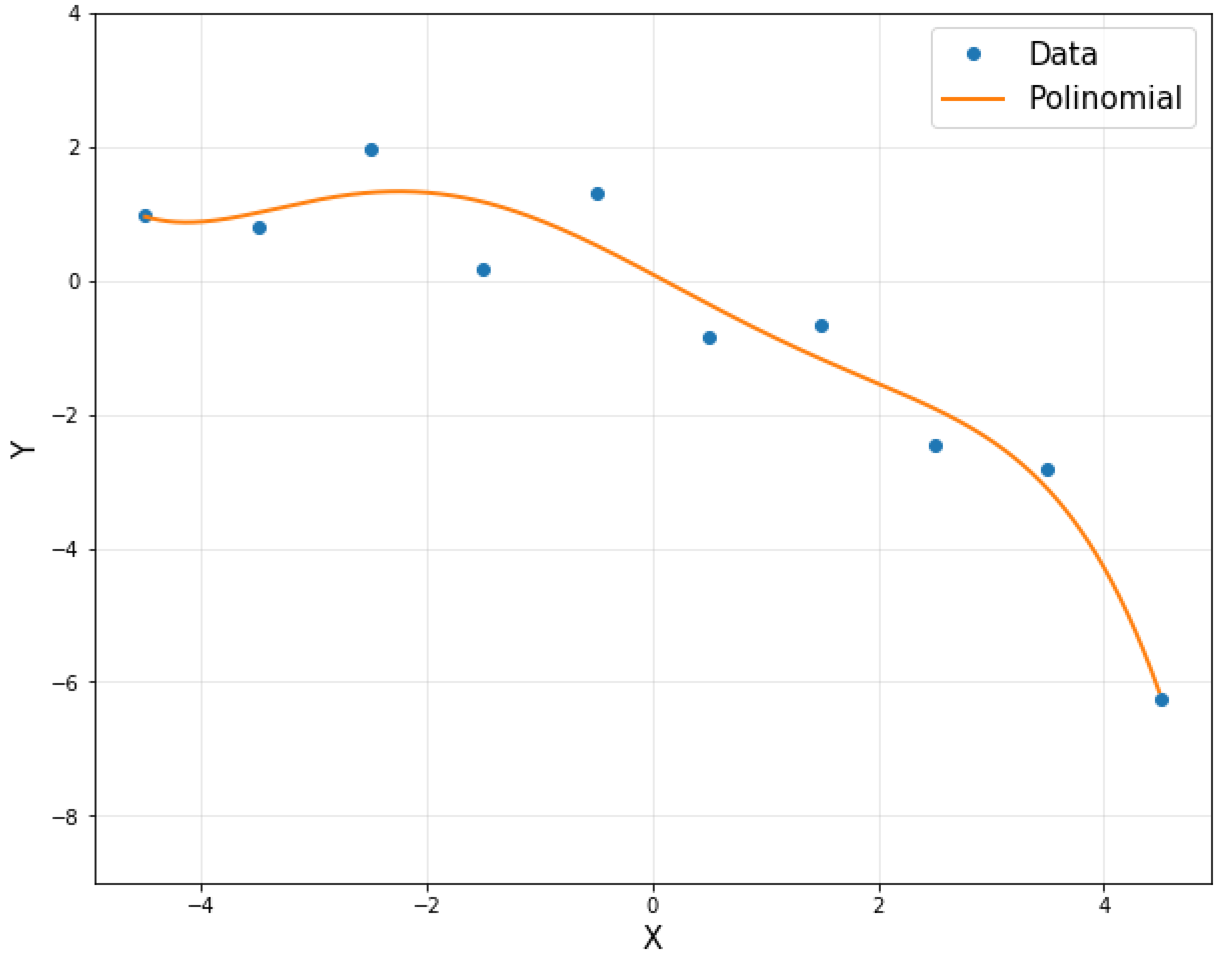
Polynomial Regression (d = 3)



