Optimization for Deep Learning: Overfitting

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Overfitting

- You want to hire someone, and you evaluate candidates by asking them ten technical yes/no questions.

- Would you feel confident if you interviewed one candidate and he makes a perfect score?

- What about interviewing ten candidates and picking the best? What about interviewing one thousand?

Overfitting Example

- A simple classification procedure is the "K-nearest neighbors."

- Given

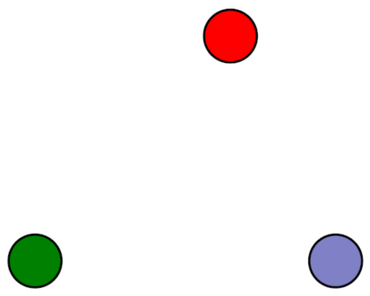
$$(x_n, y_n) \in \mathbb{R}^D \times \{1, \ldots, C\}, \; n = 1, \ldots, N$$

- to predict the y associated to a new x, take the y_n of the closest x_n:

$$\begin{aligned} n^*(x) &= \underset{n}{\operatorname{argmin}} \|x_n - x\| \\ f^*(x) &= y_{n^*(x)}. \end{aligned}$$

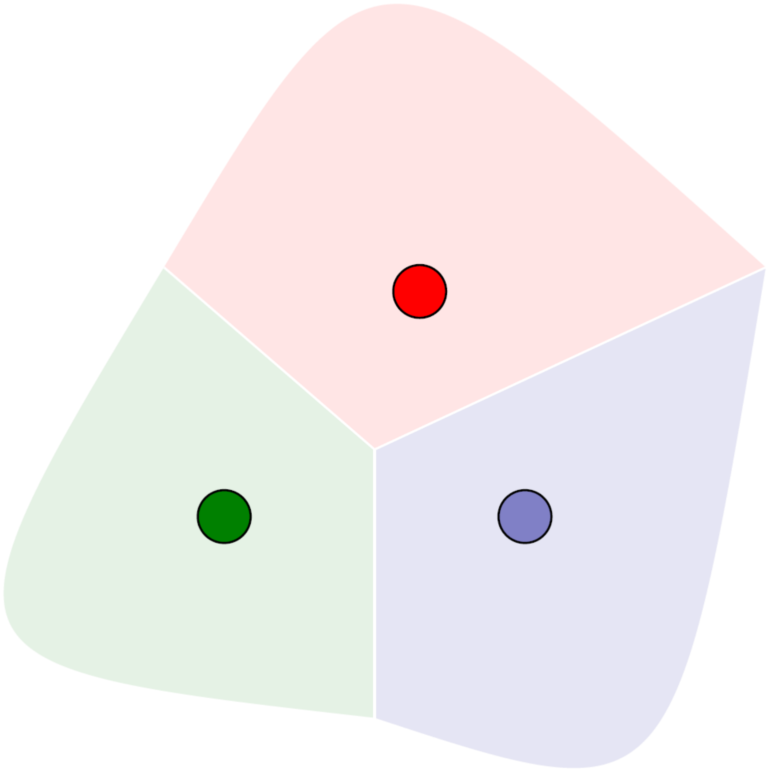
- This recipe corresponds to $K = 1$, and makes the empirical training error zero

Overfitting Example



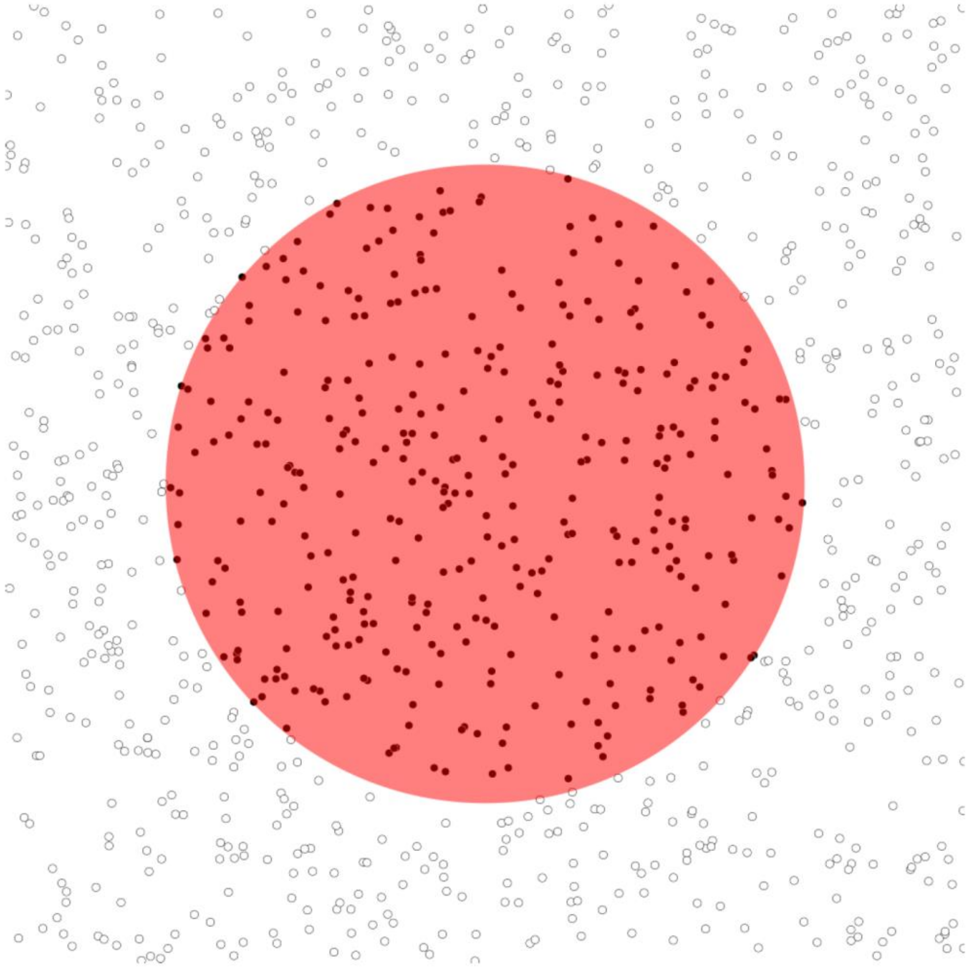
Overfitting Example

- K = 1



K = 1

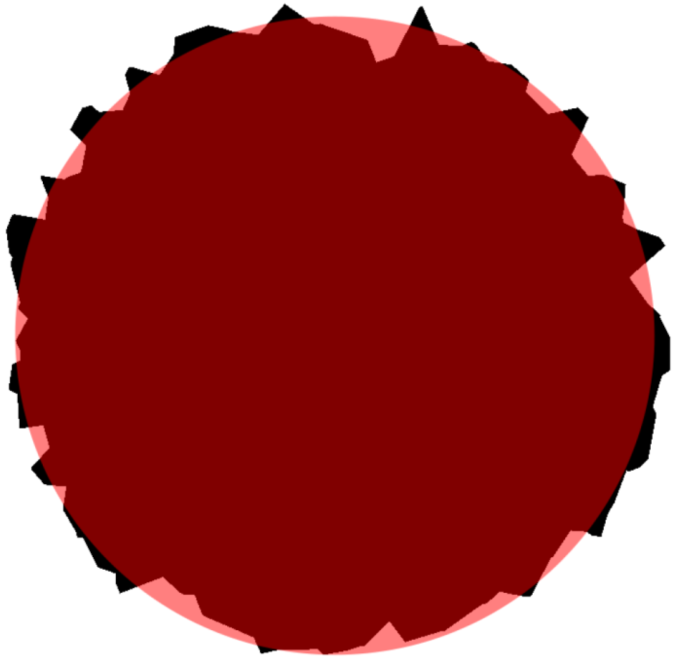
Overfitting Example



Training set

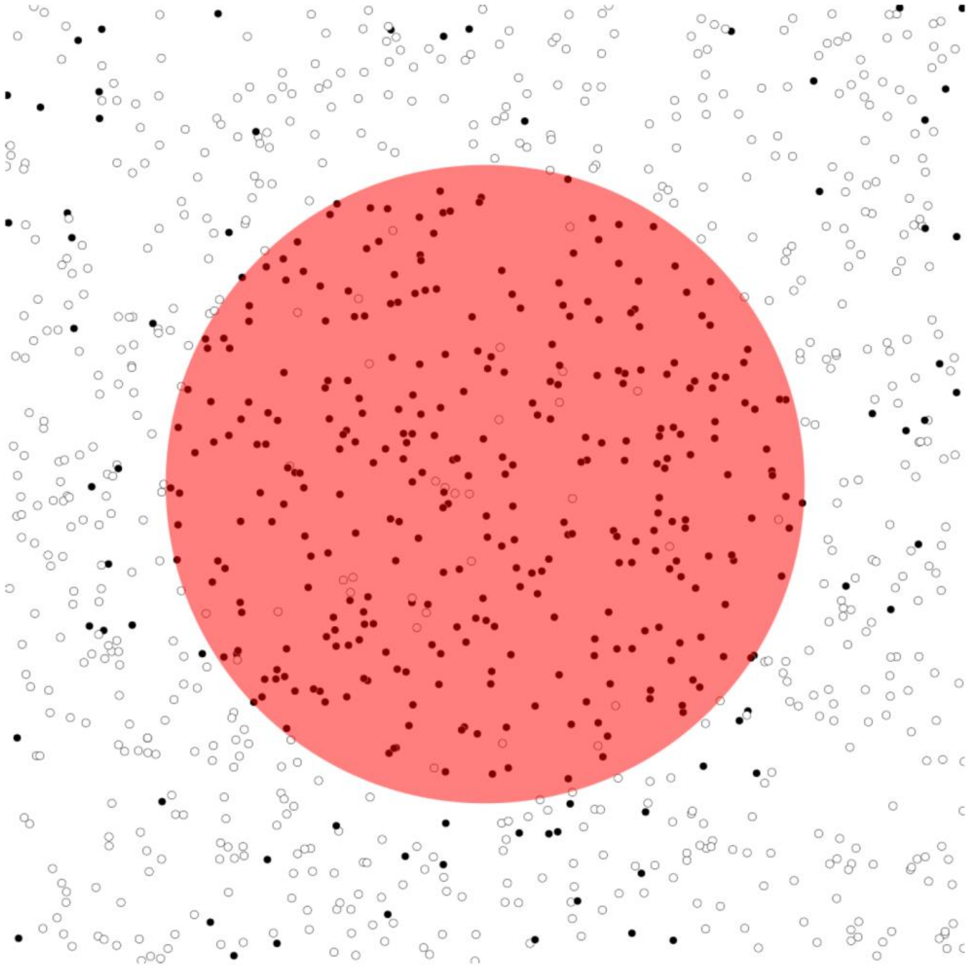
POSTECH

- K = 1
- Too noisy



Prediction (K=1)