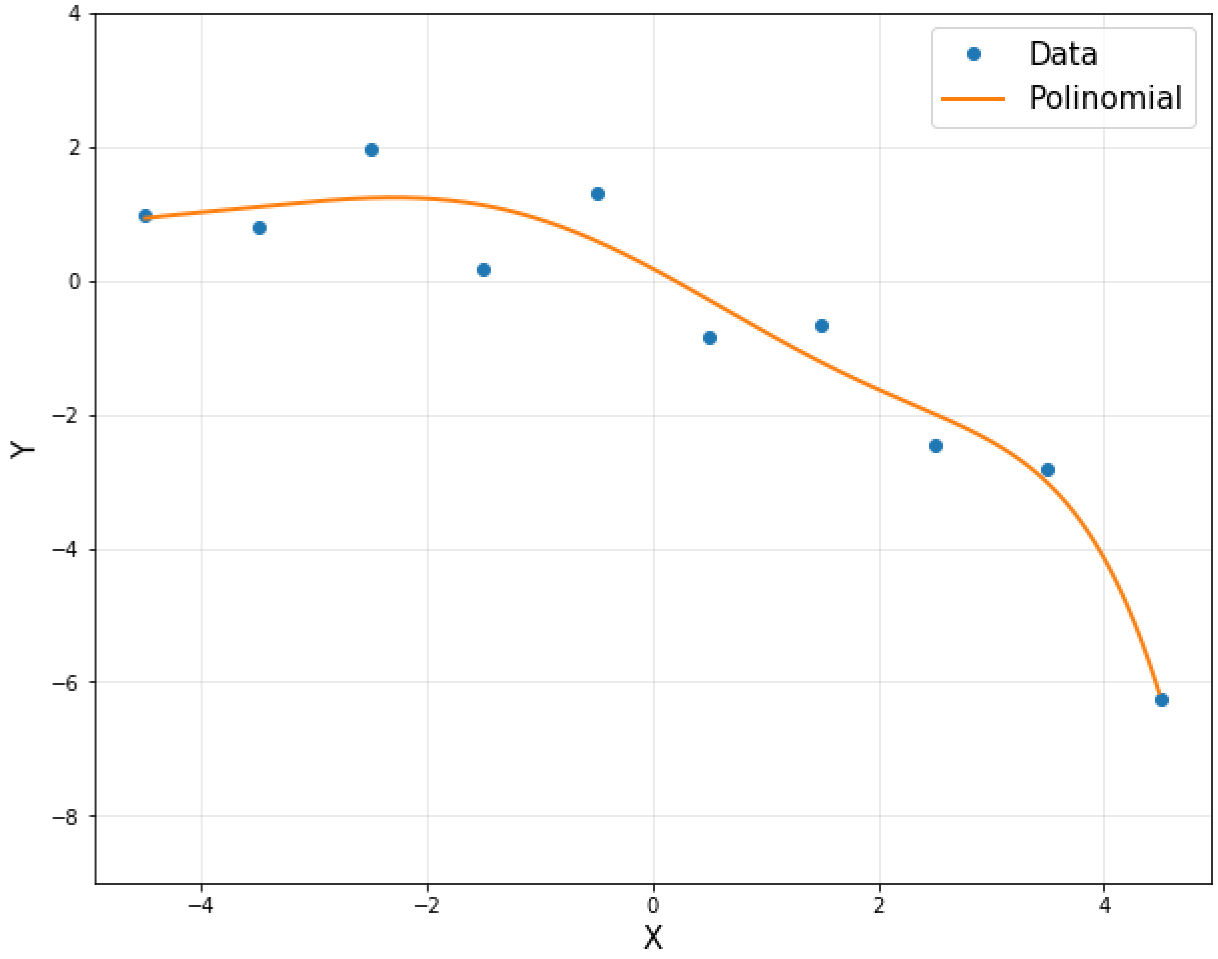
Polynomial Regression (d = 4)