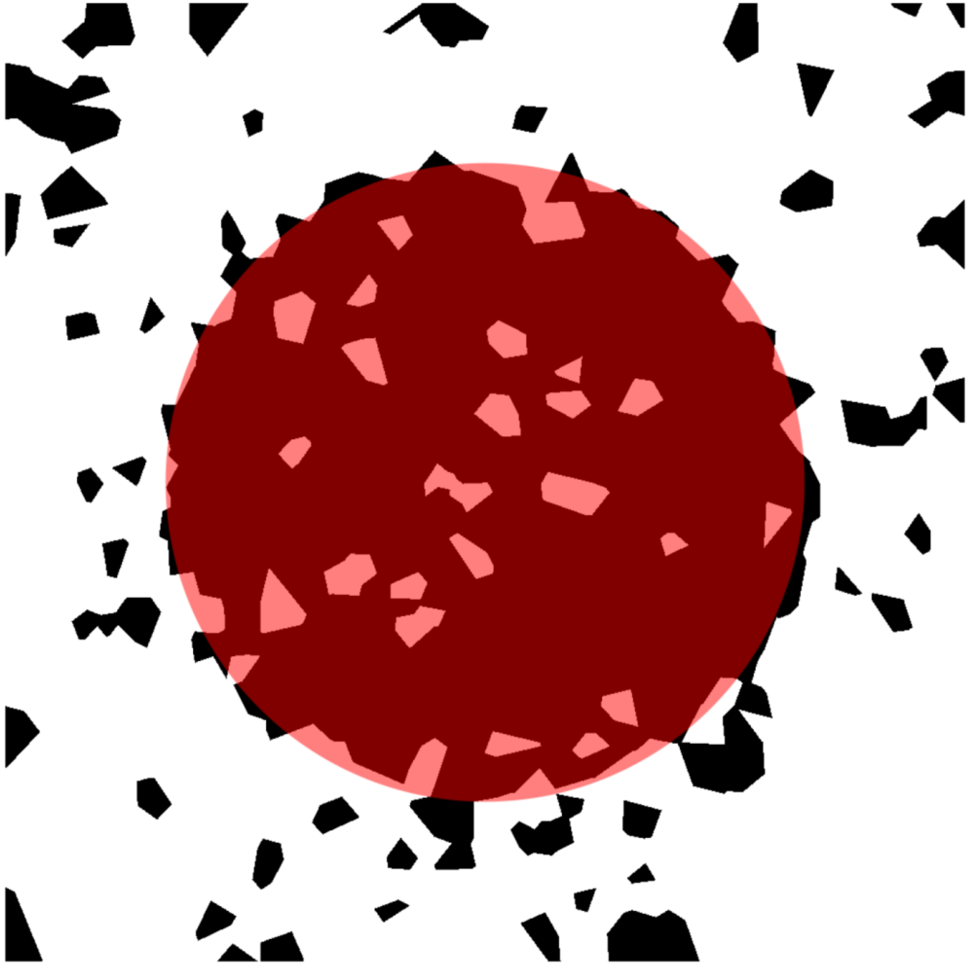
- K = 1
- With outliers



Training set

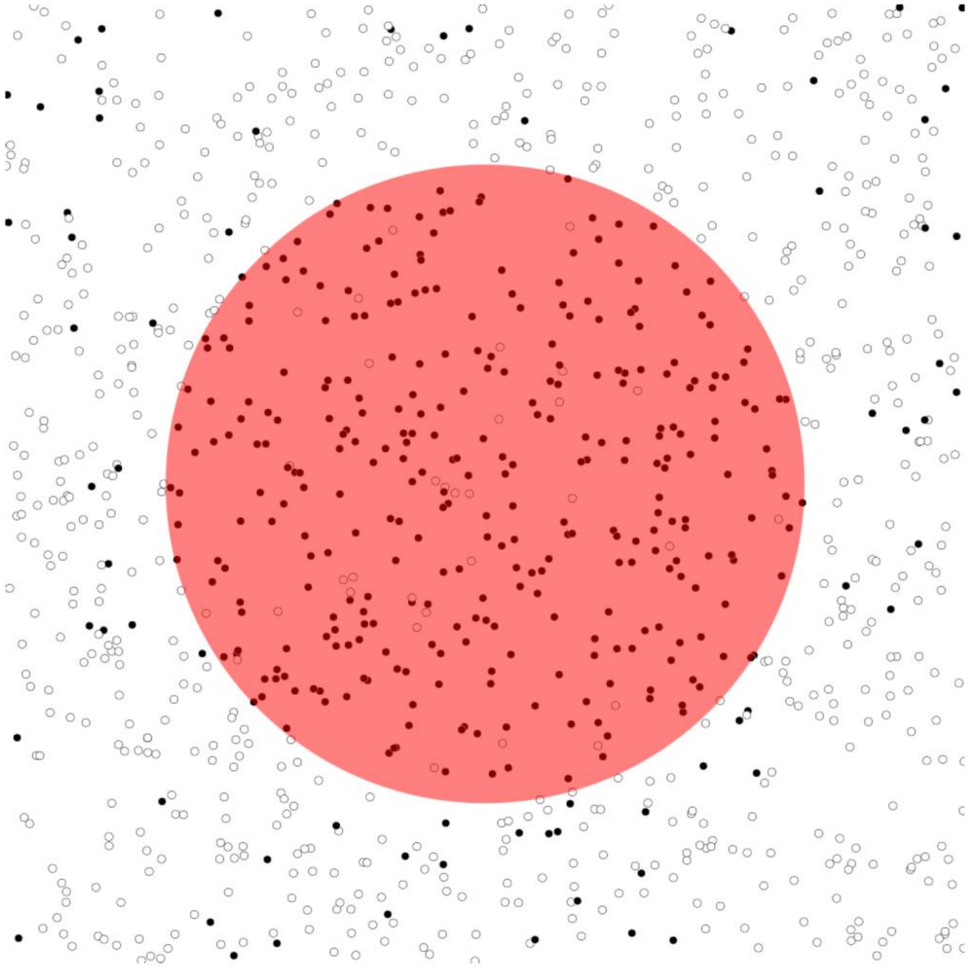
POSTECH

- K = 1
- With outliers



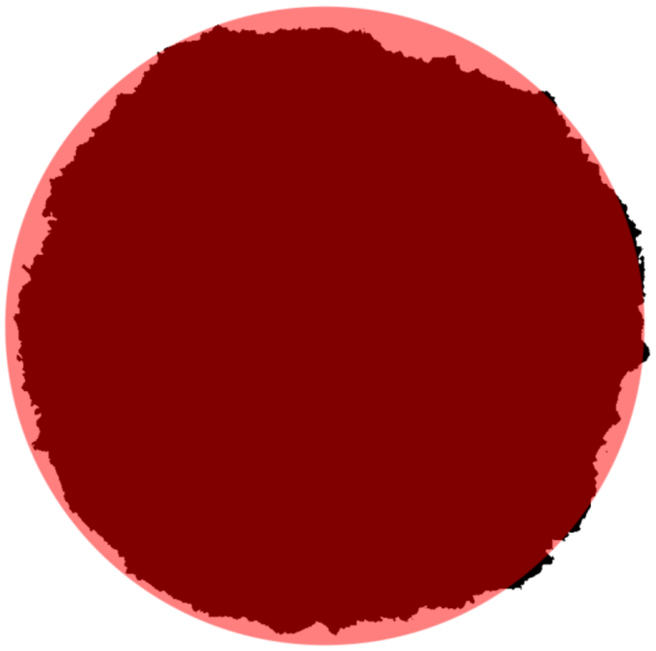
Prediction (K=1)