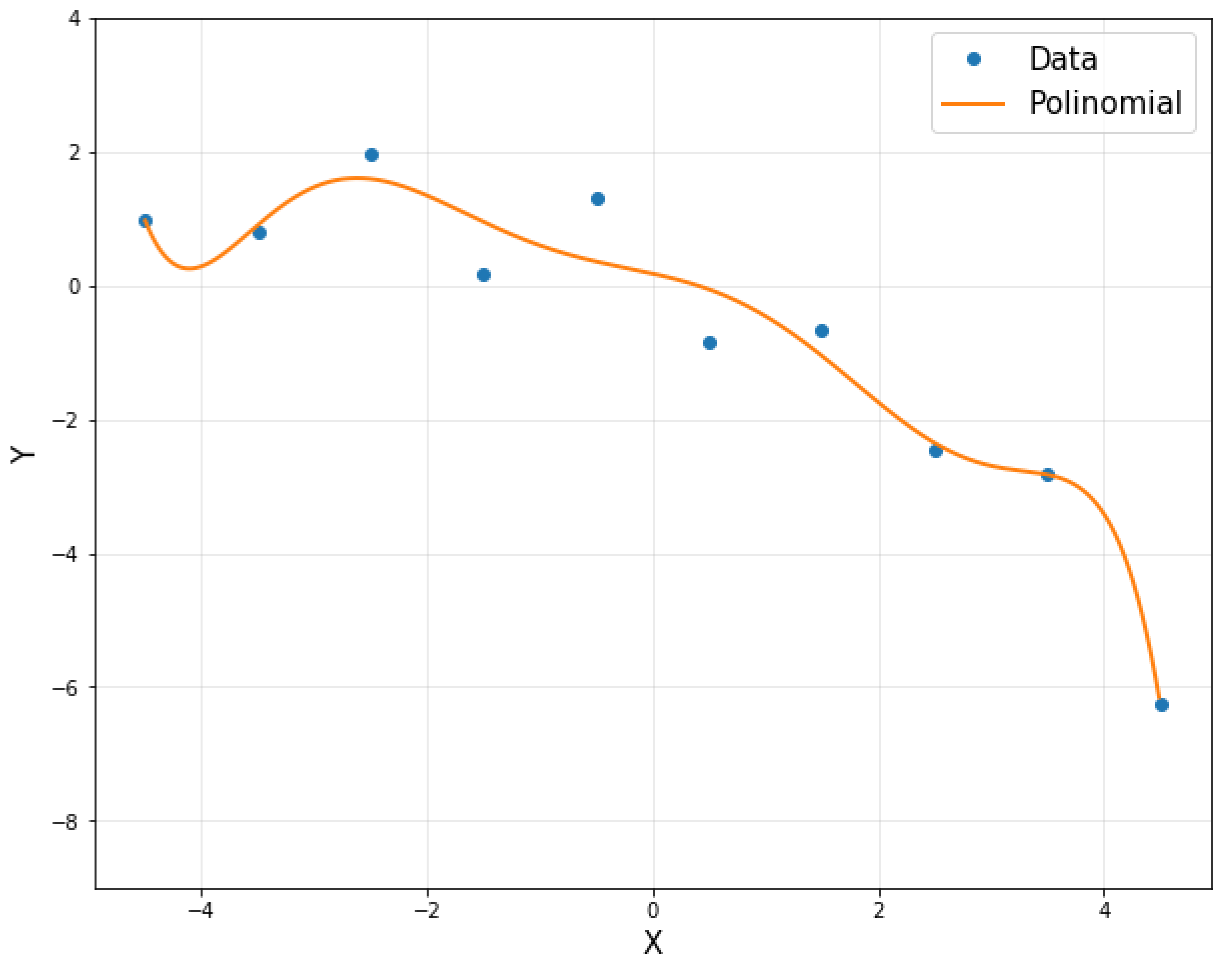
Polynomial Regression (d = 5)



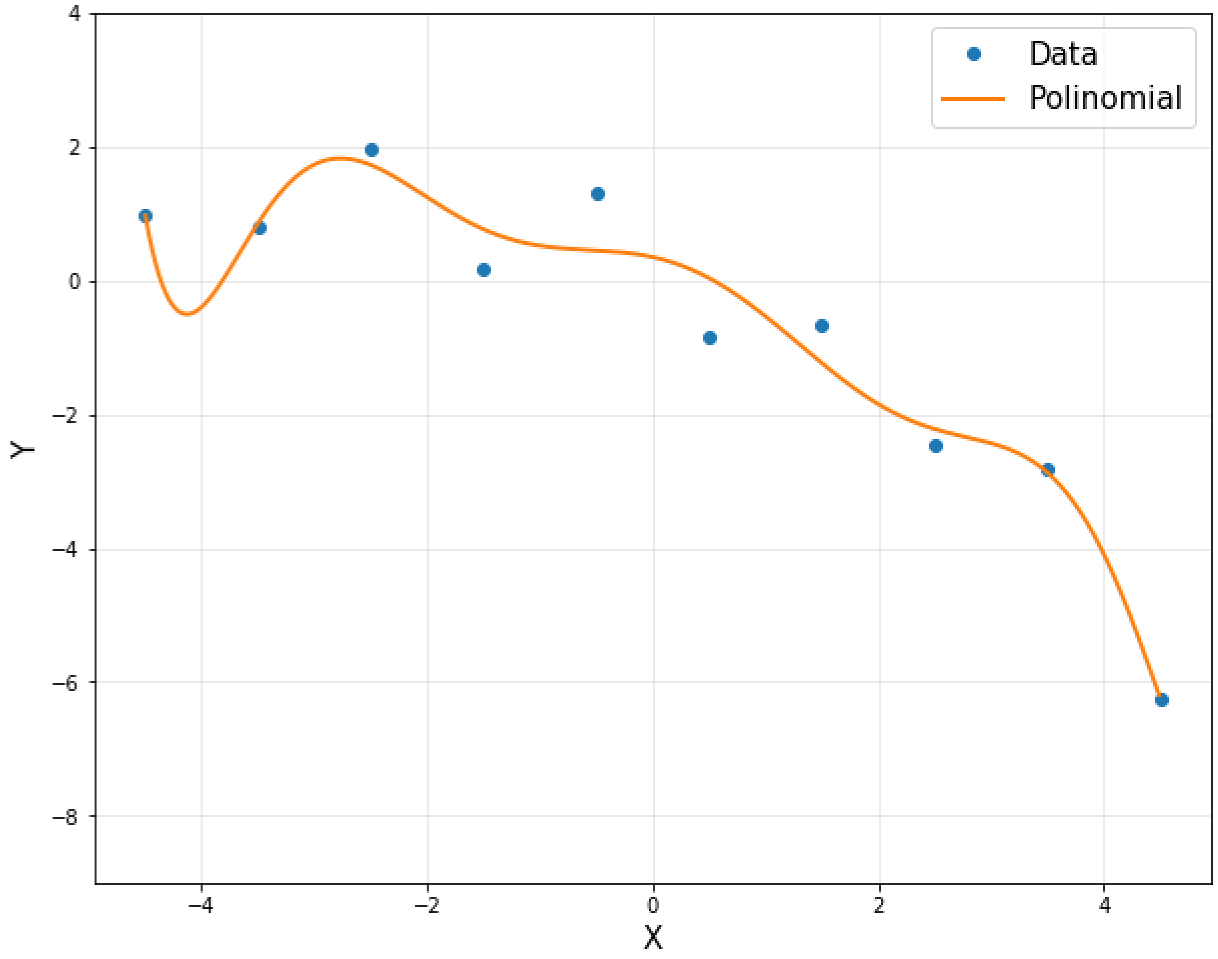
Polynomial Regression (d = 6)