- K = 51
- With outliers



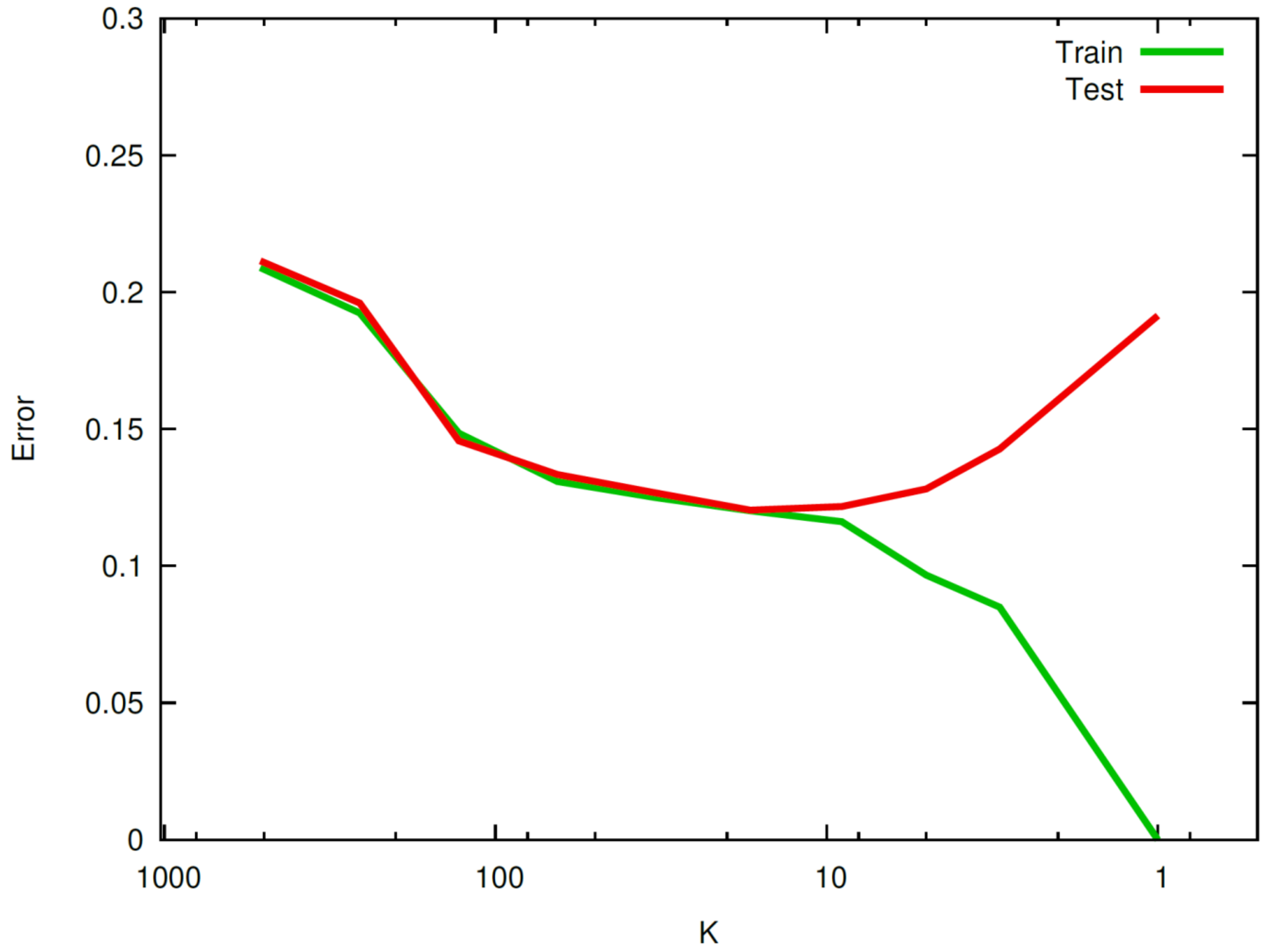
Training set

- K = 52
- With outliers
- Robust and smooth

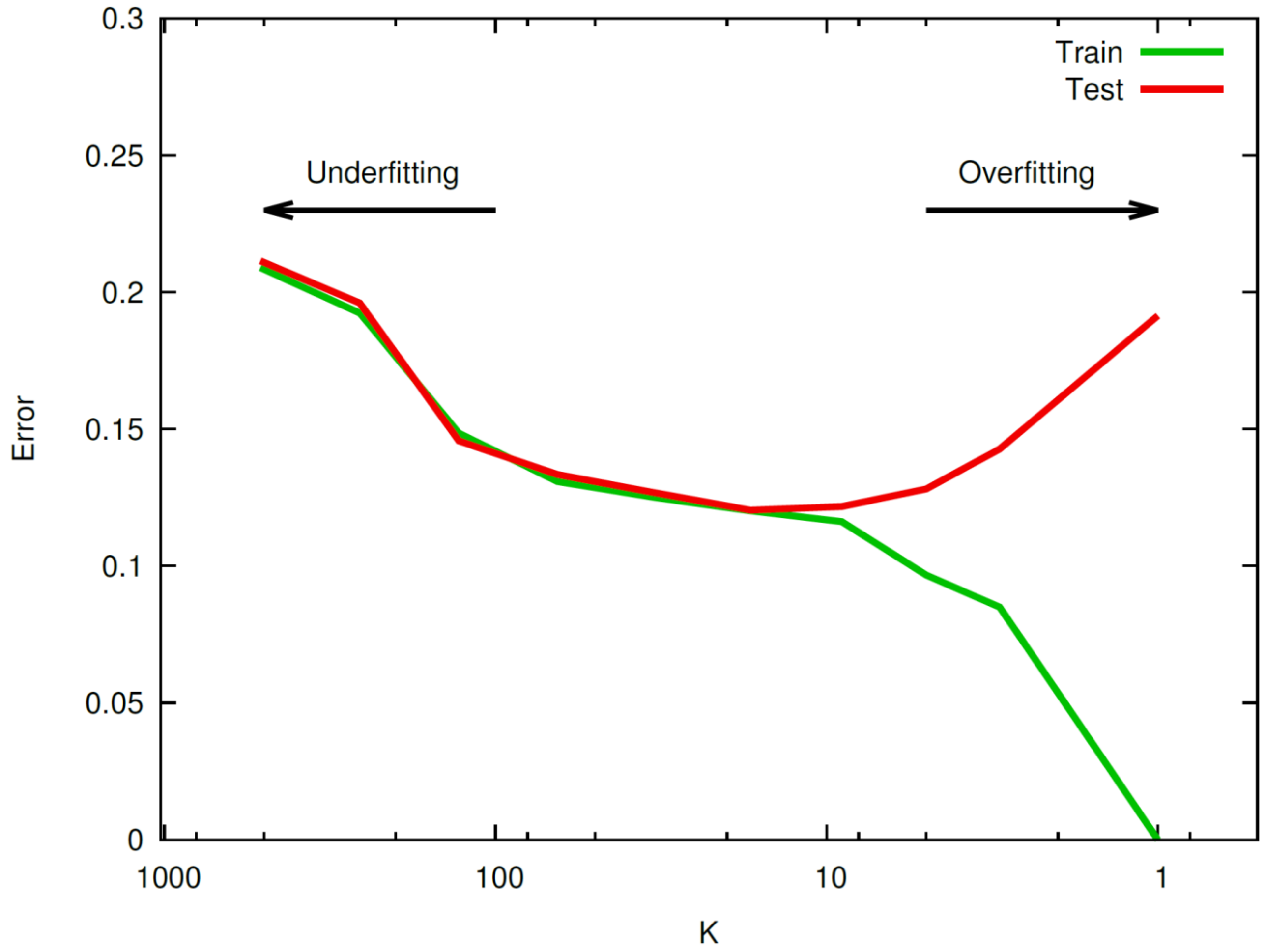


Prediction (K=51)