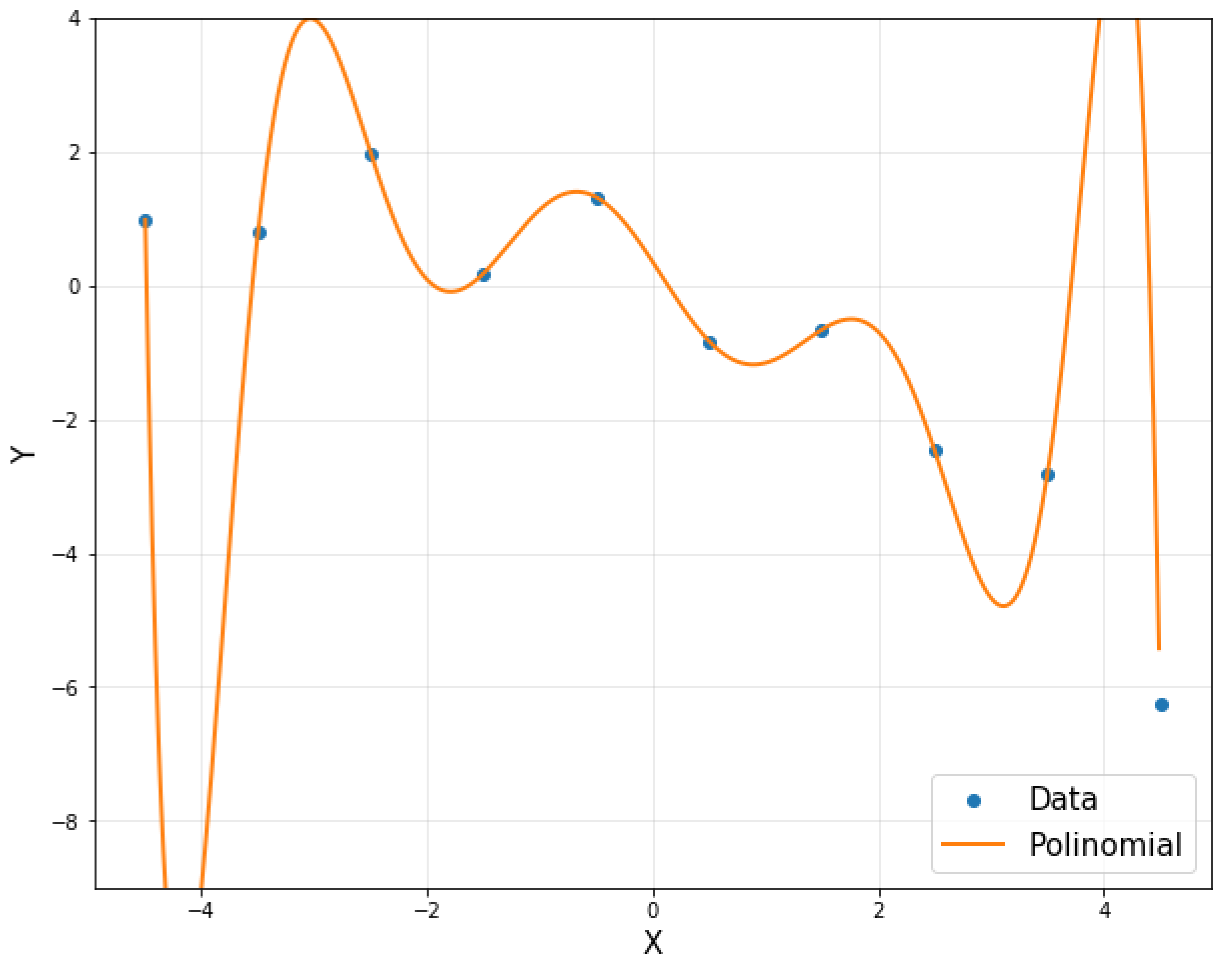
Polynomial Regression (d = 7)