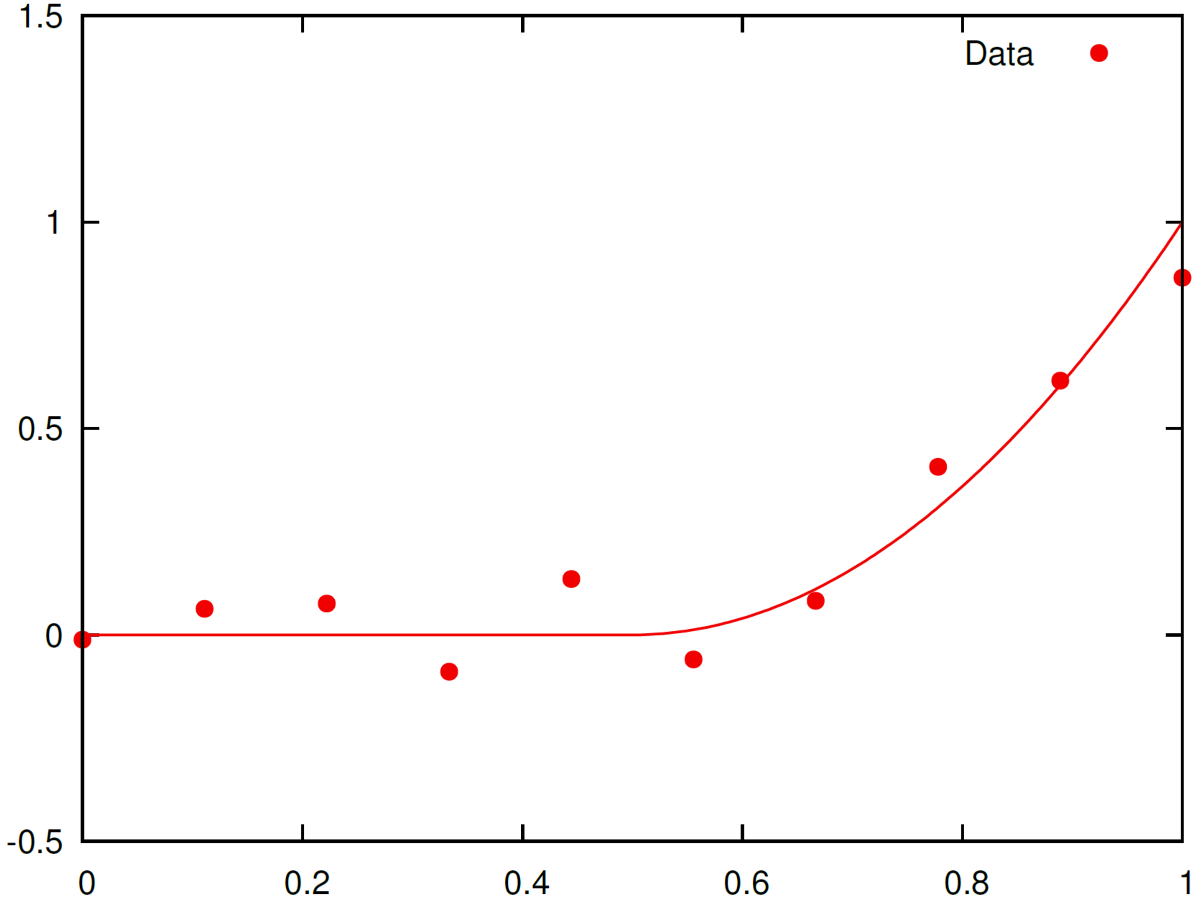
Errors on Train and Test Datasets

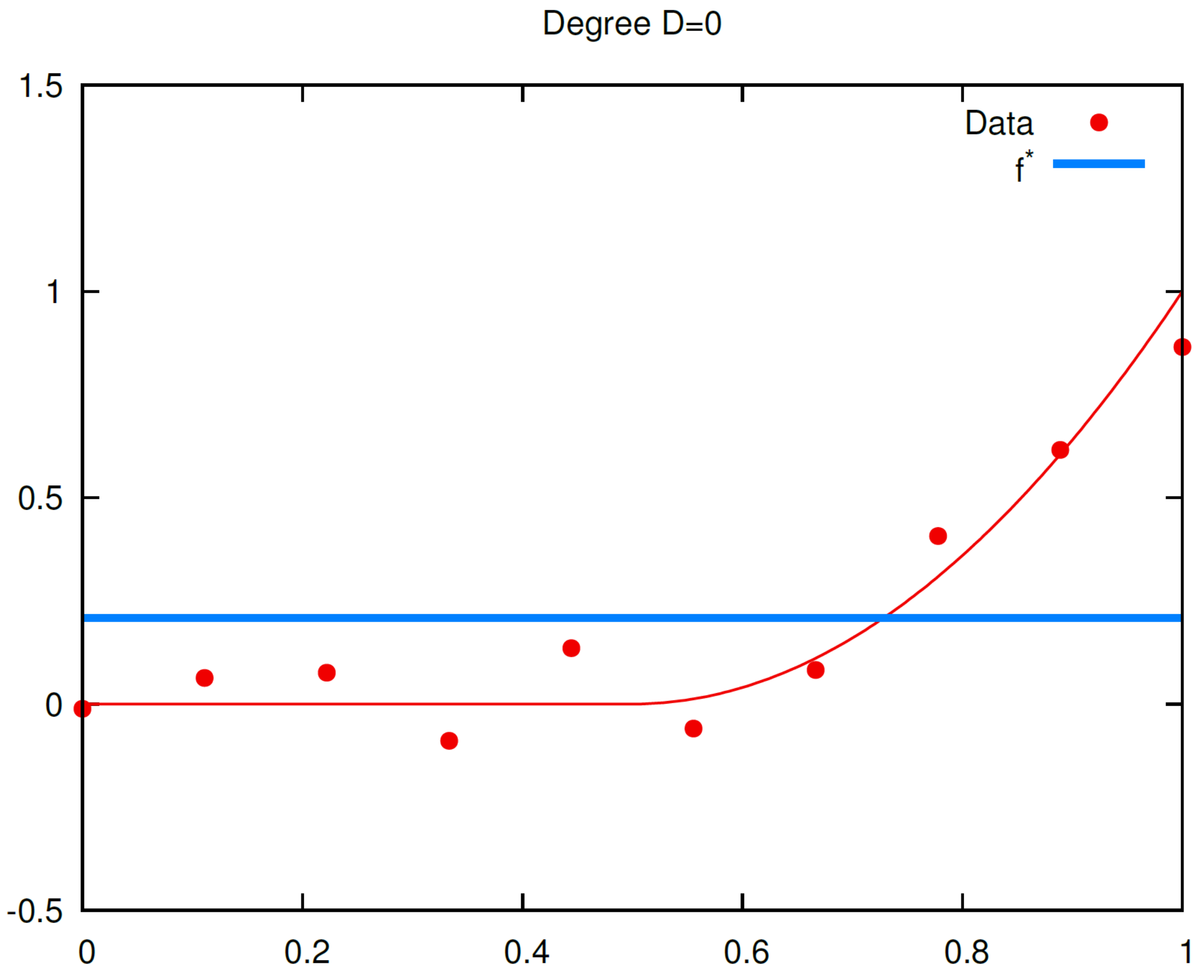


Errors on Train and Test Datasets



Polynomial Regression

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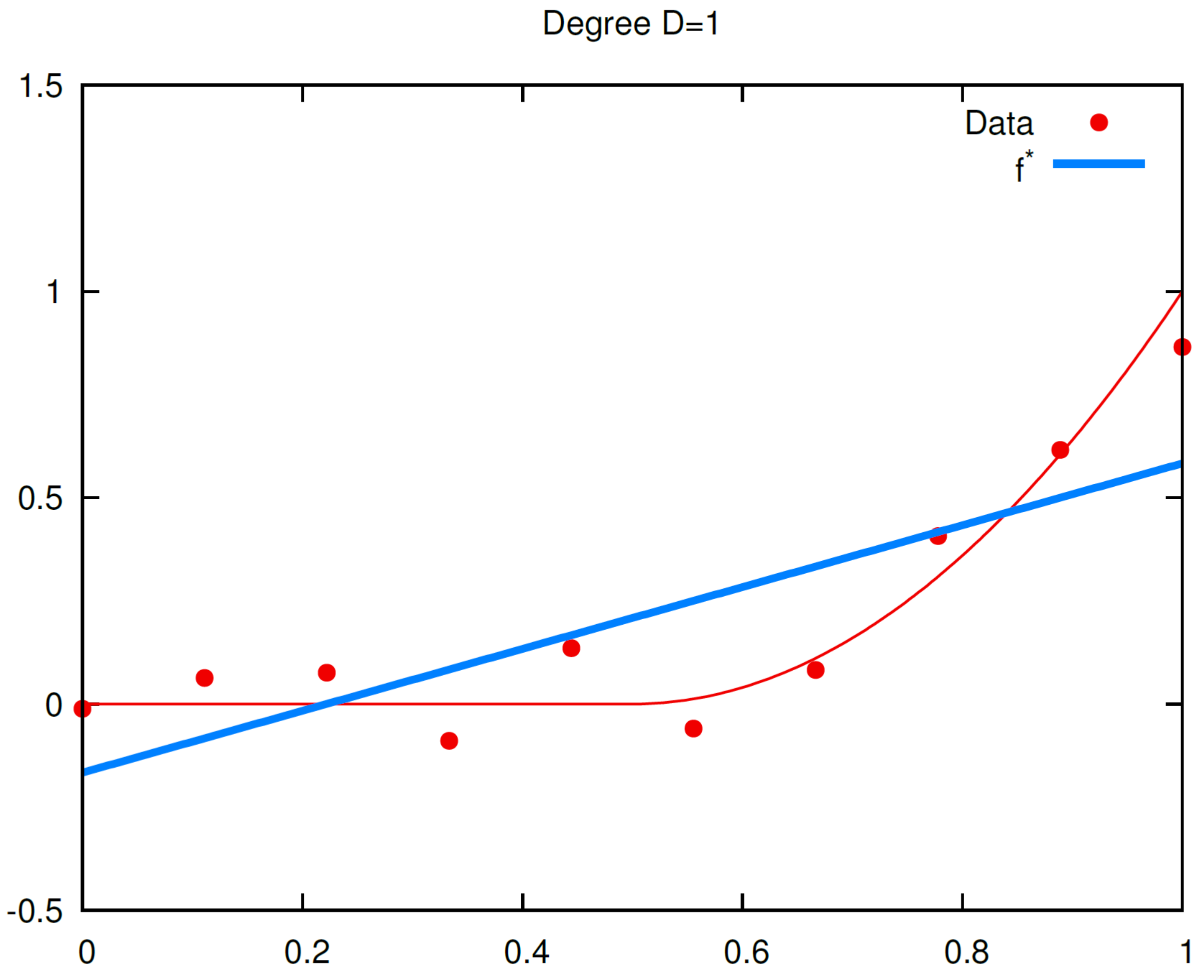
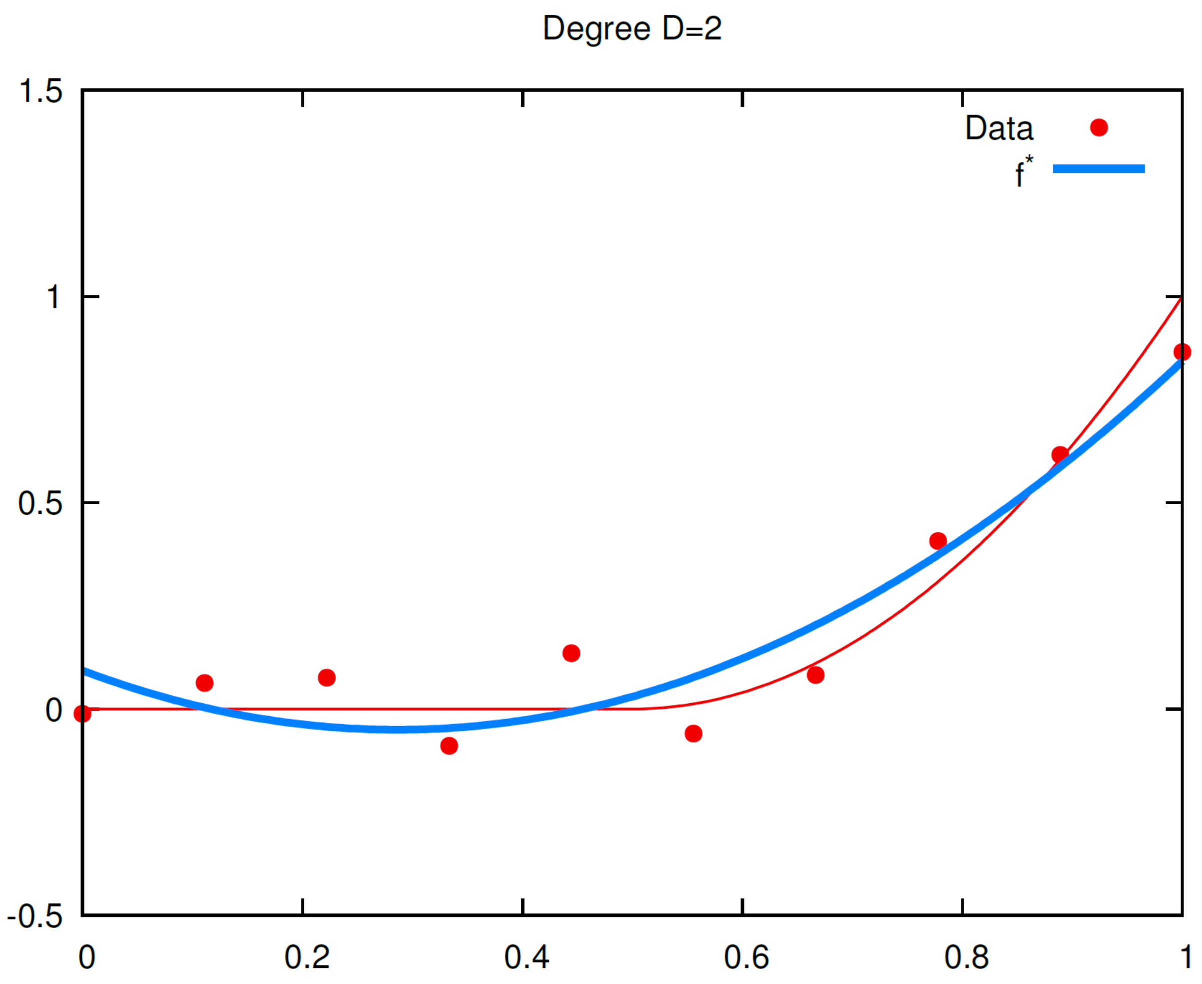
1.5
1
0.5
0
-0.5
0
0.2
0.4
0.6
0.8
1
Data
f*