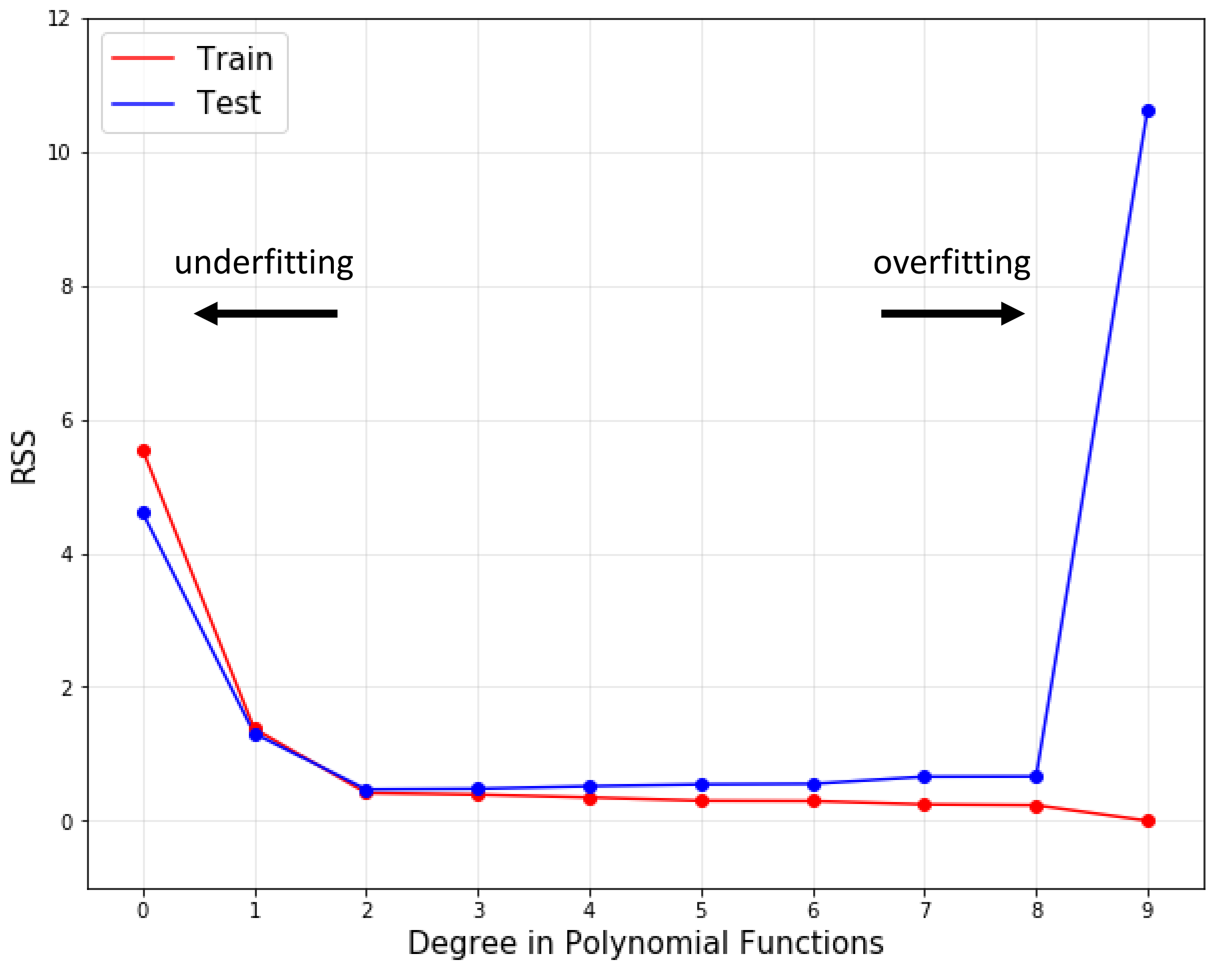
Polynomial Regression (d = 8)



Polynomial Regression (d = 9)



Errors on Train and Test Datasets



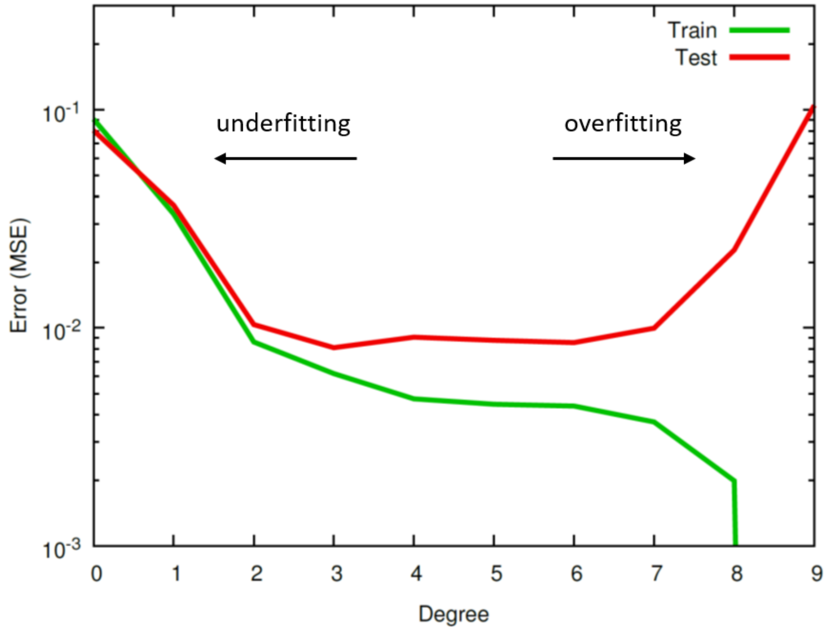
Overfitting Problem

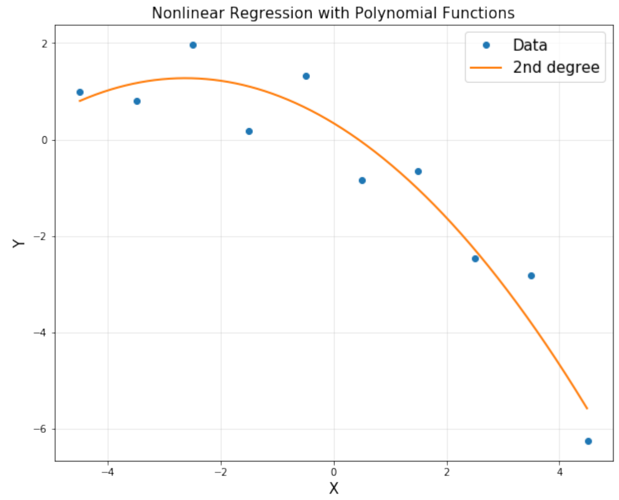
- Have you come across a situation where your model performed exceptionally well on train data, but was not able to predict test data ?

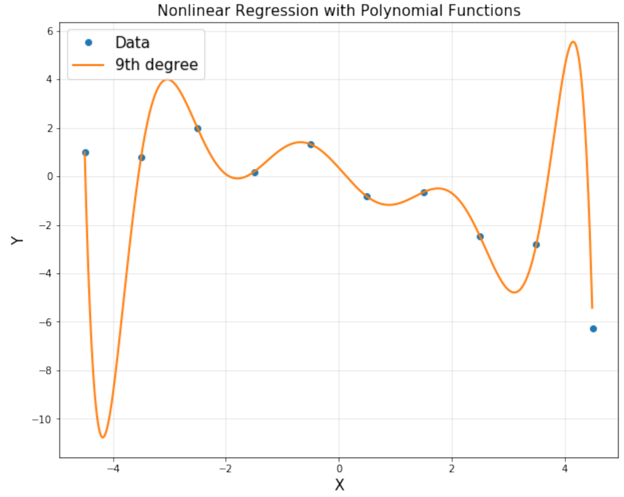
- One of the most common problem data science professionals face is to avoid overfitting.