Degree D=1
Data
f^*
1.5
1
0.5
0
-0.5
0
0.2
0.4
0.6
0.8
1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Data
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0.5
0
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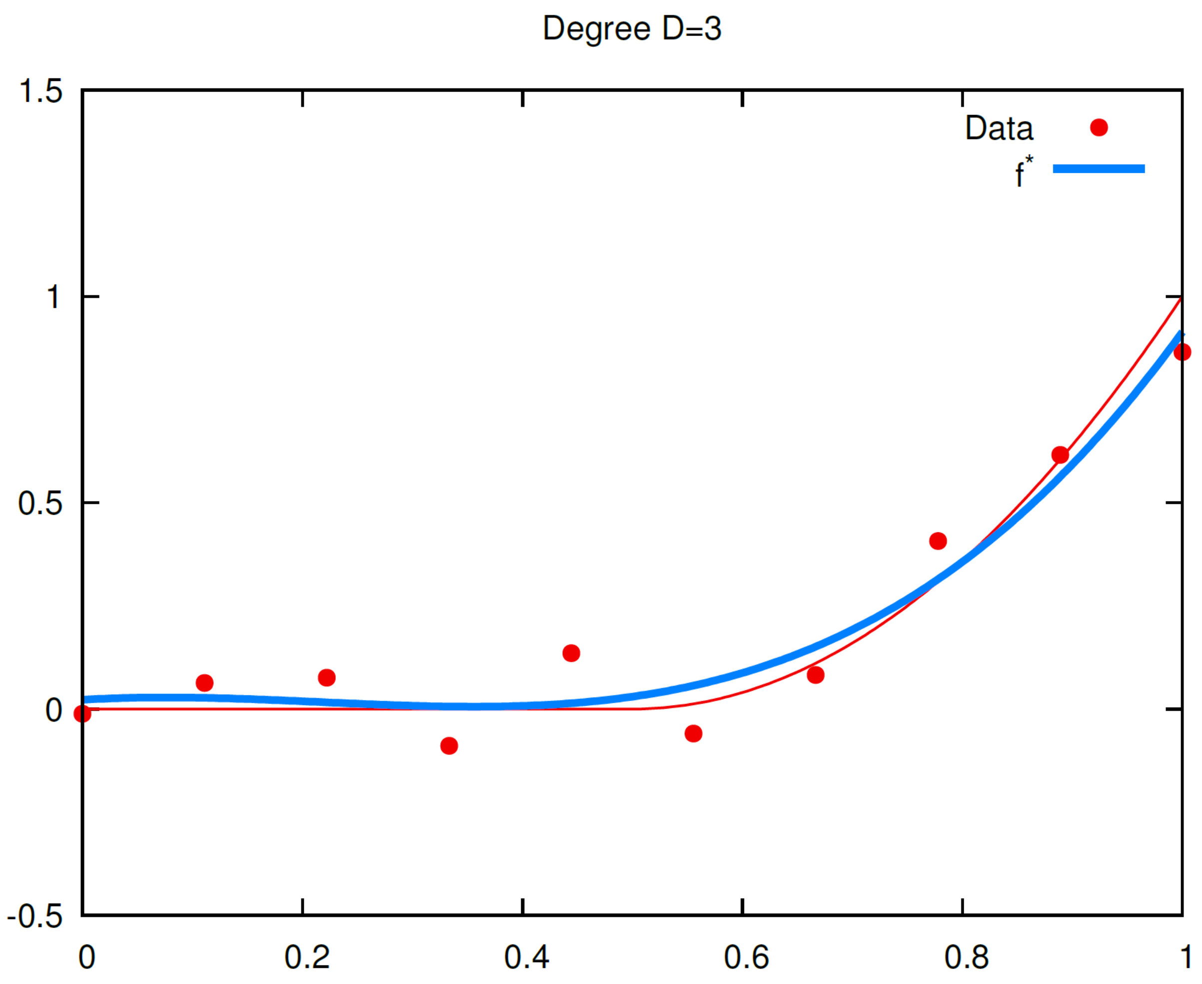
0
0.2
0.4
0.6
0.8
1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Data
f*
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1
0.5
0
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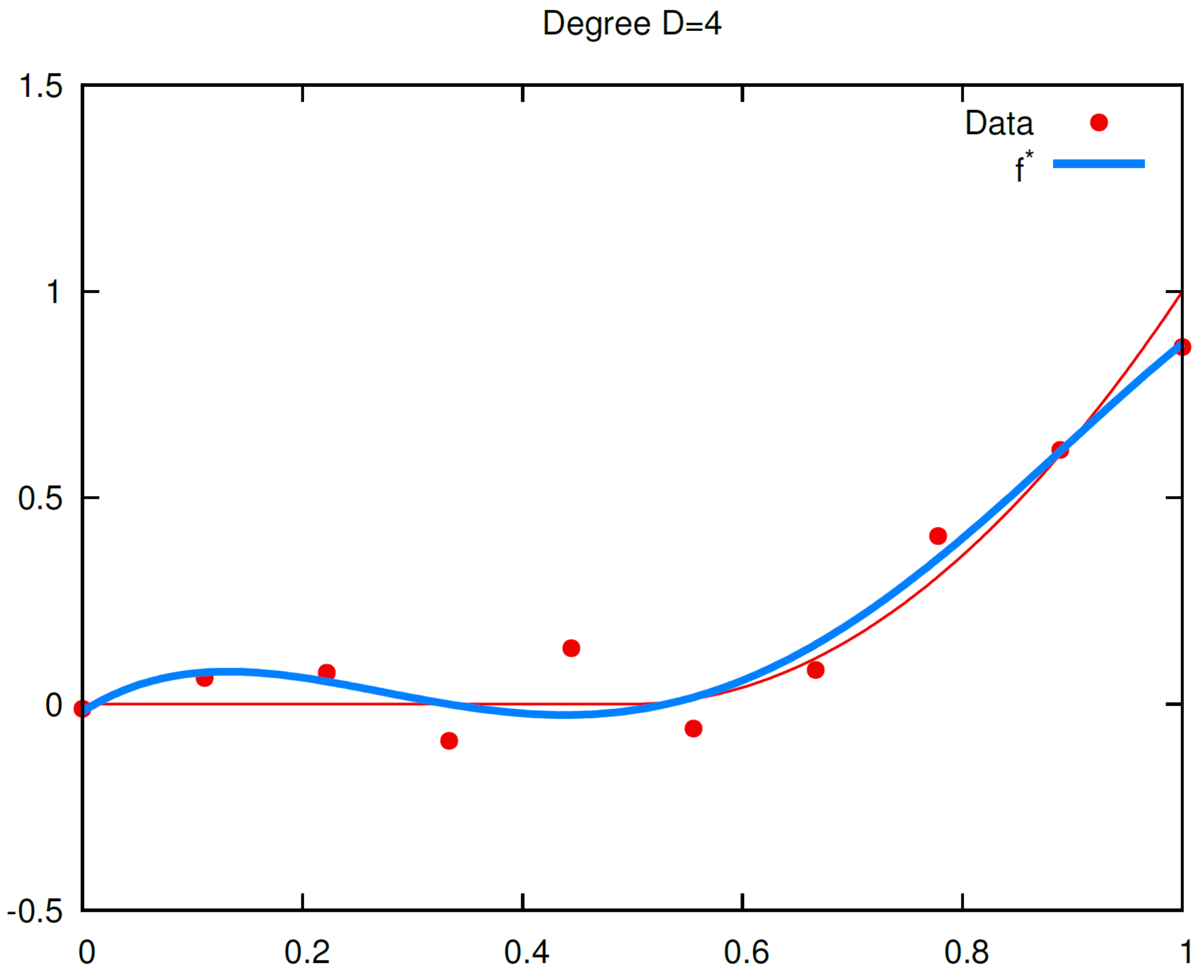
0
0.2
0.4
0.6
0.8
1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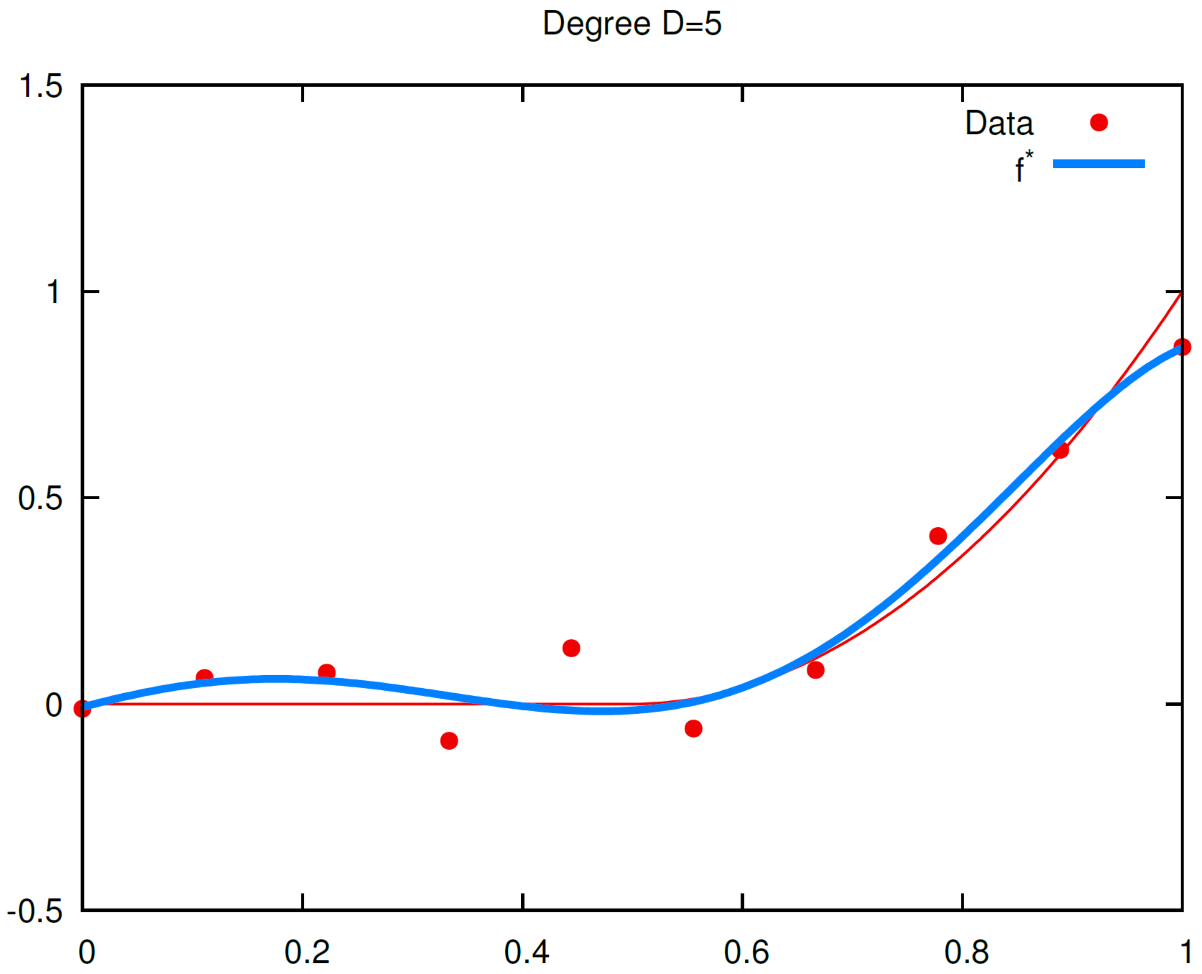
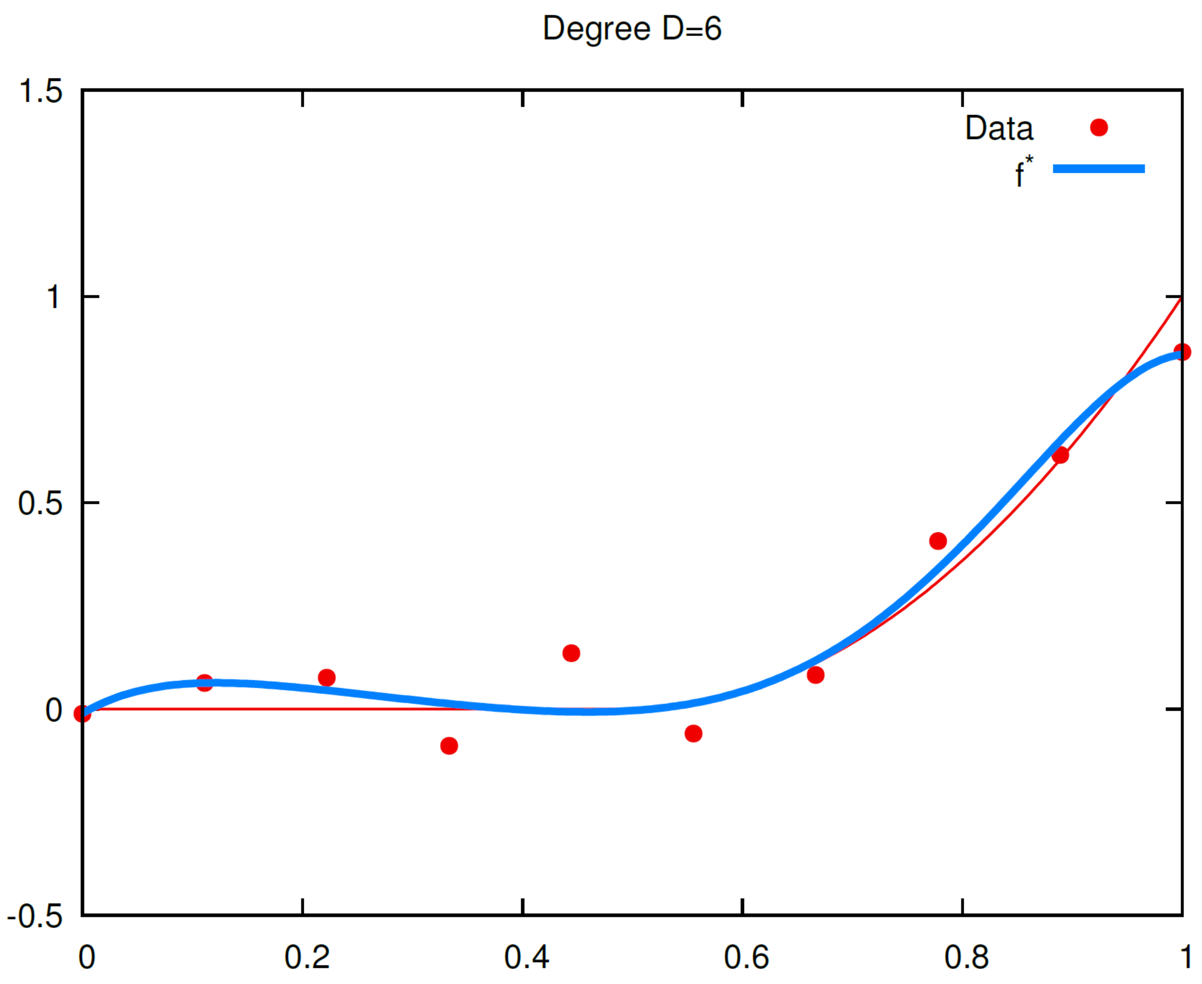
0.5
0
-0.5
0
0.2
0.4
0.6
0.8
1
Data
f*


Degree D=5
Data
f*
1.5
1
0.5
0
-0.5
0
0.2
0.4
0.6
0.8
1



Degree D=6
Data
f*
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1
0.5
0
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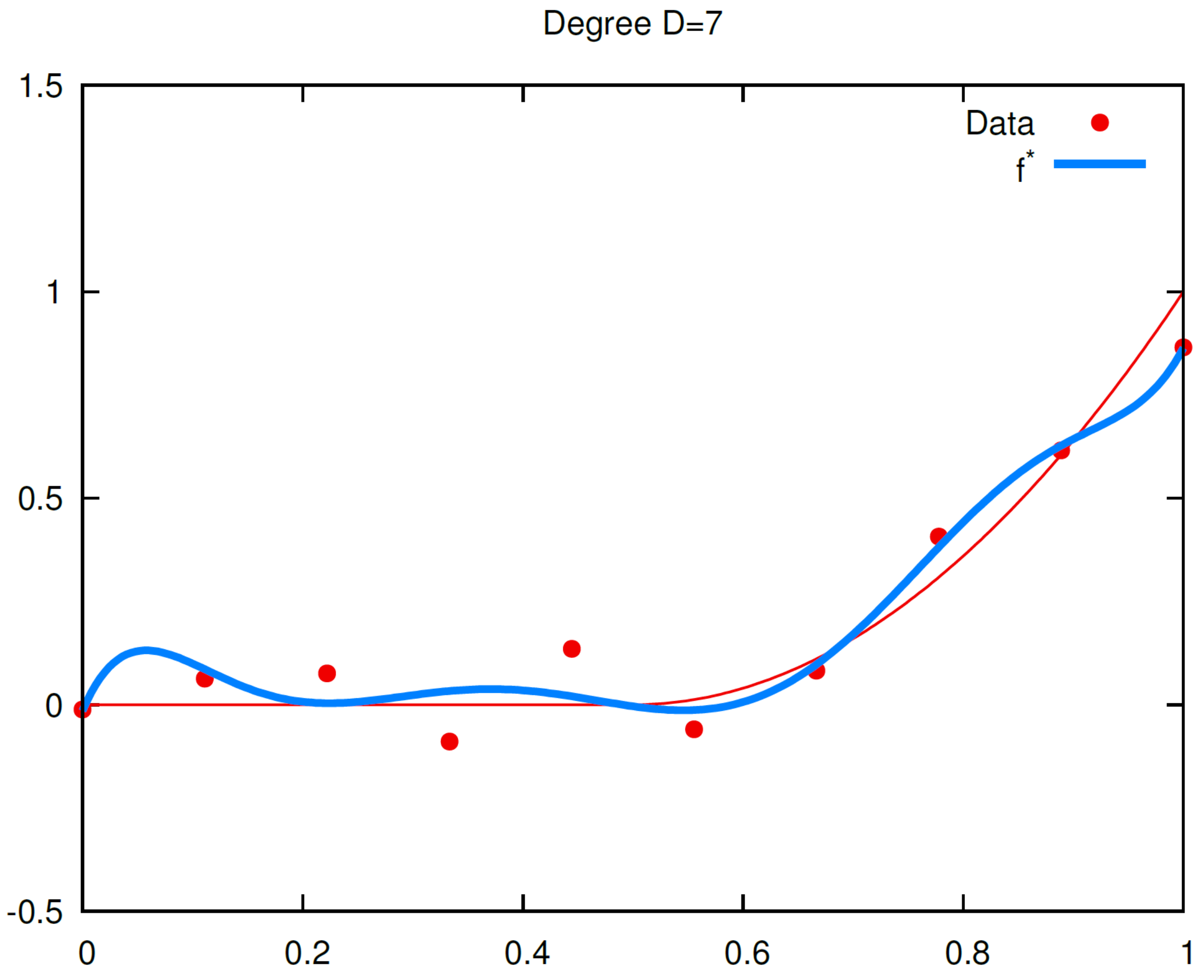
0
0.2
0.4
0.6
0.8
1