Issue with Rich Representation

- Low error on input data points, but high error nearby
- Low error on training data, but high error on testing data





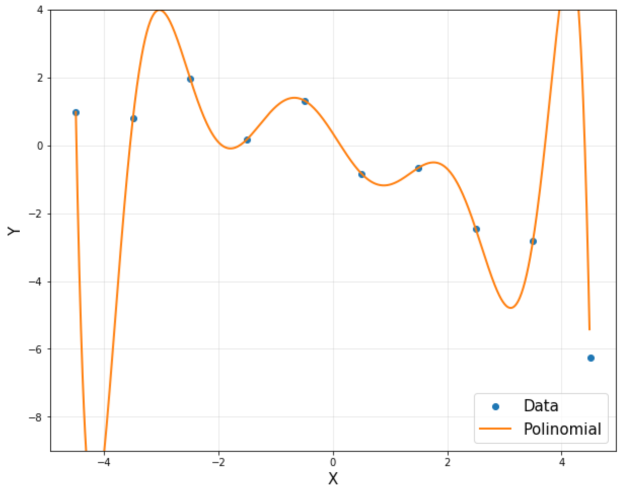


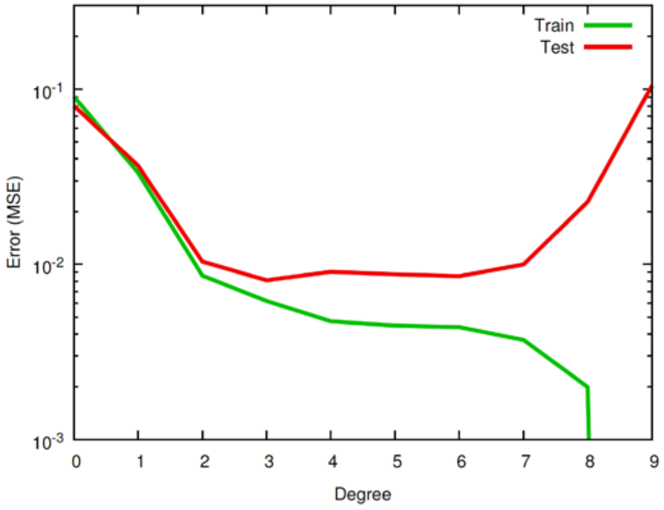
Generalization Error

- Fundamental problem: we are optimizing parameters to solve

$$\min_{\theta} \sum_{i=1}^{m} \ell(y_i, \hat{y}_i) = \min_{\theta} \sum_{i=1}^{m} \ell(y_i, \Phi\theta)$$

- But what we really care about is loss of prediction on new data (x, y)
  – also called generalization error





- Divide data into training set, and validation (testing) set

Regularization (Shrinkage Methods)

- With many features, prediction function becomes very expressive (model complexity)
  - Choose less expressive function (e.g., lower degree polynomial, fewer RBF centers, larger RBF bandwidth)
  - Keep the magnitude of the parameter small
  - Regularization: penalize large parameters θ

$$\min \; ||\Phi\theta - y||_2^2 + \lambda||\theta||_2^2$$

  - λ: regularization parameter, trades off between low loss and small values of θ

Regularization (Shrinkage Methods)

- Often, overfitting associated with very large estimated parameters
- We want to balance
  - how well function fits data
  - magnitude of coefficients

$$\text{Total cost} = \underbrace{\text{measure of fit}}_{RSS(\theta)} + \ \lambda \cdot \underbrace{\text{measure of magnitude of coefficients}}_{\lambda \cdot \|\theta\|_2^2}$$

$$\implies \min \ \|\Phi\theta - y\|_2^2 + \lambda\|\theta\|_2^2$$

  - multi-objective optimization
  - λ is a tuning parameter

Different Regularization Techniques

- Big Data
- Data augmentation
  - The simplest way to reduce overfitting is to increase the size of the training data.

Different Regularization Techniques

- Early stopping
  - When we see that the performance on the validation set is getting worse, we immediately stop the training on the model.