Degree D=7
Data
f*
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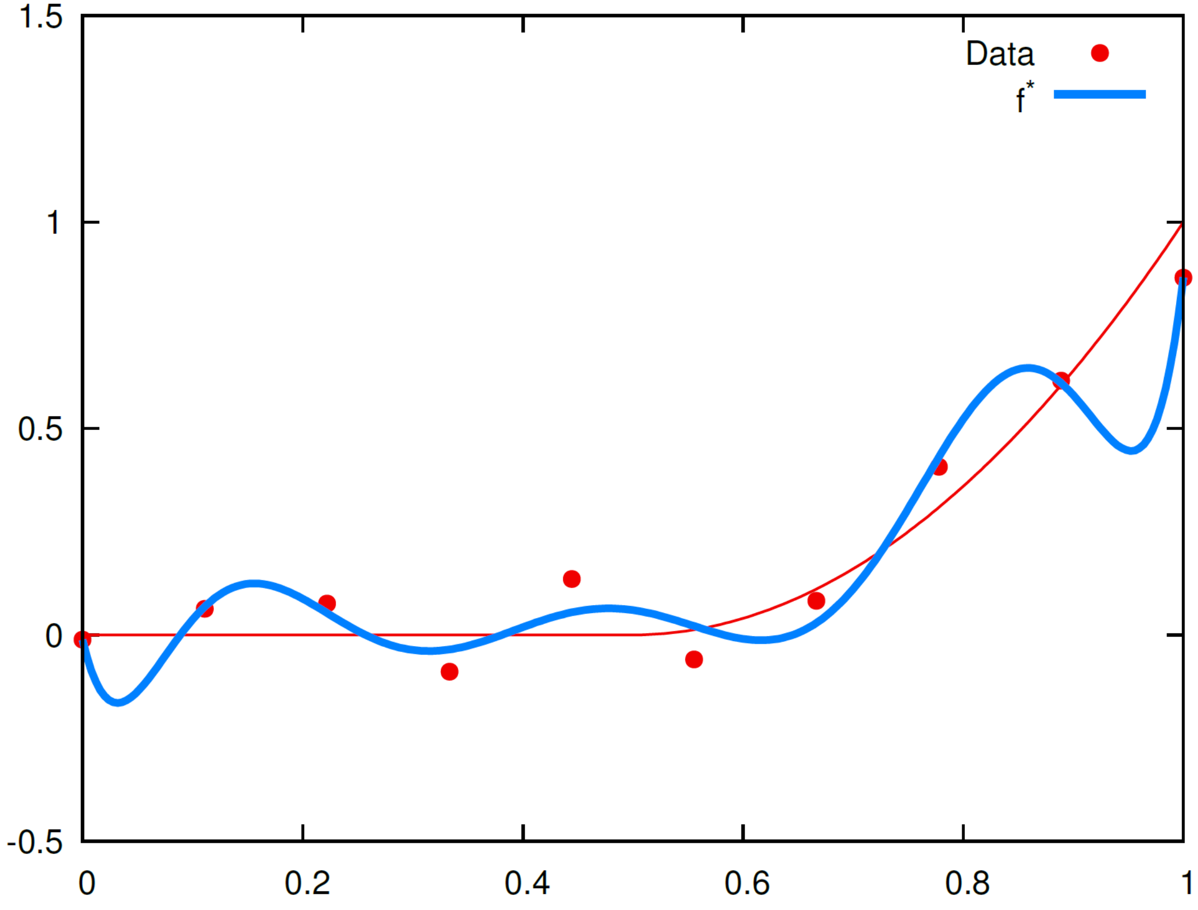
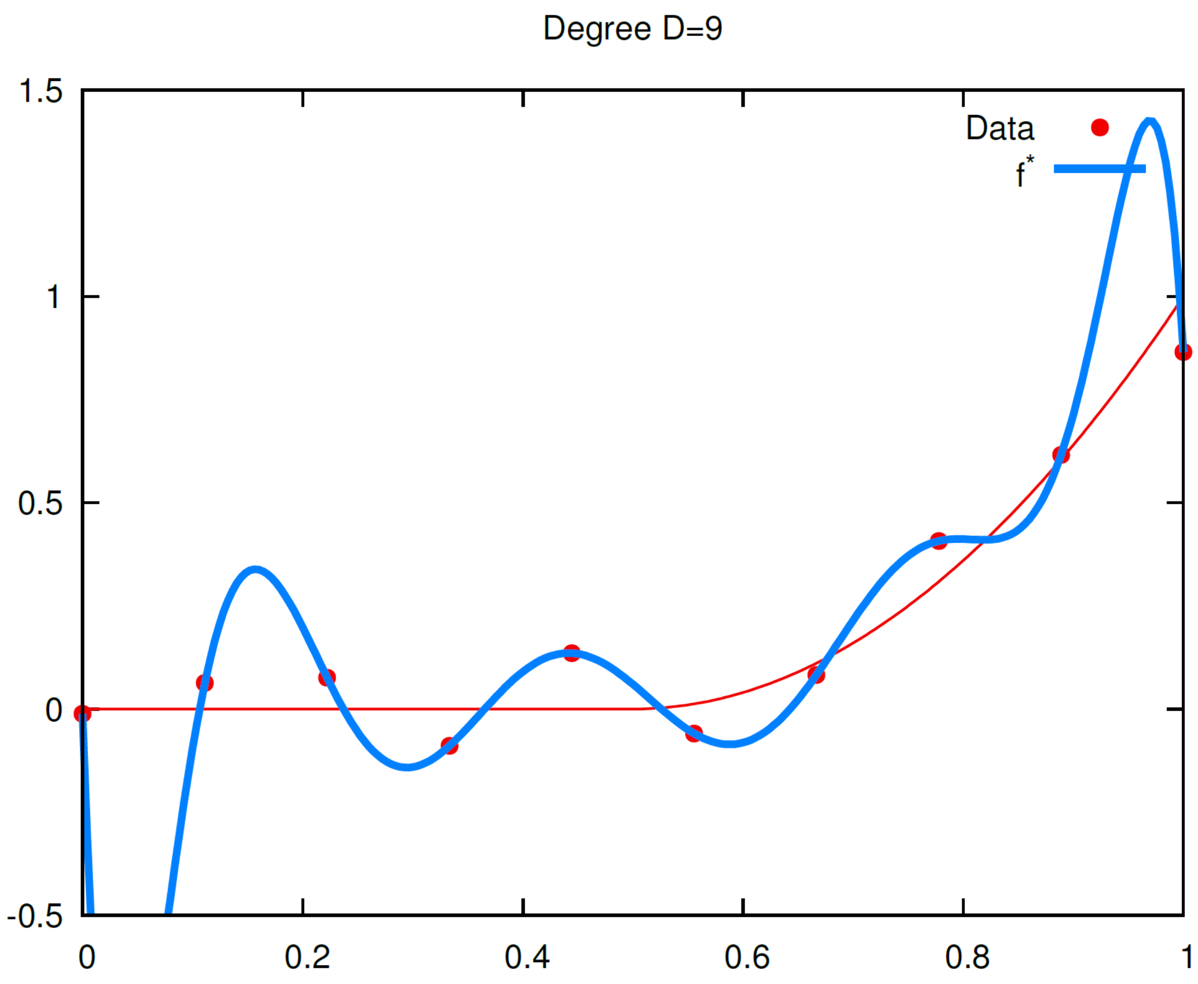
1
0.5
0
-0.5
0
0.2
0.4
0.6
0.8
1

Degree D=8




Degree D=9
Data
f^*
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0
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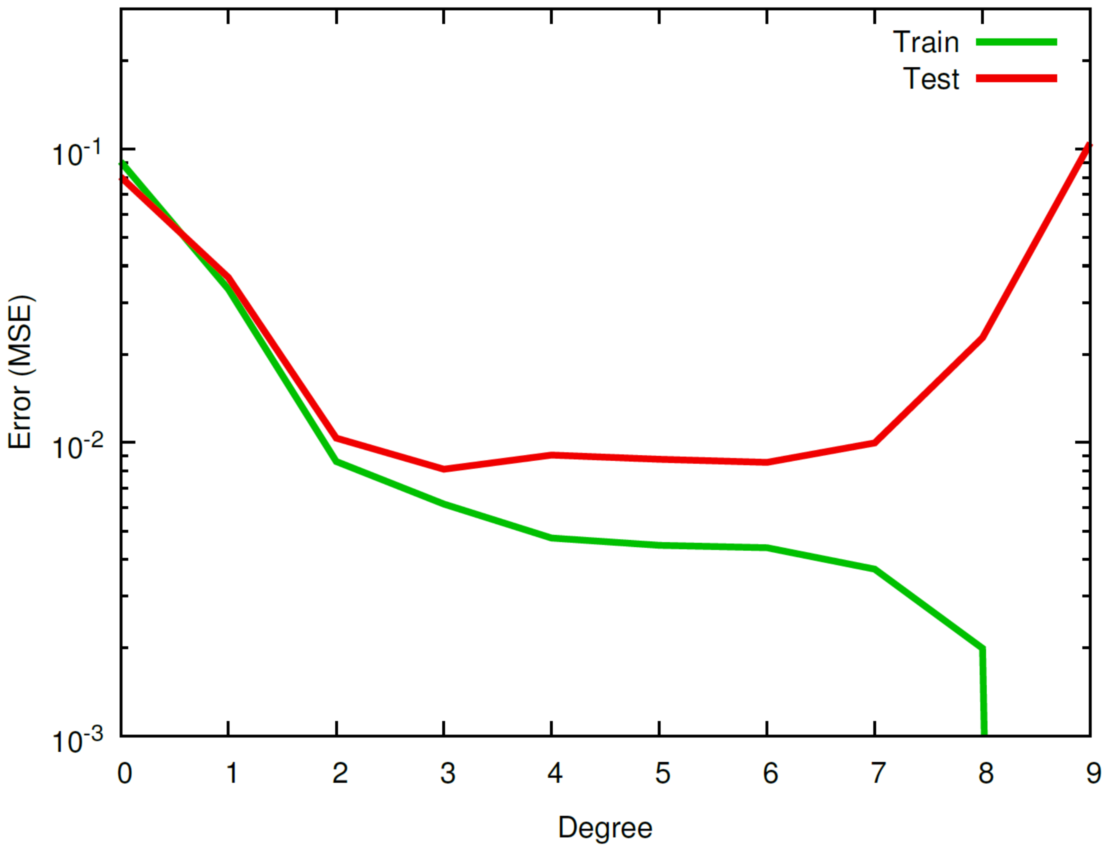
0
0.2
0.4
0.6
0.8
1

Errors on Train and Test Datasets



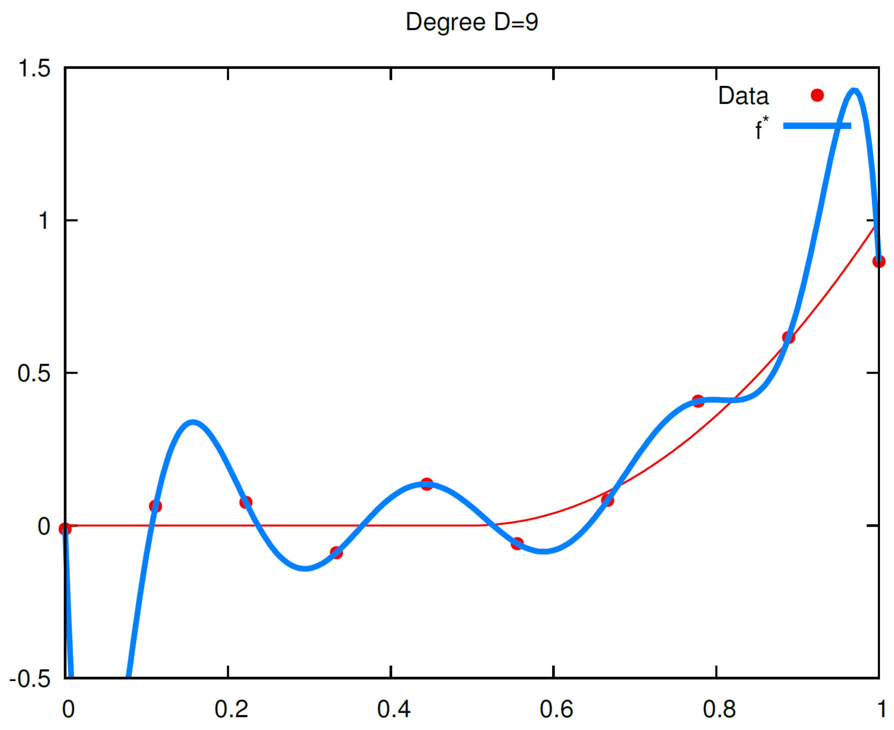
Overfitting Problem

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

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

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

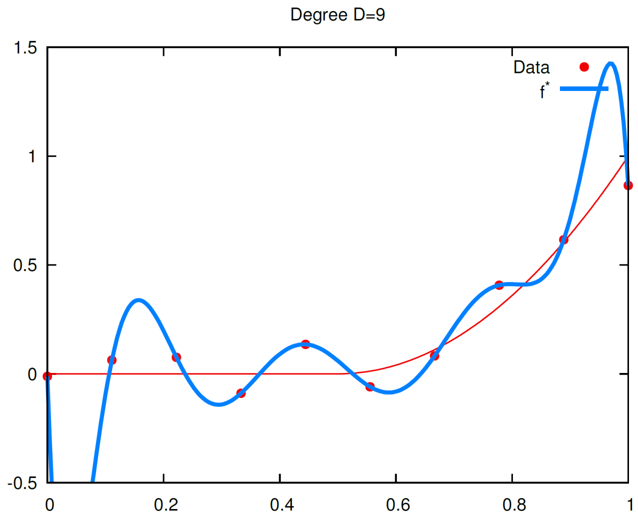


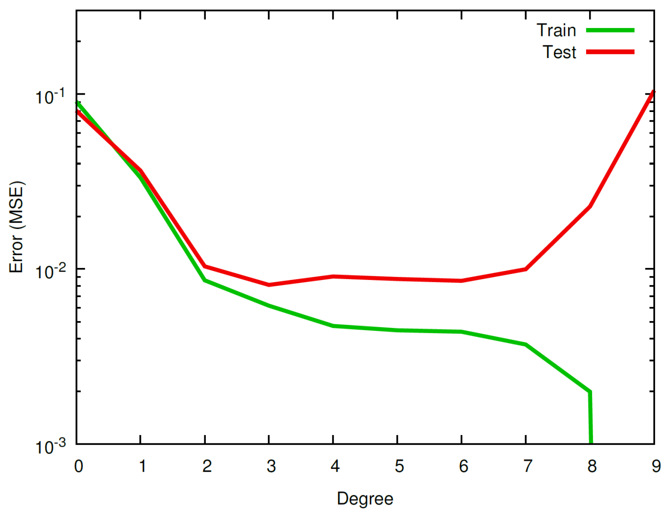
Generalization Error

- 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

Representational Difficulties

- With many features, prediction function becomes very expressive (model complexity)
  - Choose less expensive 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

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

$$\Longrightarrow \min \|\Phi\theta - y\|_2^2 + \lambda\|\theta\|_2^2 \qquad\qquad \min \|\Phi\theta - y\|_2^2 + \lambda\|\theta\|_1$$

L_2 regularization $\qquad\qquad$ L_1 regularization

  - multi-objective optimization
  - λ is a tuning parameter

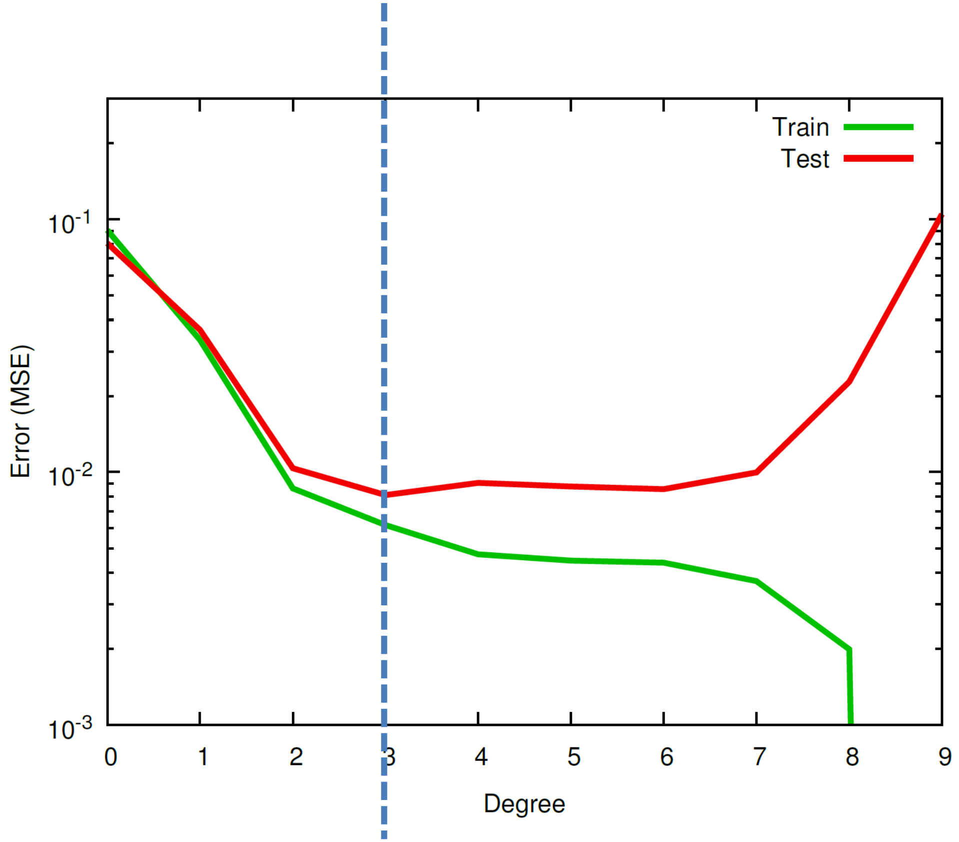
Different Regularization Techniques in Deep Learning

- L_2 and L_1 regularization

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

Different Regularization Techniques in Deep Learning

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



Early stopping

Different Regularization Techniques in Deep Learning

- Dropout
  - This is the one of the most interesting types of regularization techniques.
  - It also produces very good results and is consequently the most frequently used regularization technique in the field of deep learning.
  - At every iteration, it randomly selects some nodes and removes them.
  - It can also be thought of as an ensemble technique in machine learning.
  - (will discuss later